Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 02:38 AM JST

PDB ID	:	6KIG / pdb_00006kig
EMDB ID	:	EMD-9995
Title	:	Structure of cyanobacterial photosystem I-IsiA supercomplex
Authors	:	Cao, P.; Cao, D.F.; Si, L.; Su, X.D.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2019-07-18
Resolution	:	2.90 Å(reported)

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

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

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

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

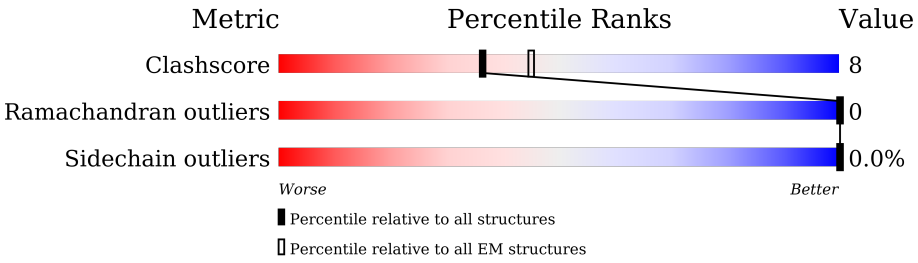
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

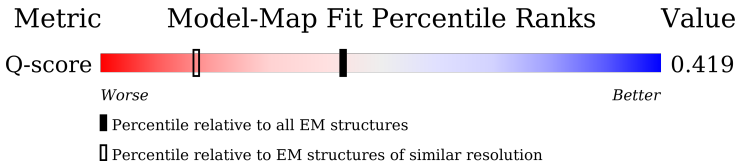
1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	763	87% 12%
1	G	763	86% 12%
1	e	763	87% 12%
2	B	734	86% 14%

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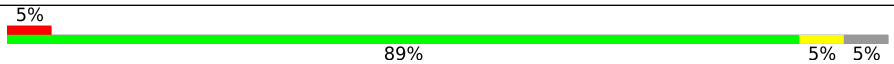
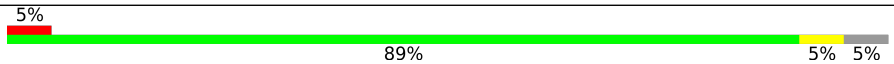
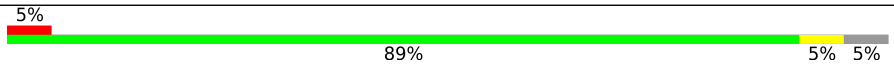
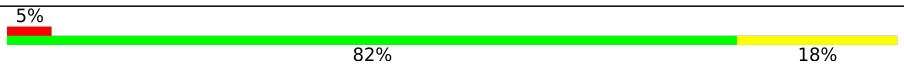
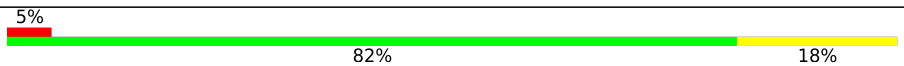
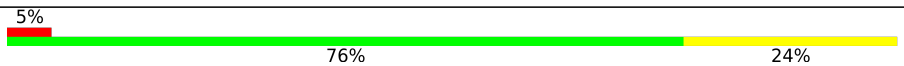
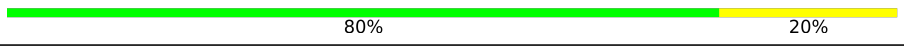
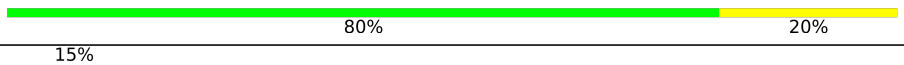
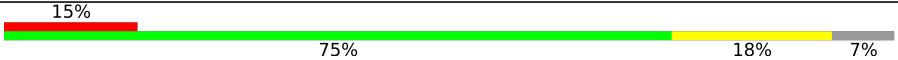
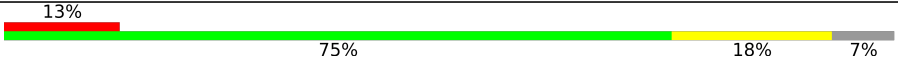
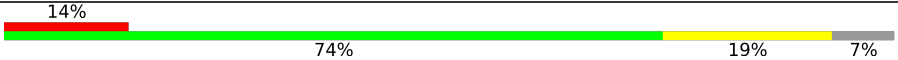
Mol	Chain	Length	Quality of chain
2	H	734	
2	f	734	
3	C	81	
3	N	81	
3	g	81	
4	D	141	
4	O	141	
4	h	141	
5	E	75	
5	Q	75	
5	i	75	
6	F	159	
6	R	159	
6	j	159	
7	I	38	
7	S	38	
7	k	38	
8	J	41	
8	T	41	
8	l	41	
9	K	84	
9	U	84	
9	m	84	
10	L	166	
10	V	166	

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Mol	Chain	Length	Quality of chain
10	n	166	87% 12%
11	M	29	86% 14%
11	W	29	86% 14%
11	o	29	86% 14%
12	1	342	49% 88% 11%
12	2	342	40% 87% 12%
12	3	342	59% 89% 10%
12	4	342	94% 87% 13%
12	5	342	98% 90% 9%
12	6	342	91% 84% 15%
12	Y	342	49% 87% 12%
12	Z	342	38% 88% 11%
12	a	342	60% 90% 9%
12	b	342	95% 87% 13%
12	c	342	98% 91% 8%
12	d	342	90% 84% 15%
12	q	342	51% 87% 12%
12	r	342	41% 87% 12%
12	s	342	59% 88% 11%
12	t	342	93% 87% 12%
12	u	342	99% 90% 9%
12	v	342	90% 86% 13%

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
13	CLA	q	505	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 143022 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	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	G	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	e	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	H	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	f	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		

- 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
			598	368	103	116	11		
3	N	80	Total	C	N	O	S	0	0
			598	368	103	116	11		
3	g	80	Total	C	N	O	S	0	0
			598	368	103	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		
4	h	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	71	Total	C	N	O	0	0
			543	343	95	105		
5	Q	71	Total	C	N	O	0	0
			543	343	95	105		
5	i	71	Total	C	N	O	0	0
			543	343	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	R	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	j	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		

- Molecule 7 is a protein called Photosystem I PsaI protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	S	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	k	38	Total	C	N	O	S	0	0
			282	191	38	51	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			335	228	52	54	1		
8	T	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	U	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	m	78	Total	C	N	O	S	0	0
			549	364	91	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	V	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	n	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		

- Molecule 11 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	W	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	o	29	Total	C	N	O	S	0	0
			228	151	36	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

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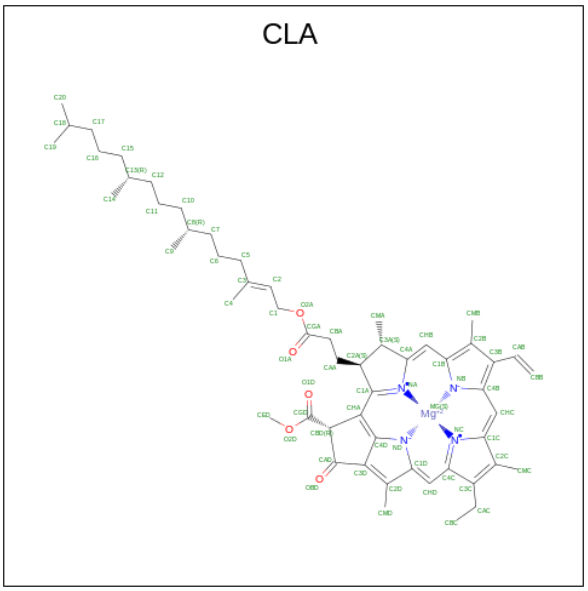
Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	5	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	6	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	Y	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	Z	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	a	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	b	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	c	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	d	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	q	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	r	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	s	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	t	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	u	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	v	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	T	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	m	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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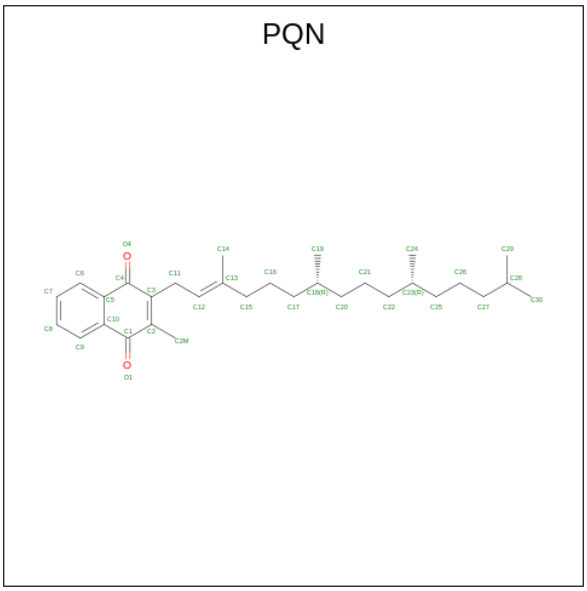
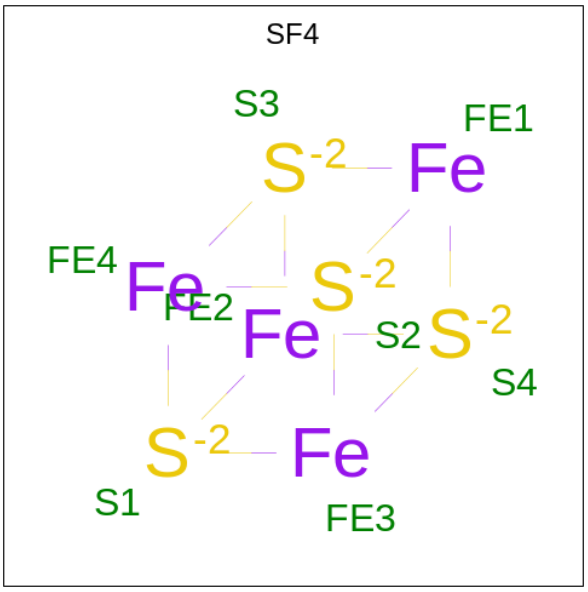
Mol	Chain	Residues	Atoms					AltConf
13	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	v	1	Total 46	C 36	Mg 1	N 4	O 5	0

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



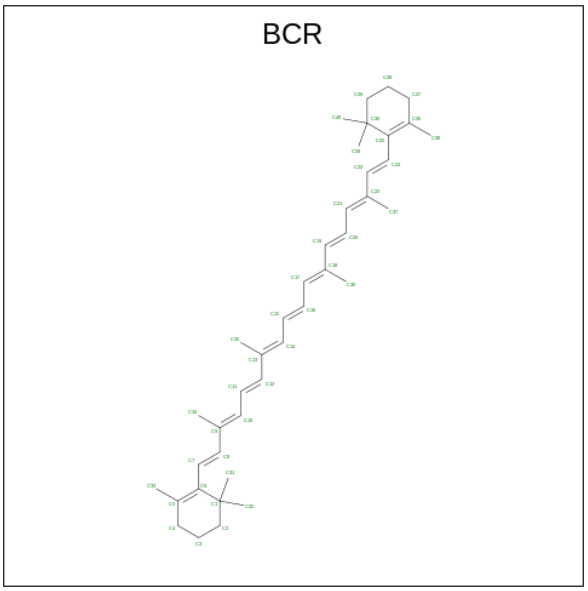
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C O 33 31 2	0
14	B	1	Total C O 33 31 2	0
14	G	1	Total C O 33 31 2	0
14	H	1	Total C O 33 31 2	0
14	e	1	Total C O 33 31 2	0
14	f	1	Total C O 33 31 2	0

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0
15	G	1	Total Fe S 8 4 4	0
15	N	1	Total Fe S 8 4 4	0
15	N	1	Total Fe S 8 4 4	0
15	e	1	Total Fe S 8 4 4	0
15	g	1	Total Fe S 8 4 4	0
15	g	1	Total Fe S 8 4 4	0

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	3	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	R	1	Total C 40 40	0
16	S	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	U	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	W	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Z	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	o	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0

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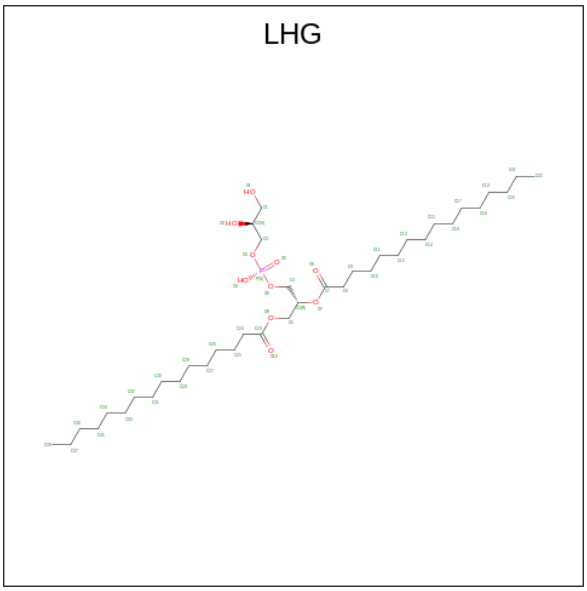
Mol	Chain	Residues	Atoms	AltConf
16	v	1	Total C 40 40	0
16	v	1	Total C 40 40	0
16	v	1	Total C 40 40	0
16	v	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C O P 39 28 10 1	0
17	A	1	Total C O P 36 25 10 1	0
17	A	1	Total C O P 45 34 10 1	0
17	A	1	Total C O P 45 34 10 1	0
17	A	1	Total C O P 47 36 10 1	0
17	A	1	Total C O P 35 24 10 1	0
17	A	1	Total C O P 49 38 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			39	28	10	1	
17	B	1	Total	C	O	P	0
			44	33	10	1	
17	I	1	Total	C	O	P	0
			44	33	10	1	
17	L	1	Total	C	O	P	0
			38	27	10	1	
17	L	1	Total	C	O	P	0
			41	30	10	1	
17	L	1	Total	C	O	P	0
			49	38	10	1	
17	G	1	Total	C	O	P	0
			39	28	10	1	
17	G	1	Total	C	O	P	0
			36	25	10	1	
17	G	1	Total	C	O	P	0
			45	34	10	1	
17	G	1	Total	C	O	P	0
			45	34	10	1	
17	G	1	Total	C	O	P	0
			47	36	10	1	
17	G	1	Total	C	O	P	0
			35	24	10	1	
17	G	1	Total	C	O	P	0
			49	38	10	1	
17	G	1	Total	C	O	P	0
			49	38	10	1	
17	G	1	Total	C	O	P	0
			41	30	10	1	
17	H	1	Total	C	O	P	0
			39	28	10	1	
17	H	1	Total	C	O	P	0
			44	33	10	1	
17	S	1	Total	C	O	P	0
			44	33	10	1	
17	V	1	Total	C	O	P	0
			38	27	10	1	

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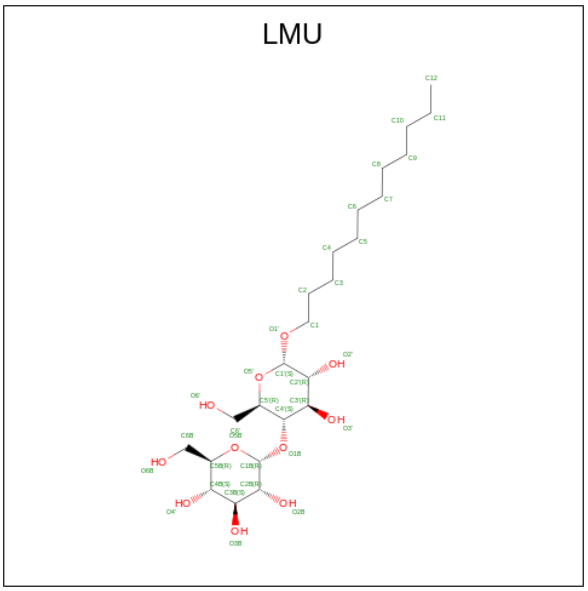
Mol	Chain	Residues	Atoms				AltConf
17	V	1	Total	C	O	P	0
			41	30	10	1	
17	V	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			39	28	10	1	
17	e	1	Total	C	O	P	0
			36	25	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			47	36	10	1	
17	e	1	Total	C	O	P	0
			35	24	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			41	30	10	1	
17	f	1	Total	C	O	P	0
			39	28	10	1	
17	f	1	Total	C	O	P	0
			44	33	10	1	
17	k	1	Total	C	O	P	0
			44	33	10	1	
17	n	1	Total	C	O	P	0
			38	27	10	1	
17	n	1	Total	C	O	P	0
			41	30	10	1	
17	n	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			23	17	6	
18	B	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			22	16	6	
18	1	1	Total	C	O	0
			19	13	6	
18	2	1	Total	C	O	0
			23	17	6	
18	G	1	Total	C	O	0
			35	24	11	
18	G	1	Total	C	O	0
			23	17	6	
18	H	1	Total	C	O	0
			35	24	11	
18	T	1	Total	C	O	0
			22	16	6	
18	Y	1	Total	C	O	0
			19	13	6	
18	Z	1	Total	C	O	0
			23	17	6	
18	e	1	Total	C	O	0
			35	24	11	
18	e	1	Total	C	O	0
			23	17	6	

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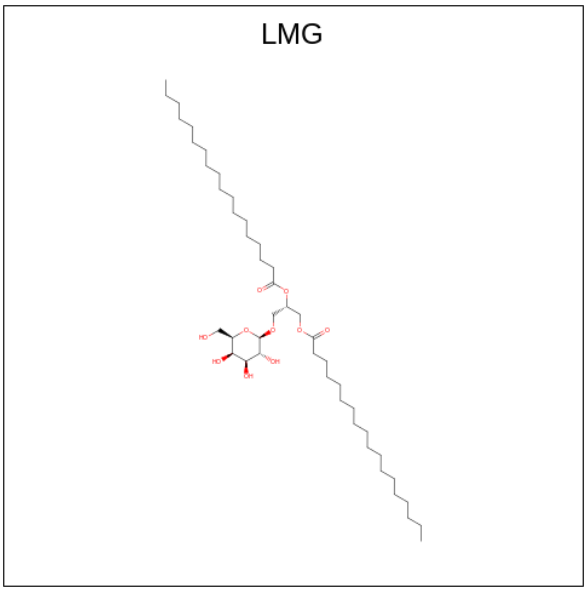
Mol	Chain	Residues	Atoms	AltConf
18	f	1	Total C O 35 24 11	0
18	l	1	Total C O 22 16 6	0
18	q	1	Total C O 19 13 6	0
18	r	1	Total C O 23 17 6	0

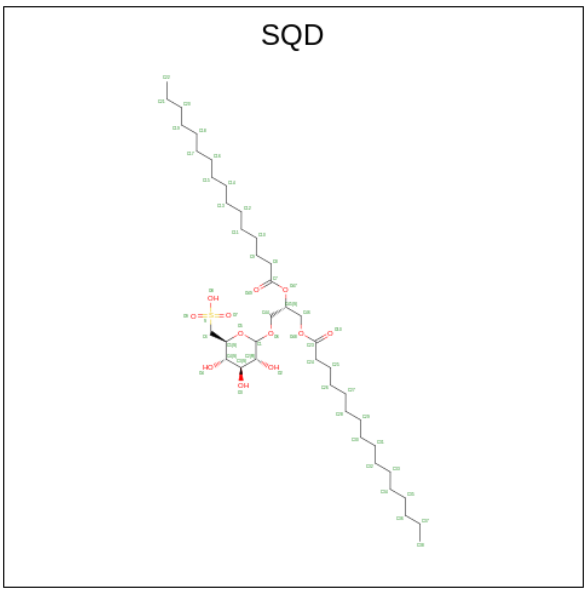
- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C O 54 44 10	0
19	J	1	Total C O 35 25 10	0
19	H	1	Total C O 54 44 10	0
19	T	1	Total C O 35 25 10	0
19	f	1	Total C O 54 44 10	0
19	l	1	Total C O 35 25 10	0

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	S	0
			45	32	12	1	
20	L	1	Total	C	O	S	0
			51	38	12	1	
20	1	1	Total	C	O	S	0
			48	35	12	1	
20	2	1	Total	C	O	S	0
			43	30	12	1	
20	3	1	Total	C	O	S	0
			43	30	12	1	
20	4	1	Total	C	O	S	0
			26	13	12	1	
20	5	1	Total	C	O	S	0
			29	16	12	1	
20	6	1	Total	C	O	S	0
			26	13	12	1	
20	H	1	Total	C	O	S	0
			45	32	12	1	
20	V	1	Total	C	O	S	0
			51	38	12	1	
20	Y	1	Total	C	O	S	0
			48	35	12	1	
20	Z	1	Total	C	O	S	0
			43	30	12	1	
20	a	1	Total	C	O	S	0
			43	30	12	1	

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Mol	Chain	Residues	Atoms				AltConf
20	b	1	Total	C	O	S	0
			26	13	12	1	
20	c	1	Total	C	O	S	0
			29	16	12	1	
20	d	1	Total	C	O	S	0
			26	13	12	1	
20	f	1	Total	C	O	S	0
			45	32	12	1	
20	n	1	Total	C	O	S	0
			51	38	12	1	
20	q	1	Total	C	O	S	0
			48	35	12	1	
20	r	1	Total	C	O	S	0
			43	30	12	1	
20	s	1	Total	C	O	S	0
			43	30	12	1	
20	t	1	Total	C	O	S	0
			26	13	12	1	
20	u	1	Total	C	O	S	0
			29	16	12	1	
20	v	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	9	Total	O	0
			9	9	
21	B	7	Total	O	0
			7	7	
21	F	1	Total	O	0
			1	1	
21	L	1	Total	O	0
			1	1	
21	G	9	Total	O	0
			9	9	
21	H	7	Total	O	0
			7	7	
21	R	1	Total	O	0
			1	1	
21	V	1	Total	O	0
			1	1	

Continued on next page...

Continued from previous page...

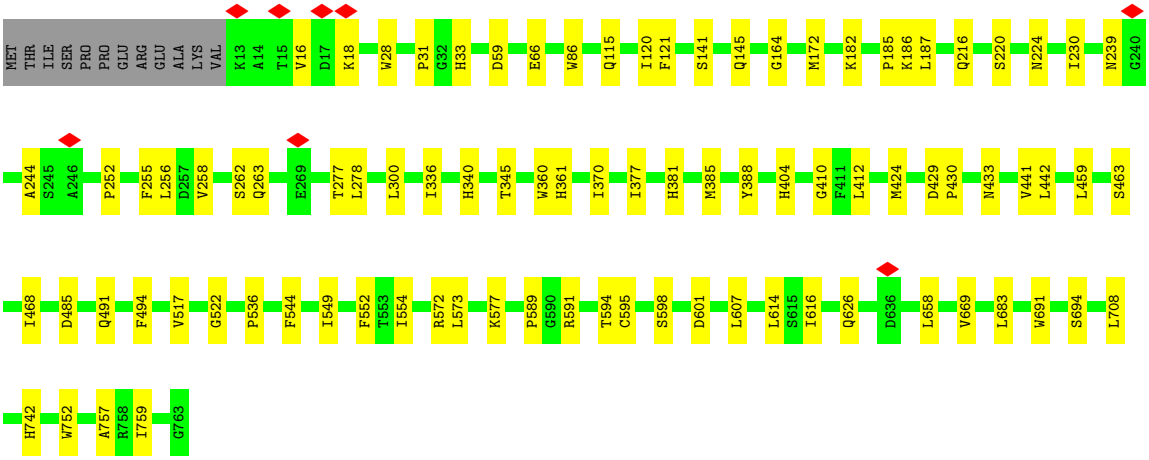
Mol	Chain	Residues	Atoms	AltConf
21	e	9	Total O 9 9	0
21	f	7	Total O 7 7	0
21	j	1	Total O 1 1	0
21	n	1	Total O 1 1	0

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.

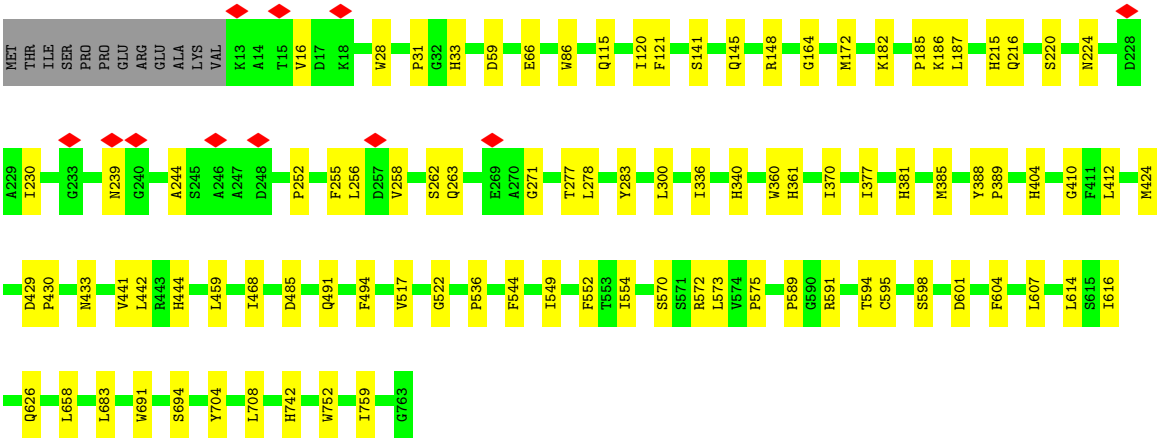
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



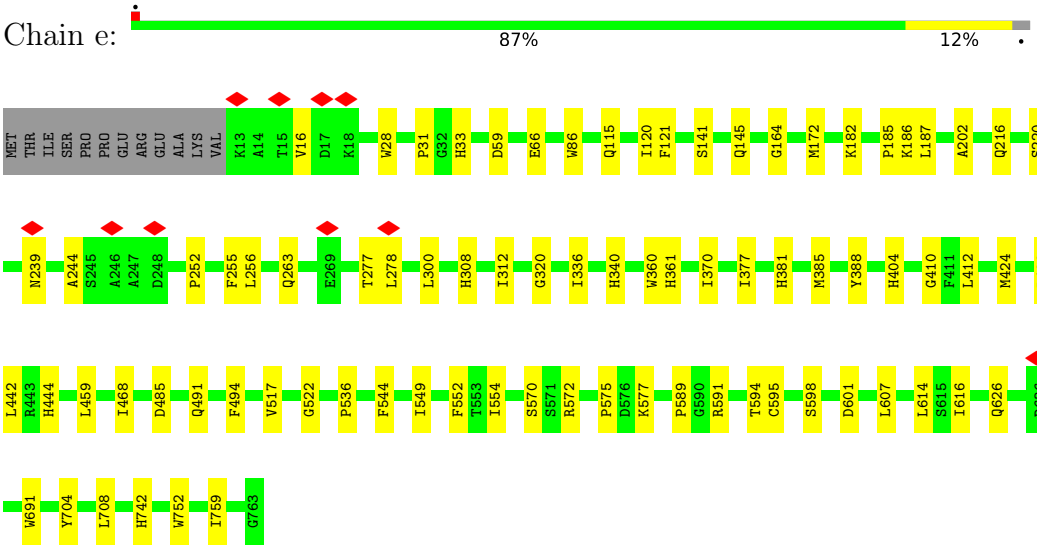
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain G:



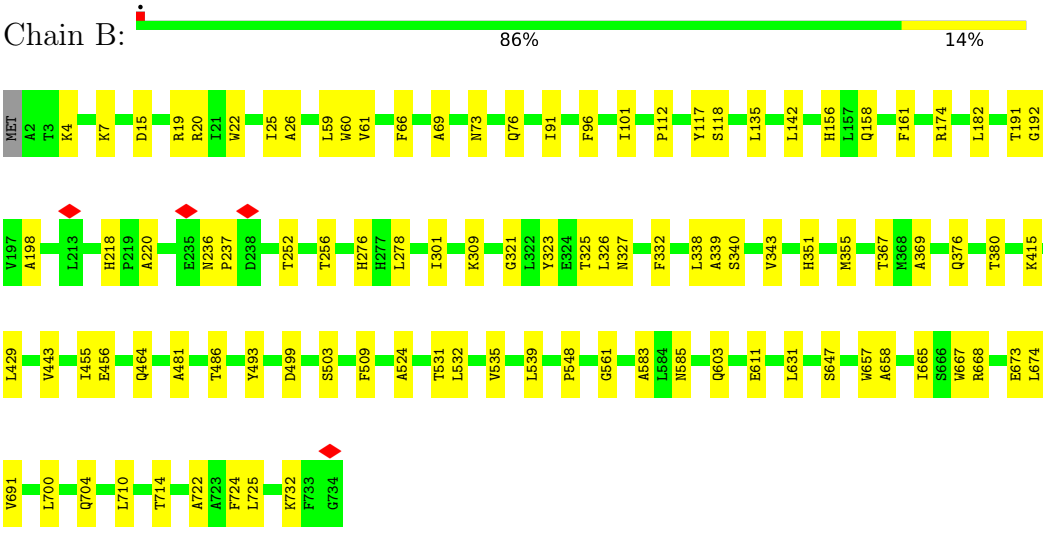
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e:



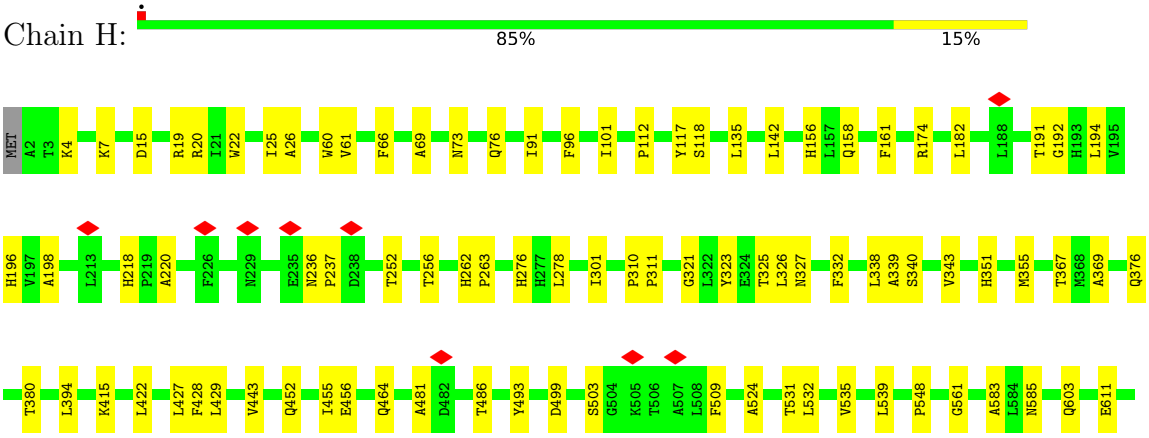
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

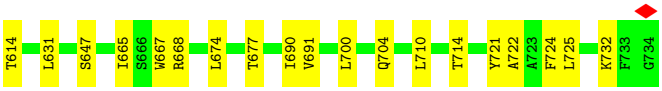
Chain B:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H:



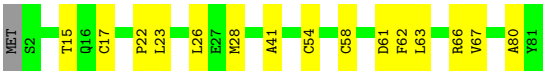


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f:

• Molecule 3: Photosystem I iron-sulfur center

Chain C:

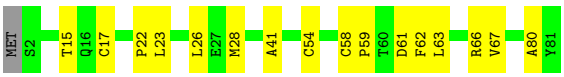


• Molecule 3: Photosystem I iron-sulfur center

Chain N:

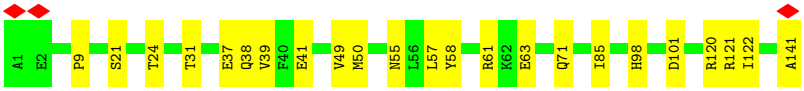
• Molecule 3: Photosystem I iron-sulfur center

Chain g:



• Molecule 4: Photosystem I reaction center subunit II

Chain D:

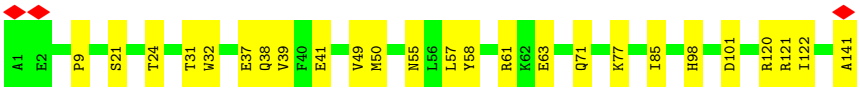


• Molecule 4: Photosystem I reaction center subunit II

Chain O:

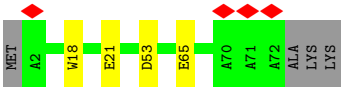
• Molecule 4: Photosystem I reaction center subunit II

Chain h:



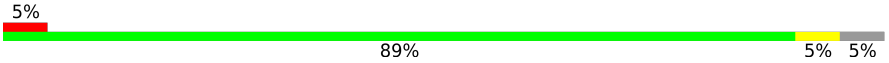
• Molecule 5: Photosystem I reaction center subunit IV

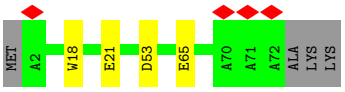
Chain E:



• Molecule 5: Photosystem I reaction center subunit IV

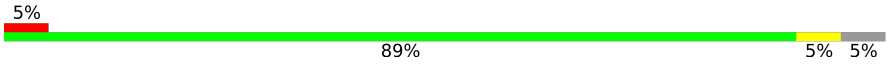
Chain Q:

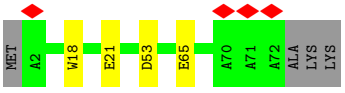




• Molecule 5: Photosystem I reaction center subunit IV

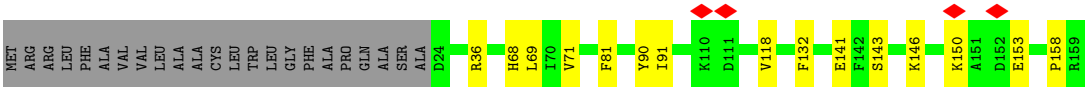
Chain i:





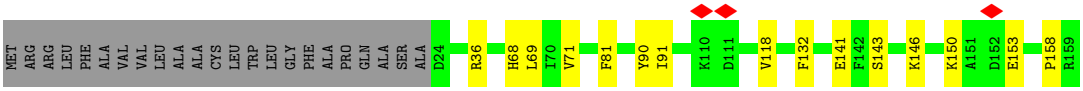
• Molecule 6: Photosystem I reaction center subunit III

Chain F:

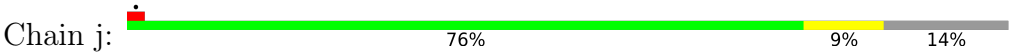


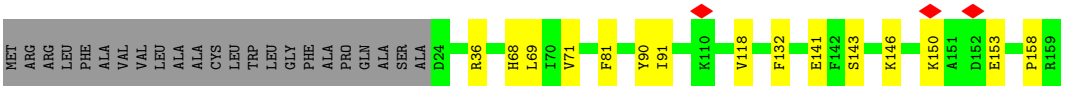
• Molecule 6: Photosystem I reaction center subunit III

Chain R:

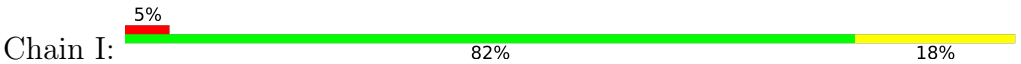


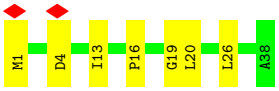
• Molecule 6: Photosystem I reaction center subunit III



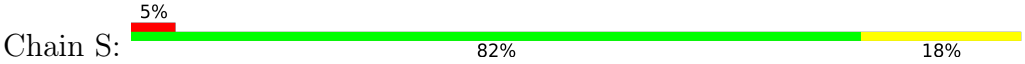


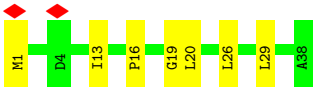
• Molecule 7: Photosystem I PsaI protein



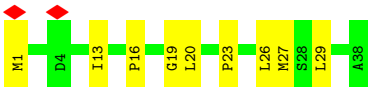


• Molecule 7: Photosystem I PsaI protein

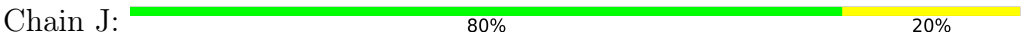


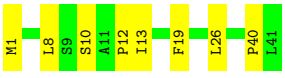


• Molecule 7: Photosystem I PsaI protein

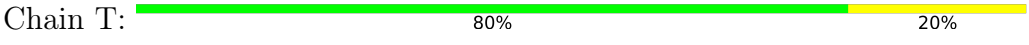


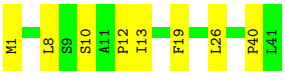
• Molecule 8: Photosystem I reaction center subunit IX





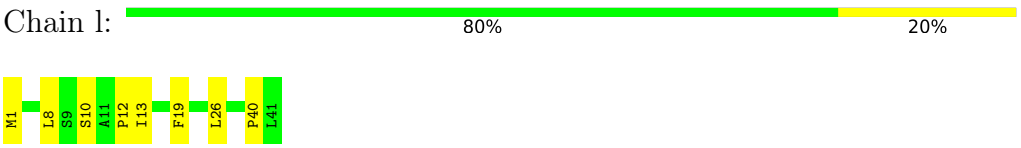
• Molecule 8: Photosystem I reaction center subunit IX





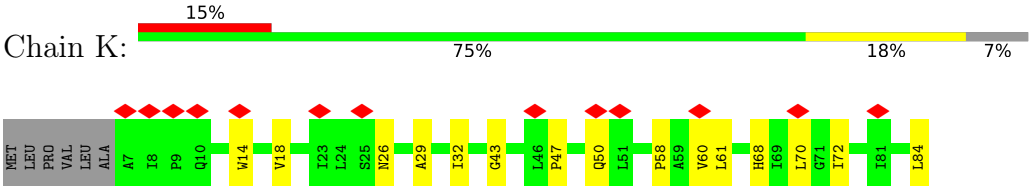
• Molecule 8: Photosystem I reaction center subunit IX

Chain l:



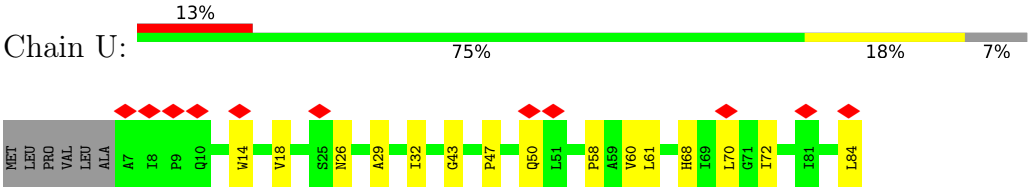
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



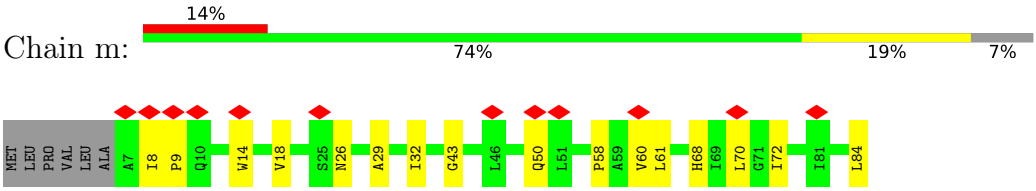
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain U:



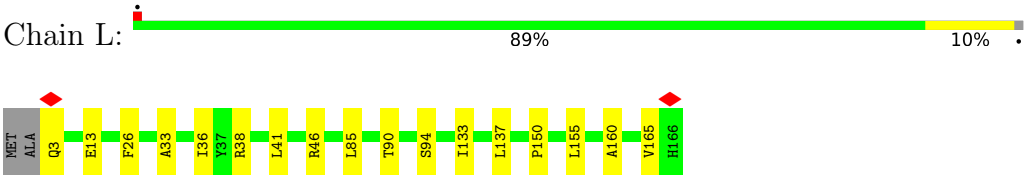
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain m:



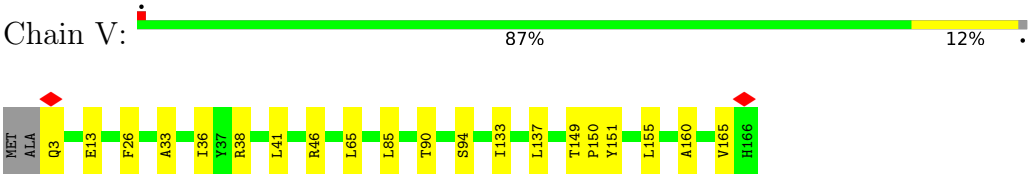
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



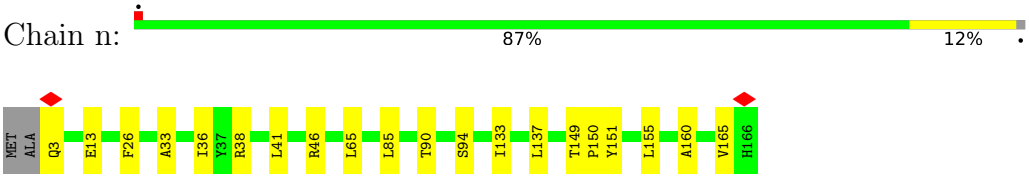
• Molecule 10: Photosystem I reaction center subunit XI

Chain V:



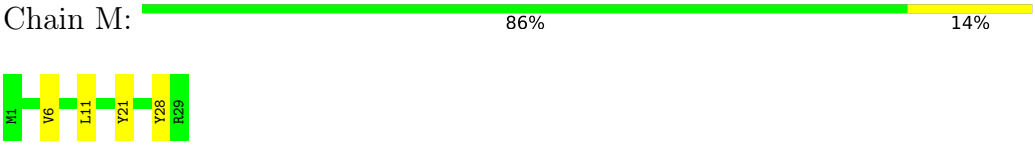
• Molecule 10: Photosystem I reaction center subunit XI

Chain n:



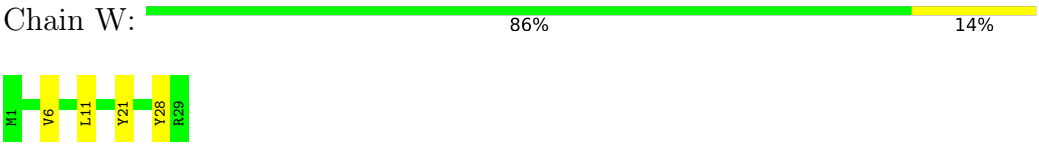
• Molecule 11: PsaM

Chain M:



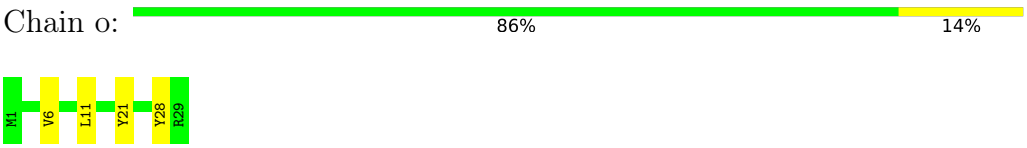
• Molecule 11: PsaM

Chain W:



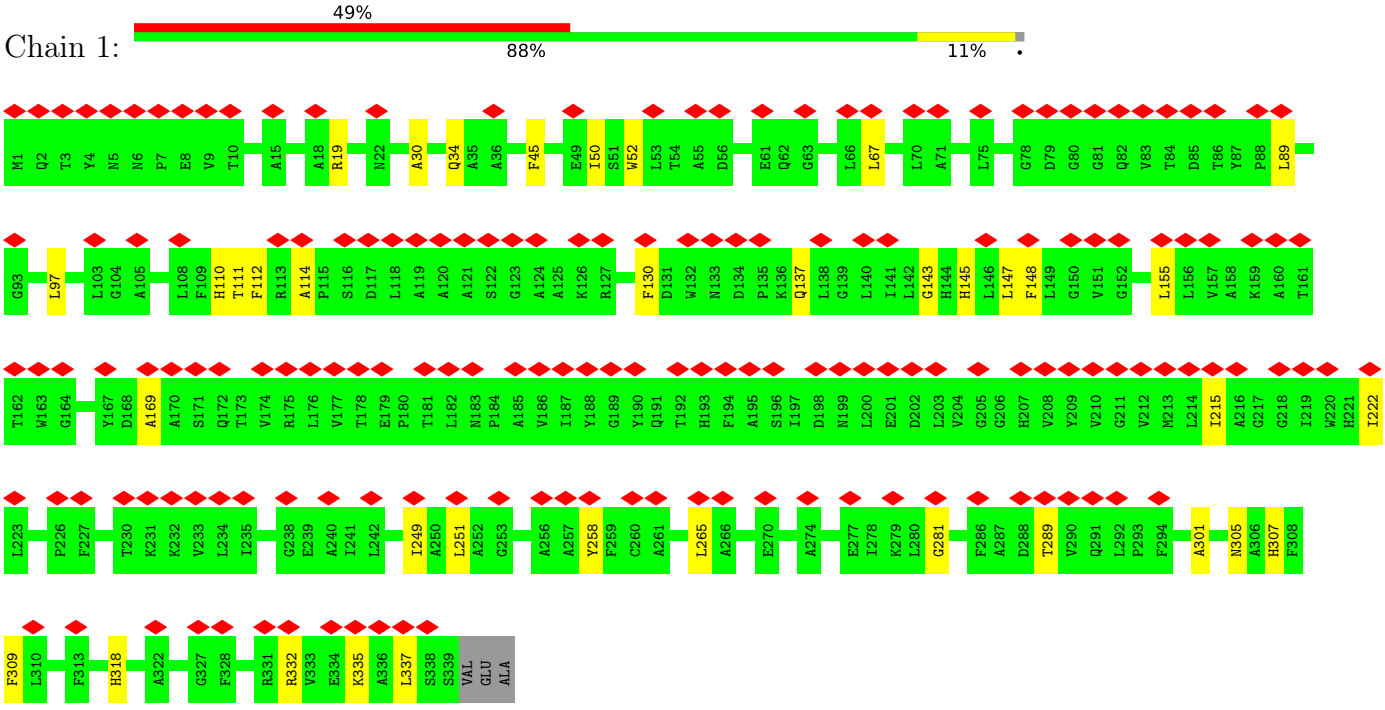
• Molecule 11: PsaM

Chain o:



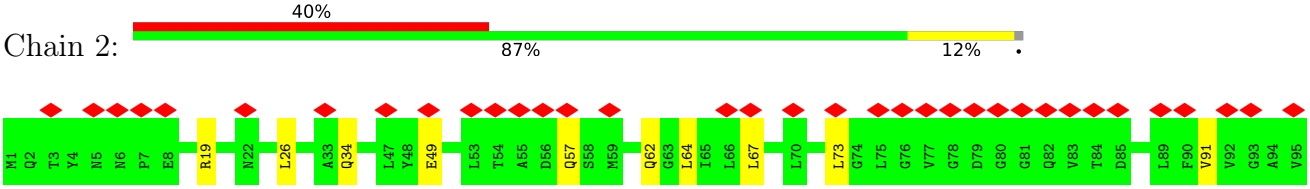
• Molecule 12: Iron stress-induced chlorophyll-binding protein

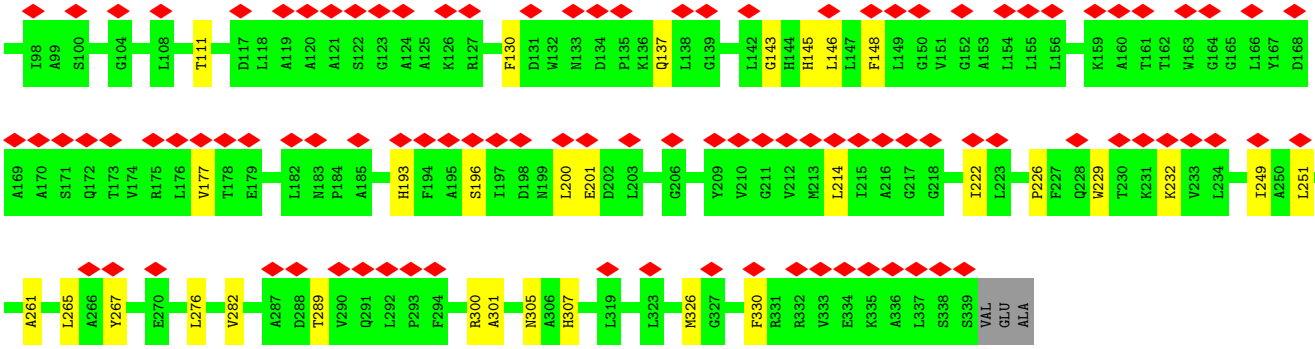
Chain 1:



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

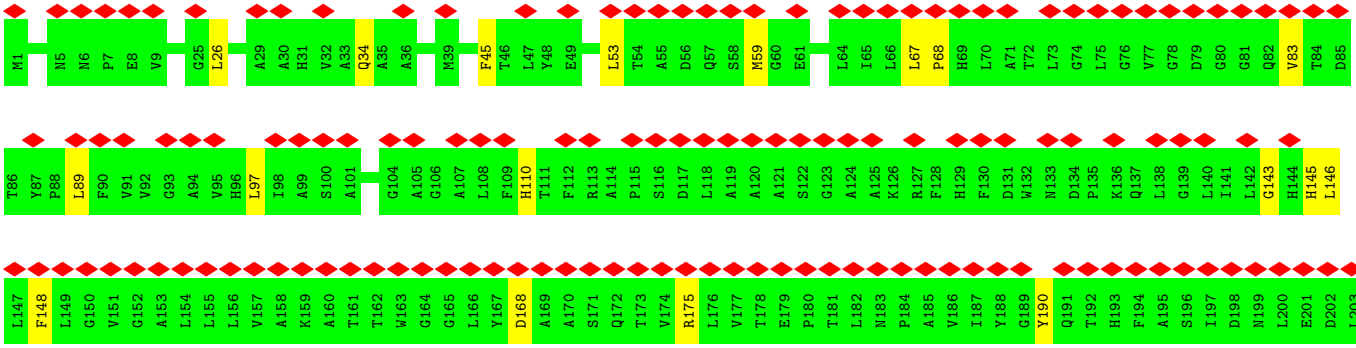
Chain 2:





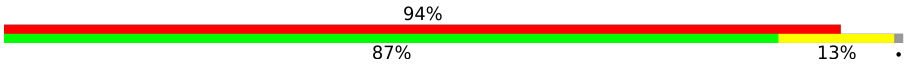
• Molecule 12: Iron stress-induced chlorophyll-binding protein

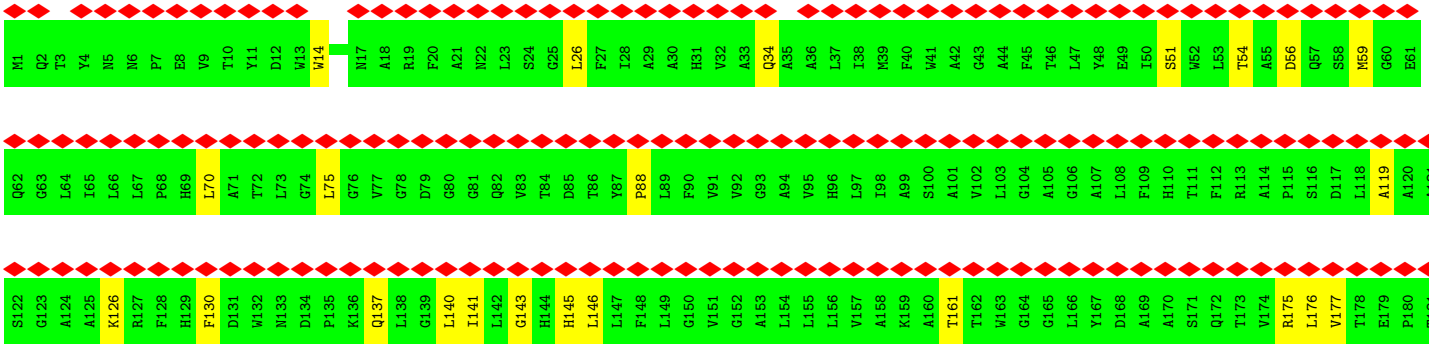
Chain 3:

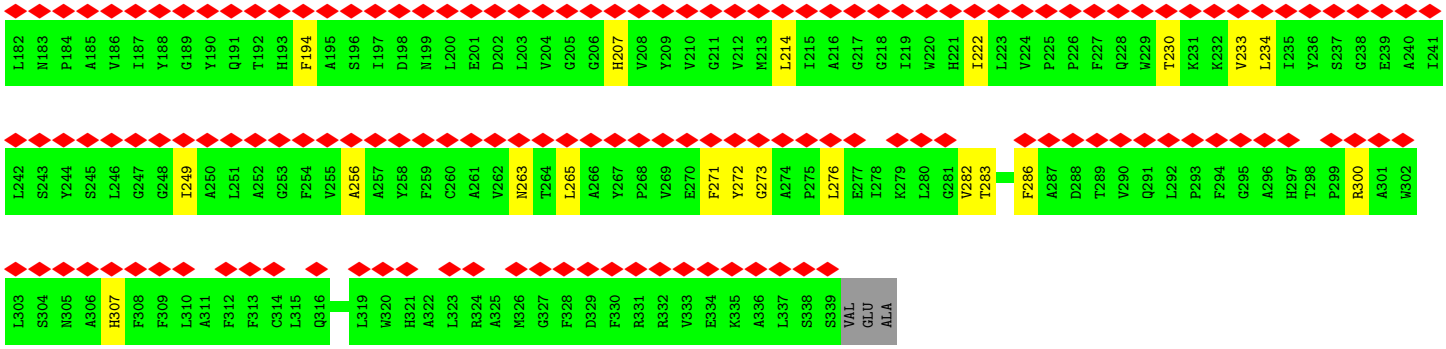


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 4:

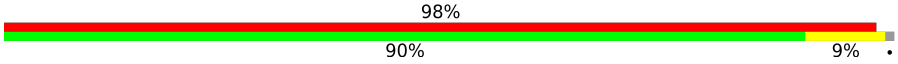


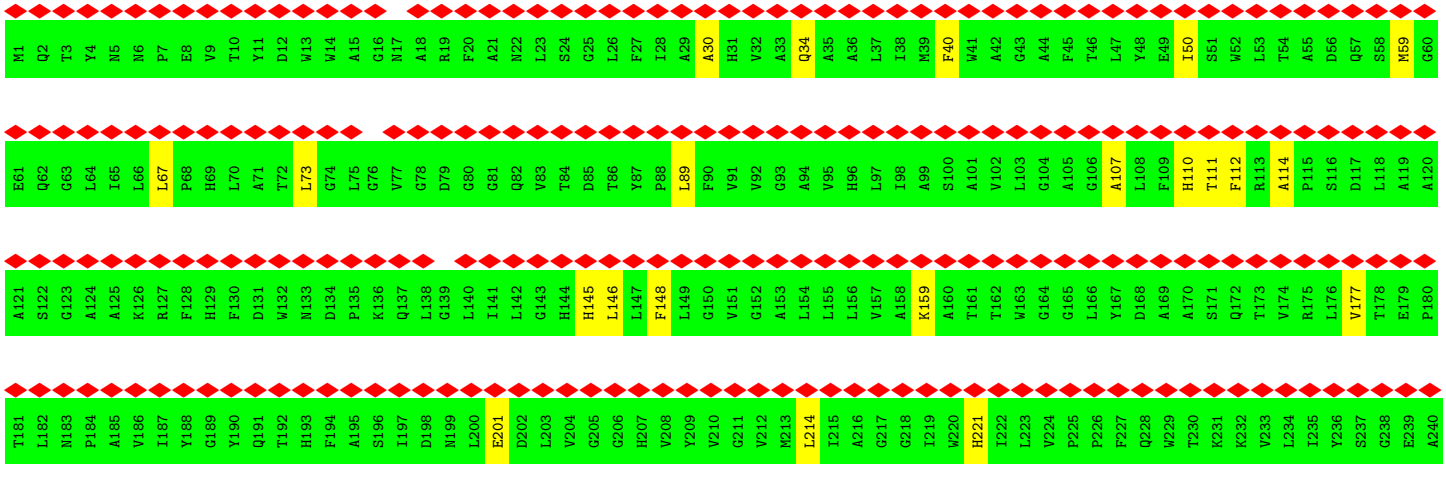


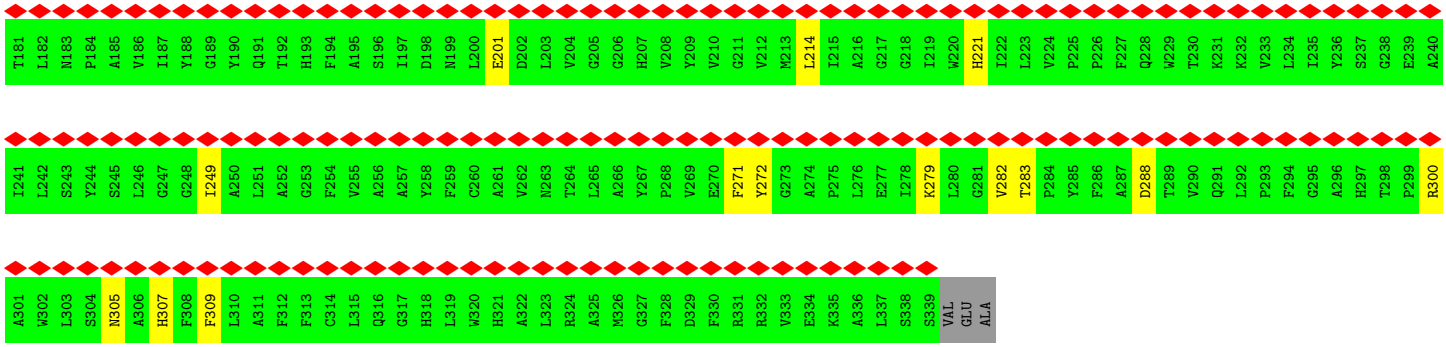


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 5:

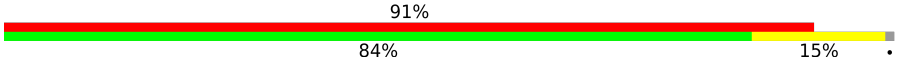


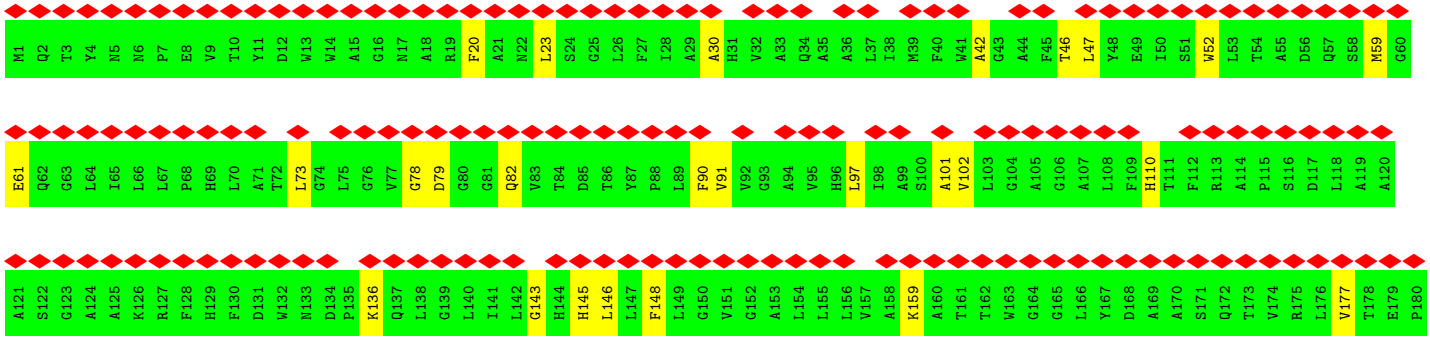


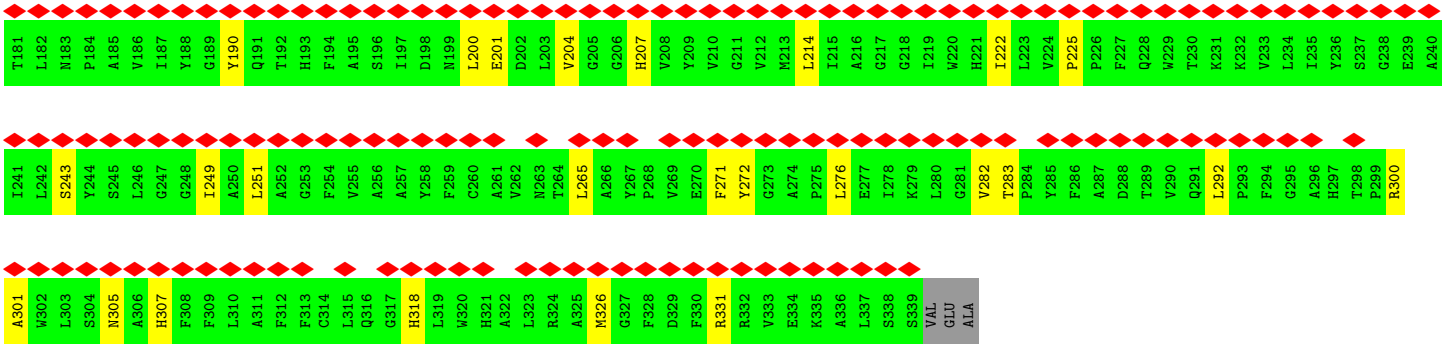


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 6:

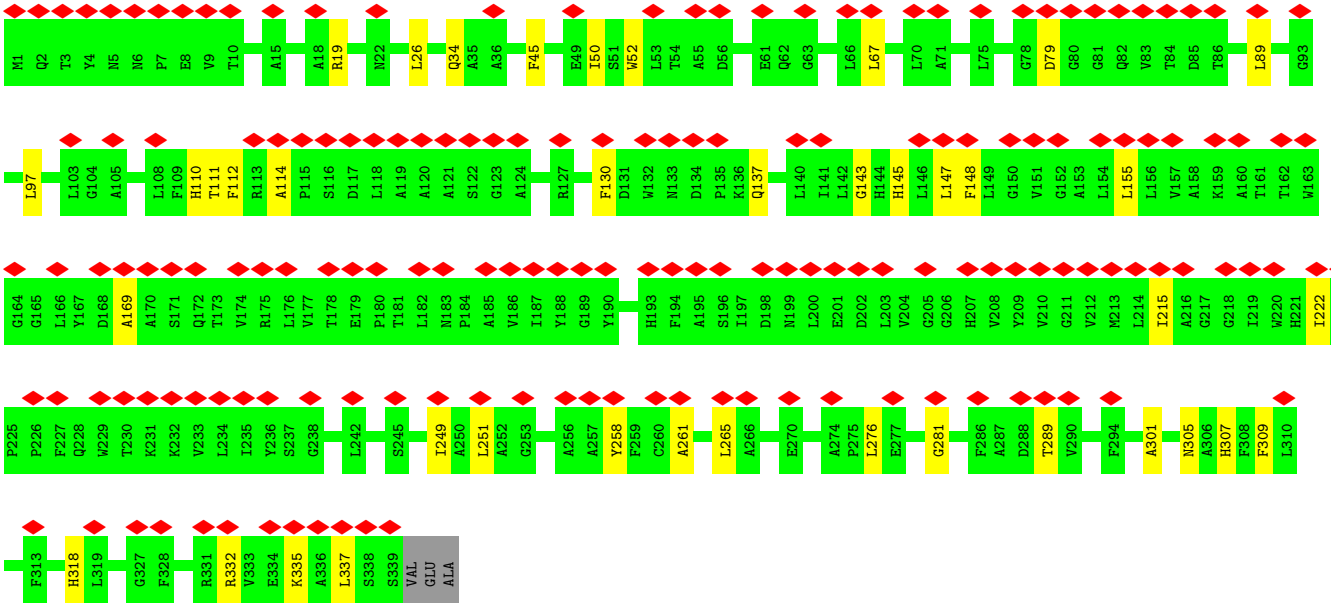






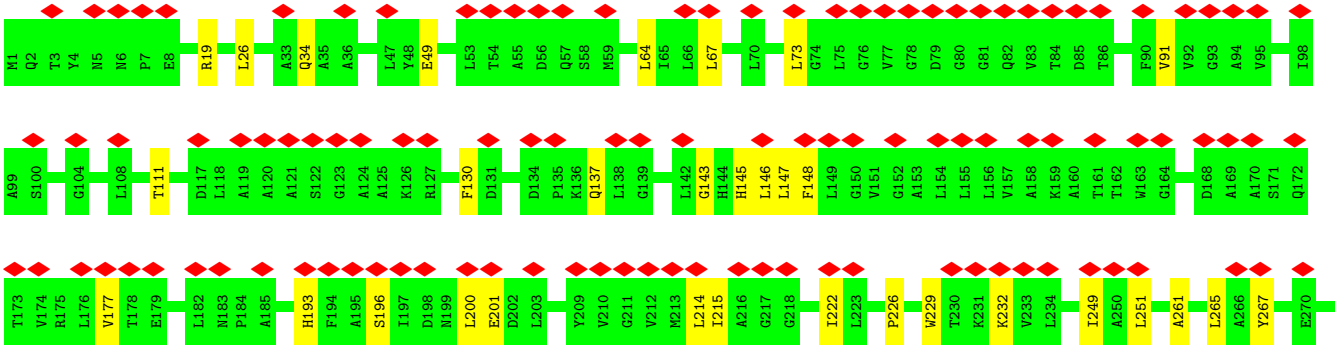
• Molecule 12: Iron stress-induced chlorophyll-binding protein

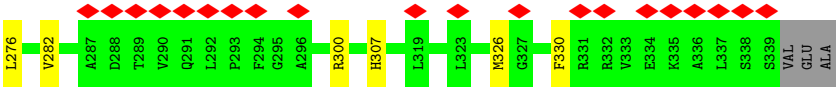
Chain Y:



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

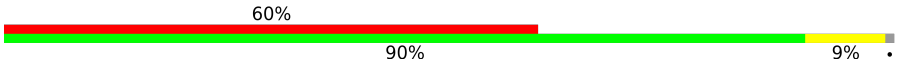
Chain Z:

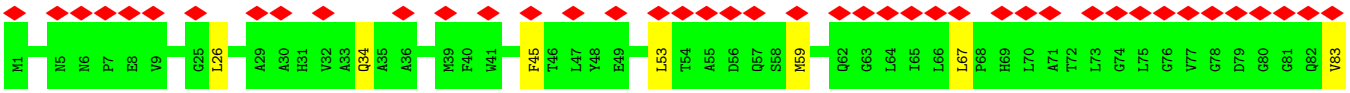


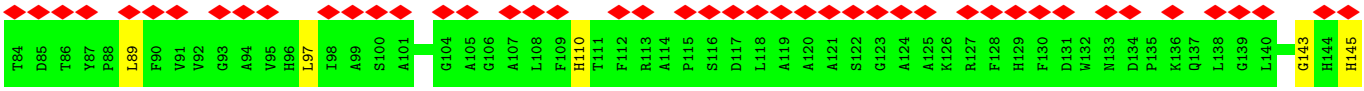


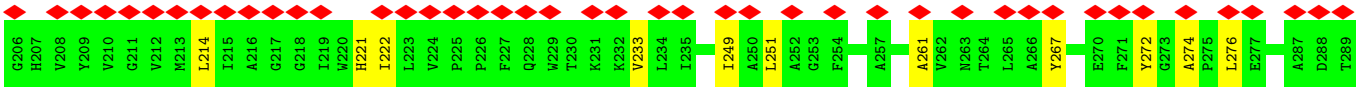
• Molecule 12: Iron stress-induced chlorophyll-binding protein

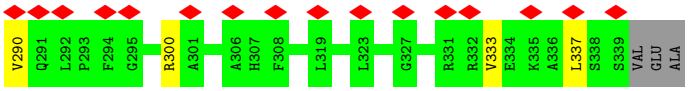
Chain a:





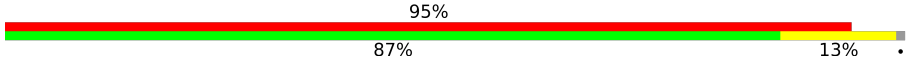


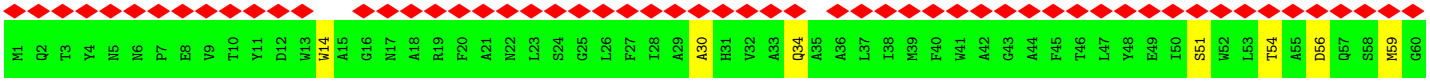


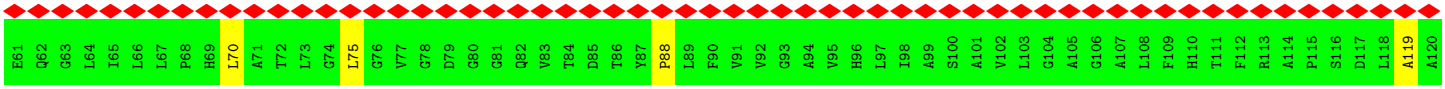


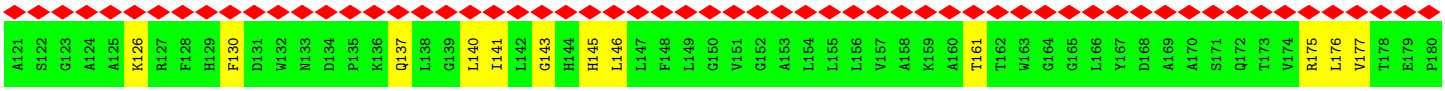
• Molecule 12: Iron stress-induced chlorophyll-binding protein

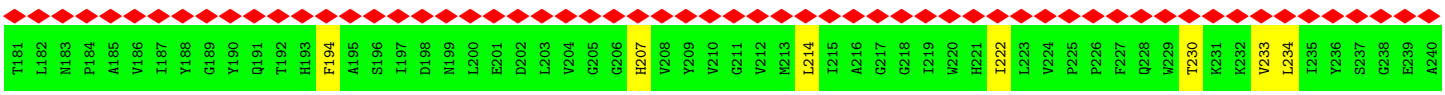
Chain b:

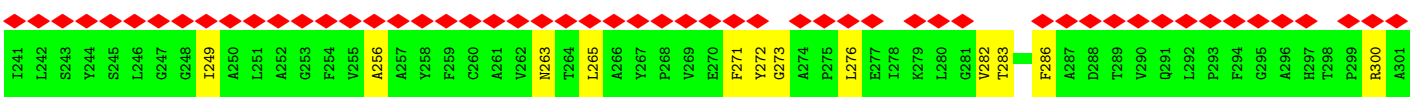


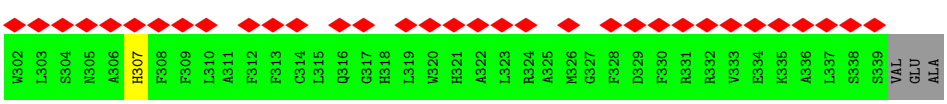






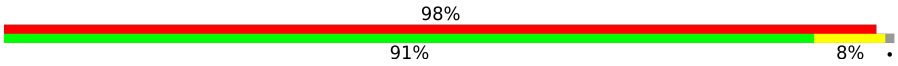


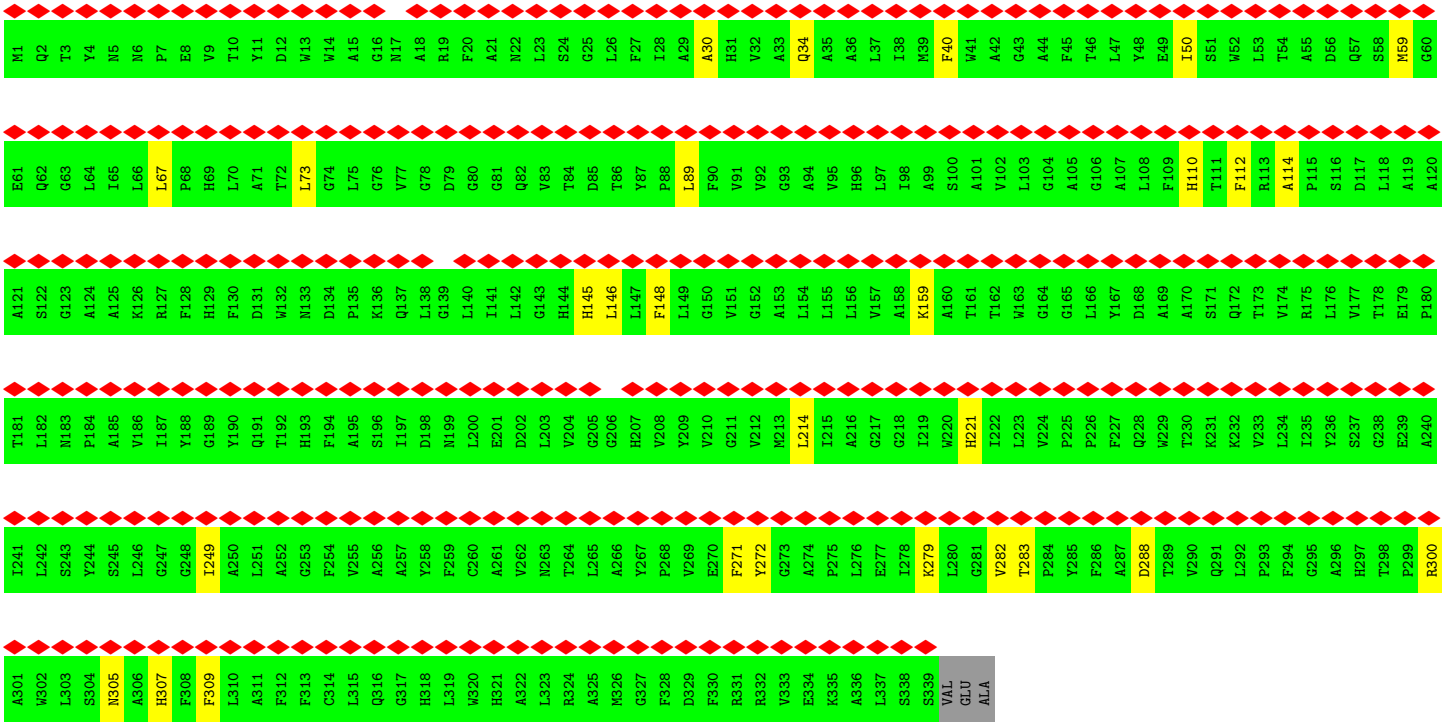




• Molecule 12: Iron stress-induced chlorophyll-binding protein

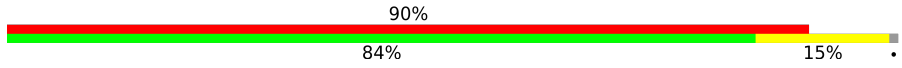
Chain c:

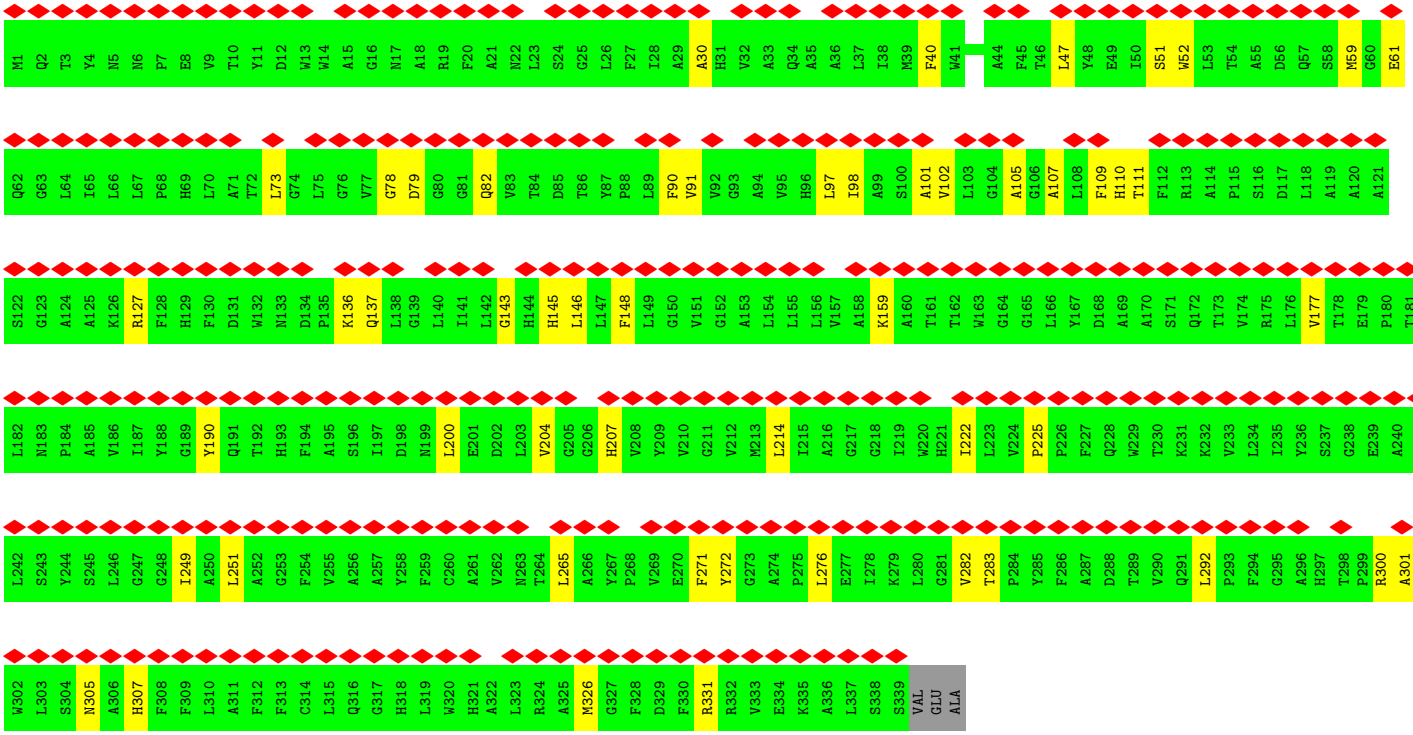




• Molecule 12: Iron stress-induced chlorophyll-binding protein

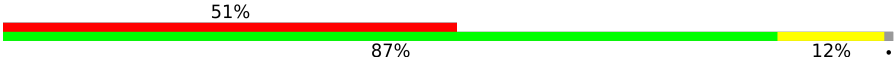
Chain d:

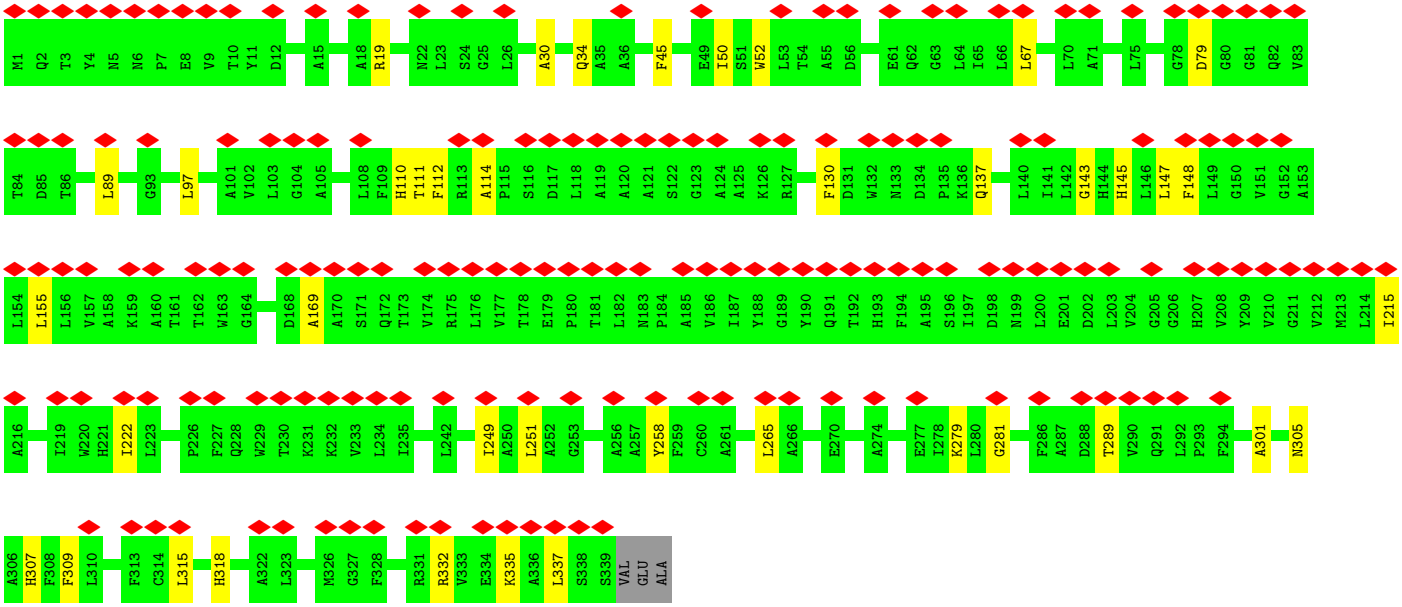




• Molecule 12: Iron stress-induced chlorophyll-binding protein

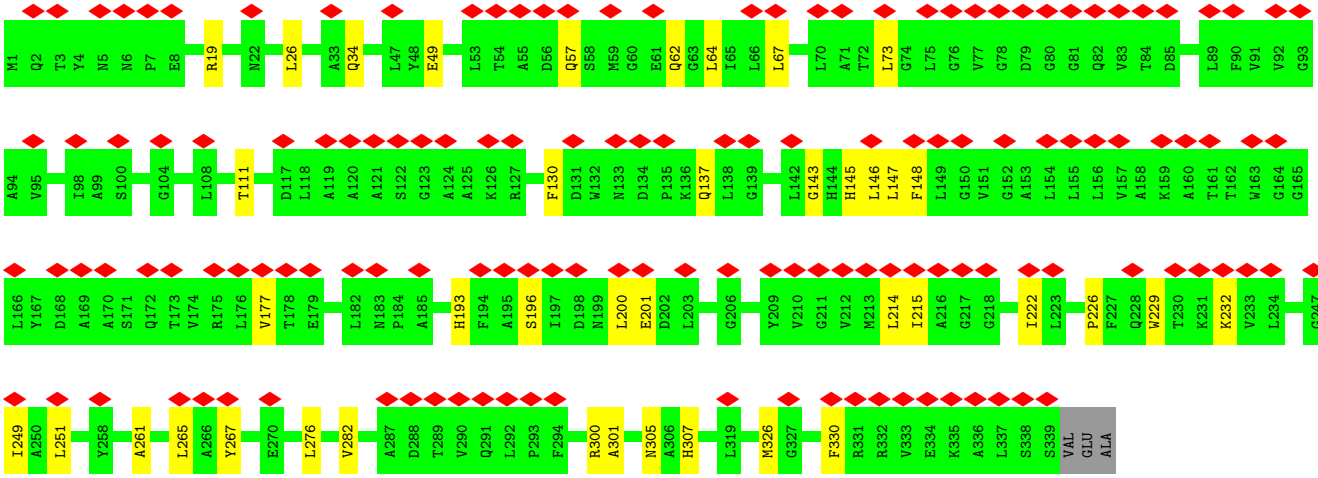
Chain q:





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

Chain r:



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

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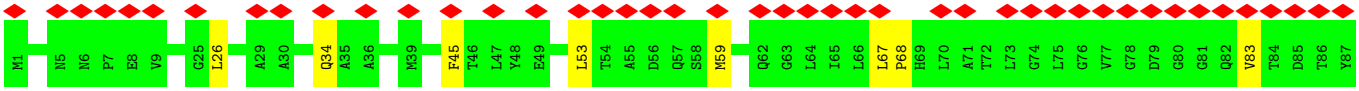
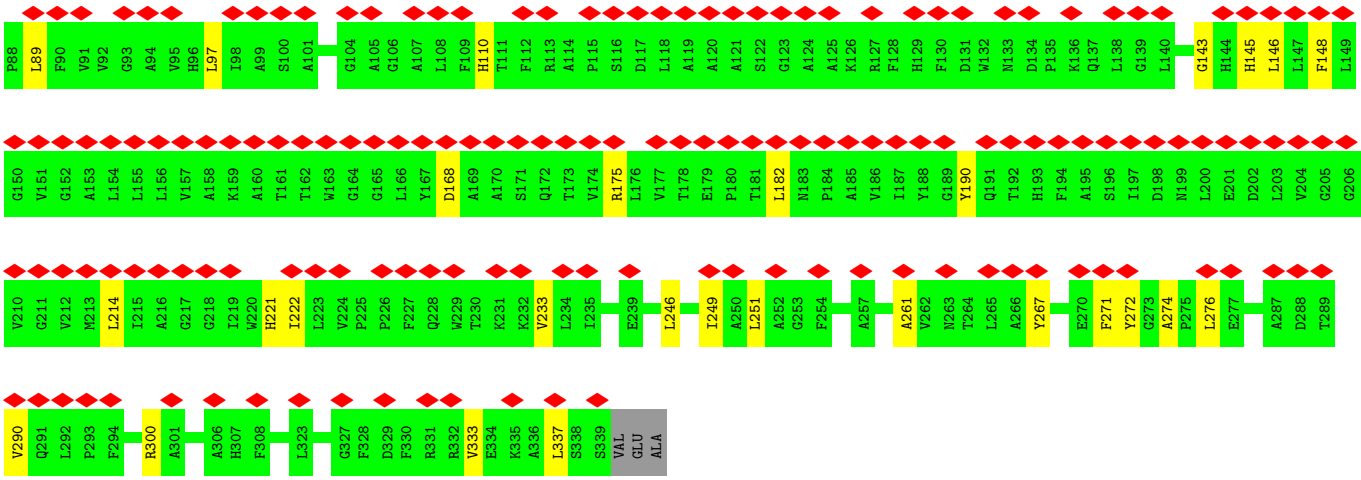
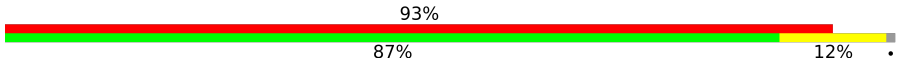
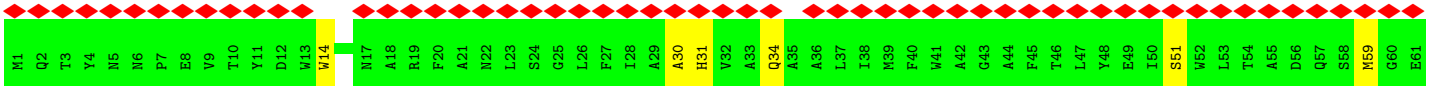


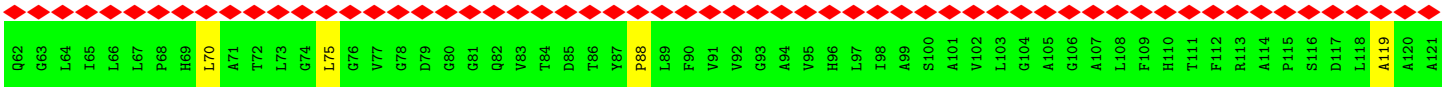


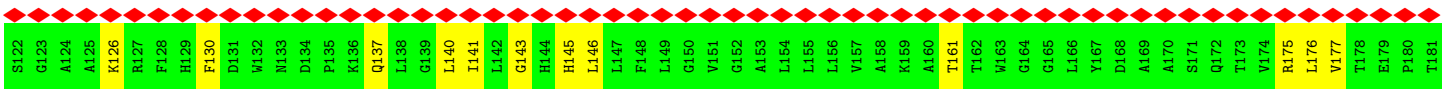
• Molecule 12: Iron stress-induced chlorophyll-binding protein

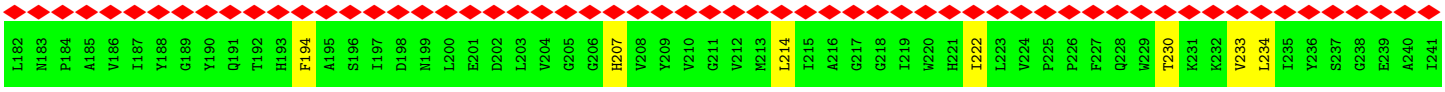
Chain t:

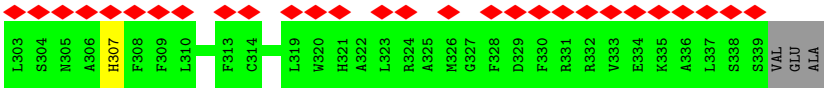






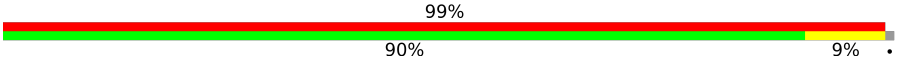


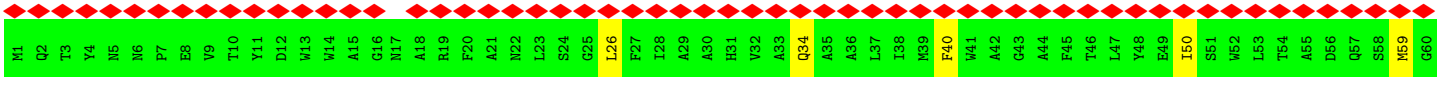


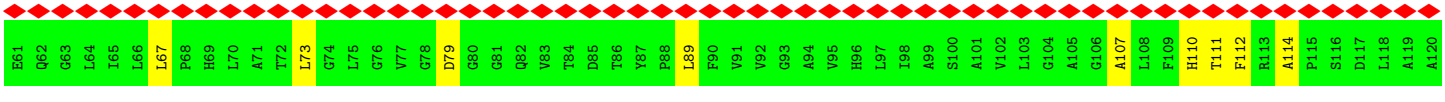


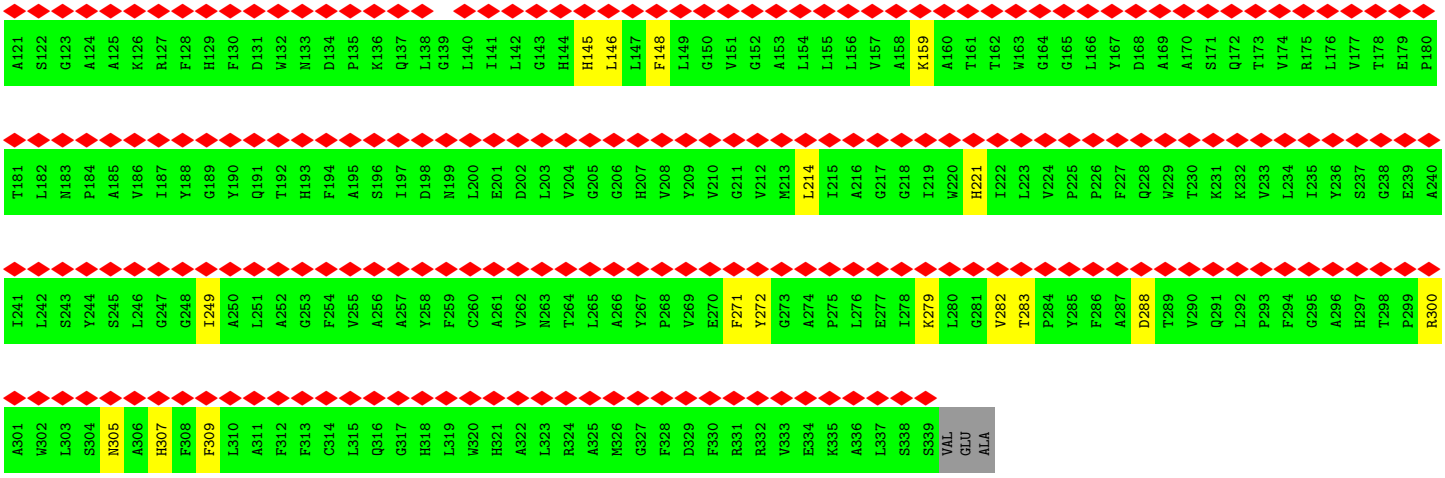
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain u:



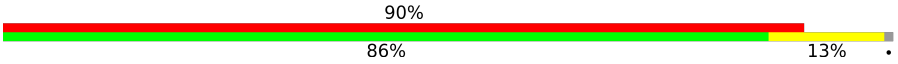


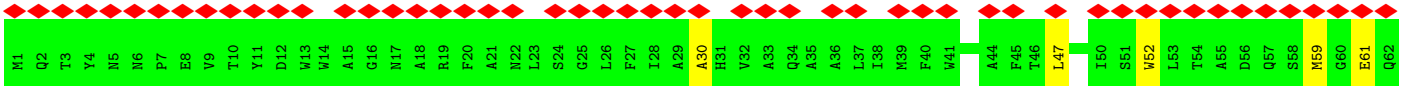


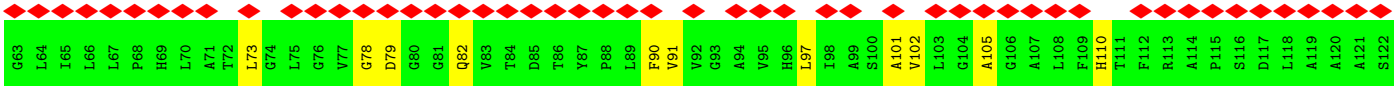


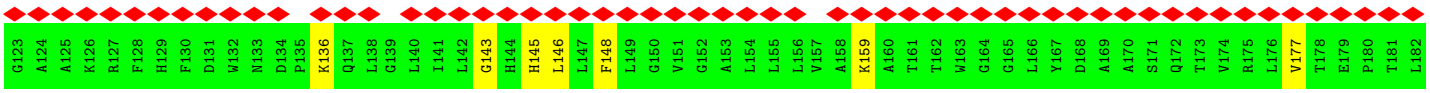
• Molecule 12: Iron stress-induced chlorophyll-binding protein

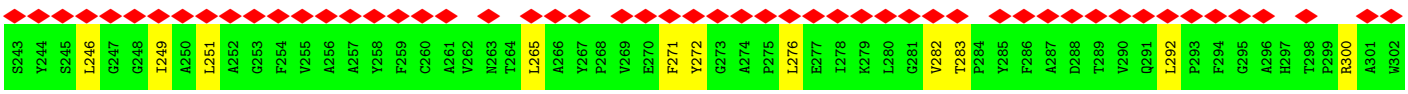
Chain v:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	63332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.37	0/6064	0.51	0/8274
1	G	0.37	0/6064	0.51	0/8274
1	e	0.37	0/6064	0.51	0/8274
2	B	0.37	0/5999	0.53	2/8199 (0.0%)
2	H	0.37	0/5999	0.53	2/8199 (0.0%)
2	f	0.37	0/5999	0.53	2/8199 (0.0%)
3	C	0.38	0/608	0.57	0/823
3	N	0.39	0/608	0.56	0/823
3	g	0.39	0/608	0.56	0/823
4	D	0.29	0/1124	0.47	0/1516
4	O	0.30	0/1124	0.47	0/1516
4	h	0.30	0/1124	0.47	0/1516
5	E	0.27	0/553	0.41	0/750
5	Q	0.27	0/553	0.41	0/750
5	i	0.27	0/553	0.42	0/750
6	F	0.30	0/1062	0.50	0/1442
6	R	0.30	0/1062	0.50	0/1442
6	j	0.30	0/1062	0.50	0/1442
7	I	0.33	0/289	0.60	0/393
7	S	0.33	0/289	0.60	0/393
7	k	0.33	0/289	0.60	0/393
8	J	0.37	0/346	0.51	0/469
8	T	0.37	0/346	0.51	0/469
8	l	0.37	0/346	0.51	0/469
9	K	0.27	0/560	0.54	0/765
9	U	0.27	0/560	0.54	0/765
9	m	0.27	0/560	0.54	0/765
10	L	0.28	0/1242	0.49	0/1696
10	V	0.28	0/1242	0.49	0/1696
10	n	0.28	0/1242	0.49	0/1696
11	M	0.33	0/231	0.53	0/314
11	W	0.33	0/231	0.53	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	o	0.33	0/231	0.53	0/314
12	1	0.20	0/2689	0.42	0/3678
12	2	0.19	0/2689	0.41	0/3678
12	3	0.18	0/2689	0.39	0/3678
12	4	0.18	0/2689	0.41	0/3678
12	5	0.17	0/2689	0.40	2/3678 (0.1%)
12	6	0.16	0/2689	0.39	0/3678
12	Y	0.21	0/2689	0.42	0/3678
12	Z	0.20	0/2689	0.41	0/3678
12	a	0.18	0/2689	0.39	0/3678
12	b	0.18	0/2689	0.41	0/3678
12	c	0.17	0/2689	0.40	2/3678 (0.1%)
12	d	0.17	0/2689	0.39	0/3678
12	q	0.21	0/2689	0.42	0/3678
12	r	0.20	0/2689	0.41	0/3678
12	s	0.18	0/2689	0.39	0/3678
12	t	0.18	0/2689	0.40	0/3678
12	u	0.17	0/2689	0.40	2/3678 (0.1%)
12	v	0.17	0/2689	0.39	0/3678
All	All	0.28	0/102636	0.46	12/140127 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	665	ILE	N-CA-C	9.10	119.65	110.82
2	f	665	ILE	N-CA-C	9.10	119.65	110.82
2	H	665	ILE	N-CA-C	9.07	119.62	110.82
2	B	668	ARG	N-CA-C	8.15	120.16	111.28
2	f	668	ARG	N-CA-C	8.13	120.14	111.28
2	H	668	ARG	N-CA-C	8.12	120.13	111.28
12	c	288	ASP	CA-C-N	5.12	131.31	121.54
12	c	288	ASP	C-N-CA	5.12	131.31	121.54
12	u	288	ASP	CA-C-N	5.11	131.31	121.54
12	u	288	ASP	C-N-CA	5.11	131.31	121.54
12	5	288	ASP	CA-C-N	5.10	131.28	121.54
12	5	288	ASP	C-N-CA	5.10	131.28	121.54

There are no chirality outliers.

There are no planarity outliers.

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	5865	0	5744	70	0
1	G	5865	0	5744	73	0
1	e	5865	0	5744	71	0
2	B	5789	0	5575	83	0
2	H	5789	0	5575	83	0
2	f	5789	0	5575	83	0
3	C	598	0	579	10	0
3	N	598	0	579	9	0
3	g	598	0	579	11	0
4	D	1098	0	1099	16	0
4	O	1098	0	1099	16	0
4	h	1098	0	1099	17	0
5	E	543	0	525	3	0
5	Q	543	0	525	3	0
5	i	543	0	525	3	0
6	F	1036	0	1031	12	0
6	R	1036	0	1031	12	0
6	j	1036	0	1031	12	0
7	I	282	0	291	10	0
7	S	282	0	291	11	0
7	k	282	0	291	11	0
8	J	335	0	344	8	0
8	T	335	0	344	8	0
8	l	335	0	344	8	0
9	K	549	0	597	13	0
9	U	549	0	597	13	0
9	m	549	0	597	13	0
10	L	1210	0	1206	15	0
10	V	1210	0	1206	17	0
10	n	1210	0	1206	16	0
11	M	228	0	246	4	0
11	W	228	0	246	4	0
11	o	228	0	246	4	0
12	1	2605	0	2564	34	0
12	2	2605	0	2564	34	0
12	3	2605	0	2564	26	0
12	4	2605	0	2564	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	5	2605	0	2564	28	0
12	6	2605	0	2564	38	0
12	Y	2605	0	2564	36	0
12	Z	2605	0	2564	32	0
12	a	2605	0	2564	25	0
12	b	2605	0	2564	35	0
12	c	2605	0	2564	26	0
12	d	2605	0	2564	54	0
12	q	2605	0	2564	36	0
12	r	2605	0	2564	33	0
12	s	2605	0	2564	28	0
12	t	2605	0	2564	35	0
12	u	2605	0	2564	27	0
12	v	2605	0	2564	38	0
13	1	951	0	894	39	0
13	2	993	0	981	34	0
13	3	950	0	900	24	0
13	4	860	0	725	20	0
13	5	857	0	721	20	0
13	6	823	0	658	21	0
13	A	2728	0	2800	99	0
13	B	2550	0	2680	93	0
13	F	110	0	105	4	0
13	G	2728	0	2800	102	0
13	H	2550	0	2680	97	0
13	J	123	0	127	5	0
13	K	150	0	121	4	0
13	L	190	0	203	10	0
13	R	110	0	105	3	0
13	T	123	0	127	3	0
13	U	150	0	121	4	0
13	V	190	0	203	11	0
13	Y	951	0	894	36	0
13	Z	993	0	981	35	0
13	a	950	0	900	23	0
13	b	860	0	725	18	0
13	c	857	0	721	21	0
13	d	823	0	658	20	0
13	e	2728	0	2800	110	0
13	f	2550	0	2680	95	0
13	j	110	0	105	4	0
13	l	123	0	127	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	150	0	121	4	0
13	n	190	0	203	11	0
13	q	951	0	894	57	0
13	r	993	0	981	37	0
13	s	950	0	900	22	0
13	t	860	0	725	20	0
13	u	857	0	721	23	0
13	v	823	0	658	18	0
14	A	33	0	46	3	0
14	B	33	0	46	2	0
14	G	33	0	46	3	0
14	H	33	0	46	4	0
14	e	33	0	46	2	0
14	f	33	0	46	3	0
15	A	8	0	0	0	0
15	C	16	0	0	1	0
15	G	8	0	0	0	0
15	N	16	0	0	1	0
15	e	8	0	0	0	0
15	g	16	0	0	1	0
16	1	160	0	224	11	0
16	2	160	0	224	13	0
16	3	160	0	224	14	0
16	4	160	0	224	6	0
16	5	160	0	224	9	0
16	6	160	0	224	16	0
16	A	240	0	336	18	0
16	B	280	0	392	29	0
16	F	40	0	56	5	0
16	G	240	0	336	17	0
16	H	280	0	392	23	0
16	I	40	0	56	3	0
16	J	120	0	168	12	0
16	K	40	0	56	7	0
16	L	160	0	224	12	0
16	M	40	0	56	2	0
16	R	40	0	56	4	0
16	S	40	0	56	5	0
16	T	120	0	168	16	0
16	U	40	0	56	6	0
16	V	160	0	224	15	0
16	W	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	160	0	224	13	0
16	Z	160	0	224	10	0
16	a	160	0	224	13	0
16	b	160	0	224	8	0
16	c	160	0	224	11	0
16	d	160	0	224	21	0
16	e	240	0	336	17	0
16	f	280	0	392	26	0
16	j	40	0	56	3	0
16	k	40	0	56	4	0
16	l	120	0	168	14	0
16	m	40	0	56	5	0
16	n	160	0	224	15	0
16	o	40	0	56	4	0
16	q	160	0	224	11	0
16	r	160	0	224	13	0
16	s	160	0	224	11	0
16	t	160	0	224	9	0
16	u	160	0	224	12	0
16	v	160	0	224	15	0
17	A	386	0	520	19	0
17	B	83	0	109	4	0
17	G	386	0	520	17	0
17	H	83	0	109	5	0
17	I	44	0	58	1	0
17	L	128	0	172	13	0
17	S	44	0	58	0	0
17	V	128	0	172	11	0
17	e	386	0	520	20	0
17	f	83	0	109	4	0
17	k	44	0	58	1	0
17	n	128	0	172	12	0
18	1	19	0	22	0	0
18	2	23	0	30	0	0
18	A	58	0	76	1	0
18	B	35	0	46	0	0
18	G	58	0	76	0	0
18	H	35	0	46	0	0
18	J	22	0	28	2	0
18	T	22	0	28	2	0
18	Y	19	0	22	0	0
18	Z	23	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	e	58	0	76	1	0
18	f	35	0	46	0	0
18	l	22	0	28	2	0
18	q	19	0	22	0	0
18	r	23	0	30	0	0
19	B	54	0	81	7	0
19	H	54	0	81	7	0
19	J	35	0	40	0	0
19	T	35	0	40	0	0
19	f	54	0	81	7	0
19	l	35	0	40	0	0
20	1	48	0	63	4	0
20	2	43	0	49	1	0
20	3	43	0	50	1	0
20	4	26	0	16	0	0
20	5	29	0	22	0	0
20	6	26	0	16	1	0
20	B	45	0	53	7	0
20	H	45	0	53	10	0
20	L	51	0	69	4	0
20	V	51	0	69	3	0
20	Y	48	0	63	5	0
20	Z	43	0	49	1	0
20	a	43	0	50	1	0
20	b	26	0	16	0	0
20	c	29	0	22	0	0
20	d	26	0	16	1	0
20	f	45	0	53	8	0
20	n	51	0	69	4	0
20	q	48	0	63	4	0
20	r	43	0	49	1	0
20	s	43	0	50	1	0
20	t	26	0	16	0	0
20	u	29	0	22	0	0
20	v	26	0	16	1	0
21	A	9	0	0	0	0
21	B	7	0	0	0	0
21	F	1	0	0	0	0
21	G	9	0	0	0	0
21	H	7	0	0	0	0
21	L	1	0	0	0	0
21	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	1	0	0	0	0
21	e	9	0	0	0	0
21	f	7	0	0	0	0
21	j	1	0	0	0	0
21	n	1	0	0	0	0
All	All	143022	0	143508	2193	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 (2193) 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)
20:H:1852:SQD:H91	17:e:5002:LHG:C23	2.07	0.84
17:L:5221:LHG:H252	13:f:1207:CLA:H42	1.60	0.83
13:B:1207:CLA:H42	17:V:5221:LHG:H252	1.58	0.83
13:H:1207:CLA:H42	17:n:5221:LHG:H252	1.59	0.83
20:H:1852:SQD:H91	17:e:5002:LHG:O10	1.81	0.81
13:B:1203:CLA:H152	13:B:1225:CLA:HBB2	1.65	0.79
13:H:1203:CLA:H152	13:H:1225:CLA:HBB2	1.65	0.77
13:a:518:CLA:HBC2	20:a:822:SQD:H282	1.67	0.77
13:f:1203:CLA:H152	13:f:1225:CLA:HBB2	1.65	0.77
13:s:518:CLA:HBC2	20:s:822:SQD:H282	1.67	0.75
12:t:75:LEU:HD12	12:t:75:LEU:O	1.87	0.75
12:4:75:LEU:HD12	12:4:75:LEU:O	1.87	0.75
13:e:1104:CLA:H42	13:e:1128:CLA:H2	1.69	0.74
17:A:5002:LHG:C23	20:f:1852:SQD:H91	2.16	0.74
12:b:75:LEU:HD12	12:b:75:LEU:O	1.87	0.74
13:3:518:CLA:HBC2	20:3:822:SQD:H282	1.67	0.74
4:O:41:GLU:H	4:O:71:GLN:HE22	1.36	0.73
13:G:1104:CLA:H42	13:G:1128:CLA:H2	1.69	0.73
13:e:1013:CLA:H111	16:e:4011:BCR:H23C	1.70	0.73
13:A:1013:CLA:H111	16:A:4011:BCR:H23C	1.70	0.73
17:L:5221:LHG:H342	13:f:1207:CLA:H142	1.68	0.73
4:D:41:GLU:H	4:D:71:GLN:HE22	1.36	0.72
13:G:1013:CLA:H111	16:G:4011:BCR:H23C	1.70	0.72
7:S:26:LEU:HD11	20:n:5216:SQD:H311	1.71	0.72
13:A:1104:CLA:H42	13:A:1128:CLA:H2	1.69	0.72
13:B:1207:CLA:H142	17:V:5221:LHG:H342	1.70	0.72
20:L:5216:SQD:H311	7:k:26:LEU:HD11	1.70	0.72
12:2:146:LEU:HD21	13:2:506:CLA:HAB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:41:GLU:H	4:h:71:GLN:HE22	1.36	0.71
12:Z:146:LEU:HD21	13:Z:506:CLA:HAB	1.72	0.71
20:B:1852:SQD:H91	17:G:5002:LHG:C23	2.20	0.71
7:I:26:LEU:HD11	20:V:5216:SQD:H311	1.73	0.70
12:r:146:LEU:HD21	13:r:506:CLA:HAB	1.72	0.69
12:4:282:VAL:O	13:4:519:CLA:NB	2.25	0.69
12:4:145:HIS:NE2	13:4:512:CLA:NA	2.40	0.69
17:A:5002:LHG:O10	20:f:1852:SQD:H91	1.92	0.69
12:b:282:VAL:O	13:b:519:CLA:NB	2.26	0.69
16:U:4104:BCR:H24C	20:Y:822:SQD:H321	1.75	0.69
12:b:145:HIS:NE2	13:b:512:CLA:NA	2.40	0.69
16:d:522:BCR:HC41	12:q:258:TYR:HB2	1.75	0.69
16:K:4104:BCR:H24C	20:1:822:SQD:H321	1.75	0.68
12:t:282:VAL:O	13:t:519:CLA:NB	2.26	0.68
16:m:4104:BCR:H24C	20:q:822:SQD:H321	1.75	0.68
12:t:145:HIS:NE2	13:t:512:CLA:NA	2.40	0.68
20:B:1852:SQD:H91	17:G:5002:LHG:O10	1.93	0.68
1:e:410:GLY:HA3	1:e:614:LEU:HD11	1.76	0.67
1:G:410:GLY:HA3	1:G:614:LEU:HD11	1.76	0.67
13:A:1130:CLA:H101	16:L:4022:BCR:H322	1.77	0.67
13:6:505:CLA:H43	16:6:524:BCR:HC7	1.76	0.67
18:T:5105:LMU:H92	16:a:521:BCR:C40	2.25	0.67
13:G:1130:CLA:H101	16:V:4022:BCR:H322	1.77	0.67
18:l:5105:LMU:H92	16:s:521:BCR:C40	2.25	0.67
18:J:5105:LMU:H92	16:3:521:BCR:C40	2.25	0.66
13:H:1207:CLA:H142	17:n:5221:LHG:H342	1.75	0.66
13:d:505:CLA:H43	16:d:524:BCR:HC7	1.76	0.66
13:e:1130:CLA:H101	16:n:4022:BCR:H322	1.77	0.66
1:A:410:GLY:HA3	1:A:614:LEU:HD11	1.77	0.66
13:A:1130:CLA:H2	13:L:1502:CLA:H43	1.78	0.66
12:d:101:ALA:HB1	13:q:505:CLA:HAB	1.76	0.66
13:e:1130:CLA:H2	13:n:1502:CLA:H43	1.78	0.66
13:v:505:CLA:H43	16:v:524:BCR:HC7	1.77	0.66
13:G:1130:CLA:H2	13:V:1502:CLA:H43	1.78	0.66
12:4:75:LEU:HD13	12:4:88:PRO:HB2	1.78	0.66
2:B:112:PRO:HD2	7:I:1:MET:HB2	1.78	0.65
13:Y:501:CLA:HBB2	13:Y:507:CLA:H92	1.79	0.65
13:q:501:CLA:HBB2	13:q:507:CLA:H92	1.79	0.65
17:H:1855:LHG:HC82	17:H:1855:LHG:H252	1.79	0.65
2:f:112:PRO:HD2	7:k:1:MET:HB2	1.78	0.65
13:B:1231:CLA:H71	16:B:4010:BCR:H313	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:PRO:HD2	7:S:1:MET:HB2	1.78	0.65
18:T:5105:LMU:H92	16:a:521:BCR:H401	1.79	0.65
12:1:145:HIS:NE2	13:1:512:CLA:NA	2.45	0.65
17:B:1855:LHG:HC82	17:B:1855:LHG:H252	1.79	0.65
13:H:1231:CLA:H71	16:H:4010:BCR:H313	1.79	0.65
12:Y:145:HIS:NE2	13:Y:512:CLA:NA	2.45	0.65
13:e:1013:CLA:HBA2	2:f:427:LEU:HD12	1.79	0.65
18:l:5105:LMU:H92	16:s:521:BCR:H401	1.79	0.65
12:q:145:HIS:NE2	13:q:512:CLA:NA	2.45	0.65
12:b:75:LEU:HD13	12:b:88:PRO:HB2	1.78	0.64
12:t:75:LEU:HD13	12:t:88:PRO:HB2	1.78	0.64
13:A:1013:CLA:HBA2	2:B:427:LEU:HD12	1.79	0.64
18:J:5105:LMU:H92	16:3:521:BCR:H401	1.79	0.64
13:f:1231:CLA:H71	16:f:4010:BCR:H313	1.79	0.63
13:1:501:CLA:HBB2	13:1:507:CLA:H92	1.79	0.63
10:n:150:PRO:HG2	17:n:5221:LHG:HC62	1.80	0.63
13:G:1013:CLA:HBA2	2:H:427:LEU:HD12	1.79	0.63
10:V:160:ALA:HB1	10:V:165:VAL:HB	1.81	0.63
10:L:160:ALA:HB1	10:L:165:VAL:HB	1.81	0.63
2:B:326:LEU:HD13	2:B:332:PHE:CD2	2.34	0.63
13:2:502:CLA:H61	13:2:512:CLA:H42	1.81	0.63
2:H:158:GLN:HB3	20:H:1852:SQD:H5	1.81	0.63
17:f:1855:LHG:HC82	17:f:1855:LHG:H252	1.79	0.62
10:L:150:PRO:HG2	17:L:5221:LHG:HC62	1.80	0.62
16:A:4011:BCR:H362	13:B:1012:CLA:H2	1.81	0.62
12:b:30:ALA:HB2	13:b:511:CLA:HMA1	1.81	0.62
13:Z:502:CLA:H61	13:Z:512:CLA:H42	1.81	0.62
13:r:502:CLA:H61	13:r:512:CLA:H42	1.81	0.62
2:f:158:GLN:HB3	20:f:1852:SQD:H5	1.81	0.62
12:3:249:ILE:HG12	13:3:502:CLA:HAC1	1.81	0.62
2:f:326:LEU:HD13	2:f:332:PHE:CD2	2.34	0.62
2:B:158:GLN:HB3	20:B:1852:SQD:H5	1.81	0.62
16:G:4011:BCR:H362	13:H:1012:CLA:H2	1.81	0.62
10:n:160:ALA:HB1	10:n:165:VAL:HB	1.81	0.62
12:s:249:ILE:HG12	13:s:502:CLA:HAC1	1.81	0.62
12:3:272:TYR:HB3	12:3:300:ARG:HB2	1.82	0.62
1:G:494:PHE:HB3	13:G:1135:CLA:H11	1.82	0.62
13:e:1126:CLA:H201	16:l:4012:BCR:H12C	1.82	0.62
16:m:4104:BCR:H392	20:q:822:SQD:H301	1.82	0.62
2:B:323:TYR:O	2:B:327:ASN:HB2	2.00	0.61
13:H:1217:CLA:HAB	13:H:1217:CLA:H93	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:26:ASN:HB3	13:U:1103:CLA:H12	1.83	0.61
13:H:1225:CLA:H12	16:H:4005:BCR:H393	1.83	0.61
10:V:150:PRO:HG2	17:V:5221:LHG:HC62	1.80	0.61
1:A:494:PHE:HB3	13:A:1135:CLA:H11	1.82	0.61
16:K:4104:BCR:H392	20:1:822:SQD:H301	1.83	0.61
1:e:494:PHE:HB3	13:e:1135:CLA:H11	1.82	0.61
12:v:30:ALA:HB2	13:v:511:CLA:HMA1	1.82	0.61
12:1:289:THR:O	12:1:289:THR:HG22	2.01	0.61
13:G:1121:CLA:HAB	13:G:1801:CLA:HAB	1.83	0.61
1:e:33:HIS:NE2	13:e:1109:CLA:O1A	2.30	0.61
9:m:26:ASN:HB3	13:m:1103:CLA:H12	1.82	0.61
12:6:249:ILE:HG12	13:6:502:CLA:HAC1	1.83	0.61
13:H:1207:CLA:H42	17:n:5221:LHG:C25	2.31	0.61
12:d:52:TRP:CZ3	17:e:5009:LHG:HC11	2.35	0.61
13:e:1121:CLA:HAB	13:e:1801:CLA:HAB	1.83	0.61
16:e:4011:BCR:H362	13:f:1012:CLA:H2	1.81	0.61
12:q:289:THR:O	12:q:289:THR:HG22	2.01	0.61
13:A:1126:CLA:H201	16:J:4012:BCR:H12C	1.82	0.61
2:H:323:TYR:O	2:H:327:ASN:HB2	2.00	0.61
2:H:326:LEU:HD13	2:H:332:PHE:CD2	2.34	0.61
12:d:30:ALA:HB2	13:d:511:CLA:HMA1	1.82	0.61
12:t:30:ALA:HB2	13:t:511:CLA:HMA1	1.81	0.61
13:f:1217:CLA:HAB	13:f:1217:CLA:H93	1.82	0.61
16:L:4022:BCR:C24	10:n:137:LEU:HD13	2.31	0.61
17:L:5221:LHG:C25	13:f:1207:CLA:H42	2.30	0.61
17:H:1855:LHG:H192	13:R:1302:CLA:HBB1	1.83	0.61
2:f:323:TYR:O	2:f:327:ASN:HB2	2.00	0.61
12:6:136:LYS:HG3	12:6:225:PRO:HB3	1.83	0.60
12:d:249:ILE:HG12	13:d:502:CLA:HAC1	1.83	0.60
13:f:1225:CLA:H12	16:f:4005:BCR:H393	1.83	0.60
12:s:272:TYR:HB3	12:s:300:ARG:HB2	1.82	0.60
12:v:136:LYS:HG3	12:v:225:PRO:HB3	1.83	0.60
9:K:26:ASN:HB3	13:K:1103:CLA:H12	1.83	0.60
12:a:249:ILE:HG12	13:a:502:CLA:HAC1	1.82	0.60
12:a:272:TYR:HB3	12:a:300:ARG:HB2	1.82	0.60
12:c:146:LEU:HD21	13:c:506:CLA:HAB	1.83	0.60
10:L:137:LEU:HD13	16:V:4022:BCR:C24	2.30	0.60
16:U:4104:BCR:H392	20:Y:822:SQD:H301	1.82	0.60
17:B:1855:LHG:H192	13:F:1302:CLA:HBB1	1.83	0.60
12:v:249:ILE:HG12	13:v:502:CLA:HAC1	1.83	0.60
1:A:278:LEU:HD21	9:K:72:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1225:CLA:H12	16:B:4005:BCR:H393	1.83	0.60
13:A:1121:CLA:HAB	13:A:1801:CLA:HAB	1.83	0.60
13:B:1217:CLA:H93	13:B:1217:CLA:HAB	1.82	0.60
12:5:146:LEU:HD21	13:5:506:CLA:HAB	1.84	0.60
12:Y:289:THR:O	12:Y:289:THR:HG22	2.01	0.60
1:A:33:HIS:NE2	13:A:1109:CLA:O1A	2.30	0.60
12:6:30:ALA:HB2	13:6:511:CLA:HMA1	1.82	0.60
12:q:52:TRP:CE3	13:q:504:CLA:HED3	2.37	0.60
13:B:1207:CLA:H42	17:V:5221:LHG:C25	2.29	0.60
12:d:102:VAL:HA	13:q:505:CLA:H61	1.84	0.60
12:d:136:LYS:HG3	12:d:225:PRO:HB3	1.83	0.60
13:G:1126:CLA:H201	16:T:4012:BCR:H12C	1.82	0.59
13:q:502:CLA:H12	13:q:503:CLA:H42	1.84	0.59
17:e:5004:LHG:H102	12:r:282:VAL:HG13	1.82	0.59
13:l:1303:CLA:H62	12:t:282:VAL:HG22	1.84	0.59
17:A:5004:LHG:H102	12:2:282:VAL:HG13	1.82	0.59
13:G:1103:CLA:H121	16:G:4002:BCR:HC41	1.84	0.59
17:G:5004:LHG:H102	12:Z:282:VAL:HG13	1.82	0.59
12:u:146:LEU:HD21	13:u:506:CLA:HAB	1.83	0.59
12:1:52:TRP:CE3	13:1:504:CLA:HED3	2.37	0.59
13:1:502:CLA:H12	13:1:503:CLA:H42	1.84	0.59
6:R:141:GLU:HG3	6:R:146:LYS:HB3	1.84	0.59
11:W:21:TYR:OH	10:n:26:PHE:HB2	2.02	0.59
12:Y:52:TRP:CE3	13:Y:504:CLA:HED3	2.37	0.59
9:U:60:VAL:HG22	13:U:1105:CLA:HAC2	1.83	0.59
17:f:1855:LHG:H192	13:j:1302:CLA:HBB1	1.83	0.59
6:j:91:ILE:HG23	13:j:1301:CLA:HAA1	1.85	0.59
13:5:501:CLA:H72	13:5:501:CLA:HBB1	1.85	0.59
1:e:577:LYS:NZ	2:f:673:GLU:OE2	2.36	0.59
12:q:251:LEU:HD13	13:q:505:CLA:H122	1.85	0.59
12:1:30:ALA:HB2	13:1:511:CLA:HMA1	1.85	0.59
1:G:278:LEU:HD21	9:U:72:ILE:HD12	1.83	0.59
9:m:60:VAL:HG22	13:m:1105:CLA:HAC2	1.83	0.59
9:K:60:VAL:HG22	13:K:1105:CLA:HAC2	1.83	0.59
6:j:141:GLU:HG3	6:j:146:LYS:HB3	1.84	0.59
6:F:91:ILE:HG23	13:F:1301:CLA:HAA1	1.85	0.59
13:Y:502:CLA:H12	13:Y:503:CLA:H42	1.84	0.59
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.85	0.58
17:A:5009:LHG:HC11	12:v:52:TRP:CZ3	2.38	0.58
13:f:1222:CLA:HMA1	16:f:4010:BCR:H14C	1.85	0.58
12:1:251:LEU:HD13	13:1:505:CLA:H122	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1222:CLA:HMA1	16:B:4010:BCR:H14C	1.85	0.58
12:Z:267:TYR:O	12:Z:300:ARG:NH2	2.37	0.58
13:c:501:CLA:H72	13:c:501:CLA:HBB1	1.85	0.58
12:s:145:HIS:NE2	13:s:512:CLA:NA	2.52	0.58
6:F:141:GLU:HG3	6:F:146:LYS:HB3	1.84	0.58
12:a:145:HIS:NE2	13:a:512:CLA:NA	2.52	0.58
12:c:30:ALA:HB2	13:c:511:CLA:HMA1	1.85	0.58
12:6:146:LEU:HD21	13:6:506:CLA:HAB	1.86	0.58
1:e:278:LEU:HD21	9:m:72:ILE:HD12	1.83	0.58
2:f:15:ASP:HB3	2:f:20:ARG:HB2	1.85	0.58
13:u:501:CLA:H72	13:u:501:CLA:HBB1	1.85	0.58
1:A:59:ASP:OD2	1:A:361:HIS:NE2	2.37	0.58
12:1:258:TYR:HB2	16:v:522:BCR:HC41	1.84	0.58
13:H:1222:CLA:HMA1	16:H:4010:BCR:H14C	1.85	0.58
12:1:110:HIS:NE2	13:1:513:CLA:NB	2.52	0.58
1:G:59:ASP:OD2	1:G:361:HIS:NE2	2.37	0.58
1:e:59:ASP:OD2	1:e:361:HIS:NE2	2.37	0.58
13:e:1103:CLA:H121	16:e:4002:BCR:HC41	1.84	0.58
13:A:1103:CLA:H121	16:A:4002:BCR:HC41	1.84	0.57
12:3:168:ASP:OD2	12:3:175:ARG:NH2	2.37	0.57
12:d:146:LEU:HD21	13:d:506:CLA:HAB	1.86	0.57
12:2:267:TYR:O	12:2:300:ARG:NH2	2.37	0.57
12:3:145:HIS:NE2	13:3:512:CLA:NA	2.52	0.57
1:e:752:TRP:NE1	13:e:1126:CLA:O1A	2.32	0.57
13:f:1239:CLA:HBB1	16:f:4017:BCR:H363	1.86	0.57
12:q:30:ALA:HB2	13:q:511:CLA:HMA1	1.85	0.57
13:T:1303:CLA:H62	12:b:282:VAL:HG22	1.84	0.57
2:f:351:HIS:ND1	13:f:1214:CLA:OBD	2.38	0.57
13:J:1303:CLA:H62	12:4:282:VAL:HG22	1.84	0.57
12:5:30:ALA:HB2	13:5:511:CLA:HMA1	1.85	0.57
12:6:251:LEU:HD13	13:6:505:CLA:H122	1.87	0.57
17:G:5006:LHG:H241	12:Y:52:TRP:CH2	2.40	0.57
2:H:15:ASP:HB3	2:H:20:ARG:HB2	1.85	0.57
10:L:26:PHE:HB2	11:o:21:TYR:OH	2.04	0.57
1:G:752:TRP:NE1	13:G:1126:CLA:O1A	2.32	0.57
2:H:351:HIS:ND1	13:H:1214:CLA:OBD	2.38	0.57
12:Y:110:HIS:NE2	13:Y:513:CLA:NB	2.52	0.57
12:v:307:HIS:NE2	13:v:502:CLA:ND	2.53	0.57
12:Y:251:LEU:HD13	13:Y:505:CLA:H122	1.85	0.57
17:e:5006:LHG:H241	12:q:52:TRP:CH2	2.40	0.57
6:R:91:ILE:HG23	13:R:1301:CLA:HAA1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:168:ASP:OD2	12:a:175:ARG:NH2	2.37	0.57
12:q:110:HIS:NE2	13:q:513:CLA:NB	2.52	0.57
12:s:168:ASP:OD2	12:s:175:ARG:NH2	2.37	0.57
12:v:146:LEU:HD21	13:v:506:CLA:HAB	1.86	0.57
17:A:5006:LHG:H241	12:1:52:TRP:CH2	2.40	0.57
12:Y:249:ILE:HG12	13:Y:502:CLA:HAC1	1.87	0.56
2:f:26:ALA:HA	13:f:1226:CLA:H43	1.87	0.56
12:r:267:TYR:O	12:r:300:ARG:NH2	2.37	0.56
9:U:18:VAL:HG22	9:U:84:LEU:HD21	1.87	0.56
9:U:50:GLN:HB2	12:Y:337:LEU:HD23	1.87	0.56
13:l:1303:CLA:H41	12:t:282:VAL:HG22	1.87	0.56
9:m:50:GLN:HB2	12:q:337:LEU:HD23	1.87	0.56
13:B:1239:CLA:HBB1	16:B:4017:BCR:H363	1.86	0.56
13:2:517:CLA:HBB1	16:2:524:BCR:H352	1.88	0.56
12:6:272:TYR:HB3	12:6:300:ARG:HB2	1.87	0.56
12:d:307:HIS:NE2	13:d:502:CLA:ND	2.53	0.56
12:v:272:TYR:HB3	12:v:300:ARG:HB2	1.87	0.56
2:B:351:HIS:ND1	13:B:1214:CLA:OBD	2.38	0.56
13:r:517:CLA:HBB1	16:r:524:BCR:H352	1.88	0.56
12:1:249:ILE:HG12	13:1:502:CLA:HAC1	1.87	0.56
12:d:102:VAL:HG22	13:q:505:CLA:H61	1.88	0.56
12:d:251:LEU:HD13	13:d:505:CLA:H122	1.87	0.56
9:K:50:GLN:HB2	12:1:337:LEU:HD23	1.87	0.56
12:d:110:HIS:NE2	13:d:513:CLA:NB	2.54	0.56
12:q:249:ILE:HG12	13:q:502:CLA:HAC1	1.87	0.56
12:v:251:LEU:HD13	13:v:505:CLA:H122	1.87	0.56
8:J:1:MET:HE3	12:3:337:LEU:HG	1.88	0.56
13:J:1303:CLA:H41	12:4:282:VAL:HG22	1.87	0.56
12:6:307:HIS:NE2	13:6:502:CLA:ND	2.53	0.56
13:Z:506:CLA:HBB2	13:Z:507:CLA:H51	1.88	0.56
13:Z:517:CLA:HBB1	16:Z:524:BCR:H352	1.88	0.56
13:A:1136:CLA:HBC1	17:L:5220:LHG:H282	1.88	0.56
11:M:21:TYR:OH	10:V:26:PHE:HB2	2.06	0.56
12:2:249:ILE:HG12	13:2:502:CLA:HAC1	1.88	0.56
13:G:1130:CLA:H121	13:V:1501:CLA:H201	1.88	0.56
13:H:1209:CLA:HBB2	13:H:1217:CLA:H102	1.88	0.56
12:d:272:TYR:HB3	12:d:300:ARG:HB2	1.87	0.56
13:e:1103:CLA:H142	16:e:4003:BCR:H372	1.88	0.56
4:h:61:ARG:NH1	4:h:63:GLU:OE1	2.39	0.56
4:D:61:ARG:NH1	4:D:63:GLU:OE1	2.39	0.55
12:6:110:HIS:NE2	13:6:513:CLA:NB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:ARG:NH1	4:O:63:GLU:OE1	2.39	0.55
6:R:143:SER:HB2	12:b:14:TRP:CH2	2.41	0.55
8:T:1:MET:HE3	12:a:337:LEU:HG	1.88	0.55
8:l:1:MET:HE3	12:s:337:LEU:HG	1.88	0.55
12:r:249:ILE:HG12	13:r:502:CLA:HAC1	1.88	0.55
12:u:249:ILE:HG12	13:u:502:CLA:HAC1	1.88	0.55
13:A:1120:CLA:HMD2	16:A:4001:BCR:H24C	1.89	0.55
13:G:1120:CLA:HMD2	16:G:4001:BCR:H24C	1.88	0.55
12:c:249:ILE:HG12	13:c:502:CLA:HAC1	1.88	0.55
13:f:1209:CLA:HBB2	13:f:1217:CLA:H102	1.87	0.55
4:h:120:ARG:HH22	4:h:141:ALA:HB3	1.72	0.55
12:r:214:LEU:HD21	13:r:507:CLA:H71	1.88	0.55
13:A:1237:CLA:H152	16:L:4020:BCR:H16C	1.89	0.55
13:B:1202:CLA:H8	13:B:1221:CLA:HBA2	1.89	0.55
4:D:120:ARG:HH22	4:D:141:ALA:HB3	1.72	0.55
9:K:18:VAL:HG22	9:K:84:LEU:HD21	1.87	0.55
12:2:214:LEU:HD21	13:2:507:CLA:H71	1.89	0.55
2:H:603:GLN:HE21	2:H:732:LYS:HD3	1.72	0.55
13:A:1103:CLA:H142	16:A:4003:BCR:H372	1.88	0.55
10:L:41:LEU:O	10:L:46:ARG:NH1	2.40	0.55
12:2:34:GLN:OE1	13:2:510:CLA:NC	2.40	0.55
13:G:1103:CLA:H142	16:G:4003:BCR:H372	1.88	0.55
13:H:1239:CLA:HBB1	16:H:4017:BCR:H363	1.86	0.55
3:N:63:LEU:HD12	3:N:66:ARG:HH21	1.71	0.55
12:Z:214:LEU:HD21	13:Z:507:CLA:H71	1.89	0.55
13:f:1023:CLA:H142	16:k:4018:BCR:H271	1.88	0.55
13:f:1202:CLA:H8	13:f:1221:CLA:HBA2	1.89	0.55
4:D:85:ILE:HB	4:D:98:HIS:HB3	1.89	0.55
13:G:1136:CLA:HBC1	17:V:5220:LHG:H282	1.88	0.55
13:e:1237:CLA:H152	16:n:4020:BCR:H16C	1.89	0.55
2:B:26:ALA:HA	13:B:1226:CLA:H43	1.87	0.55
13:6:501:CLA:H72	13:6:501:CLA:HBB1	1.89	0.55
13:e:1120:CLA:HMD2	16:e:4001:BCR:H24C	1.89	0.55
12:r:34:GLN:OE1	13:r:510:CLA:NC	2.40	0.55
2:B:603:GLN:HE21	2:B:732:LYS:HD3	1.72	0.55
6:F:143:SER:HB2	12:4:14:TRP:CH2	2.41	0.55
13:2:506:CLA:HBB2	13:2:507:CLA:H51	1.88	0.55
6:j:143:SER:HB2	12:t:14:TRP:CH2	2.41	0.55
13:v:501:CLA:H72	13:v:501:CLA:HBB1	1.89	0.55
1:G:33:HIS:NE2	13:G:1109:CLA:O1A	2.30	0.55
2:H:26:ALA:HA	13:H:1226:CLA:H43	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:85:ILE:HB	4:h:98:HIS:HB3	1.89	0.55
10:n:41:LEU:O	10:n:46:ARG:NH1	2.40	0.55
12:s:251:LEU:HD13	13:s:505:CLA:H122	1.89	0.55
13:A:1130:CLA:H121	13:L:1501:CLA:H201	1.88	0.55
13:G:1237:CLA:H152	16:V:4020:BCR:H16C	1.89	0.55
13:H:1023:CLA:H142	16:S:4018:BCR:H271	1.88	0.55
4:O:85:ILE:HB	4:O:98:HIS:HB3	1.89	0.55
13:T:1303:CLA:H41	12:b:282:VAL:HG22	1.87	0.55
12:Y:45:PHE:HE2	13:Z:519:CLA:HBA2	1.72	0.55
13:d:501:CLA:H72	13:d:501:CLA:HBB1	1.89	0.55
12:5:249:ILE:HG12	13:5:502:CLA:HAC1	1.88	0.55
13:G:1121:CLA:HHB	13:G:1801:CLA:HBC3	1.90	0.55
12:Z:34:GLN:OE1	13:Z:510:CLA:NC	2.40	0.55
12:b:146:LEU:HD21	13:b:506:CLA:HAB	1.89	0.55
12:q:45:PHE:HE2	13:r:519:CLA:HBA2	1.72	0.55
12:v:110:HIS:NE2	13:v:513:CLA:NB	2.54	0.55
13:e:1136:CLA:HBC1	17:n:5220:LHG:H282	1.88	0.54
9:m:18:VAL:HG22	9:m:84:LEU:HD21	1.88	0.54
12:1:45:PHE:HE2	13:2:519:CLA:HBA2	1.72	0.54
13:6:505:CLA:H12	16:6:524:BCR:H312	1.89	0.54
13:B:1023:CLA:H142	16:I:4018:BCR:H271	1.88	0.54
4:O:120:ARG:HH22	4:O:141:ALA:HB3	1.72	0.54
13:Z:510:CLA:HED2	13:Z:510:CLA:H2	1.89	0.54
13:r:510:CLA:HED2	13:r:510:CLA:H2	1.89	0.54
12:t:146:LEU:HD21	13:t:506:CLA:HAB	1.89	0.54
13:v:505:CLA:H12	16:v:524:BCR:H312	1.89	0.54
13:2:510:CLA:H2	13:2:510:CLA:HED2	1.89	0.54
10:V:41:LEU:O	10:V:46:ARG:NH1	2.40	0.54
3:g:63:LEU:HD12	3:g:66:ARG:HH21	1.71	0.54
13:H:1234:CLA:HMB2	13:H:1236:CLA:HED1	1.89	0.54
8:T:12:PRO:HB2	16:T:4013:BCR:H381	1.90	0.54
13:d:505:CLA:H111	13:d:517:CLA:HBB2	1.90	0.54
1:e:412:LEU:HD21	13:e:1104:CLA:H142	1.89	0.54
1:e:459:LEU:HB3	1:e:552:PHE:HB2	1.90	0.54
13:e:1130:CLA:H121	13:n:1501:CLA:H201	1.88	0.54
13:r:506:CLA:HBB2	13:r:507:CLA:H51	1.88	0.54
1:A:459:LEU:HB3	1:A:552:PHE:HB2	1.90	0.54
13:B:1204:CLA:H111	16:I:4018:BCR:HC21	1.90	0.54
13:B:1234:CLA:HMB2	13:B:1236:CLA:HED1	1.89	0.54
3:C:63:LEU:HD12	3:C:66:ARG:HH21	1.71	0.54
1:G:683:LEU:HD21	13:G:1126:CLA:H142	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:1202:CLA:H8	13:H:1221:CLA:HBA2	1.89	0.54
2:f:66:PHE:HZ	11:o:6:VAL:HG13	1.73	0.54
13:f:1234:CLA:HMB2	13:f:1236:CLA:HED1	1.89	0.54
8:J:12:PRO:HB2	16:J:4013:BCR:H381	1.90	0.54
12:4:146:LEU:HD21	13:4:506:CLA:HAB	1.89	0.54
12:Z:249:ILE:HG12	13:Z:502:CLA:HAC1	1.88	0.54
10:n:38:ARG:O	10:n:46:ARG:NH2	2.41	0.54
1:G:485:ASP:OD1	1:G:491:GLN:NE2	2.40	0.54
13:s:505:CLA:H43	16:s:524:BCR:HC7	1.90	0.54
13:v:505:CLA:H111	13:v:517:CLA:HBB2	1.90	0.54
1:A:182:LYS:NZ	17:A:5008:LHG:O2	2.41	0.54
1:A:216:GLN:HA	1:A:220:SER:HB2	1.90	0.54
1:A:616:ILE:HD12	13:A:1011:CLA:H122	1.90	0.54
13:A:1121:CLA:HHB	13:A:1801:CLA:HBC3	1.89	0.54
13:B:1209:CLA:HBB2	13:B:1217:CLA:H102	1.88	0.54
13:6:505:CLA:H111	13:6:517:CLA:HBB2	1.90	0.54
1:G:182:LYS:NZ	17:G:5008:LHG:O2	2.41	0.53
13:H:1226:CLA:H112	19:H:5002:LMG:H212	1.90	0.53
12:d:98:ILE:HG23	13:q:505:CLA:C11	2.38	0.53
1:e:683:LEU:HD21	13:e:1126:CLA:H142	1.90	0.53
13:e:1121:CLA:HHB	13:e:1801:CLA:HBC3	1.89	0.53
13:3:505:CLA:H43	16:3:524:BCR:HC7	1.90	0.53
12:4:272:TYR:HB3	12:4:300:ARG:HB2	1.90	0.53
1:G:589:PRO:HD3	2:H:561:GLY:HA2	1.90	0.53
2:H:66:PHE:HZ	11:W:6:VAL:HG13	1.73	0.53
13:d:505:CLA:H12	16:d:524:BCR:H312	1.89	0.53
2:f:61:VAL:HG21	13:f:1225:CLA:H42	1.90	0.53
2:f:603:GLN:HE21	2:f:732:LYS:HD3	1.72	0.53
4:h:39:VAL:HG22	4:h:49:VAL:HG22	1.89	0.53
13:q:509:CLA:H101	13:q:512:CLA:HBD	1.91	0.53
1:G:216:GLN:HA	1:G:220:SER:HB2	1.90	0.53
1:G:412:LEU:HD21	13:G:1104:CLA:H142	1.89	0.53
1:G:459:LEU:HB3	1:G:552:PHE:HB2	1.90	0.53
4:O:39:VAL:HG22	4:O:49:VAL:HG22	1.89	0.53
12:b:272:TYR:HB3	12:b:300:ARG:HB2	1.90	0.53
12:d:98:ILE:HG12	13:q:505:CLA:H13	1.89	0.53
12:t:272:TYR:HB3	12:t:300:ARG:HB2	1.90	0.53
1:A:752:TRP:NE1	13:A:1126:CLA:O1A	2.32	0.53
2:B:524:ALA:HB2	13:B:1235:CLA:HMA1	1.91	0.53
12:a:251:LEU:HD13	13:a:505:CLA:H122	1.89	0.53
12:c:272:TYR:HB3	12:c:300:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:182:LYS:NZ	17:e:5008:LHG:O2	2.41	0.53
1:e:616:ILE:HD12	13:e:1011:CLA:H122	1.90	0.53
1:A:708:LEU:HD21	13:A:1013:CLA:HED2	1.91	0.53
10:V:38:ARG:O	10:V:46:ARG:NH2	2.41	0.53
12:Y:26:LEU:HB3	13:Y:511:CLA:HMA1	1.90	0.53
1:A:589:PRO:HD3	2:B:561:GLY:HA2	1.90	0.53
2:B:66:PHE:HZ	11:M:6:VAL:HG13	1.73	0.53
12:5:272:TYR:HB3	12:5:300:ARG:HB2	1.91	0.53
13:f:1204:CLA:H111	16:k:4018:BCR:HC21	1.90	0.53
4:h:121:ARG:NH1	5:i:65:GLU:OE2	2.42	0.53
1:A:683:LEU:HD21	13:A:1126:CLA:H142	1.90	0.53
2:B:61:VAL:HG21	13:B:1225:CLA:H42	1.90	0.53
4:D:39:VAL:HG22	4:D:49:VAL:HG22	1.89	0.53
4:D:121:ARG:NH1	5:E:65:GLU:OE2	2.42	0.53
13:1:509:CLA:H101	13:1:512:CLA:HBD	1.90	0.53
12:3:251:LEU:HD13	13:3:505:CLA:H122	1.89	0.53
13:5:507:CLA:HED2	13:5:507:CLA:H2A	1.91	0.53
1:G:708:LEU:HD21	13:G:1013:CLA:HED2	1.90	0.53
17:G:5009:LHG:H171	12:Y:309:PHE:CZ	2.44	0.53
1:e:216:GLN:HA	1:e:220:SER:HB2	1.90	0.53
1:e:589:PRO:HD3	2:f:561:GLY:HA2	1.90	0.53
13:f:1226:CLA:H112	19:f:5002:LMG:H212	1.89	0.53
13:A:1137:CLA:H13	16:A:4007:BCR:H271	1.91	0.53
10:L:38:ARG:O	10:L:46:ARG:NH2	2.41	0.53
12:1:301:ALA:O	12:1:305:ASN:ND2	2.41	0.53
1:e:517:VAL:HG23	13:e:1133:CLA:HED3	1.91	0.53
17:e:5009:LHG:H171	12:q:309:PHE:CZ	2.44	0.53
13:B:1226:CLA:H112	19:B:5002:LMG:H212	1.90	0.53
2:H:61:VAL:HG21	13:H:1225:CLA:H42	1.91	0.53
13:H:1204:CLA:H111	16:S:4018:BCR:HC21	1.90	0.53
12:a:45:PHE:HE2	13:b:519:CLA:HAA2	1.74	0.53
13:a:505:CLA:H43	16:a:524:BCR:HC7	1.90	0.53
1:e:277:THR:HB	9:m:14:TRP:HB2	1.91	0.53
13:f:1239:CLA:HBA2	14:f:2002:PQN:H251	1.91	0.53
12:r:111:THR:HG21	16:r:522:BCR:H271	1.91	0.53
13:B:1214:CLA:HBA2	13:B:1223:CLA:HBB2	1.91	0.53
13:L:1501:CLA:H141	13:L:1503:CLA:HBC2	1.91	0.53
12:6:73:LEU:O	12:6:159:LYS:NZ	2.42	0.53
13:H:1227:CLA:H191	13:H:1236:CLA:H51	1.91	0.53
12:s:45:PHE:HE2	13:t:519:CLA:HAA2	1.74	0.53
13:B:1227:CLA:H191	13:B:1236:CLA:H51	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:1117:CLA:H8	13:G:1117:CLA:HAB	1.92	0.52
13:G:1137:CLA:H13	16:G:4007:BCR:H271	1.91	0.52
8:l:12:PRO:HB2	16:l:4013:BCR:H381	1.90	0.52
12:u:272:TYR:HB3	12:u:300:ARG:HB2	1.91	0.52
12:v:73:LEU:O	12:v:159:LYS:NZ	2.42	0.52
12:4:175:ARG:NH2	12:4:176:LEU:O	2.43	0.52
8:T:40:PRO:HD2	16:T:4015:BCR:H382	1.91	0.52
1:e:31:PRO:HB3	13:e:1101:CLA:HAC1	1.92	0.52
13:f:1227:CLA:H191	13:f:1236:CLA:H51	1.91	0.52
1:A:412:LEU:HD21	13:A:1104:CLA:H142	1.89	0.52
17:A:5009:LHG:H171	12:1:309:PHE:CZ	2.44	0.52
12:4:26:LEU:HB3	13:4:511:CLA:HMA1	1.92	0.52
13:H:1214:CLA:HBA2	13:H:1223:CLA:HBB2	1.91	0.52
10:V:137:LEU:HD13	16:n:4022:BCR:C24	2.39	0.52
12:Y:318:HIS:NE2	13:Y:505:CLA:NB	2.57	0.52
12:d:73:LEU:O	12:d:159:LYS:NZ	2.42	0.52
16:d:522:BCR:H10C	13:q:505:CLA:H161	1.91	0.52
13:A:1117:CLA:H8	13:A:1117:CLA:HAB	1.92	0.52
12:1:318:HIS:NE2	13:1:505:CLA:NB	2.57	0.52
12:2:111:THR:HG21	16:2:522:BCR:H271	1.91	0.52
4:O:121:ARG:NH1	5:Q:65:GLU:OE2	2.42	0.52
13:Y:509:CLA:H101	13:Y:512:CLA:HBD	1.90	0.52
13:Z:502:CLA:H12	13:Z:503:CLA:H42	1.92	0.52
12:b:175:ARG:NH2	12:b:176:LEU:O	2.43	0.52
13:c:507:CLA:HED2	13:c:507:CLA:H2A	1.91	0.52
13:e:1137:CLA:H13	16:e:4007:BCR:H271	1.91	0.52
12:t:175:ARG:NH2	12:t:176:LEU:O	2.43	0.52
8:J:40:PRO:HD2	16:J:4015:BCR:H382	1.91	0.52
17:L:5221:LHG:C34	13:f:1207:CLA:H142	2.40	0.52
12:3:45:PHE:HE2	13:4:519:CLA:HAA2	1.74	0.52
1:G:517:VAL:HG23	13:G:1133:CLA:HED3	1.91	0.52
13:B:1239:CLA:HBA2	14:B:2002:PQN:H251	1.91	0.52
13:L:1501:CLA:H122	16:L:4219:BCR:H372	1.92	0.52
1:G:31:PRO:HB3	13:G:1101:CLA:HAC1	1.91	0.52
2:B:339:ALA:HB2	16:B:4010:BCR:H372	1.92	0.52
1:G:277:THR:HB	9:U:14:TRP:HB2	1.90	0.52
2:H:585:ASN:HB2	13:H:1012:CLA:HBC2	1.91	0.52
13:V:1501:CLA:H141	13:V:1503:CLA:HBC2	1.91	0.52
12:q:301:ALA:O	12:q:305:ASN:ND2	2.41	0.52
12:q:318:HIS:NE2	13:q:505:CLA:NB	2.57	0.52
12:t:207:HIS:NE2	13:t:501:CLA:NB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:26:LEU:HB3	13:u:511:CLA:HMA1	1.91	0.52
1:A:517:VAL:HG23	13:A:1133:CLA:HED3	1.91	0.52
2:B:117:TYR:HA	2:B:367:THR:HG22	1.92	0.52
13:2:502:CLA:H12	13:2:503:CLA:H42	1.92	0.52
12:5:282:VAL:HG23	12:5:283:THR:HG23	1.92	0.52
8:l:40:PRO:HD2	16:l:4015:BCR:H382	1.91	0.52
13:n:1501:CLA:H122	16:n:4219:BCR:H372	1.92	0.52
12:5:67:LEU:HD22	12:5:89:LEU:HD13	1.92	0.52
2:H:524:ALA:HB2	13:H:1235:CLA:HMA1	1.91	0.52
12:b:207:HIS:NE2	13:b:501:CLA:NB	2.58	0.52
13:n:1501:CLA:H141	13:n:1503:CLA:HBC2	1.91	0.52
1:A:31:PRO:HB3	13:A:1101:CLA:HAC1	1.92	0.52
2:B:585:ASN:HB2	13:B:1012:CLA:HBC2	1.91	0.52
12:1:19:ARG:NH1	13:1:511:CLA:OBD	2.43	0.52
12:1:148:PHE:HZ	13:1:516:CLA:HBC2	1.74	0.52
1:G:616:ILE:HD12	13:G:1011:CLA:H122	1.90	0.52
1:A:277:THR:HB	9:K:14:TRP:HB2	1.90	0.51
2:B:340:SER:HB3	13:B:1221:CLA:H2	1.92	0.51
12:Y:148:PHE:HZ	13:Y:516:CLA:HBC2	1.74	0.51
13:e:1013:CLA:H142	16:e:4011:BCR:H21C	1.92	0.51
13:f:1214:CLA:HBA2	13:f:1223:CLA:HBB2	1.91	0.51
13:A:1122:CLA:HBB2	17:A:5003:LHG:HC82	1.92	0.51
2:H:422:LEU:HD13	2:H:532:LEU:HA	1.93	0.51
12:Z:64:LEU:HD13	12:Z:67:LEU:HD12	1.93	0.51
12:Z:148:PHE:HD2	13:Z:512:CLA:H3A	1.76	0.51
1:e:429:ASP:O	1:e:433:ASN:ND2	2.44	0.51
12:4:207:HIS:NE2	13:4:501:CLA:NB	2.58	0.51
17:G:5009:LHG:H241	9:U:14:TRP:HB3	1.93	0.51
12:d:145:HIS:NE2	13:d:512:CLA:NA	2.59	0.51
2:f:524:ALA:HB2	13:f:1235:CLA:HMA1	1.91	0.51
12:q:148:PHE:HZ	13:q:516:CLA:HBC2	1.74	0.51
12:Z:111:THR:HG21	16:Z:522:BCR:H271	1.91	0.51
2:f:340:SER:HB3	13:f:1221:CLA:H2	1.92	0.51
2:f:422:LEU:HD13	2:f:532:LEU:HA	1.93	0.51
2:f:585:ASN:HB2	13:f:1012:CLA:HBC2	1.91	0.51
12:v:145:HIS:NE2	13:v:512:CLA:NA	2.59	0.51
1:A:544:PHE:HZ	16:L:4219:BCR:H332	1.76	0.51
1:A:598:SER:OG	1:A:601:ASP:OD2	2.29	0.51
12:6:145:HIS:NE2	13:6:512:CLA:NA	2.59	0.51
17:G:5005:LHG:HC61	16:Z:521:BCR:HC22	1.92	0.51
13:H:1229:CLA:HBB2	16:H:4014:BCR:HC41	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:517:CLA:HED2	13:t:517:CLA:H2A	1.92	0.51
12:u:112:PHE:HB2	12:v:326:MET:HE3	1.93	0.51
12:u:282:VAL:HG23	12:u:283:THR:HG23	1.92	0.51
13:u:507:CLA:HED2	13:u:507:CLA:H2A	1.91	0.51
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.93	0.51
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.93	0.51
2:H:69:ALA:HB2	2:H:135:LEU:HB2	1.93	0.51
13:H:1239:CLA:HBA2	14:H:2002:PQN:H251	1.91	0.51
13:r:502:CLA:H12	13:r:503:CLA:H42	1.92	0.51
1:A:370:ILE:HD11	13:A:1119:CLA:H71	1.93	0.51
13:V:1501:CLA:H122	16:V:4219:BCR:H372	1.92	0.51
12:b:233:VAL:HG11	16:b:524:BCR:HC22	1.93	0.51
12:c:112:PHE:HB2	12:d:326:MET:HE3	1.93	0.51
13:e:1117:CLA:H8	13:e:1117:CLA:HAB	1.92	0.51
17:e:5008:LHG:H261	17:e:5008:LHG:HC92	1.93	0.51
13:r:505:CLA:H43	16:r:524:BCR:HC7	1.93	0.51
13:B:1229:CLA:HBB2	16:B:4014:BCR:HC41	1.92	0.51
12:6:52:TRP:CZ3	17:G:5009:LHG:HC11	2.46	0.51
16:6:522:BCR:HC41	12:Y:258:TYR:HB2	1.93	0.51
2:H:339:ALA:HB2	16:H:4010:BCR:H372	1.92	0.51
2:H:340:SER:HB3	13:H:1221:CLA:H2	1.92	0.51
12:a:53:LEU:HD21	12:a:83:VAL:HG11	1.93	0.51
1:e:370:ILE:HD11	13:e:1119:CLA:H71	1.93	0.51
1:e:708:LEU:HD21	13:e:1013:CLA:HED2	1.90	0.51
13:e:1122:CLA:HBB2	17:e:5003:LHG:HC82	1.92	0.51
13:e:1101:CLA:H91	16:l:4013:BCR:H21C	1.93	0.51
2:f:117:TYR:HA	2:f:367:THR:HG22	1.92	0.51
2:f:339:ALA:HB2	16:f:4010:BCR:H372	1.92	0.51
12:4:233:VAL:HG11	16:4:524:BCR:HC22	1.92	0.51
12:4:263:ASN:HD21	12:4:265:LEU:HB3	1.76	0.51
1:G:429:ASP:O	1:G:433:ASN:ND2	2.44	0.51
5:i:53:ASP:OD1	5:i:53:ASP:N	2.44	0.51
12:2:64:LEU:HD13	12:2:67:LEU:HD12	1.93	0.51
1:G:607:LEU:HD21	13:G:1128:CLA:HBC1	1.94	0.51
2:H:117:TYR:HA	2:H:367:THR:HG22	1.92	0.51
7:S:20:LEU:HD12	17:n:5221:LHG:H172	1.92	0.51
12:Y:148:PHE:HE2	13:Y:512:CLA:HHB	1.75	0.51
13:b:517:CLA:HED2	13:b:517:CLA:H2A	1.92	0.51
16:d:522:BCR:H323	13:q:505:CLA:H192	1.92	0.51
12:u:146:LEU:HD22	12:u:214:LEU:HD22	1.93	0.51
1:A:485:ASP:OD1	1:A:491:GLN:NE2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1237:CLA:H141	10:L:85:LEU:HD11	1.93	0.50
12:1:148:PHE:HE2	13:1:512:CLA:HHB	1.76	0.50
13:G:1122:CLA:HBB2	17:G:5003:LHG:HC82	1.92	0.50
12:b:307:HIS:NE2	13:b:502:CLA:ND	2.60	0.50
12:c:282:VAL:HG23	12:c:283:THR:HG23	1.92	0.50
1:e:86:TRP:HA	13:e:1105:CLA:HBB2	1.93	0.50
17:e:5005:LHG:HC61	16:r:521:BCR:HC22	1.92	0.50
13:q:501:CLA:C4D	13:q:503:CLA:H2	2.41	0.50
17:L:5221:LHG:H121	13:f:1207:CLA:HMA2	1.93	0.50
13:4:517:CLA:H2A	13:4:517:CLA:HED2	1.92	0.50
12:5:112:PHE:HB2	12:6:326:MET:HE3	1.93	0.50
12:Y:301:ALA:O	12:Y:305:ASN:ND2	2.41	0.50
13:Y:501:CLA:C4D	13:Y:503:CLA:H2	2.41	0.50
12:a:146:LEU:HD22	12:a:214:LEU:HD22	1.94	0.50
12:b:263:ASN:HD21	12:b:265:LEU:HB3	1.76	0.50
1:e:549:ILE:HD12	13:e:1011:CLA:H172	1.94	0.50
2:f:69:ALA:HB2	2:f:135:LEU:HB2	1.93	0.50
12:t:263:ASN:HD21	12:t:265:LEU:HB3	1.76	0.50
13:A:1101:CLA:H91	16:J:4013:BCR:H21C	1.93	0.50
17:A:5005:LHG:HC61	16:2:521:BCR:HC22	1.92	0.50
12:4:307:HIS:NE2	13:4:502:CLA:ND	2.60	0.50
12:d:109:PHE:HB2	13:q:505:CLA:CAA	2.42	0.50
1:e:485:ASP:OD1	1:e:491:GLN:NE2	2.40	0.50
1:e:544:PHE:HZ	16:n:4219:BCR:H332	1.76	0.50
17:e:5009:LHG:H241	9:m:14:TRP:HB3	1.93	0.50
12:t:51:SER:HB2	12:u:279:LYS:HG2	1.94	0.50
12:u:110:HIS:NE2	13:u:513:CLA:NB	2.60	0.50
1:A:429:ASP:O	1:A:433:ASN:ND2	2.44	0.50
13:1:501:CLA:C4D	13:1:503:CLA:H2	2.41	0.50
13:Z:505:CLA:H43	16:Z:524:BCR:HC7	1.93	0.50
1:e:598:SER:OG	1:e:601:ASP:OD2	2.29	0.50
1:e:607:LEU:HD21	13:e:1128:CLA:HBC1	1.93	0.50
13:G:1013:CLA:H142	16:G:4011:BCR:H21C	1.92	0.50
20:H:1852:SQD:O3	10:n:3:GLN:NE2	2.40	0.50
13:Y:502:CLA:HBA2	13:Y:503:CLA:H171	1.93	0.50
13:f:1229:CLA:HBB2	16:f:4014:BCR:HC41	1.92	0.50
13:2:505:CLA:H43	16:2:524:BCR:HC7	1.93	0.50
12:5:110:HIS:NE2	13:5:513:CLA:NB	2.60	0.50
12:5:146:LEU:HD22	12:5:214:LEU:HD22	1.93	0.50
1:G:336:ILE:O	1:G:340:HIS:ND1	2.37	0.50
2:H:710:LEU:HD23	19:H:5002:LMG:H362	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:1237:CLA:H141	10:n:85:LEU:HD11	1.93	0.50
1:A:16:VAL:O	1:A:186:LYS:NZ	2.43	0.50
12:4:51:SER:HB2	12:5:279:LYS:HG2	1.94	0.50
12:4:256:ALA:HB2	13:4:501:CLA:H43	1.94	0.50
13:G:1101:CLA:H91	16:T:4013:BCR:H21C	1.93	0.50
17:G:5008:LHG:H261	17:G:5008:LHG:HC92	1.93	0.50
12:q:148:PHE:HE2	13:q:512:CLA:HHB	1.76	0.50
12:r:148:PHE:HD2	13:r:512:CLA:H3A	1.76	0.50
12:u:67:LEU:HD22	12:u:89:LEU:HD13	1.92	0.50
1:G:544:PHE:HZ	16:V:4219:BCR:H332	1.76	0.50
12:c:146:LEU:HD22	12:c:214:LEU:HD22	1.92	0.50
2:B:710:LEU:HD23	19:B:5002:LMG:H362	1.93	0.50
1:G:86:TRP:HA	13:G:1105:CLA:HBB2	1.93	0.50
2:H:611:GLU:OE2	6:R:36:ARG:NH1	2.44	0.50
4:O:9:PRO:HD2	4:O:57:LEU:HD13	1.94	0.50
12:b:140:LEU:HA	12:b:222:ILE:HG22	1.94	0.50
13:c:501:CLA:C4D	13:c:503:CLA:H2	2.42	0.50
12:d:105:ALA:O	13:q:505:CLA:HBA1	2.11	0.50
2:f:161:PHE:CE2	20:f:1852:SQD:H441	2.47	0.50
2:f:429:LEU:HD11	13:f:1235:CLA:HMB2	1.94	0.50
12:t:233:VAL:HG11	16:t:524:BCR:HC22	1.93	0.50
1:A:549:ILE:HD12	13:A:1011:CLA:H172	1.94	0.49
12:2:148:PHE:HD2	13:2:512:CLA:H3A	1.76	0.49
12:3:53:LEU:HD21	12:3:83:VAL:HG11	1.93	0.49
12:4:140:LEU:HA	12:4:222:ILE:HG22	1.94	0.49
1:G:598:SER:OG	1:G:601:ASP:OD2	2.29	0.49
12:c:67:LEU:HD22	12:c:89:LEU:HD13	1.92	0.49
12:d:276:LEU:HD11	12:d:300:ARG:HG2	1.94	0.49
13:u:501:CLA:C4D	13:u:503:CLA:H2	2.42	0.49
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.94	0.49
1:G:16:VAL:O	1:G:186:LYS:NZ	2.44	0.49
1:G:66:GLU:HG3	1:G:187:LEU:HB2	1.95	0.49
20:H:1852:SQD:H242	17:e:5002:LHG:H261	1.94	0.49
12:Y:19:ARG:NH1	13:Y:511:CLA:OBD	2.43	0.49
12:b:256:ALA:HB2	13:b:501:CLA:H43	1.94	0.49
4:h:9:PRO:HD2	4:h:57:LEU:HD13	1.94	0.49
1:A:86:TRP:HA	13:A:1105:CLA:HBB2	1.93	0.49
1:A:164:GLY:HA2	17:A:5007:LHG:H332	1.94	0.49
13:A:1013:CLA:H142	16:A:4011:BCR:H21C	1.92	0.49
17:A:5009:LHG:H241	9:K:14:TRP:HB3	1.93	0.49
13:3:510:CLA:H43	13:3:510:CLA:HED3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:549:ILE:HD12	13:G:1011:CLA:H172	1.94	0.49
12:b:51:SER:HB2	12:c:279:LYS:HG2	1.94	0.49
12:b:146:LEU:HD22	12:b:214:LEU:HD22	1.94	0.49
3:g:22:PRO:HG2	3:g:23:LEU:HD12	1.94	0.49
12:r:64:LEU:HD13	12:r:67:LEU:HD12	1.93	0.49
12:t:307:HIS:NE2	13:t:502:CLA:ND	2.60	0.49
2:B:73:ASN:HB2	2:B:76:GLN:HB2	1.94	0.49
13:B:1229:CLA:HAB	16:B:4014:BCR:H323	1.95	0.49
4:D:9:PRO:HD2	4:D:57:LEU:HD13	1.94	0.49
13:1:502:CLA:HBA2	13:1:503:CLA:H171	1.93	0.49
1:G:86:TRP:NE1	13:G:1126:CLA:OBD	2.46	0.49
1:G:370:ILE:HD11	13:G:1119:CLA:H71	1.93	0.49
13:G:1237:CLA:H141	10:V:85:LEU:HD11	1.93	0.49
2:H:161:PHE:CE2	20:H:1852:SQD:H441	2.47	0.49
16:d:522:BCR:H21C	13:q:518:CLA:O1D	2.13	0.49
12:s:53:LEU:HD21	12:s:83:VAL:HG11	1.93	0.49
12:s:146:LEU:HD22	12:s:214:LEU:HD22	1.93	0.49
12:t:256:ALA:HB2	13:t:501:CLA:H43	1.94	0.49
12:v:276:LEU:HD11	12:v:300:ARG:HG2	1.94	0.49
2:B:321:GLY:O	2:B:325:THR:OG1	2.28	0.49
3:N:15:THR:HG22	3:N:28:MET:HG3	1.94	0.49
12:d:102:VAL:HG22	13:q:505:CLA:C6	2.41	0.49
1:e:164:GLY:HA2	17:e:5007:LHG:H332	1.94	0.49
13:f:1229:CLA:HAB	16:f:4014:BCR:H323	1.95	0.49
12:q:307:HIS:NE2	13:q:502:CLA:ND	2.61	0.49
1:A:381:HIS:ND1	13:A:1116:CLA:OBD	2.46	0.49
1:A:607:LEU:HD21	13:A:1128:CLA:HBC1	1.94	0.49
12:1:307:HIS:NE2	13:1:502:CLA:ND	2.61	0.49
13:5:501:CLA:C4D	13:5:503:CLA:H2	2.42	0.49
12:Z:145:HIS:NE2	13:Z:512:CLA:NA	2.60	0.49
12:a:267:TYR:O	12:a:300:ARG:NH2	2.41	0.49
12:b:276:LEU:HB3	12:b:286:PHE:HB3	1.95	0.49
2:f:710:LEU:HD23	19:f:5002:LMG:H362	1.93	0.49
17:A:5008:LHG:HC92	17:A:5008:LHG:H261	1.93	0.49
2:B:161:PHE:CE2	20:B:1852:SQD:H441	2.47	0.49
12:Y:307:HIS:NE2	13:Y:502:CLA:ND	2.61	0.49
13:Y:501:CLA:H193	13:Y:507:CLA:HBB1	1.95	0.49
12:c:110:HIS:NE2	13:c:513:CLA:NB	2.60	0.49
1:e:381:HIS:ND1	13:e:1116:CLA:OBD	2.46	0.49
1:A:577:LYS:NZ	2:B:673:GLU:OE2	2.36	0.49
2:B:722:ALA:HB2	13:B:1224:CLA:HBB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:251:LEU:HD13	13:2:505:CLA:H122	1.95	0.49
12:3:146:LEU:HD22	12:3:214:LEU:HD22	1.94	0.49
12:6:276:LEU:HD11	12:6:300:ARG:HG2	1.94	0.49
1:G:742:HIS:CE1	13:G:1140:CLA:NA	2.81	0.49
13:a:510:CLA:H43	13:a:510:CLA:HED3	1.94	0.49
17:A:5009:LHG:H291	13:K:1103:CLA:HED1	1.95	0.49
9:K:29:ALA:HA	9:K:32:ILE:HG12	1.95	0.49
2:H:722:ALA:HB2	13:H:1224:CLA:HBB1	1.95	0.49
13:H:1229:CLA:HAB	16:H:4014:BCR:H323	1.95	0.49
14:H:2002:PQN:H242	16:H:4017:BCR:H17C	1.95	0.49
13:e:1119:CLA:H61	16:e:4007:BCR:H352	1.95	0.49
10:n:33:ALA:HB1	13:n:1501:CLA:HAC1	1.94	0.49
12:r:145:HIS:NE2	13:r:512:CLA:NA	2.60	0.49
12:t:140:LEU:HA	12:t:222:ILE:HG22	1.94	0.49
1:A:66:GLU:HG3	1:A:187:LEU:HB2	1.95	0.48
3:C:15:THR:HG22	3:C:28:MET:HG3	1.94	0.48
20:L:5216:SQD:C3	2:f:4:LYS:HZ1	2.25	0.48
12:1:67:LEU:HD22	12:1:89:LEU:HD13	1.95	0.48
12:2:49:GLU:HB3	12:2:64:LEU:HD22	1.95	0.48
1:G:16:VAL:HA	1:G:185:PRO:HA	1.96	0.48
1:G:381:HIS:ND1	13:G:1116:CLA:OBD	2.46	0.48
13:G:1118:CLA:HBB1	16:U:4104:BCR:H342	1.95	0.48
12:Y:67:LEU:HD22	12:Y:89:LEU:HD13	1.95	0.48
12:d:101:ALA:HB1	13:q:505:CLA:CAB	2.42	0.48
1:e:16:VAL:O	1:e:186:LYS:NZ	2.43	0.48
1:e:16:VAL:HA	1:e:185:PRO:HA	1.95	0.48
2:f:73:ASN:HB2	2:f:76:GLN:HB2	1.94	0.48
13:f:1220:CLA:HAA1	16:f:4009:BCR:H16C	1.95	0.48
13:s:510:CLA:H43	13:s:510:CLA:HED3	1.94	0.48
12:v:331:ARG:NH2	20:v:822:SQD:O8	2.46	0.48
13:A:1103:CLA:H3A	13:A:1103:CLA:HBA1	1.54	0.48
2:B:429:LEU:HD11	13:B:1235:CLA:HMB2	1.94	0.48
13:1:501:CLA:H193	13:1:507:CLA:HBB1	1.95	0.48
12:4:276:LEU:HG	12:4:300:ARG:HD2	1.95	0.48
12:5:40:PHE:HE2	13:6:519:CLA:HBA1	1.77	0.48
17:G:5009:LHG:H291	13:U:1103:CLA:HED1	1.95	0.48
2:H:15:ASP:OD2	2:H:19:ARG:NH2	2.46	0.48
3:N:22:PRO:HG2	3:N:23:LEU:HD12	1.94	0.48
13:a:517:CLA:HBA1	13:a:517:CLA:H3A	1.50	0.48
1:e:377:ILE:HG21	13:e:1117:CLA:H201	1.95	0.48
13:e:1101:CLA:HHC	13:e:1101:CLA:HBB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:67:VAL:HG21	15:g:3002:SF4:S2	2.53	0.48
9:m:29:ALA:HA	9:m:32:ILE:HG12	1.95	0.48
12:s:148:PHE:HZ	13:s:516:CLA:HBC2	1.78	0.48
13:s:507:CLA:H112	16:s:524:BCR:H362	1.95	0.48
1:A:742:HIS:CE1	13:A:1140:CLA:NA	2.81	0.48
2:B:96:PHE:HB2	7:I:1:MET:HE1	1.96	0.48
14:B:2002:PQN:H242	16:B:4017:BCR:H17C	1.95	0.48
1:G:377:ILE:HG21	13:G:1117:CLA:H201	1.95	0.48
2:H:429:LEU:HD11	13:H:1235:CLA:HMB2	1.94	0.48
13:H:1220:CLA:HAA1	16:H:4009:BCR:H16C	1.95	0.48
13:H:1227:CLA:HAB	13:H:1236:CLA:HBB2	1.96	0.48
10:V:33:ALA:HB1	13:V:1501:CLA:HAC1	1.94	0.48
12:r:49:GLU:HB3	12:r:64:LEU:HD22	1.96	0.48
13:A:1118:CLA:HBB1	16:K:4104:BCR:H342	1.96	0.48
13:B:1226:CLA:H42	19:B:5002:LMG:H302	1.95	0.48
10:L:33:ALA:HB1	13:L:1501:CLA:HAC1	1.94	0.48
13:1:505:CLA:HAB	12:v:101:ALA:HB1	1.95	0.48
2:H:73:ASN:HB2	2:H:76:GLN:HB2	1.94	0.48
3:N:67:VAL:HG21	15:N:3002:SF4:S2	2.53	0.48
12:a:148:PHE:HZ	13:a:516:CLA:HBC2	1.78	0.48
13:a:507:CLA:H112	16:a:524:BCR:H362	1.95	0.48
12:c:40:PHE:HE2	13:d:519:CLA:HBA1	1.77	0.48
1:e:86:TRP:NE1	13:e:1126:CLA:OBD	2.46	0.48
2:f:210:ASP:OD1	2:f:210:ASP:N	2.46	0.48
3:g:15:THR:HG22	3:g:28:MET:HG3	1.94	0.48
13:q:501:CLA:HMB2	16:q:524:BCR:H23C	1.96	0.48
2:B:15:ASP:OD2	2:B:19:ARG:NH2	2.46	0.48
2:B:326:LEU:HD13	2:B:332:PHE:HD2	1.77	0.48
12:4:282:VAL:HG23	12:4:283:THR:HG23	1.95	0.48
13:H:1207:CLA:HMA2	17:n:5221:LHG:H121	1.94	0.48
13:Y:501:CLA:HMB2	16:Y:524:BCR:H23C	1.96	0.48
12:Z:49:GLU:HB3	12:Z:64:LEU:HD22	1.96	0.48
12:d:102:VAL:CG2	13:q:505:CLA:H8	2.43	0.48
14:f:2002:PQN:H242	16:f:4017:BCR:H17C	1.95	0.48
13:q:502:CLA:HBA2	13:q:503:CLA:H171	1.93	0.48
12:s:267:TYR:O	12:s:300:ARG:NH2	2.41	0.48
12:1:130:PHE:HA	12:1:137:GLN:HG2	1.96	0.48
1:e:66:GLU:HG3	1:e:187:LEU:HB2	1.95	0.48
1:e:742:HIS:CE1	13:e:1140:CLA:NA	2.81	0.48
2:f:15:ASP:OD2	2:f:19:ARG:NH2	2.46	0.48
13:f:1226:CLA:H42	19:f:5002:LMG:H302	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:m:70:LEU:HD22	13:m:1401:CLA:HMC3	1.95	0.48
12:s:34:GLN:OE1	13:s:510:CLA:NC	2.47	0.48
13:B:1219:CLA:H142	17:B:1842:LHG:C36	2.44	0.48
13:1:501:CLA:HMB2	16:1:524:BCR:H23C	1.96	0.48
13:1:512:CLA:H3A	13:1:512:CLA:HBA1	1.62	0.48
12:3:34:GLN:OE1	13:3:510:CLA:NC	2.47	0.48
12:3:148:PHE:HZ	13:3:516:CLA:HBC2	1.78	0.48
12:4:146:LEU:HD22	12:4:214:LEU:HD22	1.94	0.48
2:H:631:LEU:O	2:H:647:SER:OG	2.29	0.48
13:H:1210:CLA:H2	13:H:1210:CLA:H62	1.64	0.48
12:Z:251:LEU:HD13	13:Z:505:CLA:H122	1.95	0.48
12:d:301:ALA:O	12:d:305:ASN:ND2	2.43	0.48
2:f:96:PHE:HB2	7:k:1:MET:HE1	1.96	0.48
2:f:456:GLU:OE1	6:j:68:HIS:ND1	2.47	0.48
13:f:1203:CLA:H191	19:f:5002:LMG:H252	1.96	0.48
12:q:67:LEU:HD22	12:q:89:LEU:HD13	1.95	0.48
13:q:516:CLA:HBA1	13:q:516:CLA:H3A	1.51	0.48
12:r:330:PHE:HB3	20:r:822:SQD:H82	1.96	0.48
1:A:220:SER:O	1:A:224:ASN:HB2	2.14	0.48
13:A:1140:CLA:HBA2	17:A:5001:LHG:H171	1.96	0.48
3:C:67:VAL:HG21	15:C:3002:SF4:S2	2.53	0.48
12:Z:200:LEU:HG	12:Z:265:LEU:HD11	1.96	0.48
12:b:59:MET:HB2	12:b:271:PHE:HA	1.96	0.48
12:d:61:GLU:HG3	12:d:292:LEU:HD13	1.96	0.48
13:e:1118:CLA:HBB1	16:m:4104:BCR:H342	1.95	0.48
17:e:5009:LHG:H291	13:m:1103:CLA:HED1	1.95	0.48
12:u:40:PHE:HE2	13:v:519:CLA:HBA1	1.77	0.48
12:2:145:HIS:NE2	13:2:512:CLA:NA	2.60	0.48
1:G:164:GLY:HA2	17:G:5007:LHG:H332	1.94	0.48
13:G:1140:CLA:HBA2	17:G:5001:LHG:H171	1.96	0.48
2:H:456:GLU:OE1	6:R:68:HIS:ND1	2.47	0.48
9:U:29:ALA:HA	9:U:32:ILE:HG12	1.95	0.48
12:Z:330:PHE:HB3	20:Z:822:SQD:H82	1.96	0.48
12:a:34:GLN:OE1	13:a:510:CLA:NC	2.47	0.48
12:b:276:LEU:HG	12:b:300:ARG:HD2	1.95	0.48
12:b:282:VAL:HG23	12:b:283:THR:HG23	1.95	0.48
13:q:501:CLA:H193	13:q:507:CLA:HBB1	1.95	0.48
13:r:511:CLA:H72	12:s:333:VAL:HG13	1.96	0.48
12:t:146:LEU:HD22	12:t:214:LEU:HD22	1.94	0.48
13:B:1227:CLA:HAB	13:B:1236:CLA:HBB2	1.96	0.48
13:3:509:CLA:HBD	13:3:509:CLA:H121	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:305:ASN:HB3	16:5:521:BCR:HC8	1.96	0.48
1:G:220:SER:O	1:G:224:ASN:HB2	2.14	0.48
13:H:1219:CLA:H142	17:H:1842:LHG:C36	2.44	0.48
2:f:722:ALA:HB2	13:f:1224:CLA:HBB1	1.95	0.48
12:r:251:LEU:HD23	13:r:501:CLA:H142	1.96	0.48
12:t:282:VAL:HG23	12:t:283:THR:HG23	1.95	0.48
12:2:301:ALA:O	12:2:305:ASN:ND2	2.41	0.47
12:4:59:MET:HB2	12:4:271:PHE:HA	1.96	0.47
12:4:276:LEU:HB3	12:4:286:PHE:HB3	1.95	0.47
13:a:509:CLA:HBD	13:a:509:CLA:H121	1.96	0.47
13:f:1235:CLA:H172	16:j:4016:BCR:H272	1.96	0.47
13:s:509:CLA:HBD	13:s:509:CLA:H121	1.96	0.47
12:t:59:MET:HB2	12:t:271:PHE:HA	1.96	0.47
12:t:276:LEU:HG	12:t:300:ARG:HD2	1.95	0.47
1:A:86:TRP:NE1	13:A:1126:CLA:OBD	2.46	0.47
12:2:330:PHE:HB3	20:2:822:SQD:H82	1.96	0.47
13:G:1119:CLA:H61	16:G:4007:BCR:H352	1.95	0.47
12:d:98:ILE:HG23	13:q:505:CLA:H112	1.96	0.47
13:e:1110:CLA:HBA2	13:e:1110:CLA:H3A	1.56	0.47
1:A:377:ILE:HG21	13:A:1117:CLA:H201	1.95	0.47
2:B:4:LYS:HZ1	20:V:5216:SQD:C3	2.26	0.47
13:B:1207:CLA:H142	17:V:5221:LHG:C34	2.41	0.47
13:3:502:CLA:HBD	13:3:503:CLA:H43	1.97	0.47
13:H:1222:CLA:H52	13:H:1234:CLA:H11	1.97	0.47
12:Z:148:PHE:CD2	13:Z:512:CLA:H3A	2.50	0.47
12:a:274:ALA:HB3	12:a:290:VAL:HG22	1.97	0.47
12:d:331:ARG:NH2	20:d:822:SQD:O8	2.46	0.47
13:e:1106:CLA:H3A	13:e:1106:CLA:HBA2	1.61	0.47
12:u:305:ASN:HB3	16:u:521:BCR:HC8	1.96	0.47
13:A:1119:CLA:H61	16:A:4007:BCR:H352	1.95	0.47
12:2:200:LEU:HG	12:2:265:LEU:HD11	1.96	0.47
12:6:331:ARG:NH2	20:6:822:SQD:O8	2.46	0.47
2:H:96:PHE:HB2	7:S:1:MET:HE1	1.96	0.47
9:U:70:LEU:HD22	13:U:1401:CLA:HMC3	1.95	0.47
13:r:506:CLA:H62	13:r:506:CLA:H41	1.71	0.47
7:I:20:LEU:HD12	17:V:5221:LHG:H172	1.95	0.47
13:G:1122:CLA:H91	13:G:1122:CLA:H111	1.77	0.47
2:H:481:ALA:HA	2:H:486:THR:HG21	1.97	0.47
13:H:1226:CLA:H42	19:H:5002:LMG:H302	1.95	0.47
13:Z:518:CLA:H61	13:Z:518:CLA:H41	1.62	0.47
1:e:220:SER:O	1:e:224:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:658:LEU:HD13	13:e:1022:CLA:HED1	1.96	0.47
13:e:1140:CLA:HBA2	17:e:5001:LHG:H171	1.96	0.47
13:f:1219:CLA:H142	17:f:1842:LHG:C36	2.44	0.47
12:t:276:LEU:HB3	12:t:286:PHE:HB3	1.95	0.47
13:B:1220:CLA:HAA1	16:B:4009:BCR:H16C	1.95	0.47
13:B:1235:CLA:H172	16:F:4016:BCR:H272	1.96	0.47
13:1:516:CLA:H3A	13:1:516:CLA:HBA1	1.51	0.47
13:3:507:CLA:H112	16:3:524:BCR:H362	1.95	0.47
13:4:509:CLA:HBD	13:4:509:CLA:H121	1.96	0.47
12:5:221:HIS:CE1	13:5:506:CLA:NA	2.83	0.47
12:6:200:LEU:HG	12:6:265:LEU:HD11	1.96	0.47
13:a:502:CLA:HBD	13:a:503:CLA:H43	1.97	0.47
16:d:522:BCR:H352	12:q:315:LEU:HD21	1.96	0.47
13:A:1108:CLA:HBA2	13:A:1108:CLA:H3A	1.71	0.47
2:B:301:ILE:HG21	13:B:1221:CLA:HAC1	1.97	0.47
13:B:1207:CLA:HMA2	17:V:5221:LHG:H121	1.95	0.47
10:L:155:LEU:HD22	7:k:13:ILE:HD11	1.96	0.47
12:6:61:GLU:HG3	12:6:292:LEU:HD13	1.96	0.47
1:G:658:LEU:HD13	13:G:1022:CLA:HED1	1.96	0.47
13:H:1203:CLA:H191	19:H:5002:LMG:H252	1.96	0.47
13:H:1215:CLA:H13	13:H:1221:CLA:H162	1.97	0.47
13:H:1235:CLA:H172	16:R:4016:BCR:H272	1.96	0.47
13:Z:501:CLA:C4D	13:Z:503:CLA:H2	2.45	0.47
13:Z:511:CLA:H72	12:a:333:VAL:HG13	1.96	0.47
16:a:524:BCR:H15C	16:a:524:BCR:H351	1.78	0.47
13:b:509:CLA:HBD	13:b:509:CLA:H121	1.96	0.47
12:c:221:HIS:CE1	13:c:506:CLA:NA	2.83	0.47
1:e:522:GLY:HA2	1:e:536:PRO:HB3	1.97	0.47
13:e:1116:CLA:HBA2	13:e:1116:CLA:H3A	1.46	0.47
13:f:1227:CLA:HAB	13:f:1236:CLA:HBB2	1.96	0.47
12:r:200:LEU:HG	12:r:265:LEU:HD11	1.96	0.47
12:r:251:LEU:HD13	13:r:505:CLA:H122	1.95	0.47
12:u:221:HIS:CE1	13:u:506:CLA:NA	2.83	0.47
13:A:1139:CLA:H41	13:A:1139:CLA:H61	1.62	0.47
13:B:1203:CLA:H191	19:B:5002:LMG:H252	1.96	0.47
7:I:1:MET:HB3	7:I:1:MET:HE2	1.81	0.47
9:K:70:LEU:HD22	13:K:1401:CLA:HMC3	1.95	0.47
13:6:517:CLA:HBA1	13:6:517:CLA:H3A	1.50	0.47
13:G:1101:CLA:HHC	13:G:1101:CLA:HBB1	1.96	0.47
12:c:305:ASN:HB3	16:c:521:BCR:HC8	1.96	0.47
16:c:522:BCR:H15C	16:c:522:BCR:H351	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:1215:CLA:H13	13:f:1221:CLA:H162	1.97	0.47
13:f:1222:CLA:H52	13:f:1234:CLA:H11	1.97	0.47
4:h:21:SER:HA	4:h:24:THR:HB	1.97	0.47
13:v:519:CLA:HED2	13:v:519:CLA:H2A	1.97	0.47
4:D:21:SER:HA	4:D:24:THR:HB	1.97	0.47
16:1:522:BCR:H351	16:1:522:BCR:H15C	1.80	0.47
12:4:230:THR:HG23	12:4:234:LEU:HD12	1.97	0.47
13:H:1207:CLA:H142	17:n:5221:LHG:C34	2.44	0.47
12:q:19:ARG:NH1	13:q:511:CLA:OBD	2.43	0.47
12:q:130:PHE:HA	12:q:137:GLN:HG2	1.96	0.47
12:s:143:GLY:HA3	12:s:222:ILE:HG13	1.97	0.47
13:s:502:CLA:HBD	13:s:503:CLA:H43	1.96	0.47
13:B:1220:CLA:HED3	13:B:1220:CLA:H2A	1.97	0.47
12:6:177:VAL:HG21	12:6:204:VAL:HG21	1.96	0.47
1:G:441:VAL:HG11	13:G:1119:CLA:H192	1.97	0.47
13:G:1130:CLA:HMC1	13:V:1502:CLA:H122	1.97	0.47
12:Y:281:GLY:O	13:Y:519:CLA:HED1	2.15	0.47
2:f:481:ALA:HA	2:f:486:THR:HG21	1.97	0.47
12:q:281:GLY:O	13:q:519:CLA:HED1	2.15	0.47
13:q:510:CLA:H61	13:q:510:CLA:H41	1.61	0.47
13:A:1101:CLA:HBB1	13:A:1101:CLA:HHC	1.96	0.46
12:2:148:PHE:CD2	13:2:512:CLA:H3A	2.50	0.46
7:S:29:LEU:HB3	20:n:5216:SQD:H241	1.97	0.46
12:b:230:THR:HG23	12:b:234:LEU:HD12	1.97	0.46
13:e:1013:CLA:H203	13:e:1140:CLA:H51	1.97	0.46
12:q:111:THR:HG21	16:q:522:BCR:H271	1.97	0.46
1:A:16:VAL:HA	1:A:185:PRO:HA	1.95	0.46
13:A:1126:CLA:H3A	13:A:1126:CLA:HBA2	1.60	0.46
12:1:111:THR:HG21	16:1:522:BCR:H271	1.97	0.46
13:1:505:CLA:H43	16:1:524:BCR:HC7	1.98	0.46
13:2:501:CLA:C4D	13:2:503:CLA:H2	2.45	0.46
2:H:326:LEU:HD13	2:H:332:PHE:HD2	1.77	0.46
12:d:251:LEU:HD23	13:d:501:CLA:H142	1.97	0.46
13:e:1140:CLA:HBA2	17:e:5001:LHG:H152	1.98	0.46
12:r:148:PHE:CD2	13:r:512:CLA:H3A	2.50	0.46
13:t:509:CLA:HBD	13:t:509:CLA:H121	1.96	0.46
2:B:481:ALA:HA	2:B:486:THR:HG21	1.97	0.46
12:2:251:LEU:HD23	13:2:501:CLA:H142	1.96	0.46
13:3:501:CLA:C4D	13:3:503:CLA:H2	2.46	0.46
12:4:70:LEU:HD21	13:4:503:CLA:HED2	1.97	0.46
13:G:1110:CLA:HBA2	13:G:1110:CLA:H3A	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:26:LEU:HA	3:N:41:ALA:O	2.16	0.46
12:Z:251:LEU:HD23	13:Z:501:CLA:H142	1.96	0.46
12:b:119:ALA:O	12:b:126:LYS:NZ	2.41	0.46
12:d:200:LEU:HG	12:d:265:LEU:HD11	1.96	0.46
12:v:61:GLU:HG3	12:v:292:LEU:HD13	1.96	0.46
2:B:118:SER:HA	13:B:1224:CLA:HMA2	1.98	0.46
2:B:355:MET:HE3	2:B:355:MET:HB2	1.79	0.46
13:B:1222:CLA:H52	13:B:1234:CLA:H11	1.97	0.46
10:L:3:GLN:NE2	20:f:1852:SQD:O3	2.47	0.46
13:G:1140:CLA:HBA2	17:G:5001:LHG:H152	1.98	0.46
2:H:118:SER:HA	13:H:1224:CLA:HMA2	1.97	0.46
12:Y:130:PHE:HA	12:Y:137:GLN:HG2	1.96	0.46
12:c:307:HIS:NE2	13:c:502:CLA:NA	2.64	0.46
12:d:79:ASP:OD1	12:d:79:ASP:N	2.48	0.46
13:d:519:CLA:HED2	13:d:519:CLA:H2A	1.97	0.46
16:d:522:BCR:C23	13:q:518:CLA:HED3	2.46	0.46
3:g:62:PHE:HD2	4:h:122:ILE:HD13	1.81	0.46
16:q:524:BCR:H15C	16:q:524:BCR:H351	1.79	0.46
12:s:274:ALA:HB3	12:s:290:VAL:HG22	1.96	0.46
12:v:251:LEU:HD23	13:v:501:CLA:H142	1.98	0.46
1:A:370:ILE:HG21	13:A:1123:CLA:HMA3	1.97	0.46
13:B:1215:CLA:H13	13:B:1221:CLA:H162	1.97	0.46
13:B:1215:CLA:HBA2	13:B:1215:CLA:H3A	1.58	0.46
13:B:1224:CLA:HBA2	13:B:1224:CLA:H3A	1.65	0.46
13:J:1302:CLA:H61	13:J:1302:CLA:H2	1.73	0.46
1:G:522:GLY:HA2	1:G:536:PRO:HB3	1.97	0.46
13:G:1134:CLA:H61	13:G:1134:CLA:H41	1.83	0.46
13:a:501:CLA:C4D	13:a:503:CLA:H2	2.46	0.46
13:q:505:CLA:H43	16:q:524:BCR:HC7	1.98	0.46
13:q:508:CLA:H43	13:q:511:CLA:HAC1	1.98	0.46
12:u:307:HIS:NE2	13:u:502:CLA:NA	2.64	0.46
12:v:200:LEU:HG	12:v:265:LEU:HD11	1.96	0.46
1:A:441:VAL:HG11	13:A:1119:CLA:H192	1.97	0.46
3:C:26:LEU:HA	3:C:41:ALA:O	2.16	0.46
12:6:190:TYR:HD2	16:6:524:BCR:H401	1.81	0.46
13:G:1013:CLA:H203	13:G:1140:CLA:H51	1.97	0.46
2:H:415:LYS:HD2	2:H:539:LEU:HB3	1.98	0.46
16:U:4104:BCR:H403	20:Y:822:SQD:H332	1.98	0.46
13:b:517:CLA:H3A	13:b:517:CLA:HBA1	1.68	0.46
12:c:309:PHE:CD2	16:c:521:BCR:H10C	2.51	0.46
13:e:1130:CLA:HMC1	13:n:1502:CLA:H122	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:415:LYS:HD2	2:f:539:LEU:HB3	1.98	0.46
13:f:1023:CLA:H122	16:k:4018:BCR:H281	1.98	0.46
13:l:1302:CLA:H2	13:l:1302:CLA:H61	1.73	0.46
13:r:501:CLA:C4D	13:r:503:CLA:H2	2.45	0.46
13:u:502:CLA:HBD	13:u:503:CLA:H43	1.98	0.46
12:v:59:MET:HB2	12:v:271:PHE:HA	1.98	0.46
16:B:4005:BCR:H15C	16:B:4005:BCR:H351	1.81	0.46
3:C:62:PHE:HD2	4:D:122:ILE:HD13	1.81	0.46
13:L:1501:CLA:HMD3	10:n:94:SER:HB2	1.97	0.46
17:L:5221:LHG:H172	7:k:20:LEU:HD12	1.96	0.46
16:2:524:BCR:H15C	16:2:524:BCR:H351	1.78	0.46
12:3:274:ALA:HB3	12:3:290:VAL:HG22	1.96	0.46
1:G:370:ILE:HG21	13:G:1123:CLA:HMA3	1.97	0.46
13:G:1013:CLA:H122	13:G:1140:CLA:H101	1.98	0.46
7:S:26:LEU:HD11	20:n:5216:SQD:H282	1.97	0.46
12:c:145:HIS:NE2	13:c:512:CLA:NA	2.64	0.46
12:d:177:VAL:HG21	12:d:204:VAL:HG21	1.97	0.46
13:e:1115:CLA:H62	13:e:1115:CLA:H41	1.65	0.46
2:f:118:SER:HA	13:f:1224:CLA:HMA2	1.97	0.46
2:f:156:HIS:CE1	13:f:1208:CLA:NA	2.84	0.46
2:f:343:VAL:HG13	13:f:1222:CLA:HED1	1.97	0.46
13:r:518:CLA:H61	13:r:518:CLA:H41	1.62	0.46
13:s:501:CLA:C4D	13:s:503:CLA:H2	2.46	0.46
13:s:517:CLA:H3A	13:s:517:CLA:HBA1	1.51	0.46
13:u:509:CLA:H92	13:u:509:CLA:H62	1.81	0.46
12:v:78:GLY:N	12:v:82:GLN:O	2.49	0.46
1:A:658:LEU:HD13	13:A:1022:CLA:HED1	1.97	0.46
16:A:4007:BCR:H15C	16:A:4007:BCR:H351	1.79	0.46
2:B:611:GLU:OE2	6:F:36:ARG:NH1	2.44	0.46
10:L:90:THR:HG21	10:L:133:ILE:HD12	1.98	0.46
12:6:251:LEU:HD23	13:6:501:CLA:H142	1.98	0.46
1:G:115:GLN:NE2	13:G:1107:CLA:OBD	2.43	0.46
14:G:2001:PQN:H301	8:T:19:PHE:HZ	1.81	0.46
2:H:156:HIS:CE1	13:H:1208:CLA:NA	2.84	0.46
2:H:301:ILE:HG21	13:H:1221:CLA:HAC1	1.97	0.46
13:H:1209:CLA:H3A	13:H:1209:CLA:HBA2	1.59	0.46
13:H:1221:CLA:H112	13:H:1221:CLA:H72	1.75	0.46
16:H:4009:BCR:H351	16:H:4009:BCR:H15C	1.82	0.46
12:Y:111:THR:HG21	16:Y:522:BCR:H271	1.97	0.46
16:c:521:BCR:H24C	16:c:521:BCR:H371	1.82	0.46
2:f:326:LEU:HD13	2:f:332:PHE:HD2	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:1201:CLA:H2	16:o:4021:BCR:H323	1.98	0.46
4:h:101:ASP:OD1	4:h:101:ASP:N	2.48	0.46
13:s:501:CLA:HBB2	13:s:507:CLA:H92	1.98	0.46
16:u:521:BCR:H15C	16:u:521:BCR:H351	1.85	0.46
13:B:1221:CLA:H141	13:B:1221:CLA:H161	1.78	0.46
12:1:281:GLY:O	13:1:519:CLA:HED1	2.15	0.46
12:3:26:LEU:HB3	13:3:511:CLA:HMA1	1.98	0.46
13:Y:512:CLA:H3A	13:Y:512:CLA:HBA1	1.62	0.46
12:c:73:LEU:O	12:c:159:LYS:NZ	2.49	0.46
16:m:4104:BCR:H403	20:q:822:SQD:H332	1.98	0.46
10:n:90:THR:HG21	10:n:133:ILE:HD12	1.98	0.46
12:q:97:LEU:HG	16:q:522:BCR:H12C	1.98	0.46
13:r:501:CLA:H41	13:r:501:CLA:H62	1.61	0.46
1:A:522:GLY:HA2	1:A:536:PRO:HB3	1.97	0.46
13:A:1105:CLA:HMB3	13:A:1106:CLA:HHB	1.98	0.46
13:A:1130:CLA:HMC1	13:L:1502:CLA:H122	1.97	0.46
16:A:4003:BCR:H15C	16:A:4003:BCR:H351	1.81	0.46
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.98	0.46
7:I:13:ILE:HD11	10:V:155:LEU:HD22	1.96	0.46
13:1:508:CLA:H62	13:1:508:CLA:H41	1.62	0.46
13:3:501:CLA:HBB2	13:3:507:CLA:H92	1.98	0.46
12:5:148:PHE:HD2	13:5:512:CLA:H3A	1.81	0.46
12:5:309:PHE:HD2	16:5:521:BCR:H10C	1.81	0.46
12:6:146:LEU:HD22	12:6:214:LEU:HD22	1.98	0.46
13:G:1102:CLA:H202	13:G:1102:CLA:H161	1.82	0.46
13:H:1215:CLA:HBA2	13:H:1215:CLA:H3A	1.58	0.46
13:H:1217:CLA:HBA2	13:H:1217:CLA:H3A	1.41	0.46
12:b:70:LEU:HD21	13:b:503:CLA:HED2	1.97	0.46
12:d:146:LEU:HD22	12:d:214:LEU:HD22	1.98	0.46
1:e:360:TRP:HB3	13:e:1103:CLA:HAC1	1.98	0.46
13:e:1022:CLA:H192	13:f:1206:CLA:H51	1.98	0.46
16:l:4015:BCR:H15C	16:l:4015:BCR:H351	1.79	0.46
12:t:70:LEU:HD21	13:t:503:CLA:HED2	1.97	0.46
12:u:73:LEU:O	12:u:159:LYS:NZ	2.49	0.46
1:A:115:GLN:NE2	13:A:1107:CLA:OBD	2.43	0.45
13:A:1140:CLA:HBA2	17:A:5001:LHG:H152	1.98	0.45
2:B:343:VAL:HG13	13:B:1222:CLA:HED1	1.97	0.45
13:B:1201:CLA:H2	16:M:4021:BCR:H323	1.98	0.45
16:F:4016:BCR:H11C	16:F:4016:BCR:H341	1.77	0.45
16:1:521:BCR:H15C	16:1:521:BCR:H351	1.82	0.45
12:3:59:MET:HE2	12:3:67:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:519:CLA:HED2	13:6:519:CLA:H2A	1.97	0.45
13:H:1224:CLA:H72	13:H:1224:CLA:H111	1.68	0.45
16:H:4014:BCR:H332	16:T:4012:BCR:HC32	1.99	0.45
12:Z:226:PRO:HA	13:Z:506:CLA:HED3	1.98	0.45
12:d:102:VAL:HG22	13:q:505:CLA:C7	2.46	0.45
12:d:102:VAL:HG13	13:q:505:CLA:H52	1.98	0.45
13:f:1228:CLA:HAB	13:f:1229:CLA:H202	1.98	0.45
12:v:143:GLY:HA3	12:v:222:ILE:HG13	1.98	0.45
12:v:190:TYR:HD2	16:v:524:BCR:H401	1.81	0.45
13:A:1013:CLA:H203	13:A:1140:CLA:H51	1.97	0.45
13:A:1122:CLA:H41	13:A:1122:CLA:H62	1.68	0.45
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.99	0.45
2:B:415:LYS:HD2	2:B:539:LEU:HB3	1.98	0.45
13:B:1212:CLA:H61	13:B:1212:CLA:H41	1.70	0.45
4:D:37:GLU:HA	4:D:50:MET:O	2.16	0.45
16:1:524:BCR:H15C	16:1:524:BCR:H351	1.79	0.45
13:2:511:CLA:H72	12:3:333:VAL:HG13	1.96	0.45
13:5:512:CLA:H3A	13:5:512:CLA:HBA1	1.68	0.45
13:6:501:CLA:HMB2	16:6:524:BCR:H23C	1.98	0.45
12:b:143:GLY:HA3	12:b:222:ILE:HG23	1.98	0.45
16:c:521:BCR:H15C	16:c:521:BCR:H351	1.84	0.45
1:e:441:VAL:HG11	13:e:1119:CLA:H192	1.97	0.45
13:f:1220:CLA:H2A	13:f:1220:CLA:HED3	1.97	0.45
12:t:230:THR:HG23	12:t:234:LEU:HD12	1.97	0.45
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.99	0.45
2:B:156:HIS:CE1	13:B:1208:CLA:NA	2.84	0.45
2:B:376:GLN:O	2:B:380:THR:OG1	2.33	0.45
13:B:1219:CLA:H2	13:B:1219:CLA:H61	1.65	0.45
13:B:1222:CLA:H2	13:B:1231:CLA:HBB2	1.99	0.45
16:L:4219:BCR:H15C	16:L:4219:BCR:H351	1.78	0.45
12:2:19:ARG:NH1	13:2:511:CLA:OBD	2.50	0.45
12:2:226:PRO:HA	13:2:506:CLA:HED3	1.98	0.45
12:6:59:MET:HB2	12:6:271:PHE:HA	1.98	0.45
13:G:1139:CLA:H61	13:G:1139:CLA:H41	1.62	0.45
2:H:343:VAL:HG13	13:H:1222:CLA:HED1	1.97	0.45
13:H:1220:CLA:HED3	13:H:1220:CLA:H2A	1.97	0.45
16:T:4015:BCR:H11C	16:T:4015:BCR:H341	1.84	0.45
12:a:143:GLY:HA3	12:a:222:ILE:HG13	1.97	0.45
13:j:1301:CLA:H102	13:j:1301:CLA:H13	1.80	0.45
12:r:19:ARG:NH1	13:r:511:CLA:OBD	2.50	0.45
13:A:1013:CLA:H122	13:A:1140:CLA:H101	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:507:CLA:H62	13:2:507:CLA:H41	1.71	0.45
12:4:143:GLY:HA3	12:4:222:ILE:HG23	1.99	0.45
2:H:321:GLY:O	2:H:325:THR:OG1	2.28	0.45
13:d:501:CLA:HMB2	16:d:524:BCR:H23C	1.98	0.45
13:e:1105:CLA:HMB3	13:e:1106:CLA:HHB	1.98	0.45
13:f:1210:CLA:H112	13:f:1210:CLA:H51	1.98	0.45
16:f:4010:BCR:H351	16:f:4010:BCR:H15C	1.74	0.45
12:t:143:GLY:HA3	12:t:222:ILE:HG23	1.98	0.45
13:t:512:CLA:HAB	13:t:516:CLA:HMD2	1.99	0.45
12:u:145:HIS:NE2	13:u:512:CLA:NA	2.64	0.45
1:A:252:PRO:HA	1:A:255:PHE:HD2	1.82	0.45
16:B:4017:BCR:H15C	16:B:4017:BCR:H351	1.85	0.45
16:B:4014:BCR:H332	16:J:4012:BCR:HC32	1.99	0.45
12:2:177:VAL:HG13	12:2:201:GLU:HG3	1.98	0.45
12:5:309:PHE:CD2	16:5:521:BCR:H10C	2.51	0.45
2:H:158:GLN:HG3	20:H:1852:SQD:H1	1.98	0.45
13:H:1210:CLA:H112	13:H:1210:CLA:H51	1.99	0.45
16:H:4017:BCR:H371	16:H:4017:BCR:H24C	1.80	0.45
9:U:43:GLY:HA3	9:U:58:PRO:HG2	1.98	0.45
16:V:4219:BCR:H15C	16:V:4219:BCR:H351	1.78	0.45
16:Y:521:BCR:H15C	16:Y:521:BCR:H351	1.82	0.45
12:a:26:LEU:HB3	13:a:511:CLA:HMA1	1.98	0.45
12:d:190:TYR:HD2	16:d:524:BCR:H401	1.81	0.45
13:e:1013:CLA:H93	13:e:1013:CLA:H61	1.79	0.45
14:e:2001:PQN:H301	8:l:19:PHE:HZ	1.81	0.45
2:f:301:ILE:HG23	13:f:1216:CLA:HED3	1.98	0.45
2:f:301:ILE:HG21	13:f:1221:CLA:HAC1	1.97	0.45
4:h:37:GLU:HA	4:h:50:MET:O	2.16	0.45
12:u:309:PHE:HD2	16:u:521:BCR:H10C	1.81	0.45
13:u:509:CLA:HBA1	13:u:509:CLA:H3A	1.78	0.45
12:v:146:LEU:HD22	12:v:214:LEU:HD22	1.98	0.45
2:B:301:ILE:HG23	13:B:1216:CLA:HED3	1.98	0.45
13:1:509:CLA:H92	13:1:509:CLA:H62	1.82	0.45
13:1:518:CLA:H61	13:1:518:CLA:H41	1.73	0.45
12:3:143:GLY:HA3	12:3:222:ILE:HG13	1.97	0.45
16:6:524:BCR:H15C	16:6:524:BCR:H351	1.81	0.45
2:H:191:THR:HG21	2:H:278:LEU:HB2	1.99	0.45
2:H:301:ILE:HG23	13:H:1216:CLA:HED3	1.98	0.45
10:V:90:THR:HG21	10:V:133:ILE:HD12	1.98	0.45
13:Y:509:CLA:H92	13:Y:509:CLA:H62	1.82	0.45
13:b:512:CLA:HAB	13:b:516:CLA:HMD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:78:GLY:N	12:d:82:GLN:O	2.49	0.45
12:d:102:VAL:HG22	13:q:505:CLA:H8	1.99	0.45
12:d:105:ALA:N	13:q:505:CLA:HMB2	2.32	0.45
12:d:282:VAL:HG23	12:d:283:THR:HG23	1.98	0.45
1:e:252:PRO:HA	1:e:255:PHE:HD2	1.82	0.45
4:h:38:GLN:HG3	4:h:50:MET:HE3	1.97	0.45
12:v:282:VAL:HG23	12:v:283:THR:HG23	1.98	0.45
16:v:522:BCR:H371	16:v:522:BCR:H24C	1.82	0.45
16:A:4002:BCR:H24C	16:A:4002:BCR:H371	1.81	0.45
16:A:4011:BCR:H15C	16:A:4011:BCR:H351	1.86	0.45
3:C:17:CYS:HB2	3:C:54:CYS:HB2	1.99	0.45
4:D:38:GLN:HG3	4:D:50:MET:HE3	1.97	0.45
12:6:79:ASP:OD1	12:6:79:ASP:N	2.48	0.45
13:H:1023:CLA:H122	16:S:4018:BCR:H281	1.98	0.45
4:O:38:GLN:HG3	4:O:50:MET:HE3	1.97	0.45
12:Z:143:GLY:HA3	12:Z:222:ILE:HG13	1.99	0.45
12:d:59:MET:HB2	12:d:271:PHE:HA	1.98	0.45
2:f:191:THR:HG21	2:f:278:LEU:HB2	1.99	0.45
2:f:236:ASN:OD1	2:f:236:ASN:N	2.49	0.45
2:f:548:PRO:HB3	6:j:158:PRO:HG2	1.98	0.45
13:f:1224:CLA:H111	13:f:1224:CLA:H72	1.68	0.45
12:r:177:VAL:HG13	12:r:201:GLU:HG3	1.98	0.45
12:4:119:ALA:O	12:4:126:LYS:NZ	2.41	0.45
12:5:307:HIS:NE2	13:5:502:CLA:NA	2.64	0.45
13:5:502:CLA:HBD	13:5:503:CLA:H43	1.98	0.45
12:6:143:GLY:HA3	12:6:222:ILE:HG13	1.98	0.45
13:G:1022:CLA:H192	13:H:1206:CLA:H51	1.98	0.45
13:H:1201:CLA:H2	16:W:4021:BCR:H323	1.98	0.45
13:H:1219:CLA:HBA2	13:H:1219:CLA:H43	1.99	0.45
3:N:58:CYS:HB3	3:N:63:LEU:HD22	1.98	0.45
16:T:4015:BCR:H20C	16:T:4015:BCR:H361	1.81	0.45
16:Y:524:BCR:H15C	16:Y:524:BCR:H351	1.79	0.45
13:Z:506:CLA:H62	13:Z:506:CLA:H41	1.71	0.45
12:a:110:HIS:NE2	13:a:513:CLA:NB	2.65	0.45
12:c:309:PHE:HD2	16:c:521:BCR:H10C	1.81	0.45
12:d:98:ILE:HG23	13:q:505:CLA:H111	1.98	0.45
13:d:517:CLA:H3A	13:d:517:CLA:HBA1	1.50	0.45
1:e:554:ILE:HD11	13:e:1135:CLA:HBB1	1.99	0.45
16:e:4008:BCR:H15C	16:e:4008:BCR:H351	1.82	0.45
2:f:355:MET:HE3	2:f:355:MET:HB2	1.79	0.45
3:g:17:CYS:HB2	3:g:54:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:32:TRP:NE1	4:h:50:MET:SD	2.76	0.45
13:u:512:CLA:HBA1	13:u:512:CLA:H3A	1.68	0.45
12:v:177:VAL:HG21	12:v:204:VAL:HG21	1.96	0.45
1:A:336:ILE:O	1:A:340:HIS:ND1	2.37	0.45
1:A:360:TRP:HB3	13:A:1103:CLA:HAC1	1.98	0.45
13:B:1023:CLA:H122	16:I:4018:BCR:H281	1.98	0.45
13:B:1210:CLA:H112	13:B:1210:CLA:H51	1.98	0.45
13:1:508:CLA:H43	13:1:511:CLA:HAC1	1.98	0.45
13:1:510:CLA:H41	13:1:510:CLA:H61	1.60	0.45
12:6:301:ALA:O	12:6:305:ASN:ND2	2.43	0.45
13:G:1102:CLA:H112	13:G:1102:CLA:H151	1.73	0.45
13:G:1105:CLA:HMB3	13:G:1106:CLA:HHB	1.98	0.45
13:G:1122:CLA:H62	13:G:1122:CLA:H41	1.68	0.45
13:H:1207:CLA:HAB	7:S:19:GLY:HA3	1.99	0.45
4:O:37:GLU:HA	4:O:50:MET:O	2.16	0.45
13:Y:508:CLA:H43	13:Y:511:CLA:HAC1	1.98	0.45
12:Z:19:ARG:NH1	13:Z:511:CLA:OBD	2.50	0.45
12:a:59:MET:HE2	12:a:67:LEU:HB3	1.98	0.45
2:f:25:ILE:HA	13:f:1201:CLA:HMD2	1.99	0.45
6:j:90:TYR:OH	6:j:132:PHE:O	2.33	0.45
11:o:11:LEU:HD21	16:o:4021:BCR:H272	1.99	0.45
13:v:501:CLA:HMB2	16:v:524:BCR:H23C	1.98	0.45
13:v:517:CLA:H3A	13:v:517:CLA:HBA1	1.50	0.45
13:A:1124:CLA:H2	13:A:1124:CLA:H61	1.79	0.45
14:A:2001:PQN:H301	8:J:19:PHE:HZ	1.81	0.45
2:B:236:ASN:OD1	2:B:236:ASN:N	2.49	0.45
2:B:456:GLU:OE1	6:F:68:HIS:ND1	2.47	0.45
13:B:1224:CLA:H111	13:B:1224:CLA:H72	1.68	0.45
3:C:61:ASP:HA	3:C:62:PHE:HA	1.83	0.45
12:3:110:HIS:NE2	13:3:513:CLA:NB	2.65	0.45
12:5:73:LEU:O	12:5:159:LYS:NZ	2.49	0.45
12:5:145:HIS:NE2	13:5:512:CLA:NA	2.64	0.45
12:6:101:ALA:HB1	13:Y:505:CLA:HAB	1.99	0.45
13:6:501:CLA:H41	13:6:501:CLA:H62	1.76	0.45
1:G:252:PRO:HA	1:G:255:PHE:HD2	1.82	0.45
1:G:360:TRP:HB3	13:G:1103:CLA:HAC1	1.98	0.45
13:H:1219:CLA:H61	13:H:1219:CLA:H2	1.65	0.45
20:H:1852:SQD:O10	13:e:1801:CLA:HBD	2.17	0.45
3:N:62:PHE:HD2	4:O:122:ILE:HD13	1.81	0.45
16:Z:521:BCR:H15C	16:Z:521:BCR:H351	1.83	0.45
1:e:370:ILE:HG21	13:e:1123:CLA:HMA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:1013:CLA:H122	13:e:1140:CLA:H101	1.98	0.45
2:f:674:LEU:O	2:f:677:THR:OG1	2.34	0.45
3:g:26:LEU:HA	3:g:41:ALA:O	2.16	0.45
16:k:4018:BCR:H11C	16:k:4018:BCR:H341	1.86	0.45
13:n:1501:CLA:H41	13:n:1501:CLA:H61	1.75	0.45
16:n:4022:BCR:H11C	16:n:4022:BCR:H341	1.84	0.45
12:t:273:GLY:O	12:t:300:ARG:NH2	2.45	0.45
2:B:25:ILE:HA	13:B:1201:CLA:HMD2	1.99	0.44
20:B:1852:SQD:H252	20:B:1852:SQD:H102	1.99	0.44
5:E:53:ASP:OD1	5:E:53:ASP:N	2.44	0.44
1:G:300:LEU:HD21	1:G:385:MET:HB3	1.99	0.44
4:O:21:SER:HA	4:O:24:THR:HB	1.97	0.44
13:V:1501:CLA:HAA2	16:V:4022:BCR:H363	1.99	0.44
12:d:143:GLY:HA3	12:d:222:ILE:HG13	1.98	0.44
13:f:1212:CLA:H61	13:f:1212:CLA:H41	1.70	0.44
16:l:4015:BCR:H20C	16:l:4015:BCR:H361	1.82	0.44
12:s:26:LEU:HB3	13:s:511:CLA:HMA1	1.98	0.44
16:t:524:BCR:H351	16:t:524:BCR:H15C	1.79	0.44
12:u:309:PHE:CD2	16:u:521:BCR:H10C	2.51	0.44
13:u:505:CLA:H91	13:u:505:CLA:H112	1.81	0.44
13:A:1022:CLA:H192	13:B:1206:CLA:H51	1.98	0.44
2:B:158:GLN:HG3	20:B:1852:SQD:H1	1.98	0.44
16:K:4104:BCR:H403	20:1:822:SQD:H332	1.98	0.44
11:M:11:LEU:HD21	16:M:4021:BCR:H272	1.99	0.44
2:H:4:LYS:HZ1	20:n:5216:SQD:C3	2.29	0.44
11:W:11:LEU:HD21	16:W:4021:BCR:H272	1.99	0.44
13:c:501:CLA:HMB2	16:c:524:BCR:H23C	2.00	0.44
16:e:4002:BCR:H361	16:e:4002:BCR:H20C	1.77	0.44
13:f:1210:CLA:H2	13:f:1210:CLA:H62	1.64	0.44
13:f:1219:CLA:HBA2	13:f:1219:CLA:H43	1.99	0.44
13:B:1228:CLA:HAB	13:B:1229:CLA:H202	1.98	0.44
12:4:273:GLY:O	12:4:300:ARG:NH2	2.45	0.44
2:H:548:PRO:HB3	6:R:158:PRO:HG2	1.98	0.44
13:Y:505:CLA:H43	16:Y:524:BCR:HC7	1.98	0.44
13:c:503:CLA:H62	13:c:503:CLA:H41	1.83	0.44
16:d:524:BCR:H15C	16:d:524:BCR:H351	1.81	0.44
13:f:1221:CLA:H141	13:f:1221:CLA:H161	1.78	0.44
13:f:1207:CLA:HAB	7:k:19:GLY:HA3	1.99	0.44
12:u:148:PHE:HD2	13:u:512:CLA:H3A	1.81	0.44
1:A:595:CYS:HB2	2:B:667:TRP:HB3	2.00	0.44
2:B:674:LEU:O	2:B:677:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1202:CLA:HBD	13:B:1202:CLA:H122	2.00	0.44
16:6:522:BCR:H15C	16:6:522:BCR:H351	1.81	0.44
1:G:752:TRP:HD1	13:G:1126:CLA:HMB2	1.83	0.44
16:G:4003:BCR:H20C	16:G:4003:BCR:H361	1.88	0.44
2:H:25:ILE:HA	13:H:1201:CLA:HMD2	1.99	0.44
2:H:91:ILE:HB	2:H:112:PRO:HB2	1.99	0.44
13:H:1212:CLA:H61	13:H:1212:CLA:H41	1.70	0.44
6:R:150:LYS:HA	6:R:150:LYS:HD3	1.72	0.44
16:T:4013:BCR:H351	16:T:4013:BCR:H15C	1.82	0.44
12:Z:73:LEU:HD11	13:Z:503:CLA:HAA2	1.99	0.44
1:e:430:PRO:HG2	4:h:41:GLU:HB2	2.00	0.44
12:r:226:PRO:HA	13:r:506:CLA:HED3	1.98	0.44
13:r:507:CLA:H62	13:r:507:CLA:H41	1.71	0.44
12:s:59:MET:HE2	12:s:67:LEU:HB3	1.98	0.44
16:t:523:BCR:H11C	16:t:523:BCR:H341	1.90	0.44
13:u:501:CLA:HMB2	16:u:524:BCR:H23C	1.99	0.44
16:v:521:BCR:H15C	16:v:521:BCR:H351	1.83	0.44
13:A:1102:CLA:H141	13:A:1102:CLA:H162	1.79	0.44
12:1:97:LEU:HG	16:1:522:BCR:H12C	1.98	0.44
12:1:112:PHE:HB2	12:2:326:MET:HE3	2.00	0.44
13:5:501:CLA:HMB2	16:5:524:BCR:H23C	1.99	0.44
2:H:182:LEU:HD13	13:H:1210:CLA:HHB	1.99	0.44
2:H:674:LEU:O	2:H:677:THR:OG1	2.34	0.44
2:H:700:LEU:HD22	2:H:704:GLN:NE2	2.33	0.44
13:H:1208:CLA:H202	13:H:1208:CLA:H161	1.80	0.44
7:S:1:MET:HE2	7:S:1:MET:HB3	1.81	0.44
12:Y:112:PHE:HB2	12:Z:326:MET:HE3	2.00	0.44
12:c:148:PHE:HD2	13:c:512:CLA:H3A	1.81	0.44
13:c:502:CLA:HBD	13:c:503:CLA:H43	1.98	0.44
13:c:509:CLA:H92	13:c:509:CLA:H62	1.81	0.44
16:d:523:BCR:H15C	16:d:523:BCR:H351	1.81	0.44
16:f:4017:BCR:H24C	16:f:4017:BCR:H371	1.80	0.44
16:f:4014:BCR:H332	16:l:4012:BCR:HC32	1.98	0.44
6:j:150:LYS:HD3	6:j:150:LYS:HA	1.72	0.44
9:m:43:GLY:HA3	9:m:58:PRO:HG2	1.98	0.44
12:q:143:GLY:HA3	12:q:222:ILE:HG13	2.00	0.44
12:u:110:HIS:HA	12:u:114:ALA:HB3	2.00	0.44
13:u:501:CLA:H41	13:u:501:CLA:H62	1.70	0.44
2:B:548:PRO:HB3	6:F:158:PRO:HG2	1.98	0.44
13:B:1207:CLA:HAB	7:I:19:GLY:HA3	1.99	0.44
7:I:16:PRO:HB3	17:V:5221:LHG:H151	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:5001:LHG:H131	20:V:5216:SQD:H291	2.00	0.44
13:J:1303:CLA:HAB	13:J:1303:CLA:H161	2.00	0.44
12:2:130:PHE:HA	12:2:137:GLN:HG2	2.00	0.44
13:G:1102:CLA:H141	13:G:1102:CLA:H162	1.79	0.44
14:G:2001:PQN:H142	14:G:2001:PQN:H112	1.89	0.44
20:H:1852:SQD:H102	20:H:1852:SQD:H252	1.99	0.44
3:N:17:CYS:HB2	3:N:54:CYS:HB2	1.99	0.44
12:Y:97:LEU:HG	16:Y:522:BCR:H12C	1.98	0.44
12:Z:130:PHE:HA	12:Z:137:GLN:HG2	2.00	0.44
12:Z:177:VAL:HG13	12:Z:201:GLU:HG3	1.98	0.44
12:b:161:THR:HA	12:b:177:VAL:HB	1.99	0.44
12:c:148:PHE:CE2	13:c:512:CLA:HHB	2.53	0.44
12:d:107:ALA:O	12:d:111:THR:OG1	2.31	0.44
1:e:336:ILE:O	1:e:340:HIS:ND1	2.37	0.44
1:e:752:TRP:HD1	13:e:1126:CLA:HMB2	1.83	0.44
16:e:4003:BCR:H20C	16:e:4003:BCR:H361	1.88	0.44
2:f:158:GLN:HG3	20:f:1852:SQD:H1	1.98	0.44
13:f:1217:CLA:H3A	13:f:1217:CLA:HBA2	1.41	0.44
3:g:58:CYS:HB3	3:g:63:LEU:HD22	1.98	0.44
13:l:1303:CLA:HAB	13:l:1303:CLA:H161	2.00	0.44
12:r:130:PHE:HA	12:r:137:GLN:HG2	2.00	0.44
12:r:143:GLY:HA3	12:r:222:ILE:HG13	1.99	0.44
1:A:430:PRO:HG2	4:D:41:GLU:HB2	2.00	0.44
13:B:1219:CLA:HBA2	13:B:1219:CLA:H43	1.99	0.44
13:1:505:CLA:H61	12:v:102:VAL:HA	1.99	0.44
12:6:78:GLY:N	12:6:82:GLN:O	2.49	0.44
1:G:230:ILE:HG12	1:G:244:ALA:HA	2.00	0.44
13:H:1222:CLA:H2	13:H:1231:CLA:HBB2	1.99	0.44
4:O:31:THR:HA	4:O:55:ASN:O	2.18	0.44
13:Y:502:CLA:H61	13:Y:512:CLA:H42	1.99	0.44
16:Y:523:BCR:H15C	16:Y:523:BCR:H351	1.88	0.44
12:c:110:HIS:HA	12:c:114:ALA:HB3	1.99	0.44
2:f:91:ILE:HB	2:f:112:PRO:HB2	1.99	0.44
13:f:1209:CLA:H3A	13:f:1209:CLA:HBA2	1.59	0.44
13:f:1218:CLA:H61	13:f:1218:CLA:H2	1.72	0.44
7:k:1:MET:HE2	7:k:1:MET:HB3	1.81	0.44
12:r:301:ALA:O	12:r:305:ASN:ND2	2.41	0.44
12:t:249:ILE:HG12	13:t:502:CLA:HAC1	2.00	0.44
13:F:1302:CLA:H3A	13:F:1302:CLA:HBA1	1.70	0.44
12:6:282:VAL:HG23	12:6:283:THR:HG23	1.98	0.44
1:G:172:MET:HE1	13:G:1111:CLA:H92	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:554:ILE:HD11	13:G:1135:CLA:HBB1	1.99	0.44
7:S:16:PRO:HB3	17:n:5221:LHG:H151	2.00	0.44
2:f:700:LEU:HD22	2:f:704:GLN:NE2	2.33	0.44
16:f:4004:BCR:H11C	16:f:4004:BCR:H341	1.88	0.44
16:f:4006:BCR:H24C	16:f:4006:BCR:H371	1.75	0.44
12:q:155:LEU:HB3	13:q:502:CLA:H121	2.00	0.44
1:A:752:TRP:HD1	13:A:1126:CLA:HMB2	1.83	0.44
6:F:90:TYR:OH	6:F:132:PHE:O	2.33	0.44
16:2:521:BCR:H15C	16:2:521:BCR:H351	1.83	0.44
12:3:190:TYR:HD2	16:3:524:BCR:H401	1.83	0.44
13:3:517:CLA:H3A	13:3:517:CLA:HBA1	1.50	0.44
12:5:148:PHE:CE2	13:5:512:CLA:HHB	2.53	0.44
13:G:1013:CLA:H141	13:G:1013:CLA:H161	1.84	0.44
13:H:1205:CLA:H143	13:H:1205:CLA:H161	1.90	0.44
16:H:4004:BCR:H351	16:H:4004:BCR:H15C	1.77	0.44
16:R:4016:BCR:H24C	16:R:4016:BCR:H371	1.80	0.44
7:S:13:ILE:HD11	10:n:155:LEU:HD22	1.99	0.44
13:T:1303:CLA:HAB	13:T:1303:CLA:H161	2.00	0.44
16:e:4003:BCR:H15C	16:e:4003:BCR:H351	1.81	0.44
2:f:611:GLU:OE2	6:j:36:ARG:NH1	2.44	0.44
16:f:4004:BCR:H15C	16:f:4004:BCR:H351	1.77	0.44
3:g:58:CYS:HA	3:g:59:PRO:HD3	1.87	0.44
13:q:502:CLA:H61	13:q:512:CLA:H42	1.99	0.44
12:u:34:GLN:OE1	13:u:510:CLA:NC	2.51	0.44
12:u:148:PHE:CE2	13:u:512:CLA:HHB	2.53	0.44
1:A:172:MET:HE1	13:A:1111:CLA:H92	2.00	0.43
17:A:5002:LHG:H261	20:f:1852:SQD:H242	1.99	0.43
13:B:1213:CLA:H162	13:B:1213:CLA:H141	1.80	0.43
9:K:43:GLY:HA3	9:K:58:PRO:HG2	1.98	0.43
16:3:524:BCR:H351	16:3:524:BCR:H15C	1.78	0.43
16:5:522:BCR:H24C	16:5:522:BCR:H371	1.84	0.43
1:G:424:MET:HE1	1:G:442:LEU:HD11	2.00	0.43
1:G:595:CYS:HB2	2:H:667:TRP:HB3	2.00	0.43
2:H:332:PHE:CD1	16:H:4010:BCR:H391	2.53	0.43
13:H:1215:CLA:H142	13:H:1215:CLA:H112	1.88	0.43
13:H:1228:CLA:HAB	13:H:1229:CLA:H202	1.98	0.43
13:H:1228:CLA:HBC2	13:H:1236:CLA:HMC2	2.00	0.43
13:Y:516:CLA:H3A	13:Y:516:CLA:HBA1	1.51	0.43
13:Z:517:CLA:H3A	13:Z:517:CLA:HBA1	1.79	0.43
13:a:501:CLA:HBB2	13:a:507:CLA:H92	1.98	0.43
1:e:591:ARG:HH21	1:e:594:THR:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:1222:CLA:H2	13:f:1231:CLA:HBB2	1.99	0.43
13:f:1228:CLA:HBC2	13:f:1236:CLA:HMC2	2.00	0.43
12:r:307:HIS:NE2	13:r:502:CLA:NA	2.66	0.43
12:s:110:HIS:NE2	13:s:513:CLA:NB	2.65	0.43
1:A:554:ILE:HD11	13:A:1135:CLA:HBB1	1.99	0.43
1:A:691:TRP:O	1:A:694:SER:OG	2.30	0.43
13:A:1104:CLA:H201	17:A:5001:LHG:H221	2.00	0.43
2:B:22:TRP:HE1	13:B:1238:CLA:HBB1	1.84	0.43
4:D:31:THR:HA	4:D:55:ASN:O	2.18	0.43
6:F:71:VAL:HG12	6:F:81:PHE:HB2	2.00	0.43
16:2:521:BCR:H371	16:2:521:BCR:H24C	1.78	0.43
12:3:267:TYR:O	12:3:300:ARG:NH2	2.41	0.43
13:G:1104:CLA:H201	17:G:5001:LHG:H221	2.00	0.43
13:G:1116:CLA:H93	13:G:1116:CLA:H61	1.90	0.43
13:H:1021:CLA:H62	13:H:1021:CLA:H102	1.85	0.43
13:H:1218:CLA:H61	13:H:1218:CLA:H2	1.72	0.43
13:R:1302:CLA:HBA1	13:R:1302:CLA:H3A	1.70	0.43
12:Y:155:LEU:HB3	13:Y:502:CLA:H121	2.00	0.43
1:e:404:HIS:CE1	13:e:1126:CLA:ND	2.86	0.43
13:f:1224:CLA:H3A	13:f:1224:CLA:HBA2	1.65	0.43
13:f:1239:CLA:H91	13:f:1239:CLA:H112	1.88	0.43
16:n:4020:BCR:H371	16:n:4020:BCR:H24C	1.71	0.43
1:A:300:LEU:HD21	1:A:385:MET:HB3	1.99	0.43
1:A:404:HIS:CE1	13:A:1126:CLA:ND	2.86	0.43
13:B:1221:CLA:H72	13:B:1221:CLA:H112	1.75	0.43
10:L:85:LEU:HD12	10:L:85:LEU:HA	1.86	0.43
12:1:169:ALA:HB3	12:1:265:LEU:HD12	2.00	0.43
12:2:143:GLY:HA3	12:2:222:ILE:HG13	1.99	0.43
16:5:524:BCR:H15C	16:5:524:BCR:H351	1.80	0.43
1:G:404:HIS:CE1	13:G:1126:CLA:ND	2.86	0.43
13:Z:506:CLA:H72	16:Z:524:BCR:H10C	2.00	0.43
12:b:249:ILE:HG12	13:b:502:CLA:HAC1	2.00	0.43
13:e:1103:CLA:H3A	13:e:1103:CLA:HBA1	1.54	0.43
13:e:1122:CLA:H41	13:e:1122:CLA:H62	1.68	0.43
2:f:369:ALA:HB1	2:f:725:LEU:HD11	2.00	0.43
13:f:1234:CLA:H193	13:f:1234:CLA:H161	1.87	0.43
13:n:1501:CLA:HAA2	16:n:4022:BCR:H363	1.99	0.43
16:q:521:BCR:H11C	16:q:521:BCR:H341	1.88	0.43
12:t:161:THR:HA	12:t:177:VAL:HB	1.99	0.43
13:4:512:CLA:HAB	13:4:516:CLA:HMD2	1.99	0.43
16:4:524:BCR:H351	16:4:524:BCR:H15C	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:34:GLN:OE1	13:5:510:CLA:NC	2.51	0.43
2:H:218:HIS:HD2	2:H:220:ALA:H	1.66	0.43
13:H:1221:CLA:H141	13:H:1221:CLA:H161	1.78	0.43
13:H:1224:CLA:H141	19:H:5002:LMG:H261	2.00	0.43
16:Z:524:BCR:H15C	16:Z:524:BCR:H351	1.78	0.43
12:c:34:GLN:OE1	13:c:510:CLA:NC	2.51	0.43
16:d:522:BCR:H24C	16:d:522:BCR:H371	1.82	0.43
13:e:1104:CLA:H41	13:e:1104:CLA:H62	1.64	0.43
18:e:1849:LMU:H62	18:e:1849:LMU:H91	1.85	0.43
2:f:182:LEU:HD13	13:f:1210:CLA:HHB	2.00	0.43
13:r:501:CLA:HMB2	16:r:524:BCR:H23C	2.01	0.43
12:s:190:TYR:HD2	16:s:524:BCR:H401	1.83	0.43
13:B:1228:CLA:HBC2	13:B:1236:CLA:HMC2	2.00	0.43
16:L:4020:BCR:H24C	16:L:4020:BCR:H371	1.71	0.43
12:2:73:LEU:HD11	13:2:503:CLA:HAA2	1.99	0.43
12:2:307:HIS:NE2	13:2:502:CLA:NA	2.66	0.43
12:4:161:THR:HA	12:4:177:VAL:HB	1.99	0.43
1:G:626:GLN:HE21	1:G:759:ILE:HD13	1.83	0.43
6:R:150:LYS:HB3	6:R:153:GLU:HG3	2.01	0.43
13:Y:507:CLA:H112	16:Y:524:BCR:H362	2.00	0.43
13:Z:502:CLA:H11	13:Z:503:CLA:H161	2.01	0.43
12:a:190:TYR:HD2	16:a:524:BCR:H401	1.83	0.43
16:r:522:BCR:H24C	16:r:522:BCR:H371	1.86	0.43
2:B:182:LEU:HD13	13:B:1210:CLA:HHB	2.00	0.43
2:B:332:PHE:CD1	16:B:4010:BCR:H391	2.53	0.43
13:L:1501:CLA:HAA2	16:L:4022:BCR:H363	1.99	0.43
12:4:249:ILE:HG12	13:4:502:CLA:HAC1	2.00	0.43
2:H:22:TRP:HE1	13:H:1238:CLA:HBB1	1.84	0.43
2:H:310:PRO:HA	2:H:311:PRO:HD3	1.88	0.43
2:H:369:ALA:HB1	2:H:725:LEU:HD11	2.01	0.43
6:R:118:VAL:HA	8:T:10:SER:HA	2.01	0.43
12:d:105:ALA:HA	13:q:505:CLA:CHB	2.49	0.43
2:f:332:PHE:CD1	16:f:4010:BCR:H391	2.53	0.43
13:f:1202:CLA:H122	13:f:1202:CLA:HBD	2.00	0.43
13:f:1227:CLA:H142	16:f:4009:BCR:H17C	2.01	0.43
12:q:112:PHE:HB2	12:r:326:MET:HE3	2.00	0.43
12:r:34:GLN:HG2	13:r:509:CLA:HHB	2.00	0.43
13:r:506:CLA:H72	16:r:524:BCR:H10C	1.99	0.43
16:A:4002:BCR:H11C	16:A:4002:BCR:H341	1.82	0.43
2:B:7:LYS:HD2	11:M:28:TYR:CZ	2.54	0.43
2:B:309:LYS:HE2	2:B:309:LYS:HB2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ALA:HB1	2:B:725:LEU:HD11	2.01	0.43
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.33	0.43
13:B:1227:CLA:H142	16:B:4009:BCR:H17C	2.01	0.43
6:F:118:VAL:HA	8:J:10:SER:HA	2.01	0.43
13:1:502:CLA:H61	13:1:512:CLA:H42	1.99	0.43
13:1:509:CLA:H91	13:1:512:CLA:HAA2	2.01	0.43
13:2:506:CLA:H72	16:2:524:BCR:H10C	2.00	0.43
16:2:521:BCR:H20C	16:2:521:BCR:H361	1.87	0.43
12:3:67:LEU:HD22	12:3:89:LEU:HD13	2.01	0.43
16:4:524:BCR:H11C	16:4:524:BCR:H341	1.83	0.43
13:H:1202:CLA:HBD	13:H:1202:CLA:H122	2.00	0.43
13:H:1224:CLA:HBA2	13:H:1224:CLA:H3A	1.65	0.43
6:R:71:VAL:HG12	6:R:81:PHE:HB2	2.00	0.43
16:Y:522:BCR:H24C	16:Y:522:BCR:H371	1.84	0.43
12:Z:307:HIS:NE2	13:Z:502:CLA:NA	2.66	0.43
12:c:221:HIS:HE1	13:c:506:CLA:NA	2.17	0.43
2:f:7:LYS:HD2	11:o:28:TYR:CZ	2.54	0.43
4:h:31:THR:HA	4:h:55:ASN:O	2.17	0.43
16:l:4013:BCR:H11C	16:l:4013:BCR:H341	1.88	0.43
16:n:4022:BCR:H15C	16:n:4022:BCR:H351	1.85	0.43
16:t:524:BCR:H11C	16:t:524:BCR:H341	1.84	0.43
1:A:424:MET:HE1	1:A:442:LEU:HD11	2.00	0.43
13:A:1108:CLA:H41	13:A:1108:CLA:H61	1.78	0.43
16:A:4008:BCR:H11C	16:A:4008:BCR:H341	1.89	0.43
2:B:174:ARG:HB2	13:B:1210:CLA:HBC2	2.01	0.43
13:B:1219:CLA:HBC2	13:B:1220:CLA:HBA1	2.00	0.43
4:D:101:ASP:OD1	4:D:101:ASP:N	2.48	0.43
16:J:4015:BCR:H20C	16:J:4015:BCR:H361	1.81	0.43
10:L:94:SER:HB2	13:V:1501:CLA:HMD3	2.00	0.43
12:1:110:HIS:HA	12:1:114:ALA:HB3	2.01	0.43
12:2:261:ALA:HA	12:2:276:LEU:HD12	2.01	0.43
13:2:501:CLA:H62	13:2:501:CLA:H41	1.62	0.43
13:G:1109:CLA:H141	13:G:1109:CLA:H161	1.82	0.43
13:Y:509:CLA:H91	13:Y:512:CLA:HAA2	2.01	0.43
13:Y:518:CLA:H41	13:Y:518:CLA:H61	1.73	0.43
12:a:67:LEU:HD22	12:a:89:LEU:HD13	2.01	0.43
16:d:522:BCR:H321	13:q:505:CLA:H172	1.99	0.43
1:e:230:ILE:HG12	1:e:244:ALA:HA	2.00	0.43
1:e:595:CYS:HB2	2:f:667:TRP:HB3	2.00	0.43
12:r:193:HIS:HB2	12:r:196:SER:HB3	2.00	0.43
13:s:503:CLA:H18	13:s:510:CLA:HBB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:s:523:BCR:H11C	16:s:523:BCR:H341	1.90	0.43
16:s:523:BCR:H15C	16:s:523:BCR:H351	1.79	0.43
16:u:522:BCR:H24C	16:u:522:BCR:H371	1.84	0.43
1:A:28:TRP:CD1	13:A:1109:CLA:HBA1	2.54	0.43
2:B:531:THR:O	2:B:535:VAL:HB	2.19	0.43
13:B:1208:CLA:H202	13:B:1208:CLA:H161	1.80	0.43
13:B:1228:CLA:H12	13:B:1228:CLA:H52	1.80	0.43
16:J:4013:BCR:H11C	16:J:4013:BCR:H341	1.88	0.43
17:L:5221:LHG:H252	13:f:1207:CLA:C4	2.40	0.43
12:1:155:LEU:HB3	13:1:502:CLA:H121	2.00	0.43
13:1:505:CLA:H161	16:v:522:BCR:H10C	2.01	0.43
12:2:26:LEU:HB3	13:2:511:CLA:HMA1	2.01	0.43
13:2:501:CLA:HMB2	16:2:524:BCR:H23C	2.01	0.43
12:4:141:ILE:HD13	13:4:509:CLA:H191	2.01	0.43
1:G:430:PRO:HG2	4:O:41:GLU:HB2	2.00	0.43
13:G:1118:CLA:H3A	9:U:61:LEU:HD23	2.01	0.43
13:H:1219:CLA:HBC2	13:H:1220:CLA:HBA1	2.00	0.43
12:Y:169:ALA:HB3	12:Y:265:LEU:HD12	2.00	0.43
13:Z:501:CLA:HMB2	16:Z:524:BCR:H23C	2.01	0.43
16:Z:522:BCR:H24C	16:Z:522:BCR:H371	1.86	0.43
12:b:141:ILE:HD13	13:b:509:CLA:H191	2.01	0.43
12:d:97:LEU:HG	16:d:522:BCR:H12C	2.00	0.43
13:q:507:CLA:H112	16:q:524:BCR:H362	2.00	0.43
13:q:509:CLA:H91	13:q:512:CLA:HAA2	2.01	0.43
12:u:221:HIS:HE1	13:u:506:CLA:NA	2.17	0.43
13:A:1102:CLA:H151	13:A:1102:CLA:H112	1.73	0.43
16:B:4010:BCR:H351	16:B:4010:BCR:H15C	1.74	0.43
12:5:110:HIS:HA	12:5:114:ALA:HB3	1.99	0.43
13:G:1104:CLA:H41	13:G:1104:CLA:H62	1.64	0.43
16:G:4003:BCR:H11C	16:G:4003:BCR:H341	1.90	0.43
1:e:300:LEU:HD21	1:e:385:MET:HB3	1.99	0.43
16:n:4020:BCR:H15C	16:n:4020:BCR:H351	1.87	0.43
13:q:508:CLA:H62	13:q:508:CLA:H41	1.62	0.43
12:r:73:LEU:HD11	13:r:503:CLA:HAA2	1.99	0.43
13:r:518:CLA:H142	13:r:518:CLA:H111	1.85	0.43
12:v:148:PHE:HE2	13:v:512:CLA:HHB	1.84	0.43
1:A:239:ASN:HD22	1:A:263:GLN:HE22	1.66	0.42
1:A:691:TRP:CE2	13:A:1011:CLA:HBA2	2.54	0.42
13:A:1109:CLA:H141	13:A:1109:CLA:H161	1.82	0.42
13:A:1128:CLA:H142	13:A:1128:CLA:H111	1.87	0.42
13:A:1139:CLA:H121	13:A:1139:CLA:H161	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:HIS:HD2	2:B:220:ALA:H	1.66	0.42
2:B:493:TYR:HE2	13:B:1231:CLA:HED1	1.84	0.42
16:B:4009:BCR:H11C	16:B:4009:BCR:H341	1.86	0.42
12:1:143:GLY:HA3	12:1:222:ILE:HG13	2.00	0.42
13:1:507:CLA:H112	16:1:524:BCR:H362	2.00	0.42
13:2:502:CLA:H11	13:2:503:CLA:H161	2.00	0.42
13:G:1119:CLA:H171	13:G:1129:CLA:HBC1	2.01	0.42
12:Z:193:HIS:HB2	12:Z:196:SER:HB3	2.00	0.42
13:a:513:CLA:HBB1	16:a:523:BCR:H402	2.01	0.42
1:e:626:GLN:HE21	1:e:759:ILE:HD13	1.83	0.42
13:e:1108:CLA:H3A	13:e:1108:CLA:HBA2	1.71	0.42
2:f:22:TRP:HE1	13:f:1238:CLA:HBB1	1.84	0.42
2:f:531:THR:O	2:f:535:VAL:HB	2.19	0.42
2:f:631:LEU:O	2:f:647:SER:OG	2.29	0.42
20:f:1852:SQD:H102	20:f:1852:SQD:H252	1.99	0.42
6:j:118:VAL:HA	8:l:10:SER:HA	2.01	0.42
16:n:4019:BCR:H351	16:n:4019:BCR:H15C	1.80	0.42
12:u:107:ALA:O	12:u:111:THR:OG1	2.30	0.42
13:A:1102:CLA:H202	13:A:1102:CLA:H161	1.82	0.42
13:A:1102:CLA:HBA2	13:A:1102:CLA:H3A	1.81	0.42
13:A:1119:CLA:H171	13:A:1129:CLA:HBC1	2.01	0.42
13:A:1123:CLA:H141	13:A:1123:CLA:H161	1.80	0.42
2:B:59:LEU:HD23	2:B:59:LEU:HA	1.89	0.42
13:B:1012:CLA:H122	13:B:1012:CLA:H8	1.88	0.42
16:B:4005:BCR:H11C	16:B:4005:BCR:H341	1.86	0.42
12:1:34:GLN:OE1	13:1:510:CLA:NC	2.52	0.42
13:4:505:CLA:H112	13:4:505:CLA:H91	1.86	0.42
1:G:691:TRP:CE2	13:G:1011:CLA:HBA2	2.54	0.42
13:H:1227:CLA:H142	16:H:4009:BCR:H17C	2.01	0.42
16:T:4013:BCR:H11C	16:T:4013:BCR:H341	1.88	0.42
13:Y:502:CLA:HBD	13:Y:503:CLA:H43	2.01	0.42
13:e:1118:CLA:H3A	9:m:61:LEU:HD23	2.01	0.42
6:j:150:LYS:HB3	6:j:153:GLU:HG3	2.01	0.42
13:q:512:CLA:H3A	13:q:512:CLA:HBA1	1.62	0.42
13:s:513:CLA:HBB1	16:s:523:BCR:H402	2.01	0.42
1:A:591:ARG:HH21	1:A:594:THR:HG21	1.83	0.42
1:A:626:GLN:HE21	1:A:759:ILE:HD13	1.83	0.42
13:A:1011:CLA:H62	13:A:1011:CLA:H102	1.87	0.42
13:A:1013:CLA:H93	13:A:1013:CLA:H61	1.79	0.42
13:B:1210:CLA:H62	13:B:1210:CLA:H2	1.64	0.42
16:B:4004:BCR:H15C	16:B:4004:BCR:H351	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:4017:BCR:H371	16:B:4017:BCR:H24C	1.80	0.42
16:B:4009:BCR:H15C	16:B:4009:BCR:H351	1.82	0.42
1:G:28:TRP:CD1	13:G:1109:CLA:HBA1	2.54	0.42
2:H:101:ILE:HG12	7:S:1:MET:HE2	2.02	0.42
2:H:380:THR:HG22	2:H:583:ALA:HB1	2.02	0.42
12:Y:143:GLY:HA3	12:Y:222:ILE:HG13	2.00	0.42
1:e:28:TRP:CD1	13:e:1109:CLA:HBA1	2.54	0.42
13:e:1102:CLA:H162	13:e:1102:CLA:H141	1.79	0.42
13:e:1129:CLA:H11	13:e:1129:CLA:H51	1.80	0.42
12:q:34:GLN:OE1	13:q:510:CLA:NC	2.52	0.42
12:q:169:ALA:HB3	12:q:265:LEU:HD12	2.00	0.42
12:r:26:LEU:HB3	13:r:511:CLA:HMA1	2.01	0.42
13:t:517:CLA:H3A	13:t:517:CLA:HBA1	1.68	0.42
13:u:505:CLA:H42	16:u:524:BCR:HC7	2.02	0.42
13:B:1220:CLA:H61	13:B:1220:CLA:H2	1.85	0.42
13:3:503:CLA:H18	13:3:510:CLA:HBB2	2.00	0.42
16:3:522:BCR:H15C	16:3:522:BCR:H351	1.80	0.42
13:G:1104:CLA:H191	17:G:5001:LHG:H211	2.02	0.42
13:G:1138:CLA:HAA2	13:H:1228:CLA:HMB1	2.01	0.42
13:H:1216:CLA:H93	13:H:1216:CLA:H111	1.89	0.42
13:H:1228:CLA:H12	13:H:1228:CLA:H52	1.80	0.42
4:O:32:TRP:NE1	4:O:50:MET:SD	2.76	0.42
8:T:26:LEU:HD13	16:T:4012:BCR:HC7	2.02	0.42
9:U:68:HIS:O	9:U:72:ILE:HG12	2.20	0.42
12:Y:34:GLN:OE1	13:Y:510:CLA:NC	2.52	0.42
12:Y:147:LEU:HD12	12:Y:215:ILE:HG12	2.01	0.42
1:e:424:MET:HE1	1:e:442:LEU:HD11	2.00	0.42
13:e:1122:CLA:H91	13:e:1122:CLA:H111	1.77	0.42
13:e:1140:CLA:H11	13:e:1140:CLA:CHA	2.50	0.42
17:n:5220:LHG:H311	17:n:5220:LHG:H171	2.01	0.42
12:q:34:GLN:HG2	13:q:509:CLA:HHB	2.02	0.42
12:r:261:ALA:HA	12:r:276:LEU:HD12	2.01	0.42
13:u:503:CLA:H62	13:u:503:CLA:H41	1.83	0.42
16:B:4004:BCR:H11C	16:B:4004:BCR:H341	1.88	0.42
8:J:26:LEU:HD13	16:J:4012:BCR:HC7	2.02	0.42
16:J:4013:BCR:H15C	16:J:4013:BCR:H351	1.82	0.42
9:K:68:HIS:O	9:K:72:ILE:HG12	2.20	0.42
12:6:97:LEU:HG	16:6:522:BCR:H12C	2.00	0.42
16:Y:522:BCR:H20C	16:Y:522:BCR:H361	1.94	0.42
13:Z:501:CLA:H41	13:Z:501:CLA:H62	1.61	0.42
16:b:521:BCR:H15C	16:b:521:BCR:H351	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:50:ILE:HD11	12:c:89:LEU:HB2	2.01	0.42
12:d:40:PHE:CZ	13:q:518:CLA:C2	3.02	0.42
13:e:1116:CLA:H91	13:e:1116:CLA:H111	1.83	0.42
13:f:1219:CLA:HBC2	13:f:1220:CLA:HBA1	2.01	0.42
13:f:1224:CLA:H141	19:f:5002:LMG:H261	2.00	0.42
12:s:67:LEU:HD22	12:s:89:LEU:HD13	2.01	0.42
1:A:230:ILE:HG12	1:A:244:ALA:HA	2.00	0.42
13:B:1217:CLA:H41	13:B:1217:CLA:H61	1.73	0.42
13:L:1501:CLA:H202	13:L:1501:CLA:H161	1.88	0.42
12:2:148:PHE:CE2	13:2:512:CLA:HHB	2.55	0.42
16:3:522:BCR:H11C	16:3:522:BCR:H341	1.92	0.42
12:5:50:ILE:HD11	12:5:89:LEU:HB2	2.01	0.42
13:G:1106:CLA:H3A	13:G:1106:CLA:HBA2	1.61	0.42
2:H:7:LYS:HD2	11:W:28:TYR:CZ	2.54	0.42
2:H:236:ASN:OD1	2:H:236:ASN:N	2.49	0.42
8:T:13:ILE:HD11	16:T:4013:BCR:H281	2.02	0.42
16:T:4013:BCR:H362	16:T:4012:BCR:H17C	2.01	0.42
12:Z:26:LEU:HB3	13:Z:511:CLA:HMA1	2.01	0.42
13:a:519:CLA:HED2	13:a:519:CLA:H2A	2.02	0.42
16:a:523:BCR:H15C	16:a:523:BCR:H351	1.79	0.42
13:e:1119:CLA:H171	13:e:1129:CLA:HBC1	2.01	0.42
13:e:1138:CLA:HAA2	13:f:1228:CLA:HMB1	2.01	0.42
2:f:60:TRP:NE1	13:f:1224:CLA:OBD	2.53	0.42
2:f:174:ARG:HB2	13:f:1210:CLA:HBC2	2.01	0.42
2:f:326:LEU:HD12	2:f:326:LEU:O	2.20	0.42
2:f:338:LEU:HD21	13:f:1226:CLA:HAB	2.02	0.42
13:f:1226:CLA:H91	19:f:5002:LMG:H372	2.01	0.42
6:j:71:VAL:HG12	6:j:81:PHE:HB2	2.00	0.42
16:l:4013:BCR:H362	16:l:4012:BCR:H17C	2.01	0.42
12:q:110:HIS:HA	12:q:114:ALA:HB3	2.01	0.42
13:A:1104:CLA:H191	17:A:5001:LHG:H211	2.02	0.42
13:A:1118:CLA:H3A	9:K:61:LEU:HD23	2.01	0.42
13:A:1138:CLA:HAA2	13:B:1228:CLA:HMB1	2.01	0.42
2:B:192:GLY:O	2:B:196:HIS:HB2	2.20	0.42
13:B:1224:CLA:H141	19:B:5002:LMG:H261	2.00	0.42
17:L:5221:LHG:H151	7:k:16:PRO:HB3	2.02	0.42
12:1:34:GLN:HG2	13:1:509:CLA:HHB	2.02	0.42
12:1:289:THR:O	12:1:289:THR:CG2	2.67	0.42
16:1:523:BCR:H15C	16:1:523:BCR:H351	1.88	0.42
12:4:194:PHE:HB2	16:4:524:BCR:H391	2.01	0.42
1:G:591:ARG:HH21	1:G:594:THR:HG21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:94:SER:HB2	13:n:1501:CLA:HMD3	2.01	0.42
16:V:4020:BCR:H15C	16:V:4020:BCR:H351	1.87	0.42
16:Y:522:BCR:H15C	16:Y:522:BCR:H351	1.80	0.42
12:c:73:LEU:HD23	12:c:73:LEU:HA	1.91	0.42
13:c:512:CLA:H3A	13:c:512:CLA:HBA1	1.68	0.42
12:d:51:SER:HB2	12:q:279:LYS:HA	2.02	0.42
1:e:115:GLN:NE2	13:e:1107:CLA:OBD	2.43	0.42
13:e:1104:CLA:H193	13:e:1104:CLA:H161	1.85	0.42
13:e:1139:CLA:H41	13:e:1139:CLA:H61	1.62	0.42
2:f:101:ILE:HG12	7:k:1:MET:HE2	2.01	0.42
2:f:380:THR:HG22	2:f:583:ALA:HB1	2.01	0.42
2:f:690:ILE:HG13	10:n:36:ILE:HG12	2.02	0.42
13:f:1229:CLA:H61	16:j:4016:BCR:HC32	2.02	0.42
16:r:523:BCR:H15C	16:r:523:BCR:H351	1.85	0.42
16:v:521:BCR:H20C	16:v:521:BCR:H361	1.80	0.42
16:A:4007:BCR:H11C	16:A:4007:BCR:H341	1.88	0.42
2:B:690:ILE:HG13	10:L:36:ILE:HG12	2.02	0.42
8:J:13:ILE:HD11	16:J:4013:BCR:H281	2.02	0.42
20:L:5216:SQD:H291	17:k:5001:LHG:H131	2.02	0.42
13:3:513:CLA:HBB1	16:3:523:BCR:H402	2.01	0.42
13:5:503:CLA:H62	13:5:503:CLA:H41	1.83	0.42
12:6:102:VAL:HG22	13:Y:505:CLA:H61	2.01	0.42
14:H:2002:PQN:H261	14:H:2002:PQN:H222	1.83	0.42
16:Y:521:BCR:H11C	16:Y:521:BCR:H341	1.88	0.42
13:b:513:CLA:HBB1	16:b:523:BCR:H402	2.02	0.42
16:b:523:BCR:H15C	16:b:523:BCR:H351	1.84	0.42
13:e:1104:CLA:H201	17:e:5001:LHG:H221	2.00	0.42
13:e:1124:CLA:H2	13:e:1124:CLA:H61	1.79	0.42
13:e:1139:CLA:H101	13:e:1139:CLA:H203	2.02	0.42
2:f:218:HIS:HD2	2:f:220:ALA:H	1.66	0.42
16:n:4019:BCR:H11C	16:n:4019:BCR:H341	1.90	0.42
12:t:141:ILE:HD13	13:t:509:CLA:H191	2.01	0.42
13:t:518:CLA:C2	13:t:518:CLA:H3A	2.50	0.42
16:t:523:BCR:H15C	16:t:523:BCR:H351	1.84	0.42
16:u:522:BCR:H20C	16:u:522:BCR:H361	1.94	0.42
12:v:79:ASP:OD1	12:v:79:ASP:N	2.48	0.42
12:v:148:PHE:CE2	13:v:512:CLA:HHB	2.55	0.42
13:A:1139:CLA:H203	13:A:1139:CLA:H101	2.02	0.42
16:A:4002:BCR:H361	16:A:4002:BCR:H20C	1.77	0.42
18:A:1849:LMU:H91	18:A:1849:LMU:H62	1.85	0.42
2:B:326:LEU:O	2:B:326:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1218:CLA:HMD2	16:B:4004:BCR:H23C	2.02	0.42
13:B:1226:CLA:H91	19:B:5002:LMG:H372	2.02	0.42
16:F:4016:BCR:H371	16:F:4016:BCR:H24C	1.80	0.42
12:3:97:LEU:HG	16:3:522:BCR:H12C	2.02	0.42
12:5:221:HIS:HE1	13:5:506:CLA:NA	2.17	0.42
16:5:521:BCR:H15C	16:5:521:BCR:H351	1.85	0.42
16:6:523:BCR:H15C	16:6:523:BCR:H351	1.81	0.42
13:G:1108:CLA:HBA2	13:G:1108:CLA:H3A	1.71	0.42
12:Z:34:GLN:HG2	13:Z:509:CLA:HHB	2.00	0.42
12:a:221:HIS:CE1	13:a:506:CLA:NA	2.88	0.42
16:a:521:BCR:H24C	16:a:521:BCR:H371	1.89	0.42
16:a:524:BCR:H20C	16:a:524:BCR:H361	1.92	0.42
12:b:194:PHE:HB2	16:b:524:BCR:H391	2.01	0.42
16:b:521:BCR:H11C	16:b:521:BCR:H341	1.91	0.42
12:c:59:MET:HB2	12:c:271:PHE:HA	2.02	0.42
12:d:148:PHE:CE2	13:d:512:CLA:HHB	2.55	0.42
1:e:172:MET:HE1	13:e:1111:CLA:H92	2.00	0.42
1:e:239:ASN:HD22	1:e:263:GLN:HE22	1.67	0.42
13:e:1102:CLA:H112	13:e:1102:CLA:H151	1.73	0.42
16:e:4002:BCR:H11C	16:e:4002:BCR:H341	1.82	0.42
2:f:428:PHE:CZ	16:l:4015:BCR:HC41	2.55	0.42
13:r:502:CLA:H11	13:r:503:CLA:H161	2.00	0.42
16:r:523:BCR:H11C	16:r:523:BCR:H341	1.88	0.42
13:s:519:CLA:HED2	13:s:519:CLA:H2A	2.02	0.42
12:t:130:PHE:HA	12:t:137:GLN:HG2	2.02	0.42
13:t:505:CLA:H91	13:t:505:CLA:H112	1.86	0.42
2:B:101:ILE:HG12	7:I:1:MET:HE2	2.02	0.42
16:L:4022:BCR:H24C	16:L:4022:BCR:H371	1.85	0.42
13:4:513:CLA:HBB1	16:4:523:BCR:H402	2.02	0.42
16:6:521:BCR:H361	16:6:521:BCR:H20C	1.80	0.42
1:G:239:ASN:HD22	1:G:263:GLN:HE22	1.67	0.42
13:G:1140:CLA:H11	13:G:1140:CLA:CHA	2.50	0.42
2:H:464:GLN:HG2	2:H:509:PHE:CD1	2.55	0.42
13:Y:517:CLA:HBA1	13:Y:517:CLA:H3A	1.76	0.42
3:g:61:ASP:HA	3:g:62:PHE:HA	1.83	0.42
12:u:79:ASP:OD1	12:u:79:ASP:N	2.45	0.42
16:u:522:BCR:H351	16:u:522:BCR:H15C	1.75	0.42
12:v:97:LEU:HG	16:v:522:BCR:H12C	2.00	0.42
2:B:464:GLN:HG2	2:B:509:PHE:CD1	2.55	0.41
6:F:150:LYS:HB3	6:F:153:GLU:HG3	2.01	0.41
13:2:518:CLA:H41	13:2:518:CLA:H61	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:148:PHE:CE2	13:6:512:CLA:HHB	2.55	0.41
1:G:544:PHE:CZ	16:V:4219:BCR:H332	2.54	0.41
13:G:1116:CLA:HBA2	13:G:1116:CLA:H3A	1.46	0.41
13:G:1138:CLA:H202	13:G:1138:CLA:H162	1.88	0.41
2:H:326:LEU:HD12	2:H:326:LEU:O	2.20	0.41
2:H:376:GLN:O	2:H:380:THR:OG1	2.33	0.41
2:H:531:THR:O	2:H:535:VAL:HB	2.19	0.41
13:H:1219:CLA:H192	13:H:1219:CLA:H162	1.84	0.41
17:H:1855:LHG:HC82	17:H:1855:LHG:H112	1.93	0.41
16:V:4022:BCR:H371	16:V:4022:BCR:H24C	1.85	0.41
12:Y:34:GLN:HG2	13:Y:509:CLA:HHB	2.02	0.41
12:Y:50:ILE:HD11	12:Y:89:LEU:HB2	2.02	0.41
13:a:503:CLA:H18	13:a:510:CLA:HBB2	2.00	0.41
16:c:523:BCR:H15C	16:c:523:BCR:H351	1.79	0.41
16:c:524:BCR:H20C	16:c:524:BCR:H361	1.94	0.41
1:e:312:ILE:HD13	1:e:312:ILE:HA	1.87	0.41
1:e:704:TYR:OH	13:e:1013:CLA:OBD	2.28	0.41
13:e:1136:CLA:H92	13:e:1136:CLA:H62	1.82	0.41
2:f:493:TYR:HE2	13:f:1231:CLA:HED1	1.84	0.41
16:f:4006:BCR:H351	16:f:4006:BCR:H15C	1.83	0.41
13:q:502:CLA:HBD	13:q:503:CLA:H43	2.01	0.41
12:r:148:PHE:CE2	13:r:512:CLA:HHB	2.55	0.41
12:s:221:HIS:CE1	13:s:506:CLA:NA	2.88	0.41
16:s:521:BCR:H15C	16:s:521:BCR:H351	1.82	0.41
12:u:50:ILE:HD11	12:u:89:LEU:HB2	2.01	0.41
12:v:246:LEU:HD23	12:v:246:LEU:HA	1.92	0.41
1:A:141:SER:HB3	13:A:1126:CLA:HAA2	2.02	0.41
13:A:1104:CLA:H3A	13:A:1128:CLA:CAB	2.51	0.41
2:B:60:TRP:NE1	13:B:1224:CLA:OBD	2.53	0.41
2:B:338:LEU:HD21	13:B:1226:CLA:HAB	2.02	0.41
2:B:428:PHE:CZ	16:J:4015:BCR:HC41	2.55	0.41
2:B:631:LEU:O	2:B:647:SER:OG	2.29	0.41
16:K:4104:BCR:H11C	16:K:4104:BCR:H341	1.91	0.41
12:1:147:LEU:HD12	12:1:215:ILE:HG12	2.01	0.41
12:3:221:HIS:CE1	13:3:506:CLA:NA	2.88	0.41
12:6:42:ALA:O	12:6:46:THR:OG1	2.33	0.41
16:G:4008:BCR:H11C	16:G:4008:BCR:H341	1.89	0.41
2:H:174:ARG:HB2	13:H:1210:CLA:HBC2	2.01	0.41
2:H:338:LEU:HD21	13:H:1226:CLA:HAB	2.02	0.41
13:H:1234:CLA:H193	13:H:1234:CLA:H161	1.87	0.41
12:Y:110:HIS:HA	12:Y:114:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:518:CLA:H102	13:Y:518:CLA:H62	1.85	0.41
13:a:505:CLA:H92	13:a:505:CLA:H61	1.89	0.41
13:b:518:CLA:C2	13:b:518:CLA:H3A	2.50	0.41
1:e:570:SER:HB2	1:e:575:PRO:HA	2.03	0.41
1:e:691:TRP:CE2	13:e:1011:CLA:HBA2	2.54	0.41
13:e:1116:CLA:H93	13:e:1116:CLA:H61	1.90	0.41
17:e:5001:LHG:H372	17:e:5001:LHG:H341	1.82	0.41
2:f:464:GLN:HG2	2:f:509:PHE:CD1	2.55	0.41
14:f:2002:PQN:H211	14:f:2002:PQN:H172	1.88	0.41
16:u:524:BCR:H11C	16:u:524:BCR:H341	1.92	0.41
13:A:1106:CLA:H3A	13:A:1106:CLA:HBA2	1.61	0.41
13:A:1116:CLA:H91	13:A:1116:CLA:H111	1.83	0.41
13:A:1140:CLA:H11	13:A:1140:CLA:CHA	2.50	0.41
2:B:194:LEU:HA	2:B:198:ALA:HB3	2.02	0.41
2:B:276:HIS:HE2	13:B:1215:CLA:C2B	2.33	0.41
7:I:4:ASP:OD1	7:I:4:ASP:N	2.42	0.41
16:J:4013:BCR:H362	16:J:4012:BCR:H17C	2.01	0.41
13:3:519:CLA:HED2	13:3:519:CLA:H2A	2.02	0.41
12:6:148:PHE:HE2	13:6:512:CLA:HHB	1.84	0.41
13:G:1104:CLA:H161	13:G:1104:CLA:H193	1.85	0.41
13:G:1126:CLA:H192	13:G:1126:CLA:H161	1.96	0.41
2:H:493:TYR:HE2	13:H:1231:CLA:HED1	1.84	0.41
13:H:1226:CLA:H112	13:H:1226:CLA:H71	1.92	0.41
5:Q:53:ASP:OD1	5:Q:53:ASP:N	2.44	0.41
9:U:47:PRO:HG2	20:Y:822:SQD:H241	2.03	0.41
13:V:1503:CLA:H93	13:V:1503:CLA:H61	1.90	0.41
12:a:261:ALA:HA	12:a:276:LEU:HD12	2.02	0.41
1:e:468:ILE:HG23	13:e:1022:CLA:H61	2.02	0.41
2:f:192:GLY:O	2:f:196:HIS:HB2	2.20	0.41
2:f:237:PRO:HB3	2:f:256:THR:HG21	2.02	0.41
2:f:499:ASP:O	2:f:503:SER:HB3	2.20	0.41
13:f:1023:CLA:H202	13:f:1023:CLA:H162	1.94	0.41
13:f:1218:CLA:HMD2	16:f:4004:BCR:H23C	2.02	0.41
13:j:1301:CLA:H72	13:j:1301:CLA:H111	1.78	0.41
12:q:79:ASP:OD1	12:q:79:ASP:N	2.53	0.41
2:B:631:LEU:HD22	2:B:724:PHE:HA	2.02	0.41
16:B:4004:BCR:H361	16:B:4004:BCR:H20C	1.75	0.41
16:B:4010:BCR:H20C	16:B:4010:BCR:H361	1.92	0.41
16:K:4104:BCR:H20C	16:K:4104:BCR:H361	1.87	0.41
13:1:502:CLA:HBD	13:1:503:CLA:H43	2.01	0.41
12:2:34:GLN:HG2	13:2:509:CLA:HHB	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:193:HIS:HB2	12:2:196:SER:HB3	2.00	0.41
12:4:130:PHE:HA	12:4:137:GLN:HG2	2.02	0.41
1:G:258:VAL:O	1:G:262:SER:HB2	2.21	0.41
1:G:573:LEU:O	4:O:61:ARG:NH2	2.49	0.41
1:G:691:TRP:O	1:G:694:SER:OG	2.30	0.41
13:G:1103:CLA:H3A	13:G:1103:CLA:HBA1	1.54	0.41
14:G:2001:PQN:H162	16:H:4014:BCR:H382	2.03	0.41
16:G:4002:BCR:H24C	16:G:4002:BCR:H371	1.82	0.41
2:H:276:HIS:HE2	13:H:1215:CLA:C2B	2.34	0.41
2:H:428:PHE:CZ	16:T:4015:BCR:HC41	2.55	0.41
2:H:690:ILE:HG13	10:V:36:ILE:HG12	2.02	0.41
13:H:1203:CLA:H12	13:H:1226:CLA:HBA1	2.02	0.41
13:H:1226:CLA:H91	19:H:5002:LMG:H372	2.01	0.41
14:H:2002:PQN:H211	14:H:2002:PQN:H172	1.88	0.41
13:e:1120:CLA:C1B	13:e:1120:CLA:H2	2.50	0.41
13:e:1123:CLA:H162	13:e:1123:CLA:H193	1.83	0.41
13:e:1138:CLA:H202	13:e:1138:CLA:H162	1.88	0.41
16:e:4007:BCR:H15C	16:e:4007:BCR:H351	1.79	0.41
13:f:1204:CLA:H93	13:f:1204:CLA:H61	1.92	0.41
16:f:4009:BCR:H11C	16:f:4009:BCR:H341	1.86	0.41
12:q:147:LEU:HD12	12:q:215:ILE:HG12	2.01	0.41
16:r:521:BCR:H371	16:r:521:BCR:H24C	1.78	0.41
12:s:148:PHE:HD2	13:s:512:CLA:H3A	1.85	0.41
1:A:468:ILE:HG23	13:A:1022:CLA:H61	2.02	0.41
13:A:1129:CLA:H11	13:A:1129:CLA:H51	1.80	0.41
13:B:1229:CLA:H61	16:F:4016:BCR:HC32	2.02	0.41
12:3:261:ALA:HA	12:3:276:LEU:HD12	2.02	0.41
13:4:518:CLA:C2	13:4:518:CLA:H3A	2.50	0.41
13:G:1124:CLA:H61	13:G:1124:CLA:H2	1.79	0.41
13:H:1229:CLA:H61	16:R:4016:BCR:HC32	2.02	0.41
6:R:90:TYR:OH	6:R:132:PHE:O	2.33	0.41
12:Y:289:THR:O	12:Y:289:THR:CG2	2.67	0.41
16:Y:524:BCR:H20C	16:Y:524:BCR:H361	1.91	0.41
12:Z:148:PHE:CE2	13:Z:512:CLA:HHB	2.55	0.41
12:Z:261:ALA:HA	12:Z:276:LEU:HD12	2.01	0.41
13:a:513:CLA:H143	13:a:513:CLA:H111	1.92	0.41
13:e:1108:CLA:H41	13:e:1108:CLA:H61	1.78	0.41
13:e:1109:CLA:H141	13:e:1109:CLA:H161	1.82	0.41
13:e:1126:CLA:H3A	13:e:1126:CLA:HBA2	1.60	0.41
2:f:631:LEU:HD22	2:f:724:PHE:HA	2.02	0.41
2:f:658:ALA:HB3	13:f:1023:CLA:HBB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:696:LYS:HA	2:f:697:PRO:HD3	1.96	0.41
16:f:4017:BCR:H20C	16:f:4017:BCR:H361	1.89	0.41
16:f:4009:BCR:H15C	16:f:4009:BCR:H351	1.82	0.41
4:h:77:LYS:HD3	4:h:77:LYS:HA	1.92	0.41
9:m:68:HIS:O	9:m:72:ILE:HG12	2.20	0.41
12:q:50:ILE:HD11	12:q:89:LEU:HB2	2.02	0.41
13:r:513:CLA:H143	13:r:513:CLA:H111	1.91	0.41
12:v:91:VAL:HG22	16:v:523:BCR:HC22	2.02	0.41
1:A:258:VAL:O	1:A:262:SER:HB2	2.21	0.41
13:A:1237:CLA:HAB	2:B:691:VAL:HG11	2.03	0.41
13:B:1219:CLA:H61	13:B:1219:CLA:H92	1.91	0.41
16:B:4017:BCR:H20C	16:B:4017:BCR:H361	1.89	0.41
13:L:1501:CLA:H112	16:L:4022:BCR:H10C	2.03	0.41
16:1:522:BCR:H24C	16:1:522:BCR:H371	1.84	0.41
12:2:91:VAL:HG22	16:2:523:BCR:HC22	2.03	0.41
12:5:107:ALA:O	12:5:111:THR:OG1	2.30	0.41
1:G:271:GLY:O	1:G:283:TYR:OH	2.29	0.41
1:G:441:VAL:HA	1:G:444:HIS:CE1	2.56	0.41
2:H:192:GLY:O	2:H:196:HIS:HB2	2.20	0.41
2:H:236:ASN:OD1	2:H:252:THR:OG1	2.39	0.41
2:H:355:MET:HE3	2:H:355:MET:HB2	1.79	0.41
2:H:499:ASP:O	2:H:503:SER:HB3	2.20	0.41
2:H:714:THR:HG21	19:H:5002:LMG:H402	2.03	0.41
16:R:4016:BCR:H11C	16:R:4016:BCR:H341	1.77	0.41
13:Z:518:CLA:H111	13:Z:518:CLA:H142	1.85	0.41
12:a:97:LEU:HG	16:a:522:BCR:H12C	2.02	0.41
12:b:34:GLN:OE1	13:b:510:CLA:NC	2.54	0.41
12:d:148:PHE:HE2	13:d:512:CLA:HHB	1.84	0.41
12:d:207:HIS:CE1	16:d:524:BCR:H381	2.56	0.41
16:d:521:BCR:H20C	16:d:521:BCR:H361	1.80	0.41
13:e:1104:CLA:H3A	13:e:1128:CLA:CAB	2.51	0.41
13:e:1022:CLA:H122	16:f:4017:BCR:H12C	2.03	0.41
13:f:1219:CLA:H192	13:f:1219:CLA:H162	1.84	0.41
13:r:505:CLA:HBA2	13:r:505:CLA:H11	1.88	0.41
12:s:261:ALA:HA	12:s:276:LEU:HD12	2.02	0.41
12:t:34:GLN:OE1	13:t:510:CLA:NC	2.54	0.41
1:A:120:ILE:HG13	1:A:121:PHE:CD2	2.56	0.41
13:A:1137:CLA:H93	13:A:1137:CLA:H111	1.91	0.41
13:A:1138:CLA:H91	13:F:1301:CLA:HAC2	2.03	0.41
14:A:2001:PQN:H2M1	14:A:2001:PQN:H111	1.91	0.41
20:B:1852:SQD:O3	10:V:3:GLN:NE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:8:LEU:HA	8:J:13:ILE:HG21	2.02	0.41
16:L:4219:BCR:H393	17:L:5221:LHG:H322	2.03	0.41
17:L:5220:LHG:H311	17:L:5220:LHG:H171	2.02	0.41
13:2:505:CLA:HBC2	16:2:524:BCR:H341	2.03	0.41
13:2:506:CLA:H41	13:2:506:CLA:H62	1.71	0.41
12:3:233:VAL:HG13	16:3:524:BCR:HC21	2.03	0.41
16:5:522:BCR:H351	16:5:522:BCR:H15C	1.75	0.41
16:6:521:BCR:H15C	16:6:521:BCR:H351	1.83	0.41
16:6:522:BCR:H371	16:6:522:BCR:H24C	1.82	0.41
1:G:572:ARG:HD3	3:N:80:ALA:HB3	2.03	0.41
1:G:704:TYR:OH	13:G:1013:CLA:OBD	2.28	0.41
13:G:1131:CLA:HBB2	10:V:65:LEU:HD13	2.02	0.41
13:G:1135:CLA:H62	13:G:1135:CLA:H41	1.79	0.41
2:H:394:LEU:HD23	2:H:394:LEU:HA	1.92	0.41
17:V:5220:LHG:H311	17:V:5220:LHG:H171	2.01	0.41
16:a:522:BCR:H24C	16:a:522:BCR:H371	1.87	0.41
13:c:501:CLA:H62	13:c:501:CLA:H41	1.70	0.41
1:e:120:ILE:HG13	1:e:121:PHE:CD2	2.56	0.41
1:e:141:SER:HB3	13:e:1126:CLA:HAA2	2.02	0.41
1:e:572:ARG:HD3	3:g:80:ALA:HB3	2.03	0.41
13:e:1121:CLA:HAB	13:e:1801:CLA:CAB	2.50	0.41
2:f:714:THR:HG21	19:f:5002:LMG:H402	2.03	0.41
8:l:8:LEU:HA	8:l:13:ILE:HG21	2.02	0.41
16:q:524:BCR:H24C	16:q:524:BCR:H371	1.90	0.41
12:v:47:LEU:HD21	12:v:90:PHE:HD1	1.86	0.41
13:A:1104:CLA:H41	13:A:1104:CLA:H62	1.64	0.41
16:A:4008:BCR:H20C	16:A:4008:BCR:H361	1.84	0.41
2:B:380:THR:HG22	2:B:583:ALA:HB1	2.02	0.41
13:B:1205:CLA:H193	13:B:1205:CLA:H161	1.91	0.41
5:E:18:TRP:HB3	5:E:21:GLU:HB2	2.03	0.41
6:F:150:LYS:HD3	6:F:150:LYS:HA	1.72	0.41
17:L:5221:LHG:H121	13:f:1207:CLA:CMA	2.51	0.41
16:1:524:BCR:H20C	16:1:524:BCR:H361	1.91	0.41
12:6:47:LEU:HD21	12:6:90:PHE:HD1	1.86	0.41
16:6:524:BCR:H11C	16:6:524:BCR:H341	1.88	0.41
1:G:256:LEU:HD12	13:G:1114:CLA:HBC2	2.03	0.41
13:G:1136:CLA:H62	13:G:1136:CLA:H92	1.82	0.41
13:G:1237:CLA:HAB	2:H:691:VAL:HG11	2.03	0.41
10:V:149:THR:HG22	10:V:151:TYR:H	1.86	0.41
16:b:524:BCR:H11C	16:b:524:BCR:H341	1.83	0.41
13:c:505:CLA:H42	16:c:524:BCR:HC7	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:512:CLA:HED2	13:d:512:CLA:H2A	2.03	0.41
16:d:521:BCR:H371	16:d:521:BCR:H24C	1.82	0.41
13:e:1131:CLA:HBB2	10:n:65:LEU:HD13	2.02	0.41
13:e:1135:CLA:HAB	13:e:1135:CLA:HHC	1.87	0.41
2:f:34:HIS:HE1	13:f:1201:CLA:HED1	1.86	0.41
8:l:13:ILE:HD11	16:l:4013:BCR:H281	2.02	0.41
10:n:149:THR:HG22	10:n:151:TYR:H	1.86	0.41
16:n:4219:BCR:H393	17:n:5221:LHG:H322	2.03	0.41
16:o:4021:BCR:H15C	16:o:4021:BCR:H351	1.84	0.41
16:o:4021:BCR:H24C	16:o:4021:BCR:H371	1.85	0.41
12:r:147:LEU:HD12	12:r:215:ILE:HG12	2.03	0.41
16:r:524:BCR:H351	16:r:524:BCR:H15C	1.78	0.41
13:s:510:CLA:H143	13:s:510:CLA:H111	1.91	0.41
13:t:513:CLA:HBB1	16:t:523:BCR:H402	2.02	0.41
16:t:524:BCR:H24C	16:t:524:BCR:H371	1.92	0.41
1:A:145:GLN:HB3	1:A:388:TYR:HB3	2.02	0.41
13:A:1120:CLA:H2	13:A:1120:CLA:C1B	2.50	0.41
2:B:714:THR:HG21	19:B:5002:LMG:H402	2.03	0.41
4:D:58:TYR:H	10:L:13:GLU:HG2	1.86	0.41
9:K:47:PRO:HG2	20:1:822:SQD:H241	2.02	0.41
20:L:5216:SQD:H241	7:k:29:LEU:HB3	2.02	0.41
13:1:505:CLA:H61	12:v:102:VAL:HG22	2.02	0.41
12:2:289:THR:HG22	12:2:289:THR:O	2.21	0.41
12:3:68:PRO:HB3	12:3:271:PHE:HB3	2.03	0.41
12:3:148:PHE:HD2	13:3:512:CLA:H3A	1.85	0.41
13:3:511:CLA:H2	16:3:522:BCR:H282	2.03	0.41
16:3:522:BCR:H24C	16:3:522:BCR:H371	1.87	0.41
16:3:524:BCR:H20C	16:3:524:BCR:H361	1.91	0.41
13:5:501:CLA:H62	13:5:501:CLA:H41	1.70	0.41
12:6:177:VAL:HG13	12:6:201:GLU:HG2	2.02	0.41
13:6:512:CLA:HED2	13:6:512:CLA:H2A	2.03	0.41
1:G:145:GLN:HB3	1:G:388:TYR:HB3	2.02	0.41
1:G:601:ASP:HA	1:G:604:PHE:HB3	2.03	0.41
13:G:1120:CLA:C1B	13:G:1120:CLA:H2	2.50	0.41
13:G:1123:CLA:H141	13:G:1123:CLA:H161	1.80	0.41
2:H:262:HIS:HA	2:H:263:PRO:HD3	1.98	0.41
2:H:631:LEU:HD22	2:H:724:PHE:HA	2.02	0.41
16:H:4004:BCR:H361	16:H:4004:BCR:H20C	1.75	0.41
16:H:4005:BCR:H15C	16:H:4005:BCR:H351	1.81	0.41
4:O:58:TYR:H	10:V:13:GLU:HG2	1.86	0.41
16:S:4018:BCR:H11C	16:S:4018:BCR:H341	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:4018:BCR:H24C	16:S:4018:BCR:H371	1.90	0.41
16:U:4104:BCR:H24C	20:Y:822:SQD:H341	2.03	0.41
10:V:85:LEU:HA	10:V:85:LEU:HD12	1.86	0.41
16:W:4021:BCR:H15C	16:W:4021:BCR:H351	1.84	0.41
12:Z:229:TRP:HA	12:Z:232:LYS:HB2	2.03	0.41
12:a:233:VAL:HG13	16:a:524:BCR:HC21	2.03	0.41
12:d:47:LEU:HD21	12:d:90:PHE:HD1	1.86	0.41
1:e:145:GLN:HB3	1:e:388:TYR:HB3	2.02	0.41
13:e:1137:CLA:H93	13:e:1137:CLA:H111	1.91	0.41
2:f:142:LEU:HG	16:f:4006:BCR:H382	2.02	0.41
13:f:1203:CLA:H12	13:f:1226:CLA:HBA1	2.02	0.41
13:f:1217:CLA:H41	13:f:1217:CLA:H61	1.73	0.41
9:m:8:ILE:HA	9:m:9:PRO:HD3	1.93	0.41
16:q:522:BCR:H24C	16:q:522:BCR:H371	1.84	0.41
13:r:510:CLA:H41	13:r:510:CLA:H62	1.81	0.41
12:s:68:PRO:HB3	12:s:271:PHE:HB3	2.02	0.41
12:s:233:VAL:HG13	16:s:524:BCR:HC21	2.03	0.41
12:t:194:PHE:HB2	16:t:524:BCR:H391	2.01	0.41
12:u:59:MET:HB2	12:u:271:PHE:HA	2.02	0.41
12:v:177:VAL:HG13	12:v:201:GLU:HG2	2.02	0.41
1:A:573:LEU:O	4:D:61:ARG:NH2	2.49	0.41
13:A:1121:CLA:HAB	13:A:1801:CLA:CAB	2.50	0.41
14:A:2001:PQN:H162	16:B:4014:BCR:H382	2.03	0.41
2:B:236:ASN:OD1	2:B:252:THR:OG1	2.39	0.41
2:B:499:ASP:O	2:B:503:SER:HB3	2.20	0.41
13:B:1240:CLA:H62	13:B:1240:CLA:H41	1.88	0.41
13:J:1303:CLA:H62	13:J:1303:CLA:H41	1.83	0.41
12:5:59:MET:HB2	12:5:271:PHE:HA	2.02	0.41
13:5:505:CLA:H42	16:5:524:BCR:HC7	2.02	0.41
12:6:243:SER:O	12:6:318:HIS:ND1	2.54	0.41
1:G:148:ARG:HD3	1:G:389:PRO:HB2	2.03	0.41
13:G:1137:CLA:H93	13:G:1137:CLA:H61	1.94	0.41
13:G:1237:CLA:H202	16:V:4019:BCR:H391	2.03	0.41
13:G:1101:CLA:H102	13:G:1101:CLA:H62	1.84	0.41
2:H:142:LEU:HG	16:H:4006:BCR:H382	2.02	0.41
2:H:194:LEU:HA	2:H:198:ALA:HB3	2.02	0.41
13:H:1217:CLA:H61	13:H:1217:CLA:H41	1.73	0.41
16:T:4012:BCR:H20C	16:T:4012:BCR:H361	1.94	0.41
16:V:4022:BCR:H11C	16:V:4022:BCR:H341	1.84	0.41
12:Y:79:ASP:OD1	12:Y:79:ASP:N	2.54	0.41
12:Z:91:VAL:HG22	16:Z:523:BCR:HC22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:148:PHE:HD2	13:a:512:CLA:H3A	1.85	0.41
13:d:517:CLA:HBB1	16:d:524:BCR:H352	2.04	0.41
16:d:524:BCR:H24C	16:d:524:BCR:H371	1.87	0.41
1:e:256:LEU:HD12	13:e:1114:CLA:HBC2	2.03	0.41
1:e:308:HIS:HE2	13:e:1117:CLA:C2B	2.34	0.41
13:e:1104:CLA:H191	17:e:5001:LHG:H211	2.02	0.41
16:e:4003:BCR:H11C	16:e:4003:BCR:H341	1.90	0.41
2:f:194:LEU:HA	2:f:198:ALA:HB3	2.02	0.41
2:f:276:HIS:HE2	13:f:1215:CLA:C2B	2.33	0.41
2:f:321:GLY:O	2:f:325:THR:OG1	2.28	0.41
2:f:455:ILE:HD13	6:j:69:LEU:HB2	2.03	0.41
13:f:1223:CLA:H102	13:f:1223:CLA:H61	1.97	0.41
16:j:4016:BCR:H11C	16:j:4016:BCR:H341	1.77	0.41
8:l:26:LEU:HD13	16:l:4012:BCR:HC7	2.02	0.41
16:m:4104:BCR:H24C	20:q:822:SQD:H341	2.03	0.41
1:A:18:LYS:HA	1:A:18:LYS:HD2	1.94	0.40
1:A:459:LEU:O	1:A:463:SER:OG	2.37	0.40
2:B:142:LEU:HG	16:B:4006:BCR:H382	2.02	0.40
2:B:658:ALA:HB3	13:B:1023:CLA:HBB2	2.02	0.40
13:B:1206:CLA:H3A	13:B:1206:CLA:HBA1	1.58	0.40
16:L:4020:BCR:H20C	16:L:4020:BCR:H361	1.89	0.40
12:1:50:ILE:HD11	12:1:89:LEU:HB2	2.02	0.40
12:1:332:ARG:HA	12:1:335:LYS:HB3	2.03	0.40
13:2:518:CLA:H142	13:2:518:CLA:H111	1.85	0.40
12:5:177:VAL:HG13	12:5:201:GLU:HG2	2.04	0.40
1:G:468:ILE:HG23	13:G:1022:CLA:H61	2.02	0.40
13:G:1104:CLA:H3A	13:G:1128:CLA:CAB	2.51	0.40
16:G:4007:BCR:H371	16:G:4007:BCR:H24C	1.89	0.40
2:H:237:PRO:HB3	2:H:256:THR:HG21	2.02	0.40
13:H:1218:CLA:HMD2	16:H:4004:BCR:H23C	2.02	0.40
16:U:4104:BCR:H15C	16:U:4104:BCR:H351	1.84	0.40
16:V:4219:BCR:H393	17:V:5221:LHG:H322	2.03	0.40
12:b:130:PHE:HA	12:b:137:GLN:HG2	2.02	0.40
13:e:1126:CLA:H143	13:e:1126:CLA:H112	1.87	0.40
13:e:1128:CLA:H91	13:e:1128:CLA:H112	1.89	0.40
13:e:1137:CLA:H62	13:e:1137:CLA:H41	1.80	0.40
16:f:4009:BCR:H321	17:f:1842:LHG:H322	2.03	0.40
4:h:58:TYR:H	10:n:13:GLU:HG2	1.86	0.40
16:q:523:BCR:H15C	16:q:523:BCR:H351	1.88	0.40
12:r:229:TRP:HA	12:r:232:LYS:HB2	2.03	0.40
12:s:246:LEU:HD23	12:s:246:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:523:BCR:H351	16:u:523:BCR:H15C	1.80	0.40
16:v:523:BCR:H15C	16:v:523:BCR:H351	1.81	0.40
1:A:256:LEU:HD12	13:A:1114:CLA:HBC2	2.03	0.40
1:A:669:VAL:HG22	1:A:757:ALA:HB3	2.04	0.40
13:A:1115:CLA:H142	13:A:1115:CLA:H112	1.92	0.40
12:2:57:GLN:HB2	12:2:62:GLN:HE21	1.86	0.40
12:2:229:TRP:HA	12:2:232:LYS:HB2	2.03	0.40
12:4:34:GLN:OE1	13:4:510:CLA:NC	2.54	0.40
13:4:509:CLA:H3A	13:4:509:CLA:HBA1	1.87	0.40
1:G:141:SER:HB3	13:G:1126:CLA:HAA2	2.02	0.40
13:G:1107:CLA:H152	16:T:4012:BCR:H272	2.03	0.40
13:H:1201:CLA:H2	16:W:4021:BCR:HC31	2.03	0.40
16:H:4010:BCR:H20C	16:H:4010:BCR:H361	1.92	0.40
12:Y:332:ARG:HA	12:Y:335:LYS:HB3	2.03	0.40
16:b:524:BCR:H15C	16:b:524:BCR:H351	1.80	0.40
13:e:1107:CLA:H152	16:l:4012:BCR:H272	2.03	0.40
13:e:1128:CLA:H142	13:e:1128:CLA:H111	1.87	0.40
13:e:1237:CLA:HAB	2:f:691:VAL:HG11	2.03	0.40
7:k:23:PRO:O	7:k:27:MET:HB2	2.21	0.40
12:s:97:LEU:HG	16:s:522:BCR:H12C	2.02	0.40
13:A:1137:CLA:H122	16:A:4007:BCR:H393	2.04	0.40
13:B:1221:CLA:H112	13:B:1221:CLA:H151	1.82	0.40
13:B:1229:CLA:H192	16:F:4016:BCR:H17C	2.04	0.40
16:B:4009:BCR:H321	17:B:1842:LHG:H322	2.03	0.40
13:3:513:CLA:H143	13:3:513:CLA:H111	1.91	0.40
16:4:521:BCR:H24C	16:4:521:BCR:H371	1.91	0.40
12:6:20:PHE:HA	12:6:23:LEU:HD12	2.03	0.40
12:6:207:HIS:CE1	16:6:524:BCR:H381	2.56	0.40
1:G:120:ILE:HG13	1:G:121:PHE:CD2	2.56	0.40
1:G:570:SER:HB2	1:G:575:PRO:HA	2.03	0.40
13:G:1117:CLA:H203	13:G:1125:CLA:HAA1	2.03	0.40
13:G:1139:CLA:H101	13:G:1139:CLA:H203	2.02	0.40
16:G:4007:BCR:H11C	16:G:4007:BCR:H341	1.88	0.40
16:G:4007:BCR:H15C	16:G:4007:BCR:H351	1.79	0.40
2:H:60:TRP:NE1	13:H:1224:CLA:OBD	2.53	0.40
13:H:1213:CLA:H3A	13:H:1213:CLA:HBA2	1.84	0.40
16:H:4009:BCR:H321	17:H:1842:LHG:H322	2.03	0.40
16:T:4015:BCR:H15C	16:T:4015:BCR:H351	1.79	0.40
13:V:1501:CLA:H112	16:V:4022:BCR:H10C	2.03	0.40
16:V:4020:BCR:H24C	16:V:4020:BCR:H371	1.71	0.40
12:Y:261:ALA:HA	12:Y:276:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:147:LEU:HD12	12:Z:215:ILE:HG12	2.03	0.40
13:Z:513:CLA:H143	13:Z:513:CLA:H111	1.91	0.40
12:d:91:VAL:HG22	16:d:523:BCR:HC22	2.02	0.40
12:d:127:ARG:O	12:d:137:GLN:NE2	2.50	0.40
1:e:221:LEU:HD23	1:e:221:LEU:HA	1.89	0.40
13:e:1119:CLA:H111	13:e:1119:CLA:H152	1.87	0.40
16:e:4001:BCR:H11C	16:e:4001:BCR:H341	1.87	0.40
13:f:1234:CLA:H71	13:f:1235:CLA:H12	2.03	0.40
5:i:18:TRP:HB3	5:i:21:GLU:HB2	2.03	0.40
16:l:4013:BCR:H351	16:l:4013:BCR:H15C	1.82	0.40
13:n:1501:CLA:H102	13:n:1503:CLA:H122	2.03	0.40
17:n:5221:LHG:H241	17:n:5221:LHG:HC92	2.03	0.40
12:q:332:ARG:HA	12:q:335:LYS:HB3	2.03	0.40
13:q:518:CLA:H41	13:q:518:CLA:H61	1.73	0.40
16:q:522:BCR:H15C	16:q:522:BCR:H351	1.80	0.40
16:r:524:BCR:H11C	16:r:524:BCR:H341	1.97	0.40
12:s:182:LEU:O	12:s:209:TYR:OH	2.37	0.40
12:t:119:ALA:O	12:t:126:LYS:NZ	2.41	0.40
12:v:47:LEU:HD23	12:v:47:LEU:HA	1.94	0.40
12:v:207:HIS:CE1	16:v:524:BCR:H381	2.56	0.40
16:v:523:BCR:H20C	16:v:523:BCR:H361	1.93	0.40
16:v:524:BCR:H371	16:v:524:BCR:H24C	1.87	0.40
1:A:345:THR:HG21	17:A:5003:LHG:HC11	2.04	0.40
13:A:1022:CLA:H122	16:B:4017:BCR:H12C	2.02	0.40
2:B:455:ILE:HD13	6:F:69:LEU:HB2	2.03	0.40
13:1:505:CLA:HBA1	12:v:105:ALA:O	2.21	0.40
16:2:522:BCR:H24C	16:2:522:BCR:H371	1.86	0.40
12:6:91:VAL:HG22	16:6:523:BCR:HC22	2.02	0.40
16:G:4001:BCR:H11C	16:G:4001:BCR:H341	1.87	0.40
2:H:721:TYR:HB2	13:H:1021:CLA:HED3	2.03	0.40
20:H:1852:SQD:C9	17:e:5002:LHG:C23	2.90	0.40
8:T:8:LEU:HA	8:T:13:ILE:HG21	2.02	0.40
13:V:1501:CLA:H102	13:V:1503:CLA:H122	2.04	0.40
1:e:441:VAL:HA	1:e:444:HIS:CE1	2.56	0.40
2:f:236:ASN:OD1	2:f:252:THR:OG1	2.39	0.40
2:f:657:TRP:CZ3	13:f:1021:CLA:HHB	2.57	0.40
13:f:1213:CLA:H141	13:f:1213:CLA:H162	1.80	0.40
13:n:1501:CLA:H112	16:n:4022:BCR:H10C	2.03	0.40
16:t:521:BCR:H15C	16:t:521:BCR:H351	1.93	0.40
1:A:572:ARG:HD3	3:C:80:ALA:HB3	2.03	0.40
13:A:1128:CLA:H91	13:A:1128:CLA:H112	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:PRO:HB3	2:B:256:THR:HG21	2.02	0.40
2:B:657:TRP:CZ3	13:B:1021:CLA:HHB	2.57	0.40
13:B:1227:CLA:HMC1	13:B:1236:CLA:HAB	2.03	0.40
16:K:4104:BCR:H15C	16:K:4104:BCR:H351	1.84	0.40
13:3:503:CLA:H62	13:3:503:CLA:H101	1.89	0.40
12:4:54:THR:HG22	12:4:56:ASP:H	1.87	0.40
13:4:517:CLA:HBA1	13:4:517:CLA:H3A	1.68	0.40
12:5:73:LEU:HD23	12:5:73:LEU:HA	1.91	0.40
13:6:517:CLA:HBB1	16:6:524:BCR:H352	2.03	0.40
1:G:215:HIS:CE1	13:G:1112:CLA:NA	2.90	0.40
16:G:4002:BCR:H361	16:G:4002:BCR:H20C	1.77	0.40
2:H:452:GLN:NE2	2:H:614:THR:OG1	2.55	0.40
2:H:455:ILE:HD13	6:R:69:LEU:HB2	2.03	0.40
13:H:1206:CLA:H3A	13:H:1206:CLA:HBA1	1.58	0.40
13:H:1234:CLA:H71	13:H:1235:CLA:H12	2.03	0.40
16:H:4010:BCR:H15C	16:H:4010:BCR:H351	1.74	0.40
5:Q:18:TRP:HB3	5:Q:21:GLU:HB2	2.03	0.40
13:Z:511:CLA:H93	13:Z:511:CLA:H61	1.91	0.40
12:b:54:THR:HG22	12:b:56:ASP:H	1.87	0.40
12:b:273:GLY:O	12:b:300:ARG:NH2	2.45	0.40
16:c:522:BCR:H24C	16:c:522:BCR:H371	1.84	0.40
12:d:109:PHE:HB2	13:q:505:CLA:HAA2	2.02	0.40
1:e:202:ALA:HB2	1:e:320:GLY:HA3	2.04	0.40
1:e:278:LEU:HD23	1:e:278:LEU:HA	1.92	0.40
13:e:1137:CLA:H122	16:e:4007:BCR:H393	2.04	0.40
14:e:2001:PQN:H162	16:f:4014:BCR:H382	2.03	0.40
13:f:1202:CLA:H202	13:f:1202:CLA:H161	1.88	0.40
13:f:1220:CLA:H51	13:f:1221:CLA:H142	2.04	0.40
16:n:4219:BCR:H351	16:n:4219:BCR:H15C	1.78	0.40
12:r:57:GLN:HB2	12:r:62:GLN:HE21	1.86	0.40
13:r:505:CLA:HBC2	16:r:524:BCR:H341	2.03	0.40
12:t:31:HIS:NE2	13:t:509:CLA:NB	2.70	0.40
16:u:523:BCR:H11C	16:u:523:BCR:H341	1.98	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	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	G	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	e	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
2	B	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	H	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	f	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	g	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	O	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	h	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	Q	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	i	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
6	F	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	R	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	j	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
7	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	S	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	k	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	39/41 (95%)	39 (100%)	0	0	100	100
8	l	39/41 (95%)	39 (100%)	0	0	100	100
9	K	76/84 (90%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	U	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	m	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
10	L	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	V	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	n	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
11	M	27/29 (93%)	27 (100%)	0	0	100	100
11	W	27/29 (93%)	27 (100%)	0	0	100	100
11	o	27/29 (93%)	27 (100%)	0	0	100	100
12	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	2	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	4	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Z	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	b	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	r	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	t	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	12786/13089 (98%)	12420 (97%)	366 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/611 (98%)	600 (100%)	0	100	100
1	G	600/611 (98%)	600 (100%)	0	100	100
1	e	600/611 (98%)	600 (100%)	0	100	100
2	B	583/584 (100%)	582 (100%)	1 (0%)	87	96
2	H	583/584 (100%)	582 (100%)	1 (0%)	87	96
2	f	583/584 (100%)	582 (100%)	1 (0%)	87	96
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	g	67/68 (98%)	67 (100%)	0	100	100
4	D	114/114 (100%)	114 (100%)	0	100	100
4	O	114/114 (100%)	114 (100%)	0	100	100
4	h	114/114 (100%)	114 (100%)	0	100	100
5	E	56/59 (95%)	56 (100%)	0	100	100
5	Q	56/59 (95%)	56 (100%)	0	100	100
5	i	56/59 (95%)	56 (100%)	0	100	100
6	F	105/121 (87%)	105 (100%)	0	100	100
6	R	105/121 (87%)	105 (100%)	0	100	100
6	j	105/121 (87%)	105 (100%)	0	100	100
7	I	30/30 (100%)	30 (100%)	0	100	100
7	S	30/30 (100%)	30 (100%)	0	100	100
7	k	30/30 (100%)	30 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
8	T	35/35 (100%)	35 (100%)	0	100	100
8	l	35/35 (100%)	35 (100%)	0	100	100
9	K	56/61 (92%)	56 (100%)	0	100	100
9	U	56/61 (92%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	m	56/61 (92%)	56 (100%)	0	100	100
10	L	127/128 (99%)	127 (100%)	0	100	100
10	V	127/128 (99%)	127 (100%)	0	100	100
10	n	127/128 (99%)	127 (100%)	0	100	100
11	M	24/24 (100%)	24 (100%)	0	100	100
11	W	24/24 (100%)	24 (100%)	0	100	100
11	o	24/24 (100%)	24 (100%)	0	100	100
12	1	257/259 (99%)	257 (100%)	0	100	100
12	2	257/259 (99%)	257 (100%)	0	100	100
12	3	257/259 (99%)	257 (100%)	0	100	100
12	4	257/259 (99%)	257 (100%)	0	100	100
12	5	257/259 (99%)	257 (100%)	0	100	100
12	6	257/259 (99%)	257 (100%)	0	100	100
12	Y	257/259 (99%)	257 (100%)	0	100	100
12	Z	257/259 (99%)	257 (100%)	0	100	100
12	a	257/259 (99%)	257 (100%)	0	100	100
12	b	257/259 (99%)	257 (100%)	0	100	100
12	c	257/259 (99%)	257 (100%)	0	100	100
12	d	257/259 (99%)	257 (100%)	0	100	100
12	q	257/259 (99%)	257 (100%)	0	100	100
12	r	257/259 (99%)	257 (100%)	0	100	100
12	s	257/259 (99%)	257 (100%)	0	100	100
12	t	257/259 (99%)	257 (100%)	0	100	100
12	u	257/259 (99%)	257 (100%)	0	100	100
12	v	257/259 (99%)	257 (100%)	0	100	100
All	All	10017/10167 (98%)	10014 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	443	VAL
2	H	443	VAL
2	f	443	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	135	HIS
1	A	179	HIS
1	A	192	ASN
1	A	216	GLN
1	A	253	HIS
1	A	263	GLN
1	A	742	HIS
2	B	34	HIS
2	B	98	GLN
2	B	114	ASN
2	B	218	HIS
2	B	452	GLN
2	B	603	GLN
2	B	704	GLN
4	D	71	GLN
4	D	137	GLN
6	F	77	HIS
8	J	39	HIS
9	K	26	ASN
10	L	3	GLN
12	1	144	HIS
12	1	207	HIS
12	2	207	HIS
12	2	221	HIS
12	2	263	ASN
12	2	316	GLN
12	3	129	HIS
12	3	263	ASN
12	4	62	GLN
12	4	263	ASN
12	5	129	HIS
12	5	133	ASN
12	5	207	HIS
12	5	221	HIS
12	5	291	GLN
12	6	133	ASN
12	6	144	HIS
12	6	263	ASN
1	G	19	ASN
1	G	56	HIS

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Mol	Chain	Res	Type
1	G	135	HIS
1	G	179	HIS
1	G	192	ASN
1	G	216	GLN
1	G	253	HIS
1	G	263	GLN
1	G	742	HIS
2	H	34	HIS
2	H	98	GLN
2	H	114	ASN
2	H	218	HIS
2	H	452	GLN
2	H	603	GLN
2	H	704	GLN
4	O	71	GLN
6	R	77	HIS
8	T	39	HIS
9	U	26	ASN
12	Y	144	HIS
12	Y	207	HIS
12	Z	129	HIS
12	Z	221	HIS
12	Z	263	ASN
12	Z	316	GLN
12	a	129	HIS
12	a	263	ASN
12	b	62	GLN
12	b	263	ASN
12	c	133	ASN
12	c	207	HIS
12	c	291	GLN
12	d	133	ASN
12	d	263	ASN
1	e	19	ASN
1	e	115	GLN
1	e	135	HIS
1	e	179	HIS
1	e	192	ASN
1	e	216	GLN
1	e	253	HIS
1	e	263	GLN
1	e	294	ASN

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Mol	Chain	Res	Type
1	e	742	HIS
2	f	34	HIS
2	f	98	GLN
2	f	114	ASN
2	f	218	HIS
2	f	452	GLN
2	f	603	GLN
2	f	704	GLN
4	h	71	GLN
4	h	137	GLN
6	j	77	HIS
8	l	39	HIS
9	m	26	ASN
9	m	80	ASN
10	n	3	GLN
12	q	144	HIS
12	q	207	HIS
12	r	221	HIS
12	r	263	ASN
12	r	316	GLN
12	s	129	HIS
12	s	221	HIS
12	s	263	ASN
12	t	62	GLN
12	t	263	ASN
12	u	129	HIS
12	u	133	ASN
12	u	207	HIS
12	u	221	HIS
12	u	291	GLN
12	v	133	ASN
12	v	144	HIS
12	v	263	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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

846 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	2	505	12	69,73,73	1.23	7 (10%)	83,113,113	1.28	6 (7%)
13	CLA	3	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	5	503	12	59,63,73	1.36	8 (13%)	71,101,113	1.40	6 (8%)
16	BCR	c	524	-	41,41,41	0.69	0	56,56,56	1.67	15 (26%)
13	CLA	6	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.38	6 (8%)
13	CLA	A	1123	21	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
13	CLA	A	1115	1	64,68,73	1.26	10 (15%)	77,107,113	1.47	9 (11%)
13	CLA	V	1501	10	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	5	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	6 (8%)
13	CLA	v	504	-	49,53,73	1.48	7 (14%)	59,89,113	1.51	8 (13%)
13	CLA	G	1108	1	58,62,73	1.36	10 (17%)	69,99,113	1.35	6 (8%)
13	CLA	f	1207	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	4 (4%)
13	CLA	1	506	12	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
13	CLA	e	1126	1	69,73,73	1.20	10 (14%)	83,113,113	1.41	8 (9%)
13	CLA	a	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.35	9 (10%)
13	CLA	4	511	12	49,53,73	1.50	9 (18%)	59,89,113	1.53	7 (11%)
13	CLA	e	1138	1	69,73,73	1.21	10 (14%)	83,113,113	1.35	7 (8%)
20	SQD	2	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	c	508	12	49,53,73	1.48	9 (18%)	59,89,113	1.55	5 (8%)
20	SQD	u	822	-	28,29,54	1.26	5 (17%)	37,40,65	1.92	13 (35%)
19	LMG	B	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	c	502	12	54,58,73	1.42	10 (18%)	65,95,113	1.46	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	3	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
13	CLA	A	1110	1	55,59,73	1.40	10 (18%)	66,96,113	1.48	6 (9%)
13	CLA	d	511	12	49,53,73	1.49	9 (18%)	59,89,113	1.50	4 (6%)
18	LMU	T	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	1	513	12	59,63,73	1.35	10 (16%)	71,101,113	1.36	5 (7%)
15	SF4	g	3003	3	0,12,12	-	-	-		
13	CLA	B	1225	2	69,73,73	1.23	11 (15%)	83,113,113	1.30	8 (9%)
13	CLA	6	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.51	7 (11%)
13	CLA	f	1227	2	69,73,73	1.23	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	G	1106	1	69,73,73	1.22	11 (15%)	83,113,113	1.44	11 (13%)
13	CLA	G	1139	21	69,73,73	1.24	10 (14%)	83,113,113	1.27	8 (9%)
13	CLA	a	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.39	6 (7%)
20	SQD	6	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
17	LHG	G	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
16	BCR	F	4016	-	41,41,41	0.74	0	56,56,56	1.78	13 (23%)
16	BCR	d	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
16	BCR	H	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
16	BCR	v	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
16	BCR	B	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	H	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	9 (11%)
13	CLA	q	519	12	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
13	CLA	B	1211	2	60,64,73	1.32	8 (13%)	72,102,113	1.59	5 (6%)
16	BCR	e	4002	-	41,41,41	0.81	0	56,56,56	1.85	14 (25%)
13	CLA	B	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.70	15 (18%)
13	CLA	1	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	s	503	12	69,73,73	1.27	9 (13%)	83,113,113	1.32	7 (8%)
18	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	H	1238	21	69,73,73	1.23	9 (13%)	83,113,113	1.42	11 (13%)
20	SQD	L	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
20	SQD	r	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
20	SQD	f	1852	-	44,45,54	1.01	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	c	505	12	65,69,73	1.28	8 (12%)	78,108,113	1.27	4 (5%)
15	SF4	e	3001	2,1	0,12,12	-	-	-		
13	CLA	B	1205	2	69,73,73	1.24	10 (14%)	83,113,113	1.43	8 (9%)
13	CLA	3	513	12	69,73,73	1.24	9 (13%)	83,113,113	1.33	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	t	513	12	49,53,73	1.50	10 (20%)	59,89,113	1.47	4 (6%)
15	SF4	N	3003	3	0,12,12	-	-	-		
13	CLA	A	1109	1	69,73,73	1.23	9 (13%)	83,113,113	1.41	5 (6%)
16	BCR	u	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
13	CLA	e	1022	21	69,73,73	1.27	10 (14%)	83,113,113	1.32	9 (10%)
16	BCR	c	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
13	CLA	e	1135	1	56,60,73	1.37	9 (16%)	67,97,113	1.55	11 (16%)
13	CLA	l	1302	8	62,66,73	1.29	9 (14%)	74,104,113	1.43	6 (8%)
13	CLA	f	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	9 (11%)
13	CLA	d	501	12	64,68,73	1.29	8 (12%)	77,107,113	1.40	5 (6%)
13	CLA	L	1501	10	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	R	1302	6	49,53,73	1.46	8 (16%)	59,89,113	1.47	4 (6%)
13	CLA	d	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.48	4 (6%)
13	CLA	e	1013	-	69,73,73	1.27	11 (15%)	83,113,113	1.56	10 (12%)
16	BCR	V	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
17	LHG	A	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.34	6 (13%)
13	CLA	B	1220	2	59,63,73	1.31	9 (15%)	71,101,113	1.54	9 (12%)
13	CLA	q	513	12	59,63,73	1.34	10 (16%)	71,101,113	1.37	5 (7%)
13	CLA	s	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
13	CLA	A	1135	1	56,60,73	1.37	9 (16%)	67,97,113	1.55	11 (16%)
13	CLA	L	1502	10	69,73,73	1.23	10 (14%)	83,113,113	1.39	6 (7%)
13	CLA	6	509	12	49,53,73	1.49	8 (16%)	59,89,113	1.46	5 (8%)
13	CLA	f	1213	2	69,73,73	1.22	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	H	1217	2	61,65,73	1.31	10 (16%)	73,103,113	1.43	9 (12%)
13	CLA	B	1232	21	54,58,73	1.39	11 (20%)	65,95,113	1.60	7 (10%)
13	CLA	G	1135	1	56,60,73	1.36	9 (16%)	67,97,113	1.55	11 (16%)
13	CLA	u	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.51	5 (8%)
13	CLA	2	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.49	4 (6%)
13	CLA	q	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.54	9 (12%)
16	BCR	u	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
13	CLA	t	501	12	64,68,73	1.31	7 (10%)	77,107,113	1.34	4 (5%)
13	CLA	c	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
13	CLA	q	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.37	7 (9%)
13	CLA	u	517	-	49,53,73	1.49	10 (20%)	59,89,113	1.40	4 (6%)
13	CLA	H	1227	2	69,73,73	1.22	10 (14%)	83,113,113	1.40	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	H	1239	2	69,73,73	1.25	9 (13%)	83,113,113	1.54	12 (14%)
19	LMG	T	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
13	CLA	A	1116	1	64,68,73	1.30	9 (14%)	77,107,113	1.35	8 (10%)
13	CLA	H	1226	2	69,73,73	1.34	11 (15%)	83,113,113	1.67	15 (18%)
13	CLA	u	519	12	50,54,73	1.46	9 (18%)	60,90,113	1.46	5 (8%)
13	CLA	A	1106	1	69,73,73	1.22	11 (15%)	83,113,113	1.44	11 (13%)
13	CLA	s	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	A	1105	1	59,63,73	1.30	10 (16%)	71,101,113	1.51	10 (14%)
13	CLA	t	510	12	54,58,73	1.41	8 (14%)	65,95,113	1.49	5 (7%)
13	CLA	Z	518	12	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
13	CLA	u	508	12	49,53,73	1.49	9 (18%)	59,89,113	1.55	6 (10%)
13	CLA	c	517	-	49,53,73	1.50	8 (16%)	59,89,113	1.40	4 (6%)
14	PQN	H	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.17	4 (9%)
13	CLA	B	1230	2	64,68,73	1.30	9 (14%)	77,107,113	1.44	8 (10%)
13	CLA	c	509	12	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
13	CLA	f	1222	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	10 (12%)
13	CLA	f	1235	2	69,73,73	1.23	9 (13%)	83,113,113	1.43	8 (9%)
13	CLA	4	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.39	5 (7%)
16	BCR	v	524	-	41,41,41	0.76	0	56,56,56	1.87	13 (23%)
13	CLA	A	1124	21	60,64,73	1.36	9 (15%)	72,102,113	1.48	13 (18%)
13	CLA	H	1223	2	69,73,73	1.25	9 (13%)	83,113,113	1.40	6 (7%)
16	BCR	5	523	-	41,41,41	0.75	0	56,56,56	1.78	16 (28%)
17	LHG	V	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	G	1111	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	r	519	12	59,63,73	1.35	9 (15%)	71,101,113	1.39	8 (11%)
16	BCR	L	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
13	CLA	6	508	12	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
16	BCR	G	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	14 (25%)
13	CLA	u	503	12	59,63,73	1.37	8 (13%)	71,101,113	1.40	6 (8%)
13	CLA	B	1231	21	69,73,73	1.20	9 (13%)	83,113,113	1.41	8 (9%)
13	CLA	c	503	12	59,63,73	1.37	8 (13%)	71,101,113	1.40	6 (8%)
13	CLA	Z	507	-	69,73,73	1.23	8 (11%)	83,113,113	1.38	6 (7%)
13	CLA	F	1301	21	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
13	CLA	s	507	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	H	1230	2	64,68,73	1.30	9 (14%)	77,107,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	u	513	12	49,53,73	1.49	10 (20%)	59,89,113	1.43	6 (10%)
16	BCR	e	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	G	1133	1	69,73,73	1.20	8 (11%)	83,113,113	1.39	6 (7%)
13	CLA	2	512	12	57,61,73	1.36	8 (14%)	68,98,113	1.37	4 (5%)
16	BCR	A	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
17	LHG	S	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	u	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	7 (11%)
13	CLA	K	1103	9	54,58,73	1.40	9 (16%)	65,95,113	1.56	12 (18%)
13	CLA	A	1128	1	69,73,73	1.32	10 (14%)	83,113,113	1.53	9 (10%)
13	CLA	a	518	12	59,63,73	1.36	10 (16%)	71,101,113	1.37	5 (7%)
16	BCR	H	4017	-	41,41,41	0.79	0	56,56,56	1.58	11 (19%)
13	CLA	s	519	12	59,63,73	1.34	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	c	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	7 (9%)
13	CLA	G	1138	1	69,73,73	1.22	10 (14%)	83,113,113	1.35	7 (8%)
16	BCR	K	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
16	BCR	G	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
20	SQD	Y	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	A	1122	1	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
16	BCR	s	524	-	41,41,41	0.73	0	56,56,56	1.82	17 (30%)
13	CLA	A	1139	21	69,73,73	1.24	10 (14%)	83,113,113	1.27	8 (9%)
13	CLA	q	501	12	69,73,73	1.26	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	1	512	12	56,60,73	1.39	9 (16%)	67,97,113	1.44	5 (7%)
13	CLA	H	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.53	14 (16%)
13	CLA	6	511	12	49,53,73	1.49	9 (18%)	59,89,113	1.51	4 (6%)
16	BCR	l	4015	-	41,41,41	0.79	0	56,56,56	1.82	14 (25%)
13	CLA	2	516	12	49,53,73	1.48	8 (16%)	59,89,113	1.51	5 (8%)
13	CLA	c	506	12	49,53,73	1.49	8 (16%)	59,89,113	1.50	5 (8%)
16	BCR	a	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
13	CLA	R	1301	21	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
20	SQD	H	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	f	1236	2	59,63,73	1.35	8 (13%)	71,101,113	1.30	6 (8%)
13	CLA	6	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.30	4 (4%)
13	CLA	e	1124	21	60,64,73	1.36	9 (15%)	72,102,113	1.47	13 (18%)
13	CLA	4	503	12	59,63,73	1.38	7 (11%)	71,101,113	1.41	9 (12%)
13	CLA	A	1140	1	69,73,73	1.27	10 (14%)	83,113,113	1.39	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	H	1212	2	59,63,73	1.33	10 (16%)	71,101,113	1.47	7 (9%)
13	CLA	s	501	12	69,73,73	1.25	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	5	516	12	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
13	CLA	B	1209	2	56,60,73	1.38	9 (16%)	67,97,113	1.56	7 (10%)
18	LMU	Z	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
13	CLA	f	1217	2	61,65,73	1.30	10 (16%)	73,103,113	1.43	8 (10%)
13	CLA	u	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.37	5 (6%)
13	CLA	A	1133	1	69,73,73	1.20	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	e	1121	1	59,63,73	1.35	9 (15%)	71,101,113	1.47	10 (14%)
13	CLA	s	506	12	54,58,73	1.42	9 (16%)	65,95,113	1.47	6 (9%)
13	CLA	B	1239	2	69,73,73	1.25	8 (11%)	83,113,113	1.53	11 (13%)
13	CLA	e	1131	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
17	LHG	A	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	q	516	12	49,53,73	1.48	8 (16%)	59,89,113	1.65	8 (13%)
17	LHG	V	5220	-	40,40,48	0.64	0	43,46,54	1.23	4 (9%)
13	CLA	s	513	12	69,73,73	1.25	9 (13%)	83,113,113	1.34	5 (6%)
13	CLA	A	1138	1	69,73,73	1.21	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	u	505	12	65,69,73	1.28	7 (10%)	78,108,113	1.27	4 (5%)
13	CLA	H	1207	2	69,73,73	1.25	10 (14%)	83,113,113	1.31	4 (4%)
13	CLA	l	1303	8	69,73,73	1.23	9 (13%)	83,113,113	1.39	9 (10%)
13	CLA	A	1125	1	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)
13	CLA	e	1132	1	69,73,73	1.23	11 (15%)	83,113,113	1.38	9 (10%)
13	CLA	f	1214	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	6 (7%)
13	CLA	f	1216	21	64,68,73	1.31	10 (15%)	77,107,113	1.39	5 (6%)
13	CLA	H	1202	2	69,73,73	1.23	10 (14%)	83,113,113	1.49	9 (10%)
13	CLA	2	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.43	7 (9%)
16	BCR	V	4219	-	41,41,41	0.77	0	56,56,56	1.80	12 (21%)
13	CLA	F	1302	6	49,53,73	1.46	8 (16%)	59,89,113	1.47	4 (6%)
16	BCR	Y	522	-	41,41,41	0.73	0	56,56,56	1.91	20 (35%)
16	BCR	t	522	-	41,41,41	0.73	0	56,56,56	1.85	18 (32%)
20	SQD	Z	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
16	BCR	f	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	2	507	-	69,73,73	1.22	8 (11%)	83,113,113	1.38	6 (7%)
13	CLA	e	1801	17	49,53,73	1.51	10 (20%)	59,89,113	1.61	8 (13%)
16	BCR	l	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	PQN	f	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	u	516	12	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
13	CLA	A	1107	1	69,73,73	1.25	11 (15%)	83,113,113	1.35	10 (12%)
13	CLA	s	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.50	6 (9%)
13	CLA	Z	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
17	LHG	V	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	H	1023	-	69,73,73	1.24	11 (15%)	83,113,113	1.70	16 (19%)
13	CLA	e	1130	1	69,73,73	1.24	10 (14%)	83,113,113	1.40	11 (13%)
18	LMU	2	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
20	SQD	1	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	5	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.34	5 (7%)
13	CLA	b	510	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	2	506	12	59,63,73	1.36	10 (16%)	71,101,113	1.40	6 (8%)
13	CLA	2	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.39	8 (11%)
16	BCR	u	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
16	BCR	M	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
13	CLA	H	1231	21	69,73,73	1.20	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	b	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.49	4 (6%)
13	CLA	4	501	12	64,68,73	1.31	8 (12%)	77,107,113	1.34	4 (5%)
17	LHG	n	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
16	BCR	W	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
19	LMG	J	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
13	CLA	1	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
13	CLA	Z	510	12	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
13	CLA	b	517	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	6 (10%)
13	CLA	a	517	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	4 (6%)
13	CLA	e	1136	1	64,68,73	1.29	8 (12%)	77,107,113	1.47	10 (12%)
13	CLA	r	518	12	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
13	CLA	v	511	12	49,53,73	1.49	9 (18%)	59,89,113	1.51	4 (6%)
13	CLA	a	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.26	4 (4%)
16	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.67	12 (21%)
13	CLA	V	1502	10	69,73,73	1.23	10 (14%)	83,113,113	1.39	6 (7%)
13	CLA	v	507	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
13	CLA	Z	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.43	7 (9%)
16	BCR	H	4006	-	41,41,41	0.73	0	56,56,56	1.98	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LHG	e	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	A	1129	1	55,59,73	1.38	9 (16%)	66,96,113	1.53	10 (15%)
18	LMU	G	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	4	510	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	Y	506	12	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
13	CLA	A	1112	1	54,58,73	1.37	9 (16%)	65,95,113	1.58	10 (15%)
16	BCR	b	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
17	LHG	e	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
16	BCR	b	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	q	503	12	68,72,73	1.27	8 (11%)	81,111,113	1.34	6 (7%)
16	BCR	1	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	G	1134	1	60,64,73	1.31	8 (13%)	72,102,113	1.44	6 (8%)
20	SQD	a	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	u	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	7 (9%)
13	CLA	5	501	12	69,73,73	1.24	8 (11%)	83,113,113	1.37	5 (6%)
13	CLA	H	1224	2	64,68,73	1.27	9 (14%)	77,107,113	1.42	8 (10%)
13	CLA	H	1240	17	69,73,73	1.26	9 (13%)	83,113,113	1.34	9 (10%)
13	CLA	f	1209	2	56,60,73	1.38	9 (16%)	67,97,113	1.56	7 (10%)
20	SQD	t	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
13	CLA	c	518	12	59,63,73	1.34	9 (15%)	71,101,113	1.34	5 (7%)
16	BCR	S	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
17	LHG	n	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
16	BCR	f	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	3	511	12	54,58,73	1.43	9 (16%)	65,95,113	1.49	5 (7%)
18	LMU	e	1848	-	36,36,36	1.14	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	b	508	12	49,53,73	1.50	9 (18%)	59,89,113	1.57	9 (15%)
16	BCR	4	523	-	41,41,41	0.69	0	56,56,56	1.65	12 (21%)
17	LHG	G	5003	13	40,40,48	0.74	0	43,46,54	1.34	6 (13%)
13	CLA	f	1204	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	t	512	12	49,53,73	1.49	8 (16%)	59,89,113	1.49	4 (6%)
17	LHG	B	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	f	1208	2	69,73,73	1.21	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	G	1105	1	59,63,73	1.30	10 (16%)	71,101,113	1.52	10 (14%)
13	CLA	B	1212	2	59,63,73	1.32	9 (15%)	71,101,113	1.47	6 (8%)
13	CLA	f	1219	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	n	4022	-	41,41,41	0.75	0	56,56,56	1.90	15 (26%)
13	CLA	r	504	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	7 (10%)
16	BCR	a	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
13	CLA	G	1011	1	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
14	PQN	G	2001	-	34,34,34	2.87	11 (32%)	42,45,45	2.12	7 (16%)
20	SQD	q	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
16	BCR	G	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	a	512	12	49,53,73	1.48	9 (18%)	59,89,113	1.50	4 (6%)
13	CLA	f	1240	17	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
13	CLA	b	518	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	5 (7%)
13	CLA	B	1012	21	69,73,73	1.27	11 (15%)	83,113,113	1.38	9 (10%)
13	CLA	H	1205	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
17	LHG	G	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	e	1137	1	69,73,73	1.24	8 (11%)	83,113,113	1.42	7 (8%)
13	CLA	2	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	A	1118	1	64,68,73	1.28	9 (14%)	77,107,113	1.41	8 (10%)
16	BCR	4	524	-	41,41,41	0.67	0	56,56,56	1.84	15 (26%)
13	CLA	A	1117	1	69,73,73	1.22	11 (15%)	83,113,113	1.56	12 (14%)
13	CLA	4	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.50	4 (6%)
13	CLA	T	1303	8	69,73,73	1.24	9 (13%)	83,113,113	1.39	8 (9%)
13	CLA	Y	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.44	9 (12%)
13	CLA	B	1202	2	69,73,73	1.23	10 (14%)	83,113,113	1.49	9 (10%)
16	BCR	6	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
13	CLA	B	1226	2	69,73,73	1.34	11 (15%)	83,113,113	1.67	16 (19%)
13	CLA	A	1136	1	64,68,73	1.29	8 (12%)	77,107,113	1.47	10 (12%)
13	CLA	a	513	12	69,73,73	1.25	8 (11%)	83,113,113	1.33	5 (6%)
13	CLA	v	509	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
13	CLA	q	504	-	49,53,73	1.49	10 (20%)	59,89,113	1.49	6 (10%)
16	BCR	1	521	-	41,41,41	0.66	0	56,56,56	1.81	11 (19%)
13	CLA	b	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.27	4 (4%)
16	BCR	d	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
17	LHG	A	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	A	1121	1	59,63,73	1.34	9 (15%)	71,101,113	1.48	10 (14%)
16	BCR	T	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	e	1125	1	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LHG	L	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
18	LMU	J	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	m	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.46	7 (9%)
16	BCR	q	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	u	512	12	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
13	CLA	u	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	5 (8%)
13	CLA	A	1111	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	T	1302	8	62,66,73	1.30	9 (14%)	74,104,113	1.41	6 (8%)
13	CLA	Y	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	7 (8%)
13	CLA	d	509	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
13	CLA	1	508	12	59,63,73	1.36	9 (15%)	71,101,113	1.54	9 (12%)
13	CLA	4	508	12	49,53,73	1.51	9 (18%)	59,89,113	1.58	9 (15%)
16	BCR	e	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.02	17 (30%)
13	CLA	G	1126	1	69,73,73	1.20	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	U	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.45	8 (11%)
17	LHG	e	5008	-	34,34,48	0.77	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	Y	518	12	64,68,73	1.28	9 (14%)	77,107,113	1.42	8 (10%)
13	CLA	A	1102	1	69,73,73	1.21	9 (13%)	83,113,113	1.35	7 (8%)
16	BCR	T	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
16	BCR	U	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	6	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.47	4 (6%)
13	CLA	B	1228	2	59,63,73	1.30	9 (15%)	71,101,113	1.49	9 (12%)
16	BCR	G	4007	-	41,41,41	0.75	0	56,56,56	2.10	18 (32%)
16	BCR	a	521	-	41,41,41	0.68	0	56,56,56	1.75	10 (17%)
16	BCR	f	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	e	1104	1	69,73,73	1.23	10 (14%)	83,113,113	1.38	10 (12%)
16	BCR	n	4020	-	41,41,41	0.82	0	56,56,56	1.95	15 (26%)
19	LMG	H	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	G	1132	1	69,73,73	1.23	10 (14%)	83,113,113	1.38	9 (10%)
13	CLA	3	506	12	54,58,73	1.43	9 (16%)	65,95,113	1.47	6 (9%)
13	CLA	e	1103	1	69,73,73	1.24	8 (11%)	83,113,113	1.49	8 (9%)
13	CLA	f	1221	21	69,73,73	1.29	11 (15%)	83,113,113	1.49	13 (15%)
16	BCR	t	521	-	41,41,41	0.65	0	56,56,56	1.78	11 (19%)
13	CLA	t	517	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	6 (10%)
13	CLA	1	503	12	68,72,73	1.27	8 (11%)	81,111,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	t	524	-	41,41,41	0.68	0	56,56,56	1.84	15 (26%)
13	CLA	d	503	12	56,60,73	1.39	9 (16%)	67,97,113	1.44	7 (10%)
17	LHG	L	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	f	1239	2	69,73,73	1.25	8 (11%)	83,113,113	1.52	11 (13%)
13	CLA	6	513	12	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
13	CLA	L	1503	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	6 (7%)
13	CLA	B	1217	2	61,65,73	1.30	10 (16%)	73,103,113	1.42	8 (10%)
16	BCR	e	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
13	CLA	A	1127	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	9 (10%)
13	CLA	e	1113	1	49,53,73	1.42	9 (18%)	59,89,113	1.56	6 (10%)
13	CLA	t	508	12	49,53,73	1.51	9 (18%)	59,89,113	1.57	9 (15%)
17	LHG	G	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
16	BCR	V	4019	-	41,41,41	0.74	0	56,56,56	1.92	14 (25%)
13	CLA	3	502	12	54,58,73	1.40	8 (14%)	65,95,113	1.51	6 (9%)
16	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	1	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
16	BCR	Z	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	q	506	12	49,53,73	1.48	8 (16%)	59,89,113	1.47	5 (8%)
13	CLA	m	1103	9	54,58,73	1.40	9 (16%)	65,95,113	1.56	11 (16%)
19	LMG	f	5002	-	54,54,55	0.80	3 (5%)	62,62,63	1.43	10 (16%)
13	CLA	q	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.43	4 (6%)
17	LHG	A	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	H	1221	21	69,73,73	1.29	11 (15%)	83,113,113	1.50	13 (15%)
13	CLA	Z	516	12	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
15	SF4	G	3001	2,1	0,12,12	-	-	-		
13	CLA	B	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	c	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
13	CLA	s	516	12	49,53,73	1.50	8 (16%)	59,89,113	1.69	10 (16%)
13	CLA	H	1225	2	69,73,73	1.23	11 (15%)	83,113,113	1.30	8 (9%)
13	CLA	d	513	12	49,53,73	1.51	6 (12%)	59,89,113	1.41	4 (6%)
14	PQN	B	2002	-	34,34,34	2.88	11 (32%)	42,45,45	2.18	4 (9%)
16	BCR	L	4219	-	41,41,41	0.78	0	56,56,56	1.80	12 (21%)
16	BCR	G	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	16 (28%)
16	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.90	19 (33%)
13	CLA	e	1123	21	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SF4	C	3002	3	0,12,12	-	-	-		
13	CLA	H	1232	21	54,58,73	1.39	11 (20%)	65,95,113	1.60	7 (10%)
18	LMU	B	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
20	SQD	4	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
13	CLA	H	1213	2	69,73,73	1.22	11 (15%)	83,113,113	1.42	11 (13%)
13	CLA	G	1131	1	69,73,73	1.22	9 (13%)	83,113,113	1.35	7 (8%)
13	CLA	v	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)
13	CLA	6	501	12	64,68,73	1.29	8 (12%)	77,107,113	1.40	5 (6%)
13	CLA	A	1130	1	69,73,73	1.24	10 (14%)	83,113,113	1.41	11 (13%)
13	CLA	r	510	12	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	5	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
13	CLA	G	1119	21	69,73,73	1.27	10 (14%)	83,113,113	1.40	10 (12%)
13	CLA	G	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.56	10 (12%)
13	CLA	f	1230	2	64,68,73	1.30	9 (14%)	77,107,113	1.44	8 (10%)
20	SQD	s	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	B	1206	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	6 (7%)
13	CLA	e	1119	21	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
13	CLA	t	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.27	4 (4%)
16	BCR	e	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
13	CLA	A	1137	1	69,73,73	1.24	8 (11%)	83,113,113	1.42	7 (8%)
13	CLA	6	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	a	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	c	519	12	50,54,73	1.46	9 (18%)	60,90,113	1.46	5 (8%)
13	CLA	6	519	12	50,54,73	1.46	8 (16%)	60,90,113	1.45	4 (6%)
13	CLA	U	1105	9	49,53,73	1.50	9 (18%)	59,89,113	1.69	9 (15%)
13	CLA	4	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
14	PQN	e	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
13	CLA	e	1128	1	69,73,73	1.32	10 (14%)	83,113,113	1.53	9 (10%)
16	BCR	H	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
20	SQD	n	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
18	LMU	1	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	4	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
13	CLA	a	508	12	59,63,73	1.38	9 (15%)	71,101,113	1.45	9 (12%)
13	CLA	a	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.69	10 (16%)
13	CLA	e	1120	1	57,61,73	1.35	11 (19%)	68,98,113	1.52	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	Z	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
13	CLA	Z	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.44	9 (12%)
16	BCR	t	523	-	41,41,41	0.69	0	56,56,56	1.65	13 (23%)
16	BCR	r	522	-	41,41,41	0.70	0	56,56,56	1.75	17 (30%)
18	LMU	H	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.10	3 (6%)
13	CLA	d	518	12	59,63,73	1.36	9 (15%)	71,101,113	1.38	6 (8%)
13	CLA	A	1011	1	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
13	CLA	Z	502	12	64,68,73	1.30	8 (12%)	77,107,113	1.39	8 (10%)
13	CLA	f	1215	2	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
13	CLA	t	516	12	49,53,73	1.50	8 (16%)	59,89,113	1.44	5 (8%)
13	CLA	f	1220	2	59,63,73	1.31	9 (15%)	71,101,113	1.54	9 (12%)
13	CLA	2	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
13	CLA	J	1302	8	62,66,73	1.29	9 (14%)	74,104,113	1.41	6 (8%)
13	CLA	3	518	12	59,63,73	1.36	10 (16%)	71,101,113	1.38	5 (7%)
13	CLA	b	509	12	69,73,73	1.25	7 (10%)	83,113,113	1.38	6 (7%)
17	LHG	A	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
20	SQD	b	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.85	9 (26%)
16	BCR	6	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
16	BCR	k	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
20	SQD	v	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	B	1238	21	69,73,73	1.23	10 (14%)	83,113,113	1.42	11 (13%)
16	BCR	1	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
13	CLA	A	1108	1	58,62,73	1.36	10 (17%)	69,99,113	1.36	6 (8%)
13	CLA	H	1210	2	69,73,73	1.25	9 (13%)	83,113,113	1.41	11 (13%)
16	BCR	d	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
13	CLA	3	507	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	7 (8%)
13	CLA	H	1220	2	59,63,73	1.31	9 (15%)	71,101,113	1.54	9 (12%)
16	BCR	u	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
16	BCR	s	522	-	41,41,41	0.68	0	56,56,56	1.91	15 (26%)
13	CLA	e	1118	1	64,68,73	1.28	9 (14%)	77,107,113	1.41	8 (10%)
13	CLA	5	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
13	CLA	Y	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
13	CLA	f	1012	21	69,73,73	1.26	11 (15%)	83,113,113	1.38	9 (10%)
18	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
13	CLA	H	1021	2	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	a	507	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	7 (8%)
13	CLA	B	1221	21	69,73,73	1.28	11 (15%)	83,113,113	1.50	13 (15%)
13	CLA	5	517	-	49,53,73	1.50	9 (18%)	59,89,113	1.40	4 (6%)
13	CLA	Z	505	12	69,73,73	1.23	7 (10%)	83,113,113	1.28	6 (7%)
16	BCR	6	524	-	41,41,41	0.75	0	56,56,56	1.86	13 (23%)
18	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	e	1102	1	69,73,73	1.21	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	a	502	12	54,58,73	1.40	8 (14%)	65,95,113	1.51	6 (9%)
13	CLA	b	512	12	49,53,73	1.48	8 (16%)	59,89,113	1.50	4 (6%)
17	LHG	A	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	b	504	-	49,53,73	1.47	7 (14%)	59,89,113	1.47	5 (8%)
18	LMU	Y	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	e	1107	1	69,73,73	1.24	11 (15%)	83,113,113	1.36	11 (13%)
16	BCR	5	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
13	CLA	2	501	12	69,73,73	1.24	10 (14%)	83,113,113	1.37	6 (7%)
13	CLA	v	516	12	49,53,73	1.49	7 (14%)	59,89,113	1.46	6 (10%)
16	BCR	o	4021	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
16	BCR	A	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
13	CLA	B	1227	2	69,73,73	1.22	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	B	1214	2	69,73,73	1.25	10 (14%)	83,113,113	1.42	6 (7%)
13	CLA	r	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
16	BCR	4	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	H	1236	2	59,63,73	1.35	8 (13%)	71,101,113	1.30	6 (8%)
13	CLA	f	1203	2	69,73,73	1.26	12 (17%)	83,113,113	1.34	8 (9%)
13	CLA	Z	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.48	4 (6%)
16	BCR	L	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	e	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	e	1237	21	69,73,73	1.25	9 (13%)	83,113,113	1.43	10 (12%)
13	CLA	n	1501	10	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	Y	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.54	10 (14%)
13	CLA	e	1127	1	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
13	CLA	2	518	12	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
13	CLA	e	1140	1	69,73,73	1.27	10 (14%)	83,113,113	1.39	11 (13%)
13	CLA	f	1228	2	59,63,73	1.31	9 (15%)	71,101,113	1.49	9 (12%)
13	CLA	f	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	PQN	A	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
17	LHG	L	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
13	CLA	a	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
13	CLA	G	1113	1	49,53,73	1.43	9 (18%)	59,89,113	1.56	6 (10%)
13	CLA	5	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.50	5 (8%)
13	CLA	G	1124	21	60,64,73	1.36	9 (15%)	72,102,113	1.49	13 (18%)
13	CLA	e	1112	1	54,58,73	1.37	9 (16%)	65,95,113	1.58	9 (13%)
13	CLA	n	1502	10	69,73,73	1.23	10 (14%)	83,113,113	1.38	6 (7%)
16	BCR	J	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	H	1214	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	6 (7%)
13	CLA	f	1205	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	8 (9%)
16	BCR	j	4016	-	41,41,41	0.74	0	56,56,56	1.79	13 (23%)
13	CLA	H	1228	2	59,63,73	1.30	9 (15%)	71,101,113	1.50	10 (14%)
13	CLA	b	503	12	59,63,73	1.38	8 (13%)	71,101,113	1.42	9 (12%)
13	CLA	e	1109	1	69,73,73	1.23	9 (13%)	83,113,113	1.40	5 (6%)
13	CLA	Z	512	12	57,61,73	1.37	8 (14%)	68,98,113	1.38	4 (5%)
13	CLA	G	1114	21	54,58,73	1.42	9 (16%)	65,95,113	1.50	7 (10%)
15	SF4	N	3002	3	0,12,12	-	-	-		
13	CLA	G	1122	1	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
13	CLA	5	513	12	49,53,73	1.49	10 (20%)	59,89,113	1.43	4 (6%)
13	CLA	r	511	12	59,63,73	1.37	9 (15%)	71,101,113	1.43	7 (9%)
16	BCR	2	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
19	LMG	l	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.24	7 (16%)
13	CLA	f	1223	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	6 (7%)
13	CLA	q	518	12	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
13	CLA	r	507	-	69,73,73	1.23	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	u	502	12	54,58,73	1.42	10 (18%)	65,95,113	1.47	6 (9%)
17	LHG	e	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	e	1114	21	54,58,73	1.43	9 (16%)	65,95,113	1.50	7 (10%)
13	CLA	v	517	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
16	BCR	b	524	-	41,41,41	0.67	0	56,56,56	1.85	15 (26%)
17	LHG	f	1842	13	38,38,48	0.65	0	41,44,54	1.23	4 (9%)
16	BCR	A	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	17 (30%)
13	CLA	Z	506	12	59,63,73	1.36	10 (16%)	71,101,113	1.40	6 (8%)
13	CLA	v	513	12	49,53,73	1.50	6 (12%)	59,89,113	1.42	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	v	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.38	6 (8%)
16	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
20	SQD	3	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	H	1012	21	69,73,73	1.27	11 (15%)	83,113,113	1.38	9 (10%)
16	BCR	l	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	b	507	-	49,53,73	1.47	7 (14%)	59,89,113	1.53	7 (11%)
13	CLA	1	504	-	49,53,73	1.48	10 (20%)	59,89,113	1.49	6 (10%)
13	CLA	B	1215	2	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
13	CLA	4	504	-	49,53,73	1.48	7 (14%)	59,89,113	1.47	5 (8%)
13	CLA	d	504	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	8 (13%)
13	CLA	v	503	12	56,60,73	1.39	8 (14%)	67,97,113	1.45	7 (10%)
13	CLA	B	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	9 (11%)
13	CLA	A	1104	1	69,73,73	1.23	10 (14%)	83,113,113	1.39	10 (12%)
13	CLA	Y	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
16	BCR	B	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
13	CLA	G	1801	17	49,53,73	1.51	10 (20%)	59,89,113	1.60	8 (13%)
13	CLA	e	1122	1	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
16	BCR	Y	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	1	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.36	7 (8%)
13	CLA	4	509	12	69,73,73	1.25	8 (11%)	83,113,113	1.39	6 (7%)
13	CLA	b	502	12	54,58,73	1.41	9 (16%)	65,95,113	1.48	5 (7%)
13	CLA	a	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.36	8 (9%)
13	CLA	A	1119	21	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
13	CLA	A	1013	-	69,73,73	1.27	11 (15%)	83,113,113	1.56	10 (12%)
13	CLA	r	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	G	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	d	510	12	49,53,73	1.49	8 (16%)	59,89,113	1.41	5 (8%)
13	CLA	s	511	12	54,58,73	1.43	9 (16%)	65,95,113	1.49	5 (7%)
13	CLA	1	519	12	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
13	CLA	b	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	2	504	-	54,58,73	1.40	10 (18%)	65,95,113	1.46	7 (10%)
13	CLA	q	507	-	64,68,73	1.29	8 (12%)	77,107,113	1.41	8 (10%)
13	CLA	B	1222	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	10 (12%)
13	CLA	B	1208	2	69,73,73	1.21	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	K	1401	-	59,63,73	1.36	10 (16%)	71,101,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	3	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.35	9 (10%)
13	CLA	H	1215	2	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
13	CLA	B	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	14 (16%)
16	BCR	A	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	Z	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.39	8 (11%)
16	BCR	B	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	A	1120	1	57,61,73	1.34	11 (19%)	68,98,113	1.51	7 (10%)
13	CLA	v	512	12	49,53,73	1.48	9 (18%)	59,89,113	1.47	4 (6%)
20	SQD	B	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	A	1022	21	69,73,73	1.26	10 (14%)	83,113,113	1.32	9 (10%)
16	BCR	3	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
13	CLA	c	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	7 (11%)
13	CLA	G	1136	1	64,68,73	1.29	8 (12%)	77,107,113	1.47	10 (12%)
13	CLA	e	1106	1	69,73,73	1.21	11 (15%)	83,113,113	1.43	11 (13%)
13	CLA	e	1139	21	69,73,73	1.25	10 (14%)	83,113,113	1.28	8 (9%)
13	CLA	G	1120	1	57,61,73	1.34	11 (19%)	68,98,113	1.52	7 (10%)
13	CLA	G	1022	21	69,73,73	1.27	10 (14%)	83,113,113	1.32	9 (10%)
13	CLA	B	1218	2	64,68,73	1.27	9 (14%)	77,107,113	1.38	6 (7%)
13	CLA	H	1204	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	f	1206	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	6 (7%)
16	BCR	c	521	-	41,41,41	0.69	0	56,56,56	1.94	16 (28%)
13	CLA	r	505	12	69,73,73	1.23	8 (11%)	83,113,113	1.27	6 (7%)
13	CLA	Y	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	t	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
17	LHG	G	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
17	LHG	G	5006	-	44,44,48	0.62	0	47,50,54	1.25	5 (10%)
13	CLA	6	517	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
16	BCR	V	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
13	CLA	B	1207	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	4 (4%)
13	CLA	q	510	12	69,73,73	1.26	7 (10%)	83,113,113	1.31	7 (8%)
13	CLA	H	1208	2	69,73,73	1.21	9 (13%)	83,113,113	1.32	7 (8%)
13	CLA	Z	503	12	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	f	1218	2	64,68,73	1.27	9 (14%)	77,107,113	1.39	5 (6%)
13	CLA	1	518	12	64,68,73	1.28	10 (15%)	77,107,113	1.43	8 (10%)
13	CLA	e	1133	1	69,73,73	1.20	9 (13%)	83,113,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	f	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
13	CLA	1	507	-	64,68,73	1.29	8 (12%)	77,107,113	1.40	8 (10%)
13	CLA	r	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.39	7 (9%)
13	CLA	Z	513	12	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
16	BCR	B	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	Y	516	12	49,53,73	1.49	9 (18%)	59,89,113	1.65	8 (13%)
16	BCR	A	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	B	1235	2	69,73,73	1.23	10 (14%)	83,113,113	1.43	8 (9%)
13	CLA	4	507	-	49,53,73	1.48	7 (14%)	59,89,113	1.54	7 (11%)
13	CLA	6	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
16	BCR	I	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
13	CLA	A	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	B	1219	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
13	CLA	G	1109	1	69,73,73	1.23	9 (13%)	83,113,113	1.41	5 (6%)
13	CLA	t	509	12	69,73,73	1.26	8 (11%)	83,113,113	1.38	6 (7%)
16	BCR	4	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
13	CLA	b	501	12	64,68,73	1.31	8 (12%)	77,107,113	1.35	4 (5%)
13	CLA	G	1127	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	9 (10%)
16	BCR	J	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
17	LHG	G	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	v	501	12	64,68,73	1.29	9 (14%)	77,107,113	1.40	5 (6%)
17	LHG	I	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	e	1117	1	69,73,73	1.22	11 (15%)	83,113,113	1.56	12 (14%)
13	CLA	u	510	12	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
13	CLA	G	1104	1	69,73,73	1.23	10 (14%)	83,113,113	1.39	10 (12%)
16	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
20	SQD	d	822	-	25,26,54	1.30	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	1	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.44	8 (11%)
13	CLA	b	511	12	49,53,73	1.50	9 (18%)	59,89,113	1.53	6 (10%)
13	CLA	6	503	12	56,60,73	1.39	8 (14%)	67,97,113	1.44	7 (10%)
16	BCR	n	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	3	508	12	59,63,73	1.38	10 (16%)	71,101,113	1.44	9 (12%)
16	BCR	m	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
16	BCR	B	4014	-	41,41,41	0.74	0	56,56,56	1.85	13 (23%)
16	BCR	A	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	G	1129	1	55,59,73	1.38	9 (16%)	66,96,113	1.53	10 (15%)
13	CLA	t	519	12	59,63,73	1.36	10 (16%)	71,101,113	1.42	5 (7%)
13	CLA	A	1113	1	49,53,73	1.43	9 (18%)	59,89,113	1.56	6 (10%)
13	CLA	B	1216	21	64,68,73	1.31	10 (15%)	77,107,113	1.38	6 (7%)
13	CLA	G	1112	1	54,58,73	1.37	9 (16%)	65,95,113	1.58	10 (15%)
13	CLA	v	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
16	BCR	r	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	j	1301	21	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	4	517	-	49,53,73	1.50	8 (16%)	59,89,113	1.51	6 (10%)
13	CLA	v	519	12	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
13	CLA	n	1503	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	6 (7%)
16	BCR	r	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
13	CLA	B	1203	2	69,73,73	1.26	12 (17%)	83,113,113	1.34	8 (9%)
13	CLA	2	503	12	69,73,73	1.26	8 (11%)	83,113,113	1.33	7 (8%)
13	CLA	r	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.50	4 (6%)
15	SF4	A	3001	2,1	0,12,12	-	-	-		
13	CLA	v	506	12	49,53,73	1.50	10 (20%)	59,89,113	1.48	6 (10%)
13	CLA	4	513	12	49,53,73	1.50	9 (18%)	59,89,113	1.47	4 (6%)
13	CLA	H	1218	2	64,68,73	1.27	9 (14%)	77,107,113	1.38	5 (6%)
13	CLA	A	1114	21	54,58,73	1.42	10 (18%)	65,95,113	1.50	7 (10%)
13	CLA	v	508	12	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
18	LMU	q	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
17	LHG	G	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	B	1213	2	69,73,73	1.22	11 (15%)	83,113,113	1.42	11 (13%)
13	CLA	a	511	12	54,58,73	1.43	9 (16%)	65,95,113	1.49	5 (7%)
13	CLA	u	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.34	5 (7%)
13	CLA	e	1129	1	55,59,73	1.38	9 (16%)	66,96,113	1.52	10 (15%)
16	BCR	v	522	-	41,41,41	0.69	0	56,56,56	1.84	15 (26%)
13	CLA	4	502	12	54,58,73	1.41	9 (16%)	65,95,113	1.48	5 (7%)
16	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	G	1103	1	69,73,73	1.24	8 (11%)	83,113,113	1.50	8 (9%)
13	CLA	G	1117	1	69,73,73	1.22	11 (15%)	83,113,113	1.56	12 (14%)
13	CLA	H	1216	21	64,68,73	1.31	10 (15%)	77,107,113	1.38	5 (6%)
13	CLA	3	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.26	4 (4%)
13	CLA	G	1107	1	69,73,73	1.24	11 (15%)	83,113,113	1.35	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1110	1	55,59,73	1.40	10 (18%)	66,96,113	1.49	6 (9%)
13	CLA	3	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.69	10 (16%)
16	BCR	2	521	-	41,41,41	0.66	0	56,56,56	1.87	11 (19%)
13	CLA	r	512	12	57,61,73	1.37	8 (14%)	68,98,113	1.37	4 (5%)
13	CLA	G	1116	1	64,68,73	1.30	10 (15%)	77,107,113	1.35	8 (10%)
13	CLA	j	1302	6	49,53,73	1.47	8 (16%)	59,89,113	1.47	4 (6%)
13	CLA	B	1236	2	59,63,73	1.35	8 (13%)	71,101,113	1.30	6 (8%)
13	CLA	6	504	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	9 (15%)
13	CLA	U	1103	9	54,58,73	1.40	9 (16%)	65,95,113	1.57	11 (16%)
17	LHG	e	5007	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	r	503	12	69,73,73	1.26	9 (13%)	83,113,113	1.33	7 (8%)
13	CLA	t	503	12	59,63,73	1.38	7 (11%)	71,101,113	1.41	10 (14%)
16	BCR	e	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
16	BCR	J	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	r	506	12	59,63,73	1.35	9 (15%)	71,101,113	1.40	6 (8%)
13	CLA	f	1210	2	69,73,73	1.25	9 (13%)	83,113,113	1.41	11 (13%)
13	CLA	Y	512	12	56,60,73	1.39	9 (16%)	67,97,113	1.44	5 (7%)
13	CLA	s	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.34	9 (10%)
13	CLA	B	1240	17	69,73,73	1.26	9 (13%)	83,113,113	1.34	9 (10%)
13	CLA	5	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
13	CLA	Y	504	-	49,53,73	1.49	10 (20%)	59,89,113	1.49	6 (10%)
13	CLA	r	513	12	69,73,73	1.26	10 (14%)	83,113,113	1.30	5 (6%)
13	CLA	f	1211	2	60,64,73	1.32	8 (13%)	72,102,113	1.58	5 (6%)
13	CLA	u	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
15	SF4	C	3003	3	0,12,12	-	-	-		
13	CLA	Y	517	-	49,53,73	1.47	10 (20%)	59,89,113	1.44	4 (6%)
13	CLA	6	506	12	49,53,73	1.49	8 (16%)	59,89,113	1.49	6 (10%)
13	CLA	e	1116	1	64,68,73	1.30	10 (15%)	77,107,113	1.34	8 (10%)
13	CLA	A	1801	17	49,53,73	1.51	10 (20%)	59,89,113	1.60	8 (13%)
13	CLA	d	506	12	49,53,73	1.50	9 (18%)	59,89,113	1.48	6 (10%)
13	CLA	e	1111	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	8 (9%)
17	LHG	A	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
16	BCR	Z	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
16	BCR	q	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
16	BCR	Y	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	q	509	12	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
13	CLA	G	1118	1	64,68,73	1.28	9 (14%)	77,107,113	1.40	8 (10%)
13	CLA	G	1115	1	64,68,73	1.26	9 (14%)	77,107,113	1.47	9 (11%)
13	CLA	f	1232	21	54,58,73	1.39	11 (20%)	65,95,113	1.60	7 (10%)
17	LHG	f	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.22	5 (10%)
16	BCR	B	4006	-	41,41,41	0.72	0	56,56,56	1.99	19 (33%)
13	CLA	e	1108	1	58,62,73	1.36	10 (17%)	69,99,113	1.36	6 (8%)
20	SQD	5	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
13	CLA	H	1222	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	10 (12%)
13	CLA	3	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
13	CLA	G	1125	1	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)
13	CLA	c	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
13	CLA	H	1235	2	69,73,73	1.24	9 (13%)	83,113,113	1.43	8 (9%)
13	CLA	e	1115	1	64,68,73	1.25	9 (14%)	77,107,113	1.47	9 (11%)
13	CLA	f	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	11 (13%)
16	BCR	B	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	t	511	12	49,53,73	1.51	9 (18%)	59,89,113	1.54	7 (11%)
13	CLA	H	1211	2	60,64,73	1.32	7 (11%)	72,102,113	1.60	5 (6%)
13	CLA	f	1238	21	69,73,73	1.23	10 (14%)	83,113,113	1.42	11 (13%)
16	BCR	f	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	G	1110	1	55,59,73	1.40	10 (18%)	66,96,113	1.48	6 (9%)
13	CLA	G	1121	1	59,63,73	1.34	10 (16%)	71,101,113	1.48	10 (14%)
13	CLA	d	508	12	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
13	CLA	d	516	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	6 (10%)
13	CLA	1	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.37	7 (9%)
13	CLA	A	1237	21	69,73,73	1.25	9 (13%)	83,113,113	1.44	10 (12%)
13	CLA	d	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	f	1212	2	59,63,73	1.32	9 (15%)	71,101,113	1.48	6 (8%)
13	CLA	B	1223	2	69,73,73	1.25	9 (13%)	83,113,113	1.40	6 (7%)
13	CLA	A	1134	1	60,64,73	1.31	9 (15%)	72,102,113	1.44	6 (8%)
16	BCR	G	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
16	BCR	H	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	f	1021	2	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
16	BCR	f	4006	-	41,41,41	0.72	0	56,56,56	1.98	20 (35%)
17	LHG	B	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.76	10 (17%)
13	CLA	s	508	12	59,63,73	1.37	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	H	1203	2	69,73,73	1.26	12 (17%)	83,113,113	1.34	8 (9%)
13	CLA	H	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	a	506	12	54,58,73	1.43	9 (16%)	65,95,113	1.47	6 (9%)
13	CLA	J	1303	8	69,73,73	1.24	9 (13%)	83,113,113	1.39	10 (12%)
13	CLA	c	513	12	49,53,73	1.49	10 (20%)	59,89,113	1.44	5 (8%)
13	CLA	r	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
13	CLA	G	1128	1	69,73,73	1.32	10 (14%)	83,113,113	1.53	8 (9%)
16	BCR	H	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	t	506	12	49,53,73	1.50	9 (18%)	59,89,113	1.50	5 (8%)
17	LHG	n	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	B	1210	2	69,73,73	1.25	9 (13%)	83,113,113	1.41	11 (13%)
13	CLA	H	1219	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
13	CLA	t	518	12	59,63,73	1.36	9 (15%)	71,101,113	1.39	5 (7%)
13	CLA	A	1103	1	69,73,73	1.24	8 (11%)	83,113,113	1.49	8 (9%)
16	BCR	5	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
13	CLA	B	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
15	SF4	g	3002	3	0,12,12	-	-	-		
16	BCR	2	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	q	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.43	8 (11%)
13	CLA	G	1130	1	69,73,73	1.24	10 (14%)	83,113,113	1.40	11 (13%)
13	CLA	5	507	-	49,53,73	1.46	7 (14%)	59,89,113	1.53	7 (11%)
13	CLA	Y	507	-	64,68,73	1.29	8 (12%)	77,107,113	1.39	8 (10%)
13	CLA	f	1202	2	69,73,73	1.24	10 (14%)	83,113,113	1.48	10 (12%)
16	BCR	1	523	-	41,41,41	0.71	0	56,56,56	1.63	16 (28%)
16	BCR	R	4016	-	41,41,41	0.75	0	56,56,56	1.78	13 (23%)
16	BCR	b	523	-	41,41,41	0.70	0	56,56,56	1.65	12 (21%)
13	CLA	4	512	12	49,53,73	1.49	8 (16%)	59,89,113	1.50	4 (6%)
13	CLA	t	507	-	49,53,73	1.48	7 (14%)	59,89,113	1.55	7 (11%)
20	SQD	c	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
16	BCR	d	524	-	41,41,41	0.75	0	56,56,56	1.87	13 (23%)
13	CLA	s	518	12	59,63,73	1.36	10 (16%)	71,101,113	1.38	5 (7%)
13	CLA	b	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
16	BCR	v	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	Z	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	A	1126	1	69,73,73	1.20	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	5	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
13	CLA	c	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.37	5 (6%)
13	CLA	d	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.51	7 (11%)
13	CLA	f	1225	2	69,73,73	1.22	11 (15%)	83,113,113	1.31	8 (9%)
13	CLA	5	519	12	50,54,73	1.46	9 (18%)	60,90,113	1.45	5 (8%)
13	CLA	Y	519	12	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
13	CLA	d	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	4 (4%)
17	LHG	k	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	4	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.41	5 (7%)
16	BCR	Y	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
16	BCR	f	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
13	CLA	3	503	12	69,73,73	1.27	9 (13%)	83,113,113	1.32	7 (8%)
13	CLA	s	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.26	4 (4%)
16	BCR	L	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
16	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.76	10 (17%)
13	CLA	d	519	12	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
13	CLA	f	1226	2	69,73,73	1.34	11 (15%)	83,113,113	1.67	16 (19%)
16	BCR	H	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	H	1209	2	56,60,73	1.38	9 (16%)	67,97,113	1.56	7 (10%)
17	LHG	G	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
16	BCR	c	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
13	CLA	2	513	12	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
13	CLA	A	1131	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
13	CLA	f	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.69	15 (18%)
13	CLA	G	1102	1	69,73,73	1.21	9 (13%)	83,113,113	1.35	7 (8%)
13	CLA	c	516	12	49,53,73	1.50	9 (18%)	59,89,113	1.45	4 (6%)
13	CLA	3	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.49	4 (6%)
17	LHG	H	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	V	1503	21	64,68,73	1.28	10 (15%)	77,107,113	1.40	6 (7%)
16	BCR	T	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	3	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)
17	LHG	A	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
17	LHG	e	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LHG	A	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
17	LHG	e	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.33	6 (13%)
16	BCR	n	4219	-	41,41,41	0.78	0	56,56,56	1.81	12 (21%)
13	CLA	A	1132	1	69,73,73	1.23	11 (15%)	83,113,113	1.38	9 (10%)
13	CLA	Y	503	12	68,72,73	1.27	9 (13%)	81,111,113	1.34	6 (7%)
13	CLA	e	1105	1	59,63,73	1.30	10 (16%)	71,101,113	1.51	10 (14%)
13	CLA	2	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	Z	504	-	54,58,73	1.40	9 (16%)	65,95,113	1.46	7 (10%)
13	CLA	5	505	12	65,69,73	1.28	7 (10%)	78,108,113	1.26	4 (5%)
13	CLA	2	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.39	7 (9%)
13	CLA	q	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
16	BCR	5	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
13	CLA	f	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.42	8 (10%)
13	CLA	1	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
16	BCR	r	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
17	LHG	e	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
18	LMU	f	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
13	CLA	s	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	7 (11%)
13	CLA	1	516	12	49,53,73	1.49	9 (18%)	59,89,113	1.65	8 (13%)
13	CLA	Y	513	12	59,63,73	1.35	10 (16%)	71,101,113	1.36	5 (7%)
13	CLA	b	513	12	49,53,73	1.50	9 (18%)	59,89,113	1.48	4 (6%)
13	CLA	G	1123	21	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
13	CLA	r	516	12	49,53,73	1.47	9 (18%)	59,89,113	1.52	5 (8%)
13	CLA	e	1011	1	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
13	CLA	G	1237	21	69,73,73	1.25	9 (13%)	83,113,113	1.44	10 (12%)
16	BCR	6	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
18	LMU	e	1849	-	23,23,36	1.16	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	q	512	12	56,60,73	1.38	9 (16%)	67,97,113	1.44	5 (7%)
18	LMU	r	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
17	LHG	e	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	G	1140	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	11 (13%)
13	CLA	6	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.46	6 (10%)
13	CLA	H	1206	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	6 (7%)
16	BCR	q	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	K	1105	9	49,53,73	1.50	9 (18%)	59,89,113	1.70	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	5	508	12	49,53,73	1.49	9 (18%)	59,89,113	1.55	5 (8%)
13	CLA	f	1231	21	69,73,73	1.21	9 (13%)	83,113,113	1.42	8 (9%)
17	LHG	H	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
13	CLA	5	502	12	54,58,73	1.42	10 (18%)	65,95,113	1.46	5 (7%)
13	CLA	Y	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.38	7 (9%)
13	CLA	e	1134	1	60,64,73	1.31	9 (15%)	72,102,113	1.44	6 (8%)
13	CLA	s	517	-	49,53,73	1.47	10 (20%)	59,89,113	1.44	4 (6%)
13	CLA	m	1105	9	49,53,73	1.50	9 (18%)	59,89,113	1.69	9 (15%)
13	CLA	t	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	3	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	G	1137	1	69,73,73	1.23	8 (11%)	83,113,113	1.43	7 (8%)
13	CLA	a	503	12	69,73,73	1.27	9 (13%)	83,113,113	1.33	7 (8%)
13	CLA	B	1021	2	69,73,73	1.24	10 (14%)	83,113,113	1.37	8 (9%)
18	LMU	l	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	v	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.47	4 (6%)
13	CLA	3	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
13	CLA	d	517	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	4 (6%)
13	CLA	B	1204	2	69,73,73	1.22	9 (13%)	83,113,113	1.31	7 (8%)
20	SQD	V	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.64	10 (16%)

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
13	CLA	2	505	12	-	14/39/115/115	-
13	CLA	3	519	12	-	10/27/103/115	-
13	CLA	5	503	12	-	12/27/103/115	-
16	BCR	c	524	-	-	2/29/63/63	0/2/2/2
13	CLA	6	518	12	-	12/27/103/115	-
13	CLA	A	1123	21	-	11/39/115/115	-
13	CLA	A	1115	1	-	12/33/109/115	-
13	CLA	V	1501	10	-	20/39/115/115	-
13	CLA	5	511	12	-	7/27/103/115	-
13	CLA	v	504	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	G	1108	1	-	18/26/102/115	-
13	CLA	f	1207	2	-	16/39/115/115	-
13	CLA	1	506	12	-	6/15/91/115	-
13	CLA	e	1126	1	-	18/39/115/115	-
13	CLA	a	510	12	-	19/39/115/115	-
13	CLA	4	511	12	-	5/15/91/115	-
13	CLA	e	1138	1	-	14/39/115/115	-
20	SQD	2	822	-	-	13/38/58/69	0/1/1/1
13	CLA	c	508	12	-	6/15/91/115	-
20	SQD	u	822	-	-	7/24/44/69	0/1/1/1
19	LMG	B	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	c	502	12	-	7/21/97/115	-
16	BCR	3	522	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1110	1	-	11/23/99/115	-
13	CLA	d	511	12	-	6/15/91/115	-
18	LMU	T	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	1	513	12	-	4/27/103/115	-
15	SF4	g	3003	3	-	-	0/6/5/5
13	CLA	B	1225	2	-	8/39/115/115	-
13	CLA	6	507	-	-	6/15/91/115	-
13	CLA	f	1227	2	-	14/39/115/115	-
13	CLA	G	1106	1	-	23/39/115/115	-
13	CLA	G	1139	21	-	14/39/115/115	-
13	CLA	a	501	12	-	6/39/115/115	-
20	SQD	6	822	-	-	9/19/39/69	0/1/1/1
17	LHG	G	5007	-	-	24/51/51/53	-
16	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
16	BCR	d	523	-	-	4/29/63/63	0/2/2/2
16	BCR	H	4014	-	-	9/29/63/63	0/2/2/2
16	BCR	v	521	-	-	5/29/63/63	0/2/2/2
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	H	1201	2	-	11/33/109/115	-
13	CLA	q	519	12	-	8/21/97/115	-
13	CLA	B	1211	2	-	4/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	B	1023	-	-	10/39/115/115	-
13	CLA	1	501	12	-	20/39/115/115	-
13	CLA	s	503	12	-	9/39/115/115	-
18	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	H	1238	21	-	4/39/115/115	-
20	SQD	L	5216	-	-	17/46/66/69	0/1/1/1
20	SQD	r	822	-	-	13/38/58/69	0/1/1/1
20	SQD	f	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	c	505	12	-	16/35/111/115	-
15	SF4	e	3001	2,1	-	-	0/6/5/5
13	CLA	B	1205	2	-	12/39/115/115	-
13	CLA	3	513	12	-	15/39/115/115	-
13	CLA	t	513	12	-	9/15/91/115	-
15	SF4	N	3003	3	-	-	0/6/5/5
13	CLA	A	1109	1	-	11/39/115/115	-
16	BCR	u	523	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1022	21	-	8/39/115/115	-
16	BCR	c	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1135	1	-	10/24/100/115	-
13	CLA	l	1302	8	-	15/31/107/115	-
13	CLA	f	1201	2	-	11/33/109/115	-
13	CLA	d	501	12	-	18/33/109/115	-
13	CLA	L	1501	10	-	20/39/115/115	-
13	CLA	R	1302	6	-	10/15/91/115	-
13	CLA	d	512	12	-	8/15/91/115	-
13	CLA	e	1013	-	-	11/39/115/115	-
16	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
17	LHG	A	5003	13	-	17/45/45/53	-
13	CLA	B	1220	2	-	11/27/103/115	-
13	CLA	q	513	12	-	4/27/103/115	-
13	CLA	s	512	12	-	5/15/91/115	-
13	CLA	A	1135	1	-	10/24/100/115	-
13	CLA	L	1502	10	-	10/39/115/115	-
13	CLA	6	509	12	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1213	2	-	14/39/115/115	-
13	CLA	H	1217	2	-	14/30/106/115	-
13	CLA	B	1232	21	-	6/21/97/115	-
13	CLA	G	1135	1	-	10/24/100/115	-
13	CLA	u	506	12	-	7/15/91/115	-
13	CLA	2	517	-	-	6/15/91/115	-
13	CLA	q	508	12	-	11/27/103/115	-
16	BCR	u	521	-	-	7/29/63/63	0/2/2/2
13	CLA	t	501	12	-	14/33/109/115	-
13	CLA	c	504	-	-	5/15/91/115	-
13	CLA	q	502	12	-	16/33/109/115	-
13	CLA	u	517	-	-	11/15/91/115	-
13	CLA	H	1227	2	-	14/39/115/115	-
13	CLA	H	1239	2	-	17/39/115/115	-
19	LMG	T	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	A	1116	1	-	15/33/109/115	-
13	CLA	H	1226	2	-	12/39/115/115	-
13	CLA	u	519	12	-	10/17/93/115	-
13	CLA	A	1106	1	-	23/39/115/115	-
13	CLA	s	509	12	-	4/39/115/115	-
13	CLA	A	1105	1	-	6/27/103/115	-
13	CLA	t	510	12	-	7/21/97/115	-
13	CLA	Z	518	12	-	16/39/115/115	-
13	CLA	u	508	12	-	6/15/91/115	-
13	CLA	c	517	-	-	11/15/91/115	-
14	PQN	H	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	B	1230	2	-	12/33/109/115	-
13	CLA	c	509	12	-	12/39/115/115	-
13	CLA	f	1222	21	-	7/33/109/115	-
13	CLA	f	1235	2	-	8/39/115/115	-
13	CLA	4	518	12	-	10/27/103/115	-
16	BCR	v	524	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1124	21	-	13/29/105/115	-
13	CLA	H	1223	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	5	523	-	-	4/29/63/63	0/2/2/2
17	LHG	V	5218	-	-	23/42/42/53	-
13	CLA	G	1111	1	-	16/39/115/115	-
13	CLA	r	519	12	-	11/27/103/115	-
16	BCR	L	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	6	508	12	-	5/15/91/115	-
16	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	u	503	12	-	12/27/103/115	-
13	CLA	B	1231	21	-	8/39/115/115	-
13	CLA	c	503	12	-	12/27/103/115	-
13	CLA	Z	507	-	-	16/39/115/115	-
13	CLA	F	1301	21	-	12/39/115/115	-
13	CLA	s	507	-	-	15/39/115/115	-
13	CLA	H	1230	2	-	12/33/109/115	-
13	CLA	u	513	12	-	6/15/91/115	-
16	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	G	1133	1	-	17/39/115/115	-
13	CLA	2	512	12	-	7/25/101/115	-
16	BCR	A	4011	-	-	12/29/63/63	0/2/2/2
17	LHG	S	5001	-	-	22/48/48/53	-
13	CLA	u	507	-	-	7/15/91/115	-
13	CLA	K	1103	9	-	9/21/97/115	-
13	CLA	A	1128	1	-	12/39/115/115	-
13	CLA	a	518	12	-	12/27/103/115	-
16	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	s	519	12	-	10/27/103/115	-
13	CLA	c	511	12	-	7/27/103/115	-
13	CLA	G	1138	1	-	14/39/115/115	-
16	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
16	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
20	SQD	Y	822	-	-	20/43/63/69	0/1/1/1
13	CLA	A	1122	1	-	16/33/109/115	-
16	BCR	s	524	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1139	21	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	q	501	12	-	20/39/115/115	-
13	CLA	1	512	12	-	12/24/100/115	-
13	CLA	H	1234	2	-	13/39/115/115	-
13	CLA	6	511	12	-	6/15/91/115	-
16	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	2	516	12	-	10/15/91/115	-
13	CLA	c	506	12	-	7/15/91/115	-
16	BCR	a	522	-	-	5/29/63/63	0/2/2/2
13	CLA	R	1301	21	-	12/39/115/115	-
20	SQD	H	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	f	1236	2	-	5/27/103/115	-
13	CLA	6	505	12	-	15/39/115/115	-
13	CLA	e	1124	21	-	13/29/105/115	-
13	CLA	4	503	12	-	3/27/103/115	-
13	CLA	A	1140	1	-	13/39/115/115	-
13	CLA	H	1212	2	-	11/27/103/115	-
13	CLA	s	501	12	-	6/39/115/115	-
13	CLA	5	516	12	-	4/15/91/115	-
13	CLA	B	1209	2	-	8/24/100/115	-
18	LMU	Z	901	-	-	8/14/34/61	0/1/1/2
13	CLA	f	1217	2	-	14/30/106/115	-
13	CLA	u	501	12	-	21/39/115/115	-
13	CLA	A	1133	1	-	17/39/115/115	-
13	CLA	e	1121	1	-	8/27/103/115	-
13	CLA	s	506	12	-	5/21/97/115	-
13	CLA	B	1239	2	-	17/39/115/115	-
13	CLA	e	1131	1	-	8/39/115/115	-
17	LHG	A	5002	-	-	26/43/43/53	-
13	CLA	q	516	12	-	15/15/91/115	-
17	LHG	V	5220	-	-	24/45/45/53	-
13	CLA	s	513	12	-	15/39/115/115	-
13	CLA	A	1138	1	-	14/39/115/115	-
13	CLA	u	505	12	-	16/35/111/115	-
13	CLA	H	1207	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	l	1303	8	-	18/39/115/115	-
13	CLA	A	1125	1	-	14/39/115/115	-
13	CLA	e	1132	1	-	17/39/115/115	-
13	CLA	f	1214	2	-	15/39/115/115	-
13	CLA	f	1216	21	-	7/33/109/115	-
13	CLA	H	1202	2	-	13/39/115/115	-
13	CLA	2	511	12	-	6/27/103/115	-
16	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	F	1302	6	-	10/15/91/115	-
16	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
16	BCR	t	522	-	-	4/29/63/63	0/2/2/2
20	SQD	Z	822	-	-	13/38/58/69	0/1/1/1
16	BCR	f	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	2	507	-	-	16/39/115/115	-
13	CLA	e	1801	17	-	5/15/91/115	-
16	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
14	PQN	f	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	u	516	12	-	4/15/91/115	-
13	CLA	A	1107	1	-	16/39/115/115	-
13	CLA	s	502	12	-	6/21/97/115	-
13	CLA	Z	501	12	-	14/39/115/115	-
17	LHG	V	5221	-	-	30/53/53/53	-
13	CLA	H	1023	-	-	10/39/115/115	-
13	CLA	e	1130	1	-	9/39/115/115	-
18	LMU	2	901	-	-	8/14/34/61	0/1/1/2
20	SQD	1	822	-	-	20/43/63/69	0/1/1/1
13	CLA	5	518	12	-	13/27/103/115	-
13	CLA	b	510	12	-	7/21/97/115	-
13	CLA	2	506	12	-	8/27/103/115	-
13	CLA	2	519	12	-	11/27/103/115	-
16	BCR	u	522	-	-	5/29/63/63	0/2/2/2
16	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	H	1231	21	-	8/39/115/115	-
13	CLA	b	506	12	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	4	501	12	-	14/33/109/115	-
17	LHG	n	5220	-	-	24/45/45/53	-
16	BCR	W	4021	-	-	7/29/63/63	0/2/2/2
19	LMG	J	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	1	517	-	-	6/15/91/115	-
13	CLA	Z	510	12	-	9/39/115/115	-
13	CLA	b	517	-	-	7/15/91/115	-
13	CLA	a	517	-	-	9/15/91/115	-
13	CLA	e	1136	1	-	5/33/109/115	-
13	CLA	r	518	12	-	16/39/115/115	-
13	CLA	v	511	12	-	6/15/91/115	-
13	CLA	a	505	12	-	19/39/115/115	-
16	BCR	Z	524	-	-	2/29/63/63	0/2/2/2
13	CLA	V	1502	10	-	10/39/115/115	-
13	CLA	v	507	-	-	6/15/91/115	-
13	CLA	Z	511	12	-	6/27/103/115	-
16	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
17	LHG	e	5002	-	-	26/43/43/53	-
13	CLA	A	1129	1	-	7/23/99/115	-
18	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	4	510	12	-	7/21/97/115	-
13	CLA	Y	506	12	-	6/15/91/115	-
13	CLA	A	1112	1	-	5/21/97/115	-
16	BCR	b	522	-	-	4/29/63/63	0/2/2/2
17	LHG	e	5006	-	-	24/49/49/53	-
16	BCR	b	521	-	-	10/29/63/63	0/2/2/2
13	CLA	q	503	12	-	11/38/114/115	-
16	BCR	1	524	-	-	2/29/63/63	0/2/2/2
13	CLA	G	1134	1	-	13/29/105/115	-
20	SQD	a	822	-	-	21/38/58/69	0/1/1/1
13	CLA	u	511	12	-	7/27/103/115	-
13	CLA	5	501	12	-	21/39/115/115	-
13	CLA	H	1224	2	-	13/33/109/115	-
13	CLA	H	1240	17	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1209	2	-	8/24/100/115	-
20	SQD	t	822	-	-	8/19/39/69	0/1/1/1
13	CLA	c	518	12	-	13/27/103/115	-
16	BCR	S	4018	-	-	1/29/63/63	0/2/2/2
17	LHG	n	5218	-	-	23/42/42/53	-
16	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	3	511	12	-	7/21/97/115	-
18	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	b	508	12	-	6/15/91/115	-
16	BCR	4	523	-	-	5/29/63/63	0/2/2/2
17	LHG	G	5003	13	-	16/45/45/53	-
13	CLA	f	1204	2	-	13/39/115/115	-
13	CLA	t	512	12	-	5/15/91/115	-
17	LHG	B	1855	-	-	28/48/48/53	-
13	CLA	f	1208	2	-	17/39/115/115	-
13	CLA	G	1105	1	-	6/27/103/115	-
13	CLA	B	1212	2	-	11/27/103/115	-
13	CLA	f	1219	2	-	19/39/115/115	-
16	BCR	n	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	r	504	-	-	7/21/97/115	-
16	BCR	a	524	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1011	1	-	12/39/115/115	-
14	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
20	SQD	q	822	-	-	20/43/63/69	0/1/1/1
16	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	a	512	12	-	5/15/91/115	-
13	CLA	f	1240	17	-	15/39/115/115	-
13	CLA	b	518	12	-	10/27/103/115	-
13	CLA	B	1012	21	-	16/39/115/115	-
13	CLA	H	1205	2	-	12/39/115/115	-
17	LHG	G	5004	-	-	21/40/40/53	-
13	CLA	e	1137	1	-	19/39/115/115	-
13	CLA	2	509	12	-	6/39/115/115	-
13	CLA	A	1118	1	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	4	524	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1117	1	-	13/39/115/115	-
13	CLA	4	506	12	-	4/15/91/115	-
13	CLA	T	1303	8	-	18/39/115/115	-
13	CLA	Y	511	12	-	4/27/103/115	-
13	CLA	B	1202	2	-	13/39/115/115	-
16	BCR	6	521	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1226	2	-	12/39/115/115	-
13	CLA	A	1136	1	-	5/33/109/115	-
13	CLA	a	513	12	-	15/39/115/115	-
13	CLA	v	509	12	-	6/15/91/115	-
13	CLA	q	504	-	-	7/15/91/115	-
16	BCR	1	521	-	-	7/29/63/63	0/2/2/2
13	CLA	b	505	12	-	13/39/115/115	-
16	BCR	d	521	-	-	5/29/63/63	0/2/2/2
17	LHG	A	5001	-	-	25/53/53/53	-
13	CLA	A	1121	1	-	8/27/103/115	-
16	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	e	1125	1	-	14/39/115/115	-
17	LHG	L	5218	-	-	23/42/42/53	-
18	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	m	1401	-	-	10/27/103/115	-
16	BCR	q	524	-	-	2/29/63/63	0/2/2/2
13	CLA	u	512	12	-	7/15/91/115	-
13	CLA	u	504	-	-	5/15/91/115	-
13	CLA	A	1111	1	-	16/39/115/115	-
13	CLA	T	1302	8	-	15/31/107/115	-
13	CLA	Y	509	12	-	6/39/115/115	-
13	CLA	d	509	12	-	6/15/91/115	-
13	CLA	1	508	12	-	11/27/103/115	-
13	CLA	4	508	12	-	6/15/91/115	-
16	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	G	1126	1	-	18/39/115/115	-
13	CLA	U	1401	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	e	5008	-	-	19/39/39/53	-
13	CLA	Y	518	12	-	17/33/109/115	-
13	CLA	A	1102	1	-	11/39/115/115	-
16	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
16	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	6	512	12	-	8/15/91/115	-
13	CLA	B	1228	2	-	8/27/103/115	-
16	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
16	BCR	a	521	-	-	7/29/63/63	0/2/2/2
16	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1104	1	-	12/39/115/115	-
16	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
19	LMG	H	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	G	1132	1	-	17/39/115/115	-
13	CLA	3	506	12	-	5/21/97/115	-
13	CLA	e	1103	1	-	20/39/115/115	-
13	CLA	f	1221	21	-	14/39/115/115	-
16	BCR	t	521	-	-	10/29/63/63	0/2/2/2
13	CLA	t	517	-	-	7/15/91/115	-
13	CLA	1	503	12	-	11/38/114/115	-
16	BCR	t	524	-	-	4/29/63/63	0/2/2/2
13	CLA	d	503	12	-	10/24/100/115	-
17	LHG	L	5221	-	-	30/53/53/53	-
13	CLA	f	1239	2	-	17/39/115/115	-
13	CLA	6	513	12	-	5/15/91/115	-
13	CLA	L	1503	21	-	10/33/109/115	-
13	CLA	B	1217	2	-	14/30/106/115	-
16	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1127	1	-	12/39/115/115	-
13	CLA	e	1113	1	-	5/15/91/115	-
13	CLA	t	508	12	-	6/15/91/115	-
17	LHG	G	5001	-	-	25/53/53/53	-
16	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	3	502	12	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	a	523	-	-	4/29/63/63	0/2/2/2
13	CLA	1	505	12	-	11/39/115/115	-
16	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
13	CLA	q	506	12	-	6/15/91/115	-
13	CLA	m	1103	9	-	9/21/97/115	-
19	LMG	f	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	q	517	-	-	6/15/91/115	-
17	LHG	A	5009	-	-	28/53/53/53	-
13	CLA	H	1221	21	-	14/39/115/115	-
13	CLA	Z	516	12	-	10/15/91/115	-
15	SF4	G	3001	2,1	-	-	0/6/5/5
13	CLA	B	1229	2	-	13/39/115/115	-
13	CLA	c	510	12	-	9/15/91/115	-
13	CLA	s	516	12	-	11/15/91/115	-
13	CLA	H	1225	2	-	7/39/115/115	-
13	CLA	d	513	12	-	5/15/91/115	-
14	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
16	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
16	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
16	BCR	q	522	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1123	21	-	11/39/115/115	-
15	SF4	C	3002	3	-	-	0/6/5/5
13	CLA	H	1232	21	-	6/21/97/115	-
18	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
20	SQD	4	822	-	-	8/19/39/69	0/1/1/1
13	CLA	H	1213	2	-	14/39/115/115	-
13	CLA	G	1131	1	-	8/39/115/115	-
13	CLA	v	505	12	-	15/39/115/115	-
13	CLA	6	501	12	-	18/33/109/115	-
13	CLA	A	1130	1	-	9/39/115/115	-
13	CLA	r	510	12	-	9/39/115/115	-
13	CLA	5	512	12	-	7/15/91/115	-
13	CLA	G	1119	21	-	15/39/115/115	-
13	CLA	G	1013	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1230	2	-	12/33/109/115	-
20	SQD	s	822	-	-	21/38/58/69	0/1/1/1
13	CLA	B	1206	2	-	15/39/115/115	-
13	CLA	e	1119	21	-	15/39/115/115	-
13	CLA	t	505	12	-	13/39/115/115	-
16	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
13	CLA	A	1137	1	-	19/39/115/115	-
13	CLA	6	510	12	-	9/15/91/115	-
13	CLA	a	519	12	-	10/27/103/115	-
13	CLA	c	519	12	-	10/17/93/115	-
13	CLA	6	519	12	-	8/17/93/115	-
13	CLA	U	1105	9	-	11/15/91/115	-
13	CLA	4	505	12	-	13/39/115/115	-
14	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	e	1128	1	-	12/39/115/115	-
16	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
20	SQD	n	5216	-	-	17/46/66/69	0/1/1/1
18	LMU	1	902	-	-	6/10/30/61	0/1/1/2
13	CLA	4	516	12	-	9/15/91/115	-
13	CLA	a	508	12	-	7/27/103/115	-
13	CLA	a	516	12	-	11/15/91/115	-
13	CLA	e	1120	1	-	4/25/101/115	-
16	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
13	CLA	Z	508	12	-	8/27/103/115	-
16	BCR	t	523	-	-	5/29/63/63	0/2/2/2
16	BCR	r	522	-	-	6/29/63/63	0/2/2/2
18	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	d	518	12	-	12/27/103/115	-
13	CLA	A	1011	1	-	11/39/115/115	-
13	CLA	Z	502	12	-	13/33/109/115	-
13	CLA	f	1215	2	-	19/39/115/115	-
13	CLA	t	516	12	-	9/15/91/115	-
13	CLA	f	1220	2	-	11/27/103/115	-
13	CLA	2	510	12	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	J	1302	8	-	15/31/107/115	-
13	CLA	3	518	12	-	12/27/103/115	-
13	CLA	b	509	12	-	7/39/115/115	-
17	LHG	A	5004	-	-	21/40/40/53	-
20	SQD	b	822	-	-	8/19/39/69	0/1/1/1
16	BCR	6	522	-	-	5/29/63/63	0/2/2/2
16	BCR	k	4018	-	-	1/29/63/63	0/2/2/2
20	SQD	v	822	-	-	9/19/39/69	0/1/1/1
13	CLA	B	1238	21	-	4/39/115/115	-
16	BCR	1	522	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1108	1	-	18/26/102/115	-
13	CLA	H	1210	2	-	21/39/115/115	-
16	BCR	d	522	-	-	5/29/63/63	0/2/2/2
13	CLA	3	507	-	-	15/39/115/115	-
13	CLA	H	1220	2	-	11/27/103/115	-
16	BCR	u	524	-	-	2/29/63/63	0/2/2/2
16	BCR	s	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1118	1	-	14/33/109/115	-
13	CLA	5	510	12	-	9/15/91/115	-
13	CLA	Y	510	12	-	13/39/115/115	-
13	CLA	f	1012	21	-	16/39/115/115	-
18	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	H	1021	2	-	13/39/115/115	-
13	CLA	a	507	-	-	15/39/115/115	-
13	CLA	B	1221	21	-	14/39/115/115	-
13	CLA	5	517	-	-	11/15/91/115	-
13	CLA	Z	505	12	-	14/39/115/115	-
16	BCR	6	524	-	-	5/29/63/63	0/2/2/2
18	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	e	1102	1	-	11/39/115/115	-
13	CLA	a	502	12	-	6/21/97/115	-
13	CLA	b	512	12	-	5/15/91/115	-
17	LHG	A	5007	-	-	24/51/51/53	-
13	CLA	b	504	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMU	Y	902	-	-	6/10/30/61	0/1/1/2
13	CLA	e	1107	1	-	16/39/115/115	-
16	BCR	5	522	-	-	5/29/63/63	0/2/2/2
13	CLA	2	501	12	-	14/39/115/115	-
13	CLA	v	516	12	-	10/15/91/115	-
16	BCR	o	4021	-	-	7/29/63/63	0/2/2/2
16	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	B	1227	2	-	14/39/115/115	-
13	CLA	B	1214	2	-	15/39/115/115	-
13	CLA	r	509	12	-	6/39/115/115	-
16	BCR	4	521	-	-	10/29/63/63	0/2/2/2
13	CLA	H	1236	2	-	5/27/103/115	-
13	CLA	f	1203	2	-	18/39/115/115	-
13	CLA	Z	517	-	-	6/15/91/115	-
16	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1101	1	-	13/39/115/115	-
13	CLA	e	1237	21	-	21/39/115/115	-
13	CLA	n	1501	10	-	20/39/115/115	-
13	CLA	Y	508	12	-	11/27/103/115	-
13	CLA	e	1127	1	-	12/39/115/115	-
13	CLA	2	518	12	-	16/39/115/115	-
13	CLA	e	1140	1	-	13/39/115/115	-
13	CLA	f	1228	2	-	8/27/103/115	-
13	CLA	f	1234	2	-	13/39/115/115	-
14	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
17	LHG	L	5220	-	-	24/45/45/53	-
13	CLA	a	504	-	-	6/15/91/115	-
13	CLA	G	1113	1	-	5/15/91/115	-
13	CLA	5	506	12	-	7/15/91/115	-
13	CLA	G	1124	21	-	13/29/105/115	-
13	CLA	e	1112	1	-	5/21/97/115	-
13	CLA	n	1502	10	-	10/39/115/115	-
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	H	1214	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1205	2	-	12/39/115/115	-
16	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	H	1228	2	-	8/27/103/115	-
13	CLA	b	503	12	-	3/27/103/115	-
13	CLA	e	1109	1	-	11/39/115/115	-
13	CLA	Z	512	12	-	7/25/101/115	-
13	CLA	G	1114	21	-	2/21/97/115	-
16	BCR	2	522	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1122	1	-	16/33/109/115	-
13	CLA	5	513	12	-	6/15/91/115	-
13	CLA	r	511	12	-	6/27/103/115	-
19	LMG	l	5104	-	-	17/30/50/70	0/1/1/1
15	SF4	N	3002	3	-	-	0/6/5/5
13	CLA	f	1223	2	-	14/39/115/115	-
13	CLA	q	518	12	-	17/33/109/115	-
13	CLA	r	507	-	-	16/39/115/115	-
13	CLA	u	502	12	-	7/21/97/115	-
17	LHG	e	5005	-	-	29/49/49/53	-
13	CLA	e	1114	21	-	2/21/97/115	-
13	CLA	v	517	-	-	11/15/91/115	-
16	BCR	b	524	-	-	4/29/63/63	0/2/2/2
17	LHG	f	1842	13	-	22/43/43/53	-
16	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	Z	506	12	-	8/27/103/115	-
13	CLA	v	513	12	-	5/15/91/115	-
13	CLA	v	518	12	-	12/27/103/115	-
16	BCR	3	523	-	-	4/29/63/63	0/2/2/2
20	SQD	3	822	-	-	21/38/58/69	0/1/1/1
13	CLA	H	1012	21	-	16/39/115/115	-
16	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	b	507	-	-	8/15/91/115	-
13	CLA	1	504	-	-	7/15/91/115	-
13	CLA	B	1215	2	-	19/39/115/115	-
13	CLA	4	504	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	d	504	-	-	8/15/91/115	-
13	CLA	v	503	12	-	10/24/100/115	-
13	CLA	B	1201	2	-	11/33/109/115	-
13	CLA	A	1104	1	-	12/39/115/115	-
13	CLA	Y	505	12	-	11/39/115/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	G	1801	17	-	5/15/91/115	-
13	CLA	e	1122	1	-	16/33/109/115	-
16	BCR	Y	521	-	-	6/29/63/63	0/2/2/2
13	CLA	1	509	12	-	6/39/115/115	-
13	CLA	4	509	12	-	7/39/115/115	-
13	CLA	b	502	12	-	7/21/97/115	-
13	CLA	a	509	12	-	4/39/115/115	-
13	CLA	A	1119	21	-	15/39/115/115	-
13	CLA	A	1013	-	-	11/39/115/115	-
13	CLA	r	508	12	-	8/27/103/115	-
13	CLA	G	1101	1	-	13/39/115/115	-
13	CLA	d	510	12	-	9/15/91/115	-
13	CLA	s	511	12	-	7/21/97/115	-
13	CLA	1	519	12	-	8/21/97/115	-
13	CLA	b	519	12	-	14/27/103/115	-
13	CLA	2	504	-	-	7/21/97/115	-
13	CLA	q	507	-	-	16/33/109/115	-
13	CLA	B	1222	21	-	7/33/109/115	-
13	CLA	B	1208	2	-	17/39/115/115	-
13	CLA	K	1401	-	-	10/27/103/115	-
13	CLA	3	510	12	-	19/39/115/115	-
13	CLA	H	1215	2	-	19/39/115/115	-
13	CLA	B	1234	2	-	13/39/115/115	-
16	BCR	A	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	Z	519	12	-	11/27/103/115	-
16	BCR	B	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1120	1	-	4/25/101/115	-
13	CLA	v	512	12	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	SQD	B	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	A	1022	21	-	8/39/115/115	-
16	BCR	3	524	-	-	5/29/63/63	0/2/2/2
13	CLA	c	507	-	-	7/15/91/115	-
13	CLA	G	1136	1	-	5/33/109/115	-
13	CLA	e	1106	1	-	23/39/115/115	-
13	CLA	e	1139	21	-	14/39/115/115	-
13	CLA	G	1120	1	-	4/25/101/115	-
13	CLA	G	1022	21	-	8/39/115/115	-
13	CLA	B	1218	2	-	7/33/109/115	-
13	CLA	H	1204	2	-	13/39/115/115	-
13	CLA	f	1206	2	-	15/39/115/115	-
16	BCR	c	521	-	-	7/29/63/63	0/2/2/2
13	CLA	r	505	12	-	14/39/115/115	-
13	CLA	Y	501	12	-	20/39/115/115	-
13	CLA	t	504	-	-	7/15/91/115	-
17	LHG	G	5002	-	-	26/43/43/53	-
17	LHG	G	5006	-	-	24/49/49/53	-
13	CLA	6	517	-	-	11/15/91/115	-
16	BCR	V	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1207	2	-	16/39/115/115	-
13	CLA	q	510	12	-	13/39/115/115	-
13	CLA	H	1208	2	-	17/39/115/115	-
13	CLA	Z	503	12	-	9/39/115/115	-
13	CLA	f	1218	2	-	7/33/109/115	-
13	CLA	1	518	12	-	17/33/109/115	-
13	CLA	e	1133	1	-	17/39/115/115	-
16	BCR	f	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	1	507	-	-	16/33/109/115	-
13	CLA	r	502	12	-	13/33/109/115	-
13	CLA	Z	513	12	-	17/39/115/115	-
16	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	Y	516	12	-	15/15/91/115	-
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1235	2	-	8/39/115/115	-
13	CLA	4	507	-	-	8/15/91/115	-
13	CLA	6	502	12	-	7/21/97/115	-
16	BCR	I	4018	-	-	1/29/63/63	0/2/2/2
13	CLA	A	1101	1	-	13/39/115/115	-
13	CLA	B	1219	2	-	19/39/115/115	-
13	CLA	G	1109	1	-	11/39/115/115	-
13	CLA	t	509	12	-	7/39/115/115	-
16	BCR	4	522	-	-	4/29/63/63	0/2/2/2
13	CLA	b	501	12	-	14/33/109/115	-
13	CLA	G	1127	1	-	12/39/115/115	-
16	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
17	LHG	G	5008	-	-	19/39/39/53	-
13	CLA	v	501	12	-	18/33/109/115	-
17	LHG	I	5001	-	-	22/48/48/53	-
13	CLA	e	1117	1	-	13/39/115/115	-
13	CLA	u	510	12	-	9/15/91/115	-
13	CLA	G	1104	1	-	12/39/115/115	-
16	BCR	2	524	-	-	2/29/63/63	0/2/2/2
20	SQD	d	822	-	-	9/19/39/69	0/1/1/1
13	CLA	1	511	12	-	4/27/103/115	-
13	CLA	b	511	12	-	5/15/91/115	-
13	CLA	6	503	12	-	10/24/100/115	-
16	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	3	508	12	-	7/27/103/115	-
16	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
16	BCR	B	4014	-	-	9/29/63/63	0/2/2/2
16	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	G	1129	1	-	7/23/99/115	-
13	CLA	t	519	12	-	14/27/103/115	-
13	CLA	A	1113	1	-	5/15/91/115	-
13	CLA	B	1216	21	-	7/33/109/115	-
13	CLA	G	1112	1	-	5/21/97/115	-
13	CLA	v	510	12	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	r	523	-	-	6/29/63/63	0/2/2/2
13	CLA	j	1301	21	-	12/39/115/115	-
13	CLA	4	517	-	-	7/15/91/115	-
13	CLA	v	519	12	-	8/17/93/115	-
13	CLA	n	1503	21	-	10/33/109/115	-
16	BCR	r	521	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1203	2	-	18/39/115/115	-
13	CLA	2	503	12	-	9/39/115/115	-
13	CLA	r	517	-	-	6/15/91/115	-
15	SF4	A	3001	2,1	-	-	0/6/5/5
13	CLA	v	506	12	-	7/15/91/115	-
13	CLA	4	513	12	-	9/15/91/115	-
13	CLA	H	1218	2	-	7/33/109/115	-
13	CLA	A	1114	21	-	2/21/97/115	-
13	CLA	v	508	12	-	5/15/91/115	-
18	LMU	q	902	-	-	6/10/30/61	0/1/1/2
17	LHG	G	5005	-	-	29/49/49/53	-
13	CLA	B	1213	2	-	14/39/115/115	-
13	CLA	a	511	12	-	7/21/97/115	-
13	CLA	u	518	12	-	13/27/103/115	-
13	CLA	e	1129	1	-	7/23/99/115	-
16	BCR	v	522	-	-	5/29/63/63	0/2/2/2
13	CLA	4	502	12	-	7/21/97/115	-
16	BCR	s	523	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1103	1	-	20/39/115/115	-
13	CLA	G	1117	1	-	13/39/115/115	-
13	CLA	H	1216	21	-	7/33/109/115	-
13	CLA	3	505	12	-	19/39/115/115	-
13	CLA	G	1107	1	-	16/39/115/115	-
13	CLA	e	1110	1	-	11/23/99/115	-
13	CLA	3	516	12	-	11/15/91/115	-
16	BCR	2	521	-	-	4/29/63/63	0/2/2/2
13	CLA	r	512	12	-	7/25/101/115	-
13	CLA	G	1116	1	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	j	1302	6	-	10/15/91/115	-
13	CLA	B	1236	2	-	5/27/103/115	-
13	CLA	6	504	-	-	8/15/91/115	-
13	CLA	U	1103	9	-	9/21/97/115	-
17	LHG	e	5007	-	-	24/51/51/53	-
13	CLA	r	503	12	-	9/39/115/115	-
13	CLA	t	503	12	-	3/27/103/115	-
16	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
16	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	r	506	12	-	8/27/103/115	-
13	CLA	f	1210	2	-	21/39/115/115	-
13	CLA	Y	512	12	-	11/24/100/115	-
13	CLA	s	510	12	-	19/39/115/115	-
13	CLA	B	1240	17	-	15/39/115/115	-
13	CLA	5	504	-	-	5/15/91/115	-
13	CLA	Y	504	-	-	7/15/91/115	-
13	CLA	r	513	12	-	17/39/115/115	-
13	CLA	f	1211	2	-	4/29/105/115	-
13	CLA	u	509	12	-	12/39/115/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	Y	517	-	-	6/15/91/115	-
13	CLA	6	506	12	-	7/15/91/115	-
13	CLA	e	1116	1	-	15/33/109/115	-
13	CLA	A	1801	17	-	5/15/91/115	-
13	CLA	d	506	12	-	7/15/91/115	-
13	CLA	e	1111	1	-	16/39/115/115	-
17	LHG	A	5006	-	-	24/49/49/53	-
16	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
16	BCR	q	523	-	-	6/29/63/63	0/2/2/2
16	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
13	CLA	q	509	12	-	6/39/115/115	-
13	CLA	G	1118	1	-	14/33/109/115	-
13	CLA	G	1115	1	-	12/33/109/115	-
13	CLA	f	1232	21	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	f	1855	-	-	28/48/48/53	-
16	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1108	1	-	18/26/102/115	-
20	SQD	5	822	-	-	7/24/44/69	0/1/1/1
13	CLA	H	1222	21	-	7/33/109/115	-
13	CLA	3	517	-	-	9/15/91/115	-
13	CLA	G	1125	1	-	15/39/115/115	-
13	CLA	c	512	12	-	7/15/91/115	-
13	CLA	H	1235	2	-	8/39/115/115	-
13	CLA	e	1115	1	-	12/33/109/115	-
13	CLA	f	1229	2	-	13/39/115/115	-
16	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	t	511	12	-	5/15/91/115	-
13	CLA	H	1211	2	-	4/29/105/115	-
13	CLA	f	1238	21	-	4/39/115/115	-
16	BCR	f	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1110	1	-	11/23/99/115	-
13	CLA	G	1121	1	-	8/27/103/115	-
13	CLA	d	508	12	-	5/15/91/115	-
13	CLA	d	516	12	-	10/15/91/115	-
13	CLA	1	502	12	-	16/33/109/115	-
13	CLA	A	1237	21	-	21/39/115/115	-
13	CLA	d	502	12	-	7/21/97/115	-
13	CLA	f	1212	2	-	11/27/103/115	-
13	CLA	B	1223	2	-	14/39/115/115	-
13	CLA	A	1134	1	-	13/29/105/115	-
16	BCR	G	4011	-	-	12/29/63/63	0/2/2/2
16	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	f	1021	2	-	13/39/115/115	-
16	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
17	LHG	B	1842	13	-	22/43/43/53	-
16	BCR	3	521	-	-	7/29/63/63	0/2/2/2
13	CLA	s	508	12	-	7/27/103/115	-
13	CLA	H	1203	2	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	H	1229	2	-	13/39/115/115	-
13	CLA	a	506	12	-	5/21/97/115	-
13	CLA	J	1303	8	-	18/39/115/115	-
13	CLA	c	513	12	-	6/15/91/115	-
13	CLA	r	501	12	-	14/39/115/115	-
13	CLA	G	1128	1	-	12/39/115/115	-
16	BCR	H	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	t	506	12	-	4/15/91/115	-
17	LHG	n	5221	-	-	30/53/53/53	-
13	CLA	B	1210	2	-	21/39/115/115	-
13	CLA	H	1219	2	-	19/39/115/115	-
13	CLA	t	518	12	-	10/27/103/115	-
13	CLA	A	1103	1	-	20/39/115/115	-
16	BCR	5	524	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1224	2	-	13/33/109/115	-
15	SF4	g	3002	3	-	-	0/6/5/5
16	BCR	2	523	-	-	6/29/63/63	0/2/2/2
13	CLA	q	511	12	-	4/27/103/115	-
13	CLA	G	1130	1	-	9/39/115/115	-
13	CLA	5	507	-	-	7/15/91/115	-
13	CLA	Y	507	-	-	16/33/109/115	-
13	CLA	f	1202	2	-	13/39/115/115	-
16	BCR	1	523	-	-	6/29/63/63	0/2/2/2
16	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
16	BCR	b	523	-	-	5/29/63/63	0/2/2/2
13	CLA	4	512	12	-	5/15/91/115	-
13	CLA	t	507	-	-	8/15/91/115	-
20	SQD	c	822	-	-	7/24/44/69	0/1/1/1
16	BCR	d	524	-	-	5/29/63/63	0/2/2/2
13	CLA	s	518	12	-	12/27/103/115	-
13	CLA	b	516	12	-	9/15/91/115	-
16	BCR	v	523	-	-	4/29/63/63	0/2/2/2
13	CLA	Z	509	12	-	6/39/115/115	-
13	CLA	A	1126	1	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	5	509	12	-	12/39/115/115	-
13	CLA	c	501	12	-	21/39/115/115	-
13	CLA	d	507	-	-	6/15/91/115	-
13	CLA	f	1225	2	-	7/39/115/115	-
13	CLA	5	519	12	-	10/17/93/115	-
13	CLA	Y	519	12	-	8/21/97/115	-
13	CLA	d	505	12	-	15/39/115/115	-
17	LHG	k	5001	-	-	22/48/48/53	-
13	CLA	4	519	12	-	14/27/103/115	-
16	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
16	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	3	503	12	-	9/39/115/115	-
13	CLA	s	505	12	-	20/39/115/115	-
16	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
16	BCR	s	521	-	-	7/29/63/63	0/2/2/2
13	CLA	d	519	12	-	8/17/93/115	-
13	CLA	f	1226	2	-	12/39/115/115	-
16	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	H	1209	2	-	8/24/100/115	-
17	LHG	G	5009	-	-	28/53/53/53	-
16	BCR	c	523	-	-	4/29/63/63	0/2/2/2
13	CLA	2	513	12	-	17/39/115/115	-
13	CLA	A	1131	1	-	8/39/115/115	-
13	CLA	f	1023	-	-	10/39/115/115	-
13	CLA	G	1102	1	-	11/39/115/115	-
13	CLA	c	516	12	-	4/15/91/115	-
13	CLA	3	512	12	-	5/15/91/115	-
17	LHG	H	1855	-	-	28/48/48/53	-
13	CLA	V	1503	21	-	10/33/109/115	-
16	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	3	509	12	-	4/39/115/115	-
17	LHG	A	5008	-	-	19/39/39/53	-
17	LHG	e	5001	-	-	25/53/53/53	-
17	LHG	A	5005	-	-	29/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	e	5003	13	-	17/45/45/53	-
16	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1132	1	-	17/39/115/115	-
13	CLA	Y	503	12	-	11/38/114/115	-
13	CLA	e	1105	1	-	6/27/103/115	-
13	CLA	2	508	12	-	8/27/103/115	-
13	CLA	Z	504	-	-	7/21/97/115	-
13	CLA	5	505	12	-	16/35/111/115	-
13	CLA	2	502	12	-	13/33/109/115	-
13	CLA	q	505	12	-	11/39/115/115	-
16	BCR	5	521	-	-	7/29/63/63	0/2/2/2
13	CLA	f	1224	2	-	13/33/109/115	-
13	CLA	1	510	12	-	13/39/115/115	-
16	BCR	r	524	-	-	2/29/63/63	0/2/2/2
17	LHG	e	5009	-	-	28/53/53/53	-
18	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	s	504	-	-	6/15/91/115	-
13	CLA	1	516	12	-	15/15/91/115	-
13	CLA	Y	513	12	-	4/27/103/115	-
13	CLA	b	513	12	-	9/15/91/115	-
13	CLA	G	1123	21	-	11/39/115/115	-
13	CLA	r	516	12	-	10/15/91/115	-
13	CLA	e	1011	1	-	11/39/115/115	-
13	CLA	G	1237	21	-	20/39/115/115	-
16	BCR	6	523	-	-	4/29/63/63	0/2/2/2
18	LMU	e	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	q	512	12	-	12/24/100/115	-
18	LMU	r	901	-	-	8/14/34/61	0/1/1/2
17	LHG	e	5004	-	-	21/40/40/53	-
13	CLA	G	1140	1	-	13/39/115/115	-
13	CLA	6	516	12	-	10/15/91/115	-
13	CLA	H	1206	2	-	15/39/115/115	-
16	BCR	q	521	-	-	7/29/63/63	0/2/2/2
13	CLA	K	1105	9	-	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	5	508	12	-	6/15/91/115	-
13	CLA	f	1231	21	-	8/39/115/115	-
17	LHG	H	1842	13	-	22/43/43/53	-
13	CLA	5	502	12	-	7/21/97/115	-
13	CLA	Y	502	12	-	16/33/109/115	-
13	CLA	e	1134	1	-	13/29/105/115	-
13	CLA	s	517	-	-	9/15/91/115	-
13	CLA	m	1105	9	-	11/15/91/115	-
13	CLA	t	502	12	-	7/21/97/115	-
13	CLA	3	501	12	-	6/39/115/115	-
13	CLA	G	1137	1	-	19/39/115/115	-
13	CLA	a	503	12	-	9/39/115/115	-
13	CLA	B	1021	2	-	12/39/115/115	-
18	LMU	l	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	v	502	12	-	7/21/97/115	-
13	CLA	3	504	-	-	6/15/91/115	-
13	CLA	d	517	-	-	11/15/91/115	-
13	CLA	B	1204	2	-	13/39/115/115	-
20	SQD	V	5216	-	-	17/46/66/69	0/1/1/1

All (5705) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C12-C13	8.71	1.53	1.33
14	f	2002	PQN	C12-C13	8.70	1.53	1.33
14	H	2002	PQN	C12-C13	8.70	1.53	1.33
14	G	2001	PQN	C12-C13	8.66	1.53	1.33
14	e	2001	PQN	C12-C13	8.66	1.53	1.33
14	A	2001	PQN	C12-C13	8.65	1.53	1.33
14	f	2002	PQN	O1-C1	7.82	1.39	1.23
14	B	2002	PQN	O1-C1	7.81	1.39	1.23
14	G	2001	PQN	O1-C1	7.78	1.39	1.23
14	H	2002	PQN	O1-C1	7.77	1.39	1.23
14	e	2001	PQN	O1-C1	7.77	1.39	1.23
14	A	2001	PQN	O1-C1	7.75	1.39	1.23
14	e	2001	PQN	O4-C4	7.56	1.39	1.23
14	A	2001	PQN	O4-C4	7.56	1.39	1.23
14	G	2001	PQN	O4-C4	7.53	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	2002	PQN	O4-C4	7.43	1.38	1.23
14	f	2002	PQN	O4-C4	7.41	1.38	1.23
14	B	2002	PQN	O4-C4	7.41	1.38	1.23
14	B	2002	PQN	C2-C1	-4.90	1.37	1.48
14	f	2002	PQN	C2-C1	-4.89	1.37	1.48
14	H	2002	PQN	C2-C1	-4.86	1.37	1.48
14	e	2001	PQN	C2-C1	-4.44	1.38	1.48
14	A	2001	PQN	C2-C1	-4.42	1.38	1.48
14	G	2001	PQN	C2-C1	-4.41	1.38	1.48
13	e	1011	CLA	C1D-ND	4.37	1.43	1.37
13	A	1011	CLA	C1D-ND	4.37	1.43	1.37
13	G	1011	CLA	C1D-ND	4.35	1.43	1.37
13	b	503	CLA	C1D-ND	4.14	1.42	1.37
13	t	503	CLA	C1D-ND	4.12	1.42	1.37
13	4	503	CLA	C1D-ND	4.11	1.42	1.37
13	e	1128	CLA	CMB-C2B	-4.09	1.42	1.50
13	f	1234	CLA	C4D-ND	-4.08	1.32	1.37
13	H	1234	CLA	C4D-ND	-4.08	1.32	1.37
13	G	1128	CLA	CMB-C2B	-4.07	1.42	1.50
13	A	1128	CLA	CMB-C2B	-4.06	1.42	1.50
13	H	1226	CLA	CMB-C2B	-4.06	1.42	1.50
13	B	1226	CLA	CMB-C2B	-4.05	1.42	1.50
13	c	503	CLA	C1D-ND	4.04	1.42	1.37
13	B	1234	CLA	C4D-ND	-4.04	1.32	1.37
13	f	1226	CLA	CMB-C2B	-4.04	1.42	1.50
13	s	503	CLA	C1D-ND	4.01	1.42	1.37
13	u	503	CLA	C1D-ND	4.00	1.42	1.37
13	a	503	CLA	C1D-ND	3.99	1.42	1.37
13	5	503	CLA	C1D-ND	3.98	1.42	1.37
13	t	516	CLA	C1D-ND	3.98	1.42	1.37
13	3	503	CLA	C1D-ND	3.97	1.42	1.37
13	q	503	CLA	C1D-ND	3.94	1.42	1.37
13	b	516	CLA	C1D-ND	3.92	1.42	1.37
13	1	503	CLA	C1D-ND	3.92	1.42	1.37
13	c	517	CLA	C1D-ND	3.92	1.42	1.37
13	t	510	CLA	C1D-ND	3.92	1.42	1.37
13	d	506	CLA	C1D-ND	3.91	1.42	1.37
13	Y	506	CLA	C1D-ND	3.91	1.42	1.37
13	4	516	CLA	C1D-ND	3.90	1.42	1.37
13	b	510	CLA	C1D-ND	3.90	1.42	1.37
13	6	506	CLA	C1D-ND	3.90	1.42	1.37
13	4	517	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	506	CLA	C1D-ND	3.89	1.42	1.37
13	3	506	CLA	C1D-ND	3.88	1.42	1.37
13	a	506	CLA	C1D-ND	3.88	1.42	1.37
13	2	503	CLA	C1D-ND	3.88	1.42	1.37
13	4	510	CLA	C1D-ND	3.88	1.42	1.37
13	5	517	CLA	C1D-ND	3.88	1.42	1.37
13	r	503	CLA	C1D-ND	3.88	1.42	1.37
13	v	506	CLA	C1D-ND	3.88	1.42	1.37
13	c	516	CLA	C1D-ND	3.88	1.42	1.37
13	r	511	CLA	C1D-ND	3.88	1.42	1.37
13	Y	503	CLA	C1D-ND	3.87	1.42	1.37
13	q	506	CLA	C1D-ND	3.87	1.42	1.37
13	Z	503	CLA	C1D-ND	3.87	1.42	1.37
13	b	517	CLA	C1D-ND	3.87	1.42	1.37
13	4	507	CLA	C1D-ND	3.85	1.42	1.37
13	a	513	CLA	C1D-ND	3.85	1.42	1.37
13	d	501	CLA	C1D-ND	3.85	1.42	1.37
13	4	513	CLA	C1D-ND	3.85	1.42	1.37
13	t	502	CLA	C1D-ND	3.84	1.42	1.37
13	t	513	CLA	C1D-ND	3.84	1.42	1.37
13	s	507	CLA	C1D-ND	3.84	1.42	1.37
13	b	513	CLA	C1D-ND	3.84	1.42	1.37
13	u	517	CLA	C1D-ND	3.84	1.42	1.37
18	G	1849	LMU	O5'-C1'	3.84	1.51	1.41
13	6	503	CLA	C1D-ND	3.84	1.42	1.37
13	a	507	CLA	C1D-ND	3.84	1.42	1.37
18	A	1849	LMU	O5'-C1'	3.83	1.51	1.41
13	t	517	CLA	C1D-ND	3.83	1.42	1.37
13	s	506	CLA	C1D-ND	3.83	1.42	1.37
13	b	502	CLA	C1D-ND	3.83	1.42	1.37
13	4	501	CLA	C1D-ND	3.83	1.42	1.37
18	e	1849	LMU	O5'-C1'	3.83	1.51	1.41
13	d	513	CLA	C1D-ND	3.83	1.42	1.37
13	t	507	CLA	C1D-ND	3.83	1.42	1.37
13	Y	507	CLA	C1D-ND	3.82	1.42	1.37
13	v	501	CLA	C1D-ND	3.82	1.42	1.37
13	t	501	CLA	C1D-ND	3.82	1.42	1.37
13	b	507	CLA	C1D-ND	3.82	1.42	1.37
13	Y	513	CLA	C1D-ND	3.81	1.42	1.37
13	5	516	CLA	C1D-ND	3.81	1.42	1.37
13	v	503	CLA	C1D-ND	3.81	1.42	1.37
13	6	501	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	519	CLA	C1D-ND	3.81	1.42	1.37
13	4	502	CLA	C1D-ND	3.81	1.42	1.37
13	v	519	CLA	C1D-ND	3.80	1.42	1.37
13	u	510	CLA	C1D-ND	3.80	1.42	1.37
13	b	509	CLA	C1D-ND	3.80	1.42	1.37
13	3	513	CLA	C1D-ND	3.80	1.42	1.37
13	b	501	CLA	C1D-ND	3.80	1.42	1.37
13	q	513	CLA	C1D-ND	3.80	1.42	1.37
13	1	513	CLA	C1D-ND	3.80	1.42	1.37
13	v	502	CLA	C1D-ND	3.79	1.42	1.37
13	d	503	CLA	C1D-ND	3.79	1.42	1.37
13	r	516	CLA	C1D-ND	3.79	1.42	1.37
13	2	511	CLA	C1D-ND	3.79	1.42	1.37
13	u	508	CLA	C1D-ND	3.79	1.42	1.37
13	c	509	CLA	C1D-ND	3.79	1.42	1.37
13	5	508	CLA	C1D-ND	3.79	1.42	1.37
13	6	519	CLA	C1D-ND	3.79	1.42	1.37
13	Z	501	CLA	C1D-ND	3.79	1.42	1.37
13	f	1023	CLA	C4D-ND	-3.79	1.32	1.37
13	q	507	CLA	C1D-ND	3.79	1.42	1.37
13	s	501	CLA	C1D-ND	3.79	1.42	1.37
13	u	516	CLA	C1D-ND	3.79	1.42	1.37
13	t	509	CLA	C1D-ND	3.79	1.42	1.37
13	Z	511	CLA	C1D-ND	3.78	1.42	1.37
13	3	519	CLA	C1D-ND	3.78	1.42	1.37
13	6	513	CLA	C1D-ND	3.78	1.42	1.37
13	a	519	CLA	C1D-ND	3.78	1.42	1.37
13	v	509	CLA	C1D-ND	3.78	1.42	1.37
13	3	518	CLA	C1D-ND	3.78	1.42	1.37
13	Z	516	CLA	C1D-ND	3.78	1.42	1.37
13	a	518	CLA	C1D-ND	3.77	1.42	1.37
13	2	516	CLA	C1D-ND	3.77	1.42	1.37
13	a	501	CLA	C1D-ND	3.77	1.42	1.37
13	6	518	CLA	C1D-ND	3.77	1.42	1.37
13	s	518	CLA	C1D-ND	3.77	1.42	1.37
13	Z	513	CLA	C1D-ND	3.77	1.42	1.37
13	3	507	CLA	C1D-ND	3.77	1.42	1.37
13	6	502	CLA	C1D-ND	3.77	1.42	1.37
13	1	507	CLA	C1D-ND	3.76	1.42	1.37
13	r	501	CLA	C1D-ND	3.76	1.42	1.37
13	t	518	CLA	C1D-ND	3.76	1.42	1.37
13	d	510	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	513	CLA	C1D-ND	3.76	1.42	1.37
13	f	1229	CLA	C4D-ND	-3.76	1.32	1.37
13	4	509	CLA	C1D-ND	3.76	1.42	1.37
13	c	519	CLA	C1D-ND	3.76	1.42	1.37
13	2	506	CLA	C1D-ND	3.76	1.42	1.37
13	d	509	CLA	C1D-ND	3.76	1.42	1.37
13	G	1124	CLA	C1D-ND	3.76	1.42	1.37
13	b	518	CLA	C1D-ND	3.76	1.42	1.37
13	c	508	CLA	C1D-ND	3.75	1.42	1.37
13	d	511	CLA	C1D-ND	3.75	1.42	1.37
13	v	513	CLA	C1D-ND	3.75	1.42	1.37
13	e	1109	CLA	C4D-ND	-3.75	1.32	1.37
13	e	1135	CLA	C4D-ND	-3.75	1.32	1.37
13	s	511	CLA	C1D-ND	3.75	1.42	1.37
13	3	501	CLA	C1D-ND	3.75	1.42	1.37
13	6	511	CLA	C1D-ND	3.75	1.42	1.37
13	c	506	CLA	C1D-ND	3.75	1.42	1.37
13	6	507	CLA	C1D-ND	3.75	1.42	1.37
13	t	506	CLA	C1D-ND	3.75	1.42	1.37
13	u	504	CLA	C1D-ND	3.75	1.42	1.37
13	6	510	CLA	C1D-ND	3.74	1.42	1.37
13	5	509	CLA	C1D-ND	3.74	1.42	1.37
13	c	511	CLA	C1D-ND	3.74	1.42	1.37
13	v	517	CLA	C1D-ND	3.74	1.42	1.37
13	H	1229	CLA	C4D-ND	-3.74	1.32	1.37
13	A	1124	CLA	C1D-ND	3.74	1.42	1.37
13	5	513	CLA	C1D-ND	3.74	1.42	1.37
13	v	511	CLA	C1D-ND	3.74	1.42	1.37
13	H	1204	CLA	C4D-ND	-3.74	1.32	1.37
13	1	510	CLA	C1D-ND	3.74	1.42	1.37
13	Y	511	CLA	C1D-ND	3.74	1.42	1.37
13	d	518	CLA	C1D-ND	3.74	1.42	1.37
13	n	1502	CLA	C4D-ND	-3.74	1.32	1.37
13	Z	506	CLA	C1D-ND	3.74	1.42	1.37
13	B	1023	CLA	C4D-ND	-3.74	1.32	1.37
13	5	506	CLA	C1D-ND	3.74	1.42	1.37
13	2	501	CLA	C1D-ND	3.73	1.42	1.37
13	b	508	CLA	C1D-ND	3.73	1.42	1.37
13	s	519	CLA	C1D-ND	3.73	1.42	1.37
13	f	1204	CLA	C4D-ND	-3.73	1.32	1.37
13	6	509	CLA	C1D-ND	3.73	1.42	1.37
13	u	509	CLA	C1D-ND	3.73	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	502	CLA	C1D-ND	3.73	1.42	1.37
13	H	1023	CLA	C4D-ND	-3.73	1.32	1.37
13	B	1229	CLA	C4D-ND	-3.73	1.32	1.37
13	5	510	CLA	C1D-ND	3.73	1.42	1.37
13	4	504	CLA	C1D-ND	3.73	1.42	1.37
13	e	1124	CLA	C1D-ND	3.73	1.42	1.37
13	d	508	CLA	C1D-ND	3.72	1.42	1.37
13	4	506	CLA	C1D-ND	3.72	1.42	1.37
13	6	508	CLA	C1D-ND	3.72	1.42	1.37
13	v	518	CLA	C1D-ND	3.72	1.42	1.37
13	G	1116	CLA	C1D-ND	3.72	1.42	1.37
13	c	513	CLA	C1D-ND	3.72	1.42	1.37
13	r	506	CLA	C1D-ND	3.72	1.42	1.37
13	t	504	CLA	C1D-ND	3.72	1.42	1.37
13	t	511	CLA	C1D-ND	3.72	1.42	1.37
13	5	519	CLA	C1D-ND	3.72	1.42	1.37
13	Y	510	CLA	C1D-ND	3.72	1.42	1.37
13	b	506	CLA	C1D-ND	3.72	1.42	1.37
13	4	518	CLA	C1D-ND	3.72	1.42	1.37
13	q	501	CLA	C1D-ND	3.72	1.42	1.37
13	d	516	CLA	C1D-ND	3.72	1.42	1.37
13	u	511	CLA	C1D-ND	3.72	1.42	1.37
13	3	511	CLA	C1D-ND	3.71	1.42	1.37
13	Y	502	CLA	C1D-ND	3.71	1.42	1.37
13	v	507	CLA	C1D-ND	3.71	1.42	1.37
13	A	1109	CLA	C4D-ND	-3.71	1.32	1.37
13	5	504	CLA	C1D-ND	3.71	1.42	1.37
13	d	507	CLA	C1D-ND	3.71	1.42	1.37
13	B	1204	CLA	C4D-ND	-3.71	1.32	1.37
13	6	516	CLA	C1D-ND	3.71	1.42	1.37
13	c	504	CLA	C1D-ND	3.71	1.42	1.37
13	u	519	CLA	C1D-ND	3.71	1.42	1.37
13	G	1022	CLA	C4D-ND	-3.71	1.32	1.37
13	v	510	CLA	C1D-ND	3.71	1.42	1.37
13	A	1135	CLA	C4D-ND	-3.71	1.32	1.37
13	u	513	CLA	C1D-ND	3.70	1.42	1.37
13	G	1109	CLA	C4D-ND	-3.70	1.32	1.37
13	u	506	CLA	C1D-ND	3.70	1.42	1.37
13	4	508	CLA	C1D-ND	3.70	1.42	1.37
13	6	517	CLA	C1D-ND	3.70	1.42	1.37
13	a	508	CLA	C1D-ND	3.70	1.42	1.37
13	m	1105	CLA	C1D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	u	502	CLA	C1D-ND	3.70	1.42	1.37
13	e	1022	CLA	C4D-ND	-3.70	1.32	1.37
13	Y	501	CLA	C1D-ND	3.70	1.42	1.37
13	e	1116	CLA	C1D-ND	3.70	1.42	1.37
13	1	511	CLA	C1D-ND	3.70	1.42	1.37
13	f	1203	CLA	C4D-ND	-3.70	1.32	1.37
13	Y	517	CLA	C1D-ND	3.70	1.42	1.37
13	c	510	CLA	C1D-ND	3.70	1.42	1.37
13	v	516	CLA	C1D-ND	3.70	1.42	1.37
13	K	1105	CLA	C1D-ND	3.69	1.42	1.37
13	5	511	CLA	C1D-ND	3.69	1.42	1.37
13	a	511	CLA	C1D-ND	3.69	1.42	1.37
13	U	1105	CLA	C1D-ND	3.69	1.42	1.37
13	a	517	CLA	C1D-ND	3.69	1.42	1.37
13	4	511	CLA	C1D-ND	3.69	1.42	1.37
13	6	504	CLA	C1D-ND	3.69	1.42	1.37
13	a	510	CLA	C1D-ND	3.69	1.42	1.37
13	G	1135	CLA	C4D-ND	-3.69	1.32	1.37
13	1	517	CLA	C1D-ND	3.69	1.42	1.37
13	B	1203	CLA	C4D-ND	-3.69	1.32	1.37
13	v	508	CLA	C1D-ND	3.69	1.42	1.37
13	5	507	CLA	C1D-ND	3.68	1.42	1.37
13	1	501	CLA	C1D-ND	3.68	1.42	1.37
13	3	517	CLA	C1D-ND	3.68	1.42	1.37
13	5	502	CLA	C1D-ND	3.68	1.42	1.37
13	t	508	CLA	C1D-ND	3.68	1.42	1.37
13	2	513	CLA	C1D-ND	3.68	1.42	1.37
13	L	1502	CLA	C4D-ND	-3.68	1.32	1.37
13	2	519	CLA	C1D-ND	3.68	1.42	1.37
13	q	510	CLA	C1D-ND	3.67	1.42	1.37
13	q	517	CLA	C1D-ND	3.67	1.42	1.37
13	A	1022	CLA	C4D-ND	-3.67	1.32	1.37
13	d	504	CLA	C1D-ND	3.67	1.42	1.37
13	Z	508	CLA	C1D-ND	3.67	1.42	1.37
13	b	511	CLA	C1D-ND	3.67	1.42	1.37
13	u	518	CLA	C1D-ND	3.67	1.42	1.37
13	c	502	CLA	C1D-ND	3.67	1.42	1.37
13	s	517	CLA	C1D-ND	3.67	1.42	1.37
13	3	508	CLA	C1D-ND	3.66	1.42	1.37
13	Z	519	CLA	C1D-ND	3.66	1.42	1.37
13	b	504	CLA	C1D-ND	3.66	1.42	1.37
13	H	1203	CLA	C4D-ND	-3.66	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1116	CLA	C1D-ND	3.66	1.42	1.37
13	V	1502	CLA	C4D-ND	-3.66	1.32	1.37
13	1	502	CLA	C1D-ND	3.66	1.42	1.37
13	5	518	CLA	C1D-ND	3.66	1.42	1.37
13	n	1503	CLA	C1D-ND	3.66	1.42	1.37
13	f	1221	CLA	C4D-ND	-3.66	1.32	1.37
13	u	507	CLA	C1D-ND	3.65	1.42	1.37
13	1	509	CLA	C1D-ND	3.65	1.42	1.37
13	c	505	CLA	C1D-ND	3.65	1.42	1.37
13	H	1221	CLA	C4D-ND	-3.65	1.32	1.37
13	r	508	CLA	C1D-ND	3.65	1.42	1.37
13	2	508	CLA	C1D-ND	3.65	1.42	1.37
13	V	1503	CLA	C1D-ND	3.65	1.42	1.37
13	d	517	CLA	C1D-ND	3.65	1.42	1.37
13	e	1103	CLA	C4D-ND	-3.65	1.32	1.37
13	B	1225	CLA	C4D-ND	-3.65	1.32	1.37
13	r	519	CLA	C1D-ND	3.65	1.42	1.37
13	s	509	CLA	C1D-ND	3.65	1.42	1.37
13	d	505	CLA	C1D-ND	3.64	1.42	1.37
13	3	509	CLA	C1D-ND	3.64	1.42	1.37
13	5	501	CLA	C1D-ND	3.64	1.42	1.37
13	c	501	CLA	C1D-ND	3.64	1.42	1.37
13	r	513	CLA	C1D-ND	3.64	1.42	1.37
18	f	1843	LMU	O5'-C1'	3.64	1.51	1.41
18	H	1843	LMU	O5'-C1'	3.64	1.51	1.41
13	L	1503	CLA	C1D-ND	3.64	1.42	1.37
13	Z	510	CLA	C1D-ND	3.64	1.42	1.37
13	c	507	CLA	C1D-ND	3.64	1.42	1.37
13	Y	509	CLA	C1D-ND	3.64	1.42	1.37
13	a	509	CLA	C1D-ND	3.64	1.42	1.37
13	s	508	CLA	C1D-ND	3.64	1.42	1.37
13	4	505	CLA	C1D-ND	3.64	1.42	1.37
13	2	517	CLA	C1D-ND	3.63	1.42	1.37
13	f	1215	CLA	C4D-ND	-3.63	1.32	1.37
13	q	509	CLA	C1D-ND	3.63	1.42	1.37
13	v	505	CLA	C1D-ND	3.63	1.42	1.37
18	B	1843	LMU	O5'-C1'	3.63	1.51	1.41
13	H	1225	CLA	C4D-ND	-3.63	1.32	1.37
13	d	513	CLA	C4B-NB	3.62	1.42	1.37
13	6	505	CLA	C1D-ND	3.62	1.42	1.37
13	2	510	CLA	C1D-ND	3.62	1.42	1.37
13	b	505	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	504	CLA	C1D-ND	3.62	1.42	1.37
13	r	510	CLA	C1D-ND	3.62	1.42	1.37
13	e	1110	CLA	C1D-ND	3.62	1.42	1.37
13	5	505	CLA	C1D-ND	3.62	1.42	1.37
13	s	510	CLA	C1D-ND	3.62	1.42	1.37
13	2	518	CLA	C1D-ND	3.62	1.42	1.37
13	3	510	CLA	C1D-ND	3.62	1.42	1.37
13	r	507	CLA	C1D-ND	3.62	1.42	1.37
13	u	505	CLA	C1D-ND	3.61	1.42	1.37
13	G	1110	CLA	C1D-ND	3.61	1.42	1.37
13	f	1218	CLA	C1D-ND	3.61	1.42	1.37
13	G	1103	CLA	C4D-ND	-3.61	1.32	1.37
13	f	1223	CLA	C4D-ND	-3.61	1.32	1.37
13	q	502	CLA	C1D-ND	3.61	1.42	1.37
13	t	505	CLA	C1D-ND	3.61	1.42	1.37
13	Z	517	CLA	C1D-ND	3.61	1.42	1.37
13	H	1238	CLA	C4D-ND	-3.61	1.32	1.37
13	1	505	CLA	C1D-ND	3.61	1.42	1.37
13	q	511	CLA	C1D-ND	3.61	1.42	1.37
13	e	1120	CLA	C4D-ND	-3.61	1.32	1.37
13	A	1140	CLA	C1D-ND	3.60	1.42	1.37
13	Y	508	CLA	C1D-ND	3.60	1.42	1.37
13	A	1103	CLA	C4D-ND	-3.60	1.32	1.37
13	f	1225	CLA	C4D-ND	-3.60	1.32	1.37
13	6	513	CLA	C4B-NB	3.60	1.42	1.37
13	B	1221	CLA	C4D-ND	-3.60	1.32	1.37
13	u	501	CLA	C1D-ND	3.60	1.42	1.37
13	H	1215	CLA	C4D-ND	-3.60	1.32	1.37
13	Z	509	CLA	C1D-ND	3.60	1.42	1.37
13	B	1223	CLA	C4D-ND	-3.60	1.32	1.37
13	e	1136	CLA	C1D-ND	3.60	1.42	1.37
13	L	1501	CLA	C1D-ND	3.60	1.42	1.37
13	e	1801	CLA	C1D-ND	3.60	1.42	1.37
13	q	508	CLA	C1D-ND	3.60	1.42	1.37
13	B	1215	CLA	C4D-ND	-3.60	1.32	1.37
13	1	508	CLA	C1D-ND	3.60	1.42	1.37
13	Z	518	CLA	C1D-ND	3.60	1.42	1.37
13	A	1110	CLA	C1D-ND	3.59	1.42	1.37
13	A	1131	CLA	C1D-ND	3.59	1.42	1.37
13	2	507	CLA	C1D-ND	3.59	1.42	1.37
13	r	517	CLA	C1D-ND	3.59	1.42	1.37
13	H	1222	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1211	CLA	C1D-ND	3.59	1.42	1.37
13	V	1501	CLA	C1D-ND	3.59	1.42	1.37
13	f	1222	CLA	C1D-ND	3.59	1.42	1.37
13	H	1209	CLA	C1D-ND	3.59	1.42	1.37
13	B	1222	CLA	C1D-ND	3.59	1.42	1.37
13	e	1131	CLA	C1D-ND	3.59	1.42	1.37
13	2	509	CLA	C1D-ND	3.59	1.42	1.37
13	f	1209	CLA	C1D-ND	3.59	1.42	1.37
13	c	518	CLA	C1D-ND	3.58	1.42	1.37
13	e	1140	CLA	C1D-ND	3.58	1.42	1.37
13	B	1211	CLA	C1D-ND	3.58	1.42	1.37
13	m	1103	CLA	C1D-ND	3.58	1.42	1.37
13	H	1223	CLA	C4D-ND	-3.58	1.32	1.37
13	G	1140	CLA	C1D-ND	3.58	1.42	1.37
13	q	505	CLA	C1D-ND	3.58	1.42	1.37
13	A	1801	CLA	C4D-ND	-3.58	1.32	1.37
13	e	1801	CLA	C4D-ND	-3.58	1.32	1.37
13	G	1140	CLA	C4D-ND	-3.58	1.32	1.37
13	G	1131	CLA	C1D-ND	3.58	1.42	1.37
13	Y	505	CLA	C1D-ND	3.58	1.42	1.37
18	q	902	LMU	O5'-C1'	3.58	1.51	1.41
13	r	509	CLA	C1D-ND	3.58	1.42	1.37
13	s	502	CLA	C1D-ND	3.58	1.42	1.37
13	A	1120	CLA	C4D-ND	-3.57	1.32	1.37
13	A	1122	CLA	C1D-ND	3.57	1.42	1.37
13	H	1218	CLA	C1D-ND	3.57	1.42	1.37
18	1	902	LMU	O5'-C1'	3.57	1.50	1.41
13	u	512	CLA	C1D-ND	3.57	1.42	1.37
13	B	1236	CLA	C1D-ND	3.57	1.42	1.37
13	Z	507	CLA	C1D-ND	3.57	1.42	1.37
18	J	5105	LMU	O5'-C1'	3.57	1.50	1.41
18	l	5105	LMU	O5'-C1'	3.57	1.50	1.41
13	H	1240	CLA	C1D-ND	3.57	1.42	1.37
18	Y	902	LMU	O5'-C1'	3.57	1.50	1.41
13	5	512	CLA	C1D-ND	3.57	1.42	1.37
13	G	1136	CLA	C1D-ND	3.57	1.42	1.37
13	B	1218	CLA	C1D-ND	3.57	1.42	1.37
13	e	1137	CLA	C1D-ND	3.56	1.42	1.37
13	r	518	CLA	C1D-ND	3.56	1.42	1.37
13	G	1122	CLA	C1D-ND	3.56	1.42	1.37
13	A	1140	CLA	C4D-ND	-3.56	1.32	1.37
13	A	1801	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1211	CLA	C1D-ND	3.56	1.42	1.37
13	B	1209	CLA	C1D-ND	3.56	1.42	1.37
13	r	502	CLA	C1D-ND	3.56	1.42	1.37
13	2	504	CLA	C1D-ND	3.56	1.42	1.37
13	G	1801	CLA	C4D-ND	-3.55	1.32	1.37
13	s	505	CLA	C1D-ND	3.55	1.42	1.37
18	G	1848	LMU	O5B-C1B	3.55	1.50	1.41
13	H	1230	CLA	C4D-ND	-3.55	1.32	1.37
13	3	502	CLA	C1D-ND	3.55	1.42	1.37
18	T	5105	LMU	O5'-C1'	3.55	1.50	1.41
13	Y	516	CLA	C1D-ND	3.55	1.42	1.37
13	e	1140	CLA	C4D-ND	-3.55	1.32	1.37
13	f	1236	CLA	C1D-ND	3.55	1.42	1.37
13	G	1104	CLA	C4D-ND	-3.54	1.32	1.37
13	f	1238	CLA	C4D-ND	-3.54	1.32	1.37
13	G	1129	CLA	C4D-ND	-3.54	1.32	1.37
13	K	1401	CLA	C1D-ND	3.54	1.42	1.37
13	f	1232	CLA	C1D-ND	3.54	1.42	1.37
13	B	1238	CLA	C4D-ND	-3.54	1.32	1.37
13	l	1302	CLA	C1D-ND	3.54	1.42	1.37
13	A	1136	CLA	C1D-ND	3.54	1.42	1.37
13	U	1103	CLA	C1D-ND	3.54	1.42	1.37
13	J	1302	CLA	C1D-ND	3.54	1.42	1.37
13	e	1129	CLA	C4D-ND	-3.54	1.32	1.37
13	U	1401	CLA	C1D-ND	3.54	1.42	1.37
18	A	1848	LMU	O5B-C1B	3.54	1.50	1.41
13	3	505	CLA	C1D-ND	3.54	1.42	1.37
13	T	1302	CLA	C1D-ND	3.54	1.42	1.37
13	H	1236	CLA	C1D-ND	3.53	1.42	1.37
13	m	1401	CLA	C1D-ND	3.53	1.42	1.37
13	A	1129	CLA	C4D-ND	-3.53	1.32	1.37
13	H	1224	CLA	C4D-ND	-3.53	1.32	1.37
13	G	1111	CLA	C1D-ND	3.53	1.42	1.37
13	n	1501	CLA	C1D-ND	3.53	1.42	1.37
18	e	1848	LMU	O5B-C1B	3.53	1.50	1.41
13	c	512	CLA	C1D-ND	3.52	1.42	1.37
13	e	1122	CLA	C1D-ND	3.52	1.42	1.37
13	e	1128	CLA	C4D-ND	-3.52	1.32	1.37
13	H	1210	CLA	C1D-ND	3.52	1.42	1.37
13	Y	504	CLA	C1D-ND	3.52	1.42	1.37
13	B	1210	CLA	C1D-ND	3.52	1.42	1.37
13	d	512	CLA	C1D-ND	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1104	CLA	C4D-ND	-3.52	1.32	1.37
13	a	502	CLA	C1D-ND	3.52	1.42	1.37
13	A	1137	CLA	C1D-ND	3.52	1.42	1.37
13	K	1103	CLA	C1D-ND	3.52	1.42	1.37
13	1	516	CLA	C1D-ND	3.52	1.42	1.37
13	J	1303	CLA	C1D-ND	3.52	1.42	1.37
13	l	1303	CLA	C1D-ND	3.52	1.42	1.37
13	G	1120	CLA	C4D-ND	-3.52	1.32	1.37
13	v	513	CLA	C4B-NB	3.52	1.42	1.37
13	f	1224	CLA	C4D-ND	-3.52	1.32	1.37
13	B	1224	CLA	C4D-ND	-3.51	1.32	1.37
13	Z	504	CLA	C1D-ND	3.51	1.42	1.37
13	f	1210	CLA	C1D-ND	3.51	1.42	1.37
13	v	512	CLA	C1D-ND	3.51	1.42	1.37
13	6	512	CLA	C1D-ND	3.51	1.42	1.37
13	H	1212	CLA	C1D-ND	3.51	1.42	1.37
13	A	1111	CLA	C4D-ND	-3.51	1.32	1.37
13	B	1240	CLA	C1D-ND	3.51	1.42	1.37
13	2	502	CLA	C1D-ND	3.50	1.42	1.37
13	B	1230	CLA	C4D-ND	-3.50	1.32	1.37
13	G	1128	CLA	C4D-ND	-3.50	1.32	1.37
13	e	1104	CLA	C4D-ND	-3.50	1.32	1.37
13	H	1232	CLA	C1D-ND	3.50	1.42	1.37
13	B	1232	CLA	C1D-ND	3.50	1.42	1.37
13	A	1128	CLA	C4D-ND	-3.50	1.32	1.37
13	G	1107	CLA	C4D-ND	-3.50	1.32	1.37
13	f	1222	CLA	C4D-ND	-3.50	1.32	1.37
13	q	516	CLA	C1D-ND	3.50	1.42	1.37
13	a	505	CLA	C1D-ND	3.49	1.42	1.37
13	r	504	CLA	C1D-ND	3.49	1.42	1.37
13	H	1226	CLA	CMD-C2D	-3.49	1.43	1.50
13	A	1107	CLA	C4D-ND	-3.49	1.32	1.37
13	B	1222	CLA	C4D-ND	-3.49	1.32	1.37
13	e	1117	CLA	C1D-ND	3.49	1.42	1.37
13	G	1132	CLA	C4D-ND	-3.49	1.32	1.37
13	G	1111	CLA	C4D-ND	-3.48	1.32	1.37
13	u	513	CLA	C4B-NB	3.48	1.42	1.37
13	B	1239	CLA	C1D-ND	3.48	1.42	1.37
13	B	1226	CLA	CMD-C2D	-3.48	1.43	1.50
13	A	1106	CLA	C4D-ND	-3.48	1.32	1.37
13	e	1111	CLA	C4D-ND	-3.48	1.32	1.37
13	f	1230	CLA	C4D-ND	-3.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1236	CLA	C4D-ND	-3.48	1.32	1.37
13	T	1303	CLA	C1D-ND	3.47	1.42	1.37
13	q	519	CLA	C4D-ND	-3.47	1.32	1.37
13	G	1801	CLA	C1D-ND	3.47	1.42	1.37
13	f	1239	CLA	C1D-ND	3.47	1.42	1.37
13	B	1212	CLA	C1D-ND	3.47	1.42	1.37
13	G	1106	CLA	C4D-ND	-3.47	1.32	1.37
13	A	1117	CLA	C1D-ND	3.47	1.42	1.37
13	f	1226	CLA	CMD-C2D	-3.47	1.43	1.50
13	H	1239	CLA	C1D-ND	3.47	1.42	1.37
13	G	1137	CLA	C1D-ND	3.47	1.42	1.37
13	j	1301	CLA	C1D-ND	3.46	1.42	1.37
13	t	512	CLA	C1D-ND	3.46	1.42	1.37
13	t	519	CLA	C4D-ND	-3.46	1.32	1.37
13	e	1107	CLA	C4D-ND	-3.46	1.32	1.37
13	A	1111	CLA	C1D-ND	3.46	1.42	1.37
13	f	1240	CLA	C1D-ND	3.46	1.42	1.37
13	e	1114	CLA	C1D-ND	3.46	1.42	1.37
13	G	1119	CLA	C4D-ND	-3.45	1.32	1.37
13	1	519	CLA	C4D-ND	-3.45	1.32	1.37
13	H	1222	CLA	C4D-ND	-3.45	1.32	1.37
13	U	1401	CLA	C4D-ND	-3.45	1.32	1.37
13	a	508	CLA	C4B-NB	3.45	1.42	1.37
13	a	504	CLA	C1D-ND	3.45	1.42	1.37
13	1	504	CLA	C1D-ND	3.45	1.42	1.37
13	G	1114	CLA	C1D-ND	3.45	1.42	1.37
13	R	1301	CLA	C1D-ND	3.45	1.42	1.37
13	b	512	CLA	C1D-ND	3.45	1.42	1.37
13	G	1117	CLA	C1D-ND	3.45	1.42	1.37
13	Z	502	CLA	C1D-ND	3.45	1.42	1.37
13	B	1208	CLA	C1D-ND	3.45	1.42	1.37
13	F	1301	CLA	C1D-ND	3.45	1.42	1.37
13	f	1212	CLA	C1D-ND	3.45	1.42	1.37
13	H	1209	CLA	C4B-NB	3.45	1.42	1.37
13	s	504	CLA	C1D-ND	3.45	1.42	1.37
13	e	1105	CLA	C1D-ND	3.45	1.42	1.37
13	A	1114	CLA	C1D-ND	3.44	1.42	1.37
13	5	513	CLA	C4B-NB	3.44	1.42	1.37
13	G	1134	CLA	C1D-ND	3.44	1.42	1.37
13	K	1401	CLA	C4D-ND	-3.44	1.33	1.37
13	A	1122	CLA	C4D-ND	-3.44	1.33	1.37
13	A	1101	CLA	C3B-C4B	3.44	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1115	CLA	C4D-ND	-3.44	1.33	1.37
13	f	1208	CLA	C1D-ND	3.44	1.42	1.37
13	f	1213	CLA	C1D-ND	3.43	1.42	1.37
13	A	1134	CLA	C1D-ND	3.43	1.42	1.37
13	G	1105	CLA	C1D-ND	3.43	1.42	1.37
13	t	512	CLA	C4B-NB	3.43	1.42	1.37
13	A	1119	CLA	C4D-ND	-3.43	1.33	1.37
13	4	512	CLA	C1D-ND	3.43	1.42	1.37
13	e	1109	CLA	C1D-ND	3.43	1.42	1.37
13	H	1210	CLA	C4D-ND	-3.43	1.33	1.37
13	Y	518	CLA	C4D-ND	-3.43	1.33	1.37
13	B	1220	CLA	C1D-ND	3.43	1.42	1.37
13	f	1209	CLA	C4B-NB	3.43	1.42	1.37
18	Z	901	LMU	O5'-C1'	3.43	1.50	1.41
13	f	1201	CLA	C1D-ND	3.43	1.42	1.37
13	H	1236	CLA	C4D-ND	-3.43	1.33	1.37
13	e	1127	CLA	C4D-ND	-3.43	1.33	1.37
18	H	1843	LMU	O5B-C1B	3.43	1.50	1.41
13	B	1207	CLA	C1D-ND	3.43	1.42	1.37
13	B	1209	CLA	C4B-NB	3.42	1.42	1.37
13	f	1207	CLA	C1D-ND	3.42	1.42	1.37
13	e	1132	CLA	C4D-ND	-3.42	1.33	1.37
18	2	901	LMU	O5'-C1'	3.42	1.50	1.41
13	A	1108	CLA	C1D-ND	3.42	1.42	1.37
13	H	1207	CLA	C1D-ND	3.42	1.42	1.37
13	c	513	CLA	C4B-NB	3.42	1.42	1.37
13	H	1220	CLA	C1D-ND	3.42	1.42	1.37
18	f	1843	LMU	O5B-C1B	3.42	1.50	1.41
13	e	1134	CLA	C1D-ND	3.42	1.42	1.37
13	q	504	CLA	C1D-ND	3.42	1.42	1.37
13	B	1236	CLA	C4D-ND	-3.42	1.33	1.37
13	G	1101	CLA	C3B-C4B	3.42	1.50	1.42
13	e	1101	CLA	C3B-C4B	3.42	1.50	1.42
14	B	2002	PQN	C3-C4	-3.42	1.38	1.47
13	H	1208	CLA	C1D-ND	3.42	1.42	1.37
13	e	1136	CLA	C4D-ND	-3.42	1.33	1.37
13	e	1122	CLA	C4D-ND	-3.42	1.33	1.37
14	H	2002	PQN	C3-C4	-3.42	1.38	1.47
13	e	1137	CLA	C4D-ND	-3.42	1.33	1.37
18	B	1843	LMU	O5B-C1B	3.42	1.50	1.41
13	A	1136	CLA	C4D-ND	-3.41	1.33	1.37
13	G	1115	CLA	C4D-ND	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1106	CLA	C4D-ND	-3.41	1.33	1.37
13	A	1132	CLA	C4D-ND	-3.41	1.33	1.37
13	f	1223	CLA	C1D-ND	3.41	1.42	1.37
13	G	1122	CLA	C4D-ND	-3.41	1.33	1.37
18	r	901	LMU	O5'-C1'	3.41	1.50	1.41
13	2	505	CLA	C1D-ND	3.41	1.42	1.37
13	3	504	CLA	C1D-ND	3.41	1.42	1.37
13	4	512	CLA	C4B-NB	3.41	1.42	1.37
13	B	1201	CLA	C1D-ND	3.41	1.42	1.37
13	B	1213	CLA	C1D-ND	3.41	1.42	1.37
13	G	1127	CLA	C4D-ND	-3.41	1.33	1.37
13	f	1235	CLA	C1D-ND	3.41	1.42	1.37
13	Z	505	CLA	C1D-ND	3.41	1.42	1.37
13	c	517	CLA	C4B-NB	3.41	1.42	1.37
13	G	1125	CLA	C4D-ND	-3.41	1.33	1.37
13	e	1123	CLA	C1D-ND	3.41	1.42	1.37
13	v	517	CLA	C4B-NB	3.41	1.42	1.37
13	d	510	CLA	C4B-NB	3.41	1.42	1.37
13	v	510	CLA	C4B-NB	3.40	1.42	1.37
13	1	518	CLA	C4D-ND	-3.40	1.33	1.37
13	Y	519	CLA	C4D-ND	-3.40	1.33	1.37
13	A	1105	CLA	C1D-ND	3.40	1.42	1.37
13	f	1220	CLA	C1D-ND	3.40	1.42	1.37
13	s	516	CLA	C1D-ND	3.40	1.42	1.37
13	B	1210	CLA	C4D-ND	-3.40	1.33	1.37
13	3	508	CLA	C4B-NB	3.40	1.42	1.37
13	e	1108	CLA	C1D-ND	3.40	1.42	1.37
13	t	506	CLA	C4B-NB	3.40	1.42	1.37
13	A	1125	CLA	C4D-ND	-3.40	1.33	1.37
13	A	1123	CLA	C1D-ND	3.40	1.42	1.37
13	e	1132	CLA	C1D-ND	3.40	1.42	1.37
13	4	519	CLA	C4D-ND	-3.40	1.33	1.37
13	5	517	CLA	C4B-NB	3.40	1.42	1.37
13	e	1111	CLA	C1D-ND	3.40	1.42	1.37
13	G	1137	CLA	C4D-ND	-3.40	1.33	1.37
13	B	1202	CLA	C4D-ND	-3.40	1.33	1.37
13	b	512	CLA	C4B-NB	3.40	1.42	1.37
13	B	1223	CLA	C1D-ND	3.39	1.42	1.37
13	b	513	CLA	C4B-NB	3.39	1.42	1.37
13	6	510	CLA	C4B-NB	3.39	1.42	1.37
13	H	1235	CLA	C1D-ND	3.39	1.42	1.37
13	B	1209	CLA	C3B-C4B	3.39	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	501	CLA	C4B-NB	3.39	1.42	1.37
13	H	1213	CLA	C1D-ND	3.39	1.42	1.37
13	A	1108	CLA	C4D-ND	-3.39	1.33	1.37
13	H	1228	CLA	C4D-ND	-3.39	1.33	1.37
13	q	518	CLA	C4D-ND	-3.39	1.33	1.37
13	5	502	CLA	C4B-NB	3.39	1.42	1.37
13	3	516	CLA	C1D-ND	3.39	1.41	1.37
13	6	516	CLA	C4B-NB	3.39	1.41	1.37
13	G	1115	CLA	C1D-ND	3.39	1.41	1.37
13	a	516	CLA	C1D-ND	3.39	1.41	1.37
13	d	516	CLA	C4B-NB	3.39	1.41	1.37
14	f	2002	PQN	C3-C4	-3.39	1.38	1.47
13	A	1127	CLA	C4D-ND	-3.39	1.33	1.37
13	A	1137	CLA	C4D-ND	-3.38	1.33	1.37
13	e	1119	CLA	C4D-ND	-3.38	1.33	1.37
13	f	1210	CLA	C4D-ND	-3.38	1.33	1.37
13	A	1132	CLA	C1D-ND	3.38	1.41	1.37
13	4	506	CLA	C4B-NB	3.38	1.41	1.37
13	e	1115	CLA	C4D-ND	-3.38	1.33	1.37
13	G	1121	CLA	C1D-ND	3.38	1.41	1.37
13	B	1228	CLA	C4D-ND	-3.38	1.33	1.37
13	B	1235	CLA	C1D-ND	3.38	1.41	1.37
13	f	1209	CLA	C3B-C4B	3.38	1.50	1.42
13	A	1109	CLA	C1D-ND	3.38	1.41	1.37
13	G	1108	CLA	C1D-ND	3.38	1.41	1.37
13	f	1228	CLA	C4D-ND	-3.38	1.33	1.37
13	H	1209	CLA	C3B-C4B	3.38	1.50	1.42
13	Y	504	CLA	C4B-NB	3.38	1.41	1.37
13	4	513	CLA	C4B-NB	3.37	1.41	1.37
13	c	503	CLA	C4B-NB	3.37	1.41	1.37
13	H	1202	CLA	C4D-ND	-3.37	1.33	1.37
13	A	1130	CLA	C1D-ND	3.37	1.41	1.37
13	c	502	CLA	C4B-NB	3.37	1.41	1.37
13	m	1401	CLA	C4D-ND	-3.37	1.33	1.37
13	u	517	CLA	C4B-NB	3.37	1.41	1.37
13	H	1236	CLA	C4B-NB	3.37	1.41	1.37
13	G	1136	CLA	C4D-ND	-3.36	1.33	1.37
13	e	1108	CLA	C4D-ND	-3.36	1.33	1.37
13	r	513	CLA	C4B-NB	3.36	1.41	1.37
13	f	1235	CLA	C4D-ND	-3.36	1.33	1.37
13	e	1121	CLA	C1D-ND	3.36	1.41	1.37
13	H	1235	CLA	C4D-ND	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	2001	PQN	C3-C2	3.36	1.41	1.35
14	G	2001	PQN	C3-C2	3.36	1.41	1.35
13	H	1021	CLA	C4D-ND	-3.36	1.33	1.37
13	G	1123	CLA	C1D-ND	3.36	1.41	1.37
13	H	1223	CLA	C1D-ND	3.36	1.41	1.37
13	r	505	CLA	C1D-ND	3.36	1.41	1.37
13	H	1216	CLA	C4D-ND	-3.36	1.33	1.37
13	H	1201	CLA	C1D-ND	3.36	1.41	1.37
13	B	1021	CLA	C4D-ND	-3.36	1.33	1.37
13	B	1216	CLA	C4D-ND	-3.36	1.33	1.37
13	e	1125	CLA	C4D-ND	-3.35	1.33	1.37
13	G	1109	CLA	C1D-ND	3.35	1.41	1.37
13	H	1208	CLA	C4D-ND	-3.35	1.33	1.37
13	R	1301	CLA	C4D-ND	-3.35	1.33	1.37
13	f	1231	CLA	C4D-ND	-3.35	1.33	1.37
13	L	1503	CLA	C4D-ND	-3.35	1.33	1.37
13	G	1108	CLA	C4D-ND	-3.35	1.33	1.37
13	f	1202	CLA	C4D-ND	-3.35	1.33	1.37
13	H	1201	CLA	C4D-ND	-3.35	1.33	1.37
13	s	508	CLA	C4B-NB	3.35	1.41	1.37
13	f	1227	CLA	C4D-ND	-3.35	1.33	1.37
13	4	519	CLA	C1D-ND	3.35	1.41	1.37
13	e	1101	CLA	C4B-NB	3.34	1.41	1.37
14	G	2001	PQN	C3-C4	-3.34	1.38	1.47
13	f	1207	CLA	C4D-ND	-3.34	1.33	1.37
13	H	1203	CLA	C1D-ND	3.34	1.41	1.37
13	Z	504	CLA	C4B-NB	3.34	1.41	1.37
13	q	504	CLA	C4B-NB	3.34	1.41	1.37
13	A	1114	CLA	C4D-ND	-3.34	1.33	1.37
13	H	1214	CLA	C1D-ND	3.34	1.41	1.37
13	G	1138	CLA	C1D-ND	3.34	1.41	1.37
13	t	519	CLA	C1D-ND	3.34	1.41	1.37
13	b	519	CLA	C4D-ND	-3.34	1.33	1.37
13	B	1207	CLA	C4D-ND	-3.34	1.33	1.37
13	b	506	CLA	C4B-NB	3.34	1.41	1.37
13	v	506	CLA	C4B-NB	3.34	1.41	1.37
13	n	1503	CLA	C4D-ND	-3.34	1.33	1.37
13	t	513	CLA	C4B-NB	3.34	1.41	1.37
13	V	1503	CLA	C4D-ND	-3.34	1.33	1.37
13	G	1237	CLA	C1D-ND	3.33	1.41	1.37
14	e	2001	PQN	C3-C4	-3.33	1.38	1.47
13	6	517	CLA	C4B-NB	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1127	CLA	C1D-ND	3.33	1.41	1.37
13	e	1237	CLA	C1D-ND	3.33	1.41	1.37
13	f	1231	CLA	C1D-ND	3.33	1.41	1.37
13	A	1121	CLA	C1D-ND	3.33	1.41	1.37
13	e	1138	CLA	C1D-ND	3.33	1.41	1.37
13	H	1227	CLA	C4D-ND	-3.33	1.33	1.37
13	B	1203	CLA	C1D-ND	3.33	1.41	1.37
13	2	513	CLA	C4B-NB	3.33	1.41	1.37
13	d	517	CLA	C4B-NB	3.33	1.41	1.37
14	e	2001	PQN	C3-C2	3.33	1.41	1.35
13	F	1301	CLA	C4D-ND	-3.33	1.33	1.37
13	f	1216	CLA	C4D-ND	-3.33	1.33	1.37
13	1	501	CLA	C4B-NB	3.33	1.41	1.37
13	G	1113	CLA	C1D-ND	3.33	1.41	1.37
13	Z	513	CLA	C4B-NB	3.33	1.41	1.37
13	v	503	CLA	C4B-NB	3.33	1.41	1.37
13	A	1138	CLA	C4D-ND	-3.33	1.33	1.37
13	B	1235	CLA	C4D-ND	-3.33	1.33	1.37
13	H	1207	CLA	C4D-ND	-3.33	1.33	1.37
14	A	2001	PQN	C3-C4	-3.33	1.38	1.47
13	e	1130	CLA	C1D-ND	3.33	1.41	1.37
13	e	1114	CLA	C4D-ND	-3.33	1.33	1.37
13	G	1132	CLA	C1D-ND	3.33	1.41	1.37
13	G	1138	CLA	C4D-ND	-3.33	1.33	1.37
13	f	1021	CLA	C4D-ND	-3.33	1.33	1.37
13	b	519	CLA	C1D-ND	3.33	1.41	1.37
13	B	1236	CLA	C4B-NB	3.32	1.41	1.37
13	A	1115	CLA	C1D-ND	3.32	1.41	1.37
13	Y	501	CLA	C4B-NB	3.32	1.41	1.37
13	A	1237	CLA	C1D-ND	3.32	1.41	1.37
13	t	501	CLA	C4B-NB	3.32	1.41	1.37
13	1	504	CLA	C4B-NB	3.32	1.41	1.37
13	A	1101	CLA	C4B-NB	3.32	1.41	1.37
13	f	1236	CLA	C4B-NB	3.32	1.41	1.37
13	u	502	CLA	C4B-NB	3.32	1.41	1.37
13	u	506	CLA	C4B-NB	3.32	1.41	1.37
13	G	1130	CLA	C1D-ND	3.32	1.41	1.37
13	H	1231	CLA	C4D-ND	-3.32	1.33	1.37
13	v	512	CLA	C4B-NB	3.32	1.41	1.37
13	a	506	CLA	C4B-NB	3.31	1.41	1.37
13	j	1302	CLA	C1D-ND	3.31	1.41	1.37
13	e	1013	CLA	C4D-ND	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	517	CLA	C4B-NB	3.31	1.41	1.37
13	a	511	CLA	C4B-NB	3.31	1.41	1.37
13	b	503	CLA	C4B-NB	3.31	1.41	1.37
13	s	512	CLA	C1D-ND	3.31	1.41	1.37
13	t	511	CLA	C4B-NB	3.31	1.41	1.37
13	B	1227	CLA	C4D-ND	-3.31	1.33	1.37
13	f	1201	CLA	C4D-ND	-3.31	1.33	1.37
13	2	504	CLA	C4B-NB	3.31	1.41	1.37
13	B	1201	CLA	C4D-ND	-3.31	1.33	1.37
13	G	1013	CLA	C4D-ND	-3.31	1.33	1.37
13	3	511	CLA	C4B-NB	3.31	1.41	1.37
13	Y	513	CLA	C4B-NB	3.31	1.41	1.37
13	v	516	CLA	C4B-NB	3.31	1.41	1.37
13	B	1208	CLA	C4D-ND	-3.31	1.33	1.37
13	B	1206	CLA	C4D-ND	-3.31	1.33	1.37
13	B	1214	CLA	C1D-ND	3.31	1.41	1.37
13	u	503	CLA	C4B-NB	3.31	1.41	1.37
13	A	1138	CLA	C1D-ND	3.30	1.41	1.37
13	5	503	CLA	C4B-NB	3.30	1.41	1.37
13	6	503	CLA	C4B-NB	3.30	1.41	1.37
13	6	512	CLA	C4B-NB	3.30	1.41	1.37
13	A	1013	CLA	C4D-ND	-3.30	1.33	1.37
13	B	1231	CLA	C1D-ND	3.30	1.41	1.37
13	G	1127	CLA	C1D-ND	3.30	1.41	1.37
13	q	517	CLA	C4B-NB	3.30	1.41	1.37
13	r	504	CLA	C4B-NB	3.30	1.41	1.37
13	j	1301	CLA	C4D-ND	-3.30	1.33	1.37
13	b	501	CLA	C4B-NB	3.30	1.41	1.37
13	s	511	CLA	C4B-NB	3.30	1.41	1.37
13	u	516	CLA	C4B-NB	3.30	1.41	1.37
13	d	506	CLA	C4B-NB	3.30	1.41	1.37
13	m	1103	CLA	C4D-ND	-3.30	1.33	1.37
13	b	517	CLA	C4B-NB	3.30	1.41	1.37
13	A	1127	CLA	C1D-ND	3.30	1.41	1.37
13	H	1231	CLA	C1D-ND	3.30	1.41	1.37
13	e	1138	CLA	C4D-ND	-3.30	1.33	1.37
13	b	511	CLA	C4B-NB	3.29	1.41	1.37
13	4	511	CLA	C4B-NB	3.29	1.41	1.37
13	B	1231	CLA	C4D-ND	-3.29	1.33	1.37
13	1	512	CLA	C1D-ND	3.29	1.41	1.37
13	G	1125	CLA	C1D-ND	3.29	1.41	1.37
13	a	512	CLA	C1D-ND	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1115	CLA	C1D-ND	3.29	1.41	1.37
13	G	1126	CLA	C1D-ND	3.29	1.41	1.37
13	b	502	CLA	C4B-NB	3.29	1.41	1.37
13	G	1114	CLA	C4D-ND	-3.29	1.33	1.37
13	e	1139	CLA	C4D-ND	-3.29	1.33	1.37
13	B	1215	CLA	C1D-ND	3.29	1.41	1.37
13	f	1208	CLA	C4D-ND	-3.29	1.33	1.37
13	Y	519	CLA	C1D-ND	3.29	1.41	1.37
13	A	1126	CLA	C1D-ND	3.28	1.41	1.37
13	6	506	CLA	C4B-NB	3.28	1.41	1.37
13	G	1101	CLA	C4B-NB	3.28	1.41	1.37
13	d	519	CLA	C4B-NB	3.28	1.41	1.37
13	t	504	CLA	C4B-NB	3.28	1.41	1.37
13	H	1219	CLA	C4D-ND	-3.28	1.33	1.37
13	A	1113	CLA	C1D-ND	3.28	1.41	1.37
13	d	512	CLA	C4B-NB	3.28	1.41	1.37
13	Y	517	CLA	C4B-NB	3.28	1.41	1.37
13	u	511	CLA	C4B-NB	3.28	1.41	1.37
13	3	506	CLA	C4B-NB	3.28	1.41	1.37
13	5	506	CLA	C4B-NB	3.28	1.41	1.37
13	H	1215	CLA	C1D-ND	3.28	1.41	1.37
13	1	513	CLA	C4B-NB	3.27	1.41	1.37
13	4	501	CLA	C4B-NB	3.27	1.41	1.37
13	R	1302	CLA	C4B-NB	3.27	1.41	1.37
13	q	512	CLA	C1D-ND	3.27	1.41	1.37
13	G	1130	CLA	C4B-NB	3.27	1.41	1.37
13	f	1219	CLA	C1D-ND	3.27	1.41	1.37
13	2	511	CLA	C4B-NB	3.27	1.41	1.37
13	Y	508	CLA	C4D-ND	-3.27	1.33	1.37
13	1	517	CLA	C4B-NB	3.27	1.41	1.37
13	f	1203	CLA	C1D-ND	3.27	1.41	1.37
13	5	511	CLA	C4B-NB	3.27	1.41	1.37
13	Y	512	CLA	C1D-ND	3.27	1.41	1.37
13	A	1124	CLA	C4D-ND	-3.27	1.33	1.37
13	d	511	CLA	C4B-NB	3.27	1.41	1.37
13	e	1113	CLA	C1D-ND	3.27	1.41	1.37
13	1	519	CLA	C1D-ND	3.27	1.41	1.37
13	5	516	CLA	C4B-NB	3.27	1.41	1.37
13	H	1206	CLA	C4D-ND	-3.27	1.33	1.37
13	f	1206	CLA	C4D-ND	-3.27	1.33	1.37
13	v	509	CLA	C4B-NB	3.27	1.41	1.37
13	6	504	CLA	C4B-NB	3.27	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1124	CLA	C4D-ND	-3.27	1.33	1.37
13	Y	506	CLA	C4B-NB	3.27	1.41	1.37
13	c	516	CLA	C4B-NB	3.27	1.41	1.37
13	d	503	CLA	C4B-NB	3.27	1.41	1.37
13	u	504	CLA	C4B-NB	3.27	1.41	1.37
13	B	1219	CLA	C4D-ND	-3.27	1.33	1.37
13	e	1136	CLA	C3B-C4B	3.26	1.50	1.42
13	e	1130	CLA	C4B-NB	3.26	1.41	1.37
13	u	501	CLA	C4B-NB	3.26	1.41	1.37
13	v	519	CLA	C4B-NB	3.26	1.41	1.37
13	A	1136	CLA	C3B-C4B	3.26	1.50	1.42
13	4	502	CLA	C4B-NB	3.26	1.41	1.37
13	r	501	CLA	C4B-NB	3.26	1.41	1.37
13	G	1139	CLA	C4D-ND	-3.26	1.33	1.37
13	s	506	CLA	C4B-NB	3.26	1.41	1.37
13	G	1124	CLA	C4D-ND	-3.26	1.33	1.37
13	f	1214	CLA	C1D-ND	3.26	1.41	1.37
13	v	518	CLA	C4B-NB	3.26	1.41	1.37
13	t	518	CLA	C4B-NB	3.26	1.41	1.37
13	Z	511	CLA	C4B-NB	3.26	1.41	1.37
13	e	1126	CLA	C1D-ND	3.26	1.41	1.37
13	r	511	CLA	C4B-NB	3.26	1.41	1.37
13	b	510	CLA	C4B-NB	3.26	1.41	1.37
13	u	518	CLA	C4B-NB	3.26	1.41	1.37
13	4	503	CLA	C4B-NB	3.26	1.41	1.37
13	t	508	CLA	C4B-NB	3.26	1.41	1.37
13	B	1219	CLA	C1D-ND	3.26	1.41	1.37
13	F	1302	CLA	C1D-ND	3.26	1.41	1.37
13	A	1130	CLA	C4B-NB	3.25	1.41	1.37
13	Z	506	CLA	C4B-NB	3.25	1.41	1.37
13	f	1226	CLA	C4D-ND	-3.25	1.33	1.37
13	6	519	CLA	C4B-NB	3.25	1.41	1.37
13	a	509	CLA	C4B-NB	3.25	1.41	1.37
13	A	1139	CLA	C4D-ND	-3.25	1.33	1.37
13	Z	512	CLA	C1D-ND	3.25	1.41	1.37
13	f	1215	CLA	C1D-ND	3.25	1.41	1.37
13	3	512	CLA	C1D-ND	3.25	1.41	1.37
13	c	504	CLA	C4B-NB	3.25	1.41	1.37
13	b	518	CLA	C4B-NB	3.25	1.41	1.37
13	s	509	CLA	C4B-NB	3.25	1.41	1.37
13	c	511	CLA	C4B-NB	3.25	1.41	1.37
13	d	504	CLA	C4B-NB	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	506	CLA	C4B-NB	3.25	1.41	1.37
13	1	506	CLA	C4B-NB	3.25	1.41	1.37
13	t	503	CLA	C4B-NB	3.25	1.41	1.37
13	A	1125	CLA	C1D-ND	3.25	1.41	1.37
13	4	518	CLA	C4B-NB	3.25	1.41	1.37
13	Z	518	CLA	C4B-NB	3.25	1.41	1.37
13	G	1119	CLA	C1D-ND	3.25	1.41	1.37
13	d	518	CLA	C4B-NB	3.25	1.41	1.37
13	6	518	CLA	C4B-NB	3.25	1.41	1.37
13	A	1237	CLA	C4D-ND	-3.24	1.33	1.37
13	3	517	CLA	C4B-NB	3.24	1.41	1.37
13	4	504	CLA	C4B-NB	3.24	1.41	1.37
13	5	518	CLA	C4B-NB	3.24	1.41	1.37
13	f	1212	CLA	C4D-ND	-3.24	1.33	1.37
13	2	506	CLA	C4B-NB	3.24	1.41	1.37
13	r	517	CLA	C4B-NB	3.24	1.41	1.37
13	K	1103	CLA	C4D-ND	-3.24	1.33	1.37
13	H	1205	CLA	C4D-ND	-3.24	1.33	1.37
13	G	1101	CLA	C4D-ND	-3.24	1.33	1.37
13	4	508	CLA	C4B-NB	3.24	1.41	1.37
13	e	1125	CLA	C1D-ND	3.24	1.41	1.37
13	b	508	CLA	C4B-NB	3.24	1.41	1.37
13	A	1101	CLA	C4D-ND	-3.24	1.33	1.37
13	G	1237	CLA	C4D-ND	-3.24	1.33	1.37
13	f	1214	CLA	C4D-ND	-3.24	1.33	1.37
13	G	1116	CLA	C4D-ND	-3.24	1.33	1.37
13	j	1301	CLA	C3B-C4B	3.23	1.50	1.42
13	H	1012	CLA	C4D-ND	-3.23	1.33	1.37
13	e	1134	CLA	C4B-NB	3.23	1.41	1.37
13	a	502	CLA	C4B-NB	3.23	1.41	1.37
13	e	1118	CLA	C1D-ND	3.23	1.41	1.37
13	q	516	CLA	C4B-NB	3.23	1.41	1.37
13	1	503	CLA	C4B-NB	3.23	1.41	1.37
13	6	511	CLA	C4B-NB	3.23	1.41	1.37
13	B	1205	CLA	C4D-ND	-3.23	1.33	1.37
13	t	517	CLA	C4B-NB	3.23	1.41	1.37
13	3	502	CLA	C4B-NB	3.23	1.41	1.37
13	Y	509	CLA	C4B-NB	3.23	1.41	1.37
13	q	519	CLA	C1D-ND	3.23	1.41	1.37
13	Y	511	CLA	C4B-NB	3.23	1.41	1.37
13	B	1240	CLA	C4D-ND	-3.23	1.33	1.37
13	3	504	CLA	C4B-NB	3.23	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1221	CLA	C1D-ND	3.23	1.41	1.37
13	r	506	CLA	C4B-NB	3.23	1.41	1.37
13	s	517	CLA	C4B-NB	3.23	1.41	1.37
13	v	504	CLA	C4B-NB	3.23	1.41	1.37
13	e	1237	CLA	C4D-ND	-3.23	1.33	1.37
13	e	1101	CLA	C4D-ND	-3.23	1.33	1.37
13	3	509	CLA	C4B-NB	3.23	1.41	1.37
13	A	1102	CLA	C4D-ND	-3.23	1.33	1.37
13	e	1105	CLA	C4D-ND	-3.23	1.33	1.37
13	4	510	CLA	C4B-NB	3.23	1.41	1.37
13	f	1228	CLA	C1D-ND	3.23	1.41	1.37
13	q	513	CLA	C4B-NB	3.23	1.41	1.37
13	G	1136	CLA	C3B-C4B	3.22	1.50	1.42
13	2	501	CLA	C4B-NB	3.22	1.41	1.37
13	e	1118	CLA	C4D-ND	-3.22	1.33	1.37
13	A	1105	CLA	C4D-ND	-3.22	1.33	1.37
13	B	1212	CLA	C4D-ND	-3.22	1.33	1.37
13	1	508	CLA	C4D-ND	-3.22	1.33	1.37
13	f	1240	CLA	C4D-ND	-3.22	1.33	1.37
13	r	512	CLA	C1D-ND	3.22	1.41	1.37
13	6	509	CLA	C4B-NB	3.22	1.41	1.37
13	G	1118	CLA	C1D-ND	3.22	1.41	1.37
13	c	518	CLA	C4B-NB	3.22	1.41	1.37
13	V	1501	CLA	C4D-ND	-3.22	1.33	1.37
13	f	1012	CLA	C4D-ND	-3.22	1.33	1.37
13	B	1012	CLA	C4D-ND	-3.22	1.33	1.37
13	1	516	CLA	C4B-NB	3.22	1.41	1.37
13	f	1205	CLA	C1D-ND	3.22	1.41	1.37
13	G	1102	CLA	C4D-ND	-3.22	1.33	1.37
13	f	1219	CLA	C4D-ND	-3.22	1.33	1.37
13	B	1230	CLA	C1D-ND	3.22	1.41	1.37
13	2	512	CLA	C1D-ND	3.22	1.41	1.37
13	c	510	CLA	C4B-NB	3.22	1.41	1.37
13	H	1240	CLA	C4D-ND	-3.22	1.33	1.37
13	5	504	CLA	C4B-NB	3.22	1.41	1.37
13	q	511	CLA	C4B-NB	3.22	1.41	1.37
13	A	1116	CLA	C4D-ND	-3.22	1.33	1.37
13	j	1302	CLA	C4B-NB	3.21	1.41	1.37
13	G	1113	CLA	C4D-ND	-3.21	1.33	1.37
13	b	504	CLA	C4B-NB	3.21	1.41	1.37
13	G	1101	CLA	C1D-ND	3.21	1.41	1.37
13	q	503	CLA	C4B-NB	3.21	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	511	CLA	C4B-NB	3.21	1.41	1.37
13	f	1205	CLA	C4D-ND	-3.21	1.33	1.37
13	2	517	CLA	C4B-NB	3.21	1.41	1.37
13	6	508	CLA	C4B-NB	3.21	1.41	1.37
13	s	504	CLA	C4B-NB	3.21	1.41	1.37
13	B	1232	CLA	C4D-ND	-3.21	1.33	1.37
13	5	501	CLA	C4B-NB	3.21	1.41	1.37
13	c	506	CLA	C4B-NB	3.21	1.41	1.37
13	u	519	CLA	C4D-ND	-3.21	1.33	1.37
13	B	1224	CLA	C1D-ND	3.21	1.41	1.37
13	c	501	CLA	C4B-NB	3.21	1.41	1.37
13	d	508	CLA	C4B-NB	3.21	1.41	1.37
13	v	502	CLA	C4B-NB	3.21	1.41	1.37
13	L	1501	CLA	C4D-ND	-3.21	1.33	1.37
13	G	1133	CLA	C4D-ND	-3.21	1.33	1.37
13	R	1302	CLA	C1D-ND	3.21	1.41	1.37
13	e	1133	CLA	C1D-ND	3.21	1.41	1.37
13	B	1214	CLA	C4D-ND	-3.21	1.33	1.37
13	d	509	CLA	C4B-NB	3.21	1.41	1.37
13	5	519	CLA	C4D-ND	-3.21	1.33	1.37
13	F	1302	CLA	C4B-NB	3.21	1.41	1.37
13	G	1112	CLA	C1D-ND	3.21	1.41	1.37
13	Y	516	CLA	C4B-NB	3.21	1.41	1.37
13	H	1218	CLA	C4D-ND	-3.21	1.33	1.37
13	1	509	CLA	C4B-NB	3.21	1.41	1.37
13	1	511	CLA	C4B-NB	3.21	1.41	1.37
13	c	519	CLA	C4D-ND	-3.21	1.33	1.37
13	5	510	CLA	C4B-NB	3.21	1.41	1.37
13	G	1134	CLA	C4B-NB	3.21	1.41	1.37
13	Z	508	CLA	C4B-NB	3.21	1.41	1.37
13	H	1212	CLA	C4D-ND	-3.21	1.33	1.37
13	A	1119	CLA	C1D-ND	3.20	1.41	1.37
13	A	1134	CLA	C4B-NB	3.20	1.41	1.37
13	v	508	CLA	C4B-NB	3.20	1.41	1.37
20	b	822	SQD	O47-C7	3.20	1.42	1.35
20	v	822	SQD	O47-C7	3.20	1.42	1.35
13	H	1224	CLA	C1D-ND	3.20	1.41	1.37
13	H	1227	CLA	C1D-ND	3.20	1.41	1.37
13	F	1302	CLA	C4D-ND	-3.20	1.33	1.37
13	H	1217	CLA	C1D-ND	3.20	1.41	1.37
13	d	502	CLA	C4B-NB	3.20	1.41	1.37
13	r	503	CLA	C4B-NB	3.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	510	CLA	C4B-NB	3.20	1.41	1.37
13	F	1301	CLA	C3B-C4B	3.20	1.50	1.42
13	H	1221	CLA	C1D-ND	3.20	1.41	1.37
13	f	1232	CLA	C4D-ND	-3.20	1.33	1.37
13	u	508	CLA	C4B-NB	3.20	1.41	1.37
13	e	1116	CLA	C4D-ND	-3.20	1.33	1.37
13	e	1119	CLA	C1D-ND	3.20	1.41	1.37
13	n	1501	CLA	C4D-ND	-3.20	1.33	1.37
20	4	822	SQD	O47-C7	3.20	1.42	1.35
13	B	1205	CLA	C1D-ND	3.20	1.41	1.37
13	a	504	CLA	C4B-NB	3.20	1.41	1.37
13	a	517	CLA	C4B-NB	3.20	1.41	1.37
13	s	502	CLA	C4B-NB	3.20	1.41	1.37
13	e	1121	CLA	C4D-ND	-3.20	1.33	1.37
13	q	508	CLA	C4D-ND	-3.20	1.33	1.37
13	r	508	CLA	C4B-NB	3.20	1.41	1.37
13	e	1133	CLA	C4D-ND	-3.20	1.33	1.37
20	6	822	SQD	O47-C7	3.20	1.42	1.35
13	6	501	CLA	C4B-NB	3.20	1.41	1.37
13	Z	517	CLA	C4B-NB	3.20	1.41	1.37
13	j	1302	CLA	C4D-ND	-3.19	1.33	1.37
13	H	1205	CLA	C1D-ND	3.19	1.41	1.37
13	R	1301	CLA	C4B-NB	3.19	1.41	1.37
20	n	5216	SQD	O48-C23	3.19	1.42	1.33
13	R	1302	CLA	C4D-ND	-3.19	1.33	1.37
13	H	1238	CLA	C1D-ND	3.19	1.41	1.37
13	t	502	CLA	C4B-NB	3.19	1.41	1.37
13	G	1105	CLA	C4D-ND	-3.19	1.33	1.37
13	d	507	CLA	C4B-NB	3.19	1.41	1.37
13	r	518	CLA	C4B-NB	3.19	1.41	1.37
13	H	1220	CLA	C4D-ND	-3.19	1.33	1.37
20	d	822	SQD	O47-C7	3.19	1.42	1.35
13	A	1133	CLA	C4D-ND	-3.19	1.33	1.37
20	L	5216	SQD	O48-C23	3.19	1.42	1.33
13	A	1101	CLA	C1D-ND	3.19	1.41	1.37
13	H	1219	CLA	C1D-ND	3.19	1.41	1.37
13	d	501	CLA	C4B-NB	3.19	1.41	1.37
13	c	508	CLA	C4B-NB	3.19	1.41	1.37
13	t	509	CLA	C4B-NB	3.19	1.41	1.37
13	B	1220	CLA	C4D-ND	-3.18	1.33	1.37
13	H	1226	CLA	C4D-ND	-3.18	1.33	1.37
13	A	1112	CLA	C1D-ND	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1133	CLA	C1D-ND	3.18	1.41	1.37
13	u	512	CLA	C4B-NB	3.18	1.41	1.37
13	B	1226	CLA	C4D-ND	-3.18	1.33	1.37
13	B	1211	CLA	C4D-ND	-3.18	1.33	1.37
13	6	505	CLA	C4B-NB	3.18	1.41	1.37
13	r	502	CLA	C4B-NB	3.18	1.41	1.37
13	e	1113	CLA	C4D-ND	-3.18	1.33	1.37
13	B	1238	CLA	C1D-ND	3.18	1.41	1.37
13	a	503	CLA	C4B-NB	3.18	1.41	1.37
13	r	516	CLA	C4B-NB	3.18	1.41	1.37
13	e	1102	CLA	C4D-ND	-3.18	1.33	1.37
13	1	502	CLA	C4B-NB	3.18	1.41	1.37
13	5	508	CLA	C4B-NB	3.18	1.41	1.37
13	s	516	CLA	C4B-NB	3.18	1.41	1.37
13	B	1221	CLA	C1D-ND	3.18	1.41	1.37
13	6	502	CLA	C4B-NB	3.18	1.41	1.37
13	c	505	CLA	C4B-NB	3.18	1.41	1.37
13	v	505	CLA	C4B-NB	3.18	1.41	1.37
13	U	1103	CLA	C4D-ND	-3.18	1.33	1.37
13	2	516	CLA	C4B-NB	3.18	1.41	1.37
13	A	1118	CLA	C1D-ND	3.18	1.41	1.37
13	5	505	CLA	C4B-NB	3.18	1.41	1.37
13	H	1021	CLA	C1D-ND	3.18	1.41	1.37
13	A	1113	CLA	C4D-ND	-3.18	1.33	1.37
13	4	516	CLA	C4B-NB	3.17	1.41	1.37
13	G	1104	CLA	C1D-ND	3.17	1.41	1.37
13	v	501	CLA	C4B-NB	3.17	1.41	1.37
13	H	1214	CLA	C4D-ND	-3.17	1.33	1.37
13	Y	503	CLA	C4B-NB	3.17	1.41	1.37
13	G	1118	CLA	C4D-ND	-3.17	1.33	1.37
20	V	5216	SQD	O48-C23	3.17	1.42	1.33
13	A	1104	CLA	C1D-ND	3.17	1.41	1.37
13	B	1227	CLA	C1D-ND	3.17	1.41	1.37
13	f	1211	CLA	C4D-ND	-3.17	1.33	1.37
13	Z	516	CLA	C4B-NB	3.17	1.41	1.37
13	q	509	CLA	C4B-NB	3.17	1.41	1.37
13	u	510	CLA	C4B-NB	3.17	1.41	1.37
13	u	505	CLA	C4B-NB	3.17	1.41	1.37
13	A	1118	CLA	C4D-ND	-3.17	1.33	1.37
13	B	1218	CLA	C4D-ND	-3.17	1.33	1.37
13	Y	512	CLA	C4B-NB	3.17	1.41	1.37
13	s	516	CLA	C4D-ND	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	505	CLA	C4B-NB	3.17	1.41	1.37
13	R	1301	CLA	C3B-C4B	3.17	1.50	1.42
13	A	1137	CLA	C3B-C4B	3.17	1.50	1.42
13	H	1230	CLA	C1D-ND	3.17	1.41	1.37
13	G	1121	CLA	C4D-ND	-3.17	1.33	1.37
13	F	1301	CLA	C4B-NB	3.17	1.41	1.37
13	r	512	CLA	C4B-NB	3.17	1.41	1.37
13	b	516	CLA	C4B-NB	3.17	1.41	1.37
13	H	1228	CLA	C1D-ND	3.17	1.41	1.37
13	B	1021	CLA	C1D-ND	3.17	1.41	1.37
13	q	502	CLA	C4B-NB	3.17	1.41	1.37
13	f	1224	CLA	C1D-ND	3.16	1.41	1.37
13	t	507	CLA	C4B-NB	3.16	1.41	1.37
20	t	822	SQD	O47-C7	3.16	1.42	1.35
13	Z	503	CLA	C4B-NB	3.16	1.41	1.37
13	3	503	CLA	C4B-NB	3.16	1.41	1.37
13	r	509	CLA	C4B-NB	3.16	1.41	1.37
13	A	1110	CLA	C4D-ND	-3.16	1.33	1.37
13	H	1232	CLA	C4D-ND	-3.16	1.33	1.37
13	f	1218	CLA	C4D-ND	-3.16	1.33	1.37
13	2	508	CLA	C4B-NB	3.16	1.41	1.37
13	A	1121	CLA	C4D-ND	-3.16	1.33	1.37
13	e	1110	CLA	C4B-NB	3.16	1.41	1.37
13	f	1238	CLA	C1D-ND	3.16	1.41	1.37
13	f	1230	CLA	C1D-ND	3.16	1.41	1.37
13	Z	512	CLA	C4B-NB	3.16	1.41	1.37
13	Y	502	CLA	C4B-NB	3.16	1.41	1.37
13	B	1228	CLA	C1D-ND	3.16	1.41	1.37
13	1	512	CLA	C4B-NB	3.16	1.41	1.37
13	e	1101	CLA	C1D-ND	3.16	1.41	1.37
13	Z	519	CLA	C4D-ND	-3.15	1.33	1.37
13	Z	501	CLA	C4B-NB	3.15	1.41	1.37
13	s	510	CLA	C4B-NB	3.15	1.41	1.37
13	f	1239	CLA	C4D-ND	-3.15	1.33	1.37
13	A	1102	CLA	C1D-ND	3.15	1.41	1.37
13	2	502	CLA	C4B-NB	3.15	1.41	1.37
13	2	503	CLA	C4B-NB	3.15	1.41	1.37
13	e	1110	CLA	C4D-ND	-3.15	1.33	1.37
13	2	518	CLA	C4B-NB	3.15	1.41	1.37
13	3	516	CLA	C4B-NB	3.15	1.41	1.37
13	e	1137	CLA	C3B-C4B	3.15	1.50	1.42
13	Y	518	CLA	C1D-ND	3.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1104	CLA	C1D-ND	3.15	1.41	1.37
13	B	1217	CLA	C1D-ND	3.15	1.41	1.37
13	H	1211	CLA	C4D-ND	-3.15	1.33	1.37
13	a	518	CLA	C4B-NB	3.15	1.41	1.37
13	A	1110	CLA	C4B-NB	3.15	1.41	1.37
13	G	1133	CLA	C1D-ND	3.15	1.41	1.37
13	f	1214	CLA	C4B-NB	3.15	1.41	1.37
13	2	512	CLA	C4B-NB	3.15	1.41	1.37
13	3	518	CLA	C4B-NB	3.15	1.41	1.37
13	Z	509	CLA	C4B-NB	3.14	1.41	1.37
13	e	1112	CLA	C1D-ND	3.14	1.41	1.37
13	G	1131	CLA	C4D-ND	-3.14	1.33	1.37
13	Z	512	CLA	C4D-ND	-3.14	1.33	1.37
13	2	509	CLA	C4B-NB	3.14	1.41	1.37
13	a	519	CLA	C4B-NB	3.14	1.41	1.37
13	b	509	CLA	C4B-NB	3.14	1.41	1.37
13	j	1301	CLA	C4B-NB	3.14	1.41	1.37
13	s	503	CLA	C4B-NB	3.14	1.41	1.37
13	B	1239	CLA	C4B-NB	3.14	1.41	1.37
13	4	509	CLA	C4B-NB	3.14	1.41	1.37
13	6	507	CLA	C4B-NB	3.14	1.41	1.37
13	a	510	CLA	C4B-NB	3.14	1.41	1.37
13	f	1227	CLA	C1D-ND	3.14	1.41	1.37
13	B	1239	CLA	C4D-ND	-3.14	1.33	1.37
13	e	1117	CLA	C4D-ND	-3.14	1.33	1.37
13	e	1112	CLA	C4D-ND	-3.13	1.33	1.37
13	v	507	CLA	C4B-NB	3.13	1.41	1.37
13	A	1131	CLA	C4D-ND	-3.13	1.33	1.37
13	f	1239	CLA	C4B-NB	3.13	1.41	1.37
13	3	519	CLA	C4B-NB	3.13	1.41	1.37
13	a	516	CLA	C4B-NB	3.13	1.41	1.37
13	A	1117	CLA	C4D-ND	-3.13	1.33	1.37
13	d	513	CLA	C3B-C4B	3.13	1.50	1.42
13	f	1220	CLA	C4D-ND	-3.13	1.33	1.37
13	G	1137	CLA	C3B-C4B	3.13	1.50	1.42
13	A	1112	CLA	C4D-ND	-3.12	1.33	1.37
13	3	510	CLA	C4B-NB	3.12	1.41	1.37
13	q	510	CLA	C4B-NB	3.12	1.41	1.37
13	r	510	CLA	C4B-NB	3.12	1.41	1.37
13	H	1239	CLA	C4D-ND	-3.12	1.33	1.37
13	G	1110	CLA	C3B-C4B	3.12	1.50	1.42
20	q	822	SQD	O48-C23	3.12	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1131	CLA	C4D-ND	-3.12	1.33	1.37
13	b	505	CLA	C4B-NB	3.12	1.41	1.37
14	B	2002	PQN	C3-C2	3.12	1.40	1.35
13	G	1117	CLA	C4D-ND	-3.12	1.33	1.37
13	Z	509	CLA	C4D-ND	-3.12	1.33	1.37
13	f	1226	CLA	C1B-NB	-3.12	1.33	1.37
13	B	1214	CLA	C4B-NB	3.12	1.41	1.37
13	1	518	CLA	C1D-ND	3.12	1.41	1.37
13	Z	502	CLA	C4B-NB	3.12	1.41	1.37
13	q	504	CLA	C4D-ND	-3.12	1.33	1.37
13	r	509	CLA	C4D-ND	-3.12	1.33	1.37
13	1	505	CLA	C4B-NB	3.12	1.41	1.37
13	q	512	CLA	C4B-NB	3.12	1.41	1.37
13	Z	508	CLA	C4D-ND	-3.12	1.33	1.37
20	1	822	SQD	O48-C23	3.12	1.42	1.33
13	6	513	CLA	C3B-C4B	3.12	1.50	1.42
13	v	513	CLA	C3B-C4B	3.12	1.50	1.42
13	4	505	CLA	C4B-NB	3.12	1.41	1.37
13	H	1239	CLA	C4B-NB	3.12	1.41	1.37
13	G	1110	CLA	C4D-ND	-3.11	1.33	1.37
13	f	1213	CLA	C4D-ND	-3.11	1.33	1.37
13	G	1102	CLA	C1D-ND	3.11	1.41	1.37
13	G	1110	CLA	C4B-NB	3.11	1.41	1.37
13	r	513	CLA	C3B-C4B	3.11	1.50	1.42
13	2	519	CLA	C4D-ND	-3.11	1.33	1.37
13	4	507	CLA	C4B-NB	3.11	1.41	1.37
13	H	1219	CLA	C4B-NB	3.11	1.41	1.37
13	f	1226	CLA	C4B-NB	3.11	1.41	1.37
14	H	2002	PQN	C10-C1	-3.11	1.42	1.48
13	q	505	CLA	C4B-NB	3.11	1.41	1.37
13	e	1110	CLA	C3B-C4B	3.11	1.50	1.42
20	Y	822	SQD	O48-C23	3.11	1.42	1.33
13	t	516	CLA	C4B-NB	3.11	1.41	1.37
13	a	516	CLA	C4D-ND	-3.11	1.33	1.37
13	H	1226	CLA	C4B-NB	3.11	1.41	1.37
13	5	512	CLA	C4B-NB	3.11	1.41	1.37
13	e	1114	CLA	C4B-NB	3.11	1.41	1.37
13	3	513	CLA	C4B-NB	3.11	1.41	1.37
13	s	518	CLA	C4B-NB	3.11	1.41	1.37
13	G	1112	CLA	C4D-ND	-3.11	1.33	1.37
13	Z	510	CLA	C4B-NB	3.11	1.41	1.37
14	f	2002	PQN	C10-C1	-3.11	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	516	CLA	C4D-ND	-3.11	1.33	1.37
13	G	1013	CLA	C3B-C4B	3.11	1.50	1.42
13	a	512	CLA	C4B-NB	3.10	1.41	1.37
13	s	512	CLA	C4D-ND	-3.10	1.33	1.37
20	a	822	SQD	O48-C23	3.10	1.42	1.33
20	s	822	SQD	O48-C23	3.10	1.42	1.33
13	e	1013	CLA	C3B-C4B	3.10	1.50	1.42
13	5	509	CLA	C4B-NB	3.10	1.41	1.37
13	H	1226	CLA	C1B-NB	-3.10	1.34	1.37
13	G	1134	CLA	C4D-ND	-3.10	1.33	1.37
13	t	505	CLA	C4B-NB	3.10	1.41	1.37
20	r	822	SQD	O48-C23	3.10	1.42	1.33
13	B	1226	CLA	C1B-NB	-3.10	1.34	1.37
13	U	1105	CLA	C4B-NB	3.10	1.41	1.37
13	2	512	CLA	C4D-ND	-3.10	1.33	1.37
13	2	509	CLA	C4D-ND	-3.10	1.33	1.37
13	B	1226	CLA	C4B-NB	3.10	1.41	1.37
13	e	1102	CLA	C1D-ND	3.10	1.41	1.37
13	A	1110	CLA	C3B-C4B	3.10	1.50	1.42
13	G	1129	CLA	C1D-ND	3.10	1.41	1.37
13	f	1021	CLA	C1D-ND	3.09	1.41	1.37
13	s	519	CLA	C4B-NB	3.09	1.41	1.37
13	e	1130	CLA	C4D-ND	-3.09	1.33	1.37
13	c	509	CLA	C4B-NB	3.09	1.41	1.37
13	T	1302	CLA	C4D-ND	-3.09	1.33	1.37
13	a	503	CLA	C4D-ND	-3.09	1.33	1.37
14	B	2002	PQN	C10-C1	-3.09	1.42	1.48
13	A	1114	CLA	C4B-NB	3.09	1.41	1.37
20	2	822	SQD	O48-C23	3.09	1.42	1.33
13	A	1130	CLA	C4D-ND	-3.09	1.33	1.37
13	2	508	CLA	C4D-ND	-3.09	1.33	1.37
13	3	512	CLA	C4D-ND	-3.09	1.33	1.37
13	A	1013	CLA	C3B-C4B	3.09	1.50	1.42
13	A	1108	CLA	C4B-NB	3.09	1.41	1.37
20	Z	822	SQD	O48-C23	3.09	1.42	1.33
13	1	510	CLA	C4B-NB	3.09	1.41	1.37
13	2	519	CLA	C4B-NB	3.09	1.41	1.37
13	a	513	CLA	C4B-NB	3.09	1.41	1.37
13	e	1237	CLA	C4B-NB	3.09	1.41	1.37
13	s	507	CLA	C4B-NB	3.09	1.41	1.37
13	s	513	CLA	C4B-NB	3.08	1.41	1.37
20	3	822	SQD	O48-C23	3.08	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	519	CLA	C4D-ND	-3.08	1.33	1.37
13	K	1105	CLA	C4B-NB	3.08	1.41	1.37
13	H	1214	CLA	C4B-NB	3.08	1.41	1.37
13	B	1219	CLA	C4B-NB	3.08	1.41	1.37
13	G	1114	CLA	C4B-NB	3.08	1.41	1.37
13	2	513	CLA	C3B-C4B	3.08	1.50	1.42
13	q	506	CLA	C3B-C4B	3.08	1.50	1.42
13	f	1217	CLA	C1D-ND	3.08	1.41	1.37
13	Y	504	CLA	C4D-ND	-3.08	1.33	1.37
13	s	501	CLA	C4D-ND	-3.08	1.33	1.37
18	A	1848	LMU	O5'-C1'	3.08	1.49	1.41
14	H	2002	PQN	C3-C2	3.08	1.40	1.35
14	f	2002	PQN	C3-C2	3.08	1.40	1.35
13	Z	513	CLA	C3B-C4B	3.08	1.50	1.42
13	Y	506	CLA	C3B-C4B	3.08	1.50	1.42
13	A	1136	CLA	C4B-NB	3.08	1.41	1.37
18	G	1848	LMU	O5'-C1'	3.08	1.49	1.41
13	s	518	CLA	C4D-ND	-3.07	1.33	1.37
13	1	506	CLA	C3B-C4B	3.07	1.50	1.42
13	A	1126	CLA	C4D-ND	-3.07	1.33	1.37
13	A	1134	CLA	C4D-ND	-3.07	1.33	1.37
13	c	512	CLA	C4B-NB	3.07	1.41	1.37
13	G	1130	CLA	C4D-ND	-3.07	1.33	1.37
13	e	1126	CLA	C4D-ND	-3.07	1.33	1.37
13	B	1216	CLA	C1D-ND	3.07	1.41	1.37
13	G	1106	CLA	C1D-ND	3.07	1.41	1.37
13	r	519	CLA	C4B-NB	3.07	1.41	1.37
13	1	504	CLA	C4D-ND	-3.07	1.33	1.37
13	H	1213	CLA	C4D-ND	-3.07	1.33	1.37
13	r	502	CLA	C4D-ND	-3.07	1.33	1.37
18	e	1848	LMU	O5'-C1'	3.07	1.49	1.41
13	B	1206	CLA	C1D-ND	3.07	1.41	1.37
13	L	1501	CLA	C4B-NB	3.07	1.41	1.37
13	f	1206	CLA	C1D-ND	3.07	1.41	1.37
13	e	1123	CLA	C4D-ND	-3.07	1.33	1.37
13	e	1134	CLA	C4D-ND	-3.07	1.33	1.37
13	s	512	CLA	C4B-NB	3.07	1.41	1.37
13	r	508	CLA	C4D-ND	-3.07	1.33	1.37
13	e	1136	CLA	C4B-NB	3.07	1.41	1.37
13	e	1120	CLA	C1D-ND	3.07	1.41	1.37
13	e	1108	CLA	C4B-NB	3.07	1.41	1.37
13	G	1134	CLA	C3B-C4B	3.07	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	822	SQD	O48-C23	3.07	1.42	1.33
13	r	512	CLA	C4D-ND	-3.07	1.33	1.37
13	f	1202	CLA	C4B-NB	3.07	1.41	1.37
13	u	509	CLA	C4B-NB	3.07	1.41	1.37
13	Y	510	CLA	C4B-NB	3.06	1.41	1.37
13	f	1240	CLA	C4B-NB	3.06	1.41	1.37
13	J	1302	CLA	C4D-ND	-3.06	1.33	1.37
13	1	509	CLA	C4D-ND	-3.06	1.33	1.37
13	Z	502	CLA	C4D-ND	-3.06	1.33	1.37
13	B	1213	CLA	C4D-ND	-3.06	1.33	1.37
13	l	1303	CLA	C4D-ND	-3.06	1.33	1.37
13	f	1202	CLA	C1D-ND	3.06	1.41	1.37
13	e	1114	CLA	C3B-C4B	3.06	1.49	1.42
13	t	508	CLA	C4D-ND	-3.06	1.33	1.37
13	5	519	CLA	C4B-NB	3.06	1.41	1.37
13	G	1120	CLA	C1D-ND	3.06	1.41	1.37
13	A	1022	CLA	C1D-ND	3.06	1.41	1.37
13	G	1022	CLA	C1D-ND	3.06	1.41	1.37
13	A	1123	CLA	C4D-ND	-3.06	1.33	1.37
13	G	1126	CLA	C4D-ND	-3.06	1.33	1.37
13	G	1136	CLA	C4B-NB	3.06	1.41	1.37
13	q	508	CLA	C4B-NB	3.06	1.41	1.37
13	G	1108	CLA	C4B-NB	3.06	1.41	1.37
13	a	501	CLA	C4B-NB	3.06	1.41	1.37
13	f	1217	CLA	C4D-ND	-3.06	1.33	1.37
13	c	506	CLA	C4D-ND	-3.06	1.33	1.37
13	B	1012	CLA	C3B-C4B	3.05	1.49	1.42
13	q	509	CLA	C4D-ND	-3.05	1.33	1.37
13	B	1202	CLA	C4B-NB	3.05	1.41	1.37
13	m	1105	CLA	C4B-NB	3.05	1.41	1.37
13	s	501	CLA	C4B-NB	3.05	1.41	1.37
13	b	507	CLA	C4B-NB	3.05	1.41	1.37
13	A	1134	CLA	C3B-C4B	3.05	1.49	1.42
13	f	1012	CLA	C3B-C4B	3.05	1.49	1.42
13	A	1237	CLA	C4B-NB	3.05	1.41	1.37
13	1	507	CLA	C4B-NB	3.05	1.41	1.37
13	A	1114	CLA	C3B-C4B	3.05	1.49	1.42
13	B	1023	CLA	CMC-C2C	-3.05	1.44	1.50
13	3	501	CLA	C4D-ND	-3.05	1.33	1.37
13	3	512	CLA	C4B-NB	3.05	1.41	1.37
13	e	1022	CLA	C1D-ND	3.05	1.41	1.37
13	B	1240	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	508	CLA	C4B-NB	3.05	1.41	1.37
13	H	1216	CLA	C1D-ND	3.05	1.41	1.37
13	Y	505	CLA	C4B-NB	3.05	1.41	1.37
13	q	507	CLA	C4B-NB	3.05	1.41	1.37
13	q	518	CLA	C1D-ND	3.05	1.41	1.37
13	B	1209	CLA	C4D-ND	-3.05	1.33	1.37
13	J	1303	CLA	C4D-ND	-3.05	1.33	1.37
20	5	822	SQD	O48-C23	3.05	1.42	1.33
13	s	507	CLA	C4D-ND	-3.05	1.33	1.37
13	2	510	CLA	C4B-NB	3.05	1.41	1.37
13	V	1501	CLA	C4B-NB	3.05	1.41	1.37
13	f	1219	CLA	C4B-NB	3.05	1.41	1.37
13	H	1012	CLA	C3B-C4B	3.05	1.49	1.42
13	2	510	CLA	C4D-ND	-3.04	1.33	1.37
13	B	1217	CLA	C4D-ND	-3.04	1.33	1.37
13	G	1123	CLA	C4D-ND	-3.04	1.33	1.37
13	Z	519	CLA	C4B-NB	3.04	1.41	1.37
13	Z	501	CLA	C4D-ND	-3.04	1.33	1.37
13	f	1209	CLA	C4D-ND	-3.04	1.33	1.37
13	q	502	CLA	C4D-ND	-3.04	1.33	1.37
13	u	507	CLA	C4B-NB	3.04	1.41	1.37
13	a	508	CLA	C4D-ND	-3.04	1.33	1.37
13	A	1140	CLA	C4B-NB	3.04	1.41	1.37
20	u	822	SQD	O48-C23	3.04	1.42	1.33
13	A	1106	CLA	C1D-ND	3.04	1.41	1.37
13	n	1501	CLA	C4B-NB	3.04	1.41	1.37
13	r	513	CLA	C4D-ND	-3.04	1.33	1.37
13	H	1234	CLA	C1D-ND	3.04	1.41	1.37
13	T	1303	CLA	C4D-ND	-3.04	1.33	1.37
13	a	509	CLA	C4D-ND	-3.04	1.33	1.37
13	A	1120	CLA	C1D-ND	3.04	1.41	1.37
13	2	506	CLA	C4D-ND	-3.04	1.33	1.37
13	f	1023	CLA	CMC-C2C	-3.04	1.44	1.50
13	f	1216	CLA	C1D-ND	3.04	1.41	1.37
13	H	1217	CLA	C4D-ND	-3.04	1.33	1.37
13	v	519	CLA	C4D-ND	-3.03	1.33	1.37
13	H	1206	CLA	C1D-ND	3.03	1.41	1.37
13	u	519	CLA	C4B-NB	3.03	1.41	1.37
13	r	506	CLA	C4D-ND	-3.03	1.33	1.37
13	Y	507	CLA	C4B-NB	3.03	1.41	1.37
13	f	1221	CLA	C4B-NB	3.03	1.41	1.37
13	H	1209	CLA	C4D-ND	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	503	CLA	C4D-ND	-3.03	1.33	1.37
13	H	1202	CLA	C4B-NB	3.03	1.41	1.37
13	G	1114	CLA	C3B-C4B	3.03	1.49	1.42
13	5	507	CLA	C4B-NB	3.03	1.41	1.37
13	c	519	CLA	C4B-NB	3.03	1.41	1.37
13	2	502	CLA	C4D-ND	-3.03	1.33	1.37
13	B	1234	CLA	C1D-ND	3.03	1.41	1.37
13	3	508	CLA	C4D-ND	-3.03	1.33	1.37
13	Y	509	CLA	C4D-ND	-3.03	1.33	1.37
13	G	1140	CLA	C4B-NB	3.03	1.41	1.37
13	1	512	CLA	C4D-ND	-3.03	1.33	1.37
13	l	1302	CLA	C4D-ND	-3.03	1.33	1.37
13	6	501	CLA	C4D-ND	-3.03	1.33	1.37
13	2	504	CLA	C4D-ND	-3.03	1.33	1.37
13	a	512	CLA	C4D-ND	-3.03	1.33	1.37
13	Y	508	CLA	C4B-NB	3.03	1.41	1.37
13	B	1205	CLA	C4B-NB	3.02	1.41	1.37
13	e	1134	CLA	C3B-C4B	3.02	1.49	1.42
13	H	1023	CLA	CMC-C2C	-3.02	1.44	1.50
13	B	1202	CLA	C1D-ND	3.02	1.41	1.37
13	3	501	CLA	C4B-NB	3.02	1.41	1.37
13	3	518	CLA	C4D-ND	-3.02	1.33	1.37
13	Y	502	CLA	C4D-ND	-3.02	1.33	1.37
13	H	1205	CLA	C4B-NB	3.02	1.41	1.37
13	3	503	CLA	C4D-ND	-3.02	1.33	1.37
13	r	501	CLA	C4D-ND	-3.02	1.33	1.37
13	B	1221	CLA	C4B-NB	3.02	1.41	1.37
13	c	509	CLA	C4D-ND	-3.02	1.33	1.37
13	5	509	CLA	C4D-ND	-3.02	1.33	1.37
13	f	1234	CLA	C1D-ND	3.02	1.41	1.37
13	A	1129	CLA	C1D-ND	3.02	1.41	1.37
13	H	1240	CLA	C4B-NB	3.02	1.41	1.37
13	t	509	CLA	C4D-ND	-3.02	1.33	1.37
13	Y	512	CLA	C4D-ND	-3.01	1.33	1.37
13	e	1140	CLA	C4B-NB	3.01	1.41	1.37
13	2	513	CLA	C4D-ND	-3.01	1.33	1.37
13	a	507	CLA	C4D-ND	-3.01	1.33	1.37
13	d	516	CLA	C4D-ND	-3.01	1.33	1.37
13	e	1106	CLA	C1D-ND	3.01	1.41	1.37
13	3	509	CLA	C4D-ND	-3.01	1.33	1.37
13	a	504	CLA	C4D-ND	-3.01	1.33	1.37
13	b	509	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	504	CLA	C4D-ND	-3.01	1.33	1.37
13	q	510	CLA	C4D-ND	-3.01	1.33	1.37
13	s	502	CLA	C4D-ND	-3.01	1.33	1.37
13	a	501	CLA	C4D-ND	-3.01	1.33	1.37
13	3	507	CLA	C4B-NB	3.01	1.41	1.37
13	c	507	CLA	C4B-NB	3.01	1.41	1.37
13	3	507	CLA	C4D-ND	-3.01	1.33	1.37
13	B	1204	CLA	C1D-ND	3.01	1.41	1.37
13	Z	510	CLA	C4D-ND	-3.01	1.33	1.37
13	d	501	CLA	C4D-ND	-3.01	1.33	1.37
13	Z	507	CLA	C4D-ND	-3.01	1.33	1.37
13	r	510	CLA	C4D-ND	-3.01	1.33	1.37
13	t	516	CLA	C3B-C4B	3.01	1.49	1.42
13	1	502	CLA	C4D-ND	-3.01	1.33	1.37
13	f	1205	CLA	C4B-NB	3.00	1.41	1.37
13	s	504	CLA	C4D-ND	-3.00	1.33	1.37
13	a	505	CLA	C4B-NB	3.00	1.41	1.37
13	q	516	CLA	C4D-ND	-3.00	1.33	1.37
13	4	508	CLA	C4D-ND	-3.00	1.33	1.37
13	Y	516	CLA	C4D-ND	-3.00	1.33	1.37
13	q	518	CLA	C4B-NB	3.00	1.41	1.37
13	r	503	CLA	C4D-ND	-3.00	1.33	1.37
13	H	1221	CLA	C4B-NB	3.00	1.41	1.37
13	2	501	CLA	C4D-ND	-3.00	1.33	1.37
13	1	518	CLA	C4B-NB	3.00	1.41	1.37
13	1	516	CLA	C4D-ND	-3.00	1.33	1.37
13	Y	510	CLA	C4D-ND	-3.00	1.33	1.37
13	e	1116	CLA	C4B-NB	3.00	1.41	1.37
13	5	506	CLA	C4D-ND	-3.00	1.33	1.37
13	q	512	CLA	C4D-ND	-3.00	1.33	1.37
13	3	505	CLA	C4B-NB	3.00	1.41	1.37
13	H	1204	CLA	C1D-ND	3.00	1.41	1.37
13	s	508	CLA	C4D-ND	-3.00	1.33	1.37
13	K	1401	CLA	C4B-NB	2.99	1.41	1.37
13	a	506	CLA	C4D-ND	-2.99	1.33	1.37
13	Z	506	CLA	C4D-ND	-2.99	1.33	1.37
13	d	504	CLA	C4D-ND	-2.99	1.33	1.37
13	f	1229	CLA	C4B-NB	2.99	1.41	1.37
13	4	509	CLA	C4D-ND	-2.99	1.33	1.37
13	4	516	CLA	C3B-C4B	2.99	1.49	1.42
13	a	507	CLA	C4B-NB	2.99	1.41	1.37
13	e	1128	CLA	C1D-ND	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	u	509	CLA	C4D-ND	-2.99	1.33	1.37
13	d	517	CLA	C4D-ND	-2.99	1.33	1.37
13	5	513	CLA	C3B-C4B	2.99	1.49	1.42
13	c	513	CLA	C3B-C4B	2.99	1.49	1.42
13	d	511	CLA	C4D-ND	-2.99	1.33	1.37
13	H	1229	CLA	C3B-C4B	2.99	1.49	1.42
13	m	1401	CLA	C4B-NB	2.99	1.41	1.37
13	a	502	CLA	C4D-ND	-2.99	1.33	1.37
13	Z	505	CLA	C4B-NB	2.99	1.41	1.37
13	b	516	CLA	C3B-C4B	2.99	1.49	1.42
13	b	517	CLA	C4D-ND	-2.99	1.33	1.37
13	q	501	CLA	C4D-ND	-2.99	1.33	1.37
13	v	501	CLA	C4D-ND	-2.99	1.33	1.37
13	Z	517	CLA	C4D-ND	-2.99	1.33	1.37
13	d	510	CLA	C4D-ND	-2.99	1.33	1.37
13	e	1102	CLA	C4B-NB	2.99	1.41	1.37
13	n	1502	CLA	C1D-ND	2.99	1.41	1.37
13	Z	513	CLA	C4D-ND	-2.98	1.33	1.37
13	f	1204	CLA	C1D-ND	2.98	1.41	1.37
14	e	2001	PQN	C11-C12	2.98	1.55	1.50
13	Z	504	CLA	C4D-ND	-2.98	1.33	1.37
13	a	518	CLA	C4D-ND	-2.98	1.33	1.37
13	s	505	CLA	C4B-NB	2.98	1.41	1.37
13	6	502	CLA	C4D-ND	-2.98	1.33	1.37
13	e	1139	CLA	C4B-NB	2.98	1.41	1.37
13	v	517	CLA	C4D-ND	-2.98	1.33	1.37
13	U	1401	CLA	C4B-NB	2.98	1.41	1.37
13	5	507	CLA	C4D-ND	-2.98	1.33	1.37
13	V	1502	CLA	C1D-ND	2.98	1.41	1.37
13	e	1121	CLA	C4B-NB	2.98	1.41	1.37
13	3	506	CLA	C4D-ND	-2.98	1.33	1.37
13	s	506	CLA	C4D-ND	-2.98	1.33	1.37
13	B	1229	CLA	C3B-C4B	2.98	1.49	1.42
13	6	504	CLA	C4D-ND	-2.98	1.33	1.37
13	Y	518	CLA	C4B-NB	2.98	1.41	1.37
13	2	503	CLA	C4D-ND	-2.97	1.33	1.37
13	u	513	CLA	C3B-C4B	2.97	1.49	1.42
13	e	1139	CLA	C1D-ND	2.97	1.41	1.37
13	5	501	CLA	C4D-ND	-2.97	1.33	1.37
13	m	1105	CLA	C4D-ND	-2.97	1.33	1.37
13	A	1139	CLA	C4B-NB	2.97	1.41	1.37
13	1	501	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	504	CLA	C4D-ND	-2.97	1.33	1.37
13	2	505	CLA	C4B-NB	2.97	1.41	1.37
13	q	503	CLA	C4D-ND	-2.97	1.33	1.37
13	u	507	CLA	C4D-ND	-2.97	1.33	1.37
17	e	5001	LHG	O7-C5	-2.97	1.39	1.46
13	v	516	CLA	C3B-C4B	2.97	1.49	1.42
13	d	508	CLA	C4D-ND	-2.97	1.33	1.37
13	G	1237	CLA	C4B-NB	2.97	1.41	1.37
13	3	502	CLA	C4D-ND	-2.97	1.33	1.37
13	6	519	CLA	C4D-ND	-2.97	1.33	1.37
13	U	1105	CLA	C4D-ND	-2.97	1.33	1.37
13	A	1128	CLA	C1D-ND	2.97	1.41	1.37
13	r	505	CLA	C4B-NB	2.97	1.41	1.37
13	c	501	CLA	C4D-ND	-2.97	1.33	1.37
13	v	505	CLA	C4D-ND	-2.97	1.33	1.37
13	v	511	CLA	C4D-ND	-2.97	1.33	1.37
13	f	1216	CLA	C4B-NB	2.96	1.41	1.37
13	c	507	CLA	C4D-ND	-2.96	1.33	1.37
13	t	518	CLA	C4D-ND	-2.96	1.33	1.37
13	G	1139	CLA	C3B-C4B	2.96	1.49	1.42
13	H	1236	CLA	C3B-C4B	2.96	1.49	1.42
13	b	513	CLA	C4D-ND	-2.96	1.33	1.37
13	1	510	CLA	C4D-ND	-2.96	1.33	1.37
13	B	1236	CLA	C3B-C4B	2.96	1.49	1.42
14	A	2001	PQN	C11-C12	2.96	1.54	1.50
13	A	1116	CLA	C4B-NB	2.96	1.41	1.37
13	v	502	CLA	C4D-ND	-2.96	1.33	1.37
13	L	1502	CLA	C1D-ND	2.96	1.41	1.37
13	q	507	CLA	C4D-ND	-2.96	1.33	1.37
13	t	513	CLA	C3B-C4B	2.96	1.49	1.42
13	A	1139	CLA	C3B-C4B	2.96	1.49	1.42
13	H	1206	CLA	CMB-C2B	-2.96	1.44	1.50
13	G	1102	CLA	C4B-NB	2.96	1.41	1.37
17	G	5001	LHG	O7-C5	-2.96	1.39	1.46
13	K	1105	CLA	C4D-ND	-2.96	1.33	1.37
13	1	506	CLA	C4D-ND	-2.96	1.33	1.37
13	2	505	CLA	C4D-ND	-2.96	1.33	1.37
13	6	517	CLA	C4D-ND	-2.96	1.33	1.37
13	r	507	CLA	C4D-ND	-2.96	1.33	1.37
13	u	518	CLA	C3B-C4B	2.96	1.49	1.42
13	t	513	CLA	C4D-ND	-2.96	1.33	1.37
13	f	1229	CLA	C3B-C4B	2.96	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	516	CLA	C3B-C4B	2.95	1.49	1.42
13	d	519	CLA	C4D-ND	-2.95	1.33	1.37
13	r	505	CLA	C4D-ND	-2.95	1.33	1.37
13	H	1216	CLA	CMB-C2B	-2.95	1.44	1.50
13	6	508	CLA	C4D-ND	-2.95	1.33	1.37
13	6	511	CLA	C4D-ND	-2.95	1.33	1.37
13	G	1011	CLA	C4D-ND	-2.95	1.33	1.37
13	Z	516	CLA	C4D-ND	-2.95	1.33	1.37
17	A	5001	LHG	O7-C5	-2.95	1.39	1.46
13	4	517	CLA	C4D-ND	-2.95	1.33	1.37
13	d	505	CLA	C4D-ND	-2.95	1.33	1.37
13	B	1229	CLA	C4B-NB	2.95	1.41	1.37
13	H	1202	CLA	C1D-ND	2.95	1.41	1.37
13	u	510	CLA	C4D-ND	-2.95	1.33	1.37
13	e	1129	CLA	C1D-ND	2.95	1.41	1.37
13	b	518	CLA	C4D-ND	-2.95	1.33	1.37
13	u	512	CLA	C4D-ND	-2.95	1.33	1.37
13	r	512	CLA	C3B-C4B	2.95	1.49	1.42
13	2	512	CLA	C3B-C4B	2.95	1.49	1.42
13	Z	512	CLA	C3B-C4B	2.95	1.49	1.42
13	B	1206	CLA	CMB-C2B	-2.95	1.44	1.50
13	G	1138	CLA	C4B-NB	2.95	1.41	1.37
13	6	516	CLA	C3B-C4B	2.95	1.49	1.42
13	6	510	CLA	C4D-ND	-2.95	1.33	1.37
14	G	2001	PQN	C11-C12	2.95	1.54	1.50
13	H	1207	CLA	C4B-NB	2.95	1.41	1.37
13	r	507	CLA	C4B-NB	2.95	1.41	1.37
13	A	1011	CLA	C4D-ND	-2.95	1.33	1.37
13	q	511	CLA	C4D-ND	-2.95	1.33	1.37
13	u	506	CLA	C4D-ND	-2.95	1.33	1.37
13	u	508	CLA	C4D-ND	-2.95	1.33	1.37
13	b	504	CLA	C3B-C4B	2.95	1.49	1.42
13	b	513	CLA	C3B-C4B	2.95	1.49	1.42
13	a	519	CLA	C4D-ND	-2.95	1.33	1.37
13	d	509	CLA	C4D-ND	-2.95	1.33	1.37
13	s	509	CLA	C4D-ND	-2.95	1.33	1.37
13	t	517	CLA	C4D-ND	-2.95	1.33	1.37
13	u	509	CLA	C3B-C4B	2.95	1.49	1.42
13	A	1102	CLA	C4B-NB	2.95	1.41	1.37
13	G	1116	CLA	C4B-NB	2.95	1.41	1.37
13	s	505	CLA	C4D-ND	-2.94	1.33	1.37
13	u	501	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1139	CLA	C4B-NB	2.94	1.41	1.37
13	Y	501	CLA	C4D-ND	-2.94	1.33	1.37
13	6	509	CLA	C4D-ND	-2.94	1.33	1.37
13	v	516	CLA	C4D-ND	-2.94	1.33	1.37
13	6	516	CLA	C4D-ND	-2.94	1.33	1.37
13	v	508	CLA	C4D-ND	-2.94	1.33	1.37
13	6	506	CLA	C4D-ND	-2.94	1.33	1.37
13	Z	511	CLA	C4D-ND	-2.94	1.33	1.37
13	f	1236	CLA	C3B-C4B	2.94	1.49	1.42
13	5	509	CLA	C3B-C4B	2.94	1.49	1.42
13	v	504	CLA	C3B-C4B	2.94	1.49	1.42
13	c	518	CLA	C3B-C4B	2.94	1.49	1.42
13	G	1128	CLA	C1D-ND	2.94	1.41	1.37
13	Z	503	CLA	C4D-ND	-2.94	1.33	1.37
13	2	516	CLA	C4D-ND	-2.94	1.33	1.37
13	6	505	CLA	C4D-ND	-2.94	1.33	1.37
13	2	517	CLA	C4D-ND	-2.94	1.33	1.37
13	5	511	CLA	C4D-ND	-2.94	1.33	1.37
13	b	508	CLA	C4D-ND	-2.94	1.33	1.37
13	B	1225	CLA	C1D-ND	2.94	1.41	1.37
13	B	1012	CLA	C4B-NB	2.94	1.41	1.37
13	e	1139	CLA	C3B-C4B	2.94	1.49	1.42
13	u	511	CLA	C4D-ND	-2.94	1.33	1.37
13	s	509	CLA	C3B-C4B	2.94	1.49	1.42
13	f	1216	CLA	CMB-C2B	-2.94	1.44	1.50
13	d	502	CLA	C4D-ND	-2.94	1.33	1.37
13	q	506	CLA	C4D-ND	-2.94	1.33	1.37
13	6	506	CLA	C3B-C4B	2.93	1.49	1.42
13	t	506	CLA	C3B-C4B	2.93	1.49	1.42
13	4	513	CLA	C3B-C4B	2.93	1.49	1.42
13	d	504	CLA	C3B-C4B	2.93	1.49	1.42
13	4	513	CLA	C4D-ND	-2.93	1.33	1.37
13	Z	505	CLA	C4D-ND	-2.93	1.33	1.37
13	r	516	CLA	C4D-ND	-2.93	1.33	1.37
13	Y	506	CLA	C4D-ND	-2.93	1.33	1.37
13	v	504	CLA	C4D-ND	-2.93	1.33	1.37
13	v	510	CLA	C4D-ND	-2.93	1.33	1.37
13	4	506	CLA	C3B-C4B	2.93	1.49	1.42
13	b	506	CLA	C3B-C4B	2.93	1.49	1.42
13	A	1121	CLA	C4B-NB	2.93	1.41	1.37
13	b	511	CLA	C4D-ND	-2.93	1.33	1.37
13	G	1138	CLA	C3B-C4B	2.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	504	CLA	C3B-C4B	2.93	1.49	1.42
13	2	509	CLA	C3B-C4B	2.93	1.49	1.42
20	Z	822	SQD	O47-C7	2.93	1.42	1.34
13	r	511	CLA	C4D-ND	-2.93	1.33	1.37
13	5	518	CLA	C3B-C4B	2.93	1.49	1.42
13	d	506	CLA	C3B-C4B	2.93	1.49	1.42
13	t	504	CLA	C3B-C4B	2.93	1.49	1.42
13	v	509	CLA	C4D-ND	-2.93	1.33	1.37
13	3	509	CLA	C3B-C4B	2.93	1.49	1.42
13	A	1138	CLA	C4B-NB	2.93	1.41	1.37
13	H	1216	CLA	C4B-NB	2.93	1.41	1.37
13	Z	507	CLA	C4B-NB	2.93	1.41	1.37
13	c	509	CLA	C3B-C4B	2.93	1.49	1.42
13	4	518	CLA	C4D-ND	-2.93	1.33	1.37
13	1	507	CLA	C4D-ND	-2.93	1.33	1.37
13	6	503	CLA	C4D-ND	-2.93	1.33	1.37
13	A	1129	CLA	MG-NB	-2.93	2.00	2.05
13	a	509	CLA	C3B-C4B	2.93	1.49	1.42
13	2	507	CLA	C4D-ND	-2.93	1.33	1.37
13	1	511	CLA	C4D-ND	-2.92	1.33	1.37
13	5	502	CLA	C4D-ND	-2.92	1.33	1.37
13	v	503	CLA	C4D-ND	-2.92	1.33	1.37
13	v	506	CLA	C3B-C4B	2.92	1.49	1.42
13	t	512	CLA	C4D-ND	-2.92	1.33	1.37
13	H	1012	CLA	C4B-NB	2.92	1.41	1.37
13	1	503	CLA	C4D-ND	-2.92	1.33	1.37
13	3	519	CLA	C4D-ND	-2.92	1.33	1.37
13	s	513	CLA	C4D-ND	-2.92	1.33	1.37
13	G	1111	CLA	C4B-NB	2.92	1.41	1.37
13	c	506	CLA	C3B-C4B	2.92	1.49	1.42
13	3	505	CLA	C4D-ND	-2.92	1.33	1.37
13	u	517	CLA	C4D-ND	-2.92	1.33	1.37
13	A	1138	CLA	C3B-C4B	2.92	1.49	1.42
13	d	519	CLA	C3B-C4B	2.92	1.49	1.42
13	u	505	CLA	C3B-C4B	2.92	1.49	1.42
13	s	511	CLA	C4D-ND	-2.92	1.33	1.37
13	5	506	CLA	C3B-C4B	2.92	1.49	1.42
13	f	1012	CLA	C4B-NB	2.92	1.41	1.37
13	a	513	CLA	C4D-ND	-2.92	1.33	1.37
13	t	501	CLA	C3B-C4B	2.92	1.49	1.42
13	A	1139	CLA	C1D-ND	2.92	1.41	1.37
13	f	1201	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	506	CLA	C4D-ND	-2.92	1.33	1.37
13	u	506	CLA	C3B-C4B	2.92	1.49	1.42
13	2	518	CLA	C4D-ND	-2.92	1.33	1.37
13	4	504	CLA	C3B-C4B	2.92	1.49	1.42
13	B	1216	CLA	C4B-NB	2.92	1.41	1.37
13	G	1121	CLA	C4B-NB	2.92	1.41	1.37
13	3	513	CLA	C4D-ND	-2.91	1.33	1.37
13	Y	503	CLA	C4D-ND	-2.91	1.33	1.37
13	e	1011	CLA	C4D-ND	-2.91	1.33	1.37
13	H	1229	CLA	C4B-NB	2.91	1.41	1.37
13	2	507	CLA	C4B-NB	2.91	1.41	1.37
13	e	1129	CLA	MG-NB	-2.91	2.00	2.05
13	b	501	CLA	C3B-C4B	2.91	1.49	1.42
13	4	512	CLA	C4D-ND	-2.91	1.33	1.37
13	u	502	CLA	C4D-ND	-2.91	1.33	1.37
13	e	1140	CLA	C3B-C4B	2.91	1.49	1.42
13	t	516	CLA	C4D-ND	-2.91	1.33	1.37
13	e	1138	CLA	C3B-C4B	2.91	1.49	1.42
13	B	1207	CLA	C4B-NB	2.91	1.41	1.37
13	3	511	CLA	C4D-ND	-2.91	1.33	1.37
13	v	506	CLA	C4D-ND	-2.91	1.33	1.37
13	4	501	CLA	C3B-C4B	2.91	1.49	1.42
13	H	1225	CLA	C1D-ND	2.91	1.41	1.37
13	4	505	CLA	C4D-ND	-2.91	1.33	1.37
13	5	508	CLA	C4D-ND	-2.91	1.33	1.37
13	6	512	CLA	C3B-C4B	2.91	1.49	1.42
13	a	508	CLA	C3B-C4B	2.91	1.49	1.42
13	6	519	CLA	C3B-C4B	2.91	1.49	1.42
13	c	508	CLA	C4D-ND	-2.91	1.33	1.37
13	v	518	CLA	C4D-ND	-2.91	1.33	1.37
13	A	1140	CLA	C3B-C4B	2.91	1.49	1.42
13	5	510	CLA	C4D-ND	-2.91	1.33	1.37
13	5	517	CLA	C4D-ND	-2.91	1.33	1.37
13	a	517	CLA	C4D-ND	-2.91	1.33	1.37
13	Z	509	CLA	C3B-C4B	2.91	1.49	1.42
13	d	512	CLA	C4D-ND	-2.91	1.33	1.37
13	3	517	CLA	C4D-ND	-2.91	1.33	1.37
13	a	511	CLA	C4D-ND	-2.91	1.33	1.37
13	r	511	CLA	C3B-C4B	2.91	1.49	1.42
13	G	1103	CLA	C1D-ND	2.91	1.41	1.37
20	2	822	SQD	O47-C7	2.90	1.42	1.34
13	t	511	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1118	CLA	C4B-NB	2.90	1.41	1.37
13	l	1302	CLA	C4B-NB	2.90	1.41	1.37
13	Z	518	CLA	C4D-ND	-2.90	1.33	1.37
13	s	517	CLA	C4D-ND	-2.90	1.33	1.37
13	u	504	CLA	C4D-ND	-2.90	1.33	1.37
13	d	509	CLA	C3B-C4B	2.90	1.49	1.42
13	3	508	CLA	C3B-C4B	2.90	1.49	1.42
13	G	1140	CLA	C3B-C4B	2.90	1.49	1.42
13	Z	511	CLA	C3B-C4B	2.90	1.49	1.42
13	T	1302	CLA	C4B-NB	2.90	1.41	1.37
13	e	1111	CLA	C4B-NB	2.90	1.41	1.37
13	u	505	CLA	C4D-ND	-2.90	1.33	1.37
13	c	510	CLA	C4D-ND	-2.90	1.33	1.37
13	v	512	CLA	C3B-C4B	2.90	1.49	1.42
13	b	512	CLA	C4D-ND	-2.90	1.33	1.37
13	d	518	CLA	C4D-ND	-2.90	1.33	1.37
13	c	517	CLA	C3B-C4B	2.90	1.49	1.42
13	5	512	CLA	C4D-ND	-2.90	1.33	1.37
13	c	502	CLA	C4D-ND	-2.90	1.33	1.37
13	f	1206	CLA	CMB-C2B	-2.90	1.44	1.50
13	G	1129	CLA	MG-NB	-2.90	2.00	2.05
13	Y	511	CLA	C4D-ND	-2.90	1.33	1.37
13	s	513	CLA	C3B-C4B	2.90	1.49	1.42
13	2	511	CLA	C4D-ND	-2.89	1.33	1.37
13	r	517	CLA	C4D-ND	-2.89	1.33	1.37
13	f	1207	CLA	C4B-NB	2.89	1.41	1.37
13	r	518	CLA	C4D-ND	-2.89	1.33	1.37
13	v	512	CLA	C4D-ND	-2.89	1.33	1.37
13	1	513	CLA	C4D-ND	-2.89	1.33	1.37
13	a	505	CLA	C4D-ND	-2.89	1.33	1.37
13	a	513	CLA	C3B-C4B	2.89	1.49	1.42
13	f	1201	CLA	C3B-C4B	2.89	1.49	1.42
13	e	1135	CLA	C1D-ND	2.89	1.41	1.37
13	a	510	CLA	C4D-ND	-2.89	1.33	1.37
13	B	1216	CLA	CMB-C2B	-2.89	1.44	1.50
13	B	1201	CLA	C3B-C4B	2.89	1.49	1.42
13	Y	507	CLA	C4D-ND	-2.89	1.33	1.37
13	u	512	CLA	C3B-C4B	2.89	1.49	1.42
13	A	1128	CLA	C4B-NB	2.89	1.41	1.37
13	J	1302	CLA	C4B-NB	2.89	1.41	1.37
13	v	509	CLA	C3B-C4B	2.89	1.49	1.42
13	r	509	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	511	CLA	C4D-ND	-2.89	1.33	1.37
13	c	511	CLA	C4D-ND	-2.89	1.33	1.37
13	H	1221	CLA	C3B-C4B	2.89	1.49	1.42
13	c	505	CLA	C3B-C4B	2.89	1.49	1.42
13	q	513	CLA	C3B-C4B	2.89	1.49	1.42
13	G	1120	CLA	C4B-NB	2.89	1.41	1.37
13	2	511	CLA	C3B-C4B	2.89	1.49	1.42
13	d	503	CLA	C4D-ND	-2.89	1.33	1.37
13	5	505	CLA	C3B-C4B	2.89	1.49	1.42
20	r	822	SQD	O47-C7	2.88	1.42	1.34
13	A	1102	CLA	C3B-C4B	2.88	1.49	1.42
13	s	508	CLA	C3B-C4B	2.88	1.49	1.42
13	v	519	CLA	C3B-C4B	2.88	1.49	1.42
13	d	513	CLA	C4D-ND	-2.88	1.33	1.37
13	6	509	CLA	C3B-C4B	2.88	1.49	1.42
13	B	1201	CLA	C4B-NB	2.88	1.41	1.37
13	e	1138	CLA	C4B-NB	2.88	1.41	1.37
13	u	503	CLA	C4D-ND	-2.88	1.33	1.37
13	B	1221	CLA	C3B-C4B	2.88	1.49	1.42
13	G	1112	CLA	C3B-C4B	2.88	1.49	1.42
13	c	517	CLA	C4D-ND	-2.88	1.33	1.37
13	v	510	CLA	C3B-C4B	2.88	1.49	1.42
13	A	1111	CLA	C4B-NB	2.88	1.41	1.37
13	b	505	CLA	C4D-ND	-2.88	1.33	1.37
13	c	503	CLA	C4D-ND	-2.88	1.33	1.37
13	G	1102	CLA	C3B-C4B	2.88	1.49	1.42
13	e	1128	CLA	C4B-NB	2.88	1.41	1.37
13	5	505	CLA	C4D-ND	-2.88	1.33	1.37
13	Y	509	CLA	C3B-C4B	2.88	1.49	1.42
13	3	513	CLA	C3B-C4B	2.88	1.49	1.42
13	5	517	CLA	C3B-C4B	2.88	1.49	1.42
13	c	511	CLA	C3B-C4B	2.88	1.49	1.42
13	c	512	CLA	C3B-C4B	2.88	1.49	1.42
13	c	516	CLA	C3B-C4B	2.88	1.49	1.42
13	6	512	CLA	C4D-ND	-2.88	1.33	1.37
13	6	518	CLA	C4D-ND	-2.88	1.33	1.37
13	H	1201	CLA	C4B-NB	2.88	1.41	1.37
13	4	512	CLA	C3B-C4B	2.88	1.49	1.42
13	v	518	CLA	C3B-C4B	2.88	1.49	1.42
13	H	1201	CLA	C3B-C4B	2.88	1.49	1.42
13	f	1221	CLA	C3B-C4B	2.88	1.49	1.42
13	c	504	CLA	C4D-ND	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1107	CLA	C4B-NB	2.88	1.41	1.37
13	G	1128	CLA	C4B-NB	2.88	1.41	1.37
13	G	1111	CLA	C3B-C4B	2.88	1.49	1.42
13	A	1118	CLA	C4B-NB	2.88	1.41	1.37
13	5	512	CLA	C3B-C4B	2.88	1.49	1.42
13	Y	513	CLA	C3B-C4B	2.88	1.49	1.42
13	t	508	CLA	CMB-C2B	-2.88	1.44	1.50
13	q	510	CLA	C3B-C4B	2.88	1.49	1.42
13	q	513	CLA	C4D-ND	-2.88	1.33	1.37
13	f	1225	CLA	C1D-ND	2.88	1.41	1.37
13	3	510	CLA	C4D-ND	-2.88	1.33	1.37
13	5	518	CLA	C4D-ND	-2.88	1.33	1.37
13	5	516	CLA	C3B-C4B	2.87	1.49	1.42
13	6	513	CLA	C4D-ND	-2.87	1.33	1.37
13	J	1303	CLA	C4B-NB	2.87	1.41	1.37
13	G	1135	CLA	C1D-ND	2.87	1.41	1.37
13	d	512	CLA	C3B-C4B	2.87	1.49	1.42
13	e	1111	CLA	C3B-C4B	2.87	1.49	1.42
13	e	1102	CLA	C3B-C4B	2.87	1.49	1.42
13	u	517	CLA	C3B-C4B	2.87	1.49	1.42
20	s	822	SQD	O47-C7	2.87	1.42	1.34
13	b	506	CLA	C4D-ND	-2.87	1.33	1.37
13	f	1222	CLA	C3B-C4B	2.87	1.49	1.42
13	T	1303	CLA	C4B-NB	2.87	1.41	1.37
13	d	508	CLA	C3B-C4B	2.87	1.49	1.42
20	3	822	SQD	O47-C7	2.87	1.42	1.34
13	c	518	CLA	C4D-ND	-2.87	1.33	1.37
13	u	513	CLA	C4D-ND	-2.87	1.33	1.37
13	c	510	CLA	C3B-C4B	2.87	1.49	1.42
13	G	1139	CLA	C1D-ND	2.87	1.41	1.37
13	e	1103	CLA	C1D-ND	2.87	1.41	1.37
13	4	501	CLA	C4D-ND	-2.87	1.33	1.37
13	A	1112	CLA	C3B-C4B	2.87	1.49	1.42
13	1	513	CLA	C3B-C4B	2.87	1.49	1.42
13	5	511	CLA	C3B-C4B	2.87	1.49	1.42
13	5	504	CLA	C4D-ND	-2.87	1.33	1.37
13	B	1230	CLA	C4B-NB	2.87	1.41	1.37
13	v	508	CLA	C3B-C4B	2.87	1.49	1.42
13	5	513	CLA	C4D-ND	-2.86	1.33	1.37
13	B	1222	CLA	C3B-C4B	2.86	1.49	1.42
13	c	512	CLA	C4D-ND	-2.86	1.33	1.37
13	s	519	CLA	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1107	CLA	C4B-NB	2.86	1.41	1.37
13	u	516	CLA	C3B-C4B	2.86	1.49	1.42
13	A	1111	CLA	C3B-C4B	2.86	1.49	1.42
13	Y	513	CLA	C4D-ND	-2.86	1.33	1.37
13	G	1124	CLA	C3B-C4B	2.86	1.49	1.42
13	A	1130	CLA	C3B-C4B	2.86	1.49	1.42
13	e	1112	CLA	C3B-C4B	2.86	1.49	1.42
13	H	1232	CLA	C4B-NB	2.86	1.41	1.37
13	c	505	CLA	C4D-ND	-2.86	1.33	1.37
13	5	510	CLA	C3B-C4B	2.86	1.49	1.42
13	H	1222	CLA	C3B-C4B	2.86	1.49	1.42
13	u	511	CLA	C3B-C4B	2.86	1.49	1.42
13	Z	506	CLA	C3B-C4B	2.86	1.49	1.42
13	b	510	CLA	C3B-C4B	2.86	1.49	1.42
13	b	508	CLA	CMB-C2B	-2.86	1.44	1.50
13	6	510	CLA	C3B-C4B	2.86	1.49	1.42
13	f	1218	CLA	C4B-NB	2.86	1.41	1.37
13	a	517	CLA	C3B-C4B	2.86	1.49	1.42
13	d	510	CLA	C3B-C4B	2.86	1.49	1.42
13	t	505	CLA	C4D-ND	-2.86	1.33	1.37
13	t	512	CLA	C3B-C4B	2.86	1.49	1.42
13	G	1107	CLA	C4B-NB	2.86	1.41	1.37
13	3	510	CLA	C3B-C4B	2.86	1.49	1.42
13	4	510	CLA	C3B-C4B	2.86	1.49	1.42
13	G	1130	CLA	C3B-C4B	2.86	1.49	1.42
13	A	1128	CLA	C1B-NB	-2.86	1.34	1.37
13	A	1135	CLA	C1D-ND	2.86	1.41	1.37
13	5	503	CLA	C4D-ND	-2.86	1.33	1.37
13	q	509	CLA	C3B-C4B	2.85	1.49	1.42
13	s	510	CLA	C3B-C4B	2.85	1.49	1.42
13	a	510	CLA	C3B-C4B	2.85	1.49	1.42
13	G	1118	CLA	C4B-NB	2.85	1.41	1.37
13	d	517	CLA	C3B-C4B	2.85	1.49	1.42
13	f	1230	CLA	C4B-NB	2.85	1.41	1.37
13	U	1401	CLA	C3B-C4B	2.85	1.49	1.42
13	f	1227	CLA	C4B-NB	2.85	1.41	1.37
13	4	504	CLA	C4D-ND	-2.85	1.33	1.37
13	v	513	CLA	C4D-ND	-2.85	1.33	1.37
13	4	508	CLA	CMB-C2B	-2.85	1.44	1.50
13	s	517	CLA	C3B-C4B	2.85	1.49	1.42
13	K	1401	CLA	C3B-C4B	2.85	1.49	1.42
13	2	503	CLA	C3B-C4B	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	518	CLA	C3B-C4B	2.85	1.49	1.42
13	t	517	CLA	C3B-C4B	2.85	1.49	1.42
13	B	1232	CLA	C4B-NB	2.85	1.41	1.37
13	1	511	CLA	C3B-C4B	2.85	1.49	1.42
13	2	504	CLA	C3B-C4B	2.85	1.49	1.42
13	b	516	CLA	C4D-ND	-2.85	1.33	1.37
13	c	503	CLA	C3B-C4B	2.85	1.49	1.42
13	Z	503	CLA	C3B-C4B	2.85	1.49	1.42
13	t	510	CLA	C3B-C4B	2.85	1.49	1.42
20	u	822	SQD	O47-C7	2.85	1.42	1.34
13	t	506	CLA	C4D-ND	-2.85	1.33	1.37
13	1	509	CLA	C3B-C4B	2.85	1.49	1.42
13	u	510	CLA	C3B-C4B	2.84	1.49	1.42
13	b	512	CLA	C3B-C4B	2.84	1.49	1.42
13	m	1401	CLA	C3B-C4B	2.84	1.49	1.42
13	3	517	CLA	C3B-C4B	2.84	1.49	1.42
13	b	503	CLA	C3B-C4B	2.84	1.49	1.42
13	A	1120	CLA	C4B-NB	2.84	1.41	1.37
13	4	516	CLA	C4D-ND	-2.84	1.33	1.37
13	q	511	CLA	C3B-C4B	2.84	1.49	1.42
13	e	1124	CLA	C4B-NB	2.84	1.41	1.37
13	6	508	CLA	C3B-C4B	2.84	1.49	1.42
13	6	517	CLA	C3B-C4B	2.84	1.49	1.42
13	b	511	CLA	C3B-C4B	2.84	1.49	1.42
13	b	501	CLA	C4D-ND	-2.84	1.33	1.37
13	Z	504	CLA	C3B-C4B	2.84	1.49	1.42
13	Z	510	CLA	C3B-C4B	2.84	1.49	1.42
20	a	822	SQD	O47-C7	2.84	1.42	1.34
13	s	510	CLA	C4D-ND	-2.84	1.33	1.37
13	s	511	CLA	C3B-C4B	2.84	1.49	1.42
20	5	822	SQD	O47-C7	2.84	1.42	1.34
13	2	510	CLA	C3B-C4B	2.84	1.49	1.42
13	d	518	CLA	C3B-C4B	2.84	1.49	1.42
13	A	1103	CLA	C1D-ND	2.84	1.41	1.37
13	4	517	CLA	C3B-C4B	2.84	1.49	1.42
13	e	1120	CLA	C4B-NB	2.84	1.41	1.37
13	2	506	CLA	C3B-C4B	2.84	1.49	1.42
13	3	506	CLA	C3B-C4B	2.84	1.49	1.42
13	t	501	CLA	C4D-ND	-2.84	1.33	1.37
13	e	1128	CLA	C1B-NB	-2.84	1.34	1.37
13	H	1211	CLA	C4B-NB	2.84	1.41	1.37
13	e	1124	CLA	C3B-C4B	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1234	CLA	MG-NB	-2.83	2.00	2.05
13	r	504	CLA	C3B-C4B	2.83	1.49	1.42
13	H	1230	CLA	C4B-NB	2.83	1.41	1.37
13	1	510	CLA	C3B-C4B	2.83	1.49	1.42
20	c	822	SQD	O47-C7	2.83	1.42	1.34
13	b	504	CLA	C4D-ND	-2.83	1.33	1.37
13	3	518	CLA	C3B-C4B	2.83	1.49	1.42
13	Y	503	CLA	C3B-C4B	2.83	1.49	1.42
13	Y	511	CLA	C3B-C4B	2.83	1.49	1.42
13	r	503	CLA	C3B-C4B	2.83	1.49	1.42
13	c	513	CLA	C4D-ND	-2.83	1.33	1.37
13	H	1023	CLA	C3B-C4B	2.83	1.49	1.42
13	5	503	CLA	C3B-C4B	2.83	1.49	1.42
13	u	518	CLA	C4D-ND	-2.83	1.33	1.37
13	a	518	CLA	C3B-C4B	2.83	1.49	1.42
13	n	1502	CLA	C3B-C4B	2.83	1.49	1.42
13	4	506	CLA	C4D-ND	-2.83	1.33	1.37
13	B	1218	CLA	C4B-NB	2.83	1.41	1.37
13	H	1227	CLA	C4B-NB	2.83	1.41	1.37
13	u	503	CLA	C3B-C4B	2.83	1.49	1.42
13	H	1234	CLA	MG-NB	-2.83	2.00	2.05
13	e	1135	CLA	MG-NB	-2.83	2.00	2.05
13	1	517	CLA	C4D-ND	-2.83	1.33	1.37
13	e	1130	CLA	C3B-C4B	2.83	1.49	1.42
13	B	1023	CLA	C3B-C4B	2.83	1.49	1.42
13	H	1210	CLA	C3B-C4B	2.83	1.49	1.42
13	G	1013	CLA	C1B-NB	-2.83	1.34	1.37
13	A	1124	CLA	C3B-C4B	2.83	1.49	1.42
13	r	518	CLA	C3B-C4B	2.82	1.49	1.42
13	4	503	CLA	C3B-C4B	2.82	1.49	1.42
13	V	1502	CLA	C4B-NB	2.82	1.41	1.37
13	G	1124	CLA	C4B-NB	2.82	1.41	1.37
13	Y	512	CLA	C3B-C4B	2.82	1.49	1.42
13	G	1128	CLA	C1B-NB	-2.82	1.34	1.37
13	f	1226	CLA	C1D-ND	2.82	1.41	1.37
13	2	518	CLA	C3B-C4B	2.82	1.49	1.42
13	3	511	CLA	C3B-C4B	2.82	1.49	1.42
13	r	510	CLA	C3B-C4B	2.82	1.49	1.42
13	v	517	CLA	C3B-C4B	2.82	1.49	1.42
13	f	1232	CLA	C4B-NB	2.82	1.41	1.37
13	t	511	CLA	C3B-C4B	2.82	1.49	1.42
13	s	506	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1135	CLA	MG-NB	-2.82	2.00	2.05
13	V	1503	CLA	C4B-NB	2.82	1.41	1.37
13	4	511	CLA	C3B-C4B	2.82	1.49	1.42
13	a	504	CLA	C3B-C4B	2.82	1.49	1.42
13	s	518	CLA	C3B-C4B	2.82	1.49	1.42
13	a	511	CLA	C3B-C4B	2.82	1.49	1.42
13	u	501	CLA	C3B-C4B	2.82	1.49	1.42
13	e	1112	CLA	C4B-NB	2.82	1.41	1.37
13	e	1137	CLA	C4B-NB	2.82	1.41	1.37
13	q	517	CLA	C3B-C4B	2.82	1.49	1.42
13	1	505	CLA	C3B-C4B	2.82	1.49	1.42
13	q	505	CLA	C3B-C4B	2.82	1.49	1.42
13	s	516	CLA	C3B-C4B	2.82	1.49	1.42
13	A	1124	CLA	C4B-NB	2.81	1.41	1.37
13	B	1227	CLA	C4B-NB	2.81	1.41	1.37
13	t	507	CLA	C4D-ND	-2.81	1.33	1.37
20	Y	822	SQD	O47-C7	2.81	1.42	1.34
13	1	512	CLA	C3B-C4B	2.81	1.49	1.42
13	3	516	CLA	C3B-C4B	2.81	1.49	1.42
13	Y	505	CLA	C3B-C4B	2.81	1.49	1.42
13	L	1503	CLA	C4B-NB	2.81	1.41	1.37
13	n	1502	CLA	C4B-NB	2.81	1.41	1.37
13	r	506	CLA	C3B-C4B	2.81	1.49	1.42
13	1	505	CLA	C4D-ND	-2.81	1.33	1.37
13	b	517	CLA	C3B-C4B	2.81	1.49	1.42
13	t	503	CLA	C3B-C4B	2.81	1.49	1.42
13	5	501	CLA	C3B-C4B	2.81	1.49	1.42
13	e	1125	CLA	C3B-C4B	2.81	1.49	1.42
13	1	503	CLA	C3B-C4B	2.81	1.49	1.42
13	a	506	CLA	C3B-C4B	2.81	1.49	1.42
13	q	512	CLA	C3B-C4B	2.81	1.49	1.42
13	t	504	CLA	C4D-ND	-2.81	1.33	1.37
13	q	505	CLA	C4D-ND	-2.80	1.33	1.37
13	L	1502	CLA	C3B-C4B	2.80	1.49	1.42
13	Y	516	CLA	C3B-C4B	2.80	1.49	1.42
13	Z	518	CLA	C3B-C4B	2.80	1.49	1.42
13	a	516	CLA	C3B-C4B	2.80	1.49	1.42
13	q	508	CLA	C3B-C4B	2.80	1.49	1.42
13	t	503	CLA	C4D-ND	-2.80	1.33	1.37
13	v	507	CLA	C4D-ND	-2.80	1.33	1.37
13	f	1234	CLA	MG-NB	-2.80	2.00	2.05
13	A	1125	CLA	C3B-C4B	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	822	SQD	O47-C7	2.80	1.42	1.34
13	Y	517	CLA	C3B-C4B	2.80	1.49	1.42
20	q	822	SQD	O47-C7	2.80	1.42	1.34
13	Y	508	CLA	C3B-C4B	2.80	1.49	1.42
13	H	1217	CLA	C4B-NB	2.80	1.41	1.37
13	q	503	CLA	C3B-C4B	2.80	1.49	1.42
13	B	1210	CLA	C3B-C4B	2.80	1.49	1.42
13	G	1125	CLA	C3B-C4B	2.80	1.49	1.42
13	e	1013	CLA	C1B-NB	-2.80	1.34	1.37
13	3	504	CLA	C3B-C4B	2.80	1.49	1.42
13	G	1107	CLA	CMD-C2D	-2.80	1.44	1.50
13	Y	505	CLA	C4D-ND	-2.80	1.33	1.37
13	Y	510	CLA	C3B-C4B	2.80	1.49	1.42
13	A	1112	CLA	C4B-NB	2.80	1.41	1.37
13	G	1112	CLA	C4B-NB	2.80	1.41	1.37
13	Y	517	CLA	C4D-ND	-2.80	1.33	1.37
13	q	501	CLA	C3B-C4B	2.80	1.49	1.42
13	q	504	CLA	C3B-C4B	2.79	1.49	1.42
13	A	1119	CLA	C3B-C4B	2.79	1.49	1.42
13	e	1119	CLA	C3B-C4B	2.79	1.49	1.42
13	6	507	CLA	C4D-ND	-2.79	1.33	1.37
13	G	1113	CLA	C4B-NB	2.79	1.41	1.37
13	A	1013	CLA	C1B-NB	-2.79	1.34	1.37
13	n	1503	CLA	C4B-NB	2.79	1.41	1.37
13	G	1119	CLA	C3B-C4B	2.79	1.49	1.42
13	f	1210	CLA	C3B-C4B	2.79	1.49	1.42
13	1	517	CLA	C3B-C4B	2.79	1.49	1.42
13	G	1137	CLA	C4B-NB	2.79	1.41	1.37
13	B	1217	CLA	C4B-NB	2.79	1.41	1.37
13	f	1023	CLA	C3B-C4B	2.79	1.49	1.42
13	v	505	CLA	C3B-C4B	2.79	1.49	1.42
13	l	1303	CLA	C4B-NB	2.79	1.41	1.37
13	d	505	CLA	C3B-C4B	2.79	1.49	1.42
13	B	1226	CLA	C1D-ND	2.79	1.41	1.37
13	A	1107	CLA	CMD-C2D	-2.79	1.44	1.50
13	e	1107	CLA	CMD-C2D	-2.79	1.44	1.50
13	V	1502	CLA	C3B-C4B	2.79	1.49	1.42
13	B	1211	CLA	C4B-NB	2.79	1.41	1.37
13	b	502	CLA	C4D-ND	-2.79	1.33	1.37
13	1	504	CLA	C3B-C4B	2.78	1.49	1.42
13	4	502	CLA	C4D-ND	-2.78	1.33	1.37
13	d	503	CLA	C3B-C4B	2.78	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	u	504	CLA	C3B-C4B	2.78	1.49	1.42
13	G	1135	CLA	MG-NB	-2.78	2.00	2.05
13	5	519	CLA	C3B-C4B	2.78	1.49	1.42
13	u	519	CLA	C3B-C4B	2.78	1.49	1.42
13	b	510	CLA	C4D-ND	-2.78	1.33	1.37
13	c	516	CLA	C4D-ND	-2.78	1.33	1.37
13	s	519	CLA	C3B-C4B	2.78	1.49	1.42
13	H	1226	CLA	C1D-ND	2.78	1.41	1.37
13	1	508	CLA	C3B-C4B	2.78	1.49	1.42
13	6	503	CLA	C3B-C4B	2.78	1.49	1.42
13	b	503	CLA	C4D-ND	-2.78	1.33	1.37
13	Z	501	CLA	C3B-C4B	2.78	1.49	1.42
13	4	510	CLA	C4D-ND	-2.78	1.33	1.37
13	c	501	CLA	C3B-C4B	2.78	1.49	1.42
13	a	501	CLA	C1B-C2B	2.78	1.49	1.43
13	f	1211	CLA	C4B-NB	2.78	1.41	1.37
13	2	516	CLA	C3B-C4B	2.78	1.49	1.42
13	c	502	CLA	C3B-C4B	2.77	1.49	1.42
13	u	502	CLA	C3B-C4B	2.77	1.49	1.42
13	5	516	CLA	C4D-ND	-2.77	1.33	1.37
13	L	1502	CLA	C4B-NB	2.77	1.41	1.37
13	f	1012	CLA	C1D-ND	2.77	1.41	1.37
13	6	505	CLA	C3B-C4B	2.77	1.49	1.42
13	c	519	CLA	C3B-C4B	2.77	1.49	1.42
13	5	504	CLA	C3B-C4B	2.77	1.49	1.42
13	3	503	CLA	C3B-C4B	2.77	1.49	1.42
13	3	519	CLA	C3B-C4B	2.77	1.49	1.42
13	f	1217	CLA	C4B-NB	2.77	1.41	1.37
13	1	516	CLA	C3B-C4B	2.77	1.49	1.42
13	Y	504	CLA	C3B-C4B	2.77	1.49	1.42
13	Z	516	CLA	C3B-C4B	2.77	1.49	1.42
13	G	1131	CLA	C4B-NB	2.77	1.41	1.37
13	3	501	CLA	C1B-C2B	2.77	1.49	1.43
13	B	1205	CLA	C3B-C4B	2.77	1.49	1.42
13	s	504	CLA	C3B-C4B	2.77	1.49	1.42
13	q	516	CLA	C3B-C4B	2.77	1.49	1.42
13	G	1128	CLA	MG-NB	-2.77	2.00	2.05
13	4	503	CLA	C4D-ND	-2.77	1.33	1.37
13	f	1205	CLA	C3B-C4B	2.77	1.49	1.42
13	b	519	CLA	C3B-C4B	2.76	1.49	1.42
13	6	511	CLA	C3B-C4B	2.76	1.49	1.42
13	1	501	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	519	CLA	C3B-C4B	2.76	1.49	1.42
13	f	1021	CLA	C1B-C2B	2.76	1.49	1.43
13	4	519	CLA	C3B-C4B	2.76	1.49	1.42
13	r	516	CLA	C3B-C4B	2.76	1.49	1.42
13	A	1137	CLA	C4B-NB	2.76	1.41	1.37
13	v	511	CLA	C3B-C4B	2.76	1.49	1.42
13	q	517	CLA	C4D-ND	-2.76	1.33	1.37
13	a	519	CLA	C3B-C4B	2.76	1.49	1.42
13	H	1218	CLA	C4B-NB	2.76	1.41	1.37
13	s	501	CLA	C1B-C2B	2.76	1.49	1.43
13	u	508	CLA	C3B-C4B	2.76	1.49	1.42
13	4	502	CLA	C3B-C4B	2.76	1.49	1.42
13	G	1119	CLA	C4B-NB	2.76	1.41	1.37
13	f	1234	CLA	C3B-C4B	2.76	1.49	1.42
13	H	1205	CLA	C3B-C4B	2.75	1.49	1.42
13	Z	508	CLA	C3B-C4B	2.75	1.49	1.42
13	A	1131	CLA	C4B-NB	2.75	1.41	1.37
13	t	509	CLA	C3B-C4B	2.75	1.49	1.42
13	f	1202	CLA	C3B-C4B	2.75	1.49	1.42
13	4	507	CLA	C4D-ND	-2.75	1.33	1.37
13	s	503	CLA	C3B-C4B	2.75	1.49	1.42
13	2	501	CLA	C3B-C4B	2.75	1.49	1.42
13	q	519	CLA	C4B-NB	2.75	1.41	1.37
13	u	516	CLA	C4D-ND	-2.75	1.33	1.37
13	c	504	CLA	C3B-C4B	2.75	1.49	1.42
13	v	503	CLA	C3B-C4B	2.75	1.49	1.42
13	H	1223	CLA	C3B-C4B	2.75	1.49	1.42
13	Z	505	CLA	C3B-C4B	2.75	1.49	1.42
13	T	1302	CLA	C3B-C4B	2.75	1.49	1.42
13	t	502	CLA	C3B-C4B	2.75	1.49	1.42
13	4	505	CLA	C3B-C4B	2.75	1.49	1.42
13	t	510	CLA	C4D-ND	-2.75	1.33	1.37
13	e	1128	CLA	MG-NB	-2.75	2.00	2.05
13	A	1113	CLA	C4B-NB	2.75	1.41	1.37
13	t	502	CLA	C4D-ND	-2.75	1.33	1.37
13	B	1234	CLA	C3B-C4B	2.75	1.49	1.42
13	H	1207	CLA	C3B-C4B	2.75	1.49	1.42
13	2	508	CLA	C3B-C4B	2.75	1.49	1.42
13	b	502	CLA	C3B-C4B	2.75	1.49	1.42
13	t	519	CLA	C4B-NB	2.74	1.41	1.37
13	H	1234	CLA	C3B-C4B	2.74	1.49	1.42
13	f	1207	CLA	C3B-C4B	2.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	505	CLA	C3B-C4B	2.74	1.49	1.42
13	Y	501	CLA	C3B-C4B	2.74	1.49	1.42
13	H	1021	CLA	C1B-C2B	2.74	1.49	1.43
13	4	509	CLA	C3B-C4B	2.74	1.49	1.42
13	5	508	CLA	C3B-C4B	2.74	1.49	1.42
13	r	501	CLA	C3B-C4B	2.74	1.49	1.42
13	2	505	CLA	C3B-C4B	2.74	1.49	1.42
13	B	1021	CLA	C1B-C2B	2.74	1.49	1.43
13	e	1117	CLA	C4B-NB	2.74	1.41	1.37
13	s	512	CLA	C3B-C4B	2.74	1.49	1.42
13	b	505	CLA	C3B-C4B	2.74	1.49	1.42
13	H	1239	CLA	CMB-C2B	-2.74	1.45	1.50
13	a	503	CLA	C3B-C4B	2.74	1.49	1.42
13	G	1103	CLA	C4B-NB	2.74	1.41	1.37
13	t	507	CLA	C1B-C2B	2.74	1.49	1.43
13	B	1202	CLA	C3B-C4B	2.74	1.49	1.42
13	B	1208	CLA	C4B-NB	2.74	1.41	1.37
13	b	507	CLA	C1B-C2B	2.73	1.49	1.43
13	R	1302	CLA	C3B-C4B	2.73	1.49	1.42
13	U	1105	CLA	C3B-C4B	2.73	1.49	1.42
13	e	1113	CLA	C4B-NB	2.73	1.41	1.37
13	B	1207	CLA	C3B-C4B	2.73	1.49	1.42
13	F	1302	CLA	C3B-C4B	2.73	1.49	1.42
13	H	1232	CLA	C3B-C4B	2.73	1.49	1.42
13	q	505	CLA	C1B-C2B	2.73	1.49	1.43
13	5	502	CLA	C3B-C4B	2.73	1.49	1.42
13	A	1126	CLA	C3B-C4B	2.73	1.49	1.42
13	4	507	CLA	C1B-C2B	2.73	1.49	1.43
13	G	1126	CLA	C3B-C4B	2.73	1.49	1.42
13	H	1202	CLA	C3B-C4B	2.73	1.49	1.42
13	e	1131	CLA	C4B-NB	2.73	1.41	1.37
13	B	1223	CLA	C3B-C4B	2.73	1.49	1.42
13	c	508	CLA	C3B-C4B	2.73	1.49	1.42
13	A	1128	CLA	MG-NB	-2.73	2.00	2.05
13	3	512	CLA	C3B-C4B	2.73	1.49	1.42
13	b	507	CLA	C3B-C4B	2.73	1.49	1.42
13	B	1226	CLA	MG-NB	-2.73	2.00	2.05
13	4	518	CLA	C3B-C4B	2.73	1.49	1.42
13	H	1211	CLA	C3B-C4B	2.73	1.49	1.42
13	l	1302	CLA	C3B-C4B	2.73	1.49	1.42
13	d	507	CLA	C4D-ND	-2.73	1.33	1.37
13	H	1226	CLA	MG-NB	-2.73	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	511	CLA	C3B-C4B	2.73	1.49	1.42
13	1	519	CLA	C4B-NB	2.73	1.41	1.37
13	b	509	CLA	C3B-C4B	2.73	1.49	1.42
13	A	1125	CLA	C4B-NB	2.73	1.41	1.37
13	B	1012	CLA	C1D-ND	2.72	1.41	1.37
13	G	1011	CLA	C4B-NB	2.72	1.41	1.37
13	G	1123	CLA	C4B-NB	2.72	1.41	1.37
13	A	1119	CLA	C4B-NB	2.72	1.41	1.37
13	f	1226	CLA	MG-NB	-2.72	2.00	2.05
13	6	501	CLA	C3B-C4B	2.72	1.49	1.42
20	L	5216	SQD	O47-C7	2.72	1.42	1.34
13	H	1213	CLA	C3B-C4B	2.72	1.49	1.42
13	r	508	CLA	C3B-C4B	2.72	1.49	1.42
13	f	1232	CLA	C3B-C4B	2.72	1.49	1.42
13	f	1215	CLA	C4B-NB	2.72	1.41	1.37
13	G	1117	CLA	C4B-NB	2.72	1.41	1.37
13	u	505	CLA	C1B-C2B	2.72	1.49	1.43
13	b	518	CLA	C3B-C4B	2.72	1.49	1.42
13	f	1223	CLA	C3B-C4B	2.72	1.49	1.42
13	2	519	CLA	C3B-C4B	2.72	1.49	1.42
13	t	505	CLA	C3B-C4B	2.72	1.49	1.42
13	t	507	CLA	C3B-C4B	2.72	1.49	1.42
13	m	1105	CLA	C3B-C4B	2.72	1.49	1.42
13	5	505	CLA	C1B-C2B	2.72	1.49	1.43
13	B	1213	CLA	C3B-C4B	2.71	1.49	1.42
13	e	1131	CLA	C3B-C4B	2.71	1.49	1.42
13	e	1139	CLA	CMD-C2D	-2.71	1.45	1.50
13	e	1126	CLA	C3B-C4B	2.71	1.49	1.42
13	4	507	CLA	C3B-C4B	2.71	1.49	1.42
13	f	1213	CLA	C3B-C4B	2.71	1.49	1.42
13	B	1219	CLA	C3B-C4B	2.71	1.49	1.42
13	c	505	CLA	C1B-C2B	2.71	1.49	1.43
13	A	1131	CLA	C3B-C4B	2.71	1.49	1.42
13	B	1232	CLA	C3B-C4B	2.71	1.49	1.42
13	Z	519	CLA	C3B-C4B	2.71	1.49	1.42
13	J	1302	CLA	C3B-C4B	2.71	1.49	1.42
13	t	517	CLA	C1B-C2B	2.71	1.49	1.43
13	H	1215	CLA	C4B-NB	2.71	1.41	1.37
13	B	1211	CLA	C3B-C4B	2.71	1.49	1.42
13	G	1131	CLA	C3B-C4B	2.71	1.49	1.42
20	V	5216	SQD	O47-C7	2.71	1.41	1.34
13	f	1213	CLA	C4B-NB	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	516	CLA	C1B-C2B	2.71	1.49	1.43
13	v	501	CLA	C3B-C4B	2.71	1.49	1.42
13	j	1302	CLA	C3B-C4B	2.71	1.49	1.42
13	b	507	CLA	C4D-ND	-2.71	1.34	1.37
13	A	1103	CLA	C4B-NB	2.71	1.41	1.37
20	n	5216	SQD	O47-C7	2.71	1.41	1.34
13	Y	505	CLA	C1B-C2B	2.71	1.49	1.43
13	t	518	CLA	C3B-C4B	2.71	1.49	1.42
13	e	1103	CLA	C4B-NB	2.71	1.41	1.37
13	4	502	CLA	C1B-C2B	2.70	1.49	1.43
13	K	1105	CLA	C3B-C4B	2.70	1.49	1.42
13	s	508	CLA	CMB-C2B	-2.70	1.45	1.50
13	d	501	CLA	C3B-C4B	2.70	1.49	1.42
13	H	1012	CLA	C1D-ND	2.70	1.41	1.37
13	B	1240	CLA	C3B-C4B	2.70	1.49	1.42
13	A	1139	CLA	CMD-C2D	-2.70	1.45	1.50
13	a	512	CLA	C3B-C4B	2.70	1.49	1.42
13	f	1219	CLA	C3B-C4B	2.70	1.49	1.42
13	r	516	CLA	C1B-C2B	2.70	1.49	1.43
13	A	1117	CLA	C4B-NB	2.70	1.41	1.37
13	e	1119	CLA	C4B-NB	2.70	1.41	1.37
13	B	1239	CLA	CMB-C2B	-2.70	1.45	1.50
13	3	508	CLA	CMB-C2B	-2.70	1.45	1.50
13	f	1239	CLA	CMB-C2B	-2.70	1.45	1.50
13	2	516	CLA	C1B-C2B	2.70	1.49	1.43
13	H	1219	CLA	C3B-C4B	2.70	1.49	1.42
13	f	1211	CLA	C3B-C4B	2.70	1.49	1.42
13	1	505	CLA	C1B-C2B	2.70	1.49	1.43
13	t	502	CLA	C1B-C2B	2.70	1.49	1.43
13	a	508	CLA	CMB-C2B	-2.70	1.45	1.50
13	B	1222	CLA	C4B-NB	2.70	1.41	1.37
13	r	519	CLA	C3B-C4B	2.70	1.49	1.42
13	A	1119	CLA	CMB-C2B	-2.70	1.45	1.50
13	G	1119	CLA	CMB-C2B	-2.70	1.45	1.50
13	4	517	CLA	C1B-C2B	2.69	1.49	1.43
13	H	1225	CLA	C3B-C4B	2.69	1.49	1.42
13	G	1121	CLA	CMD-C2D	-2.69	1.45	1.50
13	m	1103	CLA	C4B-NB	2.69	1.41	1.37
13	b	502	CLA	C1B-C2B	2.69	1.49	1.43
13	e	1121	CLA	CMD-C2D	-2.69	1.45	1.50
13	f	1240	CLA	C3B-C4B	2.69	1.49	1.42
13	A	1123	CLA	C4B-NB	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1116	CLA	C3B-C4B	2.69	1.49	1.42
13	B	1215	CLA	C4B-NB	2.69	1.41	1.37
13	G	1125	CLA	C4B-NB	2.69	1.41	1.37
13	t	513	CLA	C1B-C2B	2.69	1.49	1.43
13	f	1212	CLA	C4B-NB	2.69	1.41	1.37
13	e	1119	CLA	CMB-C2B	-2.69	1.45	1.50
13	3	505	CLA	C3B-C4B	2.69	1.49	1.42
13	4	519	CLA	C4B-NB	2.69	1.41	1.37
13	H	1212	CLA	C4B-NB	2.69	1.41	1.37
13	B	1213	CLA	C4B-NB	2.69	1.41	1.37
13	f	1225	CLA	C3B-C4B	2.69	1.49	1.42
13	e	1106	CLA	C4B-NB	2.69	1.41	1.37
13	a	505	CLA	C1B-C2B	2.69	1.49	1.43
13	G	1139	CLA	CMD-C2D	-2.69	1.45	1.50
13	a	505	CLA	C3B-C4B	2.69	1.49	1.42
20	H	1852	SQD	O48-C23	2.69	1.41	1.33
13	f	1228	CLA	C4B-NB	2.69	1.41	1.37
13	B	1212	CLA	C4B-NB	2.69	1.41	1.37
13	G	1103	CLA	CMC-C2C	-2.68	1.45	1.50
13	s	516	CLA	C1B-C2B	2.68	1.49	1.43
13	G	1116	CLA	C3B-C4B	2.68	1.49	1.42
13	e	1103	CLA	CMC-C2C	-2.68	1.45	1.50
13	c	502	CLA	C1B-C2B	2.68	1.49	1.43
13	B	1228	CLA	C4B-NB	2.68	1.41	1.37
13	H	1208	CLA	C4B-NB	2.68	1.41	1.37
13	A	1108	CLA	C3B-C4B	2.68	1.49	1.42
13	6	516	CLA	C1B-C2B	2.68	1.49	1.43
13	e	1125	CLA	C4B-NB	2.68	1.41	1.37
13	b	506	CLA	C1B-C2B	2.68	1.49	1.43
13	b	517	CLA	C1B-C2B	2.68	1.49	1.43
13	u	502	CLA	C1B-C2B	2.68	1.49	1.43
13	A	1122	CLA	C4B-NB	2.68	1.41	1.37
13	a	507	CLA	C1B-C2B	2.68	1.49	1.43
13	s	507	CLA	C1B-C2B	2.68	1.49	1.43
13	e	1123	CLA	C4B-NB	2.68	1.41	1.37
13	Z	516	CLA	C1B-C2B	2.68	1.49	1.43
13	H	1240	CLA	C3B-C4B	2.68	1.49	1.42
13	e	1116	CLA	C3B-C4B	2.68	1.49	1.42
13	a	516	CLA	C1B-C2B	2.68	1.49	1.43
13	A	1011	CLA	C4B-NB	2.67	1.41	1.37
13	f	1208	CLA	C4B-NB	2.67	1.41	1.37
13	G	1114	CLA	CMB-C2B	-2.67	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	519	CLA	C4B-NB	2.67	1.41	1.37
13	H	1238	CLA	C3B-C4B	2.67	1.49	1.42
13	H	1012	CLA	CHC-C1C	2.67	1.44	1.38
13	G	1108	CLA	C3B-C4B	2.67	1.49	1.42
13	f	1222	CLA	C4B-NB	2.67	1.41	1.37
13	4	506	CLA	C1B-C2B	2.67	1.49	1.43
13	5	502	CLA	C1B-C2B	2.67	1.49	1.43
13	s	505	CLA	C3B-C4B	2.67	1.49	1.42
13	e	1114	CLA	CMB-C2B	-2.67	1.45	1.50
13	B	1225	CLA	C3B-C4B	2.67	1.49	1.42
13	v	509	CLA	C1B-C2B	2.67	1.49	1.43
13	A	1121	CLA	CMD-C2D	-2.67	1.45	1.50
13	v	516	CLA	C1B-C2B	2.67	1.49	1.43
13	2	517	CLA	C3B-C4B	2.67	1.49	1.42
13	v	502	CLA	C3B-C4B	2.67	1.49	1.42
13	6	509	CLA	C1B-C2B	2.67	1.49	1.43
13	d	516	CLA	C1B-C2B	2.67	1.49	1.43
13	3	505	CLA	C1B-C2B	2.67	1.49	1.43
13	G	1122	CLA	C4B-NB	2.67	1.41	1.37
20	B	1852	SQD	O48-C23	2.67	1.41	1.33
13	e	1108	CLA	C3B-C4B	2.66	1.49	1.42
13	5	516	CLA	C1B-C2B	2.66	1.49	1.43
13	b	519	CLA	C4B-NB	2.66	1.41	1.37
13	d	502	CLA	C1B-C2B	2.66	1.49	1.43
13	H	1228	CLA	C4B-NB	2.66	1.41	1.37
13	e	1011	CLA	C4B-NB	2.66	1.41	1.37
13	e	1022	CLA	C4B-NB	2.66	1.41	1.37
13	f	1238	CLA	C4B-NB	2.66	1.41	1.37
13	H	1213	CLA	C4B-NB	2.66	1.41	1.37
13	s	505	CLA	C1B-C2B	2.66	1.49	1.43
13	Z	517	CLA	C3B-C4B	2.66	1.49	1.42
13	e	1122	CLA	C4B-NB	2.66	1.41	1.37
13	u	516	CLA	C1B-C2B	2.66	1.49	1.43
20	f	1852	SQD	O48-C23	2.66	1.41	1.33
13	H	1021	CLA	CMD-C2D	-2.66	1.45	1.50
13	3	516	CLA	C1B-C2B	2.66	1.49	1.43
13	B	1238	CLA	C3B-C4B	2.66	1.49	1.42
13	1	502	CLA	C3B-C4B	2.66	1.49	1.42
13	a	501	CLA	C3B-C4B	2.66	1.49	1.42
13	t	506	CLA	C1B-C2B	2.66	1.49	1.43
13	H	1222	CLA	C4B-NB	2.66	1.41	1.37
13	6	502	CLA	C3B-C4B	2.66	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1103	CLA	CMC-C2C	-2.66	1.45	1.50
13	d	509	CLA	C1B-C2B	2.66	1.49	1.43
13	G	1107	CLA	CMB-C2B	-2.66	1.45	1.50
13	s	501	CLA	C3B-C4B	2.66	1.49	1.42
13	q	503	CLA	C1B-C2B	2.66	1.49	1.43
13	2	508	CLA	CMB-C2B	-2.66	1.45	1.50
13	s	502	CLA	C3B-C4B	2.66	1.49	1.42
13	Z	508	CLA	CMB-C2B	-2.65	1.45	1.50
13	G	1013	CLA	MG-NB	-2.65	2.00	2.05
13	3	502	CLA	C3B-C4B	2.65	1.49	1.42
13	b	513	CLA	C1B-C2B	2.65	1.49	1.43
13	c	517	CLA	C1B-C2B	2.65	1.49	1.43
13	d	502	CLA	C3B-C4B	2.65	1.49	1.42
13	v	507	CLA	C3B-C4B	2.65	1.49	1.42
13	3	507	CLA	C1B-C2B	2.65	1.49	1.43
13	6	502	CLA	C1B-C2B	2.65	1.49	1.43
13	G	1022	CLA	C4B-NB	2.65	1.41	1.37
13	A	1107	CLA	CMB-C2B	-2.65	1.45	1.50
13	A	1114	CLA	CMB-C2B	-2.65	1.45	1.50
13	B	1012	CLA	CHC-C1C	2.65	1.43	1.38
13	q	502	CLA	C3B-C4B	2.65	1.49	1.42
13	n	1501	CLA	C3B-C4B	2.65	1.49	1.42
13	L	1501	CLA	C3B-C4B	2.65	1.49	1.42
13	A	1106	CLA	C4B-NB	2.65	1.41	1.37
13	3	501	CLA	C3B-C4B	2.65	1.49	1.42
13	d	501	CLA	C1B-C2B	2.65	1.49	1.43
13	G	1237	CLA	CMB-C2B	-2.65	1.45	1.50
13	H	1216	CLA	C3B-C4B	2.65	1.49	1.42
13	V	1501	CLA	C3B-C4B	2.65	1.49	1.42
13	f	1238	CLA	C3B-C4B	2.65	1.49	1.42
13	4	513	CLA	C1B-C2B	2.65	1.49	1.43
13	v	502	CLA	C1B-C2B	2.65	1.49	1.43
13	u	517	CLA	C1B-C2B	2.64	1.49	1.43
13	4	516	CLA	C1B-C2B	2.64	1.49	1.43
13	6	501	CLA	C1B-C2B	2.64	1.49	1.43
13	t	518	CLA	C1B-C2B	2.64	1.49	1.43
13	H	1206	CLA	C4B-NB	2.64	1.41	1.37
19	f	5002	LMG	O8-C9	-2.64	1.39	1.45
13	e	1109	CLA	C4B-NB	2.64	1.41	1.37
13	f	1220	CLA	C4B-NB	2.64	1.41	1.37
13	r	508	CLA	CMB-C2B	-2.64	1.45	1.50
13	H	1220	CLA	C4B-NB	2.64	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	507	CLA	C3B-C4B	2.64	1.48	1.42
13	B	1229	CLA	C1D-ND	2.64	1.41	1.37
13	H	1229	CLA	C1D-ND	2.64	1.41	1.37
13	Y	502	CLA	C3B-C4B	2.64	1.48	1.42
13	f	1021	CLA	CMD-C2D	-2.64	1.45	1.50
13	e	1107	CLA	C1D-ND	2.64	1.41	1.37
13	A	1013	CLA	CMB-C2B	-2.64	1.45	1.50
13	4	518	CLA	C1B-C2B	2.64	1.49	1.43
13	B	1216	CLA	C3B-C4B	2.64	1.48	1.42
13	u	501	CLA	C1B-C2B	2.64	1.49	1.43
14	H	2002	PQN	C11-C12	2.64	1.54	1.50
13	K	1103	CLA	C4B-NB	2.64	1.41	1.37
13	A	1013	CLA	MG-NB	-2.64	2.00	2.05
13	4	508	CLA	C3B-C4B	2.64	1.48	1.42
13	f	1216	CLA	C3B-C4B	2.64	1.48	1.42
13	G	1013	CLA	CMB-C2B	-2.64	1.45	1.50
13	G	1022	CLA	MG-NB	-2.64	2.00	2.05
13	n	1503	CLA	C3B-C4B	2.64	1.48	1.42
13	b	516	CLA	C1B-C2B	2.64	1.49	1.43
13	t	516	CLA	C1B-C2B	2.63	1.49	1.43
13	f	1012	CLA	CHC-C1C	2.63	1.43	1.38
13	A	1237	CLA	CMB-C2B	-2.63	1.45	1.50
13	6	507	CLA	C3B-C4B	2.63	1.48	1.42
13	G	1105	CLA	C3B-C4B	2.63	1.48	1.42
20	H	1852	SQD	O47-C45	-2.63	1.40	1.46
13	G	1801	CLA	C3B-C4B	2.63	1.48	1.42
13	A	1022	CLA	C4B-NB	2.63	1.41	1.37
13	e	1107	CLA	CMB-C2B	-2.63	1.45	1.50
13	b	518	CLA	C1B-C2B	2.63	1.49	1.43
13	c	506	CLA	C1B-C2B	2.63	1.49	1.43
13	v	505	CLA	C1B-C2B	2.63	1.49	1.43
13	5	517	CLA	C1B-C2B	2.63	1.49	1.43
13	A	1115	CLA	C4B-NB	2.63	1.41	1.37
13	t	501	CLA	C1B-C2B	2.63	1.49	1.43
14	f	2002	PQN	C11-C12	2.63	1.54	1.50
13	G	1801	CLA	C4B-NB	2.63	1.41	1.37
13	e	1105	CLA	C4B-NB	2.63	1.41	1.37
13	4	501	CLA	C1B-C2B	2.63	1.49	1.43
13	1	517	CLA	C1B-C2B	2.63	1.49	1.43
13	5	501	CLA	C1B-C2B	2.63	1.49	1.43
13	q	517	CLA	C1B-C2B	2.63	1.49	1.43
13	b	508	CLA	C3B-C4B	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1220	CLA	C4B-NB	2.63	1.41	1.37
13	1	503	CLA	C1B-C2B	2.63	1.49	1.43
13	Z	505	CLA	C1B-C2B	2.63	1.49	1.43
13	r	517	CLA	C3B-C4B	2.63	1.48	1.42
13	F	1302	CLA	C1B-C2B	2.63	1.49	1.43
13	Y	503	CLA	C1B-C2B	2.63	1.49	1.43
13	Z	507	CLA	C1B-C2B	2.63	1.49	1.43
13	e	1105	CLA	C3B-C4B	2.63	1.48	1.42
13	L	1503	CLA	C3B-C4B	2.63	1.48	1.42
13	f	1206	CLA	C4B-NB	2.63	1.41	1.37
13	e	1115	CLA	CMC-C2C	-2.63	1.45	1.50
13	e	1104	CLA	C3B-C4B	2.63	1.48	1.42
13	G	1107	CLA	C1D-ND	2.63	1.41	1.37
13	U	1103	CLA	C4B-NB	2.63	1.41	1.37
13	e	1127	CLA	C4B-NB	2.63	1.41	1.37
13	5	503	CLA	C1B-C2B	2.63	1.49	1.43
13	e	1022	CLA	MG-NB	-2.63	2.00	2.05
13	A	1107	CLA	C1D-ND	2.63	1.41	1.37
13	v	501	CLA	C1B-C2B	2.63	1.49	1.43
13	e	1801	CLA	C3B-C4B	2.63	1.48	1.42
13	e	1013	CLA	MG-NB	-2.63	2.00	2.05
13	1	508	CLA	CMB-C2B	-2.63	1.45	1.50
13	H	1214	CLA	C3B-C4B	2.63	1.48	1.42
13	2	507	CLA	C1B-C2B	2.62	1.49	1.43
13	a	502	CLA	C3B-C4B	2.62	1.48	1.42
13	e	1123	CLA	C3B-C4B	2.62	1.48	1.42
13	6	505	CLA	C1B-C2B	2.62	1.49	1.43
13	G	1103	CLA	C3B-C4B	2.62	1.48	1.42
13	A	1022	CLA	MG-NB	-2.62	2.00	2.05
13	2	505	CLA	C1B-C2B	2.62	1.49	1.43
13	u	506	CLA	C1B-C2B	2.62	1.49	1.43
13	f	1221	CLA	CMD-C2D	-2.62	1.45	1.50
13	G	1132	CLA	C3B-C4B	2.62	1.48	1.42
13	t	509	CLA	C1B-C2B	2.62	1.49	1.43
13	G	1115	CLA	C4B-NB	2.62	1.41	1.37
13	B	1021	CLA	CMD-C2D	-2.62	1.45	1.50
13	j	1302	CLA	C1B-C2B	2.62	1.49	1.43
13	b	501	CLA	C1B-C2B	2.62	1.49	1.43
13	H	1203	CLA	C4B-NB	2.62	1.41	1.37
13	A	1105	CLA	C3B-C4B	2.62	1.48	1.42
13	4	509	CLA	C1B-C2B	2.62	1.49	1.43
13	f	1204	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	517	CLA	C1B-C2B	2.62	1.49	1.43
13	c	501	CLA	C1B-C2B	2.62	1.49	1.43
13	A	1105	CLA	C4B-NB	2.62	1.41	1.37
13	5	506	CLA	C1B-C2B	2.62	1.49	1.43
13	B	1214	CLA	C3B-C4B	2.62	1.48	1.42
13	J	1303	CLA	C3B-C4B	2.62	1.48	1.42
13	G	1104	CLA	C3B-C4B	2.62	1.48	1.42
13	B	1206	CLA	C4B-NB	2.62	1.41	1.37
13	Y	508	CLA	CMB-C2B	-2.62	1.45	1.50
13	e	1103	CLA	C3B-C4B	2.62	1.48	1.42
13	H	1204	CLA	C1B-C2B	2.62	1.49	1.43
13	c	510	CLA	C1B-C2B	2.62	1.49	1.43
13	u	503	CLA	C1B-C2B	2.62	1.49	1.43
13	R	1302	CLA	C1B-C2B	2.62	1.49	1.43
13	t	508	CLA	C3B-C4B	2.62	1.48	1.42
13	A	1801	CLA	C3B-C4B	2.62	1.48	1.42
13	t	503	CLA	C1B-C2B	2.62	1.49	1.43
13	G	1106	CLA	C4B-NB	2.62	1.41	1.37
13	f	1227	CLA	C3B-C4B	2.61	1.48	1.42
13	c	507	CLA	C1B-C2B	2.61	1.49	1.43
13	e	1115	CLA	C4B-NB	2.61	1.41	1.37
13	A	1104	CLA	C3B-C4B	2.61	1.48	1.42
20	B	1852	SQD	O47-C45	-2.61	1.40	1.46
13	e	1013	CLA	CMB-C2B	-2.61	1.45	1.50
13	V	1503	CLA	C3B-C4B	2.61	1.48	1.42
13	b	509	CLA	C1B-C2B	2.61	1.49	1.43
13	q	508	CLA	CMB-C2B	-2.61	1.45	1.50
13	u	507	CLA	C1B-C2B	2.61	1.49	1.43
13	B	1238	CLA	C4B-NB	2.61	1.41	1.37
13	a	507	CLA	C3B-C4B	2.61	1.48	1.42
13	f	1218	CLA	C3B-C4B	2.61	1.48	1.42
13	H	1220	CLA	C3B-C4B	2.61	1.48	1.42
13	l	1303	CLA	C3B-C4B	2.61	1.48	1.42
13	G	1133	CLA	C4B-NB	2.61	1.41	1.37
13	5	507	CLA	C1B-C2B	2.61	1.49	1.43
13	6	503	CLA	C1B-C2B	2.61	1.49	1.43
13	s	517	CLA	C1B-C2B	2.61	1.49	1.43
13	A	1103	CLA	C3B-C4B	2.61	1.48	1.42
13	r	505	CLA	C1B-C2B	2.61	1.49	1.43
13	G	1013	CLA	C4B-NB	2.61	1.41	1.37
13	G	1109	CLA	C4B-NB	2.61	1.41	1.37
13	f	1203	CLA	C4B-NB	2.61	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	511	CLA	C1B-C2B	2.61	1.49	1.43
13	r	507	CLA	C1B-C2B	2.61	1.49	1.43
13	A	1127	CLA	C4B-NB	2.61	1.41	1.37
13	d	503	CLA	C1B-C2B	2.61	1.49	1.43
13	A	1115	CLA	CMC-C2C	-2.61	1.45	1.50
14	B	2002	PQN	C11-C12	2.61	1.54	1.50
13	d	517	CLA	C1B-C2B	2.61	1.49	1.43
13	e	1237	CLA	CMB-C2B	-2.61	1.45	1.50
13	A	1123	CLA	C3B-C4B	2.61	1.48	1.42
13	b	512	CLA	C1B-C2B	2.61	1.49	1.43
13	d	505	CLA	C1B-C2B	2.61	1.49	1.43
13	4	503	CLA	C1B-C2B	2.61	1.49	1.43
13	G	1123	CLA	C3B-C4B	2.61	1.48	1.42
13	B	1225	CLA	CMD-C2D	-2.60	1.45	1.50
13	b	503	CLA	C1B-C2B	2.60	1.49	1.43
13	d	507	CLA	C1B-C2B	2.60	1.49	1.43
13	B	1204	CLA	C1B-C2B	2.60	1.49	1.43
13	c	503	CLA	C1B-C2B	2.60	1.49	1.43
13	r	519	CLA	C1B-C2B	2.60	1.49	1.43
13	4	512	CLA	C1B-C2B	2.60	1.49	1.43
19	B	5002	LMG	O8-C9	-2.60	1.39	1.45
13	4	504	CLA	C1B-C2B	2.60	1.49	1.43
13	G	1105	CLA	C4B-NB	2.60	1.41	1.37
14	e	2001	PQN	C11-C3	2.60	1.55	1.51
13	e	1120	CLA	C3B-C4B	2.60	1.48	1.42
13	H	1238	CLA	C4B-NB	2.60	1.41	1.37
13	2	502	CLA	CMB-C2B	-2.60	1.45	1.50
13	v	503	CLA	C1B-C2B	2.60	1.49	1.43
13	B	1227	CLA	C3B-C4B	2.60	1.48	1.42
13	A	1119	CLA	MG-NB	-2.60	2.00	2.05
13	e	1119	CLA	MG-NB	-2.60	2.00	2.05
13	A	1109	CLA	C4B-NB	2.60	1.41	1.37
13	H	1023	CLA	C1D-ND	2.60	1.41	1.37
13	A	1013	CLA	C4B-NB	2.60	1.41	1.37
13	3	503	CLA	C1B-C2B	2.60	1.49	1.43
13	B	1235	CLA	C4B-NB	2.60	1.41	1.37
13	b	504	CLA	C1B-C2B	2.60	1.49	1.43
13	H	1225	CLA	CMD-C2D	-2.60	1.45	1.50
13	f	1229	CLA	C1D-ND	2.60	1.41	1.37
13	H	1227	CLA	C3B-C4B	2.60	1.48	1.42
13	2	519	CLA	C1B-C2B	2.60	1.49	1.43
20	f	1852	SQD	O47-C45	-2.60	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	502	CLA	C3B-C4B	2.60	1.48	1.42
13	H	1230	CLA	C3B-C4B	2.60	1.48	1.42
13	5	510	CLA	C1B-C2B	2.60	1.49	1.43
13	6	517	CLA	C1B-C2B	2.60	1.49	1.43
13	G	1022	CLA	CMB-C2B	-2.59	1.45	1.50
13	r	502	CLA	CMB-C2B	-2.59	1.45	1.50
13	B	1230	CLA	C3B-C4B	2.59	1.48	1.42
13	q	519	CLA	MG-NB	-2.59	2.00	2.05
13	a	519	CLA	C1B-C2B	2.59	1.49	1.43
13	B	1221	CLA	CMD-C2D	-2.59	1.45	1.50
13	e	1129	CLA	CMD-C2D	-2.59	1.45	1.50
13	s	513	CLA	C1B-C2B	2.59	1.49	1.43
13	t	510	CLA	C1B-C2B	2.59	1.49	1.43
13	H	1218	CLA	C3B-C4B	2.59	1.48	1.42
13	H	1221	CLA	CMD-C2D	-2.59	1.45	1.50
13	H	1235	CLA	C4B-NB	2.59	1.41	1.37
13	A	1135	CLA	CMD-C2D	-2.59	1.45	1.50
13	r	502	CLA	C3B-C4B	2.59	1.48	1.42
13	G	1115	CLA	CMC-C2C	-2.59	1.45	1.50
13	3	507	CLA	C3B-C4B	2.59	1.48	1.42
13	Z	502	CLA	C3B-C4B	2.59	1.48	1.42
13	Z	519	CLA	C1B-C2B	2.59	1.49	1.43
13	u	510	CLA	C1B-C2B	2.59	1.49	1.43
13	G	1119	CLA	MG-NB	-2.59	2.00	2.05
13	3	513	CLA	C1B-C2B	2.59	1.49	1.43
13	t	512	CLA	C1B-C2B	2.59	1.49	1.43
13	Z	502	CLA	CMB-C2B	-2.59	1.45	1.50
13	A	1132	CLA	C3B-C4B	2.59	1.48	1.42
13	T	1303	CLA	C3B-C4B	2.59	1.48	1.42
13	Y	507	CLA	C1B-C2B	2.59	1.49	1.43
13	f	1224	CLA	C4B-NB	2.59	1.41	1.37
13	B	1214	CLA	CMC-C2C	-2.59	1.45	1.50
13	v	513	CLA	C1B-C2B	2.59	1.49	1.43
13	1	519	CLA	MG-NB	-2.59	2.00	2.05
19	H	5002	LMG	O8-C9	-2.59	1.39	1.45
13	b	505	CLA	C1B-C2B	2.59	1.49	1.43
13	f	1230	CLA	C3B-C4B	2.58	1.48	1.42
13	a	513	CLA	C1B-C2B	2.58	1.49	1.43
13	B	1203	CLA	C4B-NB	2.58	1.41	1.37
13	f	1214	CLA	C3B-C4B	2.58	1.48	1.42
13	6	507	CLA	C1B-C2B	2.58	1.49	1.43
13	s	511	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	507	CLA	C1B-C2B	2.58	1.49	1.43
13	q	507	CLA	C1B-C2B	2.58	1.49	1.43
13	A	1133	CLA	C4B-NB	2.58	1.41	1.37
13	A	1022	CLA	CMB-C2B	-2.58	1.45	1.50
13	B	1231	CLA	C1B-C2B	2.58	1.49	1.43
13	t	504	CLA	C1B-C2B	2.58	1.49	1.43
13	B	1218	CLA	C3B-C4B	2.58	1.48	1.42
13	G	1127	CLA	C4B-NB	2.58	1.41	1.37
13	t	505	CLA	C1B-C2B	2.58	1.49	1.43
13	f	1023	CLA	C1D-ND	2.58	1.41	1.37
13	v	517	CLA	C1B-C2B	2.58	1.49	1.43
13	H	1214	CLA	CMC-C2C	-2.58	1.45	1.50
13	4	505	CLA	C1B-C2B	2.58	1.49	1.43
13	G	1237	CLA	C3B-C4B	2.58	1.48	1.42
13	Y	519	CLA	MG-NB	-2.58	2.00	2.05
13	3	519	CLA	C1B-C2B	2.58	1.49	1.43
13	B	1203	CLA	C3B-C4B	2.58	1.48	1.42
13	s	519	CLA	C1B-C2B	2.58	1.49	1.43
13	3	517	CLA	C1B-C2B	2.57	1.49	1.43
13	4	510	CLA	C1B-C2B	2.57	1.49	1.43
13	e	1133	CLA	C4B-NB	2.57	1.40	1.37
13	B	1220	CLA	C3B-C4B	2.57	1.48	1.42
13	b	510	CLA	C1B-C2B	2.57	1.49	1.43
13	r	517	CLA	C1B-C2B	2.57	1.49	1.43
13	s	503	CLA	C1B-C2B	2.57	1.49	1.43
13	f	1220	CLA	C3B-C4B	2.57	1.48	1.42
13	2	517	CLA	C1B-C2B	2.57	1.49	1.43
13	Y	516	CLA	C1B-C2B	2.57	1.49	1.43
13	a	503	CLA	C1B-C2B	2.57	1.49	1.43
13	a	517	CLA	C1B-C2B	2.57	1.49	1.43
13	G	1113	CLA	C3B-C4B	2.57	1.48	1.42
13	e	1135	CLA	CMD-C2D	-2.57	1.45	1.50
13	e	1022	CLA	CMB-C2B	-2.57	1.45	1.50
13	f	1225	CLA	CMD-C2D	-2.57	1.45	1.50
13	A	1107	CLA	MG-NB	-2.57	2.00	2.05
13	f	1203	CLA	C3B-C4B	2.57	1.48	1.42
13	3	511	CLA	C1B-C2B	2.57	1.49	1.43
13	G	1120	CLA	C3B-C4B	2.57	1.48	1.42
13	6	513	CLA	C1B-C2B	2.57	1.49	1.43
13	A	1120	CLA	C3B-C4B	2.57	1.48	1.42
13	e	1132	CLA	C3B-C4B	2.57	1.48	1.42
13	s	507	CLA	C3B-C4B	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1127	CLA	C3B-C4B	2.57	1.48	1.42
13	f	1231	CLA	C1B-C2B	2.57	1.49	1.43
13	A	1113	CLA	C3B-C4B	2.57	1.48	1.42
13	H	1219	CLA	C1B-C2B	2.57	1.49	1.43
13	m	1105	CLA	C1B-C2B	2.57	1.49	1.43
13	f	1214	CLA	CMC-C2C	-2.57	1.45	1.50
13	G	1129	CLA	CMD-C2D	-2.57	1.45	1.50
13	A	1127	CLA	C3B-C4B	2.57	1.48	1.42
13	1	507	CLA	C1B-C2B	2.56	1.49	1.43
13	f	1235	CLA	C4B-NB	2.56	1.40	1.37
13	f	1212	CLA	C3B-C4B	2.56	1.48	1.42
13	H	1219	CLA	CMD-C2D	-2.56	1.45	1.50
13	e	1126	CLA	C4B-NB	2.56	1.40	1.37
13	T	1303	CLA	C1B-C2B	2.56	1.49	1.43
13	B	1219	CLA	C1B-C2B	2.56	1.49	1.43
13	H	1216	CLA	MG-NB	-2.56	2.00	2.05
13	A	1126	CLA	C4B-NB	2.56	1.40	1.37
13	B	1223	CLA	C4B-NB	2.56	1.40	1.37
13	1	516	CLA	C1B-C2B	2.56	1.49	1.43
13	e	1113	CLA	C3B-C4B	2.56	1.48	1.42
13	H	1203	CLA	MG-NB	-2.56	2.00	2.05
13	d	513	CLA	C1B-C2B	2.56	1.49	1.43
14	A	2001	PQN	C11-C3	2.56	1.55	1.51
13	c	518	CLA	C1B-C2B	2.56	1.49	1.43
13	A	1129	CLA	CMD-C2D	-2.56	1.45	1.50
13	B	1224	CLA	C4B-NB	2.56	1.40	1.37
13	f	1219	CLA	C1B-C2B	2.56	1.49	1.43
13	e	1107	CLA	MG-NB	-2.56	2.00	2.05
13	u	507	CLA	C3B-C4B	2.56	1.48	1.42
14	G	2001	PQN	C11-C3	2.56	1.55	1.51
13	H	1231	CLA	C1B-C2B	2.56	1.49	1.43
13	v	506	CLA	C1B-C2B	2.56	1.49	1.43
13	H	1205	CLA	CMD-C2D	-2.56	1.45	1.50
13	A	1801	CLA	C4B-NB	2.56	1.40	1.37
13	A	1104	CLA	C4B-NB	2.56	1.40	1.37
13	B	1023	CLA	C1D-ND	2.56	1.40	1.37
13	r	505	CLA	CMD-C2D	-2.56	1.45	1.50
13	G	1135	CLA	CMD-C2D	-2.56	1.45	1.50
13	Z	505	CLA	CMD-C2D	-2.55	1.45	1.50
13	H	1021	CLA	C4B-NB	2.55	1.40	1.37
13	e	1013	CLA	C4B-NB	2.55	1.40	1.37
13	d	519	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	504	CLA	C1B-C2B	2.55	1.49	1.43
13	f	1228	CLA	C3B-C4B	2.55	1.48	1.42
13	6	519	CLA	C1B-C2B	2.55	1.49	1.43
13	H	1212	CLA	CMC-C2C	-2.55	1.45	1.50
13	d	506	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1205	CLA	CMD-C2D	-2.55	1.45	1.50
13	1	504	CLA	C1B-C2B	2.55	1.49	1.43
13	l	1303	CLA	C1B-C2B	2.55	1.49	1.43
13	e	1801	CLA	C4B-NB	2.55	1.40	1.37
13	H	1203	CLA	C3B-C4B	2.55	1.48	1.42
13	Z	517	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1212	CLA	C3B-C4B	2.55	1.48	1.42
14	H	2002	PQN	C5-C4	-2.55	1.43	1.48
13	A	1237	CLA	C3B-C4B	2.55	1.48	1.42
13	B	1215	CLA	MG-NB	-2.55	2.00	2.05
13	2	505	CLA	CMD-C2D	-2.54	1.45	1.50
13	f	1203	CLA	MG-NB	-2.54	2.00	2.05
13	Y	504	CLA	C1B-C2B	2.54	1.49	1.43
13	q	505	CLA	CMD-C2D	-2.54	1.45	1.50
13	B	1234	CLA	MG-ND	-2.54	2.00	2.05
13	H	1234	CLA	MG-ND	-2.54	2.00	2.05
13	f	1223	CLA	C4B-NB	2.54	1.40	1.37
13	e	1121	CLA	C1B-C2B	2.54	1.49	1.43
13	f	1205	CLA	CMD-C2D	-2.54	1.45	1.50
13	6	511	CLA	C1B-C2B	2.54	1.49	1.43
13	H	1217	CLA	MG-NB	-2.54	2.00	2.05
13	c	507	CLA	C3B-C4B	2.54	1.48	1.42
13	s	502	CLA	C1B-C2B	2.54	1.49	1.43
13	d	512	CLA	C1B-C2B	2.54	1.49	1.43
14	f	2002	PQN	C5-C4	-2.54	1.43	1.48
13	G	1126	CLA	C4B-NB	2.54	1.40	1.37
13	G	1801	CLA	C1B-C2B	2.54	1.49	1.43
13	3	518	CLA	C1B-C2B	2.54	1.49	1.43
13	B	1203	CLA	MG-NB	-2.54	2.00	2.05
13	H	1224	CLA	C3B-C4B	2.54	1.48	1.42
13	e	1011	CLA	C1B-C2B	2.54	1.49	1.43
13	u	513	CLA	C1B-C2B	2.54	1.49	1.43
13	e	1104	CLA	C4B-NB	2.54	1.40	1.37
13	G	1123	CLA	C1B-C2B	2.54	1.49	1.43
13	c	513	CLA	C1B-C2B	2.54	1.49	1.43
13	v	511	CLA	C1B-C2B	2.54	1.49	1.43
13	B	1216	CLA	MG-NB	-2.54	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1219	CLA	CMD-C2D	-2.54	1.45	1.50
13	G	1121	CLA	C1B-C2B	2.54	1.49	1.43
13	B	1021	CLA	C4B-NB	2.54	1.40	1.37
13	a	502	CLA	C1B-C2B	2.54	1.49	1.43
13	A	1117	CLA	C3B-C4B	2.54	1.48	1.42
13	1	502	CLA	C1B-C2B	2.54	1.49	1.43
13	c	504	CLA	C1B-C2B	2.54	1.49	1.43
13	f	1218	CLA	C1B-C2B	2.54	1.49	1.43
13	u	518	CLA	C1B-C2B	2.54	1.49	1.43
13	A	1121	CLA	C1B-C2B	2.54	1.49	1.43
13	A	1801	CLA	C1B-C2B	2.54	1.49	1.43
13	H	1228	CLA	C3B-C4B	2.54	1.48	1.42
13	5	518	CLA	C1B-C2B	2.53	1.49	1.43
13	6	512	CLA	C1B-C2B	2.53	1.49	1.43
13	s	518	CLA	C1B-C2B	2.53	1.49	1.43
13	5	507	CLA	C3B-C4B	2.53	1.48	1.42
13	K	1105	CLA	C1B-C2B	2.53	1.49	1.43
13	B	1219	CLA	CMD-C2D	-2.53	1.45	1.50
13	5	504	CLA	C1B-C2B	2.53	1.49	1.43
13	e	1127	CLA	C3B-C4B	2.53	1.48	1.42
13	v	519	CLA	C1B-C2B	2.53	1.49	1.43
13	q	507	CLA	C3B-C4B	2.53	1.48	1.42
14	B	2002	PQN	C5-C4	-2.53	1.43	1.48
13	J	1303	CLA	C1B-C2B	2.53	1.49	1.43
13	H	1212	CLA	C3B-C4B	2.53	1.48	1.42
13	e	1118	CLA	C1B-C2B	2.53	1.49	1.43
13	G	1127	CLA	MG-NB	-2.53	2.00	2.05
13	A	1118	CLA	C1B-C2B	2.53	1.49	1.43
13	U	1105	CLA	C1B-C2B	2.53	1.49	1.43
13	e	1801	CLA	C1B-C2B	2.53	1.49	1.43
13	e	1117	CLA	C3B-C4B	2.53	1.48	1.42
13	B	1238	CLA	MG-NB	-2.53	2.00	2.05
13	e	1237	CLA	C3B-C4B	2.53	1.48	1.42
13	B	1228	CLA	C3B-C4B	2.53	1.48	1.42
13	u	504	CLA	C1B-C2B	2.53	1.49	1.43
13	A	1109	CLA	C3B-C4B	2.53	1.48	1.42
13	G	1117	CLA	C3B-C4B	2.53	1.48	1.42
13	f	1215	CLA	MG-NB	-2.53	2.00	2.05
13	a	512	CLA	C1B-C2B	2.52	1.49	1.43
13	a	518	CLA	C1B-C2B	2.52	1.49	1.43
13	f	1235	CLA	C3B-C4B	2.52	1.48	1.42
13	A	1011	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1234	CLA	MG-ND	-2.52	2.00	2.05
13	G	1109	CLA	C3B-C4B	2.52	1.48	1.42
13	f	1217	CLA	MG-NB	-2.52	2.00	2.05
13	6	506	CLA	C1B-C2B	2.52	1.49	1.43
13	d	510	CLA	C1B-C2B	2.52	1.49	1.43
13	H	1238	CLA	MG-NB	-2.52	2.00	2.05
13	B	1224	CLA	C3B-C4B	2.52	1.48	1.42
13	G	1011	CLA	C1B-C2B	2.52	1.49	1.43
13	G	1107	CLA	MG-NB	-2.52	2.00	2.05
13	e	1118	CLA	C3B-C4B	2.52	1.48	1.42
13	s	505	CLA	CMD-C2D	-2.52	1.45	1.50
13	f	1204	CLA	C3B-C4B	2.52	1.48	1.42
13	q	506	CLA	C1B-C2B	2.52	1.49	1.43
13	q	516	CLA	C1B-C2B	2.52	1.49	1.43
13	B	1204	CLA	C3B-C4B	2.52	1.48	1.42
13	a	504	CLA	C1B-C2B	2.52	1.49	1.43
13	G	1104	CLA	C4B-NB	2.52	1.40	1.37
13	A	1127	CLA	MG-NB	-2.52	2.00	2.05
13	3	502	CLA	C1B-C2B	2.52	1.49	1.43
13	v	512	CLA	C1B-C2B	2.52	1.49	1.43
13	1	501	CLA	C1B-C2B	2.52	1.49	1.43
13	Y	502	CLA	C1B-C2B	2.52	1.49	1.43
13	r	503	CLA	C1B-C2B	2.52	1.49	1.43
13	H	1223	CLA	C1B-C2B	2.52	1.49	1.43
13	B	1235	CLA	C3B-C4B	2.52	1.48	1.42
13	A	1132	CLA	C4B-NB	2.52	1.40	1.37
13	H	1235	CLA	C3B-C4B	2.52	1.48	1.42
13	d	504	CLA	C1B-C2B	2.52	1.49	1.43
13	B	1218	CLA	C1B-C2B	2.52	1.49	1.43
13	v	504	CLA	C1B-C2B	2.51	1.49	1.43
13	6	504	CLA	C1B-C2B	2.51	1.49	1.43
13	e	1127	CLA	MG-NB	-2.51	2.00	2.05
13	A	1107	CLA	C3B-C4B	2.51	1.48	1.42
13	6	510	CLA	C1B-C2B	2.51	1.49	1.43
13	q	502	CLA	C1B-C2B	2.51	1.49	1.43
13	G	1118	CLA	C3B-C4B	2.51	1.48	1.42
13	H	1206	CLA	MG-NB	-2.51	2.00	2.05
13	Y	513	CLA	C1B-C2B	2.51	1.49	1.43
13	d	511	CLA	C1B-C2B	2.51	1.49	1.43
13	H	1215	CLA	MG-NB	-2.51	2.00	2.05
13	f	1238	CLA	MG-NB	-2.51	2.00	2.05
13	Y	509	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1217	CLA	CMD-C2D	-2.51	1.45	1.50
13	H	1224	CLA	C4B-NB	2.51	1.40	1.37
13	B	1212	CLA	CMC-C2C	-2.51	1.45	1.50
13	A	1118	CLA	C3B-C4B	2.51	1.48	1.42
13	1	507	CLA	C3B-C4B	2.51	1.48	1.42
13	3	504	CLA	C1B-C2B	2.51	1.49	1.43
13	B	1217	CLA	MG-NB	-2.51	2.00	2.05
13	H	1218	CLA	C1B-C2B	2.51	1.49	1.43
13	a	505	CLA	CMD-C2D	-2.51	1.45	1.50
13	Y	507	CLA	C3B-C4B	2.51	1.48	1.42
13	G	1118	CLA	C1B-C2B	2.51	1.49	1.43
13	G	1013	CLA	C1D-ND	2.51	1.40	1.37
13	G	1011	CLA	C3B-C4B	2.51	1.48	1.42
13	e	1109	CLA	C3B-C4B	2.51	1.48	1.42
13	G	1109	CLA	C1B-C2B	2.51	1.49	1.43
13	B	1225	CLA	C4B-NB	2.51	1.40	1.37
13	B	1223	CLA	C1B-C2B	2.51	1.49	1.43
13	f	1217	CLA	C3B-C4B	2.50	1.48	1.42
13	A	1011	CLA	C3B-C4B	2.50	1.48	1.42
13	e	1107	CLA	C3B-C4B	2.50	1.48	1.42
13	G	1107	CLA	C3B-C4B	2.50	1.48	1.42
13	f	1216	CLA	MG-NB	-2.50	2.00	2.05
13	5	513	CLA	C1B-C2B	2.50	1.49	1.43
13	Y	501	CLA	C1B-C2B	2.50	1.49	1.43
13	A	1123	CLA	C1B-C2B	2.50	1.49	1.43
13	e	1109	CLA	C1B-C2B	2.50	1.49	1.43
13	2	503	CLA	C1B-C2B	2.50	1.49	1.43
13	f	1021	CLA	C4B-NB	2.50	1.40	1.37
13	3	505	CLA	CMD-C2D	-2.50	1.45	1.50
13	1	506	CLA	C1B-C2B	2.50	1.49	1.43
13	m	1401	CLA	C1B-C2B	2.50	1.49	1.43
13	f	1224	CLA	C3B-C4B	2.50	1.48	1.42
13	3	512	CLA	C1B-C2B	2.50	1.49	1.43
13	B	1211	CLA	C1B-C2B	2.50	1.49	1.43
13	H	1223	CLA	C4B-NB	2.50	1.40	1.37
13	e	1011	CLA	C3B-C4B	2.50	1.48	1.42
13	r	507	CLA	C3B-C4B	2.50	1.48	1.42
13	5	509	CLA	C1B-C2B	2.50	1.49	1.43
13	H	1204	CLA	C3B-C4B	2.50	1.48	1.42
13	f	1214	CLA	CMB-C2B	-2.50	1.45	1.50
13	B	1206	CLA	MG-NB	-2.50	2.00	2.05
13	e	1123	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	1302	CLA	C1B-C2B	2.50	1.49	1.43
13	1	509	CLA	C1B-C2B	2.50	1.49	1.43
13	1	505	CLA	CMD-C2D	-2.49	1.45	1.50
13	A	1013	CLA	C1D-ND	2.49	1.40	1.37
13	H	1226	CLA	MG-ND	-2.49	2.00	2.05
13	f	1223	CLA	C1B-C2B	2.49	1.49	1.43
17	A	5004	LHG	O7-C5	-2.49	1.40	1.46
13	q	501	CLA	C1B-C2B	2.49	1.49	1.43
13	r	518	CLA	C1B-C2B	2.49	1.49	1.43
13	Z	504	CLA	C1B-C2B	2.49	1.49	1.43
13	B	1217	CLA	C3B-C4B	2.49	1.48	1.42
13	B	1217	CLA	CMD-C2D	-2.49	1.45	1.50
13	e	1132	CLA	C4B-NB	2.49	1.40	1.37
13	f	1212	CLA	CMC-C2C	-2.49	1.45	1.50
13	q	509	CLA	C1B-C2B	2.49	1.49	1.43
13	s	504	CLA	C1B-C2B	2.49	1.49	1.43
13	H	1215	CLA	CMB-C2B	-2.49	1.45	1.50
13	e	1013	CLA	CMD-C2D	-2.49	1.45	1.50
17	G	5004	LHG	O7-C5	-2.49	1.40	1.46
13	e	1013	CLA	C1D-ND	2.49	1.40	1.37
13	e	1133	CLA	C3B-C4B	2.49	1.48	1.42
13	B	1226	CLA	MG-ND	-2.49	2.00	2.05
13	U	1401	CLA	C1B-C2B	2.49	1.49	1.43
13	B	1230	CLA	C1B-C2B	2.49	1.49	1.43
13	f	1206	CLA	MG-NB	-2.48	2.00	2.05
13	G	1133	CLA	C3B-C4B	2.48	1.48	1.42
13	A	1109	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1132	CLA	C4B-NB	2.48	1.40	1.37
13	B	1214	CLA	CMB-C2B	-2.48	1.45	1.50
13	Y	505	CLA	CMD-C2D	-2.48	1.45	1.50
13	K	1401	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1115	CLA	C3B-C4B	2.48	1.48	1.42
13	f	1211	CLA	C1B-C2B	2.48	1.49	1.43
17	e	5004	LHG	O7-C5	-2.48	1.40	1.46
13	A	1133	CLA	C3B-C4B	2.48	1.48	1.42
13	Z	507	CLA	C3B-C4B	2.48	1.48	1.42
13	f	1225	CLA	C4B-NB	2.48	1.40	1.37
13	s	512	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1122	CLA	C3B-C4B	2.48	1.48	1.42
13	A	1103	CLA	CMD-C2D	-2.48	1.45	1.50
13	c	509	CLA	C1B-C2B	2.48	1.49	1.43
13	v	510	CLA	C1B-C2B	2.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1217	CLA	C3B-C4B	2.48	1.48	1.42
13	s	509	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1129	CLA	CMB-C2B	-2.48	1.45	1.50
13	e	1115	CLA	C3B-C4B	2.48	1.48	1.42
13	r	504	CLA	C1B-C2B	2.48	1.49	1.43
13	A	1011	CLA	CMD-C2D	-2.48	1.45	1.50
14	B	2002	PQN	C10-C5	-2.48	1.36	1.40
13	1	513	CLA	C1B-C2B	2.48	1.49	1.43
13	2	509	CLA	C1B-C2B	2.48	1.49	1.43
13	H	1211	CLA	C1B-C2B	2.48	1.49	1.43
14	e	2001	PQN	C10-C5	-2.48	1.36	1.40
13	U	1103	CLA	MG-NB	-2.47	2.00	2.05
13	3	509	CLA	C1B-C2B	2.47	1.49	1.43
13	H	1230	CLA	C1B-C2B	2.47	1.49	1.43
13	f	1217	CLA	CMD-C2D	-2.47	1.45	1.50
13	2	504	CLA	C1B-C2B	2.47	1.49	1.43
13	a	509	CLA	C1B-C2B	2.47	1.49	1.43
13	e	1103	CLA	CMD-C2D	-2.47	1.45	1.50
13	T	1302	CLA	C1B-C2B	2.47	1.49	1.43
13	A	1115	CLA	C3B-C4B	2.47	1.48	1.42
13	e	1122	CLA	C3B-C4B	2.47	1.48	1.42
13	f	1226	CLA	MG-ND	-2.47	2.00	2.05
13	e	1129	CLA	CMB-C2B	-2.47	1.45	1.50
13	2	518	CLA	C1B-C2B	2.47	1.49	1.43
13	a	506	CLA	C1B-C2B	2.47	1.49	1.43
13	f	1230	CLA	C1B-C2B	2.47	1.49	1.43
13	Z	503	CLA	C1B-C2B	2.47	1.49	1.43
13	H	1239	CLA	C3B-C4B	2.47	1.48	1.42
13	3	510	CLA	C1B-C2B	2.47	1.49	1.43
13	Y	506	CLA	C1B-C2B	2.47	1.49	1.43
13	B	1239	CLA	C3B-C4B	2.47	1.48	1.42
13	A	1122	CLA	C3B-C4B	2.47	1.48	1.42
13	e	1011	CLA	CMD-C2D	-2.47	1.45	1.50
13	t	519	CLA	MG-NB	-2.47	2.00	2.05
13	u	509	CLA	C1B-C2B	2.47	1.49	1.43
13	a	510	CLA	C1B-C2B	2.47	1.49	1.43
13	n	1503	CLA	C1B-C2B	2.47	1.49	1.43
13	J	1302	CLA	C1B-C2B	2.47	1.49	1.43
13	2	507	CLA	C3B-C4B	2.47	1.48	1.42
13	e	1113	CLA	C1B-C2B	2.47	1.49	1.43
13	e	1013	CLA	CMC-C2C	-2.47	1.45	1.50
13	Z	518	CLA	C1B-C2B	2.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1239	CLA	C3B-C4B	2.47	1.48	1.42
13	Z	509	CLA	C1B-C2B	2.47	1.49	1.43
13	q	510	CLA	C1B-C2B	2.47	1.49	1.43
13	e	1022	CLA	CMD-C2D	-2.46	1.45	1.50
13	A	1013	CLA	CMD-C2D	-2.46	1.45	1.50
13	A	1113	CLA	C1B-C2B	2.46	1.49	1.43
13	s	510	CLA	C1B-C2B	2.46	1.49	1.43
13	f	1204	CLA	C4B-NB	2.46	1.40	1.37
13	H	1012	CLA	MG-NB	-2.46	2.00	2.05
13	f	1232	CLA	MG-NB	-2.46	2.00	2.05
13	q	513	CLA	C1B-C2B	2.46	1.49	1.43
13	f	1208	CLA	C1B-C2B	2.46	1.49	1.43
13	b	519	CLA	MG-NB	-2.46	2.00	2.05
13	B	1240	CLA	CMD-C2D	-2.46	1.45	1.50
13	V	1503	CLA	C1B-C2B	2.46	1.49	1.43
13	d	518	CLA	C1B-C2B	2.46	1.49	1.43
13	G	1139	CLA	CHC-C1C	2.46	1.43	1.38
13	4	519	CLA	MG-NB	-2.46	2.00	2.05
13	e	1022	CLA	MG-ND	-2.46	2.00	2.05
13	B	1208	CLA	C1B-C2B	2.46	1.49	1.43
13	Y	510	CLA	C1B-C2B	2.46	1.49	1.43
13	6	518	CLA	C1B-C2B	2.46	1.49	1.43
13	r	509	CLA	C1B-C2B	2.46	1.49	1.43
14	f	2002	PQN	C10-C5	-2.46	1.36	1.40
13	L	1503	CLA	C1B-C2B	2.46	1.49	1.43
13	A	1129	CLA	CMB-C2B	-2.46	1.45	1.50
13	H	1214	CLA	CMB-C2B	-2.46	1.45	1.50
13	Z	501	CLA	C1B-C2B	2.45	1.49	1.43
13	B	1215	CLA	CMB-C2B	-2.45	1.45	1.50
13	H	1220	CLA	CMC-C2C	-2.45	1.45	1.50
13	H	1210	CLA	CMC-C2C	-2.45	1.45	1.50
17	V	5221	LHG	O7-C5	-2.45	1.40	1.46
13	H	1204	CLA	C4B-NB	2.45	1.40	1.37
13	2	501	CLA	C1B-C2B	2.45	1.49	1.43
13	f	1204	CLA	MG-NB	-2.45	2.00	2.05
13	G	1013	CLA	CMD-C2D	-2.45	1.45	1.50
13	c	512	CLA	C1B-C2B	2.45	1.49	1.43
13	G	1124	CLA	CMD-C2D	-2.45	1.45	1.50
13	G	1106	CLA	C3B-C4B	2.45	1.48	1.42
13	A	1022	CLA	MG-ND	-2.45	2.00	2.05
13	B	1232	CLA	MG-NB	-2.45	2.00	2.05
13	Y	518	CLA	MG-NB	-2.45	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	513	CLA	C1B-C2B	2.45	1.49	1.43
17	L	5221	LHG	O7-C5	-2.45	1.40	1.46
13	n	1501	CLA	C1B-C2B	2.45	1.49	1.43
13	B	1012	CLA	MG-NB	-2.45	2.00	2.05
13	2	510	CLA	C1B-C2B	2.45	1.49	1.43
13	G	1118	CLA	CMD-C2D	-2.45	1.45	1.50
13	A	1106	CLA	C3B-C4B	2.45	1.48	1.42
13	1	510	CLA	C1B-C2B	2.44	1.49	1.43
13	G	1103	CLA	CMD-C2D	-2.44	1.45	1.50
13	q	519	CLA	CMC-C2C	-2.44	1.45	1.50
13	H	1232	CLA	MG-NB	-2.44	2.00	2.05
13	H	1240	CLA	CMD-C2D	-2.44	1.45	1.50
13	Z	510	CLA	C1B-C2B	2.44	1.49	1.43
13	A	1118	CLA	CMD-C2D	-2.44	1.45	1.50
13	H	1225	CLA	C4B-NB	2.44	1.40	1.37
13	3	506	CLA	C1B-C2B	2.44	1.49	1.43
13	H	1206	CLA	C1B-NB	-2.44	1.34	1.37
13	H	1204	CLA	MG-NB	-2.44	2.00	2.05
13	B	1210	CLA	CMC-C2C	-2.44	1.45	1.50
13	H	1021	CLA	CMC-C2C	-2.44	1.45	1.50
13	e	1118	CLA	CMD-C2D	-2.44	1.45	1.50
13	H	1208	CLA	C1B-C2B	2.44	1.49	1.43
14	H	2002	PQN	C10-C5	-2.44	1.36	1.40
13	m	1103	CLA	MG-NB	-2.44	2.00	2.05
13	e	1120	CLA	C1B-C2B	2.44	1.49	1.43
13	G	1121	CLA	C3B-C4B	2.44	1.48	1.42
13	A	1022	CLA	CMD-C2D	-2.44	1.45	1.50
13	B	1204	CLA	MG-NB	-2.44	2.01	2.05
13	f	1240	CLA	CMD-C2D	-2.44	1.45	1.50
13	H	1208	CLA	C3B-C4B	2.44	1.48	1.42
13	q	518	CLA	MG-NB	-2.44	2.01	2.05
13	f	1220	CLA	C1B-C2B	2.44	1.49	1.43
13	r	513	CLA	C1B-C2B	2.44	1.49	1.43
13	G	1013	CLA	CMC-C2C	-2.44	1.45	1.50
13	B	1208	CLA	C3B-C4B	2.44	1.48	1.42
13	G	1022	CLA	CMD-C2D	-2.44	1.45	1.50
13	G	1022	CLA	MG-ND	-2.43	2.01	2.05
13	A	1106	CLA	MG-NB	-2.43	2.01	2.05
13	A	1121	CLA	C3B-C4B	2.43	1.48	1.42
13	1	518	CLA	MG-NB	-2.43	2.01	2.05
13	G	1104	CLA	C1B-C2B	2.43	1.49	1.43
13	r	501	CLA	C1B-C2B	2.43	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1011	CLA	CMD-C2D	-2.43	1.45	1.50
13	K	1103	CLA	MG-NB	-2.43	2.01	2.05
13	f	1235	CLA	MG-NB	-2.43	2.01	2.05
13	5	512	CLA	C1B-C2B	2.43	1.49	1.43
13	v	518	CLA	C1B-C2B	2.43	1.49	1.43
13	B	1221	CLA	C1B-NB	-2.43	1.34	1.37
13	G	1113	CLA	C1B-C2B	2.43	1.49	1.43
13	f	1212	CLA	C1B-C2B	2.43	1.49	1.43
13	e	1106	CLA	C3B-C4B	2.43	1.48	1.42
13	B	1204	CLA	C4B-NB	2.43	1.40	1.37
13	G	1106	CLA	MG-NB	-2.43	2.01	2.05
13	e	1139	CLA	CHC-C1C	2.43	1.43	1.38
14	A	2001	PQN	C10-C5	-2.43	1.36	1.40
13	2	512	CLA	C1B-C2B	2.43	1.49	1.43
13	B	1225	CLA	MG-NB	-2.43	2.01	2.05
13	f	1210	CLA	CMC-C2C	-2.43	1.45	1.50
13	H	1224	CLA	C1B-C2B	2.43	1.49	1.43
13	e	1106	CLA	MG-NB	-2.43	2.01	2.05
13	A	1139	CLA	CHC-C1C	2.43	1.43	1.38
13	f	1206	CLA	C1B-NB	-2.43	1.34	1.37
13	A	1013	CLA	CMC-C2C	-2.43	1.45	1.50
13	f	1012	CLA	MG-NB	-2.43	2.01	2.05
13	f	1225	CLA	MG-NB	-2.43	2.01	2.05
13	B	1220	CLA	CMC-C2C	-2.43	1.45	1.50
19	T	5104	LMG	O7-C8	-2.43	1.40	1.46
13	A	1124	CLA	CMD-C2D	-2.42	1.45	1.50
13	Z	513	CLA	C1B-C2B	2.42	1.49	1.43
13	c	511	CLA	C1B-C2B	2.42	1.49	1.43
13	u	511	CLA	C1B-C2B	2.42	1.49	1.43
13	f	1223	CLA	CMC-C2C	-2.42	1.45	1.50
13	2	511	CLA	C1B-C2B	2.42	1.49	1.43
13	t	511	CLA	C1B-C2B	2.42	1.49	1.43
13	G	1103	CLA	C1B-C2B	2.42	1.49	1.43
13	H	1225	CLA	MG-NB	-2.42	2.01	2.05
13	B	1021	CLA	CMC-C2C	-2.42	1.45	1.50
13	5	511	CLA	C1B-C2B	2.42	1.49	1.43
13	r	510	CLA	C1B-C2B	2.42	1.49	1.43
13	f	1215	CLA	CMB-C2B	-2.42	1.45	1.50
13	B	1240	CLA	C1B-C2B	2.42	1.49	1.43
13	s	506	CLA	C1B-C2B	2.42	1.49	1.43
13	B	1222	CLA	CHC-C1C	2.42	1.43	1.38
13	G	1115	CLA	C1B-C2B	2.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1208	CLA	C3B-C4B	2.42	1.48	1.42
13	G	1122	CLA	C1B-C2B	2.42	1.49	1.43
13	f	1222	CLA	CHC-C1C	2.42	1.43	1.38
13	G	1116	CLA	C1B-C2B	2.42	1.49	1.43
13	Z	511	CLA	C1B-C2B	2.42	1.49	1.43
13	A	1122	CLA	C1B-C2B	2.42	1.48	1.43
13	e	1122	CLA	C1B-C2B	2.42	1.48	1.43
13	4	511	CLA	C1B-C2B	2.42	1.48	1.43
13	r	512	CLA	C1B-C2B	2.42	1.48	1.43
13	B	1206	CLA	C1B-NB	-2.42	1.34	1.37
13	H	1212	CLA	C1B-C2B	2.42	1.48	1.43
13	e	1115	CLA	C1B-C2B	2.42	1.48	1.43
13	H	1222	CLA	CHC-C1C	2.42	1.43	1.38
13	A	1104	CLA	C1B-C2B	2.42	1.48	1.43
13	Y	519	CLA	C1B-C2B	2.42	1.48	1.43
13	L	1501	CLA	C1B-C2B	2.42	1.48	1.43
13	1	512	CLA	C1B-C2B	2.42	1.48	1.43
13	b	511	CLA	C1B-C2B	2.42	1.48	1.43
13	q	511	CLA	C1B-C2B	2.41	1.48	1.43
13	5	508	CLA	C1B-C2B	2.41	1.48	1.43
14	G	2001	PQN	C10-C5	-2.41	1.36	1.40
13	f	1215	CLA	C1B-NB	-2.41	1.34	1.37
17	n	5221	LHG	O7-C5	-2.41	1.40	1.46
13	f	1224	CLA	C1B-C2B	2.41	1.48	1.43
13	f	1021	CLA	CMC-C2C	-2.41	1.45	1.50
13	q	512	CLA	C1B-C2B	2.41	1.48	1.43
13	e	1121	CLA	C3B-C4B	2.41	1.48	1.42
13	B	1224	CLA	C1B-C2B	2.41	1.48	1.43
13	f	1210	CLA	C4B-NB	2.41	1.40	1.37
13	A	1115	CLA	C1B-C2B	2.41	1.48	1.43
13	r	506	CLA	CMB-C2B	-2.41	1.45	1.50
13	u	512	CLA	C1B-C2B	2.41	1.48	1.43
13	e	1111	CLA	CMC-C2C	-2.41	1.45	1.50
13	H	1240	CLA	C1B-C2B	2.41	1.48	1.43
13	f	1023	CLA	C4B-NB	2.41	1.40	1.37
13	Z	512	CLA	C1B-C2B	2.41	1.48	1.43
13	B	1235	CLA	MG-NB	-2.41	2.01	2.05
13	e	1124	CLA	CMD-C2D	-2.41	1.45	1.50
13	u	519	CLA	C1B-C2B	2.41	1.48	1.43
13	f	1220	CLA	CMC-C2C	-2.41	1.45	1.50
13	A	1116	CLA	C1B-C2B	2.41	1.48	1.43
13	1	511	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	519	CLA	C1B-C2B	2.41	1.48	1.43
13	e	1104	CLA	C1B-C2B	2.41	1.48	1.43
13	A	1120	CLA	C1B-C2B	2.41	1.48	1.43
13	1	519	CLA	CMC-C2C	-2.41	1.45	1.50
13	B	1223	CLA	CMC-C2C	-2.41	1.45	1.50
13	f	1240	CLA	C1B-C2B	2.41	1.48	1.43
13	H	1221	CLA	C1B-NB	-2.41	1.34	1.37
13	H	1205	CLA	CMC-C2C	-2.41	1.45	1.50
13	r	517	CLA	CMC-C2C	-2.41	1.45	1.50
13	B	1220	CLA	C1B-C2B	2.40	1.48	1.43
13	5	519	CLA	C1B-C2B	2.40	1.48	1.43
13	e	1103	CLA	C1B-C2B	2.40	1.48	1.43
13	e	1134	CLA	C1B-C2B	2.40	1.48	1.43
13	f	1227	CLA	CMB-C2B	-2.40	1.45	1.50
13	e	1116	CLA	C1B-C2B	2.40	1.48	1.43
13	Z	506	CLA	CMB-C2B	-2.40	1.45	1.50
13	V	1501	CLA	C1B-C2B	2.40	1.48	1.43
13	B	1234	CLA	C4B-NB	2.40	1.40	1.37
13	G	1134	CLA	C1B-C2B	2.40	1.48	1.43
13	A	1104	CLA	MG-NB	-2.40	2.01	2.05
13	G	1117	CLA	MG-NB	-2.40	2.01	2.05
13	H	1235	CLA	MG-NB	-2.40	2.01	2.05
13	2	506	CLA	CMB-C2B	-2.40	1.45	1.50
13	H	1223	CLA	CMC-C2C	-2.40	1.45	1.50
13	A	1103	CLA	C1B-C2B	2.40	1.48	1.43
13	e	1125	CLA	MG-NB	-2.40	2.01	2.05
13	A	1125	CLA	MG-NB	-2.40	2.01	2.05
13	Y	511	CLA	C1B-C2B	2.40	1.48	1.43
13	H	1234	CLA	C4B-NB	2.40	1.40	1.37
13	H	1220	CLA	C1B-C2B	2.40	1.48	1.43
13	H	1227	CLA	CMB-C2B	-2.40	1.45	1.50
13	B	1205	CLA	CMC-C2C	-2.40	1.45	1.50
13	e	1117	CLA	MG-NB	-2.40	2.01	2.05
19	J	5104	LMG	O7-C8	-2.40	1.40	1.46
13	c	519	CLA	C1B-C2B	2.40	1.48	1.43
13	6	508	CLA	C1B-C2B	2.39	1.48	1.43
13	u	508	CLA	C1B-C2B	2.39	1.48	1.43
13	t	519	CLA	C1B-C2B	2.39	1.48	1.43
13	H	1231	CLA	C4B-NB	2.39	1.40	1.37
13	H	1239	CLA	C1B-C2B	2.39	1.48	1.43
13	G	1125	CLA	MG-NB	-2.39	2.01	2.05
13	A	1134	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1230	CLA	CMC-C2C	-2.39	1.45	1.50
13	Z	517	CLA	CMC-C2C	-2.39	1.45	1.50
13	r	502	CLA	C1B-C2B	2.39	1.48	1.43
13	B	1212	CLA	C1B-C2B	2.39	1.48	1.43
13	f	1229	CLA	CHC-C1C	2.39	1.43	1.38
13	f	1207	CLA	C1B-C2B	2.39	1.48	1.43
13	r	511	CLA	C1B-C2B	2.39	1.48	1.43
13	f	1239	CLA	C1B-C2B	2.39	1.48	1.43
13	A	1111	CLA	CMC-C2C	-2.39	1.45	1.50
13	G	1135	CLA	MG-ND	-2.39	2.01	2.05
13	B	1231	CLA	C4B-NB	2.39	1.40	1.37
13	q	519	CLA	C1B-C2B	2.38	1.48	1.43
13	A	1117	CLA	MG-NB	-2.38	2.01	2.05
13	G	1104	CLA	MG-NB	-2.38	2.01	2.05
13	G	1140	CLA	CMB-C2B	-2.38	1.45	1.50
13	G	1120	CLA	C1B-C2B	2.38	1.48	1.43
13	H	1230	CLA	CMC-C2C	-2.38	1.45	1.50
13	f	1231	CLA	C4B-NB	2.38	1.40	1.37
13	K	1103	CLA	C1B-C2B	2.38	1.48	1.43
13	G	1801	CLA	MG-NB	-2.38	2.01	2.05
13	f	1230	CLA	CMB-C2B	-2.38	1.45	1.50
13	B	1215	CLA	C1B-NB	-2.38	1.34	1.37
13	c	508	CLA	C1B-C2B	2.38	1.48	1.43
13	f	1205	CLA	CMC-C2C	-2.38	1.45	1.50
13	H	1215	CLA	C1B-NB	-2.38	1.34	1.37
13	A	1102	CLA	CHC-C1C	2.38	1.43	1.38
13	2	502	CLA	C1B-C2B	2.38	1.48	1.43
13	U	1103	CLA	C1B-C2B	2.38	1.48	1.43
13	B	1230	CLA	CMB-C2B	-2.38	1.45	1.50
13	G	1111	CLA	CMC-C2C	-2.38	1.45	1.50
13	B	1023	CLA	C4B-NB	2.38	1.40	1.37
13	f	1221	CLA	C1B-NB	-2.38	1.34	1.37
19	l	5104	LMG	O7-C8	-2.38	1.40	1.46
13	B	1227	CLA	CMB-C2B	-2.38	1.45	1.50
13	G	1101	CLA	CMD-C2D	-2.38	1.45	1.50
17	G	5005	LHG	O7-C5	-2.38	1.40	1.46
13	B	1207	CLA	C1B-C2B	2.37	1.48	1.43
13	4	519	CLA	C1B-C2B	2.37	1.48	1.43
13	A	1101	CLA	CMD-C2D	-2.37	1.45	1.50
13	2	517	CLA	CMC-C2C	-2.37	1.45	1.50
13	c	508	CLA	CMB-C2B	-2.37	1.45	1.50
13	1	512	CLA	MG-NB	-2.37	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1102	CLA	CHC-C1C	2.37	1.43	1.38
13	A	1140	CLA	CMB-C2B	-2.37	1.45	1.50
13	H	1230	CLA	CMB-C2B	-2.37	1.45	1.50
13	e	1111	CLA	MG-NB	-2.37	2.01	2.05
13	Y	512	CLA	C1B-C2B	2.37	1.48	1.43
13	B	1239	CLA	C1B-C2B	2.37	1.48	1.43
13	Y	518	CLA	C3B-C4B	2.37	1.48	1.42
13	Y	519	CLA	CMC-C2C	-2.37	1.45	1.50
13	G	1237	CLA	C1B-C2B	2.37	1.48	1.43
13	f	1230	CLA	CMC-C2C	-2.37	1.45	1.50
13	d	508	CLA	C1B-C2B	2.37	1.48	1.43
17	A	5005	LHG	O7-C5	-2.37	1.40	1.46
13	B	1210	CLA	C4B-NB	2.37	1.40	1.37
13	Z	502	CLA	C1B-C2B	2.37	1.48	1.43
13	m	1103	CLA	C1B-C2B	2.37	1.48	1.43
13	B	1238	CLA	CMB-C2B	-2.37	1.45	1.50
13	5	508	CLA	CMB-C2B	-2.37	1.45	1.50
13	A	1237	CLA	C1B-C2B	2.37	1.48	1.43
13	H	1207	CLA	C1B-C2B	2.37	1.48	1.43
13	G	1117	CLA	CMB-C2B	-2.37	1.45	1.50
13	v	508	CLA	C1B-C2B	2.37	1.48	1.43
13	e	1102	CLA	C1B-C2B	2.37	1.48	1.43
13	G	1128	CLA	CMD-C2D	-2.36	1.45	1.50
13	f	1238	CLA	CMB-C2B	-2.36	1.45	1.50
13	A	1135	CLA	MG-ND	-2.36	2.01	2.05
13	G	1120	CLA	MG-NB	-2.36	2.01	2.05
13	e	1135	CLA	MG-ND	-2.36	2.01	2.05
13	e	1125	CLA	C1B-C2B	2.36	1.48	1.43
13	B	1229	CLA	CHC-C1C	2.36	1.43	1.38
13	e	1140	CLA	CMB-C2B	-2.36	1.45	1.50
13	A	1102	CLA	C1B-C2B	2.36	1.48	1.43
13	b	519	CLA	C1B-C2B	2.36	1.48	1.43
13	3	512	CLA	MG-NB	-2.36	2.01	2.05
13	G	1125	CLA	C1B-C2B	2.36	1.48	1.43
13	e	1104	CLA	MG-NB	-2.36	2.01	2.05
13	e	1128	CLA	CMD-C2D	-2.36	1.45	1.50
13	f	1236	CLA	C1B-C2B	2.36	1.48	1.43
13	b	519	CLA	CMC-C2C	-2.36	1.45	1.50
13	G	1129	CLA	MG-ND	-2.36	2.01	2.05
13	A	1125	CLA	C1B-C2B	2.36	1.48	1.43
13	e	1237	CLA	C1B-C2B	2.36	1.48	1.43
13	f	1205	CLA	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1102	CLA	C1B-C2B	2.36	1.48	1.43
13	6	508	CLA	CMB-C2B	-2.36	1.45	1.50
13	d	508	CLA	CMB-C2B	-2.36	1.45	1.50
13	B	1236	CLA	C1B-C2B	2.36	1.48	1.43
13	d	505	CLA	CMD-C2D	-2.36	1.45	1.50
13	B	1205	CLA	CMB-C2B	-2.36	1.45	1.50
13	e	1102	CLA	CHC-C1C	2.36	1.43	1.38
13	a	506	CLA	CMB-C2B	-2.36	1.45	1.50
13	f	1205	CLA	CMB-C2B	-2.36	1.45	1.50
13	f	1234	CLA	CMD-C2D	-2.35	1.45	1.50
13	u	508	CLA	CMB-C2B	-2.35	1.45	1.50
13	H	1236	CLA	C1B-C2B	2.35	1.48	1.43
13	e	1801	CLA	MG-NB	-2.35	2.01	2.05
17	e	5005	LHG	O7-C5	-2.35	1.40	1.46
13	G	1101	CLA	CMC-C2C	-2.35	1.45	1.50
13	A	1801	CLA	MG-NB	-2.35	2.01	2.05
13	H	1023	CLA	C4B-NB	2.35	1.40	1.37
13	u	513	CLA	CHC-C1C	2.35	1.43	1.38
13	4	508	CLA	MG-NB	-2.35	2.01	2.05
13	H	1235	CLA	CMB-C2B	-2.35	1.45	1.50
13	e	1109	CLA	CMC-C2C	-2.35	1.45	1.50
13	s	512	CLA	MG-NB	-2.35	2.01	2.05
13	B	1021	CLA	MG-NB	-2.35	2.01	2.05
14	H	2002	PQN	C11-C3	2.35	1.55	1.51
13	f	1232	CLA	CMB-C2B	-2.35	1.45	1.50
13	f	1021	CLA	MG-NB	-2.35	2.01	2.05
13	K	1103	CLA	C3B-C4B	2.35	1.48	1.42
13	G	1131	CLA	C1B-C2B	2.35	1.48	1.43
13	a	512	CLA	MG-NB	-2.35	2.01	2.05
13	t	508	CLA	MG-NB	-2.35	2.01	2.05
13	B	1234	CLA	CMD-C2D	-2.35	1.45	1.50
13	f	1235	CLA	CMB-C2B	-2.35	1.45	1.50
13	3	506	CLA	CMB-C2B	-2.35	1.45	1.50
13	G	1022	CLA	CMC-C2C	-2.35	1.45	1.50
13	H	1234	CLA	CMD-C2D	-2.35	1.45	1.50
13	G	1111	CLA	MG-NB	-2.34	2.01	2.05
13	A	1117	CLA	CMB-C2B	-2.34	1.45	1.50
13	A	1101	CLA	CMC-C2C	-2.34	1.45	1.50
13	e	1022	CLA	CMC-C2C	-2.34	1.45	1.50
13	v	505	CLA	CMD-C2D	-2.34	1.45	1.50
13	b	508	CLA	MG-NB	-2.34	2.01	2.05
14	B	2002	PQN	C11-C3	2.34	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1101	CLA	CMD-C2D	-2.34	1.45	1.50
13	H	1229	CLA	CHC-C1C	2.34	1.43	1.38
13	A	1128	CLA	CMD-C2D	-2.34	1.45	1.50
13	H	1205	CLA	CMB-C2B	-2.34	1.45	1.50
13	6	505	CLA	CMD-C2D	-2.34	1.45	1.50
13	A	1120	CLA	MG-NB	-2.34	2.01	2.05
13	A	1022	CLA	CMC-C2C	-2.34	1.45	1.50
13	f	1234	CLA	C4B-NB	2.34	1.40	1.37
13	V	1503	CLA	CMD-C2D	-2.34	1.45	1.50
13	f	1224	CLA	CMD-C2D	-2.34	1.45	1.50
13	A	1116	CLA	MG-NB	-2.34	2.01	2.05
14	f	2002	PQN	C11-C3	2.34	1.55	1.51
13	U	1103	CLA	C3B-C4B	2.34	1.48	1.42
13	f	1231	CLA	C3B-C4B	2.34	1.48	1.42
13	A	1109	CLA	CMC-C2C	-2.34	1.45	1.50
13	B	1231	CLA	C3B-C4B	2.34	1.48	1.42
13	e	1116	CLA	MG-NB	-2.34	2.01	2.05
13	L	1503	CLA	CMD-C2D	-2.34	1.45	1.50
13	H	1228	CLA	MG-NB	-2.34	2.01	2.05
13	G	1135	CLA	C1B-C2B	2.34	1.48	1.43
13	G	1123	CLA	CMD-C2D	-2.34	1.45	1.50
13	1	518	CLA	C3B-C4B	2.34	1.48	1.42
13	1	518	CLA	C1B-C2B	2.34	1.48	1.43
13	A	1114	CLA	C1B-NB	-2.34	1.34	1.37
13	e	1139	CLA	C1B-C2B	2.33	1.48	1.43
13	H	1023	CLA	CMD-C2D	-2.33	1.45	1.50
13	v	508	CLA	CMB-C2B	-2.33	1.45	1.50
13	e	1101	CLA	CMC-C2C	-2.33	1.45	1.50
13	A	1139	CLA	C1B-C2B	2.33	1.48	1.43
13	B	1235	CLA	CMB-C2B	-2.33	1.45	1.50
13	H	1223	CLA	CMD-C2D	-2.33	1.45	1.50
13	q	518	CLA	C1B-C2B	2.33	1.48	1.43
13	Y	512	CLA	MG-NB	-2.33	2.01	2.05
13	H	1210	CLA	C4B-NB	2.33	1.40	1.37
13	q	512	CLA	MG-NB	-2.33	2.01	2.05
13	A	1127	CLA	CMD-C2D	-2.33	1.45	1.50
13	H	1238	CLA	CMB-C2B	-2.33	1.45	1.50
13	G	1109	CLA	CMC-C2C	-2.33	1.45	1.50
13	A	1111	CLA	MG-NB	-2.33	2.01	2.05
20	f	1852	SQD	O2-C2	-2.33	1.37	1.43
13	r	502	CLA	MG-NB	-2.33	2.01	2.05
13	B	1215	CLA	C3B-C4B	2.33	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1234	CLA	C1B-NB	-2.33	1.34	1.37
13	G	1127	CLA	CMD-C2D	-2.33	1.45	1.50
13	f	1228	CLA	MG-NB	-2.33	2.01	2.05
13	f	1215	CLA	C3B-C4B	2.33	1.48	1.42
13	n	1503	CLA	CMD-C2D	-2.33	1.45	1.50
13	A	1128	CLA	MG-ND	-2.33	2.01	2.05
13	B	1205	CLA	C1B-C2B	2.33	1.48	1.43
13	e	1117	CLA	CMB-C2B	-2.33	1.45	1.50
13	H	1021	CLA	MG-NB	-2.33	2.01	2.05
13	B	1228	CLA	MG-NB	-2.32	2.01	2.05
13	Y	518	CLA	C1B-C2B	2.32	1.48	1.43
13	2	502	CLA	MG-NB	-2.32	2.01	2.05
13	G	1106	CLA	CMB-C2B	-2.32	1.45	1.50
13	4	519	CLA	CMC-C2C	-2.32	1.45	1.50
13	H	1230	CLA	CMD-C2D	-2.32	1.45	1.50
13	G	1139	CLA	C1B-C2B	2.32	1.48	1.43
13	e	1108	CLA	C1B-C2B	2.32	1.48	1.43
13	B	1223	CLA	CMD-C2D	-2.32	1.45	1.50
13	H	1232	CLA	CMB-C2B	-2.32	1.45	1.50
13	f	1023	CLA	MG-NB	-2.32	2.01	2.05
13	f	1223	CLA	CMD-C2D	-2.32	1.45	1.50
13	q	502	CLA	CMD-C2D	-2.32	1.45	1.50
13	e	1128	CLA	MG-ND	-2.32	2.01	2.05
13	e	1129	CLA	MG-ND	-2.32	2.01	2.05
13	A	1135	CLA	C1B-C2B	2.32	1.48	1.43
13	A	1129	CLA	MG-ND	-2.32	2.01	2.05
13	B	1210	CLA	C1B-C2B	2.32	1.48	1.43
13	B	1224	CLA	CMD-C2D	-2.32	1.45	1.50
13	A	1131	CLA	C1B-C2B	2.32	1.48	1.43
13	B	1023	CLA	MG-NB	-2.32	2.01	2.05
13	q	518	CLA	CMD-C2D	-2.32	1.45	1.50
13	A	1106	CLA	CMB-C2B	-2.32	1.45	1.50
13	1	502	CLA	CMD-C2D	-2.32	1.45	1.50
13	m	1105	CLA	CMD-C2D	-2.32	1.45	1.50
13	A	1108	CLA	C1B-C2B	2.32	1.48	1.43
13	e	1132	CLA	C1B-C2B	2.32	1.48	1.43
13	e	1114	CLA	C1B-NB	-2.32	1.34	1.37
13	e	1120	CLA	MG-NB	-2.32	2.01	2.05
13	G	1118	CLA	MG-NB	-2.32	2.01	2.05
13	G	1133	CLA	MG-NB	-2.32	2.01	2.05
13	H	1023	CLA	MG-NB	-2.32	2.01	2.05
13	H	1201	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1217	CLA	C1B-C2B	2.32	1.48	1.43
13	e	1127	CLA	CMD-C2D	-2.32	1.45	1.50
13	q	519	CLA	C3B-C4B	2.32	1.48	1.42
13	G	1108	CLA	C1B-C2B	2.31	1.48	1.43
13	H	1231	CLA	C3B-C4B	2.31	1.48	1.42
13	f	1234	CLA	C1B-NB	-2.31	1.34	1.37
13	t	519	CLA	CMC-C2C	-2.31	1.45	1.50
13	A	1132	CLA	C1B-C2B	2.31	1.48	1.43
13	f	1229	CLA	C1B-NB	-2.31	1.34	1.37
13	H	1205	CLA	C1B-C2B	2.31	1.48	1.43
13	f	1023	CLA	CMD-C2D	-2.31	1.45	1.50
13	G	1133	CLA	CMB-C2B	-2.31	1.45	1.50
13	B	1232	CLA	CMB-C2B	-2.31	1.45	1.50
13	B	1227	CLA	MG-NB	-2.31	2.01	2.05
13	H	1206	CLA	C1B-C2B	2.31	1.48	1.43
13	A	1123	CLA	CMD-C2D	-2.31	1.45	1.50
13	G	1801	CLA	CAA-C2A	-2.31	1.49	1.54
20	B	1852	SQD	O2-C2	-2.31	1.37	1.43
13	e	1106	CLA	CMB-C2B	-2.31	1.45	1.50
13	Z	502	CLA	MG-NB	-2.31	2.01	2.05
13	A	1801	CLA	CAA-C2A	-2.31	1.49	1.54
13	B	1207	CLA	CMD-C2D	-2.31	1.45	1.50
13	m	1103	CLA	C3B-C4B	2.31	1.48	1.42
13	5	513	CLA	CHC-C1C	2.31	1.43	1.38
13	K	1105	CLA	CMD-C2D	-2.31	1.45	1.50
13	Y	518	CLA	CMD-C2D	-2.31	1.45	1.50
13	s	506	CLA	CMB-C2B	-2.31	1.45	1.50
13	e	1135	CLA	C1B-C2B	2.31	1.48	1.43
13	e	1131	CLA	C1B-C2B	2.30	1.48	1.43
13	f	1201	CLA	C1B-C2B	2.30	1.48	1.43
13	G	1128	CLA	MG-ND	-2.30	2.01	2.05
13	f	1227	CLA	MG-NB	-2.30	2.01	2.05
13	B	1234	CLA	C1B-NB	-2.30	1.35	1.37
13	2	506	CLA	C1B-C2B	2.30	1.48	1.43
13	m	1401	CLA	MG-NB	-2.30	2.01	2.05
13	Y	519	CLA	C3B-C4B	2.30	1.48	1.42
13	r	512	CLA	CMD-C2D	-2.30	1.45	1.50
13	H	1215	CLA	C3B-C4B	2.30	1.48	1.42
13	B	1023	CLA	CMD-C2D	-2.30	1.45	1.50
13	G	1132	CLA	C1B-C2B	2.30	1.48	1.43
13	B	1230	CLA	CMD-C2D	-2.30	1.45	1.50
13	B	1217	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1227	CLA	MG-NB	-2.30	2.01	2.05
13	G	1116	CLA	MG-NB	-2.30	2.01	2.05
13	f	1023	CLA	CHC-C1C	2.30	1.43	1.38
13	1	518	CLA	CMD-C2D	-2.30	1.45	1.50
13	H	1207	CLA	CMD-C2D	-2.30	1.45	1.50
13	u	505	CLA	CMD-C2D	-2.30	1.45	1.50
13	c	513	CLA	CHC-C1C	2.30	1.43	1.38
20	H	1852	SQD	O2-C2	-2.30	1.37	1.43
13	Z	506	CLA	C1B-C2B	2.30	1.48	1.43
13	r	506	CLA	C1B-C2B	2.30	1.48	1.43
13	q	518	CLA	C3B-C4B	2.30	1.48	1.42
13	G	1114	CLA	C1B-NB	-2.30	1.35	1.37
13	B	1201	CLA	C1B-C2B	2.30	1.48	1.43
13	e	1124	CLA	C1B-C2B	2.30	1.48	1.43
13	A	1128	CLA	C3B-C4B	2.30	1.48	1.42
13	Y	502	CLA	CMB-C2B	-2.30	1.45	1.50
13	q	502	CLA	CMB-C2B	-2.30	1.45	1.50
13	A	1133	CLA	MG-NB	-2.30	2.01	2.05
13	1	519	CLA	C3B-C4B	2.30	1.48	1.42
13	f	1210	CLA	C1B-C2B	2.30	1.48	1.43
17	e	5002	LHG	P-O6	2.30	1.68	1.59
13	f	1230	CLA	CMD-C2D	-2.30	1.45	1.50
13	B	1206	CLA	C1B-C2B	2.30	1.48	1.43
13	e	1128	CLA	C3B-C4B	2.30	1.48	1.42
13	2	512	CLA	CMD-C2D	-2.30	1.45	1.50
13	5	505	CLA	CMD-C2D	-2.29	1.45	1.50
13	s	511	CLA	CMB-C2B	-2.29	1.45	1.50
13	f	1217	CLA	C1B-C2B	2.29	1.48	1.43
13	B	1211	CLA	CMD-C2D	-2.29	1.45	1.50
13	H	1224	CLA	CMC-C2C	-2.29	1.45	1.50
13	1	502	CLA	CMB-C2B	-2.29	1.45	1.50
13	f	1012	CLA	CMC-C2C	-2.29	1.45	1.50
13	H	1224	CLA	CMD-C2D	-2.29	1.45	1.50
17	e	5008	LHG	O7-C5	-2.29	1.40	1.46
13	e	1123	CLA	C1B-NB	-2.29	1.35	1.37
13	t	511	CLA	CMD-C2D	-2.29	1.45	1.50
13	e	1140	CLA	MG-NB	-2.29	2.01	2.05
13	H	1210	CLA	C1B-C2B	2.29	1.48	1.43
13	A	1133	CLA	CMB-C2B	-2.29	1.45	1.50
13	G	1139	CLA	MG-NB	-2.29	2.01	2.05
13	B	1213	CLA	C1B-C2B	2.29	1.48	1.43
13	f	1211	CLA	CMD-C2D	-2.29	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1213	CLA	C1B-C2B	2.29	1.48	1.43
13	A	1123	CLA	C1B-NB	-2.29	1.35	1.37
13	H	1201	CLA	CMD-C2D	-2.29	1.45	1.50
13	H	1211	CLA	CMD-C2D	-2.29	1.45	1.50
13	a	511	CLA	CMB-C2B	-2.29	1.46	1.50
13	f	1207	CLA	CMD-C2D	-2.29	1.46	1.50
13	e	1140	CLA	CMC-C2C	-2.29	1.46	1.50
13	A	1124	CLA	C1B-C2B	2.29	1.48	1.43
13	f	1206	CLA	C1B-C2B	2.29	1.48	1.43
13	Y	502	CLA	CMD-C2D	-2.29	1.46	1.50
13	f	1223	CLA	MG-NB	-2.29	2.01	2.05
13	f	1212	CLA	CMD-C2D	-2.28	1.46	1.50
13	A	1112	CLA	CHC-C1C	2.28	1.43	1.38
13	f	1224	CLA	CMC-C2C	-2.28	1.46	1.50
13	Z	512	CLA	CMD-C2D	-2.28	1.46	1.50
13	1	506	CLA	CHC-C1C	2.28	1.43	1.38
13	e	1123	CLA	CMD-C2D	-2.28	1.46	1.50
13	r	508	CLA	MG-NB	-2.28	2.01	2.05
13	e	1133	CLA	CMB-C2B	-2.28	1.46	1.50
13	U	1105	CLA	CMD-C2D	-2.28	1.46	1.50
13	c	505	CLA	CMD-C2D	-2.28	1.46	1.50
13	e	1139	CLA	MG-NB	-2.28	2.01	2.05
13	B	1224	CLA	CMC-C2C	-2.28	1.46	1.50
13	Z	508	CLA	MG-NB	-2.28	2.01	2.05
13	B	1012	CLA	CMC-C2C	-2.28	1.46	1.50
13	4	511	CLA	CMD-C2D	-2.28	1.46	1.50
13	q	506	CLA	CHC-C1C	2.28	1.43	1.38
13	f	1235	CLA	C1B-C2B	2.28	1.48	1.43
13	B	1240	CLA	MG-NB	-2.28	2.01	2.05
13	A	1108	CLA	CMB-C2B	-2.28	1.46	1.50
13	3	502	CLA	CMD-C2D	-2.28	1.46	1.50
13	G	1140	CLA	CMC-C2C	-2.28	1.46	1.50
13	H	1212	CLA	CMD-C2D	-2.28	1.46	1.50
13	Z	509	CLA	CHC-C1C	2.28	1.43	1.38
13	e	1112	CLA	CHC-C1C	2.28	1.43	1.38
17	A	5002	LHG	P-O6	2.28	1.68	1.59
13	f	1226	CLA	CHC-C4B	-2.28	1.34	1.39
13	s	502	CLA	CMD-C2D	-2.28	1.46	1.50
13	G	1108	CLA	CMB-C2B	-2.28	1.46	1.50
13	H	1205	CLA	MG-NB	-2.28	2.01	2.05
13	G	1128	CLA	C3B-C4B	2.28	1.48	1.42
13	j	1301	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1110	CLA	CMD-C2D	-2.28	1.46	1.50
13	q	518	CLA	CMB-C2B	-2.28	1.46	1.50
13	G	1124	CLA	C1B-C2B	2.28	1.48	1.43
13	b	511	CLA	CMB-C2B	-2.28	1.46	1.50
13	d	504	CLA	CHC-C1C	2.27	1.43	1.38
17	G	5002	LHG	P-O6	2.27	1.68	1.59
13	A	1140	CLA	CMC-C2C	-2.27	1.46	1.50
13	6	504	CLA	CHC-C1C	2.27	1.43	1.38
13	G	1122	CLA	CMC-C2C	-2.27	1.46	1.50
13	G	1237	CLA	CMD-C2D	-2.27	1.46	1.50
13	j	1302	CLA	CMB-C2B	-2.27	1.46	1.50
13	r	501	CLA	CMD-C2D	-2.27	1.46	1.50
13	t	511	CLA	CMB-C2B	-2.27	1.46	1.50
13	A	1139	CLA	MG-NB	-2.27	2.01	2.05
13	2	512	CLA	MG-NB	-2.27	2.01	2.05
13	e	1122	CLA	CMC-C2C	-2.27	1.46	1.50
13	r	509	CLA	CHC-C1C	2.27	1.43	1.38
13	A	1122	CLA	CMC-C2C	-2.27	1.46	1.50
13	G	1123	CLA	MG-NB	-2.27	2.01	2.05
13	G	1125	CLA	CMC-C2C	-2.27	1.46	1.50
13	B	1023	CLA	CHC-C1C	2.27	1.43	1.38
13	v	516	CLA	CHC-C1C	2.27	1.43	1.38
13	3	511	CLA	CMB-C2B	-2.27	1.46	1.50
13	B	1226	CLA	CHC-C4B	-2.27	1.34	1.39
13	G	1013	CLA	CHC-C1C	2.27	1.43	1.38
13	a	502	CLA	CMD-C2D	-2.27	1.46	1.50
20	a	822	SQD	O2-C2	-2.27	1.37	1.43
13	e	1114	CLA	MG-NB	-2.27	2.01	2.05
17	A	5008	LHG	O7-C5	-2.27	1.40	1.46
17	A	5009	LHG	O7-C5	-2.27	1.40	1.46
13	F	1302	CLA	CMB-C2B	-2.27	1.46	1.50
13	q	512	CLA	CMD-C2D	-2.27	1.46	1.50
13	r	508	CLA	CMC-C2C	-2.27	1.46	1.50
13	R	1301	CLA	C1B-C2B	2.27	1.48	1.43
13	H	1240	CLA	MG-NB	-2.27	2.01	2.05
13	G	1123	CLA	C1B-NB	-2.27	1.35	1.37
13	d	516	CLA	CHC-C1C	2.27	1.43	1.38
13	B	1238	CLA	CMD-C2D	-2.27	1.46	1.50
13	B	1205	CLA	MG-NB	-2.27	2.01	2.05
13	Z	512	CLA	MG-NB	-2.27	2.01	2.05
17	G	5009	LHG	O7-C5	-2.27	1.40	1.46
13	f	1213	CLA	C1B-NB	-2.27	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	511	CLA	CMD-C2D	-2.27	1.46	1.50
13	s	502	CLA	CMB-C2B	-2.27	1.46	1.50
13	e	1801	CLA	CAA-C2A	-2.26	1.49	1.54
13	2	509	CLA	CHC-C1C	2.26	1.43	1.38
13	G	1136	CLA	C1B-C2B	2.26	1.48	1.43
13	G	1130	CLA	C1B-C2B	2.26	1.48	1.43
13	f	1219	CLA	MG-NB	-2.26	2.01	2.05
13	T	1303	CLA	CMD-C2D	-2.26	1.46	1.50
13	B	1219	CLA	MG-NB	-2.26	2.01	2.05
13	j	1301	CLA	MG-NB	-2.26	2.01	2.05
13	q	508	CLA	MG-NB	-2.26	2.01	2.05
13	H	1221	CLA	CHC-C1C	2.26	1.43	1.38
13	A	1126	CLA	CMD-C2D	-2.26	1.46	1.50
13	B	1212	CLA	CMD-C2D	-2.26	1.46	1.50
13	G	1126	CLA	MG-NB	-2.26	2.01	2.05
17	e	5009	LHG	O7-C5	-2.26	1.40	1.46
13	e	1110	CLA	CMD-C2D	-2.26	1.46	1.50
13	R	1301	CLA	MG-NB	-2.26	2.01	2.05
13	Y	518	CLA	CMB-C2B	-2.26	1.46	1.50
13	K	1401	CLA	MG-NB	-2.26	2.01	2.05
13	Y	506	CLA	CHC-C1C	2.26	1.43	1.38
13	B	1201	CLA	CMD-C2D	-2.26	1.46	1.50
13	j	1301	CLA	C1B-C2B	2.26	1.48	1.43
13	4	511	CLA	CMB-C2B	-2.26	1.46	1.50
13	A	1118	CLA	MG-NB	-2.26	2.01	2.05
13	r	512	CLA	MG-NB	-2.26	2.01	2.05
13	a	502	CLA	CMB-C2B	-2.26	1.46	1.50
13	e	1108	CLA	CMB-C2B	-2.26	1.46	1.50
13	F	1301	CLA	C1B-C2B	2.26	1.48	1.43
13	e	1123	CLA	MG-NB	-2.26	2.01	2.05
13	6	516	CLA	CHC-C1C	2.26	1.43	1.38
13	K	1103	CLA	CMB-C2B	-2.26	1.46	1.50
13	3	502	CLA	CMB-C2B	-2.26	1.46	1.50
13	A	1237	CLA	CMD-C2D	-2.26	1.46	1.50
13	f	1209	CLA	CMD-C2D	-2.26	1.46	1.50
13	A	1126	CLA	MG-NB	-2.26	2.01	2.05
13	H	1012	CLA	CMC-C2C	-2.26	1.46	1.50
13	e	1237	CLA	CMD-C2D	-2.26	1.46	1.50
13	q	510	CLA	MG-NB	-2.26	2.01	2.05
13	d	506	CLA	CHC-C1C	2.26	1.43	1.38
13	1	512	CLA	CMD-C2D	-2.26	1.46	1.50
13	R	1302	CLA	CMB-C2B	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1213	CLA	C1B-C2B	2.26	1.48	1.43
13	G	1126	CLA	CMD-C2D	-2.25	1.46	1.50
13	H	1210	CLA	CMD-C2D	-2.25	1.46	1.50
13	B	1021	CLA	C3B-C4B	2.25	1.48	1.42
13	e	1133	CLA	MG-NB	-2.25	2.01	2.05
13	A	1136	CLA	C1B-C2B	2.25	1.48	1.43
13	H	1216	CLA	CMC-C2C	-2.25	1.46	1.50
20	3	822	SQD	O2-C2	-2.25	1.37	1.43
13	H	1226	CLA	CHC-C4B	-2.25	1.34	1.39
13	f	1235	CLA	CMC-C2C	-2.25	1.46	1.50
13	B	1229	CLA	C1B-NB	-2.25	1.35	1.37
13	u	512	CLA	MG-NB	-2.25	2.01	2.05
13	A	1101	CLA	C1B-C2B	2.25	1.48	1.43
13	L	1502	CLA	C1B-C2B	2.25	1.48	1.43
13	H	1235	CLA	C1B-C2B	2.25	1.48	1.43
13	e	1136	CLA	C1B-C2B	2.25	1.48	1.43
13	B	1231	CLA	CMD-C2D	-2.25	1.46	1.50
13	Z	511	CLA	CMB-C2B	-2.25	1.46	1.50
13	e	1113	CLA	CMD-C2D	-2.25	1.46	1.50
13	e	1131	CLA	CMC-C2C	-2.25	1.46	1.50
13	A	1125	CLA	CMC-C2C	-2.25	1.46	1.50
13	f	1205	CLA	MG-NB	-2.25	2.01	2.05
13	1	518	CLA	CMB-C2B	-2.25	1.46	1.50
13	H	1213	CLA	MG-NB	-2.25	2.01	2.05
13	A	1105	CLA	C1B-C2B	2.25	1.48	1.43
13	Y	512	CLA	CMD-C2D	-2.25	1.46	1.50
13	B	1221	CLA	CHC-C1C	2.25	1.43	1.38
13	e	1130	CLA	C1B-C2B	2.25	1.48	1.43
13	G	1130	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1140	CLA	MG-NB	-2.25	2.01	2.05
13	5	512	CLA	MG-NB	-2.25	2.01	2.05
13	K	1401	CLA	CMB-C2B	-2.25	1.46	1.50
13	G	1112	CLA	CHC-C1C	2.25	1.43	1.38
13	f	1213	CLA	MG-NB	-2.25	2.01	2.05
13	6	502	CLA	CMB-C2B	-2.25	1.46	1.50
13	V	1502	CLA	C1B-C2B	2.25	1.48	1.43
13	e	1101	CLA	C1B-C2B	2.25	1.48	1.43
13	e	1105	CLA	C1B-C2B	2.25	1.48	1.43
13	G	1140	CLA	MG-NB	-2.25	2.01	2.05
13	f	1221	CLA	MG-NB	-2.25	2.01	2.05
13	e	1138	CLA	C1B-C2B	2.25	1.48	1.43
17	G	5007	LHG	O7-C5	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	516	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1114	CLA	MG-NB	-2.25	2.01	2.05
13	B	1219	CLA	CMB-C2B	-2.25	1.46	1.50
13	H	1213	CLA	CMD-C2D	-2.25	1.46	1.50
16	H	4010	BCR	C17-C18	-2.25	1.32	1.35
13	e	1126	CLA	CMD-C2D	-2.25	1.46	1.50
13	H	1231	CLA	CMD-C2D	-2.25	1.46	1.50
13	2	513	CLA	CHC-C1C	2.25	1.43	1.38
13	c	519	CLA	MG-NB	-2.25	2.01	2.05
13	6	506	CLA	CHC-C1C	2.25	1.43	1.38
13	f	1216	CLA	CMC-C2C	-2.25	1.46	1.50
13	e	1129	CLA	C4B-NB	2.25	1.40	1.37
13	f	1221	CLA	CHC-C1C	2.25	1.43	1.38
13	2	501	CLA	CMD-C2D	-2.24	1.46	1.50
13	H	1219	CLA	CMB-C2B	-2.24	1.46	1.50
13	f	1021	CLA	C3B-C4B	2.24	1.48	1.42
13	B	1213	CLA	MG-NB	-2.24	2.01	2.05
13	e	1011	CLA	CMB-C2B	-2.24	1.46	1.50
13	n	1502	CLA	C1B-C2B	2.24	1.48	1.43
13	e	1130	CLA	CHC-C1C	2.24	1.43	1.38
13	G	1114	CLA	MG-NB	-2.24	2.01	2.05
13	G	1110	CLA	CMD-C2D	-2.24	1.46	1.50
13	f	1238	CLA	CMD-C2D	-2.24	1.46	1.50
13	s	513	CLA	CHC-C1C	2.24	1.43	1.38
13	B	1235	CLA	C1B-C2B	2.24	1.48	1.43
13	A	1106	CLA	CMD-C2D	-2.24	1.46	1.50
13	H	1219	CLA	MG-NB	-2.24	2.01	2.05
13	T	1303	CLA	MG-NB	-2.24	2.01	2.05
13	f	1219	CLA	CMB-C2B	-2.24	1.46	1.50
13	A	1129	CLA	C4B-NB	2.24	1.40	1.37
13	e	1126	CLA	MG-NB	-2.24	2.01	2.05
20	s	822	SQD	O2-C2	-2.24	1.37	1.43
13	2	508	CLA	MG-NB	-2.24	2.01	2.05
13	A	1121	CLA	MG-NB	-2.24	2.01	2.05
13	A	1131	CLA	CMC-C2C	-2.24	1.46	1.50
13	2	508	CLA	CMC-C2C	-2.24	1.46	1.50
13	m	1103	CLA	CMC-C2C	-2.24	1.46	1.50
13	G	1133	CLA	C1B-C2B	2.24	1.48	1.43
13	H	1023	CLA	CHC-C1C	2.24	1.43	1.38
13	d	502	CLA	CMB-C2B	-2.24	1.46	1.50
13	J	1303	CLA	MG-NB	-2.24	2.01	2.05
13	A	1138	CLA	C1B-C2B	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1221	CLA	MG-NB	-2.24	2.01	2.05
20	2	822	SQD	O2-C2	-2.24	1.37	1.43
13	b	512	CLA	MG-NB	-2.24	2.01	2.05
13	r	513	CLA	CHC-C1C	2.24	1.43	1.38
13	G	1105	CLA	C1B-C2B	2.24	1.48	1.43
13	e	1106	CLA	CMD-C2D	-2.24	1.46	1.50
13	m	1103	CLA	CMB-C2B	-2.24	1.46	1.50
13	B	1232	CLA	C1B-NB	-2.24	1.35	1.37
13	B	1223	CLA	MG-NB	-2.24	2.01	2.05
13	G	1132	CLA	MG-NB	-2.24	2.01	2.05
13	H	1225	CLA	CMC-C2C	-2.24	1.46	1.50
13	H	1235	CLA	CMC-C2C	-2.24	1.46	1.50
13	t	513	CLA	CHC-C1C	2.24	1.43	1.38
13	v	504	CLA	CHC-C1C	2.24	1.43	1.38
13	B	1213	CLA	C1B-NB	-2.24	1.35	1.37
13	B	1209	CLA	CMD-C2D	-2.24	1.46	1.50
13	U	1401	CLA	CMB-C2B	-2.24	1.46	1.50
17	G	5008	LHG	O7-C5	-2.24	1.41	1.46
13	1	508	CLA	MG-NB	-2.24	2.01	2.05
13	d	518	CLA	CHC-C1C	2.24	1.43	1.38
13	e	1801	CLA	CMC-C2C	-2.24	1.46	1.50
13	f	1240	CLA	MG-NB	-2.24	2.01	2.05
13	r	511	CLA	CMB-C2B	-2.24	1.46	1.50
13	e	1118	CLA	MG-NB	-2.24	2.01	2.05
13	1	510	CLA	CHC-C1C	2.24	1.43	1.38
13	d	513	CLA	CHC-C1C	2.24	1.43	1.38
13	B	1235	CLA	CMC-C2C	-2.24	1.46	1.50
13	G	1138	CLA	C1B-C2B	2.24	1.48	1.43
13	A	1130	CLA	CHC-C1C	2.24	1.43	1.38
13	u	519	CLA	CHC-C1C	2.24	1.43	1.38
13	v	506	CLA	CHC-C1C	2.24	1.43	1.38
13	G	1131	CLA	CMC-C2C	-2.24	1.46	1.50
13	B	1221	CLA	MG-NB	-2.24	2.01	2.05
13	6	513	CLA	CHC-C1C	2.24	1.43	1.38
13	q	510	CLA	CHC-C1C	2.24	1.43	1.38
13	G	1801	CLA	CMC-C2C	-2.24	1.46	1.50
13	A	1123	CLA	MG-NB	-2.23	2.01	2.05
13	e	1106	CLA	MG-ND	-2.23	2.01	2.05
13	R	1301	CLA	CMB-C2B	-2.23	1.46	1.50
20	r	822	SQD	O2-C2	-2.23	1.37	1.43
13	e	1131	CLA	CMD-C2D	-2.23	1.46	1.50
13	v	518	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	822	SQD	O2-C2	-2.23	1.37	1.43
16	B	4010	BCR	C17-C18	-2.23	1.32	1.35
13	G	1140	CLA	C1B-C2B	2.23	1.48	1.43
13	q	518	CLA	CMC-C2C	-2.23	1.46	1.50
13	B	1214	CLA	MG-NB	-2.23	2.01	2.05
13	d	519	CLA	CHC-C1C	2.23	1.43	1.38
13	t	516	CLA	CHC-C1C	2.23	1.43	1.38
13	4	513	CLA	CHC-C1C	2.23	1.43	1.38
13	B	1213	CLA	CMD-C2D	-2.23	1.46	1.50
13	e	1122	CLA	CMD-C2D	-2.23	1.46	1.50
13	H	1023	CLA	MG-ND	-2.23	2.01	2.05
13	Z	517	CLA	MG-NB	-2.23	2.01	2.05
13	H	1213	CLA	C1B-NB	-2.23	1.35	1.37
13	1	518	CLA	CMC-C2C	-2.23	1.46	1.50
13	Z	501	CLA	CMD-C2D	-2.23	1.46	1.50
13	Z	507	CLA	CMD-C2D	-2.23	1.46	1.50
13	f	1213	CLA	CMD-C2D	-2.23	1.46	1.50
13	A	1111	CLA	C1B-C2B	2.23	1.48	1.43
13	F	1301	CLA	CMB-C2B	-2.23	1.46	1.50
13	U	1401	CLA	MG-NB	-2.23	2.01	2.05
13	a	508	CLA	MG-NB	-2.23	2.01	2.05
13	H	1229	CLA	C1B-NB	-2.23	1.35	1.37
13	f	1023	CLA	C1B-NB	-2.23	1.35	1.37
13	e	1138	CLA	CMD-C2D	-2.23	1.46	1.50
13	e	1101	CLA	CMB-C2B	-2.23	1.46	1.50
13	A	1130	CLA	C1B-C2B	2.23	1.48	1.43
13	n	1502	CLA	CHC-C1C	2.23	1.43	1.38
13	A	1106	CLA	MG-ND	-2.23	2.01	2.05
13	q	502	CLA	MG-NB	-2.23	2.01	2.05
13	6	518	CLA	CHC-C1C	2.23	1.43	1.38
13	H	1232	CLA	C1B-NB	-2.23	1.35	1.37
13	A	1801	CLA	CMC-C2C	-2.23	1.46	1.50
13	f	1231	CLA	CMD-C2D	-2.23	1.46	1.50
13	m	1401	CLA	CMB-C2B	-2.23	1.46	1.50
13	H	1021	CLA	C3B-C4B	2.23	1.48	1.42
13	e	1125	CLA	CMC-C2C	-2.23	1.46	1.50
13	G	1111	CLA	C1B-C2B	2.23	1.48	1.43
13	G	1011	CLA	CMB-C2B	-2.23	1.46	1.50
13	e	1122	CLA	MG-NB	-2.23	2.01	2.05
13	r	506	CLA	CMC-C2C	-2.23	1.46	1.50
13	G	1122	CLA	MG-NB	-2.23	2.01	2.05
13	G	1122	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1012	CLA	CMD-C2D	-2.23	1.46	1.50
13	e	1110	CLA	CMC-C2C	-2.23	1.46	1.50
13	v	502	CLA	CMB-C2B	-2.23	1.46	1.50
13	e	1133	CLA	C1B-C2B	2.23	1.48	1.43
13	2	510	CLA	CHC-C1C	2.23	1.43	1.38
13	e	1116	CLA	CMD-C2D	-2.23	1.46	1.50
13	q	519	CLA	CMB-C2B	-2.23	1.46	1.50
13	G	1101	CLA	C1B-C2B	2.22	1.48	1.43
13	H	1238	CLA	CMD-C2D	-2.22	1.46	1.50
13	Y	508	CLA	CMC-C2C	-2.22	1.46	1.50
13	r	501	CLA	CMC-C2C	-2.22	1.46	1.50
13	B	1212	CLA	MG-NB	-2.22	2.01	2.05
13	4	510	CLA	CHC-C1C	2.22	1.43	1.38
13	c	519	CLA	CHC-C1C	2.22	1.43	1.38
13	F	1301	CLA	MG-NB	-2.22	2.01	2.05
13	e	1125	CLA	CMB-C2B	-2.22	1.46	1.50
13	s	502	CLA	MG-NB	-2.22	2.01	2.05
13	A	1125	CLA	CMB-C2B	-2.22	1.46	1.50
13	G	1138	CLA	CMD-C2D	-2.22	1.46	1.50
13	U	1103	CLA	CMB-C2B	-2.22	1.46	1.50
13	A	1013	CLA	CHC-C1C	2.22	1.43	1.38
13	6	519	CLA	CHC-C1C	2.22	1.43	1.38
13	Y	508	CLA	MG-NB	-2.22	2.01	2.05
13	l	1303	CLA	MG-NB	-2.22	2.01	2.05
13	A	1133	CLA	C1B-C2B	2.22	1.48	1.43
13	A	1113	CLA	CMD-C2D	-2.22	1.46	1.50
13	A	1122	CLA	CMD-C2D	-2.22	1.46	1.50
13	A	1101	CLA	CMB-C2B	-2.22	1.46	1.50
13	n	1502	CLA	MG-NB	-2.22	2.01	2.05
17	A	5007	LHG	O7-C5	-2.22	1.41	1.46
13	B	1210	CLA	CMD-C2D	-2.22	1.46	1.50
13	H	1209	CLA	CMD-C2D	-2.22	1.46	1.50
13	f	1225	CLA	CMC-C2C	-2.22	1.46	1.50
13	B	1023	CLA	MG-ND	-2.22	2.01	2.05
13	G	1101	CLA	CMB-C2B	-2.22	1.46	1.50
13	j	1302	CLA	CMD-C2D	-2.22	1.46	1.50
13	5	519	CLA	MG-NB	-2.22	2.01	2.05
13	G	1121	CLA	MG-NB	-2.22	2.01	2.05
13	G	1106	CLA	CMD-C2D	-2.22	1.46	1.50
13	G	1128	CLA	CMC-C2C	-2.22	1.46	1.50
13	l	1303	CLA	CMD-C2D	-2.22	1.46	1.50
13	r	510	CLA	CHC-C1C	2.22	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	5218	LHG	O7-C5	-2.22	1.41	1.46
13	2	507	CLA	CMD-C2D	-2.22	1.46	1.50
13	2	513	CLA	CMC-C2C	-2.22	1.46	1.50
13	G	1113	CLA	CMD-C2D	-2.22	1.46	1.50
13	c	512	CLA	MG-NB	-2.22	2.01	2.05
13	B	1216	CLA	CMC-C2C	-2.22	1.46	1.50
13	J	1303	CLA	CMD-C2D	-2.22	1.46	1.50
13	2	511	CLA	CMB-C2B	-2.22	1.46	1.50
13	H	1225	CLA	CMB-C2B	-2.22	1.46	1.50
13	f	1210	CLA	CMD-C2D	-2.22	1.46	1.50
13	e	1110	CLA	C1B-C2B	2.22	1.48	1.43
13	Z	502	CLA	CMD-C2D	-2.22	1.46	1.50
13	e	1125	CLA	CMD-C2D	-2.22	1.46	1.50
13	4	516	CLA	CHC-C1C	2.22	1.43	1.38
13	L	1502	CLA	CHC-C1C	2.22	1.43	1.38
13	A	1135	CLA	C3B-C4B	2.22	1.48	1.42
13	A	1112	CLA	CMC-C2C	-2.22	1.46	1.50
13	3	508	CLA	MG-NB	-2.22	2.01	2.05
13	A	1801	CLA	C1B-NB	-2.22	1.35	1.37
13	e	1112	CLA	CMC-C2C	-2.22	1.46	1.50
13	3	504	CLA	MG-NB	-2.22	2.01	2.05
13	Y	510	CLA	CHC-C1C	2.22	1.43	1.38
13	Y	519	CLA	MG-ND	-2.22	2.01	2.05
13	4	512	CLA	CMB-C2B	-2.22	1.46	1.50
13	G	1129	CLA	CMC-C2C	-2.22	1.46	1.50
13	f	1201	CLA	CMD-C2D	-2.22	1.46	1.50
13	1	510	CLA	MG-NB	-2.22	2.01	2.05
13	4	512	CLA	MG-NB	-2.22	2.01	2.05
13	Z	513	CLA	CHC-C1C	2.22	1.43	1.38
13	f	1012	CLA	CMD-C2D	-2.22	1.46	1.50
13	1	507	CLA	MG-NB	-2.21	2.01	2.05
13	H	1202	CLA	C1B-C2B	2.21	1.48	1.43
17	n	5218	LHG	O7-C5	-2.21	1.41	1.46
13	r	513	CLA	CMC-C2C	-2.21	1.46	1.50
13	A	1140	CLA	C1B-C2B	2.21	1.48	1.43
13	A	1128	CLA	CMC-C2C	-2.21	1.46	1.50
13	B	1225	CLA	CMC-C2C	-2.21	1.46	1.50
13	e	1128	CLA	CMC-C2C	-2.21	1.46	1.50
13	e	1139	CLA	MG-ND	-2.21	2.01	2.05
13	U	1103	CLA	CMC-C2C	-2.21	1.46	1.50
13	f	1212	CLA	MG-NB	-2.21	2.01	2.05
13	s	508	CLA	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	518	CLA	CMC-C2C	-2.21	1.46	1.50
13	e	1111	CLA	C1B-C2B	2.21	1.48	1.43
13	L	1502	CLA	MG-NB	-2.21	2.01	2.05
13	f	1202	CLA	C1B-C2B	2.21	1.48	1.43
17	L	5218	LHG	O7-C5	-2.21	1.41	1.46
13	B	1239	CLA	MG-NB	-2.21	2.01	2.05
13	A	1011	CLA	CMB-C2B	-2.21	1.46	1.50
13	A	1138	CLA	CMD-C2D	-2.21	1.46	1.50
13	G	1140	CLA	CMD-C2D	-2.21	1.46	1.50
13	t	503	CLA	CMD-C2D	-2.21	1.46	1.50
13	3	513	CLA	CHC-C1C	2.21	1.43	1.38
13	c	509	CLA	CHC-C1C	2.21	1.43	1.38
13	r	507	CLA	CMD-C2D	-2.21	1.46	1.50
13	e	1140	CLA	C1B-C2B	2.21	1.48	1.43
13	F	1302	CLA	CMD-C2D	-2.21	1.46	1.50
13	V	1502	CLA	CMD-C2D	-2.21	1.46	1.50
13	H	1214	CLA	MG-NB	-2.21	2.01	2.05
13	B	1012	CLA	CMD-C2D	-2.21	1.46	1.50
13	1	508	CLA	CMC-C2C	-2.21	1.46	1.50
13	2	506	CLA	CMC-C2C	-2.21	1.46	1.50
13	v	519	CLA	CHC-C1C	2.21	1.43	1.38
13	1	502	CLA	MG-NB	-2.21	2.01	2.05
13	q	511	CLA	MG-NB	-2.21	2.01	2.05
13	G	1129	CLA	C4B-NB	2.21	1.40	1.37
13	Z	508	CLA	CMC-C2C	-2.21	1.46	1.50
13	A	1110	CLA	C1B-C2B	2.21	1.48	1.43
13	2	506	CLA	MG-NB	-2.21	2.01	2.05
13	G	1125	CLA	CMB-C2B	-2.21	1.46	1.50
13	Z	513	CLA	CMC-C2C	-2.21	1.46	1.50
13	q	508	CLA	CMC-C2C	-2.21	1.46	1.50
13	u	510	CLA	CHC-C1C	2.21	1.43	1.38
13	f	1239	CLA	MG-NB	-2.21	2.01	2.05
13	2	502	CLA	CMD-C2D	-2.21	1.46	1.50
13	e	1104	CLA	CMD-C2D	-2.21	1.46	1.50
20	t	822	SQD	O2-C2	-2.21	1.37	1.43
13	V	1502	CLA	CHC-C1C	2.21	1.43	1.38
13	Z	519	CLA	CHC-C1C	2.21	1.43	1.38
13	f	1227	CLA	CHC-C1C	2.21	1.43	1.38
13	e	1237	CLA	MG-NB	-2.21	2.01	2.05
13	s	504	CLA	MG-NB	-2.21	2.01	2.05
13	a	504	CLA	MG-NB	-2.21	2.01	2.05
13	B	1235	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1135	CLA	C3B-C4B	2.21	1.47	1.42
13	q	516	CLA	CHC-C1C	2.21	1.43	1.38
13	f	1229	CLA	MG-NB	-2.21	2.01	2.05
13	1	519	CLA	CMB-C2B	-2.21	1.46	1.50
16	f	4010	BCR	C17-C18	-2.21	1.32	1.35
13	v	513	CLA	CHC-C1C	2.21	1.43	1.38
13	G	1106	CLA	MG-ND	-2.20	2.01	2.05
13	G	1112	CLA	CMC-C2C	-2.20	1.46	1.50
13	R	1302	CLA	CMD-C2D	-2.20	1.46	1.50
13	f	1228	CLA	CMD-C2D	-2.20	1.46	1.50
13	4	505	CLA	MG-NB	-2.20	2.01	2.05
13	b	506	CLA	CHC-C1C	2.20	1.43	1.38
13	e	1119	CLA	CMD-C2D	-2.20	1.46	1.50
13	r	502	CLA	CMD-C2D	-2.20	1.46	1.50
13	a	505	CLA	MG-NB	-2.20	2.01	2.05
13	2	501	CLA	CMC-C2C	-2.20	1.46	1.50
13	5	519	CLA	CHC-C1C	2.20	1.43	1.38
13	A	1132	CLA	MG-NB	-2.20	2.01	2.05
13	B	1222	CLA	MG-NB	-2.20	2.01	2.05
13	t	506	CLA	CHC-C1C	2.20	1.43	1.38
13	H	1222	CLA	MG-NB	-2.20	2.01	2.05
13	B	1227	CLA	CHC-C1C	2.20	1.43	1.38
13	B	1214	CLA	C1B-C2B	2.20	1.48	1.43
17	e	5007	LHG	O7-C5	-2.20	1.41	1.46
13	G	1106	CLA	CMC-C2C	-2.20	1.46	1.50
13	H	1214	CLA	C1B-C2B	2.20	1.48	1.43
13	4	506	CLA	CHC-C1C	2.20	1.43	1.38
13	b	513	CLA	CHC-C1C	2.20	1.43	1.38
13	B	1228	CLA	CMD-C2D	-2.20	1.46	1.50
13	Z	506	CLA	CMC-C2C	-2.20	1.46	1.50
13	A	1116	CLA	CMD-C2D	-2.20	1.46	1.50
13	G	1130	CLA	CMB-C2B	-2.20	1.46	1.50
13	b	510	CLA	CHC-C1C	2.20	1.43	1.38
13	K	1103	CLA	CMC-C2C	-2.20	1.46	1.50
13	e	1136	CLA	CMD-C2D	-2.20	1.46	1.50
13	u	509	CLA	CHC-C1C	2.20	1.43	1.38
13	U	1103	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	512	CLA	CMB-C2B	-2.20	1.46	1.50
13	5	518	CLA	CHC-C1C	2.20	1.43	1.38
13	H	1212	CLA	MG-NB	-2.20	2.01	2.05
13	Y	510	CLA	MG-NB	-2.20	2.01	2.05
13	Z	507	CLA	MG-NB	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1119	CLA	CMC-C2C	-2.20	1.46	1.50
13	e	1137	CLA	CMB-C2B	-2.20	1.46	1.50
13	1	519	CLA	MG-ND	-2.20	2.01	2.05
13	e	1121	CLA	MG-NB	-2.20	2.01	2.05
13	e	1801	CLA	C1B-NB	-2.20	1.35	1.37
13	G	1119	CLA	CMD-C2D	-2.20	1.46	1.50
13	a	509	CLA	CHC-C1C	2.20	1.43	1.38
13	f	1230	CLA	MG-NB	-2.20	2.01	2.05
13	A	1125	CLA	CMD-C2D	-2.20	1.46	1.50
13	1	501	CLA	CMD-C2D	-2.20	1.46	1.50
14	G	2001	PQN	C10-C1	-2.20	1.44	1.48
13	1	516	CLA	CHC-C1C	2.20	1.43	1.38
13	A	1139	CLA	MG-ND	-2.20	2.01	2.05
13	2	517	CLA	MG-NB	-2.20	2.01	2.05
13	r	507	CLA	MG-NB	-2.20	2.01	2.05
13	B	1206	CLA	CMD-C2D	-2.20	1.46	1.50
13	e	1137	CLA	CMC-C2C	-2.20	1.46	1.50
13	H	1223	CLA	MG-NB	-2.20	2.01	2.05
13	a	512	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	1113	CLA	CMC-C2C	-2.20	1.46	1.50
13	B	1023	CLA	C1B-NB	-2.20	1.35	1.37
13	f	1023	CLA	MG-ND	-2.20	2.01	2.05
13	n	1501	CLA	CMB-C2B	-2.19	1.46	1.50
13	G	1122	CLA	CMB-C2B	-2.19	1.46	1.50
13	G	1110	CLA	C1B-C2B	2.19	1.48	1.43
13	3	502	CLA	MG-NB	-2.19	2.01	2.05
13	L	1501	CLA	CMB-C2B	-2.19	1.46	1.50
13	H	1231	CLA	CMC-C2C	-2.19	1.46	1.50
13	q	501	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1130	CLA	MG-NB	-2.19	2.01	2.05
13	1	511	CLA	MG-NB	-2.19	2.01	2.05
13	H	1202	CLA	CMC-C2C	-2.19	1.46	1.50
13	t	512	CLA	CMB-C2B	-2.19	1.46	1.50
13	q	507	CLA	MG-NB	-2.19	2.01	2.05
13	Z	510	CLA	CHC-C1C	2.19	1.43	1.38
13	f	1214	CLA	C1B-C2B	2.19	1.48	1.43
13	u	518	CLA	CMD-C2D	-2.19	1.46	1.50
13	c	518	CLA	CMD-C2D	-2.19	1.46	1.50
13	l	1302	CLA	CMB-C2B	-2.19	1.46	1.50
13	f	1221	CLA	CMB-C2B	-2.19	1.46	1.50
13	3	512	CLA	CMD-C2D	-2.19	1.46	1.50
13	H	1206	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1235	CLA	CMD-C2D	-2.19	1.46	1.50
13	e	1140	CLA	CMD-C2D	-2.19	1.46	1.50
13	Y	507	CLA	MG-NB	-2.19	2.01	2.05
13	f	1201	CLA	MG-NB	-2.19	2.01	2.05
13	f	1234	CLA	CMC-C2C	-2.19	1.46	1.50
13	e	1022	CLA	C3B-C4B	2.19	1.47	1.42
13	A	1127	CLA	C1B-C2B	2.19	1.48	1.43
13	f	1222	CLA	MG-NB	-2.19	2.01	2.05
13	G	1131	CLA	CMD-C2D	-2.19	1.46	1.50
13	V	1501	CLA	CMB-C2B	-2.19	1.46	1.50
13	V	1502	CLA	MG-NB	-2.19	2.01	2.05
13	e	1013	CLA	CHC-C1C	2.19	1.43	1.38
13	A	1110	CLA	CMC-C2C	-2.19	1.46	1.50
13	A	1137	CLA	CMB-C2B	-2.19	1.46	1.50
13	G	1132	CLA	CMD-C2D	-2.19	1.46	1.50
13	G	1130	CLA	MG-NB	-2.19	2.01	2.05
13	Z	506	CLA	MG-NB	-2.19	2.01	2.05
13	r	517	CLA	MG-NB	-2.19	2.01	2.05
13	u	504	CLA	MG-NB	-2.19	2.01	2.05
13	q	511	CLA	CHC-C1C	2.19	1.43	1.38
13	A	1119	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1132	CLA	CMD-C2D	-2.19	1.46	1.50
13	G	1137	CLA	CMB-C2B	-2.19	1.46	1.50
13	f	1207	CLA	CMC-C2C	-2.19	1.46	1.50
13	6	510	CLA	CHC-C1C	2.19	1.43	1.38
13	B	1202	CLA	C1B-C2B	2.19	1.48	1.43
13	A	1108	CLA	MG-NB	-2.19	2.01	2.05
13	G	1125	CLA	CMD-C2D	-2.19	1.46	1.50
13	Y	501	CLA	CMD-C2D	-2.19	1.46	1.50
13	e	1136	CLA	CMC-C2C	-2.19	1.46	1.50
13	c	518	CLA	CHC-C1C	2.19	1.43	1.38
13	v	510	CLA	CHC-C1C	2.19	1.43	1.38
13	Y	501	CLA	MG-NB	-2.19	2.01	2.05
13	e	1108	CLA	MG-NB	-2.19	2.01	2.05
13	H	1209	CLA	C1B-C2B	2.19	1.48	1.43
13	4	505	CLA	CMD-C2D	-2.19	1.46	1.50
13	u	519	CLA	MG-NB	-2.19	2.01	2.05
13	4	504	CLA	CHC-C1C	2.19	1.43	1.38
13	b	504	CLA	CHC-C1C	2.19	1.43	1.38
13	t	510	CLA	CHC-C1C	2.19	1.43	1.38
13	A	1122	CLA	MG-NB	-2.19	2.01	2.05
13	a	513	CLA	CHC-C1C	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	505	CLA	MG-NB	-2.19	2.01	2.05
13	H	1227	CLA	C1B-C2B	2.19	1.48	1.43
13	q	505	CLA	MG-NB	-2.19	2.01	2.05
13	A	1131	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1140	CLA	CMD-C2D	-2.19	1.46	1.50
13	Y	511	CLA	CHC-C1C	2.19	1.43	1.38
13	c	510	CLA	CHC-C1C	2.19	1.43	1.38
13	B	1201	CLA	MG-NB	-2.19	2.01	2.05
13	Z	501	CLA	CMC-C2C	-2.19	1.46	1.50
20	5	822	SQD	O2-C2	-2.19	1.37	1.43
13	e	1127	CLA	C1B-C2B	2.19	1.48	1.43
13	B	1234	CLA	CMC-C2C	-2.19	1.46	1.50
13	L	1502	CLA	CMD-C2D	-2.19	1.46	1.50
13	3	504	CLA	CMD-C2D	-2.19	1.46	1.50
13	e	1113	CLA	CMC-C2C	-2.19	1.46	1.50
13	Y	512	CLA	CHC-C1C	2.18	1.43	1.38
13	e	1130	CLA	MG-NB	-2.18	2.01	2.05
13	v	512	CLA	MG-NB	-2.18	2.01	2.05
13	G	1134	CLA	CMD-C2D	-2.18	1.46	1.50
13	f	1206	CLA	CMD-C2D	-2.18	1.46	1.50
13	H	1227	CLA	CHC-C1C	2.18	1.43	1.38
13	s	509	CLA	CHC-C1C	2.18	1.43	1.38
13	d	508	CLA	MG-NB	-2.18	2.01	2.05
13	e	1132	CLA	MG-NB	-2.18	2.01	2.05
13	B	1225	CLA	CMB-C2B	-2.18	1.46	1.50
13	f	1209	CLA	C1B-C2B	2.18	1.48	1.43
13	5	507	CLA	MG-NB	-2.18	2.01	2.05
13	5	511	CLA	MG-NB	-2.18	2.01	2.05
13	H	1229	CLA	MG-NB	-2.18	2.01	2.05
13	b	505	CLA	MG-NB	-2.18	2.01	2.05
13	A	1137	CLA	CMC-C2C	-2.18	1.46	1.50
13	q	511	CLA	CMB-C2B	-2.18	1.46	1.50
13	3	518	CLA	CHC-C1C	2.18	1.43	1.38
13	q	519	CLA	MG-ND	-2.18	2.01	2.05
13	A	1121	CLA	CMB-C2B	-2.18	1.46	1.50
13	A	1136	CLA	CMC-C2C	-2.18	1.46	1.50
13	A	1237	CLA	MG-NB	-2.18	2.01	2.05
13	1	511	CLA	CMB-C2B	-2.18	1.46	1.50
13	Z	503	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	504	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	518	CLA	CHC-C1C	2.18	1.43	1.38
13	2	507	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	505	CLA	MG-NB	-2.18	2.01	2.05
13	e	1135	CLA	C3B-C4B	2.18	1.47	1.42
13	G	1137	CLA	CMC-C2C	-2.18	1.46	1.50
13	2	519	CLA	CHC-C1C	2.18	1.43	1.38
13	B	1216	CLA	CMD-C2D	-2.18	1.46	1.50
13	s	505	CLA	MG-NB	-2.18	2.01	2.05
13	A	1104	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	1134	CLA	CMD-C2D	-2.18	1.46	1.50
13	B	1213	CLA	CMC-C2C	-2.18	1.46	1.50
13	e	1106	CLA	CMC-C2C	-2.18	1.46	1.50
13	Z	516	CLA	MG-NB	-2.18	2.01	2.05
13	f	1214	CLA	MG-NB	-2.18	2.01	2.05
13	5	509	CLA	CHC-C1C	2.18	1.43	1.38
13	4	503	CLA	CMD-C2D	-2.18	1.46	1.50
13	b	519	CLA	CMB-C2B	-2.18	1.46	1.50
13	B	1229	CLA	MG-NB	-2.18	2.01	2.05
13	e	1135	CLA	C4B-NB	2.18	1.40	1.37
13	A	1106	CLA	CMC-C2C	-2.18	1.46	1.50
13	2	503	CLA	CMD-C2D	-2.18	1.46	1.50
13	5	518	CLA	CMD-C2D	-2.18	1.46	1.50
13	B	1215	CLA	C1B-C2B	2.18	1.48	1.43
13	A	1133	CLA	CMD-C2D	-2.18	1.46	1.50
13	G	1121	CLA	CMB-C2B	-2.18	1.46	1.50
13	H	1216	CLA	CMD-C2D	-2.18	1.46	1.50
13	s	504	CLA	CMD-C2D	-2.18	1.46	1.50
13	Y	511	CLA	MG-NB	-2.18	2.01	2.05
13	Y	516	CLA	CHC-C1C	2.18	1.43	1.38
13	r	519	CLA	CHC-C1C	2.18	1.43	1.38
13	G	1104	CLA	CMD-C2D	-2.18	1.46	1.50
13	G	1131	CLA	CMB-C2B	-2.18	1.46	1.50
13	j	1301	CLA	CMD-C2D	-2.18	1.46	1.50
20	V	5216	SQD	O2-C2	-2.18	1.37	1.43
13	B	1230	CLA	MG-NB	-2.18	2.01	2.05
13	t	511	CLA	MG-NB	-2.18	2.01	2.05
13	H	1215	CLA	C1B-C2B	2.18	1.48	1.43
13	A	1104	CLA	CMC-C2C	-2.18	1.46	1.50
13	H	1203	CLA	CMC-C2C	-2.18	1.46	1.50
13	H	1228	CLA	CMD-C2D	-2.18	1.46	1.50
13	e	1122	CLA	CMB-C2B	-2.18	1.46	1.50
13	f	1211	CLA	CMC-C2C	-2.18	1.46	1.50
20	u	822	SQD	O2-C2	-2.18	1.37	1.43
13	6	508	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	512	CLA	MG-NB	-2.18	2.01	2.05
13	b	505	CLA	CMD-C2D	-2.18	1.46	1.50
13	e	1132	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	1129	CLA	CMC-C2C	-2.18	1.46	1.50
13	3	506	CLA	CMC-C2C	-2.18	1.46	1.50
13	G	1116	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	1116	CLA	CMC-C2C	-2.18	1.46	1.50
13	e	1133	CLA	CMD-C2D	-2.18	1.46	1.50
13	u	518	CLA	CHC-C1C	2.18	1.42	1.38
13	T	1302	CLA	MG-NB	-2.18	2.01	2.05
13	a	502	CLA	MG-NB	-2.18	2.01	2.05
13	G	1127	CLA	C1B-C2B	2.18	1.48	1.43
13	G	1116	CLA	CMC-C2C	-2.18	1.46	1.50
13	G	1132	CLA	CMC-C2C	-2.18	1.46	1.50
13	H	1239	CLA	MG-NB	-2.18	2.01	2.05
13	A	1122	CLA	CMB-C2B	-2.18	1.46	1.50
13	Y	511	CLA	CMB-C2B	-2.18	1.46	1.50
13	A	1111	CLA	CHC-C1C	2.18	1.42	1.38
13	3	519	CLA	CHC-C1C	2.18	1.42	1.38
13	e	1129	CLA	CMC-C2C	-2.18	1.46	1.50
13	q	504	CLA	CMD-C2D	-2.18	1.46	1.50
13	R	1302	CLA	MG-NB	-2.17	2.01	2.05
13	c	504	CLA	MG-NB	-2.17	2.01	2.05
13	T	1302	CLA	CMD-C2D	-2.17	1.46	1.50
13	t	518	CLA	CMD-C2D	-2.17	1.46	1.50
13	v	511	CLA	CMB-C2B	-2.17	1.46	1.50
13	A	1130	CLA	CMB-C2B	-2.17	1.46	1.50
13	f	1213	CLA	CMC-C2C	-2.17	1.46	1.50
13	1	511	CLA	CHC-C1C	2.17	1.42	1.38
13	e	1116	CLA	CHC-C1C	2.17	1.42	1.38
13	t	512	CLA	MG-NB	-2.17	2.01	2.05
13	H	1023	CLA	C1B-NB	-2.17	1.35	1.37
13	f	1232	CLA	C1B-NB	-2.17	1.35	1.37
13	B	1209	CLA	CMC-C2C	-2.17	1.46	1.50
13	1	504	CLA	CMD-C2D	-2.17	1.46	1.50
13	r	506	CLA	MG-NB	-2.17	2.01	2.05
13	u	507	CLA	MG-NB	-2.17	2.01	2.05
13	5	510	CLA	CHC-C1C	2.17	1.42	1.38
13	B	1202	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	1224	CLA	CMB-C2B	-2.17	1.46	1.50
13	J	1302	CLA	CMB-C2B	-2.17	1.46	1.50
13	Y	503	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1124	CLA	MG-NB	-2.17	2.01	2.05
13	K	1103	CLA	CMD-C2D	-2.17	1.46	1.50
13	3	509	CLA	CHC-C1C	2.17	1.42	1.38
13	c	507	CLA	MG-NB	-2.17	2.01	2.05
13	A	1134	CLA	CHC-C1C	2.17	1.42	1.38
13	H	1207	CLA	CMC-C2C	-2.17	1.46	1.50
13	Y	519	CLA	CMB-C2B	-2.17	1.46	1.50
13	r	503	CLA	CMD-C2D	-2.17	1.46	1.50
13	G	1124	CLA	MG-NB	-2.17	2.01	2.05
13	u	508	CLA	MG-NB	-2.17	2.01	2.05
20	1	822	SQD	O2-C2	-2.17	1.37	1.43
13	G	1116	CLA	CHC-C1C	2.17	1.42	1.38
13	G	1801	CLA	C1B-NB	-2.17	1.35	1.37
13	e	1138	CLA	CMB-C2B	-2.17	1.46	1.50
13	G	1112	CLA	MG-NB	-2.17	2.01	2.05
13	4	519	CLA	CMB-C2B	-2.17	1.46	1.50
13	1	505	CLA	MG-NB	-2.17	2.01	2.05
13	f	1234	CLA	CHC-C1C	2.17	1.42	1.38
13	t	504	CLA	CHC-C1C	2.17	1.42	1.38
13	B	1231	CLA	CMC-C2C	-2.17	1.46	1.50
13	b	503	CLA	CMD-C2D	-2.17	1.46	1.50
13	e	1130	CLA	CMB-C2B	-2.17	1.46	1.50
13	n	1502	CLA	CMD-C2D	-2.17	1.46	1.50
13	G	1108	CLA	MG-NB	-2.17	2.01	2.05
13	6	512	CLA	CHC-C1C	2.17	1.42	1.38
13	a	510	CLA	CHC-C1C	2.17	1.42	1.38
13	f	1209	CLA	CMC-C2C	-2.17	1.46	1.50
13	1	504	CLA	MG-NB	-2.17	2.01	2.05
13	Y	502	CLA	MG-NB	-2.17	2.01	2.05
13	e	1121	CLA	CMB-C2B	-2.17	1.46	1.50
20	Y	822	SQD	O2-C2	-2.17	1.37	1.43
13	4	508	CLA	CMC-C2C	-2.17	1.46	1.50
13	6	502	CLA	CMD-C2D	-2.17	1.46	1.50
13	H	1201	CLA	CMC-C2C	-2.17	1.46	1.50
13	e	1104	CLA	CMC-C2C	-2.17	1.46	1.50
13	A	1022	CLA	C3B-C4B	2.17	1.47	1.42
13	J	1302	CLA	MG-NB	-2.17	2.01	2.05
13	d	519	CLA	MG-NB	-2.17	2.01	2.05
13	f	1202	CLA	CMC-C2C	-2.17	1.46	1.50
13	f	1215	CLA	C1B-C2B	2.17	1.48	1.43
13	v	518	CLA	MG-NB	-2.17	2.01	2.05
13	3	516	CLA	CHC-C1C	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	512	CLA	CHC-C1C	2.17	1.42	1.38
13	l	1302	CLA	MG-NB	-2.17	2.01	2.05
13	B	1221	CLA	CMB-C2B	-2.17	1.46	1.50
13	H	1207	CLA	CMB-C2B	-2.17	1.46	1.50
13	f	1202	CLA	CMD-C2D	-2.17	1.46	1.50
13	d	510	CLA	CHC-C1C	2.17	1.42	1.38
13	H	1201	CLA	MG-NB	-2.17	2.01	2.05
20	4	822	SQD	O2-C2	-2.17	1.37	1.43
13	H	1228	CLA	C1B-C2B	2.17	1.48	1.43
13	3	512	CLA	CMB-C2B	-2.17	1.46	1.50
13	f	1207	CLA	CMB-C2B	-2.17	1.46	1.50
13	B	1234	CLA	CHC-C1C	2.17	1.42	1.38
13	s	510	CLA	CHC-C1C	2.17	1.42	1.38
13	G	1110	CLA	CMB-C2B	-2.16	1.46	1.50
13	H	1021	CLA	CMB-C2B	-2.16	1.46	1.50
13	H	1206	CLA	CMC-C2C	-2.16	1.46	1.50
13	u	511	CLA	CMB-C2B	-2.16	1.46	1.50
13	a	512	CLA	CMB-C2B	-2.16	1.46	1.50
13	d	502	CLA	CMD-C2D	-2.16	1.46	1.50
13	v	509	CLA	CHC-C1C	2.16	1.42	1.38
20	L	5216	SQD	O2-C2	-2.16	1.37	1.43
13	e	1120	CLA	CMB-C2B	-2.16	1.46	1.50
13	d	512	CLA	CHC-C1C	2.16	1.42	1.38
13	c	508	CLA	MG-NB	-2.16	2.01	2.05
13	B	1209	CLA	C1B-C2B	2.16	1.48	1.43
13	H	1209	CLA	CMB-C2B	-2.16	1.46	1.50
13	c	511	CLA	MG-NB	-2.16	2.01	2.05
13	c	502	CLA	CMB-C2B	-2.16	1.46	1.50
13	1	501	CLA	MG-NB	-2.16	2.01	2.05
13	4	511	CLA	MG-NB	-2.16	2.01	2.05
13	v	508	CLA	MG-NB	-2.16	2.01	2.05
13	f	1227	CLA	C1B-C2B	2.16	1.48	1.43
13	A	1132	CLA	CMB-C2B	-2.16	1.46	1.50
13	A	1136	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1132	CLA	CMB-C2B	-2.16	1.46	1.50
13	f	1203	CLA	CMD-C2D	-2.16	1.46	1.50
13	s	518	CLA	CHC-C1C	2.16	1.42	1.38
13	e	1105	CLA	MG-NB	-2.16	2.01	2.05
13	1	503	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1104	CLA	CMC-C2C	-2.16	1.46	1.50
13	G	1108	CLA	CMD-C2D	-2.16	1.46	1.50
13	e	1116	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1138	CLA	CHC-C1C	2.16	1.42	1.38
13	H	1234	CLA	CHC-C1C	2.16	1.42	1.38
13	q	512	CLA	CHC-C1C	2.16	1.42	1.38
13	G	1139	CLA	MG-ND	-2.16	2.01	2.05
13	u	511	CLA	MG-NB	-2.16	2.01	2.05
20	n	5216	SQD	O2-C2	-2.16	1.37	1.43
13	G	1136	CLA	CMC-C2C	-2.16	1.46	1.50
13	H	1209	CLA	CMC-C2C	-2.16	1.46	1.50
13	Y	504	CLA	CMD-C2D	-2.16	1.46	1.50
13	f	1206	CLA	CMC-C2C	-2.16	1.46	1.50
13	6	509	CLA	CHC-C1C	2.16	1.42	1.38
13	G	1111	CLA	CHC-C1C	2.16	1.42	1.38
13	d	509	CLA	CHC-C1C	2.16	1.42	1.38
20	d	822	SQD	O4-C4	-2.16	1.37	1.43
13	A	1131	CLA	CMB-C2B	-2.16	1.46	1.50
13	B	1201	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	1117	CLA	C1B-NB	-2.16	1.35	1.37
13	B	1227	CLA	C1B-C2B	2.16	1.48	1.43
13	q	512	CLA	CMB-C2B	-2.16	1.46	1.50
13	H	1211	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	1119	CLA	CMC-C2C	-2.16	1.46	1.50
13	u	511	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	1111	CLA	CMD-C2D	-2.16	1.46	1.50
13	u	507	CLA	CMD-C2D	-2.16	1.46	1.50
13	q	501	CLA	MG-NB	-2.16	2.01	2.05
13	r	510	CLA	MG-NB	-2.16	2.01	2.05
13	a	519	CLA	CHC-C1C	2.16	1.42	1.38
13	e	1111	CLA	CHC-C1C	2.16	1.42	1.38
13	f	1218	CLA	MG-NB	-2.16	2.01	2.05
13	G	1119	CLA	CMC-C2C	-2.16	1.46	1.50
13	H	1202	CLA	CMD-C2D	-2.16	1.46	1.50
13	Y	512	CLA	CMB-C2B	-2.16	1.46	1.50
13	B	1209	CLA	CHC-C1C	2.16	1.42	1.38
13	3	510	CLA	CHC-C1C	2.16	1.42	1.38
13	G	1134	CLA	CMB-C2B	-2.16	1.46	1.50
13	t	502	CLA	CMB-C2B	-2.16	1.46	1.50
13	v	517	CLA	MG-NB	-2.16	2.01	2.05
13	e	1134	CLA	CHC-C1C	2.16	1.42	1.38
13	4	518	CLA	CMD-C2D	-2.16	1.46	1.50
13	4	519	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1138	CLA	CMC-C2C	-2.16	1.46	1.50
13	Y	517	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1203	CLA	CMC-C2C	-2.16	1.46	1.50
13	r	509	CLA	CMC-C2C	-2.16	1.46	1.50
20	b	822	SQD	O2-C2	-2.16	1.37	1.43
13	B	1207	CLA	CMC-C2C	-2.16	1.46	1.50
13	1	517	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1133	CLA	CMD-C2D	-2.16	1.46	1.50
13	s	519	CLA	CHC-C1C	2.16	1.42	1.38
13	e	1115	CLA	MG-NB	-2.16	2.01	2.05
13	e	1111	CLA	CMD-C2D	-2.16	1.46	1.50
13	s	512	CLA	CMD-C2D	-2.16	1.46	1.50
13	t	508	CLA	CMD-C2D	-2.16	1.46	1.50
13	6	518	CLA	MG-NB	-2.15	2.01	2.05
13	b	511	CLA	MG-NB	-2.15	2.01	2.05
13	H	1209	CLA	CHC-C1C	2.15	1.42	1.38
13	u	501	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1203	CLA	CMD-C2D	-2.15	1.46	1.50
13	f	1225	CLA	CMB-C2B	-2.15	1.46	1.50
13	G	1107	CLA	MG-ND	-2.15	2.01	2.05
13	H	1230	CLA	MG-NB	-2.15	2.01	2.05
17	f	1855	LHG	P-O6	2.15	1.68	1.59
13	5	502	CLA	CMB-C2B	-2.15	1.46	1.50
13	m	1401	CLA	CMC-C2C	-2.15	1.46	1.50
20	6	822	SQD	O4-C4	-2.15	1.37	1.43
20	d	822	SQD	O2-C2	-2.15	1.37	1.43
20	q	822	SQD	O2-C2	-2.15	1.37	1.43
13	f	1229	CLA	C1B-C2B	2.15	1.48	1.43
13	5	508	CLA	MG-NB	-2.15	2.01	2.05
13	e	1112	CLA	MG-NB	-2.15	2.01	2.05
13	T	1302	CLA	CMB-C2B	-2.15	1.46	1.50
13	f	1021	CLA	CMB-C2B	-2.15	1.46	1.50
13	t	519	CLA	CMB-C2B	-2.15	1.46	1.50
13	H	1214	CLA	CHC-C1C	2.15	1.42	1.38
17	n	5218	LHG	P-O6	2.15	1.68	1.59
13	G	1022	CLA	C3B-C4B	2.15	1.47	1.42
13	e	1124	CLA	MG-NB	-2.15	2.01	2.05
13	f	1217	CLA	CMB-C2B	-2.15	1.46	1.50
13	A	1116	CLA	CHC-C1C	2.15	1.42	1.38
13	1	512	CLA	CHC-C1C	2.15	1.42	1.38
14	A	2001	PQN	C10-C1	-2.15	1.44	1.48
13	A	1101	CLA	MG-NB	-2.15	2.01	2.05
13	2	519	CLA	MG-NB	-2.15	2.01	2.05
13	v	502	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1138	CLA	CHC-C1C	2.15	1.42	1.38
13	Y	508	CLA	C1B-C2B	2.15	1.48	1.43
13	A	1112	CLA	MG-NB	-2.15	2.01	2.05
13	q	504	CLA	MG-NB	-2.15	2.01	2.05
13	B	1211	CLA	CMC-C2C	-2.15	1.46	1.50
13	1	508	CLA	CMD-C2D	-2.15	1.46	1.50
13	3	503	CLA	CMD-C2D	-2.15	1.46	1.50
13	m	1103	CLA	CMD-C2D	-2.15	1.46	1.50
13	r	509	CLA	CMB-C2B	-2.15	1.46	1.50
13	t	508	CLA	CMC-C2C	-2.15	1.46	1.50
13	U	1105	CLA	C3C-C2C	2.15	1.41	1.36
13	A	1138	CLA	CMB-C2B	-2.15	1.46	1.50
13	G	1138	CLA	CMB-C2B	-2.15	1.46	1.50
13	b	519	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	1202	CLA	CMC-C2C	-2.15	1.46	1.50
13	6	511	CLA	CMB-C2B	-2.15	1.46	1.50
13	f	1239	CLA	CMD-C2D	-2.15	1.46	1.50
13	t	519	CLA	CMD-C2D	-2.15	1.46	1.50
13	G	1140	CLA	CHC-C1C	2.15	1.42	1.38
13	H	1212	CLA	CMB-C2B	-2.15	1.46	1.50
13	H	1236	CLA	CMB-C2B	-2.15	1.46	1.50
13	R	1301	CLA	CMD-C2D	-2.15	1.46	1.50
13	f	1208	CLA	CMD-C2D	-2.15	1.46	1.50
13	f	1235	CLA	CMD-C2D	-2.15	1.46	1.50
13	H	1207	CLA	MG-NB	-2.15	2.01	2.05
13	d	518	CLA	MG-NB	-2.15	2.01	2.05
13	G	1129	CLA	C3B-C4B	2.15	1.47	1.42
13	B	1203	CLA	C1B-C2B	2.15	1.48	1.43
13	G	1110	CLA	CMC-C2C	-2.15	1.46	1.50
13	d	502	CLA	MG-NB	-2.15	2.01	2.05
13	a	516	CLA	CHC-C1C	2.15	1.42	1.38
20	c	822	SQD	O2-C2	-2.15	1.37	1.43
17	V	5218	LHG	P-O6	2.15	1.68	1.59
13	5	507	CLA	CMD-C2D	-2.15	1.46	1.50
13	G	1113	CLA	CMC-C2C	-2.15	1.46	1.50
13	H	1224	CLA	CMB-C2B	-2.15	1.46	1.50
13	f	1205	CLA	MG-ND	-2.15	2.01	2.05
13	s	516	CLA	CHC-C1C	2.15	1.42	1.38
13	H	1203	CLA	CMD-C2D	-2.15	1.46	1.50
20	a	822	SQD	O3-C3	-2.15	1.37	1.43
13	A	1108	CLA	CMD-C2D	-2.15	1.46	1.50
13	5	511	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V	1502	CLA	CMC-C2C	-2.15	1.46	1.50
13	c	511	CLA	CMB-C2B	-2.15	1.46	1.50
13	A	1118	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	1239	CLA	CMD-C2D	-2.15	1.46	1.50
13	G	1105	CLA	CMB-C2B	-2.15	1.46	1.50
13	s	506	CLA	CMC-C2C	-2.15	1.46	1.50
13	B	1228	CLA	C1B-C2B	2.15	1.48	1.43
13	5	504	CLA	MG-NB	-2.15	2.01	2.05
13	a	504	CLA	CHC-C1C	2.15	1.42	1.38
13	A	1129	CLA	C3B-C4B	2.15	1.47	1.42
13	A	1105	CLA	CMB-C2B	-2.15	1.46	1.50
13	A	1134	CLA	CMB-C2B	-2.15	1.46	1.50
13	G	1124	CLA	CMB-C2B	-2.15	1.46	1.50
13	v	518	CLA	CMD-C2D	-2.15	1.46	1.50
13	H	1223	CLA	C1B-NB	-2.15	1.35	1.37
13	A	1124	CLA	CMB-C2B	-2.15	1.46	1.50
13	a	506	CLA	CMC-C2C	-2.15	1.46	1.50
13	d	511	CLA	CMB-C2B	-2.15	1.46	1.50
13	e	1105	CLA	CMB-C2B	-2.15	1.46	1.50
13	s	503	CLA	CHC-C1C	2.15	1.42	1.38
13	Z	518	CLA	MG-NB	-2.15	2.01	2.05
20	6	822	SQD	O2-C2	-2.15	1.37	1.43
17	L	5218	LHG	P-O6	2.15	1.68	1.59
17	B	1855	LHG	P-O6	2.15	1.68	1.59
13	A	1105	CLA	MG-NB	-2.15	2.01	2.05
13	G	1115	CLA	MG-NB	-2.15	2.01	2.05
13	B	1209	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	1236	CLA	CMB-C2B	-2.15	1.46	1.50
13	4	502	CLA	CMB-C2B	-2.15	1.46	1.50
13	H	1234	CLA	CMC-C2C	-2.15	1.46	1.50
13	t	505	CLA	CMD-C2D	-2.15	1.46	1.50
20	b	822	SQD	O3-C3	-2.15	1.37	1.43
13	G	1138	CLA	CHC-C1C	2.15	1.42	1.38
13	J	1302	CLA	CMD-C2D	-2.15	1.46	1.50
13	H	1239	CLA	CMD-C2D	-2.15	1.46	1.50
13	e	1118	CLA	CMB-C2B	-2.15	1.46	1.50
13	f	1224	CLA	CMB-C2B	-2.15	1.46	1.50
17	H	1855	LHG	P-O6	2.15	1.68	1.59
13	5	501	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1208	CLA	MG-NB	-2.15	2.01	2.05
13	H	1218	CLA	MG-NB	-2.15	2.01	2.05
13	Y	505	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1138	CLA	CMC-C2C	-2.15	1.46	1.50
13	f	1203	CLA	C1B-NB	-2.14	1.35	1.37
13	B	1207	CLA	CMB-C2B	-2.14	1.46	1.50
13	F	1301	CLA	CMD-C2D	-2.14	1.46	1.50
13	G	1105	CLA	CMC-C2C	-2.14	1.46	1.50
13	e	1134	CLA	CMD-C2D	-2.14	1.46	1.50
13	f	1201	CLA	CMC-C2C	-2.14	1.46	1.50
13	2	504	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	503	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	506	CLA	CMB-C2B	-2.14	1.46	1.50
13	B	1207	CLA	MG-NB	-2.14	2.01	2.05
13	Z	505	CLA	MG-NB	-2.14	2.01	2.05
13	e	1110	CLA	MG-NB	-2.14	2.01	2.05
13	B	1203	CLA	C1B-NB	-2.14	1.35	1.37
13	H	1213	CLA	CMC-C2C	-2.14	1.46	1.50
13	f	1216	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	1208	CLA	CMD-C2D	-2.14	1.46	1.50
13	Z	519	CLA	CMB-C2B	-2.14	1.46	1.50
13	e	1134	CLA	CMB-C2B	-2.14	1.46	1.50
13	s	512	CLA	CMB-C2B	-2.14	1.46	1.50
13	A	1110	CLA	MG-NB	-2.14	2.01	2.05
13	2	505	CLA	MG-NB	-2.14	2.01	2.05
13	v	519	CLA	MG-NB	-2.14	2.01	2.05
14	A	2001	PQN	C5-C4	-2.14	1.44	1.48
13	A	1110	CLA	CMB-C2B	-2.14	1.46	1.50
13	1	512	CLA	CMB-C2B	-2.14	1.46	1.50
13	f	1209	CLA	CMB-C2B	-2.14	1.46	1.50
13	r	519	CLA	MG-NB	-2.14	2.01	2.05
13	G	1136	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	1117	CLA	C1B-NB	-2.14	1.35	1.37
13	u	505	CLA	CHC-C1C	2.14	1.42	1.38
13	d	512	CLA	MG-NB	-2.14	2.01	2.05
13	H	1203	CLA	C1B-C2B	2.14	1.48	1.43
13	s	503	CLA	CMD-C2D	-2.14	1.46	1.50
13	5	512	CLA	CHC-C1C	2.14	1.42	1.38
16	H	4010	BCR	C21-C22	-2.14	1.32	1.35
13	B	1203	CLA	CMC-C2C	-2.14	1.46	1.50
13	B	1206	CLA	CMC-C2C	-2.14	1.46	1.50
13	e	1124	CLA	CMB-C2B	-2.14	1.46	1.50
13	r	504	CLA	CMD-C2D	-2.14	1.46	1.50
13	3	504	CLA	CHC-C1C	2.14	1.42	1.38
13	f	1214	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1224	CLA	MG-NB	-2.14	2.01	2.05
13	f	1231	CLA	CMC-C2C	-2.14	1.46	1.50
13	c	506	CLA	CHC-C1C	2.14	1.42	1.38
13	B	1021	CLA	CMB-C2B	-2.14	1.46	1.50
13	2	509	CLA	CMB-C2B	-2.14	1.46	1.50
20	v	822	SQD	O2-C2	-2.14	1.37	1.43
13	1	513	CLA	CHC-C1C	2.14	1.42	1.38
13	3	511	CLA	CHC-C1C	2.14	1.42	1.38
13	6	517	CLA	MG-NB	-2.14	2.01	2.05
13	V	1501	CLA	CMC-C2C	-2.14	1.46	1.50
13	e	1136	CLA	CMB-C2B	-2.14	1.46	1.50
13	f	1218	CLA	CMD-C2D	-2.14	1.46	1.50
13	u	502	CLA	CMB-C2B	-2.14	1.46	1.50
13	6	517	CLA	CHC-C1C	2.14	1.42	1.38
13	A	1107	CLA	MG-ND	-2.14	2.01	2.05
13	B	1218	CLA	MG-NB	-2.14	2.01	2.05
13	Y	504	CLA	MG-NB	-2.14	2.01	2.05
20	4	822	SQD	O3-C3	-2.14	1.37	1.43
13	e	1132	CLA	CMB-C2B	-2.14	1.46	1.50
13	G	1134	CLA	CHC-C1C	2.14	1.42	1.38
13	a	503	CLA	CHC-C1C	2.14	1.42	1.38
13	u	503	CLA	CHC-C1C	2.14	1.42	1.38
13	B	1202	CLA	C1B-NB	-2.14	1.35	1.37
13	e	1107	CLA	MG-ND	-2.14	2.01	2.05
13	Z	518	CLA	CMD-C2D	-2.14	1.46	1.50
13	e	1108	CLA	CMD-C2D	-2.14	1.46	1.50
13	e	1138	CLA	CMC-C2C	-2.14	1.46	1.50
13	2	509	CLA	CMC-C2C	-2.14	1.46	1.50
13	u	506	CLA	CHC-C1C	2.14	1.42	1.38
13	2	517	CLA	CMD-C2D	-2.14	1.46	1.50
13	f	1228	CLA	C1B-C2B	2.14	1.48	1.43
13	L	1502	CLA	CMC-C2C	-2.14	1.46	1.50
13	f	1222	CLA	CMC-C2C	-2.14	1.46	1.50
13	r	519	CLA	CMC-C2C	-2.14	1.46	1.50
13	Z	519	CLA	MG-NB	-2.14	2.01	2.05
13	f	1207	CLA	MG-NB	-2.14	2.01	2.05
13	r	505	CLA	MG-NB	-2.14	2.01	2.05
13	f	1202	CLA	C1B-NB	-2.14	1.35	1.37
20	b	822	SQD	O4-C4	-2.14	1.37	1.43
20	t	822	SQD	O3-C3	-2.14	1.37	1.43
13	2	518	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	508	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	518	CLA	CMD-C2D	-2.14	1.46	1.50
13	e	1120	CLA	CMD-C2D	-2.14	1.46	1.50
13	G	1237	CLA	MG-NB	-2.14	2.01	2.05
13	H	1208	CLA	MG-NB	-2.14	2.01	2.05
13	Y	513	CLA	MG-NB	-2.14	2.01	2.05
13	e	1120	CLA	C1B-NB	-2.14	1.35	1.37
13	G	1117	CLA	CMD-C2D	-2.14	1.46	1.50
13	Z	517	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	1132	CLA	CMC-C2C	-2.14	1.46	1.50
13	4	508	CLA	CMD-C2D	-2.14	1.46	1.50
13	q	503	CLA	CMD-C2D	-2.14	1.46	1.50
20	3	822	SQD	O3-C3	-2.14	1.37	1.43
20	v	822	SQD	O4-C4	-2.14	1.37	1.43
16	B	4010	BCR	C21-C22	-2.14	1.33	1.35
13	Z	510	CLA	MG-NB	-2.14	2.01	2.05
13	a	518	CLA	CMD-C2D	-2.13	1.46	1.50
13	f	1202	CLA	MG-NB	-2.13	2.01	2.05
13	u	512	CLA	CHC-C1C	2.13	1.42	1.38
13	r	508	CLA	C1B-C2B	2.13	1.48	1.43
13	v	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	3	506	CLA	MG-NB	-2.13	2.01	2.05
14	e	2001	PQN	C10-C1	-2.13	1.44	1.48
13	5	511	CLA	CHC-C1C	2.13	1.42	1.38
13	u	511	CLA	CHC-C1C	2.13	1.42	1.38
13	v	517	CLA	CHC-C1C	2.13	1.42	1.38
13	f	1203	CLA	C1B-C2B	2.13	1.48	1.43
13	s	507	CLA	MG-NB	-2.13	2.01	2.05
20	s	822	SQD	O3-C3	-2.13	1.38	1.43
13	Y	513	CLA	CHC-C1C	2.13	1.42	1.38
13	a	508	CLA	CMD-C2D	-2.13	1.46	1.50
13	d	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	q	507	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	1135	CLA	C4B-NB	2.13	1.40	1.37
13	Z	504	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	502	CLA	CMD-C2D	-2.13	1.46	1.50
13	q	517	CLA	CMD-C2D	-2.13	1.46	1.50
13	t	506	CLA	CMB-C2B	-2.13	1.46	1.50
13	v	512	CLA	CMD-C2D	-2.13	1.46	1.50
13	5	506	CLA	MG-NB	-2.13	2.01	2.05
13	G	1111	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	1136	CLA	CMB-C2B	-2.13	1.46	1.50
13	s	518	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	511	CLA	CHC-C1C	2.13	1.42	1.38
13	e	1110	CLA	CMB-C2B	-2.13	1.46	1.50
13	f	1236	CLA	CMB-C2B	-2.13	1.46	1.50
13	F	1302	CLA	MG-NB	-2.13	2.01	2.05
13	H	1210	CLA	MG-NB	-2.13	2.01	2.05
13	u	518	CLA	MG-NB	-2.13	2.01	2.05
13	v	509	CLA	MG-NB	-2.13	2.01	2.05
13	b	508	CLA	CMC-C2C	-2.13	1.46	1.50
13	e	1130	CLA	CMC-C2C	-2.13	1.46	1.50
13	f	1222	CLA	C1B-C2B	2.13	1.48	1.43
13	H	1202	CLA	MG-NB	-2.13	2.01	2.05
13	e	1131	CLA	MG-NB	-2.13	2.01	2.05
13	f	1236	CLA	MG-NB	-2.13	2.01	2.05
13	q	517	CLA	MG-NB	-2.13	2.01	2.05
13	A	1113	CLA	MG-NB	-2.13	2.01	2.05
13	d	504	CLA	MG-NB	-2.13	2.01	2.05
13	j	1302	CLA	MG-NB	-2.13	2.01	2.05
13	3	508	CLA	CMD-C2D	-2.13	1.46	1.50
13	c	511	CLA	CHC-C1C	2.13	1.42	1.38
14	e	2001	PQN	C5-C4	-2.13	1.44	1.48
13	A	1135	CLA	C4B-NB	2.13	1.40	1.37
13	2	510	CLA	MG-NB	-2.13	2.01	2.05
13	e	1132	CLA	CMC-C2C	-2.13	1.46	1.50
13	r	517	CLA	CMD-C2D	-2.13	1.46	1.50
20	B	1852	SQD	O4-C4	-2.13	1.38	1.43
13	Z	501	CLA	CMB-C2B	-2.13	1.46	1.50
13	6	519	CLA	MG-NB	-2.13	2.01	2.05
13	v	501	CLA	MG-NB	-2.13	2.01	2.05
13	e	1129	CLA	C3B-C4B	2.13	1.47	1.42
13	e	1119	CLA	C1B-NB	-2.13	1.35	1.37
13	H	1221	CLA	CMB-C2B	-2.13	1.46	1.50
13	Y	504	CLA	CMB-C2B	-2.13	1.46	1.50
13	B	1204	CLA	MG-ND	-2.13	2.01	2.05
13	2	516	CLA	MG-NB	-2.13	2.01	2.05
13	f	1209	CLA	CHC-C1C	2.13	1.42	1.38
13	m	1105	CLA	C3C-C2C	2.13	1.41	1.36
13	G	1102	CLA	CMB-C2B	-2.13	1.46	1.50
13	q	508	CLA	CMD-C2D	-2.13	1.46	1.50
13	5	502	CLA	MG-NB	-2.13	2.01	2.05
13	G	1113	CLA	MG-NB	-2.13	2.01	2.05
13	t	507	CLA	MG-NB	-2.13	2.01	2.05
13	B	1210	CLA	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	501	CLA	CHC-C1C	2.13	1.42	1.38
13	3	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	d	512	CLA	CMD-C2D	-2.13	1.46	1.50
13	e	1130	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	1119	CLA	C1B-NB	-2.13	1.35	1.37
17	V	5221	LHG	P-O6	2.13	1.67	1.59
13	2	518	CLA	MG-NB	-2.13	2.01	2.05
13	a	513	CLA	MG-NB	-2.13	2.01	2.05
13	d	511	CLA	MG-NB	-2.13	2.01	2.05
13	Z	511	CLA	CHC-C1C	2.13	1.42	1.38
13	H	1217	CLA	CMB-C2B	-2.13	1.46	1.50
13	d	517	CLA	CHC-C1C	2.13	1.42	1.38
13	Y	508	CLA	CMD-C2D	-2.13	1.46	1.50
13	2	508	CLA	C1B-C2B	2.13	1.48	1.43
13	A	1115	CLA	MG-NB	-2.13	2.01	2.05
13	a	506	CLA	MG-NB	-2.13	2.01	2.05
13	c	507	CLA	CMD-C2D	-2.13	1.46	1.50
13	q	517	CLA	CHC-C1C	2.13	1.42	1.38
13	A	1131	CLA	MG-NB	-2.13	2.01	2.05
13	G	1117	CLA	C1B-NB	-2.13	1.35	1.37
13	A	1105	CLA	CMC-C2C	-2.13	1.46	1.50
13	G	1126	CLA	CHC-C1C	2.13	1.42	1.38
13	r	518	CLA	MG-NB	-2.13	2.01	2.05
13	3	518	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	v	502	CLA	MG-NB	-2.13	2.01	2.05
13	e	1237	CLA	CMC-C2C	-2.13	1.46	1.50
13	s	508	CLA	CMC-C2C	-2.13	1.46	1.50
13	b	501	CLA	CHC-C1C	2.12	1.42	1.38
13	A	1130	CLA	CMC-C2C	-2.12	1.46	1.50
13	5	511	CLA	CMD-C2D	-2.12	1.46	1.50
13	G	1102	CLA	CMC-C2C	-2.12	1.46	1.50
13	Z	508	CLA	C1B-C2B	2.12	1.48	1.43
13	t	512	CLA	CMD-C2D	-2.12	1.46	1.50
13	r	504	CLA	CHC-C1C	2.12	1.42	1.38
13	G	1013	CLA	MG-ND	-2.12	2.01	2.05
13	a	507	CLA	MG-NB	-2.12	2.01	2.05
13	G	1139	CLA	CMB-C2B	-2.12	1.46	1.50
13	H	1218	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	1131	CLA	CMB-C2B	-2.12	1.46	1.50
13	c	505	CLA	CHC-C1C	2.12	1.42	1.38
13	6	504	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1203	CLA	MG-ND	-2.12	2.01	2.05
13	B	1218	CLA	CMD-C2D	-2.12	1.46	1.50
13	5	506	CLA	CHC-C1C	2.12	1.42	1.38
13	c	512	CLA	CHC-C1C	2.12	1.42	1.38
13	V	1501	CLA	MG-NB	-2.12	2.01	2.05
13	4	512	CLA	CMD-C2D	-2.12	1.46	1.50
20	f	1852	SQD	O4-C4	-2.12	1.38	1.43
13	1	508	CLA	C1B-C2B	2.12	1.48	1.43
13	3	503	CLA	CHC-C1C	2.12	1.42	1.38
13	6	518	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	1105	CLA	CMC-C2C	-2.12	1.46	1.50
13	q	501	CLA	CMB-C2B	-2.12	1.46	1.50
13	s	509	CLA	CMD-C2D	-2.12	1.46	1.50
13	q	516	CLA	MG-NB	-2.12	2.01	2.05
13	K	1105	CLA	C3C-C2C	2.12	1.41	1.36
13	G	1124	CLA	CHC-C1C	2.12	1.42	1.38
13	B	1222	CLA	CMC-C2C	-2.12	1.46	1.50
13	A	1013	CLA	MG-ND	-2.12	2.01	2.05
13	B	1205	CLA	MG-ND	-2.12	2.01	2.05
13	1	513	CLA	MG-NB	-2.12	2.01	2.05
13	e	1124	CLA	CHC-C1C	2.12	1.42	1.38
13	B	1217	CLA	CMB-C2B	-2.12	1.46	1.50
13	1	501	CLA	CMB-C2B	-2.12	1.46	1.50
16	f	4010	BCR	C21-C22	-2.12	1.33	1.35
13	G	1126	CLA	C1B-C2B	2.12	1.48	1.43
13	q	513	CLA	CHC-C1C	2.12	1.42	1.38
13	G	1115	CLA	CMD-C2D	-2.12	1.46	1.50
13	6	502	CLA	MG-NB	-2.12	2.01	2.05
13	G	1110	CLA	MG-NB	-2.12	2.01	2.05
13	H	1238	CLA	C1B-NB	-2.12	1.35	1.37
13	H	1228	CLA	CMC-C2C	-2.12	1.46	1.50
13	e	1117	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	1801	CLA	CMB-C2B	-2.12	1.46	1.50
13	c	502	CLA	CHC-C1C	2.12	1.42	1.38
13	A	1119	CLA	C1B-NB	-2.12	1.35	1.37
13	a	511	CLA	MG-NB	-2.12	2.01	2.05
13	s	513	CLA	MG-NB	-2.12	2.01	2.05
13	u	506	CLA	MG-NB	-2.12	2.01	2.05
13	G	1130	CLA	CMC-C2C	-2.12	1.46	1.50
13	4	501	CLA	CHC-C1C	2.12	1.42	1.38
13	B	1224	CLA	MG-NB	-2.12	2.01	2.05
13	B	1225	CLA	MG-ND	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1105	CLA	MG-NB	-2.12	2.01	2.05
13	b	507	CLA	MG-NB	-2.12	2.01	2.05
13	c	510	CLA	MG-NB	-2.12	2.01	2.05
13	e	1011	CLA	MG-NB	-2.12	2.01	2.05
13	H	1203	CLA	C1B-NB	-2.12	1.35	1.37
13	A	1801	CLA	CMB-C2B	-2.12	1.46	1.50
13	4	506	CLA	CMB-C2B	-2.12	1.46	1.50
13	f	1220	CLA	CMB-C2B	-2.12	1.46	1.50
13	B	1229	CLA	C1B-C2B	2.12	1.48	1.43
13	3	507	CLA	MG-NB	-2.12	2.01	2.05
13	n	1502	CLA	CMC-C2C	-2.12	1.46	1.50
13	s	508	CLA	CMD-C2D	-2.12	1.46	1.50
13	1	516	CLA	MG-NB	-2.12	2.01	2.05
13	f	1208	CLA	MG-NB	-2.12	2.01	2.05
13	f	1210	CLA	MG-NB	-2.12	2.01	2.05
13	f	1225	CLA	MG-ND	-2.12	2.01	2.05
13	1	507	CLA	CMD-C2D	-2.12	1.46	1.50
13	G	1125	CLA	CHC-C1C	2.12	1.42	1.38
13	v	511	CLA	MG-NB	-2.12	2.01	2.05
13	G	1103	CLA	CMB-C2B	-2.12	1.46	1.50
13	r	518	CLA	CMB-C2B	-2.12	1.46	1.50
13	A	1124	CLA	CHC-C1C	2.12	1.42	1.38
13	c	506	CLA	MG-NB	-2.12	2.01	2.05
13	a	510	CLA	CMD-C2D	-2.12	1.46	1.50
13	f	1212	CLA	CMB-C2B	-2.12	1.46	1.50
13	4	503	CLA	CHC-C1C	2.12	1.42	1.38
13	t	511	CLA	CHC-C1C	2.12	1.42	1.38
13	H	1202	CLA	C1B-NB	-2.12	1.35	1.37
13	e	1013	CLA	MG-ND	-2.12	2.01	2.05
13	H	1222	CLA	CMB-C2B	-2.12	1.46	1.50
13	b	502	CLA	CMB-C2B	-2.12	1.46	1.50
13	B	1214	CLA	CHC-C1C	2.12	1.42	1.38
13	s	511	CLA	CHC-C1C	2.12	1.42	1.38
13	q	508	CLA	C1B-C2B	2.12	1.48	1.43
13	L	1501	CLA	MG-NB	-2.12	2.01	2.05
13	4	507	CLA	MG-NB	-2.12	2.01	2.05
13	A	1237	CLA	CMC-C2C	-2.12	1.46	1.50
13	V	1503	CLA	CHC-C1C	2.11	1.42	1.38
13	e	1140	CLA	CHC-C1C	2.11	1.42	1.38
13	H	1222	CLA	CMC-C2C	-2.11	1.46	1.50
13	d	518	CLA	CMD-C2D	-2.11	1.46	1.50
13	Y	516	CLA	MG-NB	-2.11	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1112	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	1112	CLA	CMD-C2D	-2.11	1.46	1.50
13	t	502	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1203	CLA	MG-ND	-2.11	2.01	2.05
13	3	513	CLA	MG-NB	-2.11	2.01	2.05
17	n	5221	LHG	P-O6	2.11	1.67	1.59
13	s	504	CLA	CHC-C1C	2.11	1.42	1.38
13	A	1120	CLA	CMB-C2B	-2.11	1.46	1.50
13	3	511	CLA	CMD-C2D	-2.11	1.46	1.50
13	G	1118	CLA	CMB-C2B	-2.11	1.46	1.50
13	Z	509	CLA	CMC-C2C	-2.11	1.46	1.50
13	q	519	CLA	CMD-C2D	-2.11	1.46	1.50
13	H	1229	CLA	C1B-C2B	2.11	1.48	1.43
13	e	1126	CLA	C1B-C2B	2.11	1.48	1.43
13	Z	504	CLA	MG-NB	-2.11	2.01	2.05
13	d	506	CLA	MG-NB	-2.11	2.01	2.05
13	2	504	CLA	CHC-C1C	2.11	1.42	1.38
20	d	822	SQD	O3-C3	-2.11	1.38	1.43
13	A	1117	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1212	CLA	CMB-C2B	-2.11	1.46	1.50
13	H	1203	CLA	MG-ND	-2.11	2.01	2.05
13	c	517	CLA	MG-NB	-2.11	2.01	2.05
13	d	517	CLA	MG-NB	-2.11	2.01	2.05
20	4	822	SQD	O4-C4	-2.11	1.38	1.43
13	K	1401	CLA	CMC-C2C	-2.11	1.46	1.50
13	2	511	CLA	CHC-C1C	2.11	1.42	1.38
13	2	519	CLA	CMB-C2B	-2.11	1.46	1.50
13	Y	517	CLA	MG-NB	-2.11	2.01	2.05
13	6	509	CLA	CMD-C2D	-2.11	1.46	1.50
13	2	519	CLA	CMC-C2C	-2.11	1.46	1.50
13	r	518	CLA	CMD-C2D	-2.11	1.46	1.50
20	H	1852	SQD	O4-C4	-2.11	1.38	1.43
17	L	5221	LHG	P-O6	2.11	1.67	1.59
13	6	501	CLA	MG-NB	-2.11	2.01	2.05
13	5	501	CLA	CMC-C2C	-2.11	1.46	1.50
13	Z	519	CLA	CMC-C2C	-2.11	1.46	1.50
13	a	508	CLA	CMC-C2C	-2.11	1.46	1.50
13	B	1226	CLA	C3B-C4B	2.11	1.47	1.42
13	A	1140	CLA	CHC-C1C	2.11	1.42	1.38
13	H	1229	CLA	CMD-C2D	-2.11	1.46	1.50
13	l	1302	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1202	CLA	MG-NB	-2.11	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	517	CLA	MG-NB	-2.11	2.01	2.05
13	e	1108	CLA	CHC-C1C	2.11	1.42	1.38
13	c	503	CLA	CHC-C1C	2.11	1.42	1.38
20	t	822	SQD	O4-C4	-2.11	1.38	1.43
13	A	1011	CLA	MG-NB	-2.11	2.01	2.05
13	3	511	CLA	MG-NB	-2.11	2.01	2.05
13	A	1115	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1228	CLA	CMC-C2C	-2.11	1.46	1.50
13	c	518	CLA	CMB-C2B	-2.11	1.46	1.50
20	u	822	SQD	O4-C4	-2.11	1.38	1.43
13	Z	509	CLA	CMD-C2D	-2.11	1.46	1.50
13	u	502	CLA	CMD-C2D	-2.11	1.46	1.50
13	6	511	CLA	MG-NB	-2.11	2.01	2.05
13	B	1223	CLA	C1B-NB	-2.11	1.35	1.37
13	A	1114	CLA	CMD-C2D	-2.11	1.46	1.50
13	H	1208	CLA	CMD-C2D	-2.11	1.46	1.50
13	Y	501	CLA	CMB-C2B	-2.11	1.46	1.50
13	Z	513	CLA	CMB-C2B	-2.11	1.46	1.50
13	e	1102	CLA	CMC-C2C	-2.11	1.46	1.50
13	r	519	CLA	CMB-C2B	-2.11	1.46	1.50
13	c	502	CLA	MG-NB	-2.11	2.01	2.05
13	G	1115	CLA	CMB-C2B	-2.11	1.46	1.50
13	c	512	CLA	CMB-C2B	-2.11	1.46	1.50
13	e	1139	CLA	CMB-C2B	-2.11	1.46	1.50
20	6	822	SQD	O3-C3	-2.11	1.38	1.43
13	r	511	CLA	CHC-C1C	2.11	1.42	1.38
13	G	1114	CLA	CMD-C2D	-2.11	1.46	1.50
13	r	504	CLA	MG-NB	-2.11	2.01	2.05
13	r	513	CLA	MG-NB	-2.11	2.01	2.05
13	1	517	CLA	CHC-C1C	2.11	1.42	1.38
13	b	511	CLA	CHC-C1C	2.11	1.42	1.38
13	B	1227	CLA	CMD-C2D	-2.11	1.46	1.50
13	U	1105	CLA	CMB-C2B	-2.11	1.46	1.50
13	u	518	CLA	CMB-C2B	-2.11	1.46	1.50
13	G	1107	CLA	C1B-NB	-2.11	1.35	1.37
13	e	1126	CLA	CHC-C1C	2.11	1.42	1.38
13	f	1228	CLA	CMC-C2C	-2.10	1.46	1.50
13	H	1204	CLA	MG-ND	-2.10	2.01	2.05
13	d	510	CLA	MG-NB	-2.10	2.01	2.05
13	e	1109	CLA	MG-NB	-2.10	2.01	2.05
13	B	1220	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	513	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	508	CLA	CMC-C2C	-2.10	1.46	1.50
13	a	507	CLA	CMD-C2D	-2.10	1.46	1.50
13	s	518	CLA	CMD-C2D	-2.10	1.46	1.50
13	5	510	CLA	MG-NB	-2.10	2.01	2.05
20	v	822	SQD	O3-C3	-2.10	1.38	1.43
13	A	1112	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	512	CLA	CMD-C2D	-2.10	1.46	1.50
13	c	501	CLA	CMC-C2C	-2.10	1.46	1.50
13	e	1115	CLA	CMD-C2D	-2.10	1.46	1.50
13	Z	506	CLA	CHC-C1C	2.10	1.42	1.38
13	2	504	CLA	MG-NB	-2.10	2.01	2.05
13	3	518	CLA	MG-NB	-2.10	2.01	2.05
13	U	1105	CLA	MG-NB	-2.10	2.01	2.05
13	B	1222	CLA	C1B-C2B	2.10	1.48	1.43
13	B	1238	CLA	C1B-NB	-2.10	1.35	1.37
13	3	518	CLA	CMB-C2B	-2.10	1.46	1.50
13	f	1226	CLA	C3B-C4B	2.10	1.47	1.42
13	A	1126	CLA	CHC-C1C	2.10	1.42	1.38
13	5	503	CLA	CHC-C1C	2.10	1.42	1.38
13	u	513	CLA	MG-NB	-2.10	2.01	2.05
13	A	1102	CLA	CMC-C2C	-2.10	1.46	1.50
13	4	502	CLA	CMD-C2D	-2.10	1.46	1.50
13	r	506	CLA	CHC-C1C	2.10	1.42	1.38
13	B	1217	CLA	MG-ND	-2.10	2.01	2.05
13	H	1218	CLA	CMB-C2B	-2.10	1.46	1.50
13	3	517	CLA	CHC-C1C	2.10	1.42	1.38
13	A	1120	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	1237	CLA	CMC-C2C	-2.10	1.46	1.50
13	e	1114	CLA	CMD-C2D	-2.10	1.46	1.50
13	Y	517	CLA	CHC-C1C	2.10	1.42	1.38
13	t	501	CLA	CHC-C1C	2.10	1.42	1.38
13	s	506	CLA	MG-NB	-2.10	2.01	2.05
16	G	4008	BCR	C10-C9	-2.10	1.33	1.35
13	Y	507	CLA	CMD-C2D	-2.10	1.46	1.50
13	Z	509	CLA	CMB-C2B	-2.10	1.46	1.50
13	r	501	CLA	CMB-C2B	-2.10	1.46	1.50
13	u	512	CLA	CMD-C2D	-2.10	1.46	1.50
13	Z	511	CLA	MG-NB	-2.10	2.01	2.05
13	v	505	CLA	MG-NB	-2.10	2.01	2.05
13	c	511	CLA	CMD-C2D	-2.10	1.46	1.50
13	f	1222	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	518	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1126	CLA	C1B-C2B	2.10	1.48	1.43
13	6	506	CLA	MG-NB	-2.10	2.01	2.05
13	G	1101	CLA	MG-NB	-2.10	2.01	2.05
13	2	508	CLA	CMD-C2D	-2.10	1.46	1.50
13	u	508	CLA	CMD-C2D	-2.10	1.46	1.50
13	2	509	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	1801	CLA	CMB-C2B	-2.10	1.46	1.50
13	B	1236	CLA	MG-NB	-2.10	2.01	2.05
13	u	510	CLA	MG-NB	-2.10	2.01	2.05
13	A	1139	CLA	CMB-C2B	-2.10	1.46	1.50
13	5	508	CLA	CMC-C2C	-2.10	1.46	1.50
13	f	1227	CLA	CMC-C2C	-2.10	1.46	1.50
13	r	516	CLA	MG-NB	-2.10	2.01	2.05
13	b	503	CLA	CHC-C1C	2.10	1.42	1.38
13	B	1222	CLA	CMB-C2B	-2.10	1.46	1.50
13	6	512	CLA	CMD-C2D	-2.10	1.46	1.50
13	H	1204	CLA	CMC-C2C	-2.10	1.46	1.50
13	4	511	CLA	CHC-C1C	2.10	1.42	1.38
13	c	512	CLA	CMD-C2D	-2.10	1.46	1.50
13	u	501	CLA	CMC-C2C	-2.10	1.46	1.50
13	G	1011	CLA	MG-NB	-2.10	2.01	2.05
13	H	1224	CLA	MG-NB	-2.10	2.01	2.05
13	e	1119	CLA	MG-ND	-2.10	2.01	2.05
13	e	1101	CLA	MG-NB	-2.10	2.01	2.05
13	s	510	CLA	MG-NB	-2.10	2.01	2.05
13	A	1130	CLA	CMD-C2D	-2.10	1.46	1.50
13	f	1012	CLA	CMB-C2B	-2.10	1.46	1.50
13	q	516	CLA	CMD-C2D	-2.10	1.46	1.50
13	v	504	CLA	MG-NB	-2.10	2.01	2.05
13	t	503	CLA	CHC-C1C	2.10	1.42	1.38
13	B	1012	CLA	CMB-C2B	-2.10	1.46	1.50
13	H	1222	CLA	CMD-C2D	-2.10	1.46	1.50
13	q	504	CLA	CMB-C2B	-2.10	1.46	1.50
13	A	1103	CLA	CMB-C2B	-2.10	1.46	1.50
13	A	1136	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	501	CLA	CMB-C2B	-2.10	1.46	1.50
13	5	508	CLA	CMD-C2D	-2.10	1.46	1.50
13	e	1121	CLA	CMC-C2C	-2.10	1.46	1.50
13	5	505	CLA	CHC-C1C	2.10	1.42	1.38
13	a	519	CLA	MG-NB	-2.10	2.01	2.05
13	u	517	CLA	MG-NB	-2.10	2.01	2.05
13	H	1205	CLA	MG-ND	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	1105	CLA	MG-NB	-2.10	2.01	2.05
13	L	1501	CLA	CMC-C2C	-2.10	1.46	1.50
13	c	504	CLA	CHC-C1C	2.10	1.42	1.38
13	s	517	CLA	CHC-C1C	2.10	1.42	1.38
13	6	508	CLA	CMD-C2D	-2.10	1.46	1.50
13	m	1105	CLA	CMB-C2B	-2.10	1.46	1.50
13	b	517	CLA	CHC-C1C	2.10	1.42	1.38
13	A	1109	CLA	MG-NB	-2.10	2.01	2.05
13	e	1113	CLA	MG-NB	-2.10	2.01	2.05
13	f	1238	CLA	C1B-NB	-2.10	1.35	1.37
13	K	1105	CLA	CMB-C2B	-2.10	1.46	1.50
13	H	1227	CLA	CMC-C2C	-2.10	1.46	1.50
13	n	1501	CLA	MG-NB	-2.09	2.01	2.05
13	Z	512	CLA	CMB-C2B	-2.09	1.46	1.50
13	c	502	CLA	CMD-C2D	-2.09	1.46	1.50
13	t	507	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	1213	CLA	CHC-C1C	2.09	1.42	1.38
13	A	1135	CLA	C1B-NB	-2.09	1.35	1.37
13	3	519	CLA	MG-NB	-2.09	2.01	2.05
13	f	1240	CLA	CMB-C2B	-2.09	1.46	1.50
13	s	510	CLA	CMD-C2D	-2.09	1.46	1.50
13	u	508	CLA	CMC-C2C	-2.09	1.46	1.50
13	u	502	CLA	MG-NB	-2.09	2.01	2.05
13	J	1303	CLA	CMC-C2C	-2.09	1.46	1.50
13	Y	519	CLA	CMD-C2D	-2.09	1.46	1.50
13	H	1225	CLA	MG-ND	-2.09	2.01	2.05
13	H	1236	CLA	MG-NB	-2.09	2.01	2.05
13	B	1204	CLA	CMC-C2C	-2.09	1.46	1.50
13	5	502	CLA	CMD-C2D	-2.09	1.46	1.50
13	H	1207	CLA	CHC-C1C	2.09	1.42	1.38
13	B	1234	CLA	CMB-C2B	-2.09	1.46	1.50
13	3	507	CLA	CMD-C2D	-2.09	1.46	1.50
13	H	1012	CLA	CMB-C2B	-2.09	1.46	1.50
13	B	1206	CLA	MG-ND	-2.09	2.01	2.05
13	u	519	CLA	CMC-C2C	-2.09	1.46	1.50
13	v	508	CLA	CMC-C2C	-2.09	1.46	1.50
13	f	1229	CLA	CMD-C2D	-2.09	1.46	1.50
13	r	508	CLA	CMD-C2D	-2.09	1.46	1.50
13	2	518	CLA	CMB-C2B	-2.09	1.46	1.50
13	c	501	CLA	MG-NB	-2.09	2.01	2.05
13	s	501	CLA	CMC-C2C	-2.09	1.46	1.50
13	q	503	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U	1401	CLA	CMC-C2C	-2.09	1.46	1.50
13	A	1102	CLA	MG-NB	-2.09	2.01	2.05
13	H	1206	CLA	MG-ND	-2.09	2.01	2.05
13	s	518	CLA	MG-NB	-2.09	2.01	2.05
13	v	506	CLA	MG-NB	-2.09	2.01	2.05
13	B	1227	CLA	CMC-C2C	-2.09	1.46	1.50
13	G	1120	CLA	CMB-C2B	-2.09	1.46	1.50
13	H	1234	CLA	CMB-C2B	-2.09	1.46	1.50
13	K	1105	CLA	MG-NB	-2.09	2.01	2.05
13	e	1135	CLA	C1B-NB	-2.09	1.35	1.37
13	A	1108	CLA	CHC-C1C	2.09	1.42	1.38
13	v	505	CLA	CHC-C1C	2.09	1.42	1.38
13	f	1210	CLA	CMB-C2B	-2.09	1.46	1.50
13	5	501	CLA	MG-NB	-2.09	2.01	2.05
13	t	518	CLA	MG-NB	-2.09	2.01	2.05
13	1	519	CLA	CMD-C2D	-2.09	1.46	1.50
13	3	517	CLA	CMD-C2D	-2.09	1.46	1.50
13	f	1204	CLA	CMD-C2D	-2.09	1.46	1.50
13	4	518	CLA	MG-NB	-2.09	2.01	2.05
13	5	518	CLA	MG-NB	-2.09	2.01	2.05
13	e	1102	CLA	MG-NB	-2.09	2.01	2.05
13	e	1115	CLA	CMB-C2B	-2.09	1.46	1.50
13	n	1501	CLA	CMC-C2C	-2.09	1.46	1.50
13	t	509	CLA	CMB-C2B	-2.09	1.46	1.50
14	G	2001	PQN	C5-C4	-2.09	1.44	1.48
13	H	1226	CLA	C3B-C4B	2.09	1.47	1.42
13	B	1204	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	1218	CLA	CMB-C2B	-2.09	1.46	1.50
13	v	508	CLA	CMD-C2D	-2.09	1.46	1.50
13	s	516	CLA	MG-NB	-2.09	2.01	2.05
13	v	507	CLA	MG-NB	-2.09	2.01	2.05
13	5	504	CLA	CHC-C1C	2.09	1.42	1.38
13	L	1503	CLA	CMC-C2C	-2.09	1.46	1.50
13	2	512	CLA	CMB-C2B	-2.09	1.46	1.50
13	f	1221	CLA	CMC-C2C	-2.09	1.46	1.50
20	V	5216	SQD	O4-C4	-2.09	1.38	1.43
13	A	1112	CLA	CMB-C2B	-2.09	1.46	1.50
13	B	1229	CLA	CMD-C2D	-2.09	1.46	1.50
13	3	510	CLA	CMD-C2D	-2.09	1.46	1.50
13	H	1227	CLA	CMD-C2D	-2.09	1.46	1.50
13	Z	504	CLA	CMB-C2B	-2.09	1.46	1.50
13	d	508	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1215	CLA	CMD-C2D	-2.09	1.46	1.50
13	G	1131	CLA	MG-NB	-2.09	2.01	2.05
13	H	1231	CLA	MG-NB	-2.09	2.01	2.05
13	f	1204	CLA	MG-ND	-2.09	2.01	2.05
13	n	1503	CLA	CMC-C2C	-2.09	1.46	1.50
13	G	1106	CLA	C1B-C2B	2.09	1.48	1.43
13	G	1121	CLA	CMC-C2C	-2.09	1.46	1.50
13	v	503	CLA	MG-NB	-2.09	2.01	2.05
13	K	1401	CLA	CMD-C2D	-2.08	1.46	1.50
13	H	1220	CLA	CMB-C2B	-2.08	1.46	1.50
13	V	1501	CLA	CMD-C2D	-2.08	1.46	1.50
13	c	508	CLA	CMC-C2C	-2.08	1.46	1.50
13	f	1204	CLA	CMC-C2C	-2.08	1.46	1.50
13	v	506	CLA	CMB-C2B	-2.08	1.46	1.50
20	L	5216	SQD	O4-C4	-2.08	1.38	1.43
20	5	822	SQD	O4-C4	-2.08	1.38	1.43
20	a	822	SQD	O4-C4	-2.08	1.38	1.43
13	d	507	CLA	MG-NB	-2.08	2.01	2.05
13	e	1137	CLA	MG-NB	-2.08	2.01	2.05
13	f	1221	CLA	MG-ND	-2.08	2.01	2.05
16	e	4008	BCR	C10-C9	-2.08	1.33	1.35
13	f	1203	CLA	CHC-C1C	2.08	1.42	1.38
13	v	501	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1208	CLA	CMB-C2B	-2.08	1.46	1.50
13	c	509	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	1112	CLA	CMB-C2B	-2.08	1.46	1.50
13	d	501	CLA	MG-NB	-2.08	2.01	2.05
13	5	502	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1222	CLA	CMD-C2D	-2.08	1.46	1.50
13	5	516	CLA	CHC-C1C	2.08	1.42	1.38
13	v	503	CLA	CHC-C1C	2.08	1.42	1.38
13	5	513	CLA	MG-NB	-2.08	2.01	2.05
13	b	513	CLA	MG-NB	-2.08	2.01	2.05
20	n	5216	SQD	O4-C4	-2.08	1.38	1.43
13	A	1125	CLA	CHC-C1C	2.08	1.42	1.38
13	L	1503	CLA	CHC-C1C	2.08	1.42	1.38
13	b	501	CLA	MG-NB	-2.08	2.01	2.05
13	A	1117	CLA	C1B-C2B	2.08	1.48	1.43
13	A	1102	CLA	CMB-C2B	-2.08	1.46	1.50
13	5	512	CLA	CMD-C2D	-2.08	1.46	1.50
13	5	518	CLA	CMB-C2B	-2.08	1.46	1.50
13	c	513	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1236	CLA	CMD-C2D	-2.08	1.46	1.50
13	Z	518	CLA	CHC-C1C	2.08	1.42	1.38
13	A	1119	CLA	MG-ND	-2.08	2.01	2.05
13	2	511	CLA	CMD-C2D	-2.08	1.46	1.50
13	T	1303	CLA	CMC-C2C	-2.08	1.46	1.50
13	f	1227	CLA	CMD-C2D	-2.08	1.46	1.50
13	c	508	CLA	CMD-C2D	-2.08	1.46	1.50
13	c	517	CLA	CMD-C2D	-2.08	1.46	1.50
13	s	511	CLA	CMD-C2D	-2.08	1.46	1.50
13	2	501	CLA	CHC-C1C	2.08	1.42	1.38
13	c	517	CLA	CHC-C1C	2.08	1.42	1.38
13	c	513	CLA	MG-NB	-2.08	2.01	2.05
13	A	1121	CLA	CMC-C2C	-2.08	1.46	1.50
13	5	519	CLA	CMC-C2C	-2.08	1.46	1.50
13	c	519	CLA	CMC-C2C	-2.08	1.46	1.50
13	s	509	CLA	CMB-C2B	-2.08	1.46	1.50
13	f	1217	CLA	MG-ND	-2.08	2.01	2.05
13	G	1104	CLA	CMB-C2B	-2.08	1.46	1.50
13	a	511	CLA	CMD-C2D	-2.08	1.46	1.50
13	f	1232	CLA	CMC-C2C	-2.08	1.46	1.50
20	s	822	SQD	O4-C4	-2.08	1.38	1.43
13	G	1022	CLA	C1B-C2B	2.08	1.48	1.43
13	Z	501	CLA	CHC-C1C	2.08	1.42	1.38
13	b	518	CLA	CHC-C1C	2.08	1.42	1.38
13	q	509	CLA	CHC-C1C	2.08	1.42	1.38
13	u	502	CLA	CHC-C1C	2.08	1.42	1.38
13	1	517	CLA	MG-NB	-2.08	2.01	2.05
13	G	1102	CLA	MG-NB	-2.08	2.01	2.05
13	f	1206	CLA	MG-ND	-2.08	2.01	2.05
13	q	513	CLA	MG-NB	-2.08	2.01	2.05
13	G	1111	CLA	CMB-C2B	-2.08	1.46	1.50
13	G	1112	CLA	CMB-C2B	-2.08	1.46	1.50
13	V	1503	CLA	CMC-C2C	-2.08	1.46	1.50
13	r	513	CLA	CMB-C2B	-2.08	1.46	1.50
13	1	504	CLA	CMB-C2B	-2.08	1.46	1.50
13	c	509	CLA	CMC-C2C	-2.08	1.46	1.50
13	e	1103	CLA	CMB-C2B	-2.08	1.46	1.50
13	H	1222	CLA	C1B-C2B	2.08	1.48	1.43
13	4	517	CLA	CHC-C1C	2.08	1.42	1.38
13	s	503	CLA	MG-NB	-2.08	2.01	2.05
13	A	1115	CLA	CMB-C2B	-2.08	1.46	1.50
13	f	1214	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	505	CLA	CHC-C1C	2.08	1.42	1.38
13	t	517	CLA	CHC-C1C	2.08	1.42	1.38
13	6	510	CLA	MG-NB	-2.08	2.01	2.05
13	L	1501	CLA	CMD-C2D	-2.08	1.46	1.50
13	A	1107	CLA	C1B-NB	-2.08	1.35	1.37
13	4	506	CLA	MG-NB	-2.08	2.01	2.05
13	B	1210	CLA	CMB-C2B	-2.08	1.46	1.50
13	e	1104	CLA	CMB-C2B	-2.08	1.46	1.50
13	t	513	CLA	MG-NB	-2.08	2.01	2.05
13	H	1204	CLA	CMD-C2D	-2.08	1.46	1.50
13	r	512	CLA	CMB-C2B	-2.08	1.46	1.50
13	q	504	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1240	CLA	CMB-C2B	-2.08	1.46	1.50
13	f	1226	CLA	CMC-C2C	-2.08	1.46	1.50
13	q	507	CLA	CMB-C2B	-2.08	1.46	1.50
13	r	509	CLA	CMD-C2D	-2.08	1.46	1.50
20	1	822	SQD	O3-C3	-2.08	1.38	1.43
13	s	508	CLA	C1B-C2B	2.08	1.48	1.43
13	2	517	CLA	CHC-C1C	2.08	1.42	1.38
13	G	1135	CLA	C1B-NB	-2.08	1.35	1.37
13	H	1208	CLA	CMB-C2B	-2.08	1.46	1.50
13	6	505	CLA	MG-NB	-2.08	2.01	2.05
13	e	1101	CLA	CHC-C1C	2.08	1.42	1.38
13	u	504	CLA	CHC-C1C	2.08	1.42	1.38
13	U	1401	CLA	CMD-C2D	-2.08	1.46	1.50
13	Z	508	CLA	CMD-C2D	-2.08	1.46	1.50
13	t	508	CLA	C1B-C2B	2.08	1.48	1.43
13	3	516	CLA	MG-NB	-2.08	2.01	2.05
13	3	517	CLA	MG-NB	-2.08	2.01	2.05
13	Z	516	CLA	CMD-C2D	-2.08	1.46	1.50
13	G	1106	CLA	C1B-NB	-2.08	1.35	1.37
13	B	1231	CLA	MG-NB	-2.08	2.01	2.05
13	4	518	CLA	CHC-C1C	2.08	1.42	1.38
13	d	505	CLA	CHC-C1C	2.08	1.42	1.38
13	A	1106	CLA	C1B-C2B	2.08	1.48	1.43
13	5	513	CLA	CMB-C2B	-2.08	1.46	1.50
13	G	1120	CLA	CMD-C2D	-2.08	1.46	1.50
13	l	1303	CLA	CMC-C2C	-2.08	1.46	1.50
13	q	509	CLA	CMD-C2D	-2.08	1.46	1.50
13	3	510	CLA	MG-NB	-2.08	2.01	2.05
13	a	510	CLA	MG-NB	-2.08	2.01	2.05
13	s	511	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1107	CLA	C1B-C2B	2.08	1.48	1.43
13	A	1022	CLA	C1B-C2B	2.08	1.48	1.43
13	Y	504	CLA	CHC-C1C	2.07	1.42	1.38
13	B	1221	CLA	CMC-C2C	-2.07	1.46	1.50
13	5	509	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	519	CLA	CMC-C2C	-2.07	1.46	1.50
13	u	504	CLA	CMB-C2B	-2.07	1.46	1.50
13	G	1117	CLA	MG-ND	-2.07	2.01	2.05
13	3	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	G	1107	CLA	CMC-C2C	-2.07	1.46	1.50
13	b	518	CLA	CMB-C2B	-2.07	1.46	1.50
13	B	1232	CLA	CHC-C1C	2.07	1.42	1.38
13	6	503	CLA	CHC-C1C	2.07	1.42	1.38
13	Z	504	CLA	CHC-C1C	2.07	1.42	1.38
13	B	1236	CLA	CMD-C2D	-2.07	1.46	1.50
13	5	517	CLA	CHC-C1C	2.07	1.42	1.38
13	G	1110	CLA	CHC-C1C	2.07	1.42	1.38
13	n	1503	CLA	CHC-C1C	2.07	1.42	1.38
13	r	501	CLA	CHC-C1C	2.07	1.42	1.38
20	q	822	SQD	O3-C3	-2.07	1.38	1.43
13	2	511	CLA	MG-NB	-2.07	2.01	2.05
13	G	1119	CLA	MG-ND	-2.07	2.01	2.05
20	Y	822	SQD	O3-C3	-2.07	1.38	1.43
13	a	517	CLA	MG-NB	-2.07	2.01	2.05
13	A	1107	CLA	CMC-C2C	-2.07	1.46	1.50
13	4	507	CLA	CMD-C2D	-2.07	1.46	1.50
13	6	511	CLA	CMD-C2D	-2.07	1.46	1.50
13	G	1130	CLA	CMD-C2D	-2.07	1.46	1.50
13	s	507	CLA	CMD-C2D	-2.07	1.46	1.50
13	s	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	v	511	CLA	CMD-C2D	-2.07	1.46	1.50
13	1	509	CLA	CHC-C1C	2.07	1.42	1.38
13	2	506	CLA	CHC-C1C	2.07	1.42	1.38
13	f	1213	CLA	CHC-C1C	2.07	1.42	1.38
13	v	519	CLA	CMC-C2C	-2.07	1.46	1.50
20	r	822	SQD	O3-C3	-2.07	1.38	1.43
13	r	518	CLA	CHC-C1C	2.07	1.42	1.38
13	e	1107	CLA	C1B-C2B	2.07	1.48	1.43
13	f	1208	CLA	CMB-C2B	-2.07	1.46	1.50
13	e	1117	CLA	C1B-C2B	2.07	1.48	1.43
13	H	1203	CLA	CHC-C1C	2.07	1.42	1.38
13	e	1125	CLA	CHC-C1C	2.07	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1232	CLA	CHC-C1C	2.07	1.42	1.38
20	Z	822	SQD	O4-C4	-2.07	1.38	1.43
13	G	1120	CLA	C1B-NB	-2.07	1.35	1.37
13	A	1111	CLA	CMB-C2B	-2.07	1.46	1.50
13	a	517	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	1203	CLA	CHC-C1C	2.07	1.42	1.38
13	B	1207	CLA	CHC-C1C	2.07	1.42	1.38
20	2	822	SQD	O4-C4	-2.07	1.38	1.43
13	b	518	CLA	MG-NB	-2.07	2.01	2.05
13	3	501	CLA	CMC-C2C	-2.07	1.46	1.50
13	H	1217	CLA	MG-ND	-2.07	2.01	2.05
13	Z	503	CLA	MG-NB	-2.07	2.01	2.05
13	e	1132	CLA	MG-ND	-2.07	2.01	2.05
13	2	510	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	1214	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	1226	CLA	CMC-C2C	-2.07	1.46	1.50
13	B	1232	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	518	CLA	MG-NB	-2.07	2.01	2.05
13	f	1216	CLA	MG-ND	-2.07	2.01	2.05
13	6	507	CLA	CMD-C2D	-2.07	1.46	1.50
13	6	509	CLA	MG-NB	-2.07	2.01	2.05
13	Z	503	CLA	CHC-C1C	2.07	1.42	1.38
13	c	518	CLA	MG-NB	-2.07	2.01	2.05
13	e	1022	CLA	C1B-C2B	2.07	1.48	1.43
13	6	511	CLA	CHC-C1C	2.07	1.42	1.38
13	H	1221	CLA	CMC-C2C	-2.07	1.46	1.50
13	m	1401	CLA	CMD-C2D	-2.07	1.46	1.50
13	q	504	CLA	CMC-C2C	-2.07	1.46	1.50
13	v	510	CLA	MG-NB	-2.07	2.01	2.05
13	f	1225	CLA	CHC-C1C	2.07	1.42	1.38
13	A	1120	CLA	C1B-NB	-2.07	1.35	1.37
13	3	504	CLA	CMB-C2B	-2.07	1.46	1.50
13	H	1232	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	1222	CLA	CMD-C2D	-2.07	1.46	1.50
13	u	512	CLA	CMB-C2B	-2.07	1.46	1.50
20	q	822	SQD	O4-C4	-2.07	1.38	1.43
13	A	1117	CLA	MG-ND	-2.07	2.01	2.05
13	B	1201	CLA	CHC-C1C	2.07	1.42	1.38
13	1	504	CLA	CHC-C1C	2.07	1.42	1.38
13	2	513	CLA	MG-NB	-2.07	2.01	2.05
13	G	1109	CLA	MG-NB	-2.07	2.01	2.05
13	r	509	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	509	CLA	MG-NB	-2.07	2.01	2.05
13	B	1217	CLA	C1B-NB	-2.07	1.35	1.37
13	c	516	CLA	CHC-C1C	2.07	1.42	1.38
13	H	1210	CLA	CMB-C2B	-2.07	1.46	1.50
13	s	519	CLA	CMC-C2C	-2.07	1.46	1.50
13	u	517	CLA	CMD-C2D	-2.07	1.46	1.50
13	G	1117	CLA	C1B-C2B	2.07	1.48	1.43
13	n	1503	CLA	MG-NB	-2.07	2.01	2.05
13	u	509	CLA	MG-NB	-2.07	2.01	2.05
13	6	518	CLA	CMB-C2B	-2.07	1.46	1.50
13	u	513	CLA	CMB-C2B	-2.07	1.46	1.50
13	G	1108	CLA	CHC-C1C	2.07	1.42	1.38
13	u	516	CLA	CHC-C1C	2.07	1.42	1.38
13	3	519	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	c	516	CLA	CMD-C2D	-2.07	1.46	1.50
13	G	1137	CLA	MG-NB	-2.07	2.01	2.05
13	a	512	CLA	MG-ND	-2.07	2.01	2.05
13	t	506	CLA	MG-NB	-2.07	2.01	2.05
13	q	509	CLA	CMB-C2B	-2.07	1.46	1.50
13	f	1012	CLA	MG-ND	-2.07	2.01	2.05
13	B	1225	CLA	CHC-C1C	2.07	1.42	1.38
13	5	509	CLA	CMC-C2C	-2.07	1.46	1.50
13	5	512	CLA	CMB-C2B	-2.07	1.46	1.50
13	H	1214	CLA	CMD-C2D	-2.07	1.46	1.50
13	H	1220	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	1229	CLA	CMC-C2C	-2.07	1.46	1.50
20	3	822	SQD	O4-C4	-2.07	1.38	1.43
13	A	1137	CLA	MG-NB	-2.07	2.01	2.05
13	6	503	CLA	MG-NB	-2.07	2.01	2.05
13	H	1225	CLA	CHC-C1C	2.07	1.42	1.38
13	a	518	CLA	CMC-C2C	-2.07	1.46	1.50
13	e	1102	CLA	CMB-C2B	-2.07	1.46	1.50
13	A	1104	CLA	CMB-C2B	-2.06	1.46	1.50
13	Z	507	CLA	CMB-C2B	-2.06	1.46	1.50
13	c	513	CLA	CMD-C2D	-2.06	1.46	1.50
13	d	511	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	1220	CLA	CMD-C2D	-2.06	1.46	1.50
13	s	506	CLA	CMD-C2D	-2.06	1.46	1.50
13	B	1012	CLA	MG-ND	-2.06	2.01	2.05
13	B	1203	CLA	CMB-C2B	-2.06	1.46	1.50
13	5	504	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	518	CLA	CMB-C2B	-2.06	1.46	1.50
13	1	509	CLA	CMD-C2D	-2.06	1.46	1.50
13	c	504	CLA	CMB-C2B	-2.06	1.46	1.50
13	d	506	CLA	CMB-C2B	-2.06	1.46	1.50
13	d	518	CLA	CMB-C2B	-2.06	1.46	1.50
13	s	519	CLA	CMD-C2D	-2.06	1.46	1.50
13	H	1213	CLA	CHC-C1C	2.06	1.42	1.38
13	3	508	CLA	C1B-C2B	2.06	1.48	1.43
13	H	1203	CLA	CMB-C2B	-2.06	1.46	1.50
13	Y	511	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	1232	CLA	CMD-C2D	-2.06	1.46	1.50
13	u	513	CLA	CMD-C2D	-2.06	1.46	1.50
13	G	1109	CLA	CMD-C2D	-2.06	1.46	1.50
13	e	1105	CLA	CMD-C2D	-2.06	1.46	1.50
13	H	1231	CLA	CHC-C1C	2.06	1.42	1.38
13	s	501	CLA	MG-NB	-2.06	2.01	2.05
13	e	1107	CLA	C1B-NB	-2.06	1.35	1.37
13	1	509	CLA	CMB-C2B	-2.06	1.46	1.50
13	3	507	CLA	CMB-C2B	-2.06	1.46	1.50
13	5	517	CLA	CMD-C2D	-2.06	1.46	1.50
13	e	1111	CLA	CMB-C2B	-2.06	1.46	1.50
13	f	1234	CLA	CMB-C2B	-2.06	1.46	1.50
13	d	503	CLA	CHC-C1C	2.06	1.42	1.38
13	e	1138	CLA	MG-NB	-2.06	2.01	2.05
13	u	501	CLA	MG-NB	-2.06	2.01	2.05
13	f	1201	CLA	CHC-C1C	2.06	1.42	1.38
13	u	516	CLA	MG-NB	-2.06	2.01	2.05
13	A	1108	CLA	CMC-C2C	-2.06	1.46	1.50
13	1	511	CLA	CMD-C2D	-2.06	1.46	1.50
13	q	503	CLA	CHC-C1C	2.06	1.42	1.38
20	r	822	SQD	O4-C4	-2.06	1.38	1.43
13	B	1220	CLA	MG-NB	-2.06	2.01	2.05
13	Y	506	CLA	CMC-C2C	-2.06	1.46	1.50
13	Z	510	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	1218	CLA	CMB-C2B	-2.06	1.46	1.50
13	f	1228	CLA	CMB-C2B	-2.06	1.46	1.50
13	q	501	CLA	CMC-C2C	-2.06	1.46	1.50
13	r	511	CLA	CMD-C2D	-2.06	1.46	1.50
13	H	1201	CLA	CHC-C1C	2.06	1.42	1.38
13	H	1202	CLA	CHC-C1C	2.06	1.42	1.38
13	G	1138	CLA	MG-NB	-2.06	2.01	2.05
13	r	503	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	511	CLA	CMD-C2D	-2.06	1.46	1.50
13	Z	517	CLA	CHC-C1C	2.06	1.42	1.38
13	1	503	CLA	MG-NB	-2.06	2.01	2.05
13	2	503	CLA	MG-NB	-2.06	2.01	2.05
13	3	509	CLA	MG-NB	-2.06	2.01	2.05
13	6	507	CLA	MG-NB	-2.06	2.01	2.05
13	u	519	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	510	CLA	MG-NB	-2.06	2.01	2.05
13	n	1501	CLA	CMD-C2D	-2.06	1.46	1.50
13	H	1225	CLA	C1B-C2B	2.06	1.48	1.43
13	r	517	CLA	CHC-C1C	2.06	1.42	1.38
13	Z	518	CLA	CMB-C2B	-2.06	1.46	1.50
13	s	504	CLA	CMB-C2B	-2.06	1.46	1.50
16	A	4008	BCR	C10-C9	-2.06	1.33	1.35
13	c	519	CLA	CMD-C2D	-2.06	1.46	1.50
13	q	511	CLA	CMD-C2D	-2.06	1.46	1.50
13	v	517	CLA	CMD-C2D	-2.06	1.46	1.50
13	1	503	CLA	CHC-C1C	2.06	1.42	1.38
13	d	508	CLA	CHC-C1C	2.06	1.42	1.38
13	2	501	CLA	MG-NB	-2.06	2.01	2.05
13	a	503	CLA	MG-NB	-2.06	2.01	2.05
13	e	1117	CLA	MG-ND	-2.06	2.01	2.05
13	3	506	CLA	CMD-C2D	-2.06	1.46	1.50
13	s	517	CLA	CMD-C2D	-2.06	1.46	1.50
13	t	518	CLA	CHC-C1C	2.06	1.42	1.38
13	4	501	CLA	MG-NB	-2.06	2.01	2.05
13	1	501	CLA	CMC-C2C	-2.06	1.46	1.50
13	1	516	CLA	CMD-C2D	-2.06	1.46	1.50
19	f	5002	LMG	O1-C7	-2.06	1.40	1.43
20	2	822	SQD	O3-C3	-2.06	1.38	1.43
13	e	1132	CLA	CHC-C1C	2.06	1.42	1.38
13	u	517	CLA	CHC-C1C	2.06	1.42	1.38
13	Z	513	CLA	MG-NB	-2.06	2.01	2.05
13	Y	509	CLA	CHC-C1C	2.06	1.42	1.38
13	3	503	CLA	MG-NB	-2.06	2.01	2.05
13	Z	501	CLA	MG-NB	-2.06	2.01	2.05
13	b	510	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	513	CLA	CMC-C2C	-2.06	1.46	1.50
20	c	822	SQD	O4-C4	-2.06	1.38	1.43
13	H	1240	CLA	CHC-C1C	2.06	1.42	1.38
13	2	517	CLA	CMB-C2B	-2.06	1.46	1.50
13	3	518	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	509	CLA	CMC-C2C	-2.06	1.46	1.50
13	a	519	CLA	CMB-C2B	-2.06	1.46	1.50
13	c	506	CLA	CMB-C2B	-2.06	1.46	1.50
13	v	507	CLA	CMD-C2D	-2.06	1.46	1.50
13	6	512	CLA	CMB-C2B	-2.06	1.46	1.50
13	H	1215	CLA	CMC-C2C	-2.06	1.46	1.50
13	G	1123	CLA	CMC-C2C	-2.05	1.46	1.50
13	H	1229	CLA	CMC-C2C	-2.05	1.46	1.50
13	r	510	CLA	CMD-C2D	-2.05	1.46	1.50
13	4	508	CLA	C1B-C2B	2.05	1.48	1.43
13	b	506	CLA	MG-NB	-2.05	2.01	2.05
13	a	517	CLA	CHC-C1C	2.05	1.42	1.38
13	d	512	CLA	CMB-C2B	-2.05	1.46	1.50
13	f	1231	CLA	MG-NB	-2.05	2.01	2.05
13	2	504	CLA	CMB-C2B	-2.05	1.46	1.50
13	f	1203	CLA	CMB-C2B	-2.05	1.46	1.50
13	v	518	CLA	CMB-C2B	-2.05	1.46	1.50
13	t	510	CLA	MG-NB	-2.05	2.01	2.05
13	2	516	CLA	CHC-C1C	2.05	1.42	1.38
13	3	505	CLA	CHC-C1C	2.05	1.42	1.38
13	f	1207	CLA	CHC-C1C	2.05	1.42	1.38
13	q	501	CLA	CHC-C1C	2.05	1.42	1.38
13	A	1117	CLA	CMC-C2C	-2.05	1.46	1.50
13	1	506	CLA	CMC-C2C	-2.05	1.46	1.50
13	3	503	CLA	CMB-C2B	-2.05	1.46	1.50
13	5	519	CLA	CMD-C2D	-2.05	1.46	1.50
13	Y	509	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	1138	CLA	MG-NB	-2.05	2.01	2.05
13	b	505	CLA	CHC-C1C	2.05	1.42	1.38
13	f	1202	CLA	CHC-C1C	2.05	1.42	1.38
13	5	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	c	513	CLA	CMC-C2C	-2.05	1.46	1.50
13	A	1105	CLA	CMD-C2D	-2.05	1.46	1.50
13	G	1109	CLA	CMB-C2B	-2.05	1.46	1.50
13	a	519	CLA	CMD-C2D	-2.05	1.46	1.50
13	q	506	CLA	CMC-C2C	-2.05	1.46	1.50
13	B	1221	CLA	MG-ND	-2.05	2.01	2.05
13	4	513	CLA	MG-NB	-2.05	2.01	2.05
13	s	512	CLA	MG-ND	-2.05	2.01	2.05
13	a	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	b	507	CLA	CMD-C2D	-2.05	1.46	1.50
13	e	1107	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	u	509	CLA	CMC-C2C	-2.05	1.46	1.50
13	6	508	CLA	CHC-C1C	2.05	1.42	1.38
13	c	509	CLA	MG-NB	-2.05	2.01	2.05
13	2	507	CLA	CMB-C2B	-2.05	1.46	1.50
13	4	518	CLA	CMB-C2B	-2.05	1.46	1.50
13	6	508	CLA	CMC-C2C	-2.05	1.46	1.50
13	u	509	CLA	CMD-C2D	-2.05	1.46	1.50
13	6	501	CLA	CHC-C1C	2.05	1.42	1.38
20	Y	822	SQD	O4-C4	-2.05	1.38	1.43
13	1	504	CLA	CMC-C2C	-2.05	1.46	1.50
13	H	1240	CLA	CMB-C2B	-2.05	1.46	1.50
13	s	503	CLA	CMB-C2B	-2.05	1.46	1.50
13	R	1301	CLA	CHC-C1C	2.05	1.42	1.38
13	d	511	CLA	CHC-C1C	2.05	1.42	1.38
13	3	509	CLA	CMB-C2B	-2.05	1.46	1.50
13	Y	504	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	d	519	CLA	CMC-C2C	-2.05	1.46	1.50
13	Y	505	CLA	CHC-C1C	2.05	1.42	1.38
13	V	1503	CLA	MG-NB	-2.05	2.01	2.05
13	a	504	CLA	CMB-C2B	-2.05	1.46	1.50
13	d	501	CLA	CMD-C2D	-2.05	1.46	1.50
13	s	507	CLA	CMB-C2B	-2.05	1.46	1.50
13	1	505	CLA	CHC-C1C	2.05	1.42	1.38
20	Z	822	SQD	O3-C3	-2.05	1.38	1.43
13	H	1218	CLA	CMC-C2C	-2.05	1.46	1.50
13	e	1120	CLA	CMC-C2C	-2.05	1.46	1.50
13	e	1127	CLA	CMC-C2C	-2.05	1.46	1.50
13	f	1238	CLA	CMC-C2C	-2.05	1.46	1.50
13	t	501	CLA	MG-NB	-2.05	2.01	2.05
13	H	1226	CLA	CMC-C2C	-2.05	1.46	1.50
13	Y	507	CLA	CMB-C2B	-2.05	1.46	1.50
13	d	503	CLA	CMD-C2D	-2.05	1.46	1.50
13	H	1232	CLA	CHC-C1C	2.05	1.42	1.38
13	A	1109	CLA	CMB-C2B	-2.05	1.46	1.50
13	2	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	2	503	CLA	CHC-C1C	2.05	1.42	1.38
13	a	505	CLA	CHC-C1C	2.05	1.42	1.38
13	b	508	CLA	C1B-C2B	2.05	1.48	1.43
13	6	506	CLA	CMB-C2B	-2.05	1.46	1.50
13	c	516	CLA	CMB-C2B	-2.05	1.46	1.50
13	e	1126	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	512	CLA	CMB-C2B	-2.05	1.46	1.50
13	r	516	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	501	CLA	MG-NB	-2.05	2.01	2.05
13	e	1106	CLA	C1B-NB	-2.05	1.35	1.37
13	f	1223	CLA	C1B-NB	-2.05	1.35	1.37
13	1	507	CLA	CMB-C2B	-2.05	1.46	1.50
13	3	519	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	506	CLA	CMD-C2D	-2.05	1.46	1.50
13	l	1303	CLA	CMB-C2B	-2.05	1.46	1.50
13	u	510	CLA	CMD-C2D	-2.05	1.46	1.50
13	H	1221	CLA	MG-ND	-2.05	2.01	2.05
13	A	1101	CLA	CHC-C1C	2.05	1.42	1.38
13	G	1101	CLA	CHC-C1C	2.05	1.42	1.38
13	B	1229	CLA	CMC-C2C	-2.05	1.46	1.50
13	5	509	CLA	MG-NB	-2.05	2.01	2.05
13	5	506	CLA	CMB-C2B	-2.05	1.46	1.50
13	Z	506	CLA	CMD-C2D	-2.05	1.46	1.50
13	t	518	CLA	CMB-C2B	-2.05	1.46	1.50
19	B	5002	LMG	O1-C7	-2.05	1.40	1.43
19	H	5002	LMG	O1-C7	-2.05	1.40	1.43
13	Y	509	CLA	MG-NB	-2.05	2.01	2.05
13	q	509	CLA	MG-NB	-2.05	2.01	2.05
13	e	1127	CLA	CHC-C1C	2.05	1.42	1.38
13	Y	509	CLA	CMB-C2B	-2.05	1.46	1.50
13	d	505	CLA	MG-NB	-2.05	2.01	2.05
13	t	505	CLA	CHC-C1C	2.05	1.42	1.38
13	u	503	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	1127	CLA	CHC-C1C	2.04	1.42	1.38
13	B	1225	CLA	C1B-C2B	2.04	1.48	1.43
13	d	508	CLA	CMC-C2C	-2.04	1.46	1.50
13	f	1220	CLA	MG-NB	-2.04	2.01	2.05
13	G	1108	CLA	CMC-C2C	-2.04	1.46	1.50
13	u	506	CLA	CMC-C2C	-2.04	1.46	1.50
20	1	822	SQD	O4-C4	-2.04	1.38	1.43
13	s	505	CLA	CHC-C1C	2.04	1.42	1.38
13	2	516	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	1126	CLA	CMB-C2B	-2.04	1.46	1.50
13	H	1236	CLA	CMD-C2D	-2.04	1.46	1.50
13	s	517	CLA	MG-NB	-2.04	2.01	2.05
13	b	502	CLA	CHC-C1C	2.04	1.42	1.38
13	H	1206	CLA	C3B-C4B	2.04	1.47	1.42
13	A	1123	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1232	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	1106	CLA	C1B-C2B	2.04	1.48	1.43
13	B	1216	CLA	MG-ND	-2.04	2.01	2.05
13	Y	503	CLA	MG-NB	-2.04	2.01	2.05
13	a	516	CLA	MG-NB	-2.04	2.01	2.05
13	s	519	CLA	MG-NB	-2.04	2.01	2.05
13	f	1231	CLA	CHC-C1C	2.04	1.42	1.38
13	3	501	CLA	CMD-C2D	-2.04	1.46	1.50
13	4	517	CLA	CMC-C2C	-2.04	1.46	1.50
13	H	1228	CLA	CMB-C2B	-2.04	1.46	1.50
13	Z	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	a	507	CLA	CMB-C2B	-2.04	1.46	1.50
13	t	510	CLA	CMD-C2D	-2.04	1.46	1.50
13	t	513	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	1113	CLA	CMB-C2B	-2.04	1.46	1.50
13	J	1303	CLA	CMB-C2B	-2.04	1.46	1.50
13	H	1238	CLA	CMC-C2C	-2.04	1.46	1.50
13	a	503	CLA	CMB-C2B	-2.04	1.46	1.50
13	s	513	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	1113	CLA	CMB-C2B	-2.04	1.46	1.50
13	G	1107	CLA	C1B-C2B	2.04	1.48	1.43
13	f	1215	CLA	MG-ND	-2.04	2.01	2.05
13	B	1220	CLA	CMD-C2D	-2.04	1.46	1.50
13	4	510	CLA	CMD-C2D	-2.04	1.46	1.50
13	B	1218	CLA	CMC-C2C	-2.04	1.46	1.50
13	s	518	CLA	CMC-C2C	-2.04	1.46	1.50
13	H	1217	CLA	C1B-NB	-2.04	1.35	1.37
13	f	1225	CLA	C1B-C2B	2.04	1.48	1.43
13	A	1120	CLA	CMC-C2C	-2.04	1.46	1.50
13	B	1215	CLA	CMD-C2D	-2.04	1.46	1.50
13	T	1302	CLA	CMC-C2C	-2.04	1.46	1.50
13	s	516	CLA	CMD-C2D	-2.04	1.46	1.50
13	U	1401	CLA	CHC-C1C	2.04	1.42	1.38
13	v	508	CLA	CHC-C1C	2.04	1.42	1.38
13	4	510	CLA	MG-NB	-2.04	2.01	2.05
13	v	511	CLA	CHC-C1C	2.04	1.42	1.38
13	L	1503	CLA	MG-NB	-2.04	2.01	2.05
13	5	516	CLA	MG-NB	-2.04	2.01	2.05
13	e	1133	CLA	MG-ND	-2.04	2.01	2.05
13	3	513	CLA	CMD-C2D	-2.04	1.46	1.50
13	6	503	CLA	CMD-C2D	-2.04	1.46	1.50
13	u	513	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	513	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	1113	CLA	CMB-C2B	-2.04	1.46	1.50
13	e	1117	CLA	CMC-C2C	-2.04	1.46	1.50
13	r	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	Z	516	CLA	CHC-C1C	2.04	1.42	1.38
13	d	501	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1109	CLA	CMD-C2D	-2.04	1.46	1.50
13	4	509	CLA	CMB-C2B	-2.04	1.46	1.50
13	6	517	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	1117	CLA	CMC-C2C	-2.04	1.46	1.50
13	q	509	CLA	CMC-C2C	-2.04	1.46	1.50
13	H	1220	CLA	MG-NB	-2.04	2.01	2.05
13	b	517	CLA	MG-NB	-2.04	2.01	2.05
13	e	1109	CLA	CMB-C2B	-2.04	1.46	1.50
13	A	1105	CLA	CHC-C1C	2.04	1.42	1.38
13	H	1215	CLA	MG-ND	-2.04	2.01	2.05
13	5	516	CLA	CMD-C2D	-2.04	1.46	1.50
13	s	509	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	1110	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1132	CLA	MG-ND	-2.04	2.01	2.05
13	d	509	CLA	MG-NB	-2.04	2.01	2.05
20	u	822	SQD	O3-C3	-2.04	1.38	1.43
13	H	1012	CLA	C1B-NB	-2.04	1.35	1.37
13	G	1118	CLA	CMC-C2C	-2.04	1.46	1.50
13	B	1215	CLA	CMC-C2C	-2.04	1.46	1.50
13	1	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	4	513	CLA	CMC-C2C	-2.04	1.46	1.50
13	1	501	CLA	CHC-C1C	2.04	1.42	1.38
13	c	503	CLA	CMD-C2D	-2.04	1.46	1.50
13	r	516	CLA	CHC-C1C	2.04	1.42	1.38
13	t	502	CLA	CHC-C1C	2.04	1.42	1.38
13	4	517	CLA	MG-NB	-2.04	2.01	2.05
13	5	510	CLA	CMD-C2D	-2.04	1.46	1.50
13	c	503	CLA	CMB-C2B	-2.04	1.46	1.50
13	d	507	CLA	CMD-C2D	-2.04	1.46	1.50
13	t	504	CLA	CMD-C2D	-2.04	1.46	1.50
13	F	1301	CLA	CHC-C1C	2.04	1.42	1.38
13	b	519	CLA	CHC-C1C	2.04	1.42	1.38
13	d	503	CLA	MG-NB	-2.03	2.01	2.05
13	e	1126	CLA	CMB-C2B	-2.03	1.46	1.50
13	q	513	CLA	CMB-C2B	-2.03	1.46	1.50
13	s	517	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1202	CLA	CHC-C1C	2.03	1.42	1.38
13	B	1240	CLA	CHC-C1C	2.03	1.42	1.38
13	3	501	CLA	MG-NB	-2.03	2.01	2.05
13	Y	501	CLA	CMC-C2C	-2.03	1.46	1.50
13	Y	516	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	501	CLA	CMC-C2C	-2.03	1.46	1.50
20	5	822	SQD	O3-C3	-2.03	1.38	1.43
13	6	519	CLA	CMC-C2C	-2.03	1.46	1.50
13	b	516	CLA	CMD-C2D	-2.03	1.46	1.50
13	u	516	CLA	CMD-C2D	-2.03	1.46	1.50
19	f	5002	LMG	O7-C8	-2.03	1.41	1.46
13	e	1120	CLA	CHC-C1C	2.03	1.42	1.38
13	B	1023	CLA	C1B-C2B	2.03	1.48	1.43
13	f	1218	CLA	CMC-C2C	-2.03	1.46	1.50
13	2	509	CLA	MG-NB	-2.03	2.01	2.05
13	G	1116	CLA	MG-ND	-2.03	2.01	2.05
13	v	516	CLA	MG-NB	-2.03	2.01	2.05
13	B	1206	CLA	C3B-C4B	2.03	1.47	1.42
13	4	505	CLA	CHC-C1C	2.03	1.42	1.38
13	a	516	CLA	CMD-C2D	-2.03	1.46	1.50
13	l	1302	CLA	CMC-C2C	-2.03	1.46	1.50
13	G	1127	CLA	CHC-C1C	2.03	1.42	1.38
13	m	1401	CLA	CHC-C1C	2.03	1.42	1.38
16	H	4010	BCR	C14-C13	-2.03	1.33	1.35
13	1	513	CLA	CMB-C2B	-2.03	1.46	1.50
13	3	509	CLA	CMC-C2C	-2.03	1.46	1.50
13	H	1201	CLA	CMB-C2B	-2.03	1.46	1.50
13	Y	517	CLA	CMC-C2C	-2.03	1.46	1.50
13	u	506	CLA	CMB-C2B	-2.03	1.46	1.50
13	B	1215	CLA	MG-ND	-2.03	2.01	2.05
13	3	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	r	504	CLA	CMB-C2B	-2.03	1.46	1.50
13	v	503	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	509	CLA	MG-NB	-2.03	2.01	2.05
13	B	1238	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	1109	CLA	CMD-C2D	-2.03	1.46	1.50
13	H	1021	CLA	MG-ND	-2.03	2.01	2.05
13	t	517	CLA	CMC-C2C	-2.03	1.46	1.50
13	a	508	CLA	C1B-C2B	2.03	1.48	1.43
13	f	1232	CLA	C1B-C2B	2.03	1.48	1.43
13	r	501	CLA	MG-NB	-2.03	2.01	2.05
13	s	501	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	519	CLA	CHC-C1C	2.03	1.42	1.38
13	H	1012	CLA	MG-ND	-2.03	2.01	2.05
13	A	1118	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	1108	CLA	CMC-C2C	-2.03	1.46	1.50
13	6	516	CLA	MG-NB	-2.03	2.01	2.05
13	L	1502	CLA	CMB-C2B	-2.03	1.46	1.50
13	5	516	CLA	CMB-C2B	-2.03	1.46	1.50
13	u	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	4	513	CLA	CMD-C2D	-2.03	1.46	1.50
13	H	1213	CLA	CMB-C2B	-2.03	1.46	1.50
13	1	510	CLA	CMD-C2D	-2.03	1.46	1.50
13	5	503	CLA	CMD-C2D	-2.03	1.46	1.50
13	6	510	CLA	CMD-C2D	-2.03	1.46	1.50
13	G	1114	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	1118	CLA	CMC-C2C	-2.03	1.46	1.50
13	v	506	CLA	CMC-C2C	-2.03	1.46	1.50
13	f	1240	CLA	CHC-C1C	2.03	1.42	1.38
13	G	1120	CLA	CMC-C2C	-2.03	1.46	1.50
13	Z	510	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	1114	CLA	CMC-C2C	-2.03	1.46	1.50
13	q	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	1217	CLA	C1B-NB	-2.03	1.35	1.37
13	3	519	CLA	CMB-C2B	-2.03	1.46	1.50
13	J	1302	CLA	CMC-C2C	-2.03	1.46	1.50
13	4	501	CLA	CMB-C2B	-2.03	1.46	1.50
13	B	1213	CLA	CMB-C2B	-2.02	1.46	1.50
13	T	1303	CLA	CMB-C2B	-2.02	1.46	1.50
13	Z	513	CLA	CMD-C2D	-2.02	1.46	1.50
13	f	1201	CLA	CMB-C2B	-2.02	1.46	1.50
13	v	510	CLA	CMD-C2D	-2.02	1.46	1.50
13	B	1231	CLA	CHC-C1C	2.02	1.42	1.38
13	A	1106	CLA	C1B-NB	-2.02	1.35	1.37
13	B	1228	CLA	CMB-C2B	-2.02	1.46	1.50
13	n	1502	CLA	CMB-C2B	-2.02	1.46	1.50
13	r	511	CLA	MG-NB	-2.02	2.01	2.05
13	3	501	CLA	CHC-C1C	2.02	1.42	1.38
13	3	516	CLA	CMD-C2D	-2.02	1.46	1.50
13	Y	510	CLA	CMD-C2D	-2.02	1.46	1.50
13	Y	517	CLA	CMB-C2B	-2.02	1.46	1.50
13	d	503	CLA	CMB-C2B	-2.02	1.46	1.50
13	Y	503	CLA	CHC-C1C	2.02	1.42	1.38
13	e	1105	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	506	CLA	CMD-C2D	-2.02	1.46	1.50
13	G	1105	CLA	CMD-C2D	-2.02	1.46	1.50
13	c	501	CLA	CMD-C2D	-2.02	1.46	1.50
13	u	503	CLA	CMB-C2B	-2.02	1.46	1.50
13	j	1301	CLA	CHC-C1C	2.02	1.42	1.38
13	A	1127	CLA	CMC-C2C	-2.02	1.46	1.50
13	q	513	CLA	CMC-C2C	-2.02	1.46	1.50
13	A	1137	CLA	C1B-C2B	2.02	1.48	1.43
13	e	1137	CLA	C1B-C2B	2.02	1.48	1.43
13	q	505	CLA	CHC-C1C	2.02	1.42	1.38
13	1	513	CLA	CMC-C2C	-2.02	1.46	1.50
13	Y	509	CLA	CMC-C2C	-2.02	1.46	1.50
13	s	513	CLA	CMB-C2B	-2.02	1.46	1.50
13	a	501	CLA	CHC-C1C	2.02	1.42	1.38
13	f	1012	CLA	C1B-NB	-2.02	1.35	1.37
13	5	502	CLA	CMC-C2C	-2.02	1.46	1.50
13	t	506	CLA	CMD-C2D	-2.02	1.46	1.50
13	4	509	CLA	CMD-C2D	-2.02	1.46	1.50
13	A	1133	CLA	MG-ND	-2.02	2.01	2.05
13	e	1116	CLA	MG-ND	-2.02	2.01	2.05
13	f	1238	CLA	CHC-C1C	2.02	1.42	1.38
13	4	504	CLA	CMD-C2D	-2.02	1.46	1.50
13	5	517	CLA	CMC-C2C	-2.02	1.46	1.50
13	e	1110	CLA	CHC-C1C	2.02	1.42	1.38
13	t	517	CLA	MG-NB	-2.02	2.01	2.05
13	G	1137	CLA	C1B-C2B	2.02	1.48	1.43
13	H	1239	CLA	C1B-NB	-2.02	1.35	1.37
20	L	5216	SQD	O3-C3	-2.02	1.38	1.43
13	2	519	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	509	CLA	CMB-C2B	-2.02	1.46	1.50
13	r	513	CLA	CMD-C2D	-2.02	1.46	1.50
16	G	4002	BCR	C30-C25	-2.02	1.51	1.53
16	B	4010	BCR	C14-C13	-2.02	1.33	1.35
16	f	4010	BCR	C14-C13	-2.02	1.33	1.35
20	V	5216	SQD	O3-C3	-2.02	1.38	1.43
13	A	1132	CLA	CHC-C1C	2.02	1.42	1.38
13	G	1105	CLA	CHC-C1C	2.02	1.42	1.38
13	r	503	CLA	CHC-C1C	2.02	1.42	1.38
13	d	517	CLA	CMD-C2D	-2.02	1.46	1.50
13	t	509	CLA	CMD-C2D	-2.02	1.46	1.50
13	2	508	CLA	CHC-C1C	2.02	1.42	1.38
13	1	509	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	1503	CLA	CMB-C2B	-2.02	1.46	1.50
13	3	513	CLA	CMB-C2B	-2.02	1.46	1.50
13	V	1503	CLA	CMB-C2B	-2.02	1.46	1.50
13	q	517	CLA	CMC-C2C	-2.02	1.46	1.50
13	s	519	CLA	CMB-C2B	-2.02	1.46	1.50
13	u	517	CLA	CMC-C2C	-2.02	1.46	1.50
13	K	1401	CLA	CHC-C1C	2.02	1.42	1.38
13	A	1114	CLA	CMC-C2C	-2.02	1.46	1.50
13	4	516	CLA	CMD-C2D	-2.02	1.46	1.50
13	6	501	CLA	CMD-C2D	-2.02	1.46	1.50
13	c	510	CLA	CMD-C2D	-2.02	1.46	1.50
13	r	510	CLA	CMC-C2C	-2.02	1.46	1.50
13	u	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	H	1232	CLA	C1B-C2B	2.02	1.48	1.43
13	H	1208	CLA	CHC-C1C	2.02	1.42	1.38
13	5	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	a	501	CLA	CMD-C2D	-2.02	1.46	1.50
13	B	1232	CLA	C1B-C2B	2.02	1.48	1.43
13	A	1126	CLA	CMC-C2C	-2.02	1.46	1.50
13	5	503	CLA	CMB-C2B	-2.02	1.46	1.50
13	6	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	H	1215	CLA	CMD-C2D	-2.02	1.46	1.50
13	d	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	t	513	CLA	CMD-C2D	-2.02	1.46	1.50
13	H	1023	CLA	C1B-C2B	2.02	1.48	1.43
13	4	502	CLA	MG-NB	-2.02	2.01	2.05
17	e	5003	LHG	O7-C5	-2.02	1.41	1.46
13	b	517	CLA	CMC-C2C	-2.02	1.46	1.50
13	e	1102	CLA	CMD-C2D	-2.02	1.46	1.50
13	G	1132	CLA	CHC-C1C	2.02	1.42	1.38
13	r	508	CLA	CHC-C1C	2.02	1.42	1.38
17	A	5003	LHG	O7-C5	-2.02	1.41	1.46
13	2	504	CLA	CMC-C2C	-2.02	1.46	1.50
13	5	509	CLA	CMB-C2B	-2.02	1.46	1.50
13	c	507	CLA	CMB-C2B	-2.02	1.46	1.50
13	Y	513	CLA	CMB-C2B	-2.02	1.46	1.50
13	e	1134	CLA	CMC-C2C	-2.02	1.46	1.50
13	t	517	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	502	CLA	MG-NB	-2.02	2.01	2.05
13	t	504	CLA	MG-NB	-2.02	2.01	2.05
13	b	509	CLA	CMD-C2D	-2.02	1.46	1.50
13	v	501	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	512	CLA	MG-ND	-2.02	2.01	2.05
13	d	516	CLA	MG-NB	-2.02	2.01	2.05
13	b	504	CLA	CMD-C2D	-2.01	1.46	1.50
13	e	1123	CLA	CMC-C2C	-2.01	1.46	1.50
13	v	506	CLA	CMD-C2D	-2.01	1.46	1.50
13	t	509	CLA	MG-NB	-2.01	2.01	2.05
13	1	509	CLA	CMC-C2C	-2.01	1.46	1.50
13	5	506	CLA	CMC-C2C	-2.01	1.46	1.50
13	Y	513	CLA	CMD-C2D	-2.01	1.46	1.50
13	Z	519	CLA	CMD-C2D	-2.01	1.46	1.50
13	f	1206	CLA	C3B-C4B	2.01	1.47	1.42
13	Z	509	CLA	MG-NB	-2.01	2.01	2.05
13	6	507	CLA	CMB-C2B	-2.01	1.46	1.50
13	Z	516	CLA	CMC-C2C	-2.01	1.46	1.50
13	c	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	q	508	CLA	C1B-NB	-2.01	1.35	1.37
13	3	508	CLA	CHC-C1C	2.01	1.42	1.38
13	Y	501	CLA	CHC-C1C	2.01	1.42	1.38
13	A	1126	CLA	CMB-C2B	-2.01	1.46	1.50
13	s	508	CLA	CHC-C1C	2.01	1.42	1.38
13	B	1012	CLA	C1B-NB	-2.01	1.35	1.37
13	B	1201	CLA	CMB-C2B	-2.01	1.46	1.50
13	6	513	CLA	CMB-C2B	-2.01	1.46	1.50
13	r	507	CLA	CMB-C2B	-2.01	1.46	1.50
13	B	1216	CLA	CHC-C1C	2.01	1.42	1.38
13	B	1235	CLA	C1B-NB	-2.01	1.35	1.37
13	f	1023	CLA	C1B-C2B	2.01	1.48	1.43
13	1	517	CLA	CMC-C2C	-2.01	1.46	1.50
13	u	507	CLA	CMB-C2B	-2.01	1.46	1.50
13	A	1120	CLA	CHC-C1C	2.01	1.42	1.38
13	2	506	CLA	CMD-C2D	-2.01	1.46	1.50
13	Y	516	CLA	CMB-C2B	-2.01	1.46	1.50
13	r	507	CLA	CMC-C2C	-2.01	1.46	1.50
13	Z	508	CLA	CHC-C1C	2.01	1.42	1.38
20	c	822	SQD	O3-C3	-2.01	1.38	1.43
13	H	1232	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	501	CLA	CMB-C2B	-2.01	1.46	1.50
13	u	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	4	516	CLA	MG-NB	-2.01	2.01	2.05
13	H	1212	CLA	MG-ND	-2.01	2.01	2.05
13	H	1216	CLA	CHC-C1C	2.01	1.42	1.38
13	b	509	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	506	CLA	CMD-C2D	-2.01	1.46	1.50
13	b	506	CLA	CMD-C2D	-2.01	1.46	1.50
13	r	518	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	1120	CLA	CHC-C1C	2.01	1.42	1.38
13	v	507	CLA	CMB-C2B	-2.01	1.46	1.50
13	c	516	CLA	MG-NB	-2.01	2.01	2.05
13	G	1104	CLA	C1B-NB	-2.01	1.35	1.37
20	n	5216	SQD	O3-C3	-2.01	1.38	1.43
13	A	1134	CLA	CMC-C2C	-2.01	1.46	1.50
13	d	506	CLA	CMC-C2C	-2.01	1.46	1.50
13	u	509	CLA	CMB-C2B	-2.01	1.46	1.50
13	Y	503	CLA	CMB-C2B	-2.01	1.46	1.50
13	B	1021	CLA	MG-ND	-2.01	2.01	2.05
13	b	516	CLA	MG-NB	-2.01	2.01	2.05
13	Y	513	CLA	CMC-C2C	-2.01	1.46	1.50
13	r	503	CLA	CMC-C2C	-2.01	1.46	1.50
13	u	501	CLA	CMB-C2B	-2.01	1.46	1.50
13	t	513	CLA	CMB-C2B	-2.01	1.46	1.50
13	v	501	CLA	CMD-C2D	-2.01	1.46	1.50
13	1	513	CLA	CMD-C2D	-2.01	1.46	1.50
13	f	1215	CLA	CMC-C2C	-2.01	1.46	1.50
13	r	504	CLA	CMC-C2C	-2.01	1.46	1.50
13	4	509	CLA	MG-NB	-2.01	2.01	2.05
13	V	1502	CLA	CMB-C2B	-2.01	1.46	1.50
13	a	517	CLA	CMB-C2B	-2.01	1.46	1.50
13	q	513	CLA	CMD-C2D	-2.01	1.46	1.50
13	u	504	CLA	CMD-C2D	-2.01	1.46	1.50
13	d	507	CLA	CHC-C1C	2.01	1.42	1.38
13	b	503	CLA	MG-NB	-2.01	2.01	2.05
13	c	505	CLA	MG-NB	-2.01	2.01	2.05
16	A	4002	BCR	C30-C25	-2.00	1.51	1.53
13	n	1503	CLA	CMB-C2B	-2.00	1.46	1.50
13	r	516	CLA	CMB-C2B	-2.00	1.46	1.50
13	t	516	CLA	CMD-C2D	-2.00	1.46	1.50
13	c	510	CLA	CMB-C2B	-2.00	1.46	1.50
13	H	1216	CLA	MG-ND	-2.00	2.01	2.05
13	f	1216	CLA	CHC-C1C	2.00	1.42	1.38
13	A	1114	CLA	C1B-C2B	2.00	1.48	1.43
13	t	516	CLA	MG-NB	-2.00	2.01	2.05
13	A	1115	CLA	CHC-C1C	2.00	1.42	1.38
13	4	502	CLA	CHC-C1C	2.00	1.42	1.38
13	Z	516	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	518	CLA	MG-ND	-2.00	2.01	2.05
13	f	1021	CLA	MG-ND	-2.00	2.01	2.05
13	s	501	CLA	CHC-C1C	2.00	1.42	1.38
13	1	516	CLA	CMB-C2B	-2.00	1.46	1.50
13	6	516	CLA	CMD-C2D	-2.00	1.46	1.50
13	B	1211	CLA	C1B-NB	-2.00	1.35	1.37
13	f	1211	CLA	C1B-NB	-2.00	1.35	1.37
13	6	517	CLA	CMC-C2C	-2.00	1.46	1.50
13	v	510	CLA	CMB-C2B	-2.00	1.46	1.50
13	B	1238	CLA	CHC-C1C	2.00	1.42	1.38
13	v	507	CLA	CHC-C1C	2.00	1.42	1.38
13	A	1104	CLA	C1B-NB	-2.00	1.35	1.37
13	e	1104	CLA	C1B-NB	-2.00	1.35	1.37
13	r	505	CLA	CHC-C1C	2.00	1.42	1.38
13	t	519	CLA	CHC-C1C	2.00	1.42	1.38
13	G	1127	CLA	CMC-C2C	-2.00	1.46	1.50
13	d	516	CLA	CMD-C2D	-2.00	1.46	1.50
13	d	517	CLA	CMC-C2C	-2.00	1.46	1.50
13	Y	508	CLA	C1B-NB	-2.00	1.35	1.37
13	G	1121	CLA	MG-ND	-2.00	2.01	2.05

All (6991) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
14	B	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
13	H	1211	CLA	C4A-NA-C1A	8.99	110.75	106.71
14	H	2002	PQN	C11-C12-C13	-8.98	111.85	126.79
13	B	1211	CLA	C4A-NA-C1A	8.88	110.70	106.71
13	f	1211	CLA	C4A-NA-C1A	8.84	110.68	106.71
13	G	1120	CLA	C4A-NA-C1A	8.25	110.41	106.71
13	e	1120	CLA	C4A-NA-C1A	8.21	110.40	106.71
13	A	1120	CLA	C4A-NA-C1A	8.21	110.39	106.71
13	G	1103	CLA	C4A-NA-C1A	8.20	110.39	106.71
13	A	1103	CLA	C4A-NA-C1A	8.18	110.38	106.71
13	A	1115	CLA	C4A-NA-C1A	8.15	110.37	106.71
13	e	1103	CLA	C4A-NA-C1A	8.12	110.36	106.71
13	e	1115	CLA	C4A-NA-C1A	8.12	110.36	106.71
13	B	1023	CLA	C4A-NA-C1A	8.11	110.35	106.71
13	G	1115	CLA	C4A-NA-C1A	8.11	110.35	106.71
13	f	1201	CLA	C4A-NA-C1A	8.09	110.34	106.71
13	H	1023	CLA	C4A-NA-C1A	8.09	110.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1201	CLA	C4A-NA-C1A	8.08	110.34	106.71
13	H	1201	CLA	C4A-NA-C1A	8.07	110.34	106.71
13	f	1023	CLA	C4A-NA-C1A	8.03	110.32	106.71
13	1	518	CLA	C4A-NA-C1A	7.96	110.28	106.71
13	q	518	CLA	C4A-NA-C1A	7.94	110.28	106.71
13	f	1231	CLA	C4A-NA-C1A	7.91	110.26	106.71
13	B	1224	CLA	C4A-NA-C1A	7.89	110.25	106.71
14	e	2001	PQN	C11-C12-C13	-7.88	113.67	126.79
13	f	1224	CLA	C4A-NA-C1A	7.86	110.24	106.71
14	G	2001	PQN	C11-C12-C13	-7.86	113.70	126.79
13	f	1206	CLA	C4A-NA-C1A	7.85	110.24	106.71
14	A	2001	PQN	C11-C12-C13	-7.84	113.73	126.79
13	B	1206	CLA	C4A-NA-C1A	7.84	110.23	106.71
13	A	1109	CLA	C4A-NA-C1A	7.84	110.23	106.71
13	Y	518	CLA	C4A-NA-C1A	7.82	110.22	106.71
13	G	1109	CLA	C4A-NA-C1A	7.81	110.22	106.71
13	H	1206	CLA	C4A-NA-C1A	7.80	110.21	106.71
13	B	1231	CLA	C4A-NA-C1A	7.78	110.20	106.71
13	e	1109	CLA	C4A-NA-C1A	7.78	110.20	106.71
13	H	1224	CLA	C4A-NA-C1A	7.77	110.20	106.71
13	f	1212	CLA	C4A-NA-C1A	7.74	110.18	106.71
13	H	1231	CLA	C4A-NA-C1A	7.73	110.18	106.71
13	H	1239	CLA	C4A-NA-C1A	7.73	110.18	106.71
13	B	1213	CLA	C4A-NA-C1A	7.68	110.16	106.71
13	e	1125	CLA	C4A-NA-C1A	7.68	110.16	106.71
13	B	1239	CLA	C4A-NA-C1A	7.67	110.16	106.71
13	B	1212	CLA	C4A-NA-C1A	7.66	110.15	106.71
13	V	1502	CLA	C4A-NA-C1A	7.66	110.15	106.71
13	H	1212	CLA	C4A-NA-C1A	7.65	110.15	106.71
13	H	1213	CLA	C4A-NA-C1A	7.65	110.14	106.71
13	G	1105	CLA	C4A-NA-C1A	7.65	110.14	106.71
13	L	1502	CLA	C4A-NA-C1A	7.63	110.14	106.71
13	H	1235	CLA	C4A-NA-C1A	7.62	110.13	106.71
13	f	1213	CLA	C4A-NA-C1A	7.61	110.13	106.71
13	B	1235	CLA	C4A-NA-C1A	7.61	110.13	106.71
13	a	501	CLA	C4A-NA-C1A	7.61	110.13	106.71
13	4	502	CLA	C4A-NA-C1A	7.59	110.12	106.71
13	n	1502	CLA	C4A-NA-C1A	7.59	110.12	106.71
13	A	1125	CLA	C4A-NA-C1A	7.58	110.12	106.71
13	f	1214	CLA	C4A-NA-C1A	7.58	110.11	106.71
13	A	1105	CLA	C4A-NA-C1A	7.57	110.11	106.71
13	e	1113	CLA	C4A-NA-C1A	7.56	110.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1239	CLA	C4A-NA-C1A	7.56	110.11	106.71
13	G	1125	CLA	C4A-NA-C1A	7.56	110.10	106.71
13	f	1235	CLA	C4A-NA-C1A	7.56	110.10	106.71
13	H	1208	CLA	C4A-NA-C1A	7.55	110.10	106.71
13	3	501	CLA	C4A-NA-C1A	7.54	110.10	106.71
13	t	502	CLA	C4A-NA-C1A	7.54	110.10	106.71
13	H	1228	CLA	C4A-NA-C1A	7.53	110.09	106.71
13	b	502	CLA	C4A-NA-C1A	7.53	110.09	106.71
13	A	1113	CLA	C4A-NA-C1A	7.52	110.09	106.71
13	e	1105	CLA	C4A-NA-C1A	7.52	110.09	106.71
13	f	1208	CLA	C4A-NA-C1A	7.50	110.08	106.71
13	s	501	CLA	C4A-NA-C1A	7.50	110.08	106.71
13	B	1228	CLA	C4A-NA-C1A	7.50	110.08	106.71
13	G	1113	CLA	C4A-NA-C1A	7.49	110.07	106.71
13	H	1214	CLA	C4A-NA-C1A	7.48	110.07	106.71
13	B	1208	CLA	C4A-NA-C1A	7.48	110.07	106.71
13	G	1137	CLA	C4A-NA-C1A	7.45	110.06	106.71
13	d	502	CLA	C4A-NA-C1A	7.45	110.06	106.71
13	f	1228	CLA	C4A-NA-C1A	7.45	110.06	106.71
13	6	502	CLA	C4A-NA-C1A	7.44	110.05	106.71
13	3	502	CLA	C4A-NA-C1A	7.44	110.05	106.71
13	G	1133	CLA	C4A-NA-C1A	7.44	110.05	106.71
13	V	1501	CLA	C4A-NA-C1A	7.43	110.05	106.71
13	a	502	CLA	C4A-NA-C1A	7.43	110.05	106.71
13	B	1214	CLA	C4A-NA-C1A	7.43	110.05	106.71
13	v	502	CLA	C4A-NA-C1A	7.42	110.04	106.71
14	e	2001	PQN	C15-C13-C12	-7.41	106.12	121.12
14	G	2001	PQN	C15-C13-C12	-7.41	106.13	121.12
13	L	1501	CLA	C4A-NA-C1A	7.40	110.03	106.71
13	n	1501	CLA	C4A-NA-C1A	7.40	110.03	106.71
13	f	1223	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	A	2001	PQN	C15-C13-C12	-7.39	106.16	121.12
13	A	1137	CLA	C4A-NA-C1A	7.38	110.02	106.71
13	B	1223	CLA	C4A-NA-C1A	7.36	110.02	106.71
13	V	1503	CLA	C4A-NA-C1A	7.36	110.01	106.71
13	B	1202	CLA	C4A-NA-C1A	7.36	110.01	106.71
13	t	517	CLA	C4A-NA-C1A	7.35	110.01	106.71
13	A	1133	CLA	C4A-NA-C1A	7.34	110.01	106.71
13	e	1138	CLA	C4A-NA-C1A	7.34	110.01	106.71
13	s	509	CLA	C4A-NA-C1A	7.34	110.01	106.71
13	A	1138	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	c	501	CLA	C4A-NA-C1A	7.33	110.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1215	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	f	1218	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	B	1210	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	B	1215	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	2	502	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	e	1133	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	s	502	CLA	C4A-NA-C1A	7.32	110.00	106.71
13	4	517	CLA	C4A-NA-C1A	7.32	110.00	106.71
13	H	1202	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	H	1210	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	G	1138	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	l	1302	CLA	C4A-NA-C1A	7.30	109.99	106.71
13	H	1218	CLA	C4A-NA-C1A	7.30	109.99	106.71
13	3	509	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	H	1223	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	f	1210	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	u	501	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	e	1137	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	H	1215	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	a	519	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	b	517	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	5	501	CLA	C4A-NA-C1A	7.27	109.97	106.71
13	B	1218	CLA	C4A-NA-C1A	7.26	109.97	106.71
13	b	518	CLA	C4A-NA-C1A	7.26	109.97	106.71
13	r	501	CLA	C4A-NA-C1A	7.25	109.97	106.71
13	3	519	CLA	C4A-NA-C1A	7.25	109.97	106.71
13	e	1801	CLA	C4A-NA-C1A	7.25	109.97	106.71
13	A	1118	CLA	C4A-NA-C1A	7.24	109.96	106.71
13	H	1205	CLA	C4A-NA-C1A	7.24	109.96	106.71
13	r	502	CLA	C4A-NA-C1A	7.24	109.96	106.71
13	f	1202	CLA	C4A-NA-C1A	7.24	109.96	106.71
13	s	519	CLA	C4A-NA-C1A	7.24	109.96	106.71
13	r	516	CLA	C4A-NA-C1A	7.23	109.96	106.71
13	L	1503	CLA	C4A-NA-C1A	7.23	109.96	106.71
13	Z	502	CLA	C4A-NA-C1A	7.23	109.95	106.71
13	u	502	CLA	C4A-NA-C1A	7.23	109.95	106.71
13	f	1209	CLA	C4A-NA-C1A	7.22	109.95	106.71
13	e	1112	CLA	C4A-NA-C1A	7.22	109.95	106.71
13	n	1503	CLA	C4A-NA-C1A	7.22	109.95	106.71
13	s	513	CLA	C4A-NA-C1A	7.21	109.95	106.71
13	Y	502	CLA	C4A-NA-C1A	7.21	109.95	106.71
13	A	1112	CLA	C4A-NA-C1A	7.20	109.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	509	CLA	C4A-NA-C1A	7.20	109.94	106.71
13	t	518	CLA	C4A-NA-C1A	7.20	109.94	106.71
13	B	1227	CLA	C4A-NA-C1A	7.20	109.94	106.71
13	G	1118	CLA	C4A-NA-C1A	7.20	109.94	106.71
13	Z	501	CLA	C4A-NA-C1A	7.20	109.94	106.71
13	f	1227	CLA	C4A-NA-C1A	7.19	109.94	106.71
13	H	1209	CLA	C4A-NA-C1A	7.19	109.94	106.71
13	a	513	CLA	C4A-NA-C1A	7.19	109.94	106.71
13	Z	516	CLA	C4A-NA-C1A	7.18	109.94	106.71
13	e	1118	CLA	C4A-NA-C1A	7.18	109.93	106.71
13	A	1123	CLA	C4A-NA-C1A	7.18	109.93	106.71
13	B	1209	CLA	C4A-NA-C1A	7.18	109.93	106.71
13	Z	518	CLA	C4A-NA-C1A	7.18	109.93	106.71
13	A	1801	CLA	C4A-NA-C1A	7.17	109.93	106.71
13	2	501	CLA	C4A-NA-C1A	7.17	109.93	106.71
13	a	512	CLA	C4A-NA-C1A	7.16	109.93	106.71
13	b	501	CLA	C4A-NA-C1A	7.16	109.93	106.71
14	H	2002	PQN	C15-C13-C12	-7.16	106.63	121.12
13	s	512	CLA	C4A-NA-C1A	7.16	109.92	106.71
14	B	2002	PQN	C15-C13-C12	-7.16	106.63	121.12
13	4	518	CLA	C4A-NA-C1A	7.16	109.92	106.71
13	2	516	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	f	2002	PQN	C15-C13-C12	-7.15	106.64	121.12
13	A	1101	CLA	C4A-NA-C1A	7.15	109.92	106.71
13	e	1101	CLA	C4A-NA-C1A	7.15	109.92	106.71
13	H	1227	CLA	C4A-NA-C1A	7.15	109.92	106.71
13	J	1302	CLA	C4A-NA-C1A	7.15	109.92	106.71
13	G	1104	CLA	C4A-NA-C1A	7.14	109.92	106.71
13	3	513	CLA	C4A-NA-C1A	7.14	109.92	106.71
13	G	1801	CLA	C4A-NA-C1A	7.14	109.92	106.71
13	e	1123	CLA	C4A-NA-C1A	7.14	109.92	106.71
13	5	502	CLA	C4A-NA-C1A	7.14	109.91	106.71
13	A	1117	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	G	1112	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	G	1101	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	G	1117	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	c	507	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	u	508	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	A	1104	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	1	502	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	T	1302	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	2	518	CLA	C4A-NA-C1A	7.12	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1106	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	t	506	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	5	508	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	e	1117	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	v	501	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	B	1205	CLA	C4A-NA-C1A	7.11	109.90	106.71
13	c	508	CLA	C4A-NA-C1A	7.11	109.90	106.71
13	G	1123	CLA	C4A-NA-C1A	7.11	109.90	106.71
13	u	505	CLA	C4A-NA-C1A	7.11	109.90	106.71
13	u	506	CLA	C4A-NA-C1A	7.11	109.90	106.71
13	4	509	CLA	C4A-NA-C1A	7.10	109.90	106.71
13	q	502	CLA	C4A-NA-C1A	7.10	109.90	106.71
13	r	518	CLA	C4A-NA-C1A	7.10	109.90	106.71
13	3	512	CLA	C4A-NA-C1A	7.09	109.89	106.71
13	t	509	CLA	C4A-NA-C1A	7.09	109.89	106.71
13	A	1106	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	4	506	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	B	1220	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	e	1106	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	b	509	CLA	C4A-NA-C1A	7.07	109.89	106.71
13	t	519	CLA	C4A-NA-C1A	7.07	109.89	106.71
13	A	1122	CLA	C4A-NA-C1A	7.07	109.88	106.71
13	5	507	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	e	1122	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	F	1302	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	Y	509	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	c	502	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	l	1303	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	c	505	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	r	507	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	5	505	CLA	C4A-NA-C1A	7.05	109.88	106.71
13	R	1302	CLA	C4A-NA-C1A	7.05	109.88	106.71
13	6	501	CLA	C4A-NA-C1A	7.05	109.88	106.71
13	T	1303	CLA	C4A-NA-C1A	7.05	109.88	106.71
13	5	506	CLA	C4A-NA-C1A	7.05	109.88	106.71
13	H	1220	CLA	C4A-NA-C1A	7.05	109.88	106.71
13	4	501	CLA	C4A-NA-C1A	7.05	109.87	106.71
13	G	1122	CLA	C4A-NA-C1A	7.05	109.87	106.71
13	d	501	CLA	C4A-NA-C1A	7.05	109.87	106.71
13	q	505	CLA	C4A-NA-C1A	7.04	109.87	106.71
13	c	506	CLA	C4A-NA-C1A	7.04	109.87	106.71
13	J	1303	CLA	C4A-NA-C1A	7.03	109.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	507	CLA	C4A-NA-C1A	7.03	109.87	106.71
13	H	1207	CLA	C4A-NA-C1A	7.03	109.86	106.71
13	1	505	CLA	C4A-NA-C1A	7.02	109.86	106.71
13	1	509	CLA	C4A-NA-C1A	7.02	109.86	106.71
13	r	517	CLA	C4A-NA-C1A	7.02	109.86	106.71
16	n	4019	BCR	C24-C23-C22	-7.02	115.63	126.23
13	3	518	CLA	C4A-NA-C1A	7.01	109.86	106.71
13	b	506	CLA	C4A-NA-C1A	7.01	109.86	106.71
13	e	1104	CLA	C4A-NA-C1A	7.01	109.86	106.71
13	u	507	CLA	C4A-NA-C1A	7.01	109.86	106.71
16	L	4019	BCR	C24-C23-C22	-7.00	115.65	126.23
13	4	519	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	q	509	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	r	513	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	s	518	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	t	510	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	B	1230	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	G	1134	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	f	1205	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	2	507	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	b	519	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	A	1134	CLA	C4A-NA-C1A	6.98	109.85	106.71
16	V	4019	BCR	C24-C23-C22	-6.98	115.69	126.23
13	H	1230	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	2	517	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	e	1134	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	f	1216	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	3	507	CLA	C4A-NA-C1A	6.97	109.84	106.71
13	f	1230	CLA	C4A-NA-C1A	6.97	109.84	106.71
13	t	501	CLA	C4A-NA-C1A	6.97	109.84	106.71
13	e	1136	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	j	1302	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	q	513	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	3	511	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	e	1126	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	f	1220	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	q	504	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	b	513	CLA	C4A-NA-C1A	6.96	109.83	106.71
13	Y	511	CLA	C4A-NA-C1A	6.96	109.83	106.71
13	2	504	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	Z	507	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	4	510	CLA	C4A-NA-C1A	6.95	109.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	513	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	b	510	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	b	512	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	q	507	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	A	1136	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	A	1126	CLA	C4A-NA-C1A	6.94	109.83	106.71
13	f	1021	CLA	C4A-NA-C1A	6.94	109.83	106.71
13	G	1126	CLA	C4A-NA-C1A	6.94	109.83	106.71
13	4	512	CLA	C4A-NA-C1A	6.94	109.82	106.71
13	H	1221	CLA	C4A-NA-C1A	6.94	109.82	106.71
13	Y	505	CLA	C4A-NA-C1A	6.94	109.82	106.71
13	B	1021	CLA	C4A-NA-C1A	6.93	109.82	106.71
13	2	513	CLA	C4A-NA-C1A	6.93	109.82	106.71
13	Y	508	CLA	C4A-NA-C1A	6.93	109.82	106.71
13	v	503	CLA	C4A-NA-C1A	6.93	109.82	106.71
13	B	1207	CLA	C4A-NA-C1A	6.92	109.82	106.71
13	1	504	CLA	C4A-NA-C1A	6.92	109.82	106.71
13	1	511	CLA	C4A-NA-C1A	6.92	109.82	106.71
13	e	1114	CLA	C4A-NA-C1A	6.92	109.82	106.71
13	Z	504	CLA	C4A-NA-C1A	6.92	109.82	106.71
13	s	511	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	A	1114	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	6	503	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	f	1207	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	t	513	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	B	1221	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	a	511	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	u	503	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	G	1114	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	d	512	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	a	518	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	r	504	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	4	513	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	5	503	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	3	506	CLA	C4A-NA-C1A	6.89	109.81	106.71
13	t	512	CLA	C4A-NA-C1A	6.89	109.80	106.71
13	1	503	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	1	508	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	Z	517	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	f	1221	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	u	516	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	1	513	CLA	C4A-NA-C1A	6.87	109.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1136	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	c	516	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	6	506	CLA	C4A-NA-C1A	6.87	109.79	106.71
13	a	506	CLA	C4A-NA-C1A	6.87	109.79	106.71
13	s	504	CLA	C4A-NA-C1A	6.87	109.79	106.71
13	q	508	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	q	511	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	Y	504	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	B	1232	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	q	503	CLA	C4A-NA-C1A	6.85	109.79	106.71
13	K	1105	CLA	C4A-NA-C1A	6.85	109.79	106.71
13	s	506	CLA	C4A-NA-C1A	6.85	109.79	106.71
13	1	507	CLA	C4A-NA-C1A	6.85	109.78	106.71
13	t	504	CLA	C4A-NA-C1A	6.85	109.78	106.71
13	H	1021	CLA	C4A-NA-C1A	6.85	109.78	106.71
13	H	1204	CLA	C4A-NA-C1A	6.85	109.78	106.71
13	v	512	CLA	C4A-NA-C1A	6.85	109.78	106.71
13	f	1232	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	6	507	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	6	512	CLA	C4A-NA-C1A	6.83	109.78	106.71
13	c	503	CLA	C4A-NA-C1A	6.83	109.78	106.71
13	c	513	CLA	C4A-NA-C1A	6.83	109.78	106.71
13	B	1216	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	B	1204	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	d	503	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	s	507	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	Z	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	2	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	b	504	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	H	1232	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	Y	507	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	Y	503	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	5	516	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	4	504	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	f	1204	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	t	507	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	R	1301	CLA	C4A-NA-C1A	6.80	109.77	106.71
13	v	505	CLA	C4A-NA-C1A	6.80	109.77	106.71
13	U	1105	CLA	C4A-NA-C1A	6.80	109.76	106.71
13	r	509	CLA	C4A-NA-C1A	6.80	109.76	106.71
13	3	504	CLA	C4A-NA-C1A	6.79	109.76	106.71
13	v	506	CLA	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	v	507	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	Y	513	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	d	506	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	H	1216	CLA	C4A-NA-C1A	6.77	109.75	106.71
13	5	513	CLA	C4A-NA-C1A	6.77	109.75	106.71
13	r	511	CLA	C4A-NA-C1A	6.76	109.74	106.71
13	a	504	CLA	C4A-NA-C1A	6.75	109.74	106.71
13	m	1105	CLA	C4A-NA-C1A	6.75	109.74	106.71
13	5	510	CLA	C4A-NA-C1A	6.75	109.74	106.71
13	d	507	CLA	C4A-NA-C1A	6.75	109.74	106.71
13	d	505	CLA	C4A-NA-C1A	6.74	109.74	106.71
13	2	509	CLA	C4A-NA-C1A	6.74	109.74	106.71
13	1	501	CLA	C4A-NA-C1A	6.74	109.74	106.71
13	6	505	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	s	505	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	G	1102	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	a	510	CLA	C4A-NA-C1A	6.73	109.73	106.71
13	v	504	CLA	C4A-NA-C1A	6.73	109.73	106.71
13	4	507	CLA	C4A-NA-C1A	6.73	109.73	106.71
13	Z	509	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	F	1301	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	5	504	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	6	504	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	b	503	CLA	C4A-NA-C1A	6.72	109.72	106.71
13	u	510	CLA	C4A-NA-C1A	6.71	109.72	106.71
13	c	519	CLA	C4A-NA-C1A	6.71	109.72	106.71
13	u	504	CLA	C4A-NA-C1A	6.71	109.72	106.71
13	c	510	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	1	517	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	m	1401	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	d	504	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	A	1102	CLA	C4A-NA-C1A	6.69	109.72	106.71
13	v	511	CLA	C4A-NA-C1A	6.69	109.72	106.71
13	u	513	CLA	C4A-NA-C1A	6.69	109.71	106.71
13	d	518	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	e	1102	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	4	503	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	b	507	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	d	519	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	q	501	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	v	519	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	Z	505	CLA	C4A-NA-C1A	6.67	109.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	r	506	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	6	519	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	3	510	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	u	509	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	u	519	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	Y	501	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	e	1131	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	c	509	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	v	509	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	6	511	CLA	C4A-NA-C1A	6.65	109.69	106.71
13	G	1131	CLA	C4A-NA-C1A	6.65	109.69	106.71
13	Y	517	CLA	C4A-NA-C1A	6.65	109.69	106.71
13	u	511	CLA	C4A-NA-C1A	6.65	109.69	106.71
13	2	505	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	3	505	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	2	506	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	e	1013	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	j	1301	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	c	511	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	G	1013	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	e	1110	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	v	513	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	d	508	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	2	512	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	a	505	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	5	509	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	5	519	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	a	503	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	5	511	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	A	1013	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	c	504	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	Z	506	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	U	1401	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	q	517	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	K	1401	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	v	517	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	Y	519	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	s	510	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	t	503	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	v	508	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	a	517	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	A	1131	CLA	C4A-NA-C1A	6.60	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1119	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	A	1110	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	3	517	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	6	517	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	r	512	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	3	503	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	6	508	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	v	518	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	Z	512	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	q	506	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	d	511	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	c	518	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	G	1237	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	6	518	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	s	517	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	u	518	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	A	1237	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	6	509	CLA	C4A-NA-C1A	6.56	109.66	106.71
13	d	509	CLA	C4A-NA-C1A	6.56	109.66	106.71
13	6	513	CLA	C4A-NA-C1A	6.56	109.66	106.71
13	r	503	CLA	C4A-NA-C1A	6.56	109.65	106.71
13	s	503	CLA	C4A-NA-C1A	6.56	109.65	106.71
13	A	1119	CLA	C4A-NA-C1A	6.55	109.65	106.71
13	1	519	CLA	C4A-NA-C1A	6.55	109.65	106.71
13	B	1240	CLA	C4A-NA-C1A	6.55	109.65	106.71
13	2	503	CLA	C4A-NA-C1A	6.55	109.65	106.71
13	q	519	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	G	1110	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	r	505	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	d	513	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	H	1240	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	5	518	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	1	506	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	1	512	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	H	1217	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	f	1217	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	f	1240	CLA	C4A-NA-C1A	6.51	109.64	106.71
13	t	511	CLA	C4A-NA-C1A	6.51	109.64	106.71
13	d	517	CLA	C4A-NA-C1A	6.51	109.63	106.71
13	e	1237	CLA	C4A-NA-C1A	6.51	109.63	106.71
13	Y	512	CLA	C4A-NA-C1A	6.50	109.63	106.71
13	4	511	CLA	C4A-NA-C1A	6.49	109.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	506	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	B	1217	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	q	512	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	G	1119	CLA	C4A-NA-C1A	6.47	109.61	106.71
13	Z	503	CLA	C4A-NA-C1A	6.46	109.61	106.71
13	b	505	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	b	511	CLA	C4A-NA-C1A	6.45	109.60	106.71
13	H	1236	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	v	510	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	G	1111	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	2	508	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	B	1236	CLA	C4A-NA-C1A	6.43	109.59	106.71
13	c	512	CLA	C4A-NA-C1A	6.43	109.59	106.71
13	f	1236	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	u	512	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	r	508	CLA	C4A-NA-C1A	6.40	109.58	106.71
13	e	1111	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	3	516	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	4	505	CLA	C4A-NA-C1A	6.38	109.58	106.71
13	t	505	CLA	C4A-NA-C1A	6.38	109.57	106.71
13	A	1111	CLA	C4A-NA-C1A	6.37	109.57	106.71
13	G	1116	CLA	C4A-NA-C1A	6.36	109.56	106.71
13	d	516	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	5	512	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	6	510	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	e	1127	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	G	1121	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	s	516	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	Z	508	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	a	516	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	G	1124	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	q	510	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	4	508	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	G	1127	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	A	1121	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	6	516	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	G	1129	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	f	1234	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	v	516	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	a	508	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	B	1234	CLA	C4A-NA-C1A	6.30	109.54	106.71
13	1	510	CLA	C4A-NA-C1A	6.29	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1116	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	A	1129	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	A	1124	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	u	517	CLA	C4A-NA-C1A	6.27	109.53	106.71
13	3	508	CLA	C4A-NA-C1A	6.27	109.53	106.71
13	b	508	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	5	517	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	A	1127	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	e	1129	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	t	508	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	U	1103	CLA	C4A-NA-C1A	6.25	109.51	106.71
13	d	510	CLA	C4A-NA-C1A	6.24	109.51	106.71
13	H	1238	CLA	C4A-NA-C1A	6.24	109.51	106.71
13	e	1121	CLA	C4A-NA-C1A	6.23	109.51	106.71
13	B	1238	CLA	C4A-NA-C1A	6.23	109.51	106.71
13	c	517	CLA	C4A-NA-C1A	6.23	109.51	106.71
13	A	1135	CLA	C4A-NA-C1A	6.22	109.50	106.71
13	2	519	CLA	C4A-NA-C1A	6.22	109.50	106.71
13	e	1011	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	e	1116	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	Y	510	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	A	1011	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	G	1011	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	m	1103	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	s	508	CLA	C4A-NA-C1A	6.20	109.49	106.71
16	V	4020	BCR	C24-C23-C22	-6.19	116.88	126.23
16	L	4020	BCR	C24-C23-C22	-6.19	116.89	126.23
13	K	1103	CLA	C4A-NA-C1A	6.18	109.49	106.71
13	H	1234	CLA	C4A-NA-C1A	6.18	109.48	106.71
13	f	1238	CLA	C4A-NA-C1A	6.18	109.48	106.71
16	n	4020	BCR	C24-C23-C22	-6.18	116.90	126.23
13	Z	519	CLA	C4A-NA-C1A	6.18	109.48	106.71
13	B	1229	CLA	C4A-NA-C1A	6.17	109.48	106.71
13	e	1124	CLA	C4A-NA-C1A	6.16	109.48	106.71
13	G	1135	CLA	C4A-NA-C1A	6.14	109.47	106.71
13	e	1135	CLA	C4A-NA-C1A	6.14	109.47	106.71
13	A	1130	CLA	C4A-NA-C1A	6.14	109.47	106.71
13	f	1225	CLA	C4A-NA-C1A	6.14	109.47	106.71
13	H	1229	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	r	519	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	f	1229	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	e	1108	CLA	C4A-NA-C1A	6.12	109.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	510	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	t	516	CLA	C4A-NA-C1A	6.10	109.45	106.71
16	G	4007	BCR	C3-C4-C5	-6.10	103.18	114.08
13	H	1226	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	f	1203	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	B	1226	CLA	C4A-NA-C1A	6.09	109.45	106.71
16	A	4007	BCR	C3-C4-C5	-6.09	103.20	114.08
13	B	1225	CLA	C4A-NA-C1A	6.09	109.44	106.71
13	b	516	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	G	1130	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	e	1107	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	B	1203	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	e	1130	CLA	C4A-NA-C1A	6.08	109.44	106.71
16	e	4007	BCR	C3-C4-C5	-6.08	103.22	114.08
13	4	516	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	A	1108	CLA	C4A-NA-C1A	6.07	109.43	106.71
13	H	1203	CLA	C4A-NA-C1A	6.07	109.43	106.71
13	G	1107	CLA	C4A-NA-C1A	6.06	109.43	106.71
13	H	1226	CLA	CMB-C2B-C1B	-6.06	116.14	125.37
13	f	1226	CLA	C4A-NA-C1A	6.06	109.43	106.71
13	B	1226	CLA	CMB-C2B-C1B	-6.05	116.16	125.37
13	A	1107	CLA	C4A-NA-C1A	6.03	109.42	106.71
13	f	1226	CLA	CMB-C2B-C1B	-6.03	116.19	125.37
13	G	1108	CLA	C4A-NA-C1A	6.02	109.41	106.71
13	2	510	CLA	C4A-NA-C1A	6.02	109.41	106.71
13	r	510	CLA	C4A-NA-C1A	5.99	109.40	106.71
13	1	516	CLA	C4A-NA-C1A	5.97	109.39	106.71
13	H	1225	CLA	C4A-NA-C1A	5.97	109.39	106.71
16	B	4010	BCR	C15-C14-C13	-5.93	118.84	127.31
13	q	516	CLA	C4A-NA-C1A	5.93	109.37	106.71
16	G	4008	BCR	C24-C23-C22	-5.93	117.27	126.23
16	f	4010	BCR	C15-C14-C13	-5.92	118.86	127.31
16	A	4008	BCR	C24-C23-C22	-5.92	117.29	126.23
16	H	4010	BCR	C15-C14-C13	-5.91	118.88	127.31
16	e	4008	BCR	C24-C23-C22	-5.91	117.31	126.23
13	G	1140	CLA	C4A-NA-C1A	5.89	109.36	106.71
16	l	4013	BCR	C20-C21-C22	-5.89	118.90	127.31
13	e	1022	CLA	C4A-NA-C1A	5.89	109.35	106.71
16	J	4013	BCR	C20-C21-C22	-5.89	118.91	127.31
16	T	4013	BCR	C20-C21-C22	-5.89	118.91	127.31
13	e	1140	CLA	C4A-NA-C1A	5.89	109.35	106.71
13	Y	516	CLA	C4A-NA-C1A	5.88	109.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	524	BCR	C7-C8-C9	-5.87	117.36	126.23
13	A	1022	CLA	C4A-NA-C1A	5.87	109.34	106.71
13	H	1222	CLA	C4A-NA-C1A	5.87	109.34	106.71
13	A	1140	CLA	C4A-NA-C1A	5.86	109.34	106.71
13	G	1022	CLA	C4A-NA-C1A	5.84	109.33	106.71
16	6	524	BCR	C7-C8-C9	-5.83	117.42	126.23
16	d	524	BCR	C7-C8-C9	-5.83	117.42	126.23
13	f	1219	CLA	C4A-NA-C1A	5.82	109.32	106.71
13	B	1219	CLA	C4A-NA-C1A	5.82	109.32	106.71
13	B	1222	CLA	C4A-NA-C1A	5.82	109.32	106.71
13	f	1222	CLA	C4A-NA-C1A	5.77	109.30	106.71
13	H	1219	CLA	C4A-NA-C1A	5.75	109.29	106.71
13	e	1139	CLA	C4A-NA-C1A	5.72	109.28	106.71
16	H	4006	BCR	C7-C8-C9	-5.66	117.68	126.23
16	B	4006	BCR	C7-C8-C9	-5.65	117.70	126.23
13	G	1139	CLA	C4A-NA-C1A	5.64	109.24	106.71
16	f	4006	BCR	C7-C8-C9	-5.63	117.73	126.23
13	A	1139	CLA	C4A-NA-C1A	5.59	109.22	106.71
13	A	1132	CLA	C4A-NA-C1A	5.55	109.20	106.71
13	G	1132	CLA	C4A-NA-C1A	5.50	109.18	106.71
13	G	1128	CLA	C4A-NA-C1A	5.47	109.17	106.71
13	e	1132	CLA	C4A-NA-C1A	5.45	109.16	106.71
13	A	1128	CLA	C4A-NA-C1A	5.44	109.15	106.71
13	e	1128	CLA	C4A-NA-C1A	5.44	109.15	106.71
16	G	4008	BCR	C20-C21-C22	-5.35	119.67	127.31
16	A	4008	BCR	C20-C21-C22	-5.33	119.70	127.31
16	e	4008	BCR	C20-C21-C22	-5.33	119.71	127.31
16	B	4006	BCR	C24-C23-C22	-5.32	118.19	126.23
13	e	1013	CLA	CMB-C2B-C1B	-5.32	117.27	125.37
16	H	4006	BCR	C24-C23-C22	-5.31	118.21	126.23
13	A	1013	CLA	CMB-C2B-C1B	-5.30	117.29	125.37
16	f	4006	BCR	C24-C23-C22	-5.30	118.23	126.23
16	H	4004	BCR	C20-C21-C22	-5.29	119.76	127.31
13	G	1013	CLA	CMB-C2B-C1B	-5.29	117.31	125.37
16	f	4004	BCR	C20-C21-C22	-5.28	119.77	127.31
16	B	4004	BCR	C20-C21-C22	-5.26	119.80	127.31
13	e	1128	CLA	CMB-C2B-C1B	-5.25	117.37	125.37
13	A	1128	CLA	CMB-C2B-C1B	-5.24	117.39	125.37
13	G	1128	CLA	CMB-C2B-C1B	-5.23	117.41	125.37
16	J	4015	BCR	C7-C8-C9	-5.18	118.40	126.23
16	l	4015	BCR	C7-C8-C9	-5.17	118.42	126.23
16	T	4015	BCR	C7-C8-C9	-5.17	118.42	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4022	BCR	C1-C6-C5	-5.17	115.34	122.61
16	V	4022	BCR	C1-C6-C5	-5.15	115.36	122.61
16	n	4022	BCR	C1-C6-C5	-5.14	115.37	122.61
16	R	4016	BCR	C15-C14-C13	-5.14	119.98	127.31
14	A	2001	PQN	C14-C13-C12	-5.13	110.52	123.68
16	j	4016	BCR	C15-C14-C13	-5.13	119.99	127.31
16	F	4016	BCR	C15-C14-C13	-5.12	120.00	127.31
14	e	2001	PQN	C14-C13-C12	-5.12	110.55	123.68
20	V	5216	SQD	O7-S-C6	5.12	113.02	106.94
14	G	2001	PQN	C14-C13-C12	-5.12	110.56	123.68
16	e	4011	BCR	C7-C8-C9	-5.10	118.54	126.23
20	L	5216	SQD	O7-S-C6	5.09	112.99	106.94
16	G	4011	BCR	C7-C8-C9	-5.08	118.56	126.23
16	A	4011	BCR	C7-C8-C9	-5.08	118.56	126.23
16	l	4013	BCR	C16-C17-C18	-5.07	120.07	127.31
14	H	2002	PQN	C14-C13-C12	-5.06	110.69	123.68
20	n	5216	SQD	O7-S-C6	5.06	112.95	106.94
14	B	2002	PQN	C14-C13-C12	-5.05	110.72	123.68
13	q	516	CLA	CAC-C3C-C4C	5.05	131.36	124.81
16	T	4013	BCR	C16-C17-C18	-5.04	120.11	127.31
14	f	2002	PQN	C14-C13-C12	-5.04	110.74	123.68
16	H	4014	BCR	C24-C23-C22	-5.04	118.62	126.23
16	B	4014	BCR	C24-C23-C22	-5.04	118.63	126.23
16	J	4013	BCR	C16-C17-C18	-5.03	120.12	127.31
13	1	516	CLA	CAC-C3C-C4C	5.03	131.34	124.81
16	V	4219	BCR	C15-C14-C13	-5.02	120.14	127.31
13	Y	516	CLA	CAC-C3C-C4C	5.02	131.32	124.81
16	n	4219	BCR	C15-C14-C13	-5.01	120.16	127.31
16	L	4219	BCR	C15-C14-C13	-5.00	120.18	127.31
16	f	4014	BCR	C24-C23-C22	-4.99	118.69	126.23
16	G	4007	BCR	C28-C27-C26	-4.96	105.21	114.08
16	A	4007	BCR	C28-C27-C26	-4.96	105.21	114.08
16	e	4007	BCR	C28-C27-C26	-4.96	105.22	114.08
16	G	4002	BCR	C16-C17-C18	-4.95	120.25	127.31
13	s	516	CLA	CAC-C3C-C4C	4.94	131.23	124.81
13	3	516	CLA	CAC-C3C-C4C	4.94	131.22	124.81
13	a	516	CLA	CAC-C3C-C4C	4.94	131.22	124.81
16	e	4002	BCR	C16-C17-C18	-4.93	120.28	127.31
16	V	4022	BCR	C7-C8-C9	-4.93	118.79	126.23
16	A	4002	BCR	C16-C17-C18	-4.92	120.29	127.31
13	H	1012	CLA	C4A-NA-C1A	4.92	108.92	106.71
13	f	1012	CLA	C4A-NA-C1A	4.91	108.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	4022	BCR	C7-C8-C9	-4.91	118.81	126.23
16	L	4022	BCR	C7-C8-C9	-4.90	118.83	126.23
20	B	1852	SQD	O7-S-C6	4.90	112.76	106.94
20	f	1852	SQD	O7-S-C6	4.89	112.75	106.94
20	H	1852	SQD	O7-S-C6	4.87	112.73	106.94
13	B	1012	CLA	C4A-NA-C1A	4.86	108.89	106.71
13	G	1117	CLA	O2D-CGD-O1D	-4.84	114.38	123.84
13	A	1117	CLA	O2D-CGD-O1D	-4.83	114.40	123.84
13	e	1117	CLA	O2D-CGD-O1D	-4.82	114.41	123.84
13	B	1023	CLA	CAC-C3C-C4C	4.78	131.01	124.81
13	f	1023	CLA	CAC-C3C-C4C	4.76	130.99	124.81
13	H	1023	CLA	CAC-C3C-C4C	4.75	130.97	124.81
16	G	4002	BCR	C7-C8-C9	-4.69	119.15	126.23
13	f	1226	CLA	C2D-C1D-ND	-4.68	106.65	110.10
16	A	4002	BCR	C7-C8-C9	-4.68	119.17	126.23
16	u	522	BCR	C15-C14-C13	-4.68	120.63	127.31
16	f	4010	BCR	C15-C16-C17	-4.68	113.89	123.47
16	H	4010	BCR	C15-C16-C17	-4.68	113.89	123.47
16	a	524	BCR	C15-C14-C13	-4.68	120.64	127.31
16	B	4010	BCR	C15-C16-C17	-4.67	113.90	123.47
16	c	522	BCR	C15-C14-C13	-4.66	120.65	127.31
16	e	4002	BCR	C7-C8-C9	-4.66	119.19	126.23
16	5	522	BCR	C15-C14-C13	-4.66	120.66	127.31
16	s	524	BCR	C15-C14-C13	-4.66	120.66	127.31
16	3	524	BCR	C15-C14-C13	-4.65	120.67	127.31
13	B	1226	CLA	C2D-C1D-ND	-4.62	106.70	110.10
16	H	4004	BCR	C15-C14-C13	-4.61	120.72	127.31
16	H	4010	BCR	C11-C10-C9	-4.61	120.72	127.31
16	V	4020	BCR	C16-C17-C18	-4.61	120.72	127.31
16	f	4004	BCR	C15-C14-C13	-4.61	120.73	127.31
16	B	4010	BCR	C11-C10-C9	-4.61	120.73	127.31
16	B	4004	BCR	C15-C14-C13	-4.61	120.73	127.31
16	Z	521	BCR	C28-C27-C26	-4.60	105.86	114.08
16	B	4014	BCR	C20-C21-C22	-4.60	120.75	127.31
16	f	4010	BCR	C11-C10-C9	-4.59	120.75	127.31
13	A	1011	CLA	O2D-CGD-CBD	4.59	119.43	111.27
16	n	4020	BCR	C16-C17-C18	-4.59	120.75	127.31
16	L	4020	BCR	C16-C17-C18	-4.59	120.75	127.31
16	s	523	BCR	C15-C14-C13	-4.59	120.76	127.31
16	3	523	BCR	C15-C14-C13	-4.59	120.76	127.31
16	j	4016	BCR	C11-C10-C9	-4.59	120.76	127.31
16	f	4014	BCR	C20-C21-C22	-4.59	120.76	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4014	BCR	C20-C21-C22	-4.58	120.77	127.31
16	r	521	BCR	C28-C27-C26	-4.58	105.89	114.08
13	G	1011	CLA	O2D-CGD-CBD	4.58	119.41	111.27
16	c	523	BCR	C15-C14-C13	-4.58	120.77	127.31
16	V	4019	BCR	C7-C8-C9	-4.58	119.31	126.23
16	5	523	BCR	C15-C14-C13	-4.58	120.77	127.31
16	e	4001	BCR	C16-C17-C18	-4.58	120.77	127.31
16	H	4004	BCR	C16-C17-C18	-4.58	120.77	127.31
16	2	521	BCR	C28-C27-C26	-4.58	105.90	114.08
16	F	4016	BCR	C11-C10-C9	-4.58	120.78	127.31
16	B	4004	BCR	C16-C17-C18	-4.58	120.78	127.31
13	e	1011	CLA	O2D-CGD-CBD	4.57	119.39	111.27
16	A	4001	BCR	C16-C17-C18	-4.57	120.79	127.31
16	a	523	BCR	C15-C14-C13	-4.56	120.80	127.31
16	G	4001	BCR	C16-C17-C18	-4.56	120.80	127.31
16	u	523	BCR	C15-C14-C13	-4.56	120.80	127.31
16	f	4004	BCR	C16-C17-C18	-4.56	120.81	127.31
16	R	4016	BCR	C11-C10-C9	-4.55	120.82	127.31
13	H	1226	CLA	C2D-C1D-ND	-4.55	106.75	110.10
16	L	4019	BCR	C7-C8-C9	-4.54	119.37	126.23
16	n	4019	BCR	C7-C8-C9	-4.54	119.38	126.23
16	A	4003	BCR	C7-C8-C9	-4.53	119.39	126.23
16	G	4003	BCR	C7-C8-C9	-4.53	119.40	126.23
16	H	4009	BCR	C7-C8-C9	-4.53	119.40	126.23
16	f	4014	BCR	C16-C17-C18	-4.52	120.86	127.31
16	B	4014	BCR	C16-C17-C18	-4.52	120.86	127.31
16	v	521	BCR	C16-C17-C18	-4.51	120.87	127.31
16	e	4003	BCR	C7-C8-C9	-4.51	119.42	126.23
16	6	521	BCR	C20-C21-C22	-4.51	120.88	127.31
16	v	521	BCR	C20-C21-C22	-4.50	120.88	127.31
16	6	521	BCR	C16-C17-C18	-4.50	120.89	127.31
16	B	4009	BCR	C7-C8-C9	-4.50	119.44	126.23
16	d	521	BCR	C16-C17-C18	-4.50	120.89	127.31
16	f	4009	BCR	C7-C8-C9	-4.50	119.44	126.23
16	H	4014	BCR	C16-C17-C18	-4.49	120.91	127.31
16	m	4104	BCR	C7-C8-C9	-4.49	119.45	126.23
16	d	521	BCR	C20-C21-C22	-4.48	120.92	127.31
16	s	522	BCR	C15-C14-C13	-4.47	120.93	127.31
16	K	4104	BCR	C7-C8-C9	-4.46	119.49	126.23
16	3	522	BCR	C15-C14-C13	-4.45	120.96	127.31
16	a	522	BCR	C15-C14-C13	-4.45	120.97	127.31
20	b	822	SQD	O47-C7-C8	4.44	119.26	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	822	SQD	O47-C7-C8	4.43	119.25	111.09
16	3	522	BCR	C11-C10-C9	-4.43	120.98	127.31
16	A	4003	BCR	C16-C17-C18	-4.43	120.99	127.31
13	e	1128	CLA	CHB-C1B-NB	4.43	128.95	124.26
20	t	822	SQD	O47-C7-C8	4.43	119.24	111.09
16	a	522	BCR	C11-C10-C9	-4.42	121.00	127.31
16	U	4104	BCR	C7-C8-C9	-4.42	119.55	126.23
16	l	4012	BCR	C20-C21-C22	-4.42	121.00	127.31
16	q	522	BCR	C11-C10-C9	-4.42	121.00	127.31
16	Y	522	BCR	C11-C10-C9	-4.42	121.01	127.31
16	e	4003	BCR	C16-C17-C18	-4.41	121.02	127.31
16	f	4010	BCR	C3-C4-C5	-4.40	106.21	114.08
13	G	1128	CLA	CHB-C1B-NB	4.40	128.92	124.26
16	s	522	BCR	C11-C10-C9	-4.40	121.03	127.31
16	1	522	BCR	C11-C10-C9	-4.40	121.03	127.31
13	A	1128	CLA	CHB-C1B-NB	4.40	128.92	124.26
16	B	4010	BCR	C3-C4-C5	-4.40	106.22	114.08
16	4	524	BCR	C15-C14-C13	-4.40	121.03	127.31
20	q	822	SQD	O5-C5-C4	4.40	117.68	109.69
20	1	822	SQD	O5-C5-C4	4.39	117.67	109.69
20	Y	822	SQD	O5-C5-C4	4.39	117.67	109.69
16	t	524	BCR	C15-C14-C13	-4.39	121.05	127.31
16	H	4010	BCR	C3-C4-C5	-4.39	106.24	114.08
16	S	4018	BCR	C24-C23-C22	-4.38	119.61	126.23
16	G	4003	BCR	C16-C17-C18	-4.38	121.06	127.31
20	H	1852	SQD	O5-C5-C4	4.38	117.64	109.69
16	T	4012	BCR	C20-C21-C22	-4.37	121.07	127.31
16	J	4012	BCR	C20-C21-C22	-4.37	121.07	127.31
16	b	524	BCR	C15-C14-C13	-4.36	121.08	127.31
20	B	1852	SQD	O5-C5-C4	4.36	117.61	109.69
16	d	524	BCR	C15-C14-C13	-4.36	121.09	127.31
20	f	1852	SQD	O5-C5-C4	4.36	117.61	109.69
16	I	4018	BCR	C24-C23-C22	-4.35	119.66	126.23
13	B	1232	CLA	CMB-C2B-C1B	-4.35	118.74	125.37
13	H	1232	CLA	CMB-C2B-C1B	-4.35	118.74	125.37
16	c	524	BCR	C15-C14-C13	-4.35	121.10	127.31
13	f	1232	CLA	CMB-C2B-C1B	-4.34	118.75	125.37
16	6	524	BCR	C15-C14-C13	-4.34	121.11	127.31
16	1	524	BCR	C15-C14-C13	-4.33	121.13	127.31
16	5	524	BCR	C15-C14-C13	-4.32	121.14	127.31
16	u	524	BCR	C15-C14-C13	-4.32	121.14	127.31
16	v	524	BCR	C15-C14-C13	-4.32	121.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	l	4015	BCR	C15-C14-C13	-4.32	121.14	127.31
16	T	4015	BCR	C15-C14-C13	-4.32	121.15	127.31
16	k	4018	BCR	C24-C23-C22	-4.31	119.72	126.23
13	H	1234	CLA	CMB-C2B-C1B	-4.31	118.80	125.37
13	B	1234	CLA	CMB-C2B-C1B	-4.31	118.80	125.37
16	J	4015	BCR	C15-C14-C13	-4.31	121.16	127.31
16	m	4104	BCR	C20-C21-C22	-4.31	121.16	127.31
16	q	524	BCR	C15-C14-C13	-4.30	121.17	127.31
13	f	1234	CLA	CMB-C2B-C1B	-4.30	118.82	125.37
16	v	522	BCR	C15-C14-C13	-4.30	121.18	127.31
16	Y	524	BCR	C15-C14-C13	-4.29	121.18	127.31
16	e	4011	BCR	C28-C27-C26	-4.29	106.42	114.08
16	m	4104	BCR	C15-C14-C13	-4.29	121.19	127.31
16	U	4104	BCR	C15-C14-C13	-4.29	121.19	127.31
16	U	4104	BCR	C20-C21-C22	-4.28	121.19	127.31
16	K	4104	BCR	C20-C21-C22	-4.28	121.20	127.31
16	Z	524	BCR	C15-C14-C13	-4.28	121.20	127.31
16	G	4011	BCR	C28-C27-C26	-4.28	106.43	114.08
16	A	4011	BCR	C28-C27-C26	-4.28	106.43	114.08
17	B	1842	LHG	O4-P-O5	4.28	133.40	112.24
17	f	1842	LHG	O4-P-O5	4.28	133.40	112.24
16	2	524	BCR	C15-C14-C13	-4.28	121.20	127.31
17	H	1842	LHG	O4-P-O5	4.28	133.39	112.24
16	6	522	BCR	C15-C14-C13	-4.27	121.21	127.31
16	K	4104	BCR	C15-C14-C13	-4.27	121.21	127.31
16	d	522	BCR	C15-C14-C13	-4.27	121.22	127.31
16	s	522	BCR	C3-C4-C5	-4.26	106.47	114.08
16	j	4016	BCR	C24-C23-C22	-4.26	119.80	126.23
17	A	5006	LHG	O4-P-O5	4.26	133.28	112.24
16	a	522	BCR	C3-C4-C5	-4.25	106.48	114.08
16	r	524	BCR	C15-C14-C13	-4.25	121.24	127.31
17	e	5006	LHG	O4-P-O5	4.25	133.27	112.24
16	3	522	BCR	C3-C4-C5	-4.25	106.48	114.08
16	e	4008	BCR	C16-C17-C18	-4.25	121.24	127.31
17	e	5004	LHG	O4-P-O5	4.25	133.24	112.24
16	t	521	BCR	C7-C8-C9	-4.25	119.82	126.23
16	G	4007	BCR	C15-C14-C13	-4.25	121.25	127.31
17	G	5006	LHG	O4-P-O5	4.24	133.22	112.24
17	G	5004	LHG	O4-P-O5	4.24	133.22	112.24
16	n	4019	BCR	C15-C14-C13	-4.24	121.26	127.31
16	G	4008	BCR	C16-C17-C18	-4.24	121.26	127.31
17	A	5004	LHG	O4-P-O5	4.24	133.19	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	4	521	BCR	C7-C8-C9	-4.24	119.83	126.23
16	5	521	BCR	C20-C21-C22	-4.23	121.27	127.31
16	e	4007	BCR	C15-C14-C13	-4.23	121.27	127.31
16	u	521	BCR	C20-C21-C22	-4.23	121.27	127.31
16	c	521	BCR	C20-C21-C22	-4.23	121.28	127.31
16	A	4007	BCR	C15-C14-C13	-4.23	121.28	127.31
17	G	5009	LHG	O4-P-O5	4.23	133.14	112.24
16	A	4008	BCR	C16-C17-C18	-4.23	121.28	127.31
16	2	521	BCR	C15-C14-C13	-4.23	121.28	127.31
16	L	4019	BCR	C15-C14-C13	-4.23	121.28	127.31
17	A	5009	LHG	O4-P-O5	4.22	133.12	112.24
17	e	5009	LHG	O4-P-O5	4.22	133.12	112.24
16	b	521	BCR	C7-C8-C9	-4.22	119.86	126.23
17	e	5003	LHG	O4-P-O5	4.22	133.11	112.24
17	G	5003	LHG	O4-P-O5	4.22	133.11	112.24
16	F	4016	BCR	C24-C23-C22	-4.22	119.86	126.23
17	A	5003	LHG	O4-P-O5	4.21	133.07	112.24
16	r	521	BCR	C15-C14-C13	-4.21	121.30	127.31
16	R	4016	BCR	C24-C23-C22	-4.21	119.88	126.23
16	V	4019	BCR	C15-C14-C13	-4.21	121.31	127.31
20	d	822	SQD	O47-C7-C8	4.20	118.82	111.09
17	e	5002	LHG	O4-P-O5	4.20	133.01	112.24
16	q	521	BCR	C16-C17-C18	-4.20	121.32	127.31
17	A	5002	LHG	O4-P-O5	4.20	132.99	112.24
16	k	4018	BCR	C7-C8-C9	-4.20	119.89	126.23
16	S	4018	BCR	C7-C8-C9	-4.19	119.90	126.23
17	G	5002	LHG	O4-P-O5	4.19	132.97	112.24
17	L	5218	LHG	O4-P-O5	4.19	132.97	112.24
17	n	5218	LHG	O4-P-O5	4.19	132.96	112.24
20	u	822	SQD	O9-S-C6	4.19	111.92	106.94
17	V	5218	LHG	O4-P-O5	4.19	132.95	112.24
20	c	822	SQD	O9-S-C6	4.19	111.91	106.94
16	Z	521	BCR	C15-C14-C13	-4.18	121.34	127.31
16	I	4018	BCR	C7-C8-C9	-4.18	119.92	126.23
20	5	822	SQD	O9-S-C6	4.18	111.91	106.94
16	1	521	BCR	C16-C17-C18	-4.18	121.34	127.31
13	e	1132	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
17	e	5008	LHG	O4-P-O5	4.18	132.90	112.24
13	A	1132	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
17	A	5008	LHG	O4-P-O5	4.17	132.87	112.24
17	G	5008	LHG	O4-P-O5	4.17	132.86	112.24
13	G	1132	CLA	O2D-CGD-O1D	-4.17	115.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	822	SQD	O47-C7-C8	4.17	118.76	111.09
17	n	5220	LHG	O4-P-O5	4.16	132.83	112.24
16	T	4015	BCR	C16-C17-C18	-4.16	121.37	127.31
13	e	1011	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
20	v	822	SQD	O47-C7-C8	4.16	118.75	111.09
16	Y	521	BCR	C16-C17-C18	-4.16	121.37	127.31
17	L	5220	LHG	O4-P-O5	4.16	132.81	112.24
13	B	1209	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
17	V	5220	LHG	O4-P-O5	4.16	132.79	112.24
13	G	1011	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
13	H	1209	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
16	f	4004	BCR	C24-C23-C22	-4.15	119.96	126.23
13	A	1011	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
13	f	1209	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
17	S	5001	LHG	O4-P-O5	4.15	132.76	112.24
17	I	5001	LHG	O4-P-O5	4.15	132.76	112.24
16	t	521	BCR	C16-C17-C18	-4.15	121.39	127.31
16	J	4015	BCR	C16-C17-C18	-4.15	121.39	127.31
17	k	5001	LHG	O4-P-O5	4.15	132.75	112.24
16	l	4015	BCR	C16-C17-C18	-4.14	121.40	127.31
16	b	521	BCR	C16-C17-C18	-4.14	121.40	127.31
16	e	4008	BCR	C15-C14-C13	-4.14	121.40	127.31
16	n	4022	BCR	C11-C10-C9	-4.13	121.41	127.31
20	H	1852	SQD	O47-C7-C8	4.13	120.41	111.50
16	4	522	BCR	C15-C16-C17	-4.13	115.01	123.47
16	t	522	BCR	C15-C16-C17	-4.13	115.01	123.47
17	G	5007	LHG	O4-P-O5	4.13	132.66	112.24
16	4	521	BCR	C16-C17-C18	-4.13	121.42	127.31
17	e	5007	LHG	O4-P-O5	4.13	132.64	112.24
17	A	5007	LHG	O4-P-O5	4.13	132.63	112.24
20	f	1852	SQD	O47-C7-C8	4.12	120.39	111.50
20	B	1852	SQD	O47-C7-C8	4.12	120.39	111.50
16	G	4008	BCR	C15-C14-C13	-4.12	121.43	127.31
16	H	4004	BCR	C24-C23-C22	-4.12	120.01	126.23
16	B	4004	BCR	C24-C23-C22	-4.12	120.01	126.23
16	Y	524	BCR	C16-C17-C18	-4.12	121.43	127.31
16	b	522	BCR	C15-C16-C17	-4.11	115.05	123.47
16	A	4008	BCR	C15-C14-C13	-4.11	121.44	127.31
17	e	5005	LHG	O4-P-O5	4.11	132.56	112.24
17	A	5005	LHG	O4-P-O5	4.11	132.56	112.24
16	1	524	BCR	C16-C17-C18	-4.11	121.45	127.31
17	e	5001	LHG	O4-P-O5	4.10	132.51	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	r	521	BCR	C20-C21-C22	-4.10	121.46	127.31
17	A	5001	LHG	O4-P-O5	4.10	132.50	112.24
17	G	5005	LHG	O4-P-O5	4.10	132.50	112.24
16	q	524	BCR	C16-C17-C18	-4.10	121.46	127.31
20	f	1852	SQD	C1-O5-C5	4.09	121.72	113.69
17	G	5001	LHG	O4-P-O5	4.09	132.47	112.24
17	V	5221	LHG	O4-P-O5	4.09	132.47	112.24
16	L	4022	BCR	C11-C10-C9	-4.09	121.47	127.31
17	n	5221	LHG	O4-P-O5	4.09	132.47	112.24
20	B	1852	SQD	C1-O5-C5	4.09	121.71	113.69
20	H	1852	SQD	C1-O5-C5	4.09	121.71	113.69
17	L	5221	LHG	O4-P-O5	4.09	132.45	112.24
16	d	523	BCR	C15-C14-C13	-4.09	121.48	127.31
17	H	1855	LHG	O4-P-O5	4.08	132.43	112.24
17	f	1855	LHG	O4-P-O5	4.08	132.43	112.24
17	B	1855	LHG	O4-P-O5	4.08	132.42	112.24
16	2	521	BCR	C20-C21-C22	-4.08	121.49	127.31
16	6	523	BCR	C15-C14-C13	-4.07	121.50	127.31
16	d	524	BCR	C16-C17-C18	-4.07	121.50	127.31
16	Z	521	BCR	C20-C21-C22	-4.07	121.50	127.31
16	V	4022	BCR	C11-C10-C9	-4.07	121.51	127.31
16	v	524	BCR	C16-C17-C18	-4.07	121.51	127.31
16	6	524	BCR	C16-C17-C18	-4.07	121.51	127.31
13	f	1209	CLA	O2D-CGD-CBD	4.06	118.48	111.27
13	H	1209	CLA	O2D-CGD-CBD	4.06	118.48	111.27
16	f	4010	BCR	C7-C8-C9	-4.05	120.11	126.23
16	4	522	BCR	C15-C14-C13	-4.05	121.53	127.31
13	A	1801	CLA	CAA-CBA-CGA	-4.05	101.75	112.51
13	e	1801	CLA	CAA-CBA-CGA	-4.05	101.76	112.51
16	H	4010	BCR	C7-C8-C9	-4.05	120.11	126.23
13	G	1801	CLA	CAA-CBA-CGA	-4.05	101.76	112.51
16	B	4010	BCR	C7-C8-C9	-4.05	120.11	126.23
13	B	1209	CLA	O2D-CGD-CBD	4.05	118.46	111.27
16	b	522	BCR	C15-C14-C13	-4.05	121.53	127.31
13	e	1011	CLA	C1D-ND-C4D	-4.05	103.46	106.33
16	v	523	BCR	C15-C14-C13	-4.05	121.54	127.31
16	f	4010	BCR	C24-C23-C22	-4.04	120.12	126.23
16	4	522	BCR	C24-C23-C22	-4.04	120.14	126.23
16	H	4005	BCR	C7-C8-C9	-4.04	120.14	126.23
16	t	522	BCR	C15-C14-C13	-4.04	121.55	127.31
16	H	4010	BCR	C24-C23-C22	-4.03	120.14	126.23
16	B	4010	BCR	C24-C23-C22	-4.03	120.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	n	5216	SQD	O9-S-O7	-4.03	100.01	113.95
20	V	5216	SQD	O9-S-O7	-4.03	100.01	113.95
20	L	5216	SQD	O9-S-O7	-4.02	100.02	113.95
16	A	4001	BCR	C3-C4-C5	-4.02	106.89	114.08
16	B	4005	BCR	C7-C8-C9	-4.02	120.16	126.23
16	e	4001	BCR	C3-C4-C5	-4.02	106.90	114.08
16	f	4005	BCR	C7-C8-C9	-4.02	120.16	126.23
16	t	522	BCR	C24-C23-C22	-4.01	120.17	126.23
13	H	1211	CLA	CHB-C4A-NA	4.01	130.06	124.51
13	H	1021	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
16	G	4001	BCR	C3-C4-C5	-4.01	106.92	114.08
16	b	522	BCR	C24-C23-C22	-4.01	120.18	126.23
13	B	1021	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
13	f	1021	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
13	A	1011	CLA	C1D-ND-C4D	-3.99	103.50	106.33
16	n	4022	BCR	C4-C5-C6	-3.98	116.95	122.73
16	A	4002	BCR	C24-C23-C22	-3.98	120.22	126.23
16	Y	522	BCR	C15-C14-C13	-3.98	121.63	127.31
16	c	521	BCR	C15-C14-C13	-3.98	121.63	127.31
13	B	1211	CLA	CHB-C4A-NA	3.98	130.01	124.51
16	1	522	BCR	C15-C14-C13	-3.98	121.64	127.31
16	6	521	BCR	C24-C23-C22	-3.97	120.23	126.23
16	5	521	BCR	C15-C14-C13	-3.97	121.64	127.31
16	G	4002	BCR	C24-C23-C22	-3.97	120.23	126.23
16	e	4002	BCR	C24-C23-C22	-3.97	120.23	126.23
16	q	522	BCR	C15-C14-C13	-3.97	121.65	127.31
16	v	521	BCR	C24-C23-C22	-3.97	120.24	126.23
13	f	1211	CLA	CHB-C4A-NA	3.96	129.99	124.51
16	b	524	BCR	C33-C5-C6	-3.96	120.08	124.53
16	d	521	BCR	C24-C23-C22	-3.96	120.25	126.23
16	V	4022	BCR	C4-C5-C6	-3.96	116.98	122.73
16	u	521	BCR	C15-C14-C13	-3.96	121.66	127.31
13	f	1238	CLA	CMB-C2B-C1B	-3.95	119.35	125.37
16	2	523	BCR	C7-C8-C9	-3.95	120.26	126.23
16	e	4001	BCR	C20-C21-C22	-3.95	121.67	127.31
16	L	4022	BCR	C4-C5-C6	-3.95	117.00	122.73
16	Z	523	BCR	C7-C8-C9	-3.95	120.27	126.23
16	G	4001	BCR	C15-C16-C17	-3.95	115.39	123.47
16	Z	521	BCR	C24-C23-C22	-3.95	120.27	126.23
16	L	4219	BCR	C16-C17-C18	-3.94	121.68	127.31
16	r	523	BCR	C7-C8-C9	-3.94	120.28	126.23
16	r	521	BCR	C24-C23-C22	-3.94	120.28	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1238	CLA	CMB-C2B-C1B	-3.94	119.37	125.37
16	4	524	BCR	C33-C5-C6	-3.94	120.11	124.53
13	H	1238	CLA	CMB-C2B-C1B	-3.94	119.37	125.37
16	2	521	BCR	C24-C23-C22	-3.93	120.29	126.23
16	A	4001	BCR	C20-C21-C22	-3.93	121.70	127.31
16	q	521	BCR	C15-C14-C13	-3.93	121.70	127.31
16	e	4001	BCR	C15-C16-C17	-3.93	115.43	123.47
16	n	4219	BCR	C16-C17-C18	-3.93	121.71	127.31
20	V	5216	SQD	O47-C7-C8	3.93	119.96	111.50
20	n	5216	SQD	O47-C7-C8	3.92	119.96	111.50
16	A	4001	BCR	C15-C16-C17	-3.92	115.44	123.47
16	Y	521	BCR	C15-C14-C13	-3.92	121.71	127.31
20	L	5216	SQD	O47-C7-C8	3.92	119.96	111.50
13	G	1117	CLA	O2D-CGD-CBD	3.92	118.24	111.27
16	V	4219	BCR	C16-C17-C18	-3.92	121.71	127.31
16	H	4009	BCR	C15-C14-C13	-3.92	121.72	127.31
13	G	1011	CLA	C1D-ND-C4D	-3.92	103.55	106.33
16	1	521	BCR	C15-C14-C13	-3.92	121.72	127.31
16	b	521	BCR	C15-C14-C13	-3.92	121.72	127.31
16	G	4003	BCR	C3-C4-C5	-3.92	107.08	114.08
16	5	522	BCR	C11-C10-C9	-3.91	121.72	127.31
13	e	1117	CLA	O2D-CGD-CBD	3.91	118.22	111.27
16	G	4001	BCR	C20-C21-C22	-3.91	121.73	127.31
16	c	522	BCR	C11-C10-C9	-3.91	121.73	127.31
16	t	521	BCR	C15-C14-C13	-3.91	121.73	127.31
16	a	522	BCR	C7-C8-C9	-3.91	120.33	126.23
16	f	4005	BCR	C24-C23-C22	-3.91	120.33	126.23
16	t	524	BCR	C33-C5-C6	-3.90	120.15	124.53
16	f	4009	BCR	C15-C14-C13	-3.90	121.74	127.31
13	A	1117	CLA	O2D-CGD-CBD	3.90	118.20	111.27
16	d	521	BCR	C7-C8-C9	-3.90	120.34	126.23
13	f	1226	CLA	CHB-C1B-NB	3.90	128.38	124.26
13	H	1226	CLA	CHB-C1B-NB	3.90	128.38	124.26
20	Y	822	SQD	O7-S-C6	3.89	111.57	106.94
16	I	4018	BCR	C16-C17-C18	-3.89	121.76	127.31
16	f	4005	BCR	C15-C14-C13	-3.89	121.76	127.31
20	b	822	SQD	O9-S-C6	3.89	111.56	106.94
16	B	4009	BCR	C15-C14-C13	-3.89	121.76	127.31
16	u	522	BCR	C11-C10-C9	-3.89	121.76	127.31
16	A	4003	BCR	C3-C4-C5	-3.89	107.13	114.08
16	e	4011	BCR	C20-C21-C22	-3.89	121.76	127.31
16	3	522	BCR	C7-C8-C9	-3.89	120.36	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4005	BCR	C24-C23-C22	-3.89	120.36	126.23
16	4	521	BCR	C15-C14-C13	-3.89	121.76	127.31
20	t	822	SQD	O9-S-C6	3.89	111.56	106.94
16	B	4005	BCR	C15-C14-C13	-3.89	121.77	127.31
16	S	4018	BCR	C16-C17-C18	-3.88	121.77	127.31
13	G	1121	CLA	CAA-C2A-C3A	-3.88	102.15	112.78
13	B	1226	CLA	CHB-C1B-NB	3.88	128.37	124.26
16	T	4013	BCR	C15-C14-C13	-3.88	121.77	127.31
13	Y	516	CLA	CBC-CAC-C3C	3.88	123.13	112.43
13	A	1121	CLA	CAA-C2A-C3A	-3.88	102.16	112.78
16	k	4018	BCR	C16-C17-C18	-3.88	121.77	127.31
13	U	1103	CLA	C1-C2-C3	-3.88	120.48	126.75
13	e	1121	CLA	CAA-C2A-C3A	-3.88	102.17	112.78
16	H	4005	BCR	C15-C14-C13	-3.88	121.78	127.31
16	6	521	BCR	C7-C8-C9	-3.88	120.38	126.23
16	e	4003	BCR	C3-C4-C5	-3.87	107.16	114.08
16	J	4013	BCR	C15-C14-C13	-3.87	121.78	127.31
20	4	822	SQD	O9-S-C6	3.87	111.54	106.94
16	A	4011	BCR	C20-C21-C22	-3.87	121.79	127.31
16	G	4011	BCR	C20-C21-C22	-3.87	121.79	127.31
20	1	822	SQD	O7-S-C6	3.87	111.54	106.94
13	1	516	CLA	CBC-CAC-C3C	3.87	123.10	112.43
16	H	4005	BCR	C24-C23-C22	-3.86	120.40	126.23
16	l	4013	BCR	C15-C14-C13	-3.86	121.80	127.31
16	s	522	BCR	C7-C8-C9	-3.86	120.40	126.23
16	6	521	BCR	C11-C10-C9	-3.86	121.80	127.31
13	q	516	CLA	CBC-CAC-C3C	3.86	123.06	112.43
16	v	521	BCR	C7-C8-C9	-3.85	120.42	126.23
13	K	1103	CLA	C1-C2-C3	-3.85	120.52	126.75
16	W	4021	BCR	C11-C10-C9	-3.85	121.82	127.31
13	m	1103	CLA	C1-C2-C3	-3.84	120.53	126.75
16	v	521	BCR	C11-C10-C9	-3.84	121.83	127.31
16	o	4021	BCR	C11-C10-C9	-3.84	121.83	127.31
20	q	822	SQD	O7-S-C6	3.84	111.50	106.94
16	d	521	BCR	C11-C10-C9	-3.84	121.83	127.31
16	c	521	BCR	C16-C17-C18	-3.83	121.84	127.31
16	b	524	BCR	C11-C10-C9	-3.83	121.84	127.31
16	3	521	BCR	C16-C17-C18	-3.83	121.84	127.31
16	M	4021	BCR	C11-C10-C9	-3.83	121.85	127.31
16	4	523	BCR	C16-C17-C18	-3.83	121.85	127.31
16	t	523	BCR	C16-C17-C18	-3.83	121.85	127.31
16	j	4016	BCR	C7-C8-C9	-3.83	120.45	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	q	822	SQD	C4-C3-C2	3.83	117.50	110.82
16	4	524	BCR	C11-C10-C9	-3.82	121.85	127.31
16	s	521	BCR	C16-C17-C18	-3.82	121.85	127.31
20	Y	822	SQD	C4-C3-C2	3.82	117.50	110.82
13	U	1105	CLA	CMC-C2C-C1C	-3.82	119.22	125.04
13	K	1105	CLA	CMC-C2C-C1C	-3.82	119.22	125.04
16	t	524	BCR	C11-C10-C9	-3.82	121.86	127.31
16	T	4015	BCR	C20-C21-C22	-3.82	121.86	127.31
16	J	4015	BCR	C20-C21-C22	-3.81	121.87	127.31
20	r	822	SQD	O9-S-C6	3.81	111.47	106.94
16	l	4015	BCR	C20-C21-C22	-3.81	121.87	127.31
20	s	822	SQD	O9-S-C6	3.81	111.47	106.94
16	G	4011	BCR	C34-C9-C10	-3.81	117.59	122.92
16	2	522	BCR	C15-C14-C13	-3.81	121.88	127.31
13	G	1129	CLA	C3B-C4B-NB	-3.81	106.98	110.52
16	V	4019	BCR	C16-C17-C18	-3.80	121.88	127.31
16	1	521	BCR	C3-C4-C5	-3.80	107.28	114.08
16	Y	521	BCR	C3-C4-C5	-3.80	107.28	114.08
20	2	822	SQD	O9-S-C6	3.80	111.46	106.94
16	v	521	BCR	C15-C14-C13	-3.80	121.88	127.31
20	3	822	SQD	O9-S-C6	3.80	111.46	106.94
16	q	521	BCR	C3-C4-C5	-3.80	107.29	114.08
13	e	1137	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
16	r	522	BCR	C15-C14-C13	-3.80	121.89	127.31
20	1	822	SQD	C4-C3-C2	3.80	117.46	110.82
16	v	521	BCR	C28-C27-C26	-3.80	107.29	114.08
13	G	1137	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
16	b	523	BCR	C16-C17-C18	-3.80	121.89	127.31
16	u	521	BCR	C16-C17-C18	-3.80	121.89	127.31
13	m	1105	CLA	CMC-C2C-C1C	-3.80	119.26	125.04
16	5	521	BCR	C16-C17-C18	-3.80	121.89	127.31
16	F	4016	BCR	C7-C8-C9	-3.80	120.50	126.23
16	L	4019	BCR	C16-C17-C18	-3.79	121.89	127.31
20	a	822	SQD	O9-S-C6	3.79	111.45	106.94
16	Z	522	BCR	C15-C14-C13	-3.79	121.90	127.31
16	H	4017	BCR	C24-C23-C22	-3.79	120.51	126.23
16	a	521	BCR	C16-C17-C18	-3.79	121.90	127.31
16	R	4016	BCR	C7-C8-C9	-3.79	120.51	126.23
16	A	4011	BCR	C34-C9-C10	-3.79	117.62	122.92
16	d	521	BCR	C15-C14-C13	-3.79	121.90	127.31
16	n	4019	BCR	C16-C17-C18	-3.79	121.90	127.31
16	6	521	BCR	C28-C27-C26	-3.79	107.32	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	t	523	BCR	C15-C14-C13	-3.79	121.91	127.31
20	Z	822	SQD	O9-S-C6	3.78	111.44	106.94
16	d	521	BCR	C28-C27-C26	-3.78	107.32	114.08
16	Z	523	BCR	C15-C14-C13	-3.78	121.91	127.31
13	A	1137	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
16	6	521	BCR	C15-C14-C13	-3.78	121.92	127.31
16	r	523	BCR	C15-C14-C13	-3.78	121.92	127.31
16	o	4021	BCR	C24-C23-C22	-3.77	120.53	126.23
16	W	4021	BCR	C24-C23-C22	-3.77	120.54	126.23
16	e	4011	BCR	C34-C9-C10	-3.77	117.64	122.92
16	2	521	BCR	C16-C17-C18	-3.77	121.93	127.31
16	J	4013	BCR	C24-C23-C22	-3.77	120.54	126.23
16	r	521	BCR	C16-C17-C18	-3.77	121.93	127.31
16	Z	521	BCR	C16-C17-C18	-3.77	121.94	127.31
16	M	4021	BCR	C24-C23-C22	-3.77	120.55	126.23
16	B	4006	BCR	C15-C14-C13	-3.76	121.94	127.31
16	f	4017	BCR	C24-C23-C22	-3.76	120.55	126.23
13	e	1139	CLA	C3B-C4B-NB	-3.76	107.02	110.52
16	B	4017	BCR	C24-C23-C22	-3.76	120.55	126.23
20	1	822	SQD	O47-C7-C8	3.76	119.60	111.50
20	q	822	SQD	O47-C7-C8	3.76	119.60	111.50
16	4	523	BCR	C15-C14-C13	-3.76	121.95	127.31
16	a	521	BCR	C28-C27-C26	-3.76	107.37	114.08
16	2	523	BCR	C15-C14-C13	-3.76	121.95	127.31
13	A	1129	CLA	C3B-C4B-NB	-3.76	107.03	110.52
16	n	4219	BCR	C33-C5-C6	-3.76	120.31	124.53
16	T	4013	BCR	C24-C23-C22	-3.76	120.56	126.23
16	f	4006	BCR	C15-C14-C13	-3.76	121.95	127.31
16	3	521	BCR	C28-C27-C26	-3.75	107.37	114.08
16	e	4007	BCR	C11-C10-C9	-3.75	121.95	127.31
16	b	524	BCR	C16-C17-C18	-3.75	121.95	127.31
16	n	4219	BCR	C7-C8-C9	-3.75	120.57	126.23
20	Y	822	SQD	O47-C7-C8	3.75	119.59	111.50
20	Z	822	SQD	O47-C7-C8	3.75	119.58	111.50
20	r	822	SQD	O47-C7-C8	3.75	119.58	111.50
16	V	4219	BCR	C7-C8-C9	-3.75	120.57	126.23
16	s	521	BCR	C28-C27-C26	-3.75	107.38	114.08
16	H	4009	BCR	C21-C20-C19	-3.74	111.53	123.22
16	a	521	BCR	C15-C14-C13	-3.74	121.97	127.31
16	m	4104	BCR	C38-C26-C25	-3.74	120.33	124.53
16	b	523	BCR	C15-C14-C13	-3.74	121.97	127.31
16	v	524	BCR	C11-C10-C9	-3.74	121.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4219	BCR	C33-C5-C6	-3.74	120.33	124.53
16	B	4009	BCR	C21-C20-C19	-3.74	111.55	123.22
13	e	1129	CLA	C3B-C4B-NB	-3.74	107.05	110.52
20	2	822	SQD	O47-C7-C8	3.74	119.56	111.50
16	H	4006	BCR	C15-C14-C13	-3.73	121.98	127.31
13	A	1139	CLA	C3B-C4B-NB	-3.73	107.05	110.52
16	t	524	BCR	C16-C17-C18	-3.73	121.98	127.31
16	4	524	BCR	C16-C17-C18	-3.73	121.98	127.31
16	l	4013	BCR	C24-C23-C22	-3.73	120.60	126.23
13	H	1221	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
20	v	822	SQD	O7-S-C6	3.73	111.37	106.94
16	A	4007	BCR	C11-C10-C9	-3.73	121.99	127.31
16	f	4009	BCR	C21-C20-C19	-3.73	111.58	123.22
13	B	1221	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
16	f	4005	BCR	C33-C5-C6	-3.73	120.34	124.53
13	G	1139	CLA	C3B-C4B-NB	-3.73	107.06	110.52
16	3	521	BCR	C15-C14-C13	-3.72	122.00	127.31
16	L	4219	BCR	C7-C8-C9	-3.72	120.61	126.23
16	K	4104	BCR	C38-C26-C25	-3.72	120.35	124.53
20	6	822	SQD	O7-S-C6	3.72	111.36	106.94
16	s	521	BCR	C15-C14-C13	-3.71	122.01	127.31
13	f	1221	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
16	H	4005	BCR	C33-C5-C6	-3.71	120.36	124.53
16	G	4002	BCR	C11-C10-C9	-3.71	122.02	127.31
16	Z	522	BCR	C11-C10-C9	-3.71	122.02	127.31
16	V	4219	BCR	C33-C5-C6	-3.71	120.36	124.53
16	q	522	BCR	C7-C8-C9	-3.70	120.64	126.23
16	q	524	BCR	C33-C5-C6	-3.70	120.37	124.53
16	B	4005	BCR	C33-C5-C6	-3.70	120.37	124.53
20	d	822	SQD	O7-S-C6	3.70	111.34	106.94
16	2	522	BCR	C11-C10-C9	-3.70	122.03	127.31
16	6	524	BCR	C11-C10-C9	-3.70	122.03	127.31
16	d	524	BCR	C11-C10-C9	-3.70	122.04	127.31
20	d	822	SQD	O9-S-O7	-3.70	101.16	113.95
16	G	4007	BCR	C11-C10-C9	-3.69	122.04	127.31
13	H	1229	CLA	CHD-C1D-ND	-3.69	121.06	124.45
13	f	1229	CLA	CHD-C1D-ND	-3.69	121.06	124.45
20	6	822	SQD	O9-S-O7	-3.69	101.18	113.95
20	v	822	SQD	O9-S-O7	-3.69	101.18	113.95
16	r	523	BCR	C16-C17-C18	-3.69	122.05	127.31
16	U	4104	BCR	C38-C26-C25	-3.69	120.39	124.53
20	3	822	SQD	O9-S-O7	-3.69	101.19	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	524	BCR	C33-C5-C6	-3.68	120.39	124.53
16	A	4002	BCR	C11-C10-C9	-3.68	122.05	127.31
16	r	522	BCR	C11-C10-C9	-3.68	122.05	127.31
16	B	4005	BCR	C11-C10-C9	-3.68	122.05	127.31
20	a	822	SQD	O9-S-O7	-3.68	101.21	113.95
16	H	4005	BCR	C11-C10-C9	-3.68	122.06	127.31
16	1	522	BCR	C7-C8-C9	-3.68	120.67	126.23
16	B	4005	BCR	C20-C21-C22	-3.68	122.06	127.31
13	K	1401	CLA	CAA-C2A-C3A	-3.68	102.70	112.78
13	B	1229	CLA	CHD-C1D-ND	-3.68	121.07	124.45
20	s	822	SQD	O9-S-O7	-3.67	101.23	113.95
16	Z	523	BCR	C16-C17-C18	-3.67	122.07	127.31
16	Y	524	BCR	C33-C5-C6	-3.67	120.40	124.53
16	f	4005	BCR	C20-C21-C22	-3.67	122.07	127.31
16	v	522	BCR	C15-C16-C17	-3.67	115.95	123.47
13	U	1401	CLA	CAA-C2A-C3A	-3.67	102.73	112.78
16	2	523	BCR	C16-C17-C18	-3.67	122.07	127.31
20	Z	822	SQD	O7-S-C6	3.67	111.30	106.94
16	f	4005	BCR	C11-C10-C9	-3.67	122.08	127.31
16	l	4012	BCR	C3-C4-C5	-3.67	107.53	114.08
13	m	1401	CLA	CAA-C2A-C3A	-3.67	102.74	112.78
20	a	822	SQD	O7-S-C6	3.67	111.30	106.94
16	Y	522	BCR	C7-C8-C9	-3.66	120.70	126.23
16	J	4012	BCR	C3-C4-C5	-3.66	107.54	114.08
16	J	4013	BCR	C3-C4-C5	-3.66	107.55	114.08
16	H	4005	BCR	C20-C21-C22	-3.66	122.09	127.31
16	6	522	BCR	C15-C16-C17	-3.66	115.98	123.47
16	a	521	BCR	C7-C8-C9	-3.66	120.71	126.23
16	s	521	BCR	C7-C8-C9	-3.65	120.71	126.23
20	5	822	SQD	O9-S-O7	-3.65	101.31	113.95
20	2	822	SQD	O7-S-C6	3.65	111.28	106.94
20	u	822	SQD	O9-S-O7	-3.65	101.32	113.95
16	A	4003	BCR	C15-C14-C13	-3.65	122.10	127.31
16	G	4003	BCR	C15-C14-C13	-3.65	122.10	127.31
20	c	822	SQD	O9-S-O7	-3.65	101.33	113.95
16	d	522	BCR	C15-C16-C17	-3.65	116.00	123.47
16	3	521	BCR	C7-C8-C9	-3.65	120.73	126.23
16	l	4013	BCR	C3-C4-C5	-3.64	107.57	114.08
16	T	4012	BCR	C3-C4-C5	-3.64	107.57	114.08
20	3	822	SQD	O7-S-C6	3.64	111.27	106.94
13	A	1132	CLA	O2D-CGD-CBD	3.64	117.74	111.27
13	e	1132	CLA	O2D-CGD-CBD	3.64	117.74	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	822	SQD	O9-S-O7	-3.64	101.36	113.95
20	s	822	SQD	O7-S-C6	3.64	111.26	106.94
13	e	1106	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
20	t	822	SQD	O9-S-O7	-3.63	101.38	113.95
20	4	822	SQD	O9-S-O7	-3.63	101.38	113.95
16	e	4002	BCR	C11-C10-C9	-3.63	122.13	127.31
16	e	4003	BCR	C15-C14-C13	-3.63	122.13	127.31
13	G	1132	CLA	O2D-CGD-CBD	3.63	117.72	111.27
20	r	822	SQD	O9-S-O7	-3.63	101.39	113.95
16	T	4013	BCR	C3-C4-C5	-3.63	107.60	114.08
16	W	4021	BCR	C38-C26-C25	-3.63	120.46	124.53
13	A	1106	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
16	2	524	BCR	C16-C17-C18	-3.62	122.14	127.31
20	2	822	SQD	O9-S-O7	-3.62	101.42	113.95
20	r	822	SQD	O7-S-C6	3.62	111.24	106.94
13	G	1106	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
20	Y	822	SQD	O9-S-O7	-3.62	101.43	113.95
20	Z	822	SQD	O9-S-O7	-3.61	101.44	113.95
13	e	1011	CLA	CGD-CBD-CAD	3.61	122.44	110.73
20	f	1852	SQD	O9-S-O7	-3.61	101.44	113.95
20	1	822	SQD	O9-S-O7	-3.61	101.45	113.95
13	G	1011	CLA	CGD-CBD-CAD	3.61	122.43	110.73
16	r	524	BCR	C16-C17-C18	-3.61	122.16	127.31
13	A	1011	CLA	CGD-CBD-CAD	3.61	122.42	110.73
13	B	1012	CLA	CMB-C2B-C1B	-3.61	119.87	125.37
20	H	1852	SQD	O9-S-O7	-3.61	101.46	113.95
13	H	1012	CLA	CMB-C2B-C1B	-3.61	119.88	125.37
20	v	822	SQD	O9-S-C6	3.61	111.22	106.94
20	B	1852	SQD	O9-S-O7	-3.61	101.47	113.95
16	o	4021	BCR	C15-C14-C13	-3.60	122.17	127.31
20	q	822	SQD	O9-S-O7	-3.60	101.49	113.95
13	f	1012	CLA	CMB-C2B-C1B	-3.60	119.89	125.37
16	Z	524	BCR	C16-C17-C18	-3.60	122.18	127.31
16	M	4021	BCR	C38-C26-C25	-3.59	120.49	124.53
13	H	1221	CLA	CMB-C2B-C1B	-3.59	119.90	125.37
16	t	521	BCR	C20-C21-C22	-3.59	122.19	127.31
20	d	822	SQD	O9-S-C6	3.58	111.20	106.94
16	Y	524	BCR	C7-C8-C9	-3.58	120.82	126.23
16	Y	523	BCR	C15-C14-C13	-3.58	122.20	127.31
16	n	4020	BCR	C16-C15-C14	-3.58	116.14	123.47
16	u	521	BCR	C28-C27-C26	-3.58	107.68	114.08
16	Z	521	BCR	C11-C10-C9	-3.58	122.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	822	SQD	O9-S-C6	3.58	111.20	106.94
16	2	521	BCR	C11-C10-C9	-3.58	122.20	127.31
16	L	4020	BCR	C16-C15-C14	-3.58	116.14	123.47
13	G	1013	CLA	CAA-C2A-C1A	-3.58	100.25	111.97
13	e	1126	CLA	CMB-C2B-C1B	-3.58	119.92	125.37
13	A	1107	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
13	e	1013	CLA	CAA-C2A-C1A	-3.57	100.26	111.97
16	o	4021	BCR	C38-C26-C25	-3.57	120.52	124.53
13	A	1013	CLA	CAA-C2A-C1A	-3.57	100.27	111.97
16	V	4020	BCR	C16-C15-C14	-3.57	116.16	123.47
13	B	1221	CLA	CMB-C2B-C1B	-3.57	119.93	125.37
13	2	507	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
16	H	4009	BCR	C3-C4-C5	-3.57	107.71	114.08
16	H	4017	BCR	C16-C17-C18	-3.57	122.22	127.31
13	Z	507	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
13	G	1107	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
16	5	521	BCR	C28-C27-C26	-3.56	107.72	114.08
13	H	1229	CLA	CMB-C2B-C1B	-3.56	119.94	125.37
13	e	1107	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
13	f	1221	CLA	CMB-C2B-C1B	-3.56	119.95	125.37
16	W	4021	BCR	C15-C14-C13	-3.56	122.23	127.31
16	M	4021	BCR	C15-C14-C13	-3.56	122.23	127.31
13	B	1229	CLA	CMB-C2B-C1B	-3.56	119.95	125.37
13	A	1126	CLA	CMB-C2B-C1B	-3.56	119.95	125.37
16	G	4008	BCR	C7-C8-C9	-3.56	120.86	126.23
16	A	4008	BCR	C7-C8-C9	-3.56	120.86	126.23
16	1	524	BCR	C7-C8-C9	-3.56	120.86	126.23
16	r	521	BCR	C11-C10-C9	-3.56	122.24	127.31
16	c	521	BCR	C28-C27-C26	-3.56	107.73	114.08
16	1	523	BCR	C15-C14-C13	-3.55	122.24	127.31
16	v	522	BCR	C24-C23-C22	-3.55	120.87	126.23
16	b	521	BCR	C20-C21-C22	-3.55	122.24	127.31
13	G	1126	CLA	CMB-C2B-C1B	-3.55	119.96	125.37
16	q	523	BCR	C15-C14-C13	-3.55	122.24	127.31
16	4	521	BCR	C20-C21-C22	-3.55	122.25	127.31
16	6	524	BCR	C33-C5-C6	-3.55	120.55	124.53
13	f	1229	CLA	CMB-C2B-C1B	-3.54	119.97	125.37
16	B	4009	BCR	C3-C4-C5	-3.54	107.75	114.08
16	f	4017	BCR	C16-C17-C18	-3.54	122.26	127.31
16	B	4017	BCR	C16-C17-C18	-3.54	122.26	127.31
16	v	524	BCR	C33-C5-C6	-3.54	120.56	124.53
13	T	1302	CLA	O2D-CGD-O1D	-3.54	116.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	524	BCR	C7-C8-C9	-3.53	120.90	126.23
13	l	1302	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
16	v	521	BCR	C3-C4-C5	-3.53	107.78	114.08
13	r	507	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
16	e	4008	BCR	C7-C8-C9	-3.53	120.91	126.23
16	f	4009	BCR	C3-C4-C5	-3.52	107.78	114.08
16	d	524	BCR	C33-C5-C6	-3.52	120.57	124.53
16	6	522	BCR	C24-C23-C22	-3.52	120.91	126.23
13	a	508	CLA	CMB-C2B-C1B	-3.52	120.00	125.37
16	6	521	BCR	C3-C4-C5	-3.52	107.79	114.08
16	d	521	BCR	C3-C4-C5	-3.52	107.79	114.08
16	d	522	BCR	C24-C23-C22	-3.52	120.92	126.23
13	3	508	CLA	CMB-C2B-C1B	-3.52	120.01	125.37
13	f	1222	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
13	J	1302	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
16	a	522	BCR	C28-C27-C26	-3.51	107.81	114.08
16	5	522	BCR	C24-C23-C22	-3.51	120.93	126.23
16	v	523	BCR	C16-C17-C18	-3.51	122.30	127.31
16	1	521	BCR	C28-C27-C26	-3.51	107.81	114.08
13	B	1222	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
16	H	4010	BCR	C39-C30-C25	-3.50	104.61	110.30
16	B	4010	BCR	C39-C30-C25	-3.50	104.62	110.30
16	6	523	BCR	C16-C17-C18	-3.50	122.31	127.31
16	3	522	BCR	C28-C27-C26	-3.50	107.82	114.08
16	Y	521	BCR	C28-C27-C26	-3.50	107.82	114.08
16	f	4010	BCR	C39-C30-C25	-3.50	104.62	110.30
16	u	522	BCR	C24-C23-C22	-3.50	120.95	126.23
16	q	521	BCR	C11-C10-C9	-3.50	122.32	127.31
16	b	522	BCR	C28-C27-C26	-3.50	107.84	114.08
16	c	522	BCR	C24-C23-C22	-3.49	120.96	126.23
16	t	522	BCR	C28-C27-C26	-3.49	107.84	114.08
16	B	4014	BCR	C20-C19-C18	-3.49	116.61	126.42
16	Y	521	BCR	C11-C10-C9	-3.49	122.33	127.31
16	H	4014	BCR	C20-C19-C18	-3.49	116.62	126.42
16	q	521	BCR	C28-C27-C26	-3.49	107.85	114.08
16	4	522	BCR	C28-C27-C26	-3.49	107.85	114.08
16	s	522	BCR	C28-C27-C26	-3.49	107.85	114.08
16	n	4020	BCR	C15-C14-C13	-3.49	122.33	127.31
13	e	1137	CLA	O2D-CGD-CBD	3.49	117.46	111.27
16	c	521	BCR	C7-C8-C9	-3.49	120.97	126.23
13	s	508	CLA	CMB-C2B-C1B	-3.48	120.06	125.37
16	1	521	BCR	C11-C10-C9	-3.48	122.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1220	CLA	CAA-C2A-C1A	-3.48	100.56	111.97
16	l	4013	BCR	C11-C10-C9	-3.48	122.34	127.31
16	f	4014	BCR	C20-C19-C18	-3.48	116.64	126.42
16	d	523	BCR	C16-C17-C18	-3.48	122.35	127.31
13	G	1137	CLA	O2D-CGD-CBD	3.48	117.45	111.27
16	L	4020	BCR	C15-C14-C13	-3.48	122.35	127.31
13	B	1220	CLA	CAA-C2A-C1A	-3.48	100.58	111.97
13	H	1220	CLA	CAA-C2A-C1A	-3.47	100.59	111.97
13	H	1222	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
16	V	4020	BCR	C15-C14-C13	-3.47	122.35	127.31
16	d	522	BCR	C11-C10-C9	-3.47	122.36	127.31
16	e	4007	BCR	C20-C21-C22	-3.47	122.36	127.31
13	A	1137	CLA	O2D-CGD-CBD	3.47	117.43	111.27
16	T	4013	BCR	C11-C10-C9	-3.47	122.36	127.31
16	6	522	BCR	C3-C4-C5	-3.46	107.89	114.08
16	d	522	BCR	C3-C4-C5	-3.46	107.89	114.08
13	t	507	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
20	n	5216	SQD	C4-C3-C2	3.46	116.87	110.82
16	v	522	BCR	C11-C10-C9	-3.46	122.37	127.31
16	v	522	BCR	C3-C4-C5	-3.46	107.90	114.08
16	5	521	BCR	C7-C8-C9	-3.46	121.01	126.23
13	b	507	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
16	s	524	BCR	C7-C8-C9	-3.46	121.01	126.23
13	f	1234	CLA	CHB-C1B-NB	3.46	127.92	124.26
16	u	521	BCR	C7-C8-C9	-3.46	121.01	126.23
13	4	507	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
16	6	522	BCR	C11-C10-C9	-3.45	122.38	127.31
16	J	4013	BCR	C11-C10-C9	-3.45	122.38	127.31
16	G	4007	BCR	C20-C21-C22	-3.45	122.38	127.31
16	H	4017	BCR	C10-C11-C12	-3.45	112.45	123.22
16	A	4007	BCR	C27-C26-C25	-3.45	117.72	122.73
16	o	4021	BCR	C20-C21-C22	-3.45	122.39	127.31
16	J	4015	BCR	C32-C1-C6	-3.45	104.71	110.30
16	M	4021	BCR	C20-C21-C22	-3.45	122.39	127.31
16	o	4021	BCR	C28-C27-C26	-3.45	107.92	114.08
16	W	4021	BCR	C20-C21-C22	-3.45	122.39	127.31
16	W	4021	BCR	C28-C27-C26	-3.44	107.93	114.08
16	t	524	BCR	C7-C8-C9	-3.44	121.03	126.23
16	A	4007	BCR	C20-C21-C22	-3.44	122.39	127.31
16	a	521	BCR	C20-C21-C22	-3.44	122.39	127.31
16	H	4017	BCR	C15-C14-C13	-3.44	122.39	127.31
20	L	5216	SQD	C4-C3-C2	3.44	116.83	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	4015	BCR	C32-C1-C6	-3.44	104.71	110.30
16	S	4018	BCR	C27-C26-C25	-3.44	117.73	122.73
16	B	4009	BCR	C11-C10-C9	-3.44	122.40	127.31
16	B	4017	BCR	C10-C11-C12	-3.44	112.48	123.22
16	5	523	BCR	C15-C16-C17	-3.44	116.43	123.47
13	H	1228	CLA	CMB-C2B-C1B	-3.44	120.13	125.37
13	B	1228	CLA	CMB-C2B-C1B	-3.44	120.13	125.37
16	G	4007	BCR	C27-C26-C25	-3.44	117.74	122.73
16	3	524	BCR	C7-C8-C9	-3.44	121.04	126.23
16	H	4009	BCR	C11-C10-C9	-3.43	122.41	127.31
16	M	4021	BCR	C28-C27-C26	-3.43	107.94	114.08
13	f	1235	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
16	H	4010	BCR	C16-C17-C18	-3.43	122.41	127.31
13	B	1234	CLA	CHB-C1B-NB	3.43	127.89	124.26
16	B	4009	BCR	C24-C23-C22	-3.43	121.05	126.23
16	b	524	BCR	C7-C8-C9	-3.43	121.05	126.23
16	3	521	BCR	C20-C21-C22	-3.43	122.41	127.31
20	V	5216	SQD	C4-C3-C2	3.43	116.81	110.82
16	3	524	BCR	C33-C5-C6	-3.43	120.67	124.53
16	f	4017	BCR	C10-C11-C12	-3.43	112.51	123.22
16	s	524	BCR	C33-C5-C6	-3.43	120.68	124.53
16	B	4010	BCR	C16-C17-C18	-3.43	122.42	127.31
13	H	1201	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
13	H	1235	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
16	H	4009	BCR	C24-C23-C22	-3.43	121.06	126.23
16	a	524	BCR	C7-C8-C9	-3.43	121.06	126.23
16	l	4015	BCR	C32-C1-C6	-3.43	104.74	110.30
16	c	523	BCR	C15-C16-C17	-3.42	116.46	123.47
16	l	4013	BCR	C2-C1-C6	3.42	115.75	110.48
13	B	1235	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
16	I	4018	BCR	C27-C26-C25	-3.42	117.76	122.73
16	4	524	BCR	C7-C8-C9	-3.42	121.06	126.23
20	c	822	SQD	O47-C7-C8	3.42	118.87	111.50
16	f	4009	BCR	C24-C23-C22	-3.42	121.07	126.23
16	v	524	BCR	C20-C21-C22	-3.42	122.43	127.31
16	u	523	BCR	C15-C16-C17	-3.42	116.47	123.47
16	e	4007	BCR	C27-C26-C25	-3.42	117.77	122.73
16	6	524	BCR	C20-C21-C22	-3.42	122.43	127.31
16	f	4010	BCR	C16-C17-C18	-3.42	122.43	127.31
16	f	4017	BCR	C15-C14-C13	-3.42	122.43	127.31
13	f	1201	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
16	G	4008	BCR	C33-C5-C6	-3.42	120.69	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	k	4018	BCR	C27-C26-C25	-3.41	117.77	122.73
13	f	1228	CLA	CMB-C2B-C1B	-3.41	120.17	125.37
16	B	4017	BCR	C15-C14-C13	-3.41	122.44	127.31
13	B	1227	CLA	C3B-C4B-NB	-3.41	107.35	110.52
16	d	524	BCR	C20-C21-C22	-3.41	122.44	127.31
16	f	4009	BCR	C11-C10-C9	-3.41	122.44	127.31
16	s	521	BCR	C20-C21-C22	-3.41	122.44	127.31
13	f	1227	CLA	C3B-C4B-NB	-3.41	107.35	110.52
16	J	4013	BCR	C2-C1-C6	3.41	115.73	110.48
16	e	4008	BCR	C33-C5-C6	-3.41	120.70	124.53
13	H	1234	CLA	CHB-C1B-NB	3.41	127.86	124.26
13	B	1201	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
13	A	1128	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
13	H	1202	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
20	u	822	SQD	O47-C7-C8	3.41	118.84	111.50
13	e	1128	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
20	5	822	SQD	O47-C7-C8	3.40	118.84	111.50
14	f	2002	PQN	C14-C13-C15	-3.40	109.55	115.27
13	U	1105	CLA	CBC-CAC-C3C	3.40	121.81	112.43
16	A	4008	BCR	C33-C5-C6	-3.40	120.71	124.53
16	a	524	BCR	C33-C5-C6	-3.40	120.71	124.53
16	T	4013	BCR	C2-C1-C6	3.40	115.72	110.48
13	B	1012	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
13	H	1227	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
13	A	1123	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
13	f	1227	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
16	c	521	BCR	C11-C10-C9	-3.40	122.46	127.31
16	f	4006	BCR	C33-C5-C6	-3.40	120.71	124.53
13	f	1202	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
16	U	4104	BCR	C16-C17-C18	-3.39	122.47	127.31
13	B	1202	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
13	f	1012	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
16	B	4006	BCR	C33-C5-C6	-3.39	120.72	124.53
20	b	822	SQD	O7-S-C6	3.39	110.97	106.94
13	H	1012	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
16	1	521	BCR	C20-C21-C22	-3.39	122.47	127.31
13	G	1128	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
14	B	2002	PQN	C14-C13-C15	-3.39	109.58	115.27
13	K	1105	CLA	CBC-CAC-C3C	3.39	121.77	112.43
13	m	1105	CLA	CBC-CAC-C3C	3.39	121.77	112.43
16	3	524	BCR	C16-C17-C18	-3.39	122.48	127.31
16	f	4006	BCR	C16-C17-C18	-3.39	122.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1023	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
13	G	1123	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
13	H	1227	CLA	C3B-C4B-NB	-3.38	107.38	110.52
13	B	1227	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
13	e	1123	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
16	v	522	BCR	C28-C27-C26	-3.38	108.04	114.08
16	H	4006	BCR	C33-C5-C6	-3.38	120.73	124.53
16	a	524	BCR	C16-C17-C18	-3.38	122.49	127.31
13	B	1023	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
16	c	522	BCR	C7-C8-C9	-3.38	121.13	126.23
16	B	4006	BCR	C16-C17-C18	-3.38	122.49	127.31
16	G	4007	BCR	C24-C23-C22	-3.38	121.13	126.23
16	K	4104	BCR	C16-C17-C18	-3.38	122.49	127.31
16	u	521	BCR	C11-C10-C9	-3.38	122.49	127.31
16	5	522	BCR	C7-C8-C9	-3.38	121.13	126.23
20	u	822	SQD	O7-S-C6	3.38	110.95	106.94
16	T	4015	BCR	C11-C10-C9	-3.38	122.49	127.31
13	f	1216	CLA	C3B-C4B-NB	-3.37	107.38	110.52
13	u	519	CLA	C3B-C4B-NB	-3.37	107.38	110.52
13	H	1205	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
16	5	521	BCR	C11-C10-C9	-3.37	122.49	127.31
20	5	822	SQD	O7-S-C6	3.37	110.95	106.94
20	c	822	SQD	O7-S-C6	3.37	110.95	106.94
16	q	521	BCR	C20-C21-C22	-3.37	122.50	127.31
14	H	2002	PQN	C14-C13-C15	-3.37	109.60	115.27
13	G	1013	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
16	s	523	BCR	C7-C8-C9	-3.37	121.14	126.23
20	t	822	SQD	O7-S-C6	3.37	110.94	106.94
16	d	522	BCR	C28-C27-C26	-3.37	108.06	114.08
16	A	4007	BCR	C24-C23-C22	-3.37	121.15	126.23
16	e	4007	BCR	C16-C17-C18	-3.37	122.51	127.31
20	4	822	SQD	O7-S-C6	3.36	110.94	106.94
16	Y	521	BCR	C20-C21-C22	-3.36	122.51	127.31
16	6	522	BCR	C28-C27-C26	-3.36	108.07	114.08
16	s	523	BCR	C11-C10-C9	-3.36	122.51	127.31
16	H	4014	BCR	C16-C15-C14	-3.36	116.59	123.47
16	u	522	BCR	C7-C8-C9	-3.36	121.16	126.23
13	B	1205	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
16	3	523	BCR	C7-C8-C9	-3.36	121.16	126.23
13	f	1222	CLA	CAA-C2A-C1A	-3.36	100.98	111.97
16	r	522	BCR	C7-C8-C9	-3.36	121.17	126.23
16	e	4007	BCR	C24-C23-C22	-3.35	121.17	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1023	CLA	CMB-C2B-C1B	-3.35	120.26	125.37
16	m	4104	BCR	C16-C17-C18	-3.35	122.52	127.31
16	2	522	BCR	C7-C8-C9	-3.35	121.17	126.23
16	f	4014	BCR	C16-C15-C14	-3.35	116.61	123.47
16	s	524	BCR	C16-C17-C18	-3.35	122.53	127.31
13	f	1205	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
13	B	1222	CLA	CAA-C2A-C1A	-3.35	100.99	111.97
16	B	4014	BCR	C16-C15-C14	-3.35	116.61	123.47
13	e	1101	CLA	C3B-C4B-NB	-3.35	107.41	110.52
13	A	1013	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
13	H	1222	CLA	CAA-C2A-C1A	-3.35	101.00	111.97
16	J	4015	BCR	C11-C10-C9	-3.35	122.53	127.31
16	A	4007	BCR	C16-C17-C18	-3.35	122.53	127.31
16	Z	522	BCR	C7-C8-C9	-3.35	121.18	126.23
13	B	1216	CLA	C3B-C4B-NB	-3.35	107.41	110.52
16	a	523	BCR	C11-C10-C9	-3.35	122.53	127.31
13	5	519	CLA	C3B-C4B-NB	-3.34	107.41	110.52
16	G	4007	BCR	C16-C17-C18	-3.34	122.54	127.31
16	l	4015	BCR	C11-C10-C9	-3.34	122.54	127.31
16	H	4006	BCR	C16-C17-C18	-3.34	122.54	127.31
13	e	1013	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
16	2	524	BCR	C7-C8-C9	-3.34	121.19	126.23
16	a	523	BCR	C7-C8-C9	-3.34	121.19	126.23
16	5	522	BCR	C28-C27-C26	-3.34	108.12	114.08
16	r	524	BCR	C7-C8-C9	-3.34	121.19	126.23
16	3	523	BCR	C11-C10-C9	-3.34	122.55	127.31
13	H	1216	CLA	C3B-C4B-NB	-3.34	107.42	110.52
16	Z	524	BCR	C7-C8-C9	-3.33	121.20	126.23
13	H	1202	CLA	CMB-C2B-C1B	-3.33	120.29	125.37
16	u	522	BCR	C28-C27-C26	-3.33	108.13	114.08
14	G	2001	PQN	C14-C13-C15	-3.33	109.67	115.27
13	e	1013	CLA	CMB-C2B-C3B	3.33	134.65	126.59
13	A	1013	CLA	CMB-C2B-C3B	3.33	134.65	126.59
13	f	1202	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
13	e	1112	CLA	CHB-C4A-NA	3.33	129.11	124.51
16	c	522	BCR	C28-C27-C26	-3.32	108.14	114.08
16	L	4022	BCR	C20-C21-C22	-3.32	122.57	127.31
16	4	521	BCR	C11-C10-C9	-3.32	122.57	127.31
16	5	521	BCR	C24-C23-C22	-3.32	121.22	126.23
13	H	1012	CLA	C3B-C4B-NB	-3.32	107.43	110.52
13	q	519	CLA	C3B-C4B-NB	-3.32	107.44	110.52
13	e	1112	CLA	C3B-C4B-NB	-3.32	107.44	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	2001	PQN	C14-C13-C15	-3.32	109.69	115.27
16	V	4022	BCR	C20-C21-C22	-3.32	122.58	127.31
13	A	1101	CLA	C3B-C4B-NB	-3.31	107.44	110.52
13	G	1112	CLA	CHB-C4A-NA	3.31	129.09	124.51
16	n	4022	BCR	C20-C21-C22	-3.31	122.58	127.31
13	B	1204	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
16	s	522	BCR	C24-C23-C22	-3.31	121.23	126.23
13	A	1101	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
13	A	1112	CLA	C3B-C4B-NB	-3.31	107.44	110.52
13	G	1013	CLA	CMB-C2B-C3B	3.31	134.60	126.59
13	B	1202	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
13	G	1101	CLA	C3B-C4B-NB	-3.31	107.45	110.52
13	c	519	CLA	C3B-C4B-NB	-3.31	107.45	110.52
13	f	1012	CLA	C3B-C4B-NB	-3.31	107.45	110.52
16	b	521	BCR	C11-C10-C9	-3.31	122.59	127.31
13	Y	501	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
13	B	1012	CLA	C3B-C4B-NB	-3.30	107.45	110.52
13	A	1112	CLA	CHB-C4A-NA	3.30	129.08	124.51
16	a	523	BCR	C16-C17-C18	-3.30	122.60	127.31
16	n	4219	BCR	C24-C23-C22	-3.30	121.24	126.23
16	u	521	BCR	C24-C23-C22	-3.30	121.24	126.23
13	H	1234	CLA	CMB-C2B-C3B	3.30	134.59	126.59
13	G	1101	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
13	f	1204	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
16	m	4104	BCR	C11-C10-C9	-3.30	122.60	127.31
20	V	5216	SQD	O9-S-C6	3.30	110.86	106.94
13	G	1112	CLA	C3B-C4B-NB	-3.30	107.45	110.52
14	e	2001	PQN	C14-C13-C15	-3.30	109.72	115.27
13	H	1204	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
16	t	521	BCR	C11-C10-C9	-3.30	122.60	127.31
13	1	519	CLA	C3B-C4B-NB	-3.30	107.46	110.52
13	B	1234	CLA	CMB-C2B-C3B	3.30	134.57	126.59
13	1	501	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
16	U	4104	BCR	C11-C10-C9	-3.29	122.61	127.31
13	e	1101	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	L	5216	SQD	O9-S-C6	3.29	110.85	106.94
16	K	4104	BCR	C11-C10-C9	-3.29	122.61	127.31
16	V	4219	BCR	C24-C23-C22	-3.29	121.27	126.23
16	s	523	BCR	C16-C17-C18	-3.29	122.62	127.31
16	c	521	BCR	C24-C23-C22	-3.28	121.27	126.23
16	L	4219	BCR	C24-C23-C22	-3.28	121.28	126.23
20	a	822	SQD	O47-C7-C8	3.28	118.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1101	CLA	O2D-CGD-CBD	3.28	117.09	111.27
13	q	501	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
16	u	524	BCR	C16-C17-C18	-3.28	122.63	127.31
13	F	1301	CLA	C3B-C4B-NB	-3.28	107.47	110.52
13	f	1234	CLA	CMB-C2B-C3B	3.28	134.52	126.59
16	V	4022	BCR	C15-C14-C13	-3.28	122.64	127.31
16	Y	522	BCR	C24-C23-C22	-3.27	121.29	126.23
16	1	522	BCR	C24-C23-C22	-3.27	121.29	126.23
16	q	522	BCR	C28-C27-C26	-3.27	108.23	114.08
13	Y	519	CLA	C3B-C4B-NB	-3.27	107.48	110.52
16	3	523	BCR	C16-C17-C18	-3.27	122.64	127.31
16	a	522	BCR	C24-C23-C22	-3.27	121.30	126.23
13	a	516	CLA	CBC-CAC-C3C	3.27	121.44	112.43
13	G	1106	CLA	O2A-CGA-O1A	-3.27	115.35	123.59
20	1	822	SQD	C3-C4-C5	3.27	116.06	110.24
16	1	521	BCR	C7-C8-C9	-3.27	121.30	126.23
13	B	1239	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
13	H	1239	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
13	j	1301	CLA	C3B-C4B-NB	-3.27	107.49	110.52
16	1	522	BCR	C28-C27-C26	-3.26	108.25	114.08
13	f	1239	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
16	c	524	BCR	C16-C17-C18	-3.26	122.65	127.31
20	3	822	SQD	O47-C7-C8	3.26	118.53	111.50
13	R	1301	CLA	C3B-C4B-NB	-3.26	107.49	110.52
16	q	521	BCR	C7-C8-C9	-3.26	121.31	126.23
20	n	5216	SQD	O9-S-C6	3.26	110.82	106.94
20	c	822	SQD	C1-O5-C5	3.26	120.09	113.69
13	f	1230	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
16	3	522	BCR	C24-C23-C22	-3.26	121.31	126.23
16	n	4020	BCR	C20-C21-C22	-3.26	122.66	127.31
13	G	1124	CLA	CAA-C2A-C1A	-3.26	101.29	111.97
13	B	1223	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
16	b	524	BCR	C20-C21-C22	-3.26	122.66	127.31
16	a	521	BCR	C24-C23-C22	-3.26	121.31	126.23
16	Z	524	BCR	C33-C5-C6	-3.26	120.87	124.53
16	3	521	BCR	C24-C23-C22	-3.26	121.31	126.23
13	A	1101	CLA	O2D-CGD-CBD	3.26	117.06	111.27
13	e	1106	CLA	O2A-CGA-O1A	-3.26	115.38	123.59
13	G	1118	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
13	G	1137	CLA	CHB-C4A-NA	3.25	129.01	124.51
16	L	4020	BCR	C20-C21-C22	-3.25	122.67	127.31
13	3	516	CLA	CBC-CAC-C3C	3.25	121.40	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1124	CLA	CAA-C2A-C1A	-3.25	101.32	111.97
13	e	1101	CLA	O2D-CGD-CBD	3.25	117.05	111.27
13	s	516	CLA	CBC-CAC-C3C	3.25	121.39	112.43
20	H	1852	SQD	O8-S-C6	3.25	110.92	105.74
16	5	524	BCR	C16-C17-C18	-3.25	122.67	127.31
13	f	1223	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
13	e	1124	CLA	CAA-C2A-C1A	-3.25	101.33	111.97
13	f	1213	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
16	Y	521	BCR	C7-C8-C9	-3.25	121.33	126.23
16	q	522	BCR	C24-C23-C22	-3.25	121.33	126.23
16	G	4001	BCR	C24-C23-C22	-3.25	121.33	126.23
16	V	4020	BCR	C20-C21-C22	-3.25	122.67	127.31
16	4	524	BCR	C20-C21-C22	-3.25	122.68	127.31
16	t	524	BCR	C20-C21-C22	-3.25	122.68	127.31
13	G	1119	CLA	CHB-C1B-NB	3.25	127.69	124.26
20	s	822	SQD	O47-C7-C8	3.24	118.49	111.50
13	A	1106	CLA	O2A-CGA-O1A	-3.24	115.40	123.59
20	Y	822	SQD	C3-C4-C5	3.24	116.03	110.24
20	q	822	SQD	C3-C4-C5	3.24	116.03	110.24
16	Y	522	BCR	C28-C27-C26	-3.24	108.29	114.08
13	G	1135	CLA	CMB-C2B-C1B	-3.24	120.43	125.37
13	B	1230	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
16	t	522	BCR	C20-C21-C22	-3.24	122.69	127.31
13	G	1110	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
13	A	1118	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
13	B	1213	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
13	A	1137	CLA	CHB-C4A-NA	3.24	128.99	124.51
13	H	1223	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
16	4	522	BCR	C20-C21-C22	-3.24	122.69	127.31
13	H	1213	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
20	5	822	SQD	C1-O5-C5	3.24	120.04	113.69
13	A	1110	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
13	H	1202	CLA	CHB-C4A-NA	3.24	128.99	124.51
13	B	1202	CLA	CHB-C4A-NA	3.23	128.99	124.51
13	B	1023	CLA	C3B-C4B-NB	-3.23	107.52	110.52
16	r	524	BCR	C33-C5-C6	-3.23	120.90	124.53
16	L	4022	BCR	C15-C14-C13	-3.23	122.70	127.31
13	e	1137	CLA	CHB-C4A-NA	3.23	128.98	124.51
16	2	524	BCR	C33-C5-C6	-3.23	120.90	124.53
13	e	1102	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
13	2	516	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
13	d	501	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	522	BCR	C20-C21-C22	-3.23	122.70	127.31
16	e	4001	BCR	C24-C23-C22	-3.23	121.36	126.23
13	G	1102	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
13	r	516	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
13	A	1102	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
13	f	1202	CLA	CHB-C4A-NA	3.22	128.97	124.51
13	A	1119	CLA	CHB-C1B-NB	3.22	127.67	124.26
16	m	4104	BCR	C30-C25-C26	-3.22	118.07	122.61
13	A	1135	CLA	CMB-C2B-C1B	-3.22	120.46	125.37
20	B	1852	SQD	O8-S-C6	3.22	110.88	105.74
13	e	1110	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
16	u	523	BCR	C28-C27-C26	-3.22	108.32	114.08
13	G	1105	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
13	f	1221	CLA	CHB-C4A-NA	3.22	128.97	124.51
16	f	4009	BCR	C33-C5-C6	-3.22	120.91	124.53
16	A	4001	BCR	C24-C23-C22	-3.22	121.37	126.23
16	s	521	BCR	C24-C23-C22	-3.22	121.37	126.23
13	f	1023	CLA	C3B-C4B-NB	-3.22	107.53	110.52
13	e	1118	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
13	a	510	CLA	CHB-C4A-NA	3.22	128.97	124.51
13	T	1303	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
16	Z	521	BCR	C7-C8-C9	-3.22	121.37	126.23
13	J	1303	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
20	u	822	SQD	C1-O5-C5	3.22	120.00	113.69
16	2	522	BCR	C28-C27-C26	-3.22	108.33	114.08
16	r	521	BCR	C7-C8-C9	-3.22	121.38	126.23
13	e	1105	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
16	n	4022	BCR	C15-C14-C13	-3.22	122.72	127.31
13	B	1221	CLA	CHB-C4A-NA	3.21	128.96	124.51
13	e	1135	CLA	CMB-C2B-C1B	-3.21	120.47	125.37
13	Z	516	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
20	f	1852	SQD	O8-S-C6	3.21	110.86	105.74
13	A	1105	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
16	3	521	BCR	C11-C10-C9	-3.21	122.73	127.31
13	H	1230	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
16	s	521	BCR	C11-C10-C9	-3.21	122.73	127.31
16	r	522	BCR	C28-C27-C26	-3.21	108.35	114.08
16	5	523	BCR	C28-C27-C26	-3.21	108.35	114.08
13	B	1214	CLA	C3B-C4B-NB	-3.21	107.54	110.52
16	2	521	BCR	C7-C8-C9	-3.21	121.39	126.23
13	s	510	CLA	CHB-C4A-NA	3.20	128.94	124.51
13	e	1139	CLA	O2D-CGD-O1D	-3.20	117.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	510	CLA	CHB-C4A-NA	3.20	128.94	124.51
13	f	1214	CLA	C3B-C4B-NB	-3.20	107.55	110.52
16	a	521	BCR	C11-C10-C9	-3.20	122.74	127.31
13	Z	501	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
16	K	4104	BCR	C30-C25-C26	-3.20	118.11	122.61
16	u	521	BCR	C3-C4-C5	-3.20	108.37	114.08
13	H	1221	CLA	CHB-C4A-NA	3.20	128.93	124.51
13	A	1139	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
13	H	1023	CLA	C3B-C4B-NB	-3.19	107.55	110.52
16	5	521	BCR	C3-C4-C5	-3.19	108.38	114.08
13	G	1139	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
16	H	4009	BCR	C33-C5-C6	-3.19	120.94	124.53
16	Z	522	BCR	C28-C27-C26	-3.19	108.38	114.08
13	G	1134	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
13	6	501	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
13	l	1303	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
16	e	4007	BCR	C7-C8-C9	-3.19	121.42	126.23
16	c	523	BCR	C28-C27-C26	-3.19	108.38	114.08
16	e	4003	BCR	C20-C21-C22	-3.19	122.76	127.31
16	n	4019	BCR	C28-C27-C26	-3.19	108.39	114.08
13	2	501	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
16	A	4007	BCR	C7-C8-C9	-3.19	121.42	126.23
13	f	1215	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
16	V	4020	BCR	C37-C22-C21	-3.18	118.46	122.92
13	f	1226	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
16	G	4003	BCR	C20-C21-C22	-3.18	122.77	127.31
13	A	1134	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
16	d	524	BCR	C15-C16-C17	-3.18	116.96	123.47
16	L	4020	BCR	C37-C22-C21	-3.18	118.47	122.92
13	B	1226	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
16	V	4019	BCR	C28-C27-C26	-3.18	108.40	114.08
16	G	4007	BCR	C7-C8-C9	-3.18	121.43	126.23
16	Y	523	BCR	C28-C27-C26	-3.18	108.40	114.08
13	G	1112	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
13	v	501	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
16	v	524	BCR	C15-C16-C17	-3.18	116.96	123.47
13	q	512	CLA	C6-C5-C3	-3.18	109.42	114.62
13	H	1226	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
16	G	4001	BCR	C11-C10-C9	-3.18	122.78	127.31
16	c	521	BCR	C3-C4-C5	-3.17	108.41	114.08
16	n	4020	BCR	C37-C22-C21	-3.17	118.48	122.92
16	1	524	BCR	C24-C23-C22	-3.17	121.44	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1131	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
16	c	521	BCR	C38-C26-C27	3.17	119.71	113.62
16	B	4009	BCR	C33-C5-C6	-3.17	120.97	124.53
13	H	1216	CLA	CHB-C1B-NB	3.17	127.62	124.26
13	A	1112	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
13	f	1023	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
13	r	501	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
16	6	524	BCR	C15-C16-C17	-3.17	116.97	123.47
13	e	1112	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
16	U	4104	BCR	C30-C25-C26	-3.17	118.15	122.61
16	5	521	BCR	C38-C26-C27	3.17	119.71	113.62
16	L	4019	BCR	C28-C27-C26	-3.17	108.42	114.08
13	e	1134	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
16	1	523	BCR	C28-C27-C26	-3.17	108.42	114.08
13	H	1214	CLA	C3B-C4B-NB	-3.17	107.58	110.52
16	A	4003	BCR	C20-C21-C22	-3.17	122.79	127.31
13	e	1119	CLA	CHB-C1B-NB	3.17	127.61	124.26
13	A	1131	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
13	B	1215	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
16	e	4001	BCR	C11-C10-C9	-3.17	122.79	127.31
13	Y	508	CLA	CMB-C2B-C1B	-3.17	120.55	125.37
13	H	1215	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
16	v	522	BCR	C20-C21-C22	-3.17	122.79	127.31
16	Y	522	BCR	C20-C21-C22	-3.16	122.79	127.31
13	6	512	CLA	C3B-C4B-NB	-3.16	107.58	110.52
16	A	4001	BCR	C11-C10-C9	-3.16	122.80	127.31
13	G	1103	CLA	CHB-C4A-NA	3.16	128.88	124.51
16	f	4010	BCR	C28-C27-C26	-3.16	108.43	114.08
13	B	1023	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
13	f	1214	CLA	CHB-C4A-NA	3.16	128.88	124.51
16	q	524	BCR	C24-C23-C22	-3.16	121.46	126.23
13	V	1502	CLA	C3B-C4B-NB	-3.16	107.58	110.52
13	1	508	CLA	CMB-C2B-C1B	-3.16	120.56	125.37
13	H	1023	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
13	A	1103	CLA	CHB-C4A-NA	3.16	128.88	124.51
13	d	512	CLA	C3B-C4B-NB	-3.16	107.59	110.52
16	H	4005	BCR	C16-C17-C18	-3.16	122.81	127.31
16	q	523	BCR	C28-C27-C26	-3.15	108.44	114.08
13	q	508	CLA	CMB-C2B-C1B	-3.15	120.56	125.37
13	f	1207	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
16	Y	524	BCR	C24-C23-C22	-3.15	121.47	126.23
13	e	1131	CLA	O2D-CGD-O1D	-3.15	117.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4005	BCR	C16-C17-C18	-3.15	122.81	127.31
13	V	1501	CLA	CHB-C4A-NA	3.15	128.87	124.51
16	t	521	BCR	C3-C4-C5	-3.15	108.45	114.08
13	A	1136	CLA	C3B-C4B-NB	-3.15	107.59	110.52
13	n	1502	CLA	C3B-C4B-NB	-3.15	107.59	110.52
16	f	4004	BCR	C33-C5-C6	-3.15	120.99	124.53
16	B	4005	BCR	C16-C17-C18	-3.15	122.81	127.31
16	1	522	BCR	C20-C21-C22	-3.15	122.81	127.31
13	l	1302	CLA	CHB-C4A-NA	3.15	128.87	124.51
13	A	1103	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
13	1	512	CLA	C6-C5-C3	-3.15	109.47	114.62
13	t	519	CLA	C3B-C4B-NB	-3.15	107.60	110.52
13	v	512	CLA	C3B-C4B-NB	-3.15	107.60	110.52
13	e	1135	CLA	C1-C2-C3	-3.14	120.60	126.04
16	H	4010	BCR	C28-C27-C26	-3.14	108.46	114.08
13	G	1135	CLA	C1-C2-C3	-3.14	120.61	126.04
13	f	1216	CLA	CHB-C4A-NA	3.14	128.86	124.51
16	B	4010	BCR	C28-C27-C26	-3.14	108.46	114.08
13	e	1136	CLA	C3B-C4B-NB	-3.14	107.60	110.52
16	u	521	BCR	C38-C26-C27	3.14	119.65	113.62
13	f	1217	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
13	e	1119	CLA	CMB-C2B-C1B	-3.14	120.58	125.37
16	V	4022	BCR	C16-C17-C18	-3.14	122.83	127.31
16	q	522	BCR	C20-C21-C22	-3.14	122.83	127.31
13	f	1240	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
13	2	519	CLA	C3B-C4B-NB	-3.14	107.60	110.52
16	2	523	BCR	C28-C27-C26	-3.14	108.47	114.08
16	4	521	BCR	C3-C4-C5	-3.14	108.47	114.08
13	f	1207	CLA	C3B-C4B-NB	-3.14	107.60	110.52
13	Y	512	CLA	C6-C5-C3	-3.14	109.49	114.62
16	L	4219	BCR	C15-C16-C17	-3.14	117.05	123.47
16	r	523	BCR	C28-C27-C26	-3.14	108.48	114.08
13	B	1217	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
13	e	1103	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
16	6	522	BCR	C20-C21-C22	-3.14	122.83	127.31
13	f	1216	CLA	CHB-C1B-NB	3.14	127.58	124.26
13	e	1103	CLA	CHB-C4A-NA	3.13	128.85	124.51
16	Z	523	BCR	C28-C27-C26	-3.13	108.48	114.08
16	5	524	BCR	C33-C5-C6	-3.13	121.01	124.53
13	G	1136	CLA	C3B-C4B-NB	-3.13	107.61	110.52
16	b	523	BCR	C33-C5-C6	-3.13	121.01	124.53
16	J	4013	BCR	C32-C1-C6	-3.13	105.22	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	522	BCR	C20-C21-C22	-3.13	122.84	127.31
13	L	1501	CLA	CHB-C4A-NA	3.13	128.84	124.51
13	B	1216	CLA	CHB-C1B-NB	3.13	127.57	124.26
13	r	519	CLA	C3B-C4B-NB	-3.13	107.61	110.52
13	B	1214	CLA	CHB-C4A-NA	3.13	128.84	124.51
13	A	1135	CLA	C1-C2-C3	-3.13	120.63	126.04
16	n	4219	BCR	C15-C16-C17	-3.13	117.06	123.47
16	T	4013	BCR	C32-C1-C6	-3.13	105.22	110.30
13	H	1207	CLA	C3B-C4B-NB	-3.13	107.61	110.52
13	A	1119	CLA	CMB-C2B-C1B	-3.13	120.61	125.37
13	G	1103	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
13	B	1207	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
13	G	1116	CLA	CMB-C2B-C1B	-3.13	120.61	125.37
13	H	1214	CLA	CHB-C4A-NA	3.13	128.83	124.51
16	s	524	BCR	C15-C16-C17	-3.13	117.07	123.47
16	G	4011	BCR	C8-C9-C10	3.12	123.73	118.94
13	s	508	CLA	CHB-C1B-NB	3.12	127.56	124.26
13	G	1119	CLA	CMB-C2B-C1B	-3.12	120.61	125.37
16	B	4004	BCR	C33-C5-C6	-3.12	121.02	124.53
16	H	4004	BCR	C33-C5-C6	-3.12	121.02	124.53
16	c	524	BCR	C33-C5-C6	-3.12	121.02	124.53
16	V	4219	BCR	C15-C16-C17	-3.12	117.08	123.47
16	1	521	BCR	C24-C23-C22	-3.12	121.52	126.23
16	b	521	BCR	C3-C4-C5	-3.12	108.50	114.08
13	n	1501	CLA	CHB-C4A-NA	3.12	128.83	124.51
16	A	4011	BCR	C8-C9-C10	3.12	123.73	118.94
16	T	4012	BCR	C7-C8-C9	-3.12	121.52	126.23
16	a	524	BCR	C15-C16-C17	-3.12	117.08	123.47
16	I	4018	BCR	C11-C10-C9	-3.12	122.86	127.31
16	u	524	BCR	C33-C5-C6	-3.12	121.02	124.53
16	J	4012	BCR	C7-C8-C9	-3.12	121.52	126.23
13	B	1207	CLA	C3B-C4B-NB	-3.12	107.62	110.52
16	4	523	BCR	C33-C5-C6	-3.12	121.03	124.53
16	k	4018	BCR	C11-C10-C9	-3.12	122.86	127.31
13	Z	519	CLA	C3B-C4B-NB	-3.12	107.62	110.52
16	Y	521	BCR	C24-C23-C22	-3.12	121.52	126.23
13	B	1240	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
13	H	1205	CLA	O2A-CGA-O1A	-3.12	115.73	123.59
16	5	522	BCR	C38-C26-C25	-3.12	121.03	124.53
13	q	509	CLA	CHB-C4A-NA	3.12	128.82	124.51
16	u	522	BCR	C38-C26-C25	-3.12	121.03	124.53
16	2	522	BCR	C24-C23-C22	-3.11	121.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	522	BCR	C24-C23-C22	-3.11	121.53	126.23
16	l	4013	BCR	C32-C1-C6	-3.11	105.25	110.30
16	q	521	BCR	C24-C23-C22	-3.11	121.53	126.23
16	l	4013	BCR	C20-C19-C18	-3.11	117.67	126.42
16	b	523	BCR	C28-C27-C26	-3.11	108.52	114.08
16	3	524	BCR	C15-C16-C17	-3.11	117.10	123.47
13	A	1116	CLA	CMB-C2B-C1B	-3.11	120.63	125.37
16	W	4021	BCR	C10-C11-C12	-3.11	113.51	123.22
13	L	1502	CLA	C3B-C4B-NB	-3.11	107.63	110.52
13	H	1207	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
16	e	4011	BCR	C8-C9-C10	3.11	123.71	118.94
13	B	1205	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
13	e	1110	CLA	C3B-C4B-NB	-3.11	107.63	110.52
13	H	1217	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
16	L	4022	BCR	C16-C17-C18	-3.11	122.87	127.31
16	t	523	BCR	C33-C5-C6	-3.11	121.04	124.53
13	H	1232	CLA	CMB-C2B-C3B	3.11	134.12	126.59
16	S	4018	BCR	C11-C10-C9	-3.11	122.87	127.31
16	t	523	BCR	C28-C27-C26	-3.11	108.53	114.08
16	4	521	BCR	C24-C23-C22	-3.11	121.54	126.23
16	b	523	BCR	C24-C23-C22	-3.11	121.54	126.23
13	B	1216	CLA	CHB-C4A-NA	3.11	128.81	124.51
16	b	521	BCR	C24-C23-C22	-3.11	121.54	126.23
16	n	4022	BCR	C16-C17-C18	-3.10	122.88	127.31
13	Y	509	CLA	CHB-C4A-NA	3.10	128.80	124.51
16	t	523	BCR	C24-C23-C22	-3.10	121.55	126.23
13	G	1140	CLA	C3B-C4B-NB	-3.10	107.64	110.52
20	Y	822	SQD	O9-S-C6	3.10	110.63	106.94
16	M	4021	BCR	C15-C16-C17	-3.10	117.12	123.47
13	f	1205	CLA	O2A-CGA-O1A	-3.10	115.76	123.59
20	1	822	SQD	O9-S-C6	3.10	110.62	106.94
13	e	1116	CLA	CMB-C2B-C1B	-3.10	120.65	125.37
13	T	1302	CLA	CHB-C4A-NA	3.10	128.80	124.51
16	W	4021	BCR	C15-C16-C17	-3.10	117.12	123.47
16	c	522	BCR	C20-C21-C22	-3.10	122.89	127.31
16	o	4021	BCR	C15-C16-C17	-3.10	117.12	123.47
13	B	1232	CLA	CMB-C2B-C3B	3.10	134.09	126.59
16	t	521	BCR	C28-C27-C26	-3.10	108.55	114.08
16	l	4012	BCR	C7-C8-C9	-3.10	121.56	126.23
16	r	522	BCR	C24-C23-C22	-3.10	121.56	126.23
16	u	522	BCR	C20-C21-C22	-3.10	122.89	127.31
13	f	1232	CLA	CMB-C2B-C3B	3.10	134.09	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	509	CLA	CHB-C4A-NA	3.10	128.79	124.51
13	A	1107	CLA	C3B-C4B-NB	-3.10	107.64	110.52
13	H	1240	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
13	G	1136	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
13	4	519	CLA	C3B-C4B-NB	-3.09	107.64	110.52
13	H	1216	CLA	CHB-C4A-NA	3.09	128.79	124.51
16	4	523	BCR	C24-C23-C22	-3.09	121.56	126.23
13	c	512	CLA	C3B-C4B-NB	-3.09	107.65	110.52
16	a	523	BCR	C15-C16-C17	-3.09	117.14	123.47
16	4	523	BCR	C28-C27-C26	-3.09	108.56	114.08
13	J	1302	CLA	CHB-C4A-NA	3.09	128.78	124.51
16	b	524	BCR	C33-C5-C4	3.09	119.55	113.62
16	4	524	BCR	C33-C5-C4	3.09	119.55	113.62
16	M	4021	BCR	C10-C11-C12	-3.09	113.58	123.22
16	J	4013	BCR	C20-C19-C18	-3.09	117.74	126.42
13	B	1209	CLA	C3B-C4B-NB	-3.09	107.65	110.52
13	b	519	CLA	C3B-C4B-NB	-3.09	107.65	110.52
16	4	521	BCR	C28-C27-C26	-3.09	108.56	114.08
16	T	4013	BCR	C20-C19-C18	-3.09	117.74	126.42
16	b	522	BCR	C7-C8-C9	-3.09	121.57	126.23
16	b	521	BCR	C28-C27-C26	-3.09	108.56	114.08
13	f	1225	CLA	CMB-C2B-C1B	-3.09	120.67	125.37
16	4	524	BCR	C1-C6-C5	-3.09	118.27	122.61
16	t	521	BCR	C24-C23-C22	-3.08	121.57	126.23
13	f	1219	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
16	V	4219	BCR	C10-C11-C12	-3.08	113.60	123.22
16	o	4021	BCR	C10-C11-C12	-3.08	113.60	123.22
16	t	524	BCR	C33-C5-C4	3.08	119.54	113.62
16	4	522	BCR	C7-C8-C9	-3.08	121.58	126.23
13	f	1205	CLA	CBA-CAA-C2A	3.08	122.96	113.86
20	q	822	SQD	C1-O5-C5	3.08	119.73	113.69
13	m	1401	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
20	Y	822	SQD	C1-O5-C5	3.08	119.73	113.69
16	q	523	BCR	C21-C20-C19	-3.08	113.61	123.22
13	G	1110	CLA	C3B-C4B-NB	-3.08	107.66	110.52
13	f	1209	CLA	C3B-C4B-NB	-3.08	107.66	110.52
13	B	1205	CLA	CBA-CAA-C2A	3.08	122.94	113.86
20	H	1852	SQD	O6-C1-C2	3.08	113.11	108.30
13	G	1125	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
16	3	523	BCR	C15-C16-C17	-3.08	117.17	123.47
16	s	523	BCR	C15-C16-C17	-3.08	117.17	123.47
20	q	822	SQD	O9-S-C6	3.08	110.59	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	4219	BCR	C10-C11-C12	-3.08	113.62	123.22
13	H	1225	CLA	CMB-C2B-C1B	-3.07	120.69	125.37
20	B	1852	SQD	O6-C1-C2	3.07	113.10	108.30
13	G	1107	CLA	C3B-C4B-NB	-3.07	107.66	110.52
13	G	1133	CLA	CHB-C4A-NA	3.07	128.76	124.51
16	2	523	BCR	C33-C5-C6	-3.07	121.08	124.53
16	c	522	BCR	C38-C26-C25	-3.07	121.08	124.53
16	T	4012	BCR	C11-C10-C9	-3.07	122.92	127.31
13	3	508	CLA	CHB-C1B-NB	3.07	127.51	124.26
16	5	523	BCR	C10-C11-C12	-3.07	113.63	123.22
13	e	1107	CLA	C3B-C4B-NB	-3.07	107.66	110.52
16	t	522	BCR	C7-C8-C9	-3.07	121.59	126.23
13	A	1136	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
13	A	1125	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
16	b	524	BCR	C1-C6-C5	-3.07	118.29	122.61
13	K	1401	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
16	L	4219	BCR	C10-C11-C12	-3.07	113.64	123.22
13	H	1205	CLA	CBA-CAA-C2A	3.07	122.92	113.86
16	c	521	BCR	C38-C26-C25	-3.07	121.08	124.53
13	B	1235	CLA	CHB-C4A-NA	3.07	128.75	124.51
16	u	523	BCR	C10-C11-C12	-3.07	113.64	123.22
13	B	1225	CLA	CMB-C2B-C1B	-3.07	120.70	125.37
13	H	1209	CLA	CHB-C4A-NA	3.07	128.75	124.51
20	f	1852	SQD	O9-S-C6	3.07	110.58	106.94
13	A	1140	CLA	C3B-C4B-NB	-3.07	107.67	110.52
20	f	1852	SQD	O6-C1-C2	3.07	113.09	108.30
16	J	4012	BCR	C11-C10-C9	-3.06	122.94	127.31
16	5	522	BCR	C20-C21-C22	-3.06	122.94	127.31
20	1	822	SQD	C1-O5-C5	3.06	119.70	113.69
13	5	512	CLA	C3B-C4B-NB	-3.06	107.67	110.52
13	u	512	CLA	C3B-C4B-NB	-3.06	107.67	110.52
16	Y	523	BCR	C21-C20-C19	-3.06	113.66	123.22
13	H	1235	CLA	CHB-C4A-NA	3.06	128.75	124.51
16	S	4018	BCR	C15-C16-C17	-3.06	117.20	123.47
13	Z	519	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
13	B	1219	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
16	1	523	BCR	C21-C20-C19	-3.06	113.66	123.22
13	B	1218	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
16	l	4015	BCR	C38-C26-C25	-3.06	121.09	124.53
13	A	1013	CLA	CHB-C1B-NB	3.06	127.50	124.26
16	3	521	BCR	C3-C4-C5	-3.06	108.61	114.08
16	c	523	BCR	C10-C11-C12	-3.06	113.67	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1125	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
13	a	506	CLA	CMB-C2B-C1B	-3.06	120.71	125.37
16	k	4018	BCR	C15-C16-C17	-3.06	117.21	123.47
16	s	521	BCR	C3-C4-C5	-3.06	108.62	114.08
13	A	1130	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
16	t	524	BCR	C1-C6-C5	-3.06	118.31	122.61
13	A	1110	CLA	C3B-C4B-NB	-3.05	107.68	110.52
16	I	4018	BCR	C15-C16-C17	-3.05	117.22	123.47
16	l	4012	BCR	C11-C10-C9	-3.05	122.95	127.31
13	B	1220	CLA	CHB-C4A-NA	3.05	128.74	124.51
16	Y	523	BCR	C15-C16-C17	-3.05	117.22	123.47
13	f	1232	CLA	CHB-C1B-NB	3.05	127.49	124.26
13	H	1209	CLA	C3B-C4B-NB	-3.05	107.68	110.52
13	A	1133	CLA	CHB-C4A-NA	3.05	128.73	124.51
13	B	1232	CLA	CHB-C1B-NB	3.05	127.49	124.26
13	G	1130	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
16	e	4011	BCR	C15-C14-C13	-3.05	122.95	127.31
13	G	1013	CLA	CHB-C1B-NB	3.05	127.49	124.26
13	G	1106	CLA	C3B-C4B-NB	-3.05	107.69	110.52
13	e	1136	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	f	1209	CLA	CHB-C4A-NA	3.05	128.73	124.51
16	A	4011	BCR	C15-C14-C13	-3.05	122.96	127.31
20	B	1852	SQD	O9-S-C6	3.05	110.56	106.94
13	H	1219	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
16	5	521	BCR	C38-C26-C25	-3.05	121.11	124.53
13	e	1013	CLA	CHB-C1B-NB	3.05	127.48	124.26
13	f	1203	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	e	1133	CLA	CHB-C4A-NA	3.05	128.72	124.51
13	U	1401	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	f	1235	CLA	CHB-C4A-NA	3.05	128.72	124.51
16	a	521	BCR	C3-C4-C5	-3.04	108.64	114.08
13	B	1209	CLA	CHB-C4A-NA	3.04	128.72	124.51
13	3	510	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	H	1218	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	f	1218	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	b	509	CLA	CHB-C4A-NA	3.04	128.72	124.51
13	a	510	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	H	1220	CLA	CHB-C4A-NA	3.04	128.72	124.51
16	Z	523	BCR	C33-C5-C6	-3.04	121.11	124.53
20	H	1852	SQD	O9-S-C6	3.04	110.55	106.94
13	Z	512	CLA	C3B-C4B-NB	-3.04	107.69	110.52
16	1	523	BCR	C15-C16-C17	-3.04	117.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1129	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
13	r	513	CLA	C3B-C4B-NB	-3.04	107.70	110.52
13	2	519	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
13	e	1106	CLA	C3B-C4B-NB	-3.04	107.70	110.52
13	e	1140	CLA	C3B-C4B-NB	-3.04	107.70	110.52
13	e	1126	CLA	CMB-C2B-C3B	3.04	133.94	126.59
13	f	1231	CLA	CHB-C4A-NA	3.04	128.71	124.51
13	e	1129	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
13	e	1130	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
13	A	1124	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
13	u	512	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
13	A	1140	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
13	A	1129	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
13	f	1227	CLA	CHB-C4A-NA	3.03	128.71	124.51
13	e	1140	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
16	G	4008	BCR	C11-C10-C9	-3.03	122.98	127.31
13	G	1140	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
16	c	522	BCR	C33-C5-C6	-3.03	121.12	124.53
16	T	4015	BCR	C38-C26-C25	-3.03	121.12	124.53
13	a	508	CLA	CHB-C1B-NB	3.03	127.46	124.26
16	A	4008	BCR	C11-C10-C9	-3.03	122.99	127.31
16	G	4011	BCR	C15-C14-C13	-3.03	122.99	127.31
13	3	506	CLA	CMB-C2B-C1B	-3.03	120.76	125.37
13	G	1124	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
13	c	512	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
16	6	523	BCR	C33-C5-C6	-3.02	121.13	124.53
13	e	1127	CLA	CMB-C2B-C1B	-3.02	120.76	125.37
13	B	1227	CLA	CHB-C4A-NA	3.02	128.69	124.51
13	B	1203	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
13	t	509	CLA	CHB-C4A-NA	3.02	128.69	124.51
13	s	519	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
13	G	1138	CLA	C3B-C4B-NB	-3.02	107.71	110.52
16	v	523	BCR	C33-C5-C6	-3.02	121.13	124.53
13	5	512	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
13	a	513	CLA	CHB-C4A-NA	3.02	128.69	124.51
13	H	1214	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
13	s	510	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
16	r	523	BCR	C33-C5-C6	-3.02	121.14	124.53
13	A	1106	CLA	C3B-C4B-NB	-3.02	107.71	110.52
13	H	1203	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
16	u	521	BCR	C38-C26-C25	-3.02	121.14	124.53
13	s	506	CLA	CMB-C2B-C1B	-3.02	120.77	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4006	BCR	C11-C10-C9	-3.02	123.00	127.31
13	4	509	CLA	CHB-C4A-NA	3.02	128.69	124.51
13	2	513	CLA	C3B-C4B-NB	-3.02	107.72	110.52
13	e	1137	CLA	C3B-C4B-NB	-3.02	107.72	110.52
13	B	1214	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
13	r	519	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
13	f	1220	CLA	CHB-C4A-NA	3.02	128.69	124.51
16	Z	523	BCR	C11-C10-C9	-3.02	123.00	127.31
13	H	1232	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
13	H	1227	CLA	CHB-C4A-NA	3.02	128.68	124.51
16	J	4015	BCR	C38-C26-C25	-3.02	121.14	124.53
16	r	523	BCR	C24-C23-C22	-3.02	121.68	126.23
13	e	1120	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
13	G	1127	CLA	CMB-C2B-C1B	-3.02	120.78	125.37
16	q	523	BCR	C15-C16-C17	-3.01	117.30	123.47
13	A	1127	CLA	CMB-C2B-C1B	-3.01	120.78	125.37
13	A	1126	CLA	CMB-C2B-C3B	3.01	133.89	126.59
13	H	1232	CLA	CHB-C1B-NB	3.01	127.45	124.26
16	e	4002	BCR	C16-C15-C14	-3.01	117.30	123.47
16	2	523	BCR	C24-C23-C22	-3.01	121.68	126.23
13	Z	513	CLA	C3B-C4B-NB	-3.01	107.72	110.52
13	r	512	CLA	C3B-C4B-NB	-3.01	107.72	110.52
16	Z	523	BCR	C24-C23-C22	-3.01	121.69	126.23
13	G	1121	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	G	1126	CLA	CMB-C2B-C3B	3.01	133.88	126.59
16	A	4002	BCR	C16-C15-C14	-3.01	117.31	123.47
16	H	4014	BCR	C2-C1-C6	3.01	115.11	110.48
13	G	1105	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
16	n	4219	BCR	C21-C20-C19	-3.01	113.83	123.22
16	d	523	BCR	C7-C8-C9	-3.01	121.69	126.23
16	6	523	BCR	C7-C8-C9	-3.01	121.69	126.23
13	3	519	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
16	G	4002	BCR	C16-C15-C14	-3.01	117.32	123.47
13	2	512	CLA	C3B-C4B-NB	-3.01	107.73	110.52
16	e	4001	BCR	C2-C1-C6	3.00	115.11	110.48
16	B	4014	BCR	C2-C1-C6	3.00	115.11	110.48
13	A	1113	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
13	B	1231	CLA	CHB-C4A-NA	3.00	128.66	124.51
13	A	1137	CLA	C3B-C4B-NB	-3.00	107.73	110.52
13	e	1133	CLA	C3B-C4B-NB	-3.00	107.73	110.52
13	e	1124	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
16	G	4001	BCR	C2-C1-C6	3.00	115.10	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4014	BCR	C2-C1-C6	3.00	115.10	110.48
16	B	4006	BCR	C11-C10-C9	-3.00	123.03	127.31
16	L	4219	BCR	C21-C20-C19	-3.00	113.86	123.22
16	u	522	BCR	C33-C5-C6	-3.00	121.16	124.53
13	G	1111	CLA	C3B-C4B-NB	-3.00	107.73	110.52
16	5	522	BCR	C33-C5-C6	-3.00	121.16	124.53
13	A	1105	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
16	A	4001	BCR	C2-C1-C6	3.00	115.09	110.48
13	H	1206	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
16	V	4219	BCR	C21-C20-C19	-3.00	113.87	123.22
16	A	4002	BCR	C20-C21-C22	-3.00	123.03	127.31
16	d	523	BCR	C24-C23-C22	-3.00	121.71	126.23
16	e	4008	BCR	C11-C10-C9	-3.00	123.03	127.31
13	A	1120	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
13	e	1105	CLA	CMB-C2B-C1B	-2.99	120.81	125.37
13	e	1113	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
13	f	1214	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
13	A	1121	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
16	d	523	BCR	C33-C5-C6	-2.99	121.17	124.53
13	A	1138	CLA	C3B-C4B-NB	-2.99	107.74	110.52
16	v	523	BCR	C7-C8-C9	-2.99	121.72	126.23
16	H	4014	BCR	C3-C4-C5	-2.99	108.74	114.08
16	r	523	BCR	C11-C10-C9	-2.99	123.04	127.31
13	A	1111	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
16	e	4002	BCR	C20-C21-C22	-2.99	123.04	127.31
13	s	513	CLA	CHB-C4A-NA	2.99	128.65	124.51
16	B	4014	BCR	C3-C4-C5	-2.99	108.74	114.08
13	G	1113	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	a	519	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	3	513	CLA	CHB-C4A-NA	2.99	128.64	124.51
13	a	504	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	A	1111	CLA	C3B-C4B-NB	-2.99	107.75	110.52
16	j	4016	BCR	C28-C27-C26	-2.99	108.75	114.08
13	Z	504	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	e	1121	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	f	1232	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	3	504	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	B	1232	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	e	1111	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
16	V	4020	BCR	C7-C8-C9	-2.98	121.73	126.23
16	F	4016	BCR	C28-C27-C26	-2.98	108.75	114.08
16	L	4020	BCR	C7-C8-C9	-2.98	121.73	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	r	822	SQD	O6-C1-C2	2.98	112.96	108.30
13	G	1108	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
13	e	1138	CLA	C3B-C4B-NB	-2.98	107.75	110.52
13	s	509	CLA	CHB-C4A-NA	2.98	128.63	124.51
16	v	523	BCR	C24-C23-C22	-2.98	121.73	126.23
13	H	1231	CLA	CHB-C4A-NA	2.98	128.63	124.51
16	R	4016	BCR	C28-C27-C26	-2.98	108.76	114.08
13	f	1206	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
16	f	4014	BCR	C3-C4-C5	-2.98	108.76	114.08
13	Y	512	CLA	C3B-C4B-NB	-2.98	107.75	110.52
13	B	1206	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
16	2	523	BCR	C11-C10-C9	-2.98	123.06	127.31
16	G	4002	BCR	C20-C21-C22	-2.98	123.06	127.31
17	V	5221	LHG	O8-C23-C24	2.98	121.25	111.91
16	t	522	BCR	C38-C26-C25	-2.98	121.18	124.53
13	s	504	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
13	f	1201	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
20	5	822	SQD	O8-S-C6	2.98	110.48	105.74
20	u	822	SQD	O8-S-C6	2.98	110.48	105.74
13	G	1109	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
13	G	1111	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
13	A	1123	CLA	CHB-C4A-NA	2.98	128.63	124.51
17	L	5221	LHG	O8-C23-C24	2.98	121.25	111.91
16	f	4009	BCR	C33-C5-C4	2.98	119.33	113.62
13	r	504	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
16	6	523	BCR	C24-C23-C22	-2.98	121.74	126.23
16	e	4002	BCR	C15-C14-C13	-2.98	123.06	127.31
16	4	522	BCR	C38-C26-C25	-2.97	121.19	124.53
13	G	1137	CLA	C3B-C4B-NB	-2.97	107.76	110.52
17	n	5221	LHG	O8-C23-C24	2.97	121.24	111.91
13	H	1201	CLA	CMB-C2B-C1B	-2.97	120.84	125.37
13	B	1229	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
16	H	4006	BCR	C11-C10-C9	-2.97	123.07	127.31
16	n	4020	BCR	C7-C8-C9	-2.97	121.75	126.23
20	c	822	SQD	O8-S-C6	2.97	110.47	105.74
13	H	1226	CLA	CMB-C2B-C3B	2.97	133.78	126.59
13	A	1109	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
13	f	1229	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
13	H	1213	CLA	CHB-C4A-NA	2.97	128.62	124.51
13	f	1223	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
13	A	1108	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
13	H	1229	CLA	O2D-CGD-O1D	-2.97	118.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1102	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
13	2	504	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
13	A	1102	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
20	6	822	SQD	O8-S-C6	2.97	110.47	105.74
13	e	1111	CLA	C3B-C4B-NB	-2.97	107.76	110.52
13	B	1201	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
13	3	509	CLA	CHB-C4A-NA	2.97	128.61	124.51
20	q	822	SQD	O6-C1-C2	2.97	112.93	108.30
13	V	1502	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
13	s	513	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
13	B	1226	CLA	CMB-C2B-C3B	2.96	133.77	126.59
13	e	1108	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
16	b	522	BCR	C38-C26-C25	-2.96	121.20	124.53
16	q	524	BCR	C11-C10-C9	-2.96	123.08	127.31
13	Z	509	CLA	CHB-C4A-NA	2.96	128.61	124.51
13	G	1120	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
16	A	4002	BCR	C15-C14-C13	-2.96	123.08	127.31
16	Y	524	BCR	C11-C10-C9	-2.96	123.08	127.31
20	2	822	SQD	O6-C1-C2	2.96	112.93	108.30
20	d	822	SQD	O8-S-C6	2.96	110.46	105.74
13	q	519	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
13	s	512	CLA	C3B-C4B-NB	-2.96	107.77	110.52
13	U	1105	CLA	CMC-C2C-C3C	2.96	134.15	126.12
13	t	506	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
13	G	1121	CLA	CHB-C4A-NA	2.96	128.60	124.51
13	e	1123	CLA	CHB-C4A-NA	2.96	128.60	124.51
13	K	1105	CLA	CMC-C2C-C3C	2.96	134.14	126.12
13	G	1125	CLA	C3B-C4B-NB	-2.96	107.77	110.52
13	a	509	CLA	CHB-C4A-NA	2.96	128.60	124.51
13	G	1133	CLA	C3B-C4B-NB	-2.95	107.77	110.52
20	u	822	SQD	O5-C5-C4	2.95	115.06	109.69
13	H	1228	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
13	G	1123	CLA	CHB-C4A-NA	2.95	128.60	124.51
13	H	1012	CLA	CMB-C2B-C3B	2.95	133.74	126.59
13	B	1202	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
13	H	1202	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
20	1	822	SQD	O6-C1-C2	2.95	112.91	108.30
20	5	822	SQD	O5-C5-C4	2.95	115.05	109.69
13	n	1502	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
13	f	1012	CLA	CMB-C2B-C3B	2.95	133.73	126.59
13	q	512	CLA	C3B-C4B-NB	-2.95	107.78	110.52
13	e	1109	CLA	O2A-CGA-O1A	-2.95	116.15	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1126	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
13	f	1202	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
13	B	1012	CLA	CMB-C2B-C3B	2.95	133.73	126.59
16	v	522	BCR	C33-C5-C6	-2.95	121.22	124.53
20	v	822	SQD	O8-S-C6	2.95	110.44	105.74
16	Y	523	BCR	C16-C17-C18	-2.95	123.10	127.31
13	B	1223	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
13	f	1226	CLA	CMB-C2B-C3B	2.95	133.73	126.59
13	m	1105	CLA	CMC-C2C-C3C	2.95	134.12	126.12
20	Z	822	SQD	O6-C1-C2	2.95	112.91	108.30
13	2	502	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
13	1	512	CLA	C3B-C4B-NB	-2.95	107.78	110.52
20	Y	822	SQD	O6-C1-C2	2.95	112.90	108.30
16	1	524	BCR	C11-C10-C9	-2.95	123.11	127.31
16	k	4018	BCR	C20-C21-C22	-2.95	123.11	127.31
13	B	1213	CLA	CHB-C4A-NA	2.95	128.59	124.51
13	4	506	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
13	B	1228	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
16	G	4002	BCR	C15-C14-C13	-2.94	123.11	127.31
13	H	1223	CLA	CMB-C2B-C1B	-2.94	120.88	125.37
13	f	1238	CLA	CMB-C2B-C3B	2.94	133.72	126.59
13	b	506	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
20	c	822	SQD	O5-C5-C4	2.94	115.04	109.69
16	a	523	BCR	C24-C23-C22	-2.94	121.79	126.23
13	f	1234	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
13	A	1104	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
13	1	519	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
13	u	507	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
13	B	1220	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	A	1121	CLA	CHB-C4A-NA	2.94	128.58	124.51
13	r	509	CLA	CHB-C4A-NA	2.94	128.58	124.51
13	e	1130	CLA	C3B-C4B-NB	-2.94	107.79	110.52
13	B	1224	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	d	512	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	3	512	CLA	C3B-C4B-NB	-2.94	107.79	110.52
13	B	1238	CLA	CMB-C2B-C3B	2.94	133.71	126.59
13	G	1102	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
20	f	1852	SQD	C44-O6-C1	2.94	119.48	113.74
16	I	4018	BCR	C20-C21-C22	-2.94	123.12	127.31
13	B	1236	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	3	513	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	5	501	CLA	O2D-CGD-O1D	-2.94	118.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4009	BCR	C33-C5-C4	2.94	119.26	113.62
13	r	502	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
13	e	1104	CLA	CAA-C2A-C3A	-2.94	104.74	112.78
16	s	523	BCR	C24-C23-C22	-2.94	121.80	126.23
13	H	1238	CLA	CMB-C2B-C3B	2.94	133.70	126.59
13	A	1133	CLA	C3B-C4B-NB	-2.94	107.79	110.52
13	5	507	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
13	a	513	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
16	6	523	BCR	C28-C27-C26	-2.93	108.84	114.08
13	B	1234	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
13	A	1125	CLA	C3B-C4B-NB	-2.93	107.79	110.52
13	G	1104	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
13	6	512	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
16	6	522	BCR	C33-C5-C6	-2.93	121.23	124.53
16	H	4009	BCR	C33-C5-C4	2.93	119.25	113.62
13	f	1220	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	f	1228	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	f	1213	CLA	CHB-C4A-NA	2.93	128.56	124.51
13	Z	513	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	u	501	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
16	d	523	BCR	C28-C27-C26	-2.93	108.84	114.08
20	B	1852	SQD	C44-O6-C1	2.93	119.46	113.74
16	S	4018	BCR	C20-C21-C22	-2.93	123.13	127.31
16	q	524	BCR	C33-C5-C4	2.93	119.25	113.62
13	e	1237	CLA	C4-C3-C5	2.93	120.20	115.27
13	G	1126	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	H	1224	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	Z	502	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	2	509	CLA	CHB-C4A-NA	2.93	128.56	124.51
13	f	1236	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	v	511	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
16	3	523	BCR	C24-C23-C22	-2.93	121.81	126.23
16	1	522	BCR	C38-C26-C25	-2.93	121.24	124.53
16	u	522	BCR	C38-C26-C27	2.93	119.24	113.62
13	c	507	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	A	1130	CLA	C3B-C4B-NB	-2.93	107.80	110.52
13	G	1130	CLA	C3B-C4B-NB	-2.93	107.80	110.52
13	L	1502	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
20	H	1852	SQD	C44-O6-C1	2.93	119.45	113.74
13	2	513	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
13	f	1224	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
13	A	1237	CLA	C4-C3-C5	2.92	120.19	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1121	CLA	CHB-C4A-NA	2.92	128.56	124.51
13	q	510	CLA	C3B-C4B-NB	-2.92	107.80	110.52
13	G	1237	CLA	C4-C3-C5	2.92	120.19	115.27
13	Y	519	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
13	A	1126	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
13	a	512	CLA	C3B-C4B-NB	-2.92	107.80	110.52
16	S	4018	BCR	C1-C6-C5	-2.92	118.50	122.61
16	q	522	BCR	C3-C4-C5	-2.92	108.86	114.08
13	d	513	CLA	C3B-C4B-NB	-2.92	107.80	110.52
13	G	1105	CLA	CHB-C4A-NA	2.92	128.55	124.51
16	1	524	BCR	C33-C5-C4	2.92	119.23	113.62
13	c	509	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
13	H	1236	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
13	e	1105	CLA	CHB-C4A-NA	2.92	128.55	124.51
13	A	1140	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
13	b	510	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
16	s	523	BCR	C33-C5-C6	-2.92	121.25	124.53
16	Y	522	BCR	C3-C4-C5	-2.92	108.86	114.08
13	H	1220	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
16	v	523	BCR	C28-C27-C26	-2.92	108.87	114.08
16	5	522	BCR	C38-C26-C27	2.92	119.22	113.62
13	r	511	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
13	G	1140	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
13	e	1140	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
13	q	508	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
13	d	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
16	u	523	BCR	C16-C17-C18	-2.91	123.15	127.31
13	t	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
16	1	523	BCR	C16-C17-C18	-2.91	123.15	127.31
16	d	524	BCR	C24-C23-C22	-2.91	121.83	126.23
13	4	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	c	501	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	6	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	2	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	Z	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	t	519	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	A	1105	CLA	CHB-C4A-NA	2.91	128.54	124.51
13	Y	512	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	v	512	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
16	k	4018	BCR	C1-C6-C5	-2.91	118.51	122.61
13	K	1401	CLA	C3B-C4B-NB	-2.91	107.81	110.52
13	1	510	CLA	C3B-C4B-NB	-2.91	107.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1135	CLA	C3B-C4B-NB	-2.91	107.81	110.52
16	Y	522	BCR	C38-C26-C25	-2.91	121.26	124.53
16	a	523	BCR	C33-C5-C6	-2.91	121.26	124.53
16	W	4021	BCR	C20-C19-C18	-2.91	118.24	126.42
16	d	522	BCR	C33-C5-C6	-2.91	121.26	124.53
13	r	513	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	U	1401	CLA	C3B-C4B-NB	-2.91	107.82	110.52
16	1	522	BCR	C3-C4-C5	-2.91	108.89	114.08
13	H	1234	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
16	q	523	BCR	C16-C17-C18	-2.91	123.16	127.31
13	d	503	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
13	e	1109	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	f	5002	LMG	O6-C1-O1	-2.91	103.09	109.97
13	e	1128	CLA	C2B-C1B-NB	-2.91	108.28	110.23
13	e	1110	CLA	CHB-C4A-NA	2.91	128.53	124.51
16	v	524	BCR	C24-C23-C22	-2.91	121.84	126.23
16	c	522	BCR	C38-C26-C27	2.91	119.20	113.62
13	Y	508	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
13	v	503	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
16	f	4004	BCR	C11-C10-C9	-2.91	123.16	127.31
13	4	510	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
20	5	822	SQD	O48-C23-C24	2.90	119.00	111.38
13	u	509	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
13	f	1229	CLA	CMB-C2B-C3B	2.90	133.62	126.59
16	B	4006	BCR	C37-C22-C21	-2.90	118.86	122.92
20	u	822	SQD	O48-C23-C24	2.90	119.00	111.38
16	H	4006	BCR	C37-C22-C21	-2.90	118.86	122.92
13	B	1229	CLA	CMB-C2B-C3B	2.90	133.62	126.59
13	s	519	CLA	C3B-C4B-NB	-2.90	107.82	110.52
16	6	524	BCR	C24-C23-C22	-2.90	121.85	126.23
16	t	524	BCR	C8-C7-C6	-2.90	119.05	127.20
13	b	519	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	B	5002	LMG	O6-C1-O1	-2.90	103.11	109.97
16	Y	524	BCR	C33-C5-C4	2.90	119.19	113.62
16	M	4021	BCR	C20-C19-C18	-2.90	118.27	126.42
13	1	508	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	5	822	SQD	C44-O6-C1	2.90	119.40	113.74
13	5	509	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
13	b	508	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
13	B	1238	CLA	CHB-C1B-NB	2.90	127.33	124.26
16	H	4017	BCR	C34-C9-C8	2.90	122.64	118.08
13	t	510	CLA	O2D-CGD-O1D	-2.90	118.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	d	513	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
16	q	522	BCR	C38-C26-C25	-2.90	121.28	124.53
16	5	523	BCR	C16-C17-C18	-2.90	123.18	127.31
13	r	508	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	c	822	SQD	O48-C23-C24	2.90	118.97	111.38
13	a	519	CLA	CHB-C4A-NA	2.90	128.52	124.51
16	H	4004	BCR	C11-C10-C9	-2.90	123.18	127.31
13	Y	502	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
13	H	1229	CLA	CMB-C2B-C3B	2.90	133.60	126.59
13	Y	510	CLA	C3B-C4B-NB	-2.90	107.83	110.52
16	B	4004	BCR	C11-C10-C9	-2.90	123.18	127.31
16	L	4019	BCR	C11-C10-C9	-2.89	123.18	127.31
16	V	4019	BCR	C11-C10-C9	-2.89	123.18	127.31
13	b	508	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
20	c	822	SQD	C44-O6-C1	2.89	119.39	113.74
20	u	822	SQD	C44-O6-C1	2.89	119.39	113.74
13	G	1104	CLA	CHB-C4A-NA	2.89	128.51	124.51
16	b	524	BCR	C8-C7-C6	-2.89	119.08	127.20
16	3	523	BCR	C33-C5-C6	-2.89	121.28	124.53
13	b	511	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	a	507	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	H	5002	LMG	O6-C1-O1	-2.89	103.12	109.97
13	1	512	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	A	1128	CLA	C2B-C1B-NB	-2.89	108.29	110.23
16	4	524	BCR	C8-C7-C6	-2.89	119.08	127.20
13	a	518	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	c	521	BCR	C30-C25-C26	-2.89	118.54	122.61
13	s	518	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	A	1136	CLA	CHB-C4A-NA	2.89	128.51	124.51
13	3	519	CLA	CHB-C4A-NA	2.89	128.51	124.51
13	H	1238	CLA	CHB-C1B-NB	2.89	127.32	124.26
16	o	4021	BCR	C20-C19-C18	-2.89	118.30	126.42
13	e	1125	CLA	C3B-C4B-NB	-2.89	107.83	110.52
13	m	1401	CLA	C3B-C4B-NB	-2.89	107.83	110.52
13	4	519	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	508	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	6	503	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	n	4019	BCR	C11-C10-C9	-2.89	123.19	127.31
13	f	1201	CLA	CHB-C4A-NA	2.89	128.50	124.51
13	3	518	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	q	512	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	c	523	BCR	C16-C17-C18	-2.89	123.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1115	CLA	CHB-C4A-NA	2.89	128.50	124.51
16	I	4018	BCR	C1-C6-C5	-2.88	118.55	122.61
13	A	1237	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
13	H	1023	CLA	CHB-C4A-NA	2.88	128.50	124.51
13	B	1234	CLA	C3B-C4B-NB	-2.88	107.84	110.52
13	c	509	CLA	CHB-C4A-NA	2.88	128.50	124.51
13	4	511	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
16	H	4017	BCR	C21-C20-C19	-2.88	114.22	123.22
13	H	1234	CLA	C3B-C4B-NB	-2.88	107.84	110.52
16	B	4017	BCR	C34-C9-C8	2.88	122.62	118.08
13	s	506	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
13	q	502	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
16	1	522	BCR	C33-C5-C6	-2.88	121.30	124.53
13	A	1109	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
16	Y	522	BCR	C33-C5-C6	-2.88	121.30	124.53
13	v	513	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
16	F	4016	BCR	C11-C12-C13	-2.88	118.33	126.42
13	e	1115	CLA	CHB-C4A-NA	2.88	128.49	124.51
16	B	4017	BCR	C21-C20-C19	-2.88	114.24	123.22
16	u	521	BCR	C30-C25-C26	-2.88	118.56	122.61
13	A	1104	CLA	CHB-C4A-NA	2.88	128.49	124.51
16	A	4011	BCR	C20-C19-C18	-2.88	118.33	126.42
13	e	1135	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
13	b	503	CLA	CHB-C4A-NA	2.88	128.49	124.51
13	a	519	CLA	C3B-C4B-NB	-2.88	107.85	110.52
16	f	4009	BCR	C15-C16-C17	-2.88	117.58	123.47
16	n	4022	BCR	C28-C27-C26	-2.88	108.94	114.08
16	5	521	BCR	C30-C25-C26	-2.88	118.56	122.61
13	4	508	CLA	CMB-C2B-C1B	-2.88	120.99	125.37
16	G	4011	BCR	C20-C19-C18	-2.88	118.34	126.42
16	Y	522	BCR	C38-C26-C27	2.88	119.14	113.62
13	A	1135	CLA	C3B-C4B-NB	-2.87	107.85	110.52
13	e	1135	CLA	C3B-C4B-NB	-2.87	107.85	110.52
13	1	502	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	Z	508	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	b	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
16	R	4016	BCR	C11-C12-C13	-2.87	118.34	126.42
13	1	513	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	t	508	CLA	CMB-C2B-C1B	-2.87	120.99	125.37
13	3	507	CLA	CHB-C4A-NA	2.87	128.49	124.51
13	G	1115	CLA	CHB-C4A-NA	2.87	128.49	124.51
13	G	1136	CLA	CHB-C4A-NA	2.87	128.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	505	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	A	1122	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	4	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	f	1212	CLA	CHB-C4A-NA	2.87	128.48	124.51
13	4	518	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	B	1023	CLA	CHB-C4A-NA	2.87	128.48	124.51
13	2	508	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	e	1237	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
16	r	521	BCR	C3-C4-C5	-2.87	108.95	114.08
16	G	4008	BCR	C16-C15-C14	-2.87	117.59	123.47
13	6	513	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	A	1110	CLA	CHB-C4A-NA	2.87	128.48	124.51
13	s	519	CLA	CHB-C4A-NA	2.87	128.48	124.51
13	t	511	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	f	1234	CLA	C3B-C4B-NB	-2.87	107.85	110.52
13	3	508	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	a	506	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
16	f	4017	BCR	C21-C20-C19	-2.87	114.26	123.22
16	j	4016	BCR	C11-C12-C13	-2.87	118.36	126.42
13	e	1136	CLA	CHB-C4A-NA	2.87	128.48	124.51
16	Z	521	BCR	C3-C4-C5	-2.87	108.95	114.08
13	f	1023	CLA	CHB-C4A-NA	2.87	128.48	124.51
16	A	4008	BCR	C16-C15-C14	-2.87	117.60	123.47
13	f	1238	CLA	CHB-C1B-NB	2.87	127.29	124.26
13	H	1212	CLA	CHB-C4A-NA	2.87	128.48	124.51
16	V	4022	BCR	C28-C27-C26	-2.87	108.96	114.08
13	s	508	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	B	1201	CLA	CHB-C4A-NA	2.87	128.48	124.51
13	Y	513	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	v	518	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
16	3	524	BCR	C24-C23-C22	-2.87	121.91	126.23
16	s	524	BCR	C24-C23-C22	-2.87	121.91	126.23
16	H	4009	BCR	C15-C16-C17	-2.87	117.60	123.47
13	q	513	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
16	f	4006	BCR	C37-C22-C21	-2.86	118.91	122.92
13	t	511	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	G	1122	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	t	512	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	6	519	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	c	511	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	e	4008	BCR	C16-C15-C14	-2.86	117.61	123.47
16	f	4017	BCR	C34-C9-C8	2.86	122.59	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1135	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	G	1237	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	e	4011	BCR	C20-C19-C18	-2.86	118.38	126.42
13	v	513	CLA	C3B-C4B-NB	-2.86	107.86	110.52
16	A	4002	BCR	C3-C4-C5	-2.86	108.97	114.08
13	d	507	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	b	511	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	6	518	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	B	1212	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	4	505	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	5	509	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	3	519	CLA	C3B-C4B-NB	-2.86	107.86	110.52
13	G	1109	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	G	1128	CLA	C2B-C1B-NB	-2.86	108.31	110.23
13	q	507	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
16	1	522	BCR	C38-C26-C27	2.86	119.11	113.62
13	H	1201	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	f	1218	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	3	506	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
16	q	523	BCR	C33-C5-C6	-2.86	121.32	124.53
16	2	521	BCR	C3-C4-C5	-2.86	108.97	114.08
13	c	508	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	A	1102	CLA	C3B-C4B-NB	-2.86	107.86	110.52
13	G	1115	CLA	C3B-C4B-NB	-2.86	107.86	110.52
13	e	1122	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	Y	507	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	4	503	CLA	CHB-C4A-NA	2.86	128.46	124.51
13	e	1118	CLA	C3B-C4B-NB	-2.86	107.87	110.52
13	b	518	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
13	t	518	CLA	CHB-C4A-NA	2.86	128.46	124.51
13	6	513	CLA	C3B-C4B-NB	-2.85	107.87	110.52
13	A	1114	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	B	1218	CLA	CHB-C4A-NA	2.85	128.46	124.51
13	4	511	CLA	CHB-C4A-NA	2.85	128.46	124.51
13	e	1114	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
16	f	4010	BCR	C8-C7-C6	-2.85	119.19	127.20
16	L	4022	BCR	C28-C27-C26	-2.85	108.98	114.08
13	5	508	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	t	505	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
16	B	4009	BCR	C15-C16-C17	-2.85	117.63	123.47
13	b	510	CLA	CHB-C4A-NA	2.85	128.46	124.51
13	v	501	CLA	CHB-C4A-NA	2.85	128.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	v	518	CLA	C3B-C4B-NB	-2.85	107.87	110.52
13	6	516	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	u	508	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
16	e	4002	BCR	C3-C4-C5	-2.85	108.99	114.08
13	F	1302	CLA	CHB-C4A-NA	2.85	128.45	124.51
13	b	518	CLA	CHB-C4A-NA	2.85	128.45	124.51
13	H	1218	CLA	CHB-C4A-NA	2.85	128.45	124.51
13	u	509	CLA	CHB-C4A-NA	2.85	128.45	124.51
16	G	4002	BCR	C3-C4-C5	-2.85	108.99	114.08
13	1	507	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	d	516	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
16	1	522	BCR	C11-C12-C13	-2.85	118.41	126.42
16	q	522	BCR	C38-C26-C27	2.85	119.09	113.62
13	6	507	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	u	511	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	B	1023	CLA	CMB-C2B-C3B	2.85	133.48	126.59
16	a	524	BCR	C24-C23-C22	-2.85	121.93	126.23
13	b	508	CLA	CHB-C1B-NB	2.85	127.27	124.26
13	t	508	CLA	CHB-C1B-NB	2.85	127.27	124.26
16	B	4010	BCR	C8-C7-C6	-2.85	119.21	127.20
13	a	501	CLA	CHB-C4A-NA	2.85	128.45	124.51
13	5	511	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	G	1135	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	t	518	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
16	Y	522	BCR	C11-C12-C13	-2.85	118.42	126.42
13	G	1135	CLA	CMB-C2B-C3B	2.85	133.48	126.59
13	G	1131	CLA	CHB-C4A-NA	2.84	128.45	124.51
13	d	518	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	B	1215	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
13	4	508	CLA	CHB-C1B-NB	2.84	127.27	124.26
13	G	1114	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	4	502	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	G	1110	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	A	1133	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	v	516	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	a	502	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	5	518	CLA	C3B-C4B-NB	-2.84	107.88	110.52
13	R	1302	CLA	CHB-C4A-NA	2.84	128.44	124.51
16	H	4010	BCR	C8-C7-C6	-2.84	119.22	127.20
13	e	1135	CLA	CMB-C2B-C3B	2.84	133.47	126.59
13	c	517	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	v	519	CLA	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	511	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	4	518	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	3	502	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	4	509	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	r	503	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	f	1215	CLA	CMB-C2B-C1B	-2.84	121.05	125.37
16	V	4219	BCR	C28-C27-C26	-2.84	109.01	114.08
13	A	1118	CLA	C3B-C4B-NB	-2.84	107.88	110.52
13	G	1108	CLA	C3B-C4B-NB	-2.84	107.88	110.52
13	s	511	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	u	513	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	H	1023	CLA	CMB-C2B-C3B	2.84	133.46	126.59
13	f	1023	CLA	CMB-C2B-C3B	2.84	133.46	126.59
16	L	4219	BCR	C28-C27-C26	-2.84	109.01	114.08
13	s	511	CLA	CHB-C4A-NA	2.84	128.44	124.51
13	u	518	CLA	C3B-C4B-NB	-2.84	107.88	110.52
16	r	523	BCR	C20-C21-C22	-2.84	123.26	127.31
13	Y	508	CLA	CHB-C4A-NA	2.84	128.43	124.51
13	q	508	CLA	CHB-C4A-NA	2.84	128.43	124.51
13	r	516	CLA	CHB-C4A-NA	2.84	128.43	124.51
13	t	510	CLA	CHB-C4A-NA	2.84	128.43	124.51
13	b	509	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	V	1502	CLA	CHB-C4A-NA	2.84	128.43	124.51
13	A	1135	CLA	CMB-C2B-C3B	2.84	133.46	126.59
13	d	519	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
13	e	1104	CLA	CHB-C4A-NA	2.83	128.43	124.51
13	4	502	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
13	1	508	CLA	C4-C3-C5	2.83	120.04	115.27
13	t	502	CLA	CHB-C4A-NA	2.83	128.43	124.51
20	L	5216	SQD	O8-S-C6	2.83	110.25	105.74
13	A	1115	CLA	C3B-C4B-NB	-2.83	107.89	110.52
13	m	1103	CLA	CHB-C4A-NA	2.83	128.43	124.51
16	q	522	BCR	C11-C12-C13	-2.83	118.46	126.42
13	e	1123	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
13	e	1133	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
13	3	501	CLA	CHB-C4A-NA	2.83	128.43	124.51
16	H	4010	BCR	C20-C21-C22	-2.83	123.27	127.31
13	u	517	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	4	501	CLA	CHB-C4A-NA	2.83	128.43	124.51
13	u	506	CLA	CHB-C4A-NA	2.83	128.43	124.51
13	e	1102	CLA	C3B-C4B-NB	-2.83	107.89	110.52
16	s	524	BCR	C33-C5-C4	2.83	119.05	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	522	BCR	C38-C26-C25	-2.83	121.35	124.53
13	3	511	CLA	CHB-C4A-NA	2.83	128.42	124.51
13	Z	511	CLA	CHB-C4A-NA	2.83	128.42	124.51
13	t	509	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	r	508	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
13	A	1108	CLA	C3B-C4B-NB	-2.83	107.89	110.52
13	Z	507	CLA	CHB-C4A-NA	2.83	128.42	124.51
16	n	4219	BCR	C28-C27-C26	-2.83	109.03	114.08
13	2	508	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
13	q	508	CLA	C4-C3-C5	2.83	120.03	115.27
16	q	522	BCR	C33-C5-C6	-2.83	121.35	124.53
13	Y	508	CLA	C4-C3-C5	2.83	120.03	115.27
20	V	5216	SQD	O8-S-C6	2.83	110.24	105.74
13	G	1130	CLA	CHB-C1B-NB	2.83	127.25	124.26
20	b	822	SQD	C44-O6-C1	2.83	119.26	113.74
13	G	1133	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	A	1131	CLA	CHB-C4A-NA	2.83	128.42	124.51
13	e	1115	CLA	C3B-C4B-NB	-2.83	107.89	110.52
13	5	513	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
13	G	1119	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
16	3	524	BCR	C33-C5-C4	2.82	119.04	113.62
13	Z	501	CLA	CHB-C4A-NA	2.82	128.42	124.51
13	r	507	CLA	CHB-C4A-NA	2.82	128.42	124.51
16	G	4008	BCR	C38-C26-C25	-2.82	121.36	124.53
13	H	1215	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
13	e	1108	CLA	C3B-C4B-NB	-2.82	107.90	110.52
16	4	522	BCR	C38-C26-C27	2.82	119.04	113.62
13	j	1302	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	r	511	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	u	519	CLA	CHB-C4A-NA	2.82	128.41	124.51
16	J	4012	BCR	C23-C22-C21	2.82	123.27	118.94
13	v	507	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
16	A	4008	BCR	C38-C26-C25	-2.82	121.36	124.53
13	G	1130	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
19	f	5002	LMG	O1-C7-C8	-2.82	104.09	110.90
20	n	5216	SQD	O8-S-C6	2.82	110.24	105.74
13	5	517	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	6	501	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	r	501	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	G	1102	CLA	C3B-C4B-NB	-2.82	107.90	110.52
16	b	522	BCR	C38-C26-C27	2.82	119.03	113.62
13	t	503	CLA	CHB-C4A-NA	2.82	128.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	503	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	b	502	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	s	507	CLA	CHB-C4A-NA	2.82	128.41	124.51
20	4	822	SQD	C44-O6-C1	2.82	119.25	113.74
16	6	522	BCR	C38-C26-C25	-2.82	121.36	124.53
13	4	510	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	e	1131	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	Z	506	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
16	t	522	BCR	C38-C26-C27	2.82	119.03	113.62
16	H	4010	BCR	C33-C5-C4	2.82	119.03	113.62
13	3	511	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
13	Y	503	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
13	e	1119	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
16	a	522	BCR	C20-C21-C22	-2.82	123.29	127.31
16	1	523	BCR	C33-C5-C6	-2.82	121.36	124.53
16	a	524	BCR	C33-C5-C4	2.82	119.03	113.62
13	b	501	CLA	CHB-C4A-NA	2.82	128.41	124.51
13	n	1503	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	e	5002	LHG	O8-C23-C24	2.82	120.75	111.91
13	5	516	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
13	A	1123	CLA	CMB-C2B-C1B	-2.82	121.08	125.37
13	1	508	CLA	CHB-C4A-NA	2.82	128.41	124.51
16	u	524	BCR	C15-C16-C17	-2.82	117.71	123.47
17	A	5002	LHG	O8-C23-C24	2.82	120.74	111.91
16	5	521	BCR	C23-C24-C25	-2.82	119.29	127.20
16	f	4010	BCR	C33-C5-C4	2.82	119.03	113.62
13	B	1220	CLA	O2A-CGA-O1A	-2.82	116.49	123.59
13	d	518	CLA	C3B-C4B-NB	-2.82	107.90	110.52
16	n	4020	BCR	C10-C11-C12	-2.82	114.43	123.22
19	B	5002	LMG	O1-C7-C8	-2.82	104.11	110.90
16	u	521	BCR	C23-C24-C25	-2.81	119.30	127.20
16	Y	523	BCR	C33-C5-C6	-2.81	121.37	124.53
13	2	507	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	Z	518	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	c	518	CLA	C3B-C4B-NB	-2.81	107.90	110.52
16	c	521	BCR	C23-C24-C25	-2.81	119.30	127.20
13	Z	508	CLA	CMB-C2B-C1B	-2.81	121.08	125.37
16	B	4010	BCR	C33-C5-C4	2.81	119.02	113.62
13	a	511	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	c	519	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	s	502	CLA	CHB-C4A-NA	2.81	128.40	124.51
16	v	522	BCR	C38-C26-C25	-2.81	121.37	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4020	BCR	C10-C11-C12	-2.81	114.44	123.22
13	e	1130	CLA	CHB-C1B-NB	2.81	127.23	124.26
13	2	516	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	1	503	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	H	1220	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
16	Z	523	BCR	C20-C21-C22	-2.81	123.30	127.31
13	c	513	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	f	1231	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
16	T	4012	BCR	C23-C22-C21	2.81	123.25	118.94
13	4	510	CLA	C3B-C4B-NB	-2.81	107.91	110.52
13	6	518	CLA	C3B-C4B-NB	-2.81	107.91	110.52
16	3	522	BCR	C20-C21-C22	-2.81	123.30	127.31
19	H	5002	LMG	O1-C7-C8	-2.81	104.12	110.90
13	b	502	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	u	501	CLA	CHB-C4A-NA	2.81	128.40	124.51
16	2	522	BCR	C33-C5-C6	-2.81	121.37	124.53
16	e	4008	BCR	C38-C26-C25	-2.81	121.37	124.53
13	t	502	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	U	1103	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	d	501	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	c	510	CLA	C3B-C4B-NB	-2.81	107.91	110.52
13	f	1240	CLA	C3B-C4B-NB	-2.81	107.91	110.52
16	2	523	BCR	C20-C21-C22	-2.81	123.30	127.31
13	6	505	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	f	1220	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
13	B	1208	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	L	1502	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	6	507	CLA	CHB-C4A-NA	2.81	128.40	124.51
13	B	1222	CLA	C3B-C4B-NB	-2.81	107.91	110.52
13	Z	503	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
16	B	4010	BCR	C20-C21-C22	-2.81	123.30	127.31
13	f	1206	CLA	CMB-C2B-C1B	-2.81	121.09	125.37
13	v	505	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	u	502	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
20	t	822	SQD	C44-O6-C1	2.81	119.22	113.74
13	s	501	CLA	CHB-C4A-NA	2.81	128.39	124.51
13	G	1123	CLA	CMB-C2B-C1B	-2.81	121.09	125.37
13	2	506	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	5	502	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	a	517	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	Z	516	CLA	CHB-C4A-NA	2.81	128.39	124.51
13	d	502	CLA	CHB-C4A-NA	2.80	128.39	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1208	CLA	CHB-C4A-NA	2.80	128.39	124.51
13	r	506	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
16	r	522	BCR	C33-C5-C6	-2.80	121.38	124.53
13	c	503	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
13	5	501	CLA	CHB-C4A-NA	2.80	128.39	124.51
13	L	1503	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
13	c	516	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
13	u	516	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	G	5002	LHG	O8-C23-C24	2.80	120.70	111.91
13	A	1130	CLA	CMB-C2B-C1B	-2.80	121.10	125.37
13	e	1130	CLA	CMB-C2B-C1B	-2.80	121.10	125.37
16	Z	522	BCR	C33-C5-C6	-2.80	121.38	124.53
13	6	502	CLA	CHB-C4A-NA	2.80	128.39	124.51
16	5	524	BCR	C20-C21-C22	-2.80	123.31	127.31
13	a	511	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
13	c	502	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
16	c	524	BCR	C15-C16-C17	-2.80	117.74	123.47
13	l	1303	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	A	1130	CLA	CHB-C1B-NB	2.80	127.22	124.26
16	u	524	BCR	C20-C21-C22	-2.80	123.31	127.31
13	K	1103	CLA	CHB-C4A-NA	2.80	128.38	124.51
16	u	523	BCR	C21-C20-C19	-2.80	114.48	123.22
13	2	501	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	A	1119	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
16	5	523	BCR	C21-C20-C19	-2.80	114.48	123.22
13	5	506	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	5	508	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	H	1228	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	s	518	CLA	C3B-C4B-NB	-2.80	107.92	110.52
13	3	517	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	H	1023	CLA	CBC-CAC-C3C	2.80	120.14	112.43
13	c	504	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	b	517	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	a	505	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
16	V	4020	BCR	C10-C11-C12	-2.80	114.49	123.22
13	a	518	CLA	C3B-C4B-NB	-2.80	107.92	110.52
13	b	510	CLA	C3B-C4B-NB	-2.80	107.92	110.52
16	4	523	BCR	C20-C21-C22	-2.80	123.32	127.31
13	c	506	CLA	CHB-C4A-NA	2.80	128.38	124.51
13	d	510	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	q	503	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	v	502	CLA	CHB-C4A-NA	2.79	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	5003	LHG	C11-C10-C9	-2.79	100.24	114.42
13	B	1231	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
13	s	517	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
13	5	519	CLA	CHB-C4A-NA	2.79	128.38	124.51
13	t	501	CLA	CHB-C4A-NA	2.79	128.38	124.51
13	3	505	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	d	505	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	d	507	CLA	CHB-C4A-NA	2.79	128.38	124.51
13	v	503	CLA	CHB-C4A-NA	2.79	128.38	124.51
13	3	518	CLA	C3B-C4B-NB	-2.79	107.92	110.52
13	q	506	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	u	503	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	n	1502	CLA	CHB-C4A-NA	2.79	128.37	124.51
16	c	523	BCR	C21-C20-C19	-2.79	114.50	123.22
17	e	5003	LHG	C11-C10-C9	-2.79	100.25	114.42
13	H	1222	CLA	C3B-C4B-NB	-2.79	107.92	110.52
17	G	5003	LHG	C11-C10-C9	-2.79	100.25	114.42
13	6	503	CLA	CHB-C4A-NA	2.79	128.37	124.51
16	b	523	BCR	C20-C21-C22	-2.79	123.33	127.31
13	H	1204	CLA	CHB-C4A-NA	2.79	128.37	124.51
13	H	1208	CLA	CHB-C4A-NA	2.79	128.37	124.51
16	R	4016	BCR	C16-C17-C18	-2.79	123.33	127.31
13	4	516	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
16	f	4006	BCR	C34-C9-C10	-2.79	119.02	122.92
13	J	1303	CLA	CHB-C4A-NA	2.79	128.37	124.51
16	c	524	BCR	C20-C21-C22	-2.79	123.33	127.31
13	f	1222	CLA	C3B-C4B-NB	-2.79	107.93	110.52
13	1	506	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
16	5	524	BCR	C15-C16-C17	-2.79	117.76	123.47
13	d	506	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
13	1	518	CLA	CHB-C4A-NA	2.79	128.37	124.51
13	T	1303	CLA	CHB-C4A-NA	2.79	128.37	124.51
13	f	1207	CLA	CHB-C4A-NA	2.79	128.37	124.51
16	B	4006	BCR	C34-C9-C10	-2.79	119.02	122.92
13	v	506	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
13	v	517	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
16	1	524	BCR	C20-C21-C22	-2.79	123.33	127.31
13	B	1023	CLA	CBC-CAC-C3C	2.79	120.11	112.43
13	B	1228	CLA	CHB-C4A-NA	2.79	128.37	124.51
13	G	1117	CLA	CHB-C4A-NA	2.79	128.37	124.51
16	f	4010	BCR	C20-C21-C22	-2.79	123.33	127.31
16	W	4021	BCR	C38-C26-C27	2.79	118.97	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c	508	CLA	CHB-C4A-NA	2.79	128.36	124.51
13	u	508	CLA	CHB-C4A-NA	2.79	128.36	124.51
13	t	510	CLA	C3B-C4B-NB	-2.79	107.93	110.52
13	6	517	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
13	H	1231	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
13	v	507	CLA	CHB-C4A-NA	2.78	128.36	124.51
13	G	1801	CLA	CMB-C2B-C1B	-2.78	121.13	125.37
13	V	1503	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
13	A	1134	CLA	C3B-C4B-NB	-2.78	107.93	110.52
16	H	4006	BCR	C15-C16-C17	-2.78	117.77	123.47
13	B	1206	CLA	CMB-C2B-C1B	-2.78	121.13	125.37
13	t	516	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
13	f	1208	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
20	b	822	SQD	O8-S-C6	2.78	110.17	105.74
13	c	501	CLA	CHB-C4A-NA	2.78	128.36	124.51
16	B	4014	BCR	C28-C27-C26	-2.78	109.11	114.08
13	A	1011	CLA	C2A-C1A-CHA	2.78	128.72	123.86
13	c	507	CLA	CHB-C4A-NA	2.78	128.36	124.51
16	s	522	BCR	C20-C21-C22	-2.78	123.34	127.31
13	H	1202	CLA	CMB-C2B-C3B	2.78	133.32	126.59
13	f	1023	CLA	CBC-CAC-C3C	2.78	120.09	112.43
13	e	1011	CLA	C2A-C1A-CHA	2.78	128.72	123.86
16	A	4001	BCR	C11-C12-C13	-2.78	118.61	126.42
13	A	1801	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
13	s	505	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
13	B	1207	CLA	CHB-C4A-NA	2.78	128.35	124.51
13	B	1240	CLA	C3B-C4B-NB	-2.78	107.94	110.52
13	6	506	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	5	507	CLA	CHB-C4A-NA	2.78	128.35	124.51
16	f	4014	BCR	C28-C27-C26	-2.78	109.12	114.08
13	6	510	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
16	f	4006	BCR	C15-C16-C17	-2.78	117.78	123.47
13	q	506	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
13	a	503	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
16	e	4001	BCR	C11-C12-C13	-2.78	118.61	126.42
16	F	4016	BCR	C16-C17-C18	-2.78	123.35	127.31
13	s	503	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	Y	506	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	q	518	CLA	CHB-C4A-NA	2.77	128.35	124.51
13	u	504	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
13	G	1118	CLA	C3B-C4B-NB	-2.77	107.94	110.52
16	M	4021	BCR	C38-C26-C27	2.77	118.95	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	503	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
13	B	1205	CLA	CHB-C4A-NA	2.77	128.35	124.51
13	H	1207	CLA	CHB-C4A-NA	2.77	128.35	124.51
16	B	4006	BCR	C15-C16-C17	-2.77	117.79	123.47
13	B	1208	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	u	505	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
16	H	4006	BCR	C34-C9-C10	-2.77	119.04	122.92
16	Y	524	BCR	C20-C21-C22	-2.77	123.35	127.31
13	4	517	CLA	CHB-C4A-NA	2.77	128.35	124.51
13	e	1117	CLA	CHB-C4A-NA	2.77	128.35	124.51
13	e	1801	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
16	j	4016	BCR	C16-C17-C18	-2.77	123.35	127.31
13	2	513	CLA	CHB-C4A-NA	2.77	128.35	124.51
13	2	518	CLA	CHB-C4A-NA	2.77	128.35	124.51
13	q	507	CLA	CHB-C4A-NA	2.77	128.35	124.51
20	4	822	SQD	O8-S-C6	2.77	110.16	105.74
13	5	504	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	3	518	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	s	518	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	t	517	CLA	CHB-C4A-NA	2.77	128.34	124.51
16	S	4018	BCR	C21-C20-C19	-2.77	114.57	123.22
13	5	505	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	B	1203	CLA	C3B-C4B-NB	-2.77	107.94	110.52
13	5	503	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	t	501	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	H	1205	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	f	1228	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	U	1103	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	e	1120	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	r	518	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	Z	513	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	b	501	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
16	G	4001	BCR	C11-C12-C13	-2.77	118.64	126.42
13	G	1122	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	H	1208	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
16	L	4019	BCR	C20-C21-C22	-2.77	123.36	127.31
16	l	4012	BCR	C23-C22-C21	2.77	123.19	118.94
13	G	1120	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	b	516	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	5	510	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	B	1204	CLA	CHB-C4A-NA	2.77	128.34	124.51
16	J	4013	BCR	C16-C15-C14	-2.77	117.81	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	822	SQD	O8-S-C6	2.77	110.15	105.74
13	H	1203	CLA	C3B-C4B-NB	-2.77	107.95	110.52
17	S	5001	LHG	O8-C23-C24	2.77	120.59	111.91
13	v	510	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	e	1122	CLA	CHB-C4A-NA	2.77	128.34	124.51
13	H	1240	CLA	C3B-C4B-NB	-2.77	107.95	110.52
13	Y	506	CLA	CMB-C2B-C1B	-2.77	121.16	125.37
13	L	1501	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
16	H	4014	BCR	C28-C27-C26	-2.77	109.14	114.08
16	k	4018	BCR	C21-C20-C19	-2.77	114.59	123.22
13	1	506	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
16	l	4013	BCR	C16-C15-C14	-2.76	117.81	123.47
13	A	1117	CLA	CHB-C4A-NA	2.76	128.33	124.51
13	e	1134	CLA	C3B-C4B-NB	-2.76	107.95	110.52
16	T	4013	BCR	C16-C15-C14	-2.76	117.81	123.47
20	t	822	SQD	O8-S-C6	2.76	110.14	105.74
13	f	1203	CLA	C3B-C4B-NB	-2.76	107.95	110.52
13	a	509	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
16	t	523	BCR	C20-C21-C22	-2.76	123.37	127.31
13	4	513	CLA	CHB-C4A-NA	2.76	128.33	124.51
13	c	516	CLA	CHB-C4A-NA	2.76	128.33	124.51
17	I	5001	LHG	O8-C23-C24	2.76	120.57	111.91
16	I	4018	BCR	C21-C20-C19	-2.76	114.60	123.22
16	o	4021	BCR	C38-C26-C27	2.76	118.92	113.62
13	c	505	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
13	n	1501	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
13	u	510	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
13	f	1202	CLA	CMB-C2B-C3B	2.76	133.27	126.59
13	G	1011	CLA	C2A-C1A-CHA	2.76	128.68	123.86
16	G	4011	BCR	C16-C17-C18	-2.76	123.37	127.31
16	q	524	BCR	C20-C21-C22	-2.76	123.37	127.31
20	a	822	SQD	O8-S-C6	2.76	110.14	105.74
13	A	1122	CLA	CHB-C4A-NA	2.76	128.33	124.51
17	k	5001	LHG	O8-C23-C24	2.76	120.56	111.91
13	3	509	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
16	Z	521	BCR	C33-C5-C6	-2.76	121.43	124.53
13	d	517	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
13	H	1221	CLA	O2D-CGD-CBD	2.76	116.17	111.27
13	d	503	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	u	516	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	4	501	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
13	B	1229	CLA	CHB-C4A-NA	2.76	128.32	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	1503	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	f	1229	CLA	CHB-C4A-NA	2.76	128.32	124.51
20	s	822	SQD	O8-S-C6	2.76	110.13	105.74
13	5	503	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	s	503	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	B	1202	CLA	CMB-C2B-C3B	2.76	133.26	126.59
13	Y	508	CLA	CHB-C1B-NB	2.76	127.17	124.26
13	r	513	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	t	507	CLA	CHB-C4A-NA	2.76	128.32	124.51
13	K	1103	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
13	4	506	CLA	CHB-C4A-NA	2.75	128.32	124.51
13	G	1116	CLA	CHB-C4A-NA	2.75	128.32	124.51
13	m	1103	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
13	u	507	CLA	CHB-C4A-NA	2.75	128.32	124.51
13	b	517	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
13	c	510	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	H	1217	CLA	CHB-C4A-NA	2.75	128.32	124.51
13	5	510	CLA	C3B-C4B-NB	-2.75	107.96	110.52
13	G	1134	CLA	C3B-C4B-NB	-2.75	107.96	110.52
13	r	512	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
16	f	4004	BCR	C28-C27-C26	-2.75	109.16	114.08
16	u	522	BCR	C15-C16-C17	-2.75	117.84	123.47
20	v	822	SQD	C44-O6-C1	2.75	119.11	113.74
16	A	4008	BCR	C10-C11-C12	-2.75	114.63	123.22
16	B	4004	BCR	C28-C27-C26	-2.75	109.17	114.08
16	n	4019	BCR	C20-C21-C22	-2.75	123.39	127.31
13	b	513	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	f	1204	CLA	CHB-C4A-NA	2.75	128.31	124.51
16	e	4007	BCR	C15-C16-C17	-2.75	117.84	123.47
16	e	4011	BCR	C16-C17-C18	-2.75	123.39	127.31
13	5	516	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	H	1229	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	t	506	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	u	510	CLA	C3B-C4B-NB	-2.75	107.97	110.52
13	R	1302	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	a	512	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
20	2	822	SQD	C4-C3-C2	2.75	115.62	110.82
13	2	512	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	V	1501	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	H	1206	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
13	f	1221	CLA	O2D-CGD-CBD	2.75	116.15	111.27
20	d	822	SQD	C44-O6-C1	2.75	119.11	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	u	510	CLA	CHB-C4A-NA	2.75	128.31	124.51
20	3	822	SQD	C44-O6-C1	2.75	119.10	113.74
13	F	1302	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	H	1212	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
20	2	822	SQD	O8-S-C6	2.75	110.12	105.74
13	q	508	CLA	CHB-C1B-NB	2.75	127.16	124.26
13	1	507	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	q	503	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	3	512	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	s	512	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	6	502	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
13	r	518	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
13	t	517	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
13	G	1111	CLA	CHB-C4A-NA	2.74	128.31	124.51
13	Y	511	CLA	CHB-C4A-NA	2.74	128.31	124.51
13	u	518	CLA	CHB-C4A-NA	2.74	128.31	124.51
13	s	509	CLA	CMB-C2B-C1B	-2.74	121.19	125.37
13	4	517	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
20	6	822	SQD	C44-O6-C1	2.74	119.10	113.74
20	s	822	SQD	C44-O6-C1	2.74	119.10	113.74
16	m	4104	BCR	C3-C4-C5	-2.74	109.18	114.08
16	U	4104	BCR	C15-C16-C17	-2.74	117.86	123.47
13	f	1212	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
13	B	1221	CLA	O2D-CGD-CBD	2.74	116.14	111.27
20	r	822	SQD	O8-S-C6	2.74	110.11	105.74
13	t	504	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	v	502	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
16	G	4008	BCR	C10-C11-C12	-2.74	114.67	123.22
13	Y	507	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	Z	512	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
13	d	502	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
13	f	1230	CLA	O2D-CGD-CBD	2.74	116.14	111.27
13	f	1205	CLA	CHB-C4A-NA	2.74	128.30	124.51
20	Z	822	SQD	C4-C3-C2	2.74	115.61	110.82
16	U	4104	BCR	C3-C4-C5	-2.74	109.19	114.08
13	1	503	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	f	1217	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	r	508	CLA	CHB-C1B-NB	2.74	127.16	124.26
13	u	503	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	j	1302	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
16	c	523	BCR	C7-C8-C9	-2.74	122.10	126.23
16	n	4020	BCR	C3-C4-C5	-2.74	109.19	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4008	BCR	C10-C11-C12	-2.74	114.68	123.22
17	e	5005	LHG	C11-C10-C9	-2.74	100.53	114.42
16	r	521	BCR	C33-C5-C6	-2.74	121.45	124.53
13	G	1135	CLA	CHC-C4B-NB	2.74	127.15	124.26
13	j	1301	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
13	A	1120	CLA	CHB-C4A-NA	2.74	128.29	124.51
13	L	1503	CLA	CHB-C4A-NA	2.74	128.29	124.51
16	2	521	BCR	C33-C5-C6	-2.74	121.46	124.53
16	c	524	BCR	C8-C7-C6	-2.74	119.52	127.20
13	B	1222	CLA	O2D-CGD-CBD	2.74	116.13	111.27
16	u	523	BCR	C7-C8-C9	-2.73	122.10	126.23
13	a	518	CLA	CHB-C4A-NA	2.73	128.29	124.51
16	m	4104	BCR	C15-C16-C17	-2.73	117.87	123.47
16	u	522	BCR	C16-C17-C18	-2.73	123.41	127.31
13	B	1212	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
13	t	512	CLA	C3B-C4B-NB	-2.73	107.98	110.52
13	c	503	CLA	CHB-C4A-NA	2.73	128.29	124.51
13	B	1211	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
16	V	4019	BCR	C20-C21-C22	-2.73	123.41	127.31
16	c	522	BCR	C16-C17-C18	-2.73	123.41	127.31
17	A	5005	LHG	C11-C10-C9	-2.73	100.55	114.42
13	e	1124	CLA	C2D-C1D-ND	-2.73	108.09	110.10
16	c	522	BCR	C15-C16-C17	-2.73	117.88	123.47
13	A	1113	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
16	5	523	BCR	C7-C8-C9	-2.73	122.11	126.23
13	Y	518	CLA	CHB-C4A-NA	2.73	128.29	124.51
16	K	4104	BCR	C3-C4-C5	-2.73	109.20	114.08
13	e	1113	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
13	Y	503	CLA	CHB-C4A-NA	2.73	128.29	124.51
16	K	4104	BCR	C15-C16-C17	-2.73	117.88	123.47
13	1	504	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
20	Z	822	SQD	O8-S-C6	2.73	110.09	105.74
13	m	1105	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	1	511	CLA	CHB-C4A-NA	2.73	128.29	124.51
13	A	1138	CLA	CHB-C4A-NA	2.73	128.29	124.51
13	n	1503	CLA	CHB-C4A-NA	2.73	128.29	124.51
13	u	511	CLA	CHB-C4A-NA	2.73	128.29	124.51
13	F	1301	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	H	1222	CLA	O2D-CGD-CBD	2.73	116.12	111.27
17	G	5005	LHG	C11-C10-C9	-2.73	100.57	114.42
16	H	4004	BCR	C28-C27-C26	-2.73	109.20	114.08
16	A	4011	BCR	C16-C17-C18	-2.73	123.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1222	CLA	O2D-CGD-CBD	2.73	116.12	111.27
16	4	523	BCR	C11-C10-C9	-2.73	123.42	127.31
20	a	822	SQD	C44-O6-C1	2.73	119.07	113.74
13	t	513	CLA	CHB-C4A-NA	2.73	128.28	124.51
13	q	510	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	G	1124	CLA	C2D-C1D-ND	-2.73	108.09	110.10
13	2	518	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
13	5	518	CLA	CHB-C4A-NA	2.73	128.28	124.51
13	a	503	CLA	CHB-C4A-NA	2.73	128.28	124.51
16	A	4007	BCR	C15-C16-C17	-2.73	117.89	123.47
16	5	522	BCR	C15-C16-C17	-2.73	117.89	123.47
13	Z	518	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
16	Z	524	BCR	C11-C10-C9	-2.73	123.42	127.31
13	r	516	CLA	O2D-CGD-CBD	2.73	116.11	111.27
13	H	1221	CLA	CMB-C2B-C3B	2.73	133.19	126.59
13	Y	504	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
13	c	502	CLA	C3B-C4B-NB	-2.72	107.99	110.52
16	r	524	BCR	C11-C10-C9	-2.72	123.42	127.31
13	A	1116	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	B	1217	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	e	1127	CLA	CHB-C4A-NA	2.72	128.28	124.51
20	r	822	SQD	C4-C3-C2	2.72	115.58	110.82
13	4	504	CLA	CHB-C4A-NA	2.72	128.28	124.51
16	L	4020	BCR	C3-C4-C5	-2.72	109.21	114.08
13	u	502	CLA	C3B-C4B-NB	-2.72	107.99	110.52
13	4	504	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
16	V	4020	BCR	C3-C4-C5	-2.72	109.21	114.08
13	f	1225	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
13	4	507	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	c	511	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	e	1138	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	K	1105	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	5	518	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	c	518	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	5	510	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	d	504	CLA	C3B-C4B-NB	-2.72	107.99	110.52
13	Z	516	CLA	O2D-CGD-CBD	2.72	116.10	111.27
13	A	1118	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	5	502	CLA	C3B-C4B-NB	-2.72	107.99	110.52
13	e	1125	CLA	CHB-C4A-NA	2.72	128.27	124.51
13	G	1129	CLA	CHC-C4B-NB	2.72	127.14	124.26
16	5	524	BCR	C8-C7-C6	-2.72	119.56	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	q	504	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	3	503	CLA	CHB-C4A-NA	2.72	128.27	124.51
20	1	822	SQD	O8-S-C6	2.72	110.07	105.74
16	3	522	BCR	C11-C12-C13	-2.72	118.78	126.42
16	s	522	BCR	C11-C12-C13	-2.72	118.78	126.42
13	a	502	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	G	1113	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
13	H	1211	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
13	G	1104	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	3	517	CLA	CHB-C4A-NA	2.72	128.27	124.51
13	q	511	CLA	CHB-C4A-NA	2.72	128.27	124.51
16	2	524	BCR	C11-C10-C9	-2.72	123.43	127.31
13	B	1225	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	f	1221	CLA	CMB-C2B-C3B	2.72	133.17	126.59
13	1	517	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
13	r	505	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
16	5	522	BCR	C16-C17-C18	-2.72	123.43	127.31
13	c	518	CLA	CHB-C4A-NA	2.72	128.27	124.51
13	2	508	CLA	CHB-C1B-NB	2.72	127.13	124.26
20	Y	822	SQD	O8-S-C6	2.72	110.07	105.74
13	u	518	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
13	B	1221	CLA	CMB-C2B-C3B	2.72	133.17	126.59
13	b	506	CLA	CHB-C4A-NA	2.72	128.27	124.51
16	H	4010	BCR	C33-C5-C6	-2.72	121.48	124.53
16	A	4007	BCR	C38-C26-C27	2.72	118.83	113.62
20	V	5216	SQD	O6-C1-C2	2.72	112.54	108.30
13	f	1211	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
13	3	502	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
13	6	509	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
13	s	502	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
13	A	1135	CLA	CHC-C4B-NB	2.71	127.13	124.26
13	1	508	CLA	CHB-C1B-NB	2.71	127.13	124.26
13	d	506	CLA	CHB-C4A-NA	2.71	128.27	124.51
13	4	513	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
16	B	4010	BCR	C33-C5-C6	-2.71	121.48	124.53
13	r	503	CLA	CHB-C4A-NA	2.71	128.26	124.51
13	s	517	CLA	CHB-C4A-NA	2.71	128.26	124.51
16	e	4007	BCR	C38-C26-C27	2.71	118.83	113.62
13	t	504	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
16	f	4010	BCR	C33-C5-C6	-2.71	121.48	124.53
13	t	513	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
13	B	1230	CLA	O2D-CGD-CBD	2.71	116.09	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	524	BCR	C8-C7-C6	-2.71	119.59	127.20
13	2	516	CLA	O2D-CGD-CBD	2.71	116.08	111.27
13	n	1502	CLA	O2D-CGD-CBD	2.71	116.08	111.27
20	n	5216	SQD	O6-C1-C2	2.71	112.53	108.30
13	6	506	CLA	CHB-C4A-NA	2.71	128.26	124.51
13	1	510	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	e	1104	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	H	1230	CLA	O2D-CGD-CBD	2.71	116.08	111.27
17	n	5218	LHG	O8-C23-C24	2.71	120.41	111.91
16	A	4001	BCR	C35-C13-C12	2.71	122.35	118.08
13	q	517	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	q	822	SQD	O8-S-C6	2.71	110.06	105.74
17	V	5218	LHG	O8-C23-C24	2.71	120.41	111.91
16	l	4015	BCR	C2-C1-C6	2.71	114.65	110.48
13	Y	517	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	A	1111	CLA	CHB-C4A-NA	2.71	128.26	124.51
13	a	516	CLA	CAC-C3C-C2C	-2.71	122.90	127.53
13	f	1223	CLA	CHB-C4A-NA	2.71	128.25	124.51
13	R	1301	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
16	b	523	BCR	C11-C10-C9	-2.71	123.45	127.31
13	A	1127	CLA	CHB-C4A-NA	2.71	128.25	124.51
13	G	1138	CLA	CHB-C4A-NA	2.71	128.25	124.51
16	G	4007	BCR	C15-C16-C17	-2.71	117.93	123.47
13	2	503	CLA	CHB-C4A-NA	2.71	128.25	124.51
13	d	509	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
16	e	4001	BCR	C35-C13-C12	2.71	122.34	118.08
13	B	1232	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	Z	510	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	a	517	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	b	519	CLA	CHB-C4A-NA	2.70	128.25	124.51
17	L	5218	LHG	O8-C23-C24	2.70	120.39	111.91
13	f	1201	CLA	C3B-C4B-NB	-2.70	108.01	110.52
20	L	5216	SQD	O6-C1-C2	2.70	112.53	108.30
13	H	1225	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
16	a	522	BCR	C11-C12-C13	-2.70	118.82	126.42
13	5	511	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	r	510	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	v	506	CLA	CHB-C4A-NA	2.70	128.25	124.51
16	G	4007	BCR	C38-C26-C27	2.70	118.81	113.62
13	Y	510	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	f	1234	CLA	CBC-CAC-C3C	2.70	119.88	112.43
13	b	504	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1118	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	Y	511	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	B	1234	CLA	CBC-CAC-C3C	2.70	119.88	112.43
13	q	516	CLA	CAC-C3C-C2C	-2.70	122.91	127.53
20	s	822	SQD	O5-C5-C4	2.70	114.60	109.69
13	c	506	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	c	510	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	3	516	CLA	CAC-C3C-C2C	-2.70	122.91	127.53
13	A	1104	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	A	1125	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	b	507	CLA	CHB-C4A-NA	2.70	128.25	124.51
16	H	4010	BCR	C38-C26-C25	-2.70	121.50	124.53
20	3	822	SQD	O5-C5-C4	2.70	114.60	109.69
13	Z	502	CLA	C3B-C4B-NB	-2.70	108.01	110.52
13	H	1228	CLA	CMB-C2B-C3B	2.70	133.13	126.59
13	4	519	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	e	1136	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
20	a	822	SQD	O5-C5-C4	2.70	114.59	109.69
13	G	1125	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	v	511	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	4	512	CLA	C3B-C4B-NB	-2.70	108.01	110.52
13	2	505	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	q	511	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	V	1502	CLA	O2D-CGD-CBD	2.70	116.06	111.27
13	e	1135	CLA	CHC-C4B-NB	2.70	127.11	124.26
13	B	1210	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	v	509	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	A	1116	CLA	C3B-C4B-NB	-2.70	108.01	110.52
13	Y	517	CLA	C3B-C4B-NB	-2.70	108.01	110.52
13	b	504	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
13	U	1105	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
13	G	1127	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	s	501	CLA	CMB-C2B-C1B	-2.70	121.26	125.37
13	s	504	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	d	519	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	q	504	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	A	1136	CLA	O2A-CGA-O1A	-2.69	116.79	123.59
13	3	501	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
13	2	504	CLA	CHB-C4A-NA	2.69	128.24	124.51
13	f	1232	CLA	CHB-C4A-NA	2.69	128.24	124.51
13	v	519	CLA	CHB-C4A-NA	2.69	128.24	124.51
13	A	1129	CLA	CHC-C4B-NB	2.69	127.11	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1210	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	G	1124	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	Z	505	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	b	513	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
20	s	822	SQD	O6-C1-C2	2.69	112.51	108.30
16	J	4015	BCR	C2-C1-C6	2.69	114.63	110.48
13	b	505	CLA	CHB-C4A-NA	2.69	128.24	124.51
13	H	1234	CLA	CBC-CAC-C3C	2.69	119.86	112.43
13	H	1210	CLA	CHB-C4A-NA	2.69	128.24	124.51
13	L	1502	CLA	O2D-CGD-CBD	2.69	116.05	111.27
13	e	1129	CLA	CHC-C4B-NB	2.69	127.11	124.26
13	G	1113	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	A	1127	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	B	1201	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	H	1201	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	H	1225	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	q	501	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	s	517	CLA	C3B-C4B-NB	-2.69	108.02	110.52
16	T	4012	BCR	C33-C5-C6	-2.69	121.51	124.53
13	e	1111	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	A	1124	CLA	C2D-C1D-ND	-2.69	108.12	110.10
16	t	523	BCR	C11-C10-C9	-2.69	123.47	127.31
13	3	516	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
13	t	505	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	Z	503	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	1	516	CLA	CAC-C3C-C2C	-2.69	122.93	127.53
13	e	1106	CLA	O2D-CGD-CBD	2.69	116.05	111.27
13	m	1401	CLA	O2D-CGD-CBD	2.69	116.05	111.27
13	2	502	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	Z	504	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	B	1228	CLA	CMB-C2B-C3B	2.69	133.10	126.59
13	G	1136	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
13	4	505	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	6	519	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	e	1127	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	5	506	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
13	q	518	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
13	s	516	CLA	CAC-C3C-C2C	-2.69	122.93	127.53
13	a	501	CLA	CMB-C2B-C1B	-2.69	121.28	125.37
13	5	513	CLA	C3B-C4B-NB	-2.69	108.02	110.52
13	d	519	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	A	1106	CLA	O2D-CGD-CBD	2.69	116.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	902	LMU	O5'-C5'-C4'	2.69	114.57	109.69
13	u	513	CLA	CHB-C4A-NA	2.69	128.23	124.51
20	3	822	SQD	O6-C1-C2	2.69	112.50	108.30
18	Y	902	LMU	O5'-C5'-C4'	2.69	114.57	109.69
13	f	1238	CLA	C3B-C4B-NB	-2.69	108.02	110.52
18	G	1848	LMU	C1B-O1B-C4'	-2.69	111.32	117.96
16	J	4012	BCR	C33-C5-C6	-2.68	121.51	124.53
13	6	519	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	6	504	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	e	1116	CLA	C3B-C4B-NB	-2.68	108.03	110.52
16	l	4012	BCR	C33-C5-C6	-2.68	121.51	124.53
18	e	1848	LMU	C1B-O1B-C4'	-2.68	111.32	117.96
13	G	1140	CLA	CHB-C1B-NB	2.68	127.10	124.26
13	r	510	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
13	Y	516	CLA	CAC-C3C-C2C	-2.68	122.94	127.53
13	H	1238	CLA	C3B-C4B-NB	-2.68	108.03	110.52
16	G	4001	BCR	C35-C13-C12	2.68	122.30	118.08
13	f	1210	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	t	519	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	1	511	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	1	518	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	s	516	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	2	510	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	6	511	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	d	518	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	1848	LMU	C1B-O1B-C4'	-2.68	111.33	117.96
13	2	510	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	G	1013	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	2	502	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	Y	504	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	Y	518	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	3	504	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	G	1118	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	a	504	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	G	1106	CLA	O2D-CGD-CBD	2.68	116.03	111.27
13	U	1401	CLA	O2D-CGD-CBD	2.68	116.03	111.27
16	q	523	BCR	C10-C11-C12	-2.68	114.86	123.22
13	u	506	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	b	512	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	H	1232	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	1	517	CLA	C3B-C4B-NB	-2.68	108.03	110.52
20	a	822	SQD	O6-C1-C2	2.68	112.48	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	q	902	LMU	O5'-C5'-C4'	2.68	114.56	109.69
13	Y	501	CLA	CHB-C4A-NA	2.68	128.21	124.51
13	u	513	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	a	516	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
13	R	1302	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	a	517	CLA	C3B-C4B-NB	-2.68	108.03	110.52
13	f	1228	CLA	CMB-C2B-C3B	2.67	133.07	126.59
16	f	4010	BCR	C38-C26-C25	-2.67	121.53	124.53
16	f	4017	BCR	C33-C5-C6	-2.67	121.53	124.53
13	6	504	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	e	1013	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	2	510	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
16	q	523	BCR	C24-C23-C22	-2.67	122.20	126.23
13	d	511	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	B	1238	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	F	1302	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	B	1203	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	A	1022	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
16	H	4017	BCR	C20-C21-C22	-2.67	123.50	127.31
13	B	1225	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	A	1113	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	e	1116	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	G	1131	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	H	1217	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	A	1013	CLA	CHB-C4A-NA	2.67	128.20	124.51
16	Y	523	BCR	C10-C11-C12	-2.67	114.89	123.22
13	B	1210	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
13	r	504	CLA	CHB-C4A-NA	2.67	128.20	124.51
16	B	4005	BCR	C28-C27-C26	-2.67	109.31	114.08
13	e	1124	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	G	1022	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
13	Z	508	CLA	CHB-C1B-NB	2.67	127.08	124.26
13	e	1129	CLA	CHB-C1B-NB	2.67	127.08	124.26
13	5	513	CLA	CHB-C4A-NA	2.67	128.20	124.51
16	1	523	BCR	C10-C11-C12	-2.67	114.89	123.22
18	e	1848	LMU	C2'-C3'-C4'	2.67	115.77	109.68
13	K	1401	CLA	O2D-CGD-CBD	2.67	116.01	111.27
13	r	502	CLA	C3B-C4B-NB	-2.67	108.04	110.52
16	T	4015	BCR	C2-C1-C6	2.67	114.59	110.48
13	H	1223	CLA	CHB-C4A-NA	2.67	128.20	124.51
13	f	1203	CLA	CHB-C4A-NA	2.67	128.20	124.51
16	s	521	BCR	C33-C5-C6	-2.67	121.53	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	r	506	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
13	f	1217	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	q	517	CLA	C3B-C4B-NB	-2.67	108.04	110.52
18	A	1848	LMU	C2'-C3'-C4'	2.67	115.77	109.68
13	1	501	CLA	CHB-C4A-NA	2.67	128.20	124.51
13	d	504	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
13	3	517	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	B	1223	CLA	CHB-C4A-NA	2.67	128.20	124.51
13	4	505	CLA	CHB-C4A-NA	2.67	128.20	124.51
13	e	1132	CLA	CAC-C3C-C4C	2.67	128.27	124.81
17	A	5001	LHG	C20-C19-C18	-2.66	100.90	114.42
13	v	516	CLA	C3B-C4B-NB	-2.66	108.04	110.52
13	q	513	CLA	CHB-C4A-NA	2.66	128.20	124.51
13	v	504	CLA	CHB-C4A-NA	2.66	128.20	124.51
13	G	1136	CLA	CHB-C1B-NB	2.66	127.08	124.26
13	r	517	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
13	G	1132	CLA	CAC-C3C-C4C	2.66	128.27	124.81
17	e	5001	LHG	C20-C19-C18	-2.66	100.90	114.42
13	G	1116	CLA	C3B-C4B-NB	-2.66	108.04	110.52
16	f	4005	BCR	C28-C27-C26	-2.66	109.32	114.08
13	q	501	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	1	504	CLA	C3B-C4B-NB	-2.66	108.05	110.52
13	v	504	CLA	C3B-C4B-NB	-2.66	108.05	110.52
13	6	504	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
16	c	524	BCR	C11-C10-C9	-2.66	123.51	127.31
13	A	1106	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	r	510	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
13	Z	510	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
16	s	522	BCR	C15-C16-C17	-2.66	118.02	123.47
17	G	5001	LHG	C20-C19-C18	-2.66	100.92	114.42
16	5	523	BCR	C33-C5-C6	-2.66	121.54	124.53
16	3	522	BCR	C15-C16-C17	-2.66	118.02	123.47
16	f	4017	BCR	C20-C21-C22	-2.66	123.51	127.31
13	j	1302	CLA	C3B-C4B-NB	-2.66	108.05	110.52
16	B	4017	BCR	C20-C21-C22	-2.66	123.51	127.31
13	c	513	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	d	504	CLA	CHB-C4A-NA	2.66	128.19	124.51
16	f	4006	BCR	C31-C1-C6	-2.66	105.98	110.30
16	B	4010	BCR	C38-C26-C25	-2.66	121.54	124.53
16	B	4006	BCR	C31-C1-C6	-2.66	105.99	110.30
13	5	504	CLA	CHB-C4A-NA	2.66	128.19	124.51
16	B	4017	BCR	C33-C5-C6	-2.66	121.54	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	516	CLA	C3B-C4B-NB	-2.66	108.05	110.52
13	1	516	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
13	A	1135	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	u	504	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	B	1217	CLA	C3B-C4B-NB	-2.66	108.05	110.52
13	Y	516	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
13	H	1203	CLA	CHB-C4A-NA	2.66	128.19	124.51
16	H	4005	BCR	C28-C27-C26	-2.66	109.33	114.08
13	l	1302	CLA	C3B-C4B-NB	-2.66	108.05	110.52
16	1	523	BCR	C24-C23-C22	-2.66	122.22	126.23
16	c	522	BCR	C1-C6-C5	-2.66	118.87	122.61
13	a	501	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
13	v	519	CLA	C3B-C4B-NB	-2.65	108.05	110.52
13	A	1140	CLA	CHB-C1B-NB	2.65	127.07	124.26
16	H	4006	BCR	C31-C1-C6	-2.65	105.99	110.30
13	v	504	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
13	Z	506	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
13	e	1113	CLA	CHB-C4A-NA	2.65	128.18	124.51
13	e	1801	CLA	CHD-C1D-ND	-2.65	122.02	124.45
13	b	505	CLA	C3B-C4B-NB	-2.65	108.05	110.52
13	2	506	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
16	H	4017	BCR	C33-C5-C6	-2.65	121.55	124.53
13	A	1104	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
13	e	1104	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
13	Z	502	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	G	1848	LMU	C2'-C3'-C4'	2.65	115.73	109.68
13	c	513	CLA	C3B-C4B-NB	-2.65	108.06	110.52
13	3	501	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	c	504	CLA	CHB-C4A-NA	2.65	128.18	124.51
13	Z	510	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
13	v	517	CLA	CHB-C4A-NA	2.65	128.18	124.51
13	A	1114	CLA	CHB-C1B-NB	2.65	127.06	124.26
13	e	1022	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	A	1132	CLA	CAC-C3C-C4C	2.65	128.25	124.81
13	2	517	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	e	1140	CLA	CHB-C1B-NB	2.65	127.06	124.26
13	G	1127	CLA	C3B-C4B-NB	-2.65	108.06	110.52
13	B	1224	CLA	CHB-C4A-NA	2.65	128.17	124.51
13	5	502	CLA	CHB-C4A-NA	2.65	128.17	124.51
13	s	501	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	u	502	CLA	CHB-C4A-NA	2.65	128.17	124.51
13	T	1302	CLA	C3B-C4B-NB	-2.65	108.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	510	CLA	C3B-C4B-NB	-2.65	108.06	110.52
13	Z	517	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
13	a	507	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
13	f	1210	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
16	a	522	BCR	C15-C16-C17	-2.65	118.06	123.47
16	H	4004	BCR	C20-C19-C18	-2.64	118.99	126.42
16	1	524	BCR	C15-C16-C17	-2.64	118.06	123.47
13	e	1106	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	s	507	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
13	1	513	CLA	CHB-C4A-NA	2.64	128.17	124.51
16	3	521	BCR	C33-C5-C6	-2.64	121.56	124.53
13	e	1135	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	t	505	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	3	510	CLA	C3B-C4B-NB	-2.64	108.06	110.52
13	f	1215	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	6	517	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	v	518	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	H	1210	CLA	C3B-C4B-NB	-2.64	108.06	110.52
16	Y	524	BCR	C15-C16-C17	-2.64	118.06	123.47
13	H	1224	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	G	1121	CLA	C3B-C4B-NB	-2.64	108.07	110.52
13	G	1106	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	G	1104	CLA	CMB-C2B-C1B	-2.64	121.35	125.37
13	s	510	CLA	C3B-C4B-NB	-2.64	108.07	110.52
13	3	507	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
16	v	523	BCR	C10-C11-C12	-2.64	114.98	123.22
13	e	1126	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	A	1129	CLA	CHB-C1B-NB	2.64	127.05	124.26
17	G	5004	LHG	O8-C23-C24	2.64	120.18	111.91
13	H	1230	CLA	C3B-C4B-NB	-2.64	108.07	110.52
13	e	1121	CLA	C3B-C4B-NB	-2.64	108.07	110.52
17	A	5008	LHG	C11-C10-C9	-2.64	101.04	114.42
16	q	524	BCR	C1-C6-C5	-2.64	118.90	122.61
13	B	1213	CLA	C1-C2-C3	-2.64	121.48	126.04
13	r	502	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	B	1215	CLA	CHB-C4A-NA	2.63	128.16	124.51
13	f	1224	CLA	CHB-C4A-NA	2.63	128.16	124.51
13	B	1210	CLA	C3B-C4B-NB	-2.63	108.07	110.52
16	c	523	BCR	C33-C5-C6	-2.63	121.57	124.53
13	H	1239	CLA	CHB-C4A-NA	2.63	128.15	124.51
13	f	1213	CLA	C1-C2-C3	-2.63	121.49	126.04
13	3	504	CLA	C3B-C4B-NB	-2.63	108.07	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	513	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	a	511	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	f	1210	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	q	516	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
13	G	1130	CLA	CHB-C4A-NA	2.63	128.15	124.51
13	G	1013	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
13	H	1213	CLA	C1-C2-C3	-2.63	121.49	126.04
16	u	523	BCR	C33-C5-C6	-2.63	121.57	124.53
13	A	1124	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	G	1119	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	s	511	CLA	C3B-C4B-NB	-2.63	108.07	110.52
17	e	5008	LHG	C11-C10-C9	-2.63	101.06	114.42
13	e	1013	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
13	1	501	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	a	503	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	r	510	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	u	506	CLA	C3B-C4B-NB	-2.63	108.07	110.52
16	k	4018	BCR	C4-C5-C6	-2.63	118.91	122.73
16	f	4004	BCR	C20-C19-C18	-2.63	119.03	126.42
17	G	5008	LHG	C11-C10-C9	-2.63	101.07	114.42
16	I	4018	BCR	C4-C5-C6	-2.63	118.91	122.73
13	d	516	CLA	C3B-C4B-NB	-2.63	108.08	110.52
13	G	1801	CLA	CHD-C1D-ND	-2.63	122.04	124.45
16	q	524	BCR	C15-C16-C17	-2.63	118.09	123.47
13	6	518	CLA	CHB-C4A-NA	2.63	128.15	124.51
16	6	523	BCR	C10-C11-C12	-2.63	115.01	123.22
16	5	524	BCR	C11-C10-C9	-2.63	123.56	127.31
13	Y	513	CLA	CHB-C4A-NA	2.63	128.15	124.51
16	B	4004	BCR	C20-C19-C18	-2.63	119.03	126.42
16	d	523	BCR	C33-C5-C4	2.63	118.67	113.62
13	A	1131	CLA	C3B-C4B-NB	-2.63	108.08	110.52
16	5	522	BCR	C1-C6-C5	-2.63	118.91	122.61
16	a	521	BCR	C33-C5-C6	-2.63	121.58	124.53
13	G	1114	CLA	CHB-C1B-NB	2.63	127.04	124.26
13	1	504	CLA	CHB-C4A-NA	2.63	128.14	124.51
13	G	1135	CLA	CHB-C4A-NA	2.63	128.14	124.51
16	r	522	BCR	C21-C20-C19	-2.63	115.02	123.22
13	B	1230	CLA	C3B-C4B-NB	-2.63	108.08	110.52
13	3	511	CLA	C3B-C4B-NB	-2.63	108.08	110.52
13	f	1225	CLA	C3B-C4B-NB	-2.63	108.08	110.52
16	2	522	BCR	C21-C20-C19	-2.63	115.02	123.22
16	v	523	BCR	C20-C21-C22	-2.62	123.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	513	CLA	C3B-C4B-NB	-2.62	108.08	110.52
13	A	1130	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	s	504	CLA	C3B-C4B-NB	-2.62	108.08	110.52
13	A	1126	CLA	CHB-C4A-NA	2.62	128.14	124.51
16	f	4009	BCR	C16-C17-C18	-2.62	123.57	127.31
16	u	524	BCR	C11-C10-C9	-2.62	123.57	127.31
13	A	1013	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
13	A	1136	CLA	CHB-C1B-NB	2.62	127.03	124.26
16	d	523	BCR	C10-C11-C12	-2.62	115.03	123.22
16	Y	523	BCR	C24-C23-C22	-2.62	122.27	126.23
16	Z	522	BCR	C21-C20-C19	-2.62	115.03	123.22
13	Y	505	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
13	Y	509	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
13	r	517	CLA	CHB-C4A-NA	2.62	128.14	124.51
16	v	523	BCR	C33-C5-C4	2.62	118.65	113.62
16	1	522	BCR	C23-C24-C25	-2.62	119.84	127.20
13	s	516	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	A	5004	LHG	O8-C23-C24	2.62	120.13	111.91
13	d	517	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	a	504	CLA	C3B-C4B-NB	-2.62	108.08	110.52
13	G	1126	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	e	1132	CLA	CHD-C1D-ND	-2.62	122.05	124.45
13	1	505	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
17	e	5004	LHG	O8-C23-C24	2.62	120.12	111.91
13	H	1215	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	Y	504	CLA	CHB-C4A-NA	2.62	128.13	124.51
16	Y	522	BCR	C23-C24-C25	-2.62	119.85	127.20
16	6	523	BCR	C33-C5-C4	2.62	118.64	113.62
13	t	513	CLA	C3B-C4B-NB	-2.62	108.09	110.52
13	Z	509	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
13	c	502	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	2	509	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
13	r	508	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	e	1127	CLA	CMB-C2B-C3B	2.62	132.93	126.59
13	A	1801	CLA	CHD-C1D-ND	-2.62	122.05	124.45
13	a	516	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	5	506	CLA	C3B-C4B-NB	-2.62	108.09	110.52
13	G	1011	CLA	C3B-C4B-NB	-2.62	108.09	110.52
13	3	516	CLA	CHB-C4A-NA	2.61	128.13	124.51
13	t	516	CLA	CHB-C4A-NA	2.61	128.13	124.51
13	A	1129	CLA	CHB-C4A-NA	2.61	128.13	124.51
20	v	822	SQD	C1-O5-C5	2.61	118.82	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	q	504	CLA	CHB-C4A-NA	2.61	128.13	124.51
13	r	509	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	A	1138	CLA	C1-C2-C3	-2.61	121.52	126.04
13	e	1136	CLA	CHB-C1B-NB	2.61	127.02	124.26
13	B	1239	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	1	517	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	G	1138	CLA	C1-C2-C3	-2.61	121.53	126.04
16	Y	524	BCR	C1-C6-C5	-2.61	118.94	122.61
13	J	1302	CLA	C3B-C4B-NB	-2.61	108.09	110.52
13	e	1131	CLA	C3B-C4B-NB	-2.61	108.09	110.52
13	Y	509	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
13	A	1132	CLA	CHD-C1D-ND	-2.61	122.06	124.45
13	e	1114	CLA	CHB-C1B-NB	2.61	127.02	124.26
13	G	1101	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	d	517	CLA	C3B-C4B-NB	-2.61	108.09	110.52
13	d	516	CLA	CHB-C4A-NA	2.61	128.12	124.51
16	q	522	BCR	C23-C24-C25	-2.61	119.88	127.20
16	u	522	BCR	C1-C6-C5	-2.61	118.94	122.61
13	b	504	CLA	C3B-C4B-NB	-2.61	108.09	110.52
13	f	1230	CLA	C3B-C4B-NB	-2.61	108.09	110.52
13	V	1502	CLA	CHD-C1D-ND	-2.61	122.06	124.45
16	d	522	BCR	C38-C26-C27	2.61	118.63	113.62
20	Z	822	SQD	O5-C5-C4	2.61	114.43	109.69
13	c	506	CLA	C3B-C4B-NB	-2.61	108.10	110.52
20	d	822	SQD	C1-O5-C5	2.61	118.81	113.69
13	2	517	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	4	516	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	Y	517	CLA	CHB-C4A-NA	2.61	128.12	124.51
16	1	524	BCR	C1-C6-C5	-2.61	118.94	122.61
13	A	1127	CLA	CMB-C2B-C3B	2.61	132.90	126.59
13	r	509	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
13	G	1129	CLA	CHB-C1B-NB	2.61	127.02	124.26
13	q	509	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
13	H	1221	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	Z	510	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	G	1102	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	2	510	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	3	503	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	H	1205	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	G	1127	CLA	CMB-C2B-C3B	2.60	132.89	126.59
13	H	1219	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	q	505	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	6	522	BCR	C38-C26-C27	2.60	118.61	113.62
16	4	523	BCR	C7-C8-C9	-2.60	122.30	126.23
16	S	4018	BCR	C4-C5-C6	-2.60	118.95	122.73
13	H	1213	CLA	O2D-CGD-CBD	2.60	115.89	111.27
16	b	522	BCR	C33-C5-C6	-2.60	121.61	124.53
13	1	509	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
13	u	504	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	c	509	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
13	4	516	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	r	516	CLA	C3B-C4B-NB	-2.60	108.10	110.52
16	B	4009	BCR	C16-C17-C18	-2.60	123.60	127.31
13	A	1106	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
16	t	522	BCR	C33-C5-C6	-2.60	121.61	124.53
13	A	1138	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
20	6	822	SQD	C1-O5-C5	2.60	118.79	113.69
16	k	4018	BCR	C33-C5-C4	2.60	118.61	113.62
16	H	4017	BCR	C8-C9-C10	-2.60	114.96	118.94
16	b	523	BCR	C7-C8-C9	-2.60	122.31	126.23
13	s	503	CLA	C3B-C4B-NB	-2.60	108.11	110.52
13	A	1121	CLA	C3B-C4B-NB	-2.60	108.11	110.52
13	5	504	CLA	C3B-C4B-NB	-2.60	108.11	110.52
13	b	516	CLA	C3B-C4B-NB	-2.60	108.11	110.52
13	G	1116	CLA	CMB-C2B-C3B	2.60	132.87	126.59
16	4	522	BCR	C33-C5-C6	-2.59	121.61	124.53
13	e	1109	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	q	502	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	v	516	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	c	504	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	1	506	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	G	1129	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	b	516	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	f	1213	CLA	O2D-CGD-CBD	2.59	115.88	111.27
13	H	1213	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	u	511	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	A	1109	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	f	1225	CLA	CHB-C4A-NA	2.59	128.10	124.51
19	f	5002	LMG	O7-C10-O9	-2.59	117.44	123.70
13	1	509	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
16	Y	524	BCR	C8-C7-C6	-2.59	119.92	127.20
16	c	523	BCR	C20-C21-C22	-2.59	123.61	127.31
13	e	1102	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	e	1130	CLA	CHB-C4A-NA	2.59	128.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	r	822	SQD	O5-C5-C4	2.59	114.40	109.69
13	G	1106	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
20	2	822	SQD	O5-C5-C4	2.59	114.40	109.69
13	e	1103	CLA	CAC-C3C-C4C	2.59	128.17	124.81
16	6	523	BCR	C20-C21-C22	-2.59	123.61	127.31
13	3	509	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
16	f	4014	BCR	C34-C9-C8	2.59	122.16	118.08
20	H	1852	SQD	C26-C25-C24	-2.59	103.88	113.19
13	Z	504	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	f	1204	CLA	O2D-CGD-CBD	2.59	115.87	111.27
13	B	1205	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	v	517	CLA	C3B-C4B-NB	-2.59	108.11	110.52
20	B	1852	SQD	C26-C25-C24	-2.59	103.88	113.19
13	G	1138	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
13	u	519	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
13	B	1213	CLA	O2D-CGD-CBD	2.59	115.87	111.27
13	B	1206	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	Z	505	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	s	509	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
13	e	1116	CLA	CMB-C2B-C3B	2.59	132.86	126.59
19	B	5002	LMG	O7-C10-O9	-2.59	117.44	123.70
13	2	509	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
16	B	4014	BCR	C34-C9-C8	2.59	122.16	118.08
16	d	523	BCR	C20-C21-C22	-2.59	123.62	127.31
13	e	1106	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
16	I	4018	BCR	C33-C5-C4	2.59	118.59	113.62
13	2	508	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	G	1109	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	Y	502	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	r	511	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	e	1138	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
16	B	4010	BCR	C21-C20-C19	-2.59	115.14	123.22
13	A	1116	CLA	CMB-C2B-C3B	2.59	132.85	126.59
20	f	1852	SQD	C26-C25-C24	-2.59	103.89	113.19
16	a	524	BCR	C20-C21-C22	-2.59	123.62	127.31
16	v	522	BCR	C38-C26-C27	2.59	118.58	113.62
13	U	1401	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	Z	517	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	e	1119	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	q	517	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	e	1138	CLA	C1-C2-C3	-2.59	121.57	126.04
13	5	519	CLA	O2D-CGD-O1D	-2.58	118.78	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	509	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
13	6	517	CLA	C3B-C4B-NB	-2.58	108.12	110.52
13	B	1204	CLA	O2D-CGD-CBD	2.58	115.86	111.27
13	H	1206	CLA	CHB-C4A-NA	2.58	128.09	124.51
13	f	1239	CLA	CHB-C4A-NA	2.58	128.09	124.51
13	G	1122	CLA	CHD-C1D-ND	-2.58	122.08	124.45
13	H	1227	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
13	e	1119	CLA	C3B-C4B-NB	-2.58	108.12	110.52
16	f	4010	BCR	C21-C20-C19	-2.58	115.15	123.22
16	S	4018	BCR	C33-C5-C4	2.58	118.58	113.62
16	H	4010	BCR	C21-C20-C19	-2.58	115.16	123.22
13	u	509	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
13	t	516	CLA	C3B-C4B-NB	-2.58	108.12	110.52
16	1	524	BCR	C8-C7-C6	-2.58	119.95	127.20
13	e	1129	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	f	1234	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	A	1011	CLA	C3B-C4B-NB	-2.58	108.12	110.52
13	5	509	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
13	B	1234	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	L	1502	CLA	CHD-C1D-ND	-2.58	122.08	124.45
13	6	516	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	f	1205	CLA	C3B-C4B-NB	-2.58	108.12	110.52
13	A	1119	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	f	1206	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	2	504	CLA	C3B-C4B-NB	-2.58	108.12	110.52
13	A	1102	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	A	1101	CLA	CHB-C4A-NA	2.58	128.08	124.51
16	H	4009	BCR	C16-C17-C18	-2.58	123.63	127.31
13	q	509	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
13	Y	506	CLA	CHB-C4A-NA	2.58	128.07	124.51
13	Z	508	CLA	CHB-C4A-NA	2.58	128.07	124.51
16	s	521	BCR	C29-C30-C25	2.58	114.45	110.48
16	3	524	BCR	C20-C21-C22	-2.58	123.63	127.31
13	a	513	CLA	C3B-C4B-NB	-2.58	108.13	110.52
16	s	524	BCR	C20-C21-C22	-2.58	123.64	127.31
16	3	523	BCR	C33-C5-C4	2.57	118.56	113.62
16	q	524	BCR	C8-C7-C6	-2.57	119.97	127.20
13	A	1119	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	3	513	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	B	1021	CLA	CHC-C4B-NB	2.57	126.98	124.26
16	H	4014	BCR	C34-C9-C8	2.57	122.13	118.08
13	H	1230	CLA	CAA-C2A-C1A	-2.57	103.54	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1230	CLA	CAA-C2A-C1A	-2.57	103.54	111.97
16	3	521	BCR	C29-C30-C25	2.57	114.44	110.48
13	1	502	CLA	CHB-C4A-NA	2.57	128.07	124.51
13	B	1227	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
13	4	504	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	Y	501	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	f	1213	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	q	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
13	f	1229	CLA	CHB-C1B-NB	2.57	126.98	124.26
16	a	521	BCR	C29-C30-C25	2.57	114.44	110.48
16	a	523	BCR	C33-C5-C4	2.57	118.55	113.62
13	A	1117	CLA	C1-C2-C3	-2.57	121.60	126.04
19	H	5002	LMG	O7-C10-O9	-2.57	117.49	123.70
16	f	4010	BCR	C10-C11-C12	-2.57	115.20	123.22
16	B	4017	BCR	C8-C9-C10	-2.57	115.00	118.94
13	f	1227	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
13	b	501	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	u	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
16	6	523	BCR	C15-C16-C17	-2.57	118.21	123.47
16	t	523	BCR	C7-C8-C9	-2.57	122.36	126.23
13	H	1204	CLA	O2D-CGD-CBD	2.57	115.83	111.27
13	c	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	B	1221	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	4	501	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	v	506	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	c	519	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
13	B	1230	CLA	CAA-C2A-C1A	-2.57	103.57	111.97
13	T	1303	CLA	O2A-CGA-O1A	-2.57	117.12	123.59
13	d	513	CLA	CHB-C4A-NA	2.57	128.06	124.51
16	1	521	BCR	C33-C5-C6	-2.57	121.65	124.53
13	G	1115	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
13	Z	509	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
13	f	1021	CLA	CHC-C4B-NB	2.57	126.97	124.26
16	s	523	BCR	C33-C5-C4	2.57	118.54	113.62
16	l	4015	BCR	C24-C23-C22	-2.57	122.36	126.23
13	2	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	H	1234	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	A	1103	CLA	CAC-C3C-C4C	2.56	128.14	124.81
18	H	1843	LMU	O5B-C5B-C4B	2.56	114.35	109.69
13	e	1237	CLA	C3B-C4B-NB	-2.56	108.14	110.52
16	G	4011	BCR	C23-C24-C25	-2.56	120.00	127.20
13	B	1225	CLA	CHB-C4A-NA	2.56	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1843	LMU	O5B-C5B-C4B	2.56	114.35	109.69
16	L	4020	BCR	C38-C26-C25	-2.56	121.65	124.53
16	v	523	BCR	C15-C16-C17	-2.56	118.22	123.47
13	B	1213	CLA	C3B-C4B-NB	-2.56	108.14	110.52
13	2	516	CLA	C3B-C4B-NB	-2.56	108.14	110.52
13	H	1201	CLA	CMB-C2B-C3B	2.56	132.80	126.59
16	S	4018	BCR	C38-C26-C27	2.56	118.54	113.62
16	Z	524	BCR	C33-C5-C4	2.56	118.54	113.62
13	n	1502	CLA	CHD-C1D-ND	-2.56	122.10	124.45
16	H	4010	BCR	C10-C11-C12	-2.56	115.22	123.22
13	e	1114	CLA	C3B-C4B-NB	-2.56	108.14	110.52
16	q	521	BCR	C33-C5-C6	-2.56	121.65	124.53
13	J	1303	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
20	r	822	SQD	C44-O6-C1	2.56	118.74	113.74
16	3	523	BCR	C20-C21-C22	-2.56	123.65	127.31
16	A	4008	BCR	C38-C26-C27	2.56	118.54	113.62
13	m	1401	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	f	1231	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
13	4	512	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	5	505	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	f	1201	CLA	CMB-C2B-C3B	2.56	132.79	126.59
16	s	523	BCR	C20-C21-C22	-2.56	123.66	127.31
13	r	505	CLA	CHB-C4A-NA	2.56	128.05	124.51
16	B	4010	BCR	C10-C11-C12	-2.56	115.23	123.22
13	v	509	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	t	504	CLA	C3B-C4B-NB	-2.56	108.14	110.52
13	b	512	CLA	CHB-C4A-NA	2.56	128.05	124.51
16	a	523	BCR	C21-C20-C19	-2.56	115.23	123.22
13	B	1219	CLA	C3B-C4B-NB	-2.56	108.14	110.52
20	2	822	SQD	C44-O6-C1	2.56	118.74	113.74
16	3	523	BCR	C21-C20-C19	-2.56	115.23	123.22
13	e	1116	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
16	d	522	BCR	C11-C12-C13	-2.56	119.23	126.42
16	e	4008	BCR	C38-C26-C27	2.56	118.53	113.62
13	A	1115	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
16	v	522	BCR	C11-C12-C13	-2.56	119.23	126.42
13	e	1117	CLA	C1-C2-C3	-2.56	121.62	126.04
13	t	501	CLA	C3B-C4B-NB	-2.56	108.14	110.52
16	H	4014	BCR	C10-C11-C12	-2.56	115.24	123.22
16	s	523	BCR	C21-C20-C19	-2.56	115.24	123.22
13	K	1401	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	e	5001	LHG	C11-C10-C9	-2.55	101.46	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1122	CLA	CHD-C1D-ND	-2.55	122.11	124.45
13	H	1223	CLA	CMB-C2B-C3B	2.55	132.77	126.59
13	G	1140	CLA	C2A-C1A-CHA	2.55	128.32	123.86
13	6	508	CLA	CMB-C2B-C1B	-2.55	121.48	125.37
13	A	1114	CLA	C3B-C4B-NB	-2.55	108.15	110.52
13	B	1223	CLA	CMB-C2B-C3B	2.55	132.77	126.59
13	a	505	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	A	4011	BCR	C23-C24-C25	-2.55	120.04	127.20
13	c	512	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	2	524	BCR	C33-C5-C4	2.55	118.52	113.62
16	5	523	BCR	C20-C21-C22	-2.55	123.67	127.31
16	B	4014	BCR	C10-C11-C12	-2.55	115.26	123.22
13	f	1223	CLA	CMB-C2B-C3B	2.55	132.77	126.59
13	A	1140	CLA	C2A-C1A-CHA	2.55	128.32	123.86
13	H	1225	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	u	512	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	l	1303	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
13	H	1021	CLA	CHC-C4B-NB	2.55	126.96	124.26
18	f	1843	LMU	O5B-C5B-C4B	2.55	114.33	109.69
13	H	1224	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
16	f	4017	BCR	C8-C9-C10	-2.55	115.03	118.94
17	A	5001	LHG	C11-C10-C9	-2.55	101.48	114.42
13	A	1116	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
16	k	4018	BCR	C38-C26-C27	2.55	118.51	113.62
16	r	521	BCR	C29-C30-C25	2.55	114.41	110.48
16	d	523	BCR	C15-C16-C17	-2.55	118.25	123.47
16	K	4104	BCR	C38-C26-C27	2.55	118.51	113.62
13	e	1107	CLA	CHB-C1B-NB	2.55	126.95	124.26
16	u	523	BCR	C20-C21-C22	-2.55	123.67	127.31
13	G	1114	CLA	C3B-C4B-NB	-2.55	108.15	110.52
13	H	1021	CLA	C3B-C4B-NB	-2.55	108.15	110.52
16	n	4020	BCR	C38-C26-C25	-2.55	121.67	124.53
13	G	1119	CLA	CHB-C4A-NA	2.55	128.03	124.51
16	I	4018	BCR	C38-C26-C27	2.55	118.51	113.62
16	G	4008	BCR	C38-C26-C27	2.55	118.51	113.62
13	e	1101	CLA	CHB-C4A-NA	2.55	128.03	124.51
13	v	508	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
13	e	1101	CLA	CHB-C1B-NB	2.55	126.95	124.26
13	v	508	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
20	Z	822	SQD	C44-O6-C1	2.55	118.71	113.74
16	e	4011	BCR	C23-C24-C25	-2.55	120.05	127.20
16	a	523	BCR	C20-C21-C22	-2.55	123.68	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	s	513	CLA	C3B-C4B-NB	-2.55	108.15	110.52
16	6	522	BCR	C11-C12-C13	-2.55	119.26	126.42
13	f	1238	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
13	v	508	CLA	CHB-C4A-NA	2.55	128.03	124.51
13	B	1231	CLA	CMB-C2B-C1B	-2.54	121.49	125.37
16	U	4104	BCR	C38-C26-C27	2.54	118.50	113.62
17	G	5001	LHG	C11-C10-C9	-2.54	101.51	114.42
13	B	1201	CLA	CMB-C2B-C3B	2.54	132.75	126.59
13	q	505	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	H	1220	CLA	CAA-CBA-CGA	-2.54	105.82	113.25
13	H	1229	CLA	CHB-C1B-NB	2.54	126.95	124.26
13	d	506	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	H	1225	CLA	CMB-C2B-C3B	2.54	132.75	126.59
13	A	1022	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
16	3	522	BCR	C16-C17-C18	-2.54	123.68	127.31
13	A	1101	CLA	CHB-C1B-NB	2.54	126.95	124.26
13	6	508	CLA	CHB-C4A-NA	2.54	128.03	124.51
16	s	522	BCR	C16-C17-C18	-2.54	123.68	127.31
16	u	521	BCR	C33-C5-C6	-2.54	121.67	124.53
13	B	1240	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	f	1219	CLA	O2D-CGD-CBD	2.54	115.78	111.27
13	G	1237	CLA	C6-C5-C3	2.54	120.12	113.45
13	r	504	CLA	C3B-C4B-NB	-2.54	108.16	110.52
16	r	524	BCR	C33-C5-C4	2.54	118.49	113.62
13	G	1107	CLA	CHB-C1B-NB	2.54	126.94	124.26
13	6	513	CLA	CHB-C4A-NA	2.54	128.02	124.51
13	q	510	CLA	CHB-C4A-NA	2.54	128.02	124.51
13	t	512	CLA	CHB-C4A-NA	2.54	128.02	124.51
16	V	4020	BCR	C38-C26-C25	-2.54	121.68	124.53
16	m	4104	BCR	C38-C26-C27	2.54	118.49	113.62
16	Z	521	BCR	C29-C30-C25	2.54	114.39	110.48
13	B	1021	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	2	517	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	d	508	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
16	c	523	BCR	C34-C9-C8	2.54	122.08	118.08
13	e	1115	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
13	H	1231	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
16	f	4014	BCR	C10-C11-C12	-2.54	115.30	123.22
13	A	1237	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	Y	511	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	6	508	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
13	B	1220	CLA	CAA-CBA-CGA	-2.54	105.84	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1205	CLA	C1-C2-C3	-2.54	121.66	126.04
16	a	524	BCR	C11-C10-C9	-2.54	123.69	127.31
13	e	1135	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
16	Y	521	BCR	C33-C5-C6	-2.54	121.68	124.53
16	L	4020	BCR	C34-C9-C8	2.54	122.07	118.08
13	e	1121	CLA	C2D-C1D-ND	-2.54	108.23	110.10
16	c	522	BCR	C33-C5-C4	2.54	118.49	113.62
13	B	1238	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
13	5	511	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	e	1011	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	B	1224	CLA	CMB-C2B-C1B	-2.54	121.51	125.37
13	A	1135	CLA	O2A-CGA-O1A	-2.53	117.19	123.59
13	B	1225	CLA	CMB-C2B-C3B	2.53	132.73	126.59
13	d	510	CLA	C3B-C4B-NB	-2.53	108.16	110.52
16	s	523	BCR	C28-C27-C26	-2.53	109.55	114.08
13	G	1103	CLA	CAC-C3C-C4C	2.53	128.10	124.81
16	5	522	BCR	C33-C5-C4	2.53	118.48	113.62
13	H	1240	CLA	CHB-C4A-NA	2.53	128.02	124.51
13	e	1801	CLA	CHB-C4A-NA	2.53	128.02	124.51
16	V	4020	BCR	C34-C9-C8	2.53	122.07	118.08
13	G	1116	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
13	6	506	CLA	C3B-C4B-NB	-2.53	108.17	110.52
16	5	521	BCR	C33-C5-C6	-2.53	121.68	124.53
13	G	1117	CLA	C1-C2-C3	-2.53	121.66	126.04
13	G	1132	CLA	CHD-C1D-ND	-2.53	122.13	124.45
13	f	1219	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	f	1221	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	d	508	CLA	CMB-C2B-C1B	-2.53	121.51	125.37
13	e	1022	CLA	CMB-C2B-C1B	-2.53	121.51	125.37
13	G	1135	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
13	f	1230	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
13	G	1237	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	Z	516	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	c	511	CLA	C3B-C4B-NB	-2.53	108.17	110.52
16	J	4015	BCR	C24-C23-C22	-2.53	122.41	126.23
13	G	1101	CLA	CHB-C1B-NB	2.53	126.94	124.26
13	A	1114	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	1	510	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	A	1237	CLA	C6-C5-C3	2.53	120.09	113.45
16	u	522	BCR	C33-C5-C4	2.53	118.48	113.62
13	B	1229	CLA	CHB-C1B-NB	2.53	126.94	124.26
16	U	4104	BCR	C24-C23-C22	-2.53	122.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1205	CLA	C1-C2-C3	-2.53	121.67	126.04
13	H	1230	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
16	3	524	BCR	C11-C10-C9	-2.53	123.70	127.31
13	B	1230	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
13	e	1237	CLA	C6-C5-C3	2.53	120.08	113.45
16	2	521	BCR	C29-C30-C25	2.53	114.37	110.48
13	3	505	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	v	513	CLA	CHB-C4A-NA	2.53	128.01	124.51
16	5	522	BCR	C11-C12-C13	-2.53	119.31	126.42
20	d	822	SQD	C4-C3-C2	2.53	115.24	110.82
13	e	1140	CLA	C2A-C1A-CHA	2.53	128.28	123.86
13	t	508	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	f	1220	CLA	CAA-CBA-CGA	-2.53	105.87	113.25
13	H	1234	CLA	CBA-CAA-C2A	-2.53	106.40	113.86
13	1	511	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	Z	517	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	r	517	CLA	C3B-C4B-NB	-2.53	108.17	110.52
13	q	519	CLA	CHB-C4A-NA	2.53	128.00	124.51
13	f	1224	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
16	c	522	BCR	C11-C12-C13	-2.53	119.32	126.42
13	2	511	CLA	C3B-C4B-NB	-2.53	108.17	110.52
16	V	4020	BCR	C11-C10-C9	-2.53	123.71	127.31
13	e	1103	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
13	5	512	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	e	1114	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	f	1225	CLA	CMB-C2B-C3B	2.52	132.70	126.59
13	f	1234	CLA	CBA-CAA-C2A	-2.52	106.41	113.86
13	2	506	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	1	505	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	f	1240	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	H	1842	LHG	O8-C23-C24	2.52	119.83	111.91
20	6	822	SQD	C4-C3-C2	2.52	115.23	110.82
13	G	1022	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
16	3	523	BCR	C28-C27-C26	-2.52	109.57	114.08
17	V	5221	LHG	C20-C19-C18	-2.52	101.62	114.42
16	u	523	BCR	C34-C9-C8	2.52	122.05	118.08
13	Y	505	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	d	508	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	s	505	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	B	1219	CLA	O2D-CGD-CBD	2.52	115.75	111.27
20	v	822	SQD	C4-C3-C2	2.52	115.22	110.82
13	v	510	CLA	C3B-C4B-NB	-2.52	108.18	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	s	522	BCR	C38-C26-C25	-2.52	121.70	124.53
13	A	1107	CLA	CHB-C1B-NB	2.52	126.92	124.26
16	L	4020	BCR	C11-C10-C9	-2.52	123.72	127.31
13	G	1114	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	H	1238	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
16	T	4015	BCR	C24-C23-C22	-2.52	122.43	126.23
16	m	4104	BCR	C24-C23-C22	-2.52	122.43	126.23
13	B	1234	CLA	CBA-CAA-C2A	-2.52	106.43	113.86
13	H	1219	CLA	O2D-CGD-CBD	2.52	115.74	111.27
16	K	4104	BCR	C24-C23-C22	-2.52	122.43	126.23
16	5	523	BCR	C34-C9-C8	2.52	122.04	118.08
16	s	524	BCR	C11-C10-C9	-2.52	123.72	127.31
13	r	506	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	L	5221	LHG	C20-C19-C18	-2.52	101.65	114.42
13	6	509	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	H	1201	CLA	O2D-CGD-CBD	2.52	115.74	111.27
16	a	522	BCR	C16-C17-C18	-2.52	123.72	127.31
13	B	1203	CLA	CMB-C2B-C1B	-2.52	121.54	125.37
17	n	5221	LHG	C20-C19-C18	-2.52	101.66	114.42
13	4	508	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	6	510	CLA	C3B-C4B-NB	-2.51	108.18	110.52
13	Y	511	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
16	u	522	BCR	C11-C12-C13	-2.51	119.35	126.42
13	G	1801	CLA	CHB-C4A-NA	2.51	127.99	124.51
13	A	1102	CLA	CMB-C2B-C3B	2.51	132.68	126.59
16	c	521	BCR	C20-C19-C18	-2.51	119.36	126.42
16	f	4010	BCR	C31-C1-C6	-2.51	106.22	110.30
16	m	4104	BCR	C28-C27-C26	-2.51	109.59	114.08
13	A	1136	CLA	C1-C2-C3	-2.51	121.70	126.04
13	d	509	CLA	CHB-C4A-NA	2.51	127.99	124.51
16	c	521	BCR	C33-C5-C6	-2.51	121.71	124.53
13	f	1212	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
20	1	822	SQD	C44-O6-C1	2.51	118.65	113.74
17	B	1842	LHG	O8-C23-C24	2.51	119.79	111.91
20	s	822	SQD	O48-C23-C24	2.51	119.79	111.91
16	n	4020	BCR	C34-C9-C8	2.51	122.03	118.08
13	b	508	CLA	CHB-C4A-NA	2.51	127.98	124.51
16	u	521	BCR	C20-C19-C18	-2.51	119.36	126.42
20	3	822	SQD	O48-C23-C24	2.51	119.79	111.91
13	f	1205	CLA	C1-C2-C3	-2.51	121.70	126.04
13	A	1801	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	f	1842	LHG	O8-C23-C24	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1103	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
16	a	522	BCR	C38-C26-C25	-2.51	121.71	124.53
13	4	506	CLA	C3B-C4B-NB	-2.51	108.19	110.52
16	m	4104	BCR	C30-C25-C24	2.51	122.87	115.78
13	B	1201	CLA	O2D-CGD-CBD	2.51	115.72	111.27
13	H	1239	CLA	CAC-C3C-C4C	-2.51	121.56	124.81
16	n	4020	BCR	C11-C10-C9	-2.51	123.73	127.31
13	A	1121	CLA	C2D-C1D-ND	-2.51	108.26	110.10
13	G	1103	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
13	f	1021	CLA	C3B-C4B-NB	-2.51	108.19	110.52
20	Y	822	SQD	C44-O6-C1	2.51	118.64	113.74
13	d	505	CLA	CHB-C4A-NA	2.51	127.98	124.51
16	H	4010	BCR	C31-C1-C6	-2.51	106.23	110.30
13	e	1102	CLA	CMB-C2B-C3B	2.51	132.66	126.59
13	e	1122	CLA	CHD-C1D-ND	-2.50	122.15	124.45
13	f	1203	CLA	CMB-C2B-C1B	-2.50	121.55	125.37
17	n	5221	LHG	C27-C26-C25	-2.50	101.71	114.42
13	B	1212	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
13	b	518	CLA	C3B-C4B-NB	-2.50	108.19	110.52
16	5	521	BCR	C20-C19-C18	-2.50	119.38	126.42
20	a	822	SQD	O48-C23-C24	2.50	119.77	111.91
13	f	1201	CLA	O2D-CGD-CBD	2.50	115.72	111.27
17	L	5221	LHG	C27-C26-C25	-2.50	101.72	114.42
13	G	1121	CLA	C2D-C1D-ND	-2.50	108.26	110.10
13	Y	510	CLA	CHB-C4A-NA	2.50	127.97	124.51
16	a	523	BCR	C28-C27-C26	-2.50	109.61	114.08
13	B	1222	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
13	Z	506	CLA	CHB-C4A-NA	2.50	127.97	124.51
16	t	522	BCR	C1-C6-C5	-2.50	119.09	122.61
16	B	4010	BCR	C31-C1-C6	-2.50	106.24	110.30
16	2	524	BCR	C8-C7-C6	-2.50	120.18	127.20
13	q	511	CLA	C3B-C4B-NB	-2.50	108.19	110.52
16	e	4003	BCR	C38-C26-C25	-2.50	121.72	124.53
20	q	822	SQD	C44-O6-C1	2.50	118.62	113.74
13	G	1102	CLA	CMB-C2B-C3B	2.50	132.64	126.59
13	1	512	CLA	CHB-C4A-NA	2.50	127.97	124.51
16	K	4104	BCR	C30-C25-C24	2.50	122.85	115.78
16	b	522	BCR	C1-C6-C5	-2.50	119.09	122.61
17	V	5221	LHG	C27-C26-C25	-2.50	101.74	114.42
13	B	1239	CLA	CAC-C3C-C4C	-2.50	121.57	124.81
13	a	516	CLA	C3B-C4B-NB	-2.50	108.20	110.52
13	B	1211	CLA	O2D-CGD-O1D	-2.50	118.95	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	519	CLA	CHB-C4A-NA	2.50	127.97	124.51
13	v	505	CLA	CHB-C4A-NA	2.50	127.97	124.51
16	G	4011	BCR	C10-C11-C12	-2.50	115.42	123.22
16	A	4003	BCR	C38-C26-C25	-2.50	121.72	124.53
13	t	506	CLA	C3B-C4B-NB	-2.50	108.20	110.52
16	a	522	BCR	C33-C5-C6	-2.50	121.72	124.53
13	e	1136	CLA	C1-C2-C3	-2.50	121.73	126.04
13	1	519	CLA	CHB-C4A-NA	2.50	127.96	124.51
13	t	509	CLA	O2A-CGA-O1A	-2.50	117.30	123.59
16	2	522	BCR	C3-C4-C5	-2.49	109.62	114.08
13	G	1136	CLA	C1-C2-C3	-2.49	121.73	126.04
13	f	1222	CLA	CMB-C2B-C1B	-2.49	121.57	125.37
13	4	509	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
13	A	1134	CLA	CHD-C1D-ND	-2.49	122.16	124.45
16	5	522	BCR	C23-C24-C25	-2.49	120.20	127.20
13	R	1301	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	q	512	CLA	CHB-C4A-NA	2.49	127.96	124.51
16	Z	524	BCR	C8-C7-C6	-2.49	120.20	127.20
16	B	4014	BCR	C35-C13-C12	2.49	122.00	118.08
13	t	518	CLA	C3B-C4B-NB	-2.49	108.20	110.52
16	u	522	BCR	C23-C24-C25	-2.49	120.20	127.20
13	Y	518	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
13	f	1211	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
13	q	507	CLA	C2A-C1A-CHA	2.49	128.22	123.86
13	2	501	CLA	C3B-C4B-NB	-2.49	108.20	110.52
13	d	509	CLA	C3B-C4B-NB	-2.49	108.20	110.52
13	b	509	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
13	H	1212	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
16	K	4104	BCR	C28-C27-C26	-2.49	109.63	114.08
13	Y	512	CLA	CHB-C4A-NA	2.49	127.95	124.51
13	6	505	CLA	CHB-C4A-NA	2.49	127.95	124.51
13	4	518	CLA	C3B-C4B-NB	-2.49	108.21	110.52
16	r	524	BCR	C8-C7-C6	-2.49	120.21	127.20
16	U	4104	BCR	C30-C25-C24	2.49	122.82	115.78
16	f	4014	BCR	C35-C13-C12	2.49	122.00	118.08
13	H	1211	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
16	Z	522	BCR	C3-C4-C5	-2.49	109.64	114.08
13	H	1203	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
13	Z	519	CLA	CHB-C4A-NA	2.49	127.95	124.51
16	4	522	BCR	C1-C6-C5	-2.49	119.11	122.61
13	u	501	CLA	C3B-C4B-NB	-2.49	108.21	110.52
17	A	5008	LHG	O8-C23-C24	2.49	119.71	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	5001	LHG	O8-C23-C24	2.49	119.71	111.91
16	c	524	BCR	C33-C5-C4	2.49	118.39	113.62
17	G	5008	LHG	O8-C23-C24	2.48	119.71	111.91
13	1	518	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
13	r	501	CLA	C3B-C4B-NB	-2.48	108.21	110.52
13	e	1022	CLA	C2D-C1D-ND	-2.48	108.27	110.10
13	G	1134	CLA	CHD-C1D-ND	-2.48	122.17	124.45
16	5	524	BCR	C33-C5-C4	2.48	118.39	113.62
16	3	522	BCR	C38-C26-C25	-2.48	121.74	124.53
17	A	5007	LHG	O8-C23-C24	2.48	119.70	111.91
17	G	5007	LHG	O8-C23-C24	2.48	119.70	111.91
16	r	522	BCR	C11-C12-C13	-2.48	119.44	126.42
13	A	1120	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
16	2	522	BCR	C11-C12-C13	-2.48	119.44	126.42
13	e	1106	CLA	C1-C2-C3	-2.48	121.75	126.04
13	B	1023	CLA	CHB-C1B-NB	2.48	126.89	124.26
16	A	4011	BCR	C10-C11-C12	-2.48	115.47	123.22
16	u	524	BCR	C33-C5-C4	2.48	118.38	113.62
13	H	1023	CLA	CHB-C1B-NB	2.48	126.88	124.26
13	3	516	CLA	C3B-C4B-NB	-2.48	108.21	110.52
13	Z	509	CLA	C3B-C4B-NB	-2.48	108.21	110.52
16	U	4104	BCR	C28-C27-C26	-2.48	109.65	114.08
17	A	5001	LHG	O8-C23-C24	2.48	119.69	111.91
17	e	5007	LHG	O8-C23-C24	2.48	119.69	111.91
20	q	822	SQD	O48-C23-C24	2.48	119.69	111.91
13	1	511	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
13	3	506	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	G	5001	LHG	O8-C23-C24	2.48	119.69	111.91
13	q	511	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
16	3	522	BCR	C33-C5-C6	-2.48	121.74	124.53
13	A	1022	CLA	C2D-C1D-ND	-2.48	108.28	110.10
13	G	1022	CLA	C2D-C1D-ND	-2.48	108.28	110.10
13	e	1134	CLA	CHB-C4A-NA	2.48	127.94	124.51
16	e	4011	BCR	C10-C11-C12	-2.48	115.48	123.22
16	H	4014	BCR	C35-C13-C12	2.48	121.98	118.08
13	s	506	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	U	1105	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	Y	822	SQD	O48-C23-C24	2.48	119.68	111.91
13	b	506	CLA	C3B-C4B-NB	-2.48	108.22	110.52
13	1	507	CLA	C2A-C1A-CHA	2.48	128.19	123.86
20	6	822	SQD	O5-C5-C4	2.48	114.19	109.69
13	A	1134	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1114	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
16	c	524	BCR	C7-C8-C9	-2.48	122.49	126.23
20	1	822	SQD	O48-C23-C24	2.48	119.68	111.91
13	f	1239	CLA	CAC-C3C-C4C	-2.48	121.60	124.81
13	H	1216	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
13	f	1021	CLA	O1D-CGD-CBD	2.48	129.55	124.48
13	G	1134	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	f	1216	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
13	Z	501	CLA	C3B-C4B-NB	-2.47	108.22	110.52
13	G	1120	CLA	CMB-C2B-C1B	-2.47	121.60	125.37
17	A	5003	LHG	C20-C19-C18	-2.47	101.87	114.42
16	Z	522	BCR	C11-C12-C13	-2.47	119.47	126.42
16	u	523	BCR	C8-C7-C6	-2.47	120.25	127.20
13	e	1134	CLA	CHD-C1D-ND	-2.47	122.18	124.45
17	G	5003	LHG	C20-C19-C18	-2.47	101.87	114.42
17	e	5003	LHG	C20-C19-C18	-2.47	101.87	114.42
13	H	1021	CLA	O1D-CGD-CBD	2.47	129.54	124.48
13	r	519	CLA	CHB-C4A-NA	2.47	127.93	124.51
16	c	522	BCR	C23-C24-C25	-2.47	120.26	127.20
13	A	1123	CLA	C2A-C1A-CHA	2.47	128.18	123.86
13	e	1134	CLA	O2D-CGD-CBD	2.47	115.66	111.27
13	H	1222	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
13	a	506	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	Y	507	CLA	C2A-C1A-CHA	2.47	128.18	123.86
16	s	522	BCR	C38-C26-C27	2.47	118.36	113.62
13	Y	519	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	s	508	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	e	1120	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
13	B	1021	CLA	O1D-CGD-CBD	2.47	129.54	124.48
13	Z	511	CLA	C3B-C4B-NB	-2.47	108.22	110.52
13	A	1106	CLA	C1-C2-C3	-2.47	121.77	126.04
16	M	4021	BCR	C33-C5-C6	-2.47	121.75	124.53
13	3	508	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	e	5008	LHG	O8-C23-C24	2.47	119.66	111.91
16	a	522	BCR	C38-C26-C27	2.47	118.36	113.62
13	K	1105	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	V	5216	SQD	O5-C5-C4	2.47	114.17	109.69
16	s	522	BCR	C33-C5-C6	-2.47	121.76	124.53
20	d	822	SQD	O5-C5-C4	2.47	114.17	109.69
13	f	1023	CLA	CHB-C1B-NB	2.47	126.87	124.26
16	S	4018	BCR	C30-C25-C26	-2.47	119.14	122.61
19	f	5002	LMG	O1-C1-C2	-2.47	104.45	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1102	CLA	O2D-CGD-CBD	2.47	115.65	111.27
17	V	5220	LHG	C11-C10-C9	-2.47	101.91	114.42
16	3	522	BCR	C38-C26-C27	2.47	118.35	113.62
16	d	524	BCR	C38-C26-C25	-2.46	121.76	124.53
13	q	518	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
13	e	1123	CLA	C2A-C1A-CHA	2.46	128.17	123.86
13	d	512	CLA	CHB-C4A-NA	2.46	127.92	124.51
13	e	1102	CLA	O2D-CGD-CBD	2.46	115.65	111.27
13	u	507	CLA	C2A-C1A-CHA	2.46	128.17	123.86
16	o	4021	BCR	C33-C5-C6	-2.46	121.76	124.53
13	A	1134	CLA	O2D-CGD-CBD	2.46	115.65	111.27
16	b	524	BCR	C3-C4-C5	-2.46	109.68	114.08
13	G	1106	CLA	C1-C2-C3	-2.46	121.78	126.04
13	2	509	CLA	C3B-C4B-NB	-2.46	108.23	110.52
13	6	509	CLA	C3B-C4B-NB	-2.46	108.23	110.52
13	B	1235	CLA	C3B-C4B-NB	-2.46	108.23	110.52
17	L	5220	LHG	C11-C10-C9	-2.46	101.93	114.42
16	5	523	BCR	C8-C7-C6	-2.46	120.29	127.20
16	1	524	BCR	C21-C20-C19	-2.46	115.54	123.22
16	d	521	BCR	C20-C19-C18	-2.46	119.50	126.42
13	v	509	CLA	C3B-C4B-NB	-2.46	108.23	110.52
13	6	510	CLA	CHB-C4A-NA	2.46	127.92	124.51
13	B	1216	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
16	V	4019	BCR	C38-C26-C25	-2.46	121.77	124.53
20	L	5216	SQD	O5-C5-C4	2.46	114.16	109.69
16	c	523	BCR	C8-C7-C6	-2.46	120.29	127.20
13	e	1128	CLA	CMB-C2B-C3B	2.46	132.54	126.59
13	A	1111	CLA	CHB-C1B-NB	2.46	126.86	124.26
13	5	501	CLA	C3B-C4B-NB	-2.46	108.23	110.52
13	G	1132	CLA	C3B-C4B-NB	-2.46	108.23	110.52
17	n	5220	LHG	C11-C10-C9	-2.46	101.94	114.42
16	r	522	BCR	C3-C4-C5	-2.46	109.69	114.08
19	B	5002	LMG	O1-C1-C2	-2.46	104.47	108.30
13	A	1132	CLA	C3B-C4B-NB	-2.46	108.23	110.52
13	A	1114	CLA	CMB-C2B-C1B	-2.46	121.63	125.37
19	T	5104	LMG	O1-C1-C2	-2.46	104.47	108.30
16	6	521	BCR	C20-C19-C18	-2.46	119.51	126.42
13	G	1123	CLA	C2A-C1A-CHA	2.46	128.16	123.86
13	a	508	CLA	CHB-C4A-NA	2.46	127.91	124.51
17	G	5009	LHG	C11-C10-C9	-2.46	101.95	114.42
13	F	1301	CLA	CHB-C4A-NA	2.46	127.91	124.51
13	H	1206	CLA	CHC-C4B-NB	2.46	126.86	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	r	523	BCR	C21-C20-C19	-2.46	115.55	123.22
13	d	510	CLA	CHB-C4A-NA	2.46	127.91	124.51
16	5	521	BCR	C27-C26-C25	-2.45	119.17	122.73
13	A	1132	CLA	CHB-C4A-NA	2.45	127.91	124.51
13	G	1134	CLA	O2D-CGD-CBD	2.45	115.63	111.27
20	V	5216	SQD	C44-O6-C1	2.45	118.53	113.74
17	A	5009	LHG	C11-C10-C9	-2.45	101.97	114.42
19	H	5002	LMG	O1-C1-C2	-2.45	104.47	108.30
13	G	1102	CLA	O2D-CGD-CBD	2.45	115.63	111.27
20	n	5216	SQD	C44-O6-C1	2.45	118.53	113.74
16	q	524	BCR	C21-C20-C19	-2.45	115.56	123.22
16	G	4003	BCR	C38-C26-C25	-2.45	121.77	124.53
19	J	5104	LMG	O1-C1-C2	-2.45	104.47	108.30
17	A	5003	LHG	O8-C23-C24	2.45	119.60	111.91
16	W	4021	BCR	C33-C5-C6	-2.45	121.78	124.53
16	n	4019	BCR	C38-C26-C25	-2.45	121.78	124.53
16	I	4018	BCR	C30-C25-C26	-2.45	119.16	122.61
20	n	5216	SQD	O5-C5-C4	2.45	114.14	109.69
18	B	1843	LMU	C1B-O1B-C4'	-2.45	111.90	117.96
13	e	1114	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
13	b	511	CLA	C3B-C4B-NB	-2.45	108.24	110.52
13	s	516	CLA	C3B-C4B-NB	-2.45	108.24	110.52
17	V	5220	LHG	O8-C23-C24	2.45	119.60	111.91
16	Z	523	BCR	C21-C20-C19	-2.45	115.57	123.22
13	6	508	CLA	CHB-C1B-NB	2.45	126.85	124.26
20	v	822	SQD	O5-C5-C4	2.45	114.14	109.69
16	6	524	BCR	C38-C26-C25	-2.45	121.78	124.53
17	G	5003	LHG	O8-C23-C24	2.45	119.59	111.91
13	c	507	CLA	C2A-C1A-CHA	2.45	128.14	123.86
16	2	523	BCR	C21-C20-C19	-2.45	115.58	123.22
16	L	4019	BCR	C38-C26-C25	-2.45	121.78	124.53
13	H	1236	CLA	C3B-C4B-NB	-2.45	108.24	110.52
13	c	501	CLA	C3B-C4B-NB	-2.45	108.24	110.52
16	Y	524	BCR	C21-C20-C19	-2.45	115.58	123.22
14	e	2001	PQN	C2M-C2-C3	-2.45	120.41	124.40
13	c	517	CLA	CHB-C4A-NA	2.45	127.90	124.51
14	A	2001	PQN	C2M-C2-C3	-2.45	120.41	124.40
16	5	524	BCR	C7-C8-C9	-2.45	122.54	126.23
13	5	517	CLA	CHB-C4A-NA	2.45	127.89	124.51
17	e	5003	LHG	O8-C23-C24	2.45	119.58	111.91
13	A	1114	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
18	f	1843	LMU	C1B-O1B-C4'	-2.45	111.91	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	5009	LHG	C11-C10-C9	-2.44	102.01	114.42
13	A	1111	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
16	t	524	BCR	C3-C4-C5	-2.44	109.71	114.08
13	G	1128	CLA	CMB-C2B-C3B	2.44	132.51	126.59
13	f	1239	CLA	CAC-C3C-C2C	2.44	131.71	127.53
18	H	1843	LMU	C1B-O1B-C4'	-2.44	111.92	117.96
16	r	524	BCR	C21-C20-C19	-2.44	115.59	123.22
16	v	521	BCR	C20-C19-C18	-2.44	119.55	126.42
13	e	1120	CLA	C3B-C4B-NB	-2.44	108.25	110.52
13	A	1128	CLA	CMB-C2B-C3B	2.44	132.50	126.59
20	V	5216	SQD	O48-C23-C24	2.44	119.57	111.91
19	l	5104	LMG	O1-C1-C2	-2.44	104.49	108.30
16	c	521	BCR	C27-C26-C25	-2.44	119.19	122.73
13	G	1114	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
13	G	1111	CLA	CHB-C1B-NB	2.44	126.84	124.26
20	n	5216	SQD	O48-C23-C24	2.44	119.57	111.91
16	B	4009	BCR	C10-C11-C12	-2.44	115.60	123.22
13	H	1229	CLA	C3B-C4B-NB	-2.44	108.25	110.52
16	n	4020	BCR	C31-C1-C6	-2.44	106.34	110.30
13	v	510	CLA	CHB-C4A-NA	2.44	127.89	124.51
13	d	508	CLA	CHB-C1B-NB	2.44	126.84	124.26
16	4	524	BCR	C3-C4-C5	-2.44	109.72	114.08
13	s	504	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
16	2	524	BCR	C21-C20-C19	-2.44	115.61	123.22
13	r	518	CLA	C3B-C4B-NB	-2.44	108.25	110.52
16	v	524	BCR	C38-C26-C25	-2.44	121.79	124.53
16	Z	524	BCR	C21-C20-C19	-2.44	115.61	123.22
13	H	1213	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
16	u	521	BCR	C27-C26-C25	-2.44	119.19	122.73
13	G	1111	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
13	f	1210	CLA	C1-C2-C3	-2.44	121.83	126.04
13	e	1132	CLA	CHB-C4A-NA	2.44	127.88	124.51
13	u	517	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	L	5218	LHG	C11-C10-C9	-2.44	102.06	114.42
16	u	524	BCR	C7-C8-C9	-2.44	122.56	126.23
16	L	4020	BCR	C31-C1-C6	-2.44	106.35	110.30
17	L	5220	LHG	O8-C23-C24	2.43	119.55	111.91
13	e	1124	CLA	CMB-C2B-C1B	-2.43	121.66	125.37
16	r	524	BCR	C37-C22-C23	2.43	121.91	118.08
13	5	507	CLA	C2A-C1A-CHA	2.43	128.12	123.86
13	e	1132	CLA	C3B-C4B-NB	-2.43	108.26	110.52
13	t	511	CLA	C3B-C4B-NB	-2.43	108.26	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	2001	PQN	C2M-C2-C3	-2.43	120.43	124.40
16	A	4003	BCR	C24-C23-C22	-2.43	122.56	126.23
17	e	5009	LHG	O8-C23-C24	2.43	119.54	111.91
13	H	1217	CLA	O2D-CGD-CBD	2.43	115.59	111.27
13	B	1217	CLA	O2D-CGD-CBD	2.43	115.59	111.27
13	K	1103	CLA	C5-C3-C4	2.43	119.97	114.60
16	k	4018	BCR	C30-C25-C26	-2.43	119.19	122.61
13	v	512	CLA	CHB-C4A-NA	2.43	127.88	124.51
17	H	1842	LHG	C11-C10-C9	-2.43	102.08	114.42
20	L	5216	SQD	C44-O6-C1	2.43	118.49	113.74
20	5	822	SQD	C4-C3-C2	2.43	115.07	110.82
17	n	5218	LHG	C11-C10-C9	-2.43	102.08	114.42
17	A	5009	LHG	O8-C23-C24	2.43	119.54	111.91
13	B	1213	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
13	5	508	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
13	f	1213	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
13	G	1114	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
13	B	1239	CLA	CAC-C3C-C2C	2.43	131.69	127.53
13	A	1122	CLA	C3B-C4B-NB	-2.43	108.26	110.52
13	H	1220	CLA	C3B-C4B-NB	-2.43	108.26	110.52
13	c	516	CLA	C3B-C4B-NB	-2.43	108.26	110.52
13	U	1103	CLA	C5-C3-C4	2.43	119.97	114.60
13	6	512	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	V	5218	LHG	C11-C10-C9	-2.43	102.09	114.42
17	G	5009	LHG	O8-C23-C24	2.43	119.53	111.91
13	B	1238	CLA	CHD-C1D-ND	-2.43	122.22	124.45
13	H	1239	CLA	CAC-C3C-C2C	2.43	131.69	127.53
13	H	1210	CLA	C1-C2-C3	-2.43	121.84	126.04
20	L	5216	SQD	O48-C23-C24	2.43	119.53	111.91
13	e	1117	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
17	B	1842	LHG	C11-C10-C9	-2.43	102.09	114.42
13	B	1210	CLA	C1-C2-C3	-2.43	121.84	126.04
13	m	1105	CLA	CHB-C4A-NA	2.43	127.87	124.51
13	H	1239	CLA	CMC-C2C-C3C	2.43	132.71	126.12
17	n	5220	LHG	O8-C23-C24	2.43	119.53	111.91
17	f	1842	LHG	C11-C10-C9	-2.43	102.10	114.42
16	V	4020	BCR	C31-C1-C6	-2.43	106.36	110.30
13	f	1206	CLA	CHC-C4B-NB	2.43	126.83	124.26
13	e	1111	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
16	f	4009	BCR	C10-C11-C12	-2.43	115.64	123.22
13	G	1136	CLA	CHD-C1D-ND	-2.43	122.22	124.45
13	A	1117	CLA	CMB-C2B-C1B	-2.43	121.67	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1124	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
13	f	1217	CLA	O2D-CGD-CBD	2.42	115.58	111.27
13	B	1206	CLA	CHC-C4B-NB	2.42	126.82	124.26
16	G	4003	BCR	C24-C23-C22	-2.42	122.57	126.23
13	G	1132	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	f	1236	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	u	508	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
13	G	1127	CLA	C1-C2-C3	-2.42	121.85	126.04
13	4	511	CLA	C3B-C4B-NB	-2.42	108.27	110.52
20	u	822	SQD	C4-C3-C2	2.42	115.05	110.82
13	G	1117	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
16	n	4022	BCR	C33-C5-C4	2.42	118.27	113.62
16	H	4009	BCR	C10-C11-C12	-2.42	115.66	123.22
16	G	4007	BCR	C29-C30-C25	2.42	114.21	110.48
17	S	5001	LHG	C11-C10-C9	-2.42	102.13	114.42
16	t	521	BCR	C33-C5-C6	-2.42	121.81	124.53
13	e	1111	CLA	CHB-C1B-NB	2.42	126.82	124.26
13	b	503	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
20	a	822	SQD	C4-C3-C2	2.42	115.05	110.82
13	H	1235	CLA	C3B-C4B-NB	-2.42	108.27	110.52
17	k	5001	LHG	C11-C10-C9	-2.42	102.14	114.42
13	A	1124	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	j	1301	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	B	1239	CLA	CMC-C2C-C3C	2.42	132.68	126.12
13	B	1229	CLA	C3B-C4B-NB	-2.42	108.27	110.52
17	I	5001	LHG	C11-C10-C9	-2.42	102.15	114.42
16	4	521	BCR	C33-C5-C6	-2.42	121.81	124.53
16	b	521	BCR	C33-C5-C6	-2.42	121.81	124.53
13	m	1103	CLA	C5-C3-C4	2.42	119.94	114.60
16	e	4007	BCR	C29-C30-C25	2.42	114.20	110.48
20	s	822	SQD	C4-C3-C2	2.42	115.04	110.82
13	H	1238	CLA	CHB-C4A-NA	2.42	127.86	124.51
20	3	822	SQD	C4-C3-C2	2.42	115.04	110.82
13	A	1112	CLA	CHB-C1B-NB	2.42	126.82	124.26
13	G	1011	CLA	CHC-C4B-NB	2.42	126.82	124.26
16	A	4007	BCR	C29-C30-C25	2.42	114.20	110.48
16	A	4007	BCR	C33-C5-C4	2.42	118.26	113.62
16	Z	522	BCR	C38-C26-C25	-2.42	121.81	124.53
13	r	509	CLA	C3B-C4B-NB	-2.42	108.27	110.52
16	e	4003	BCR	C24-C23-C22	-2.42	122.58	126.23
13	G	1107	CLA	CHB-C4A-NA	2.41	127.85	124.51
16	e	4007	BCR	C33-C5-C4	2.41	118.25	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	5004	LHG	C11-C10-C9	-2.41	102.17	114.42
13	4	503	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
13	b	509	CLA	C2A-C1A-CHA	2.41	128.08	123.86
17	G	5004	LHG	C11-C10-C9	-2.41	102.17	114.42
13	3	504	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
13	5	516	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	f	1235	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	f	1239	CLA	CMC-C2C-C3C	2.41	132.67	126.12
17	A	5004	LHG	C11-C10-C9	-2.41	102.18	114.42
17	A	5005	LHG	O8-C23-C24	2.41	119.48	111.91
13	e	1104	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	a	504	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
16	Y	522	BCR	C15-C16-C17	-2.41	118.53	123.47
16	2	522	BCR	C38-C26-C25	-2.41	121.82	124.53
13	H	1227	CLA	CHD-C1D-ND	-2.41	122.24	124.45
13	B	1236	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	v	508	CLA	CHB-C1B-NB	2.41	126.81	124.26
13	B	1023	CLA	CAC-C3C-C2C	-2.41	123.41	127.53
13	f	1226	CLA	C3B-C2B-C1B	2.41	110.07	107.16
16	Z	524	BCR	C20-C21-C22	-2.41	123.87	127.31
17	G	5005	LHG	O8-C23-C24	2.41	119.47	111.91
16	1	522	BCR	C15-C16-C17	-2.41	118.54	123.47
16	r	522	BCR	C38-C26-C25	-2.41	121.82	124.53
13	G	1124	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
13	e	1137	CLA	CHB-C1B-NB	2.41	126.81	124.26
13	f	1023	CLA	CAC-C3C-C2C	-2.41	123.41	127.53
20	c	822	SQD	C4-C3-C2	2.41	115.03	110.82
13	c	508	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
13	f	1238	CLA	CHD-C1D-ND	-2.41	122.24	124.45
13	A	1137	CLA	CHB-C1B-NB	2.41	126.81	124.26
13	1	513	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	A	1136	CLA	CHD-C1D-ND	-2.41	122.24	124.45
13	G	1129	CLA	C2D-C1D-ND	-2.41	108.33	110.10
13	Y	519	CLA	CHC-C4B-NB	2.41	126.80	124.26
13	B	1236	CLA	CHB-C4A-NA	2.41	127.84	124.51
13	G	1124	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	e	5005	LHG	O8-C23-C24	2.41	119.45	111.91
16	H	4010	BCR	C38-C26-C27	2.40	118.24	113.62
13	q	513	CLA	C3B-C4B-NB	-2.40	108.28	110.52
13	q	516	CLA	CHB-C4A-NA	2.40	127.84	124.51
16	G	4007	BCR	C33-C5-C4	2.40	118.23	113.62
17	A	5007	LHG	C11-C10-C9	-2.40	102.22	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	519	CLA	CHC-C4B-NB	2.40	126.80	124.26
13	H	1236	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	H	1226	CLA	C3B-C2B-C1B	2.40	110.06	107.16
16	r	522	BCR	C1-C6-C5	-2.40	119.23	122.61
16	2	524	BCR	C20-C21-C22	-2.40	123.88	127.31
13	e	1127	CLA	C1-C2-C3	-2.40	121.89	126.04
17	G	5007	LHG	C11-C10-C9	-2.40	102.24	114.42
16	L	4022	BCR	C33-C5-C4	2.40	118.23	113.62
13	H	1238	CLA	CHD-C1D-ND	-2.40	122.25	124.45
13	4	509	CLA	C2A-C1A-CHA	2.40	128.06	123.86
16	e	4011	BCR	C15-C16-C17	-2.40	118.56	123.47
13	H	1023	CLA	CAC-C3C-C2C	-2.40	123.42	127.53
17	e	5007	LHG	C11-C10-C9	-2.40	102.24	114.42
13	G	1011	CLA	C4D-C3D-CAD	-2.40	105.27	108.10
13	B	1226	CLA	C3B-C2B-C1B	2.40	110.06	107.16
16	r	522	BCR	C38-C26-C27	2.40	118.22	113.62
13	2	518	CLA	C3B-C4B-NB	-2.40	108.29	110.52
13	6	511	CLA	C3B-C4B-NB	-2.40	108.29	110.52
13	G	1122	CLA	C3B-C4B-NB	-2.40	108.29	110.52
13	m	1105	CLA	C2D-C1D-ND	-2.40	108.34	110.10
13	e	1011	CLA	C4D-C3D-CAD	-2.40	105.27	108.10
16	B	4010	BCR	C38-C26-C27	2.40	118.22	113.62
13	e	1112	CLA	CHB-C1B-NB	2.40	126.80	124.26
13	t	509	CLA	C2A-C1A-CHA	2.40	128.05	123.86
13	e	1136	CLA	CHD-C1D-ND	-2.40	122.25	124.45
13	t	503	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
16	Z	522	BCR	C38-C26-C27	2.40	118.22	113.62
13	q	516	CLA	C3B-C4B-NB	-2.40	108.29	110.52
13	f	1227	CLA	CHD-C1D-ND	-2.40	122.25	124.45
16	q	522	BCR	C15-C16-C17	-2.40	118.57	123.47
13	A	1127	CLA	C1-C2-C3	-2.40	121.90	126.04
13	Y	513	CLA	C3B-C4B-NB	-2.40	108.29	110.52
13	e	1124	CLA	CHB-C4A-NA	2.40	127.82	124.51
13	B	1227	CLA	CHD-C1D-ND	-2.40	122.25	124.45
13	1	516	CLA	CHB-C4A-NA	2.39	127.82	124.51
16	2	524	BCR	C37-C22-C23	2.39	121.85	118.08
13	G	1112	CLA	CHB-C1B-NB	2.39	126.79	124.26
13	e	1140	CLA	CBA-CAA-C2A	2.39	120.93	113.86
16	f	4006	BCR	C3-C4-C5	-2.39	109.80	114.08
13	6	501	CLA	C3B-C4B-NB	-2.39	108.30	110.52
13	d	501	CLA	C3B-C4B-NB	-2.39	108.30	110.52
13	r	505	CLA	C1-C2-C3	-2.39	121.91	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	2	522	BCR	C38-C26-C27	2.39	118.21	113.62
16	q	523	BCR	C20-C21-C22	-2.39	123.90	127.31
16	5	523	BCR	C33-C5-C4	2.39	118.21	113.62
16	4	522	BCR	C36-C18-C19	2.39	121.84	118.08
16	b	522	BCR	C36-C18-C19	2.39	121.84	118.08
16	R	4016	BCR	C33-C5-C6	-2.39	121.84	124.53
13	A	1140	CLA	CBA-CAA-C2A	2.39	120.92	113.86
16	Y	522	BCR	C16-C17-C18	-2.39	123.90	127.31
13	f	1229	CLA	C3B-C4B-NB	-2.39	108.30	110.52
20	d	822	SQD	C45-O47-C7	2.39	122.35	117.90
13	H	1231	CLA	CMB-C2B-C3B	2.39	132.37	126.59
13	f	1220	CLA	C3B-C4B-NB	-2.39	108.30	110.52
13	A	1120	CLA	C3B-C4B-NB	-2.39	108.30	110.52
13	v	508	CLA	C3B-C4B-NB	-2.39	108.30	110.52
13	B	1238	CLA	CHB-C4A-NA	2.39	127.81	124.51
16	v	523	BCR	C21-C20-C19	-2.39	115.77	123.22
13	B	1231	CLA	CMB-C2B-C3B	2.39	132.37	126.59
16	2	522	BCR	C1-C6-C5	-2.39	119.25	122.61
16	G	4007	BCR	C30-C25-C26	-2.39	119.25	122.61
16	e	4007	BCR	C30-C25-C26	-2.39	119.25	122.61
16	F	4016	BCR	C33-C5-C6	-2.38	121.85	124.53
13	q	506	CLA	CMB-C2B-C3B	2.38	132.36	126.59
13	e	1125	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
16	6	523	BCR	C21-C20-C19	-2.38	115.78	123.22
16	B	4006	BCR	C3-C4-C5	-2.38	109.82	114.08
13	e	1107	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
13	Y	516	CLA	C3B-C4B-NB	-2.38	108.30	110.52
13	A	1011	CLA	CHC-C4B-NB	2.38	126.78	124.26
16	V	4022	BCR	C33-C5-C4	2.38	118.19	113.62
16	f	4009	BCR	C29-C30-C25	2.38	114.15	110.48
16	u	523	BCR	C33-C5-C4	2.38	118.19	113.62
13	B	1220	CLA	C3B-C4B-NB	-2.38	108.31	110.52
13	e	1237	CLA	CHB-C4A-NA	2.38	127.81	124.51
16	B	4009	BCR	C29-C30-C25	2.38	114.15	110.48
13	d	508	CLA	C3B-C4B-NB	-2.38	108.31	110.52
16	r	524	BCR	C20-C21-C22	-2.38	123.91	127.31
16	c	523	BCR	C33-C5-C4	2.38	118.19	113.62
13	A	1123	CLA	CMB-C2B-C3B	2.38	132.35	126.59
16	H	4006	BCR	C3-C4-C5	-2.38	109.83	114.08
13	1	516	CLA	C3B-C4B-NB	-2.38	108.31	110.52
13	e	1122	CLA	C3B-C4B-NB	-2.38	108.31	110.52
13	v	511	CLA	C3B-C4B-NB	-2.38	108.31	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1140	CLA	CBA-CAA-C2A	2.38	120.89	113.86
13	G	1123	CLA	CMB-C2B-C3B	2.38	132.35	126.59
16	d	523	BCR	C21-C20-C19	-2.38	115.79	123.22
16	t	522	BCR	C36-C18-C19	2.38	121.83	118.08
13	u	516	CLA	C3B-C4B-NB	-2.38	108.31	110.52
20	6	822	SQD	C45-O47-C7	2.38	122.33	117.90
13	e	1105	CLA	CMB-C2B-C3B	2.38	132.35	126.59
13	A	1107	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	G	1125	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
16	3	523	BCR	C8-C7-C6	-2.38	120.53	127.20
13	Z	518	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
13	A	1104	CLA	C3B-C4B-NB	-2.38	108.31	110.52
13	G	1126	CLA	C2A-C1A-CHA	2.38	128.01	123.86
13	e	1123	CLA	CMB-C2B-C3B	2.38	132.34	126.59
13	r	507	CLA	C3B-C4B-NB	-2.38	108.31	110.52
20	v	822	SQD	C45-O47-C7	2.38	122.32	117.90
16	f	4006	BCR	C1-C6-C5	-2.38	119.27	122.61
13	A	1237	CLA	CHB-C4A-NA	2.37	127.80	124.51
13	G	1120	CLA	C3B-C4B-NB	-2.37	108.31	110.52
13	G	1107	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
16	s	523	BCR	C8-C7-C6	-2.37	120.53	127.20
16	A	4011	BCR	C15-C16-C17	-2.37	118.61	123.47
16	a	523	BCR	C8-C7-C6	-2.37	120.53	127.20
13	A	1011	CLA	C4D-C3D-CAD	-2.37	105.30	108.10
13	A	1126	CLA	C2A-C1A-CHA	2.37	128.01	123.86
16	Z	524	BCR	C37-C22-C23	2.37	121.82	118.08
13	1	506	CLA	CMB-C2B-C3B	2.37	132.34	126.59
13	f	1236	CLA	C3B-C4B-NB	-2.37	108.31	110.52
16	G	4011	BCR	C15-C16-C17	-2.37	118.61	123.47
19	f	5002	LMG	C38-C37-C36	-2.37	102.38	114.42
16	H	4006	BCR	C1-C6-C5	-2.37	119.27	122.61
16	r	522	BCR	C15-C16-C17	-2.37	118.61	123.47
16	G	4002	BCR	C38-C26-C27	2.37	118.17	113.62
16	V	4219	BCR	C20-C21-C22	-2.37	123.92	127.31
13	e	1129	CLA	O2D-CGD-CBD	2.37	115.48	111.27
13	A	1105	CLA	CMB-C2B-C3B	2.37	132.33	126.59
19	B	5002	LMG	C38-C37-C36	-2.37	102.39	114.42
13	Z	507	CLA	C3B-C4B-NB	-2.37	108.31	110.52
13	r	503	CLA	C3B-C4B-NB	-2.37	108.31	110.52
16	B	4006	BCR	C1-C6-C5	-2.37	119.27	122.61
13	B	1211	CLA	CMB-C2B-C3B	2.37	132.33	126.59
16	1	522	BCR	C16-C17-C18	-2.37	123.93	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4009	BCR	C29-C30-C25	2.37	114.13	110.48
13	G	1105	CLA	CMB-C2B-C3B	2.37	132.33	126.59
13	G	1129	CLA	O2D-CGD-CBD	2.37	115.48	111.27
16	Z	522	BCR	C15-C16-C17	-2.37	118.62	123.47
16	e	4007	BCR	C4-C5-C6	-2.37	119.29	122.73
13	f	1211	CLA	CMB-C2B-C3B	2.37	132.33	126.59
13	e	1107	CLA	CHB-C4A-NA	2.37	127.79	124.51
16	f	4010	BCR	C38-C26-C27	2.37	118.17	113.62
13	r	518	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
13	2	505	CLA	C1-C2-C3	-2.37	121.95	126.04
13	H	1211	CLA	CMB-C2B-C3B	2.37	132.32	126.59
16	1	523	BCR	C34-C9-C8	2.37	121.81	118.08
16	A	4007	BCR	C4-C5-C6	-2.37	119.29	122.73
13	Y	506	CLA	CMB-C2B-C3B	2.37	132.32	126.59
13	f	1231	CLA	CMB-C2B-C3B	2.37	132.32	126.59
13	Z	505	CLA	C1-C2-C3	-2.37	121.95	126.04
13	A	1129	CLA	O2D-CGD-CBD	2.37	115.47	111.27
13	A	1107	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
13	B	1231	CLA	CMA-C3A-C2A	-2.37	104.28	113.83
13	B	1209	CLA	CHB-C1B-NB	2.37	126.76	124.26
19	l	5104	LMG	C6-C5-C4	-2.37	107.46	113.00
16	Y	523	BCR	C34-C9-C8	2.37	121.81	118.08
13	K	1105	CLA	C2D-C1D-ND	-2.37	108.36	110.10
13	e	1110	CLA	CHB-C1B-NB	2.37	126.76	124.26
13	e	1126	CLA	C2A-C1A-CHA	2.37	128.00	123.86
13	d	504	CLA	CMB-C2B-C1B	-2.37	121.77	125.37
16	A	4007	BCR	C30-C25-C26	-2.37	119.28	122.61
19	J	5104	LMG	C6-C5-C4	-2.37	107.46	113.00
13	f	1231	CLA	CMA-C3A-C2A	-2.37	104.29	113.83
13	A	1129	CLA	C2D-C1D-ND	-2.37	108.36	110.10
19	H	5002	LMG	C38-C37-C36	-2.36	102.42	114.42
13	f	1236	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
13	f	1238	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	c	517	CLA	C3B-C4B-NB	-2.36	108.32	110.52
16	e	4002	BCR	C38-C26-C27	2.36	118.15	113.62
16	q	522	BCR	C16-C17-C18	-2.36	123.94	127.31
13	6	508	CLA	C3B-C4B-NB	-2.36	108.32	110.52
13	d	511	CLA	C3B-C4B-NB	-2.36	108.32	110.52
13	G	1137	CLA	CHB-C1B-NB	2.36	126.76	124.26
13	5	509	CLA	CMB-C2B-C3B	2.36	132.31	126.59
13	f	1234	CLA	CAC-C3C-C4C	2.36	127.87	124.81
13	A	1125	CLA	CMB-C2B-C1B	-2.36	121.77	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	516	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	Z	518	CLA	C3B-C4B-NB	-2.36	108.33	110.52
13	G	1801	CLA	CMB-C2B-C3B	2.36	132.30	126.59
13	2	503	CLA	C3B-C4B-NB	-2.36	108.33	110.52
13	B	1222	CLA	CMB-C2B-C3B	2.36	132.30	126.59
13	G	1237	CLA	CHB-C4A-NA	2.36	127.77	124.51
13	f	1209	CLA	CHB-C1B-NB	2.36	126.75	124.26
13	H	1235	CLA	O2D-CGD-CBD	2.36	115.46	111.27
13	H	1231	CLA	CMA-C3A-C2A	-2.36	104.32	113.83
13	q	519	CLA	CHC-C4B-NB	2.36	126.75	124.26
13	c	509	CLA	CMB-C2B-C3B	2.36	132.30	126.59
13	u	509	CLA	CMB-C2B-C3B	2.36	132.30	126.59
13	Z	501	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
13	f	1204	CLA	C3B-C4B-NB	-2.36	108.33	110.52
16	j	4016	BCR	C33-C5-C6	-2.36	121.88	124.53
13	A	1801	CLA	CMB-C2B-C3B	2.36	132.29	126.59
20	s	822	SQD	C1-O5-C5	2.36	118.31	113.69
16	T	4012	BCR	C2-C1-C6	2.36	114.11	110.48
13	5	517	CLA	C3B-C4B-NB	-2.36	108.33	110.52
13	v	501	CLA	C3B-C4B-NB	-2.36	108.33	110.52
13	2	518	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
19	T	5104	LMG	C6-C5-C4	-2.35	107.49	113.00
13	f	1222	CLA	CMB-C2B-C3B	2.35	132.29	126.59
13	H	1209	CLA	CHB-C1B-NB	2.35	126.75	124.26
16	Z	522	BCR	C1-C6-C5	-2.35	119.30	122.61
16	e	4003	BCR	C21-C20-C19	-2.35	115.87	123.22
16	2	522	BCR	C15-C16-C17	-2.35	118.65	123.47
13	B	1236	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
16	L	4219	BCR	C20-C21-C22	-2.35	123.95	127.31
16	e	4003	BCR	C11-C10-C9	-2.35	123.95	127.31
16	A	4008	BCR	C34-C9-C8	2.35	121.78	118.08
13	e	1108	CLA	CHB-C1B-NB	2.35	126.75	124.26
16	c	524	BCR	C10-C11-C12	-2.35	115.88	123.22
13	r	501	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
16	l	4012	BCR	C2-C1-C6	2.35	114.10	110.48
13	H	1236	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
16	B	4006	BCR	C33-C5-C4	2.35	118.13	113.62
16	n	4219	BCR	C20-C21-C22	-2.35	123.96	127.31
13	A	1110	CLA	CHB-C1B-NB	2.35	126.74	124.26
13	e	1011	CLA	CHC-C4B-NB	2.35	126.74	124.26
13	b	510	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
13	2	501	CLA	CAA-C2A-C3A	-2.35	106.35	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4006	BCR	C33-C5-C4	2.35	118.13	113.62
13	6	504	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
16	A	4002	BCR	C38-C26-C27	2.35	118.13	113.62
16	G	4007	BCR	C4-C5-C6	-2.35	119.32	122.73
16	j	4016	BCR	C21-C20-C19	-2.35	115.89	123.22
16	q	523	BCR	C34-C9-C8	2.35	121.77	118.08
13	H	1208	CLA	CHC-C4B-NB	2.35	126.74	124.26
16	u	524	BCR	C10-C11-C12	-2.35	115.89	123.22
19	B	5002	LMG	C40-C39-C38	-2.35	102.52	114.42
16	f	4006	BCR	C33-C5-C4	2.35	118.12	113.62
13	H	1202	CLA	O2D-CGD-CBD	2.35	115.44	111.27
16	Z	524	BCR	C15-C16-C17	-2.35	118.67	123.47
16	H	4009	BCR	C37-C22-C23	2.35	121.77	118.08
16	R	4016	BCR	C21-C20-C19	-2.34	115.90	123.22
16	e	4008	BCR	C34-C9-C8	2.34	121.77	118.08
13	f	1222	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	H	5002	LMG	C40-C39-C38	-2.34	102.52	114.42
17	e	5006	LHG	O8-C23-C24	2.34	119.26	111.91
16	H	4010	BCR	C23-C24-C25	-2.34	120.62	127.20
19	f	5002	LMG	C40-C39-C38	-2.34	102.53	114.42
16	A	4003	BCR	C21-C20-C19	-2.34	115.91	123.22
16	f	4005	BCR	C15-C16-C17	-2.34	118.67	123.47
13	H	1222	CLA	CMB-C2B-C3B	2.34	132.26	126.59
16	f	4010	BCR	C23-C24-C25	-2.34	120.62	127.20
19	T	5104	LMG	O2-C2-C1	-2.34	104.36	110.05
13	G	1104	CLA	C3B-C4B-NB	-2.34	108.34	110.52
13	e	1801	CLA	CMB-C2B-C3B	2.34	132.26	126.59
13	B	1202	CLA	O2D-CGD-CBD	2.34	115.43	111.27
16	5	524	BCR	C10-C11-C12	-2.34	115.91	123.22
13	H	1215	CLA	C3B-C4B-NB	-2.34	108.34	110.52
13	H	1222	CLA	CHB-C4A-NA	2.34	127.75	124.51
16	H	4004	BCR	C15-C16-C17	-2.34	118.68	123.47
17	A	5006	LHG	O8-C23-C24	2.34	119.25	111.91
16	F	4016	BCR	C21-C20-C19	-2.34	115.92	123.22
13	U	1105	CLA	C2D-C1D-ND	-2.34	108.38	110.10
13	H	1234	CLA	CAC-C3C-C4C	2.34	127.84	124.81
16	Y	523	BCR	C20-C21-C22	-2.34	123.97	127.31
16	2	524	BCR	C15-C16-C17	-2.34	118.68	123.47
16	B	4009	BCR	C37-C22-C23	2.34	121.76	118.08
13	4	510	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
13	B	1234	CLA	CAC-C3C-C4C	2.34	127.84	124.81
13	f	1235	CLA	O2D-CGD-CBD	2.34	115.42	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	502	CLA	C3B-C4B-NB	-2.34	108.35	110.52
13	4	517	CLA	C3B-C4B-NB	-2.34	108.35	110.52
13	Z	503	CLA	C3B-C4B-NB	-2.34	108.35	110.52
16	G	4003	BCR	C21-C20-C19	-2.34	115.92	123.22
16	f	4009	BCR	C36-C18-C19	2.34	121.76	118.08
16	J	4012	BCR	C2-C1-C6	2.34	114.08	110.48
16	4	521	BCR	C29-C30-C25	2.34	114.08	110.48
16	B	4010	BCR	C23-C24-C25	-2.34	120.64	127.20
13	e	1124	CLA	CHB-C1B-NB	2.34	126.73	124.26
16	r	522	BCR	C33-C5-C4	2.34	118.10	113.62
13	H	1226	CLA	C2B-C1B-NB	-2.34	108.67	110.23
16	b	521	BCR	C29-C30-C25	2.34	114.08	110.48
13	B	1222	CLA	CHB-C4A-NA	2.34	127.74	124.51
16	d	522	BCR	C30-C25-C26	-2.34	119.32	122.61
13	G	1110	CLA	CHB-C1B-NB	2.34	126.73	124.26
13	v	504	CLA	CMB-C2B-C1B	-2.33	121.81	125.37
16	1	523	BCR	C20-C21-C22	-2.33	123.98	127.31
16	H	4005	BCR	C15-C16-C17	-2.33	118.69	123.47
16	G	4008	BCR	C34-C9-C8	2.33	121.75	118.08
16	f	4010	BCR	C36-C18-C19	2.33	121.75	118.08
16	l	4012	BCR	C28-C27-C26	-2.33	109.91	114.08
16	B	4005	BCR	C15-C16-C17	-2.33	118.69	123.47
16	Z	522	BCR	C33-C5-C4	2.33	118.10	113.62
13	e	1130	CLA	CMB-C2B-C3B	2.33	132.24	126.59
13	B	1235	CLA	O2D-CGD-CBD	2.33	115.41	111.27
16	B	4004	BCR	C15-C16-C17	-2.33	118.70	123.47
20	3	822	SQD	C1-O5-C5	2.33	118.27	113.69
13	Z	509	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
13	q	508	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
13	t	510	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
16	b	522	BCR	C33-C5-C4	2.33	118.09	113.62
13	a	509	CLA	C3B-C4B-NB	-2.33	108.35	110.52
16	H	4009	BCR	C36-C18-C19	2.33	121.75	118.08
13	e	1129	CLA	C2D-C1D-ND	-2.33	108.39	110.10
16	u	522	BCR	C3-C4-C5	-2.33	109.92	114.08
19	J	5104	LMG	O2-C2-C1	-2.33	104.39	110.05
13	A	1125	CLA	CAA-CBA-CGA	-2.33	106.45	113.25
13	A	1118	CLA	O2D-CGD-CBD	2.33	115.41	111.27
13	1	518	CLA	CHB-C1B-NB	2.33	126.72	124.26
16	f	4009	BCR	C37-C22-C23	2.33	121.75	118.08
16	t	522	BCR	C33-C5-C4	2.33	118.09	113.62
13	G	1118	CLA	O2D-CGD-CBD	2.33	115.40	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1108	CLA	CHB-C1B-NB	2.33	126.72	124.26
13	G	1124	CLA	C3C-C4C-NC	-2.33	107.96	110.57
13	2	503	CLA	CMB-C2B-C1B	-2.33	121.83	125.37
16	t	524	BCR	C1-C6-C7	2.33	122.36	115.78
16	A	4007	BCR	C2-C1-C6	2.33	114.06	110.48
16	e	4007	BCR	C2-C1-C6	2.33	114.06	110.48
13	B	1204	CLA	C3B-C4B-NB	-2.33	108.36	110.52
16	B	4009	BCR	C36-C18-C19	2.33	121.74	118.08
16	l	4013	BCR	C29-C30-C25	2.33	114.06	110.48
13	A	1124	CLA	C3C-C4C-NC	-2.33	107.96	110.57
16	2	522	BCR	C33-C5-C4	2.33	118.08	113.62
20	a	822	SQD	C1-O5-C5	2.33	118.25	113.69
13	A	1013	CLA	C3B-C4B-NB	-2.33	108.36	110.52
13	f	1215	CLA	C3B-C4B-NB	-2.33	108.36	110.52
13	A	1128	CLA	C3B-C2B-C1B	2.33	109.97	107.16
16	5	522	BCR	C3-C4-C5	-2.32	109.93	114.08
13	f	1225	CLA	CHB-C1B-NB	2.32	126.72	124.26
13	H	1210	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
16	J	4012	BCR	C28-C27-C26	-2.32	109.93	114.08
16	v	521	BCR	C33-C5-C6	-2.32	121.92	124.53
16	4	524	BCR	C1-C6-C7	2.32	122.35	115.78
13	G	1125	CLA	CAA-CBA-CGA	-2.32	106.46	113.25
13	b	507	CLA	O2D-CGD-CBD	2.32	115.40	111.27
16	T	4012	BCR	C28-C27-C26	-2.32	109.93	114.08
13	a	502	CLA	C3B-C4B-NB	-2.32	108.36	110.52
13	F	1301	CLA	CHB-C1B-NB	2.32	126.72	124.26
16	s	524	BCR	C23-C24-C25	-2.32	120.68	127.20
13	e	1125	CLA	CAA-CBA-CGA	-2.32	106.47	113.25
13	R	1301	CLA	CHB-C1B-NB	2.32	126.72	124.26
17	V	5221	LHG	C11-C10-C9	-2.32	102.64	114.42
16	t	521	BCR	C29-C30-C25	2.32	114.06	110.48
17	G	5006	LHG	O8-C23-C24	2.32	119.19	111.91
16	3	524	BCR	C23-C24-C25	-2.32	120.68	127.20
13	e	1118	CLA	O2D-CGD-CBD	2.32	115.39	111.27
13	f	1202	CLA	O2D-CGD-CBD	2.32	115.39	111.27
16	Y	522	BCR	C30-C25-C26	-2.32	119.34	122.61
13	G	1130	CLA	CMB-C2B-C3B	2.32	132.21	126.59
13	a	505	CLA	C3B-C4B-NB	-2.32	108.36	110.52
13	1	508	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
13	r	508	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
16	f	4004	BCR	C15-C16-C17	-2.32	118.72	123.47
16	1	522	BCR	C30-C25-C26	-2.32	119.35	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	509	CLA	C3B-C4B-NB	-2.32	108.36	110.52
16	4	522	BCR	C33-C5-C4	2.32	118.07	113.62
13	A	1124	CLA	CHB-C1B-NB	2.32	126.71	124.26
16	r	524	BCR	C15-C16-C17	-2.32	118.72	123.47
13	G	1013	CLA	C3B-C4B-NB	-2.32	108.36	110.52
16	G	4007	BCR	C2-C1-C6	2.32	114.05	110.48
17	L	5221	LHG	C11-C10-C9	-2.32	102.66	114.42
20	r	822	SQD	O48-C23-C24	2.32	119.18	111.91
13	r	503	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
20	2	822	SQD	O48-C23-C24	2.32	119.18	111.91
13	H	1223	CLA	C3B-C4B-NB	-2.32	108.37	110.52
13	u	507	CLA	CHC-C4B-NB	2.32	126.71	124.26
20	b	822	SQD	C1-O5-C5	2.32	118.23	113.69
16	v	522	BCR	C30-C25-C26	-2.32	119.35	122.61
13	s	510	CLA	C2A-C1A-CHA	2.32	127.91	123.86
13	Y	508	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
13	B	1215	CLA	C3B-C4B-NB	-2.32	108.37	110.52
13	q	518	CLA	CHB-C1B-NB	2.32	126.71	124.26
13	f	1210	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
16	r	523	BCR	C15-C16-C17	-2.31	118.73	123.47
13	Z	507	CLA	C2A-C1A-CHA	2.31	127.91	123.86
13	d	507	CLA	C2A-C1A-CHA	2.31	127.91	123.86
13	B	1210	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
16	T	4013	BCR	C7-C8-C9	-2.31	122.74	126.23
13	2	509	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
16	d	521	BCR	C33-C5-C6	-2.31	121.93	124.53
20	t	822	SQD	C1-O5-C5	2.31	118.23	113.69
13	A	1108	CLA	CHB-C1B-NB	2.31	126.71	124.26
13	2	507	CLA	C2A-C1A-CHA	2.31	127.90	123.86
13	2	507	CLA	C3B-C4B-NB	-2.31	108.37	110.52
17	n	5221	LHG	C11-C10-C9	-2.31	102.68	114.42
16	T	4013	BCR	C35-C13-C12	2.31	121.72	118.08
13	6	507	CLA	C2A-C1A-CHA	2.31	127.90	123.86
19	l	5104	LMG	O2-C2-C1	-2.31	104.43	110.05
20	Z	822	SQD	O48-C23-C24	2.31	119.17	111.91
17	A	5009	LHG	C20-C19-C18	-2.31	102.69	114.42
16	c	522	BCR	C3-C4-C5	-2.31	109.95	114.08
13	Z	508	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
13	4	507	CLA	O2D-CGD-CBD	2.31	115.38	111.27
13	v	507	CLA	C2A-C1A-CHA	2.31	127.90	123.86
13	A	1130	CLA	CMB-C2B-C3B	2.31	132.19	126.59
13	2	508	CLA	O2A-CGA-O1A	-2.31	117.76	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	J	4013	BCR	C35-C13-C12	2.31	121.72	118.08
19	H	5002	LMG	C42-C41-C40	-2.31	102.69	114.42
13	2	519	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
16	6	521	BCR	C33-C5-C6	-2.31	121.93	124.53
13	u	517	CLA	C3B-C4B-NB	-2.31	108.37	110.52
13	H	1225	CLA	CHB-C1B-NB	2.31	126.70	124.26
13	j	1301	CLA	CHB-C1B-NB	2.31	126.70	124.26
13	r	519	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
13	f	1202	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	e	5009	LHG	C20-C19-C18	-2.31	102.70	114.42
16	B	4010	BCR	C36-C18-C19	2.31	121.72	118.08
16	b	524	BCR	C1-C6-C7	2.31	122.31	115.78
16	H	4005	BCR	C33-C5-C4	2.31	118.05	113.62
13	r	509	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
16	A	4003	BCR	C11-C10-C9	-2.31	124.02	127.31
13	b	517	CLA	C3B-C4B-NB	-2.31	108.37	110.52
13	1	501	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
16	V	4019	BCR	C15-C16-C17	-2.31	118.75	123.47
16	4	523	BCR	C21-C20-C19	-2.31	116.02	123.22
13	Z	508	CLA	C3B-C4B-NB	-2.31	108.38	110.52
13	B	1226	CLA	C3C-C4C-NC	-2.31	107.98	110.57
13	B	1225	CLA	CHB-C1B-NB	2.31	126.70	124.26
13	5	508	CLA	CHB-C1B-NB	2.31	126.70	124.26
16	U	4104	BCR	C10-C11-C12	-2.31	116.02	123.22
13	Z	519	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
17	G	5009	LHG	C20-C19-C18	-2.31	102.72	114.42
13	r	519	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
13	Y	518	CLA	CHB-C1B-NB	2.31	126.70	124.26
13	s	502	CLA	C3B-C4B-NB	-2.31	108.38	110.52
16	2	523	BCR	C15-C16-C17	-2.31	118.75	123.47
16	n	4019	BCR	C15-C16-C17	-2.31	118.75	123.47
16	a	524	BCR	C23-C24-C25	-2.31	120.73	127.20
19	B	5002	LMG	C42-C41-C40	-2.31	102.72	114.42
19	f	5002	LMG	C42-C41-C40	-2.31	102.72	114.42
13	Y	501	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
13	c	508	CLA	CHB-C1B-NB	2.30	126.70	124.26
13	s	512	CLA	CHB-C4A-NA	2.30	127.70	124.51
13	q	501	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
16	l	4013	BCR	C7-C8-C9	-2.30	122.75	126.23
16	6	522	BCR	C30-C25-C26	-2.30	119.37	122.61
13	Z	503	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
13	A	1106	CLA	CHB-C1B-NB	2.30	126.70	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4022	BCR	C29-C28-C27	-2.30	106.23	111.38
13	e	1105	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
13	Z	519	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
16	M	4021	BCR	C3-C4-C5	-2.30	109.96	114.08
16	T	4013	BCR	C29-C30-C25	2.30	114.03	110.48
20	4	822	SQD	C1-O5-C5	2.30	118.21	113.69
16	n	4019	BCR	C33-C5-C6	-2.30	121.94	124.53
13	t	507	CLA	C3B-C4B-NB	-2.30	108.38	110.52
13	2	519	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
13	G	1128	CLA	C3B-C2B-C1B	2.30	109.94	107.16
13	e	1128	CLA	C3B-C2B-C1B	2.30	109.94	107.16
16	L	4019	BCR	C15-C16-C17	-2.30	118.76	123.47
13	e	1013	CLA	C3B-C4B-NB	-2.30	108.38	110.52
13	3	510	CLA	C2A-C1A-CHA	2.30	127.88	123.86
16	e	4002	BCR	C33-C5-C6	-2.30	121.94	124.53
13	3	512	CLA	CHB-C4A-NA	2.30	127.69	124.51
13	3	505	CLA	C3B-C4B-NB	-2.30	108.38	110.52
13	t	517	CLA	C3B-C4B-NB	-2.30	108.38	110.52
16	b	523	BCR	C21-C20-C19	-2.30	116.04	123.22
20	4	822	SQD	O5-C5-C4	2.30	113.87	109.69
16	K	4104	BCR	C10-C11-C12	-2.30	116.04	123.22
13	e	1124	CLA	C3C-C4C-NC	-2.30	107.99	110.57
13	5	507	CLA	CHC-C4B-NB	2.30	126.69	124.26
13	t	507	CLA	O2D-CGD-CBD	2.30	115.35	111.27
16	s	524	BCR	C34-C9-C8	2.30	121.70	118.08
16	V	4022	BCR	C29-C28-C27	-2.30	106.24	111.38
13	u	508	CLA	CHB-C1B-NB	2.30	126.69	124.26
16	f	4005	BCR	C33-C5-C4	2.30	118.03	113.62
13	v	503	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	t	822	SQD	C4-C3-C2	2.30	114.83	110.82
20	t	822	SQD	O5-C5-C4	2.30	113.86	109.69
13	B	1208	CLA	CHC-C4B-NB	2.30	126.69	124.26
16	W	4021	BCR	C3-C4-C5	-2.30	109.98	114.08
13	a	512	CLA	CHB-C4A-NA	2.30	127.69	124.51
16	L	4019	BCR	C33-C5-C6	-2.30	121.95	124.53
13	H	1226	CLA	CHC-C1C-NC	2.30	127.69	124.20
16	n	4219	BCR	C36-C18-C19	2.30	121.69	118.08
13	r	507	CLA	C2A-C1A-CHA	2.30	127.87	123.86
16	t	523	BCR	C21-C20-C19	-2.29	116.06	123.22
16	Z	523	BCR	C15-C16-C17	-2.29	118.77	123.47
16	V	4219	BCR	C36-C18-C19	2.29	121.69	118.08
13	H	1227	CLA	O2D-CGD-CBD	2.29	115.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1239	CLA	CMC-C2C-C1C	-2.29	121.55	125.04
13	H	1226	CLA	C3C-C4C-NC	-2.29	108.00	110.57
13	G	1105	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
16	n	4020	BCR	C21-C20-C19	-2.29	116.06	123.22
13	1	516	CLA	CHD-C1D-ND	-2.29	122.35	124.45
13	B	1223	CLA	C3B-C4B-NB	-2.29	108.39	110.52
16	J	4013	BCR	C29-C30-C25	2.29	114.01	110.48
16	R	4016	BCR	C16-C15-C14	-2.29	118.78	123.47
13	H	1202	CLA	CHD-C1D-ND	-2.29	122.35	124.45
13	K	1103	CLA	C3B-C4B-NB	-2.29	108.39	110.52
13	2	508	CLA	C3B-C4B-NB	-2.29	108.39	110.52
13	s	509	CLA	C3B-C4B-NB	-2.29	108.39	110.52
13	f	1208	CLA	CHC-C4B-NB	2.29	126.68	124.26
20	b	822	SQD	O5-C5-C4	2.29	113.86	109.69
13	H	1221	CLA	C2A-C1A-CHA	2.29	127.87	123.86
13	B	1239	CLA	CMC-C2C-C1C	-2.29	121.55	125.04
16	G	4003	BCR	C11-C10-C9	-2.29	124.04	127.31
16	J	4013	BCR	C7-C8-C9	-2.29	122.77	126.23
16	B	4005	BCR	C33-C5-C4	2.29	118.02	113.62
16	n	4022	BCR	C29-C28-C27	-2.29	106.26	111.38
13	a	510	CLA	C2A-C1A-CHA	2.29	127.86	123.86
13	G	1119	CLA	C2D-C1D-ND	-2.29	108.42	110.10
16	A	4002	BCR	C33-C5-C6	-2.29	121.96	124.53
16	m	4104	BCR	C10-C11-C12	-2.29	116.08	123.22
13	s	510	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
16	j	4016	BCR	C16-C15-C14	-2.29	118.79	123.47
16	L	4219	BCR	C36-C18-C19	2.29	121.68	118.08
13	f	1202	CLA	C3B-C4B-NB	-2.29	108.39	110.52
13	H	1228	CLA	CHC-C4B-NB	2.29	126.68	124.26
13	e	1118	CLA	CHC-C4B-NB	2.29	126.68	124.26
13	f	1226	CLA	C2B-C1B-NB	-2.29	108.70	110.23
13	a	510	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
13	G	1106	CLA	CHB-C1B-NB	2.29	126.68	124.26
16	n	4022	BCR	C29-C30-C25	2.29	114.00	110.48
13	a	508	CLA	C3B-C4B-NB	-2.29	108.39	110.52
13	f	1218	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
16	H	4010	BCR	C36-C18-C19	2.28	121.68	118.08
16	c	523	BCR	C37-C22-C23	2.28	121.68	118.08
17	e	5007	LHG	C18-C17-C16	-2.28	102.83	114.42
13	r	507	CLA	CHC-C4B-NB	2.28	126.67	124.26
13	B	1226	CLA	C2B-C1B-NB	-2.28	108.70	110.23
13	H	1238	CLA	O2A-CGA-O1A	-2.28	117.83	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	1501	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
16	V	4019	BCR	C33-C5-C6	-2.28	121.96	124.53
20	4	822	SQD	C4-C3-C2	2.28	114.81	110.82
13	H	1239	CLA	CMC-C2C-C1C	-2.28	121.56	125.04
16	V	4020	BCR	C21-C20-C19	-2.28	116.09	123.22
13	H	1204	CLA	C3B-C4B-NB	-2.28	108.40	110.52
13	s	508	CLA	C3B-C4B-NB	-2.28	108.40	110.52
13	B	1202	CLA	CHD-C1D-ND	-2.28	122.36	124.45
17	G	5007	LHG	C18-C17-C16	-2.28	102.84	114.42
16	F	4016	BCR	C16-C15-C14	-2.28	118.80	123.47
13	A	1105	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
13	b	503	CLA	C3B-C4B-NB	-2.28	108.40	110.52
13	f	1227	CLA	O2D-CGD-CBD	2.28	115.32	111.27
13	e	1105	CLA	CHD-C1D-ND	-2.28	122.36	124.45
13	f	1226	CLA	C3C-C4C-NC	-2.28	108.01	110.57
17	G	5005	LHG	C18-C17-C16	-2.28	102.84	114.42
20	b	822	SQD	C4-C3-C2	2.28	114.81	110.82
17	A	5007	LHG	C18-C17-C16	-2.28	102.84	114.42
13	2	506	CLA	CHB-C1B-NB	2.28	126.67	124.26
13	Z	511	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
13	n	1501	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
16	l	4013	BCR	C35-C13-C12	2.28	121.67	118.08
13	a	501	CLA	CMB-C2B-C3B	2.28	132.11	126.59
13	G	1124	CLA	CHB-C1B-NB	2.28	126.67	124.26
13	f	1221	CLA	C2A-C1A-CHA	2.28	127.84	123.86
13	e	1106	CLA	CHB-C1B-NB	2.28	126.67	124.26
16	L	4020	BCR	C21-C20-C19	-2.28	116.10	123.22
16	d	523	BCR	C8-C7-C6	-2.28	120.80	127.20
17	A	5005	LHG	C18-C17-C16	-2.28	102.86	114.42
13	4	507	CLA	C3B-C4B-NB	-2.28	108.40	110.52
20	B	1852	SQD	C4-C3-C2	2.28	114.80	110.82
17	e	5005	LHG	C18-C17-C16	-2.28	102.86	114.42
13	2	511	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
13	r	511	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
13	r	506	CLA	CHB-C1B-NB	2.28	126.67	124.26
13	B	1226	CLA	CHC-C1C-NC	2.28	127.66	124.20
16	V	4022	BCR	C29-C30-C25	2.28	113.99	110.48
16	u	523	BCR	C37-C22-C23	2.28	121.66	118.08
13	f	1228	CLA	C1-C2-C3	-2.28	122.11	126.04
13	L	1501	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
16	4	522	BCR	C3-C4-C5	-2.28	110.01	114.08
13	B	1238	CLA	O2A-CGA-O1A	-2.28	117.85	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	f	1852	SQD	C4-C3-C2	2.28	114.80	110.82
13	B	1227	CLA	O2D-CGD-CBD	2.28	115.31	111.27
13	B	1221	CLA	C2A-C1A-CHA	2.28	127.84	123.86
16	G	4002	BCR	C33-C5-C6	-2.28	121.97	124.53
13	e	1801	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
16	3	524	BCR	C34-C9-C8	2.27	121.66	118.08
16	a	524	BCR	C34-C9-C8	2.27	121.66	118.08
16	n	4022	BCR	C24-C23-C22	-2.27	122.80	126.23
16	L	4022	BCR	C29-C30-C25	2.27	113.98	110.48
16	6	523	BCR	C8-C7-C6	-2.27	120.82	127.20
13	b	507	CLA	C3B-C4B-NB	-2.27	108.41	110.52
13	s	505	CLA	C3B-C4B-NB	-2.27	108.41	110.52
13	3	510	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
13	H	1218	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
13	B	1221	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
13	B	1219	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
16	o	4021	BCR	C3-C4-C5	-2.27	110.02	114.08
17	G	5003	LHG	C18-C17-C16	-2.27	102.89	114.42
13	H	1228	CLA	C1-C2-C3	-2.27	122.11	126.04
16	U	4104	BCR	C37-C22-C21	-2.27	119.74	122.92
13	t	503	CLA	C3B-C4B-NB	-2.27	108.41	110.52
17	A	5003	LHG	C18-C17-C16	-2.27	102.89	114.42
13	B	1228	CLA	C1-C2-C3	-2.27	122.11	126.04
13	H	1221	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
16	T	4013	BCR	C10-C11-C12	-2.27	116.13	123.22
13	t	503	CLA	C2D-C1D-ND	-2.27	108.43	110.10
13	3	508	CLA	C3B-C4B-NB	-2.27	108.41	110.52
13	U	1103	CLA	C3B-C4B-NB	-2.27	108.41	110.52
13	f	1238	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
16	l	4012	BCR	C16-C17-C18	-2.27	124.07	127.31
13	3	501	CLA	CMB-C2B-C3B	2.27	132.09	126.59
13	e	1113	CLA	CMB-C2B-C3B	2.27	132.09	126.59
13	H	1219	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
16	5	523	BCR	C37-C22-C23	2.27	121.65	118.08
17	A	5007	LHG	C27-C26-C25	-2.27	102.90	114.42
17	e	5003	LHG	C18-C17-C16	-2.27	102.90	114.42
13	B	1202	CLA	C3B-C4B-NB	-2.27	108.41	110.52
17	G	5007	LHG	C27-C26-C25	-2.27	102.90	114.42
13	H	1012	CLA	CHB-C1B-NB	2.27	126.66	124.26
13	G	1121	CLA	C2A-C1A-CHA	2.27	127.83	123.86
13	A	1113	CLA	CMB-C2B-C3B	2.27	132.09	126.59
16	q	522	BCR	C30-C25-C26	-2.27	119.42	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	1843	LMU	C6B-C5B-C4B	-2.27	107.69	113.00
13	B	1234	CLA	O2D-CGD-CBD	2.27	115.30	111.27
20	H	1852	SQD	C4-C3-C2	2.27	114.78	110.82
16	K	4104	BCR	C37-C22-C21	-2.27	119.75	122.92
16	b	522	BCR	C3-C4-C5	-2.27	110.03	114.08
13	H	1228	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
16	m	4104	BCR	C37-C22-C21	-2.27	119.75	122.92
17	e	5007	LHG	C27-C26-C25	-2.27	102.91	114.42
13	m	1103	CLA	C3B-C4B-NB	-2.27	108.41	110.52
13	G	1121	CLA	CHC-C4B-NB	2.27	126.66	124.26
13	f	1228	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
13	B	1218	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
13	2	510	CLA	CMB-C2B-C3B	2.27	132.08	126.59
18	f	1843	LMU	C6B-C5B-C4B	-2.27	107.70	113.00
13	u	519	CLA	CHB-C1B-NB	2.27	126.66	124.26
13	1	503	CLA	C3B-C4B-NB	-2.26	108.41	110.52
16	J	4013	BCR	C10-C11-C12	-2.26	116.15	123.22
13	H	1210	CLA	CBC-CAC-C3C	2.26	118.67	112.43
16	Z	523	BCR	C10-C11-C12	-2.26	116.15	123.22
16	l	4013	BCR	C10-C11-C12	-2.26	116.15	123.22
16	v	523	BCR	C8-C7-C6	-2.26	120.84	127.20
18	B	1843	LMU	C6B-C5B-C4B	-2.26	107.70	113.00
19	T	5104	LMG	C1-C2-C3	-2.26	105.28	110.00
13	A	1140	CLA	O2D-CGD-CBD	2.26	115.29	111.27
13	A	1118	CLA	CHC-C4B-NB	2.26	126.65	124.26
13	e	1140	CLA	O2D-CGD-CBD	2.26	115.29	111.27
13	A	1022	CLA	CMB-C2B-C3B	2.26	132.07	126.59
13	s	501	CLA	CMB-C2B-C3B	2.26	132.07	126.59
16	T	4012	BCR	C16-C17-C18	-2.26	124.08	127.31
13	j	1301	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
13	A	1801	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
13	G	1801	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
13	f	1210	CLA	CBC-CAC-C3C	2.26	118.67	112.43
13	Z	507	CLA	CHC-C4B-NB	2.26	126.65	124.26
13	c	507	CLA	CHC-C4B-NB	2.26	126.65	124.26
13	n	1501	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
13	G	1140	CLA	O2D-CGD-CBD	2.26	115.28	111.27
13	f	1234	CLA	O2D-CGD-CBD	2.26	115.28	111.27
13	6	503	CLA	C3B-C4B-NB	-2.26	108.42	110.52
13	A	1117	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
16	2	523	BCR	C33-C5-C4	2.26	117.96	113.62
13	G	1117	CLA	O2A-CGA-O1A	-2.26	117.89	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1119	CLA	C2D-C1D-ND	-2.26	108.44	110.10
13	r	510	CLA	CMB-C2B-C3B	2.26	132.06	126.59
16	V	4022	BCR	C3-C4-C5	-2.26	110.04	114.08
16	J	4012	BCR	C16-C17-C18	-2.26	124.09	127.31
13	A	1121	CLA	C2A-C1A-CHA	2.26	127.81	123.86
13	H	1240	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
13	e	1117	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
16	V	4022	BCR	C24-C23-C22	-2.26	122.82	126.23
13	f	1228	CLA	CHC-C4B-NB	2.26	126.65	124.26
16	A	4001	BCR	C34-C9-C8	2.26	121.63	118.08
13	L	1503	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
13	n	1503	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
13	4	503	CLA	C3B-C4B-NB	-2.26	108.42	110.52
16	G	4001	BCR	C34-C9-C8	2.26	121.63	118.08
13	H	1226	CLA	CAC-C3C-C4C	2.26	127.74	124.81
13	A	1139	CLA	CHB-C1B-NB	2.26	126.64	124.26
16	T	4015	BCR	C21-C20-C19	-2.26	116.18	123.22
13	f	1219	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
13	L	1501	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
13	f	1221	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
13	G	1113	CLA	CMB-C2B-C3B	2.25	132.05	126.59
13	B	1228	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
13	J	1303	CLA	CAA-C2A-C1A	2.25	119.36	111.97
16	e	4001	BCR	C34-C9-C8	2.25	121.63	118.08
13	G	1022	CLA	CMB-C2B-C3B	2.25	132.04	126.59
13	f	1210	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
13	6	516	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
13	R	1301	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
13	f	1221	CLA	C6-C7-C8	-2.25	108.64	115.92
17	e	5006	LHG	O8-C23-O10	-2.25	117.91	123.59
16	t	522	BCR	C3-C4-C5	-2.25	110.06	114.08
16	2	523	BCR	C10-C11-C12	-2.25	116.19	123.22
16	G	4002	BCR	C10-C11-C12	-2.25	116.19	123.22
13	d	516	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
13	f	1238	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
13	Z	510	CLA	CMB-C2B-C3B	2.25	132.04	126.59
13	B	1240	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
13	e	1117	CLA	C3B-C4B-NB	-2.25	108.43	110.52
17	A	5006	LHG	O8-C23-O10	-2.25	117.91	123.59
13	T	1303	CLA	CAA-C2A-C1A	2.25	119.35	111.97
16	r	523	BCR	C10-C11-C12	-2.25	116.19	123.22
13	e	1121	CLA	C2A-C1A-CHA	2.25	127.79	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1210	CLA	CBC-CAC-C3C	2.25	118.64	112.43
13	B	1221	CLA	C6-C7-C8	-2.25	108.65	115.92
13	H	1221	CLA	C6-C7-C8	-2.25	108.65	115.92
13	e	1022	CLA	CMB-C2B-C3B	2.25	132.04	126.59
13	A	1139	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
13	H	1202	CLA	C3B-C4B-NB	-2.25	108.43	110.52
13	f	1218	CLA	C3B-C4B-NB	-2.25	108.43	110.52
16	Z	523	BCR	C33-C5-C4	2.25	117.94	113.62
13	A	1131	CLA	CHD-C1D-ND	-2.25	122.39	124.45
13	F	1301	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
13	V	1503	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
13	f	1223	CLA	C3B-C4B-NB	-2.25	108.43	110.52
13	f	1240	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
13	B	1226	CLA	CAC-C3C-C4C	2.25	127.73	124.81
13	G	1139	CLA	CHB-C1B-NB	2.25	126.64	124.26
16	f	4010	BCR	C4-C5-C6	-2.25	119.47	122.73
13	H	1238	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
18	Y	902	LMU	C1'-C2'-C3'	2.25	114.68	110.00
13	B	1230	CLA	CHB-C4A-NA	2.25	127.62	124.51
13	B	1218	CLA	C3B-C4B-NB	-2.25	108.43	110.52
13	r	508	CLA	C3B-C4B-NB	-2.25	108.43	110.52
13	e	1107	CLA	CHC-C4B-NB	2.25	126.64	124.26
13	Y	516	CLA	CHD-C1D-ND	-2.25	122.39	124.45
13	B	1210	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
17	H	1855	LHG	C20-C19-C18	-2.25	103.02	114.42
19	H	5002	LMG	O2-C2-C1	-2.25	104.59	110.05
17	e	5006	LHG	C27-C26-C25	-2.25	103.02	114.42
16	L	4022	BCR	C3-C4-C5	-2.25	110.07	114.08
13	Z	506	CLA	CHB-C1B-NB	2.25	126.64	124.26
13	l	1303	CLA	CAA-C2A-C1A	2.25	119.34	111.97
13	B	1238	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
13	H	1230	CLA	CHB-C4A-NA	2.25	127.62	124.51
16	H	4010	BCR	C4-C5-C6	-2.25	119.47	122.73
13	f	1226	CLA	CAC-C3C-C4C	2.25	127.72	124.81
13	H	1201	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
19	J	5104	LMG	C1-C2-C3	-2.25	105.32	110.00
17	f	1855	LHG	C20-C19-C18	-2.25	103.03	114.42
13	f	1230	CLA	CHB-C4A-NA	2.25	127.62	124.51
13	d	503	CLA	C3B-C4B-NB	-2.25	108.43	110.52
13	e	1121	CLA	CHC-C4B-NB	2.25	126.63	124.26
17	G	5006	LHG	C27-C26-C25	-2.24	103.03	114.42
13	A	1107	CLA	CMB-C2B-C1B	-2.24	121.95	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	5006	LHG	C27-C26-C25	-2.24	103.03	114.42
17	B	1855	LHG	C20-C19-C18	-2.24	103.03	114.42
19	f	5002	LMG	O2-C2-C1	-2.24	104.59	110.05
13	q	503	CLA	C3B-C4B-NB	-2.24	108.43	110.52
16	r	523	BCR	C33-C5-C4	2.24	117.93	113.62
16	l	4015	BCR	C21-C20-C19	-2.24	116.21	123.22
13	v	516	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
16	L	4022	BCR	C24-C23-C22	-2.24	122.84	126.23
16	B	4010	BCR	C4-C5-C6	-2.24	119.47	122.73
16	J	4015	BCR	C21-C20-C19	-2.24	116.22	123.22
13	2	505	CLA	C2D-C1D-ND	-2.24	108.45	110.10
13	B	1012	CLA	CHB-C1B-NB	2.24	126.63	124.26
13	H	1227	CLA	CHB-C1B-NB	2.24	126.63	124.26
16	B	4009	BCR	C8-C7-C6	-2.24	120.90	127.20
13	A	1022	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
13	V	1501	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
13	A	1107	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
13	A	1105	CLA	CHD-C1D-ND	-2.24	122.39	124.45
13	G	1107	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
16	n	4022	BCR	C3-C4-C5	-2.24	110.08	114.08
20	H	1852	SQD	O6-C44-C45	2.24	116.31	110.90
13	3	509	CLA	CMB-C2B-C3B	2.24	132.02	126.59
13	a	506	CLA	CMB-C2B-C3B	2.24	132.02	126.59
19	B	5002	LMG	O2-C2-C1	-2.24	104.60	110.05
13	A	1117	CLA	C3B-C4B-NB	-2.24	108.44	110.52
13	e	1013	CLA	C3C-C4C-NC	-2.24	108.06	110.57
13	G	1118	CLA	CHC-C4B-NB	2.24	126.63	124.26
13	e	1139	CLA	CHB-C1B-NB	2.24	126.63	124.26
13	B	1229	CLA	C6-C7-C8	-2.24	108.68	115.92
13	G	1107	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
13	G	1139	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
13	e	1107	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
16	H	4009	BCR	C8-C7-C6	-2.24	120.91	127.20
16	A	4002	BCR	C10-C11-C12	-2.24	116.23	123.22
20	f	1852	SQD	O6-C44-C45	2.24	116.30	110.90
13	e	1022	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
13	e	1139	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
13	B	1219	CLA	CHC-C4B-NB	2.24	126.63	124.26
13	e	1237	CLA	CHB-C1B-NB	2.24	126.63	124.26
13	e	1119	CLA	C2D-C1D-ND	-2.24	108.45	110.10
13	a	509	CLA	CMB-C2B-C3B	2.24	132.01	126.59
13	f	1226	CLA	CHC-C1C-NC	2.24	127.60	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1214	CLA	CHB-C1B-NB	2.24	126.62	124.26
13	B	1228	CLA	CHC-C4B-NB	2.24	126.62	124.26
13	B	1201	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
19	l	5104	LMG	C1-C2-C3	-2.24	105.34	110.00
16	q	522	BCR	C1-C6-C7	2.24	122.11	115.78
13	G	1105	CLA	CHD-C1D-ND	-2.24	122.40	124.45
13	A	1107	CLA	CHC-C4B-NB	2.24	126.62	124.26
13	B	1221	CLA	CHB-C1B-NB	2.24	126.62	124.26
13	H	1234	CLA	O2D-CGD-CBD	2.24	115.24	111.27
13	Z	506	CLA	C3B-C4B-NB	-2.24	108.44	110.52
16	5	524	BCR	C38-C26-C25	-2.24	122.02	124.53
19	B	5002	LMG	O3-C3-C2	-2.23	105.18	110.35
20	B	1852	SQD	O6-C44-C45	2.23	116.29	110.90
13	e	1108	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	f	5002	LMG	O3-C3-C2	-2.23	105.18	110.35
16	u	524	BCR	C38-C26-C25	-2.23	122.02	124.53
13	G	1131	CLA	CHD-C1D-ND	-2.23	122.40	124.45
16	5	522	BCR	C30-C25-C26	-2.23	119.47	122.61
13	A	1108	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	e	5009	LHG	C27-C26-C25	-2.23	103.08	114.42
13	a	503	CLA	C2D-C1D-ND	-2.23	108.46	110.10
13	e	1131	CLA	CHD-C1D-ND	-2.23	122.40	124.45
13	A	1135	CLA	O2A-C1-C2	2.23	114.50	108.64
13	4	503	CLA	C2D-C1D-ND	-2.23	108.46	110.10
13	H	1229	CLA	C6-C7-C8	-2.23	108.70	115.92
13	H	1210	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
13	A	1121	CLA	CHC-C4B-NB	2.23	126.62	124.26
16	5	522	BCR	C1-C6-C7	2.23	122.09	115.78
16	f	4009	BCR	C8-C7-C6	-2.23	120.94	127.20
13	s	509	CLA	CMB-C2B-C3B	2.23	131.99	126.59
16	1	522	BCR	C1-C6-C7	2.23	122.09	115.78
13	A	1124	CLA	CHD-C1D-ND	-2.23	122.40	124.45
13	q	516	CLA	CHD-C1D-ND	-2.23	122.40	124.45
16	c	524	BCR	C21-C20-C19	-2.23	116.26	123.22
16	u	524	BCR	C21-C20-C19	-2.23	116.26	123.22
13	Y	502	CLA	C3B-C4B-NB	-2.23	108.45	110.52
13	f	1219	CLA	CHC-C4B-NB	2.23	126.62	124.26
16	Y	522	BCR	C1-C6-C7	2.23	122.09	115.78
17	G	5006	LHG	O8-C23-O10	-2.23	117.96	123.59
13	f	1229	CLA	C6-C7-C8	-2.23	108.71	115.92
13	2	510	CLA	CHB-C1B-NB	2.23	126.62	124.26
16	c	524	BCR	C38-C26-C25	-2.23	122.03	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	5003	LHG	C27-C26-C25	-2.23	103.11	114.42
13	B	1012	CLA	O2D-CGD-CBD	2.23	115.23	111.27
13	H	1217	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
13	G	1013	CLA	C3C-C4C-NC	-2.23	108.07	110.57
13	A	1127	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
13	A	1115	CLA	C4-C3-C5	2.23	119.02	115.27
13	f	1201	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
13	t	511	CLA	C2D-C1D-ND	-2.23	108.46	110.10
13	A	1013	CLA	C3C-C4C-NC	-2.23	108.07	110.57
13	G	1106	CLA	CHC-C4B-NB	2.23	126.61	124.26
13	e	1115	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
16	u	522	BCR	C30-C25-C26	-2.23	119.48	122.61
16	4	523	BCR	C10-C11-C12	-2.23	116.27	123.22
13	f	1204	CLA	CHD-C1D-ND	-2.23	122.41	124.45
13	G	1127	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
17	A	5009	LHG	C27-C26-C25	-2.22	103.13	114.42
17	G	5003	LHG	C27-C26-C25	-2.22	103.13	114.42
13	1	502	CLA	C3B-C4B-NB	-2.22	108.45	110.52
13	H	1208	CLA	C3B-C4B-NB	-2.22	108.45	110.52
13	G	1135	CLA	O2A-C1-C2	2.22	114.48	108.64
17	e	5003	LHG	C27-C26-C25	-2.22	103.13	114.42
13	A	1115	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
16	Y	524	BCR	C37-C22-C23	2.22	121.58	118.08
13	e	1115	CLA	C4-C3-C5	2.22	119.01	115.27
13	f	1012	CLA	C4-C3-C5	2.22	119.01	115.27
16	e	4002	BCR	C10-C11-C12	-2.22	116.28	123.22
13	G	1109	CLA	C3B-C4B-NB	-2.22	108.45	110.52
13	f	1208	CLA	C3B-C4B-NB	-2.22	108.45	110.52
13	H	1214	CLA	CHB-C1B-NB	2.22	126.61	124.26
13	f	1217	CLA	CHC-C4B-NB	2.22	126.61	124.26
16	a	524	BCR	C8-C7-C6	-2.22	120.96	127.20
16	t	523	BCR	C10-C11-C12	-2.22	116.28	123.22
13	A	1140	CLA	CHA-C1A-NA	-2.22	121.31	126.40
13	B	1208	CLA	C3B-C4B-NB	-2.22	108.45	110.52
13	G	1117	CLA	C3B-C4B-NB	-2.22	108.45	110.52
13	H	1218	CLA	C3B-C4B-NB	-2.22	108.45	110.52
16	5	524	BCR	C21-C20-C19	-2.22	116.28	123.22
19	T	5104	LMG	O3-C3-C2	-2.22	105.21	110.35
13	e	1127	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
17	V	5218	LHG	C27-C26-C25	-2.22	103.15	114.42
13	e	1135	CLA	O2A-C1-C2	2.22	114.47	108.64
18	1	902	LMU	C1'-C2'-C3'	2.22	114.62	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	522	BCR	C1-C6-C7	2.22	122.06	115.78
13	s	503	CLA	C2D-C1D-ND	-2.22	108.47	110.10
16	e	4003	BCR	C10-C11-C12	-2.22	116.28	123.22
13	e	1107	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
13	G	1022	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
13	5	519	CLA	CHB-C1B-NB	2.22	126.61	124.26
13	f	1012	CLA	O2D-CGD-CBD	2.22	115.21	111.27
13	G	1123	CLA	O2D-CGD-CBD	2.22	115.21	111.27
13	G	1140	CLA	CHA-C1A-NA	-2.22	121.31	126.40
13	G	1124	CLA	CHD-C1D-ND	-2.22	122.41	124.45
13	3	506	CLA	CMB-C2B-C3B	2.22	131.96	126.59
16	c	522	BCR	C1-C6-C7	2.22	122.06	115.78
16	H	4006	BCR	C21-C20-C19	-2.22	116.29	123.22
13	Z	510	CLA	CHB-C1B-NB	2.22	126.61	124.26
17	G	5009	LHG	C27-C26-C25	-2.22	103.16	114.42
17	f	1855	LHG	C11-C10-C9	-2.22	103.16	114.42
16	q	524	BCR	C37-C22-C23	2.22	121.57	118.08
13	B	1203	CLA	CHB-C1B-NB	2.22	126.61	124.26
13	G	1115	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
16	1	524	BCR	C37-C22-C23	2.22	121.57	118.08
16	3	524	BCR	C8-C7-C6	-2.22	120.97	127.20
13	Y	503	CLA	C3B-C4B-NB	-2.22	108.46	110.52
13	q	502	CLA	C3B-C4B-NB	-2.22	108.46	110.52
13	e	1128	CLA	O2D-CGD-CBD	2.22	115.21	111.27
13	f	1234	CLA	C3A-C2A-C1A	2.22	104.66	101.34
17	L	5218	LHG	C27-C26-C25	-2.22	103.17	114.42
13	B	1219	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	B	1855	LHG	C11-C10-C9	-2.22	103.17	114.42
13	A	1123	CLA	O2D-CGD-CBD	2.22	115.21	111.27
13	A	1128	CLA	O2D-CGD-CBD	2.22	115.21	111.27
13	2	507	CLA	CHC-C4B-NB	2.22	126.60	124.26
19	H	5002	LMG	O3-C3-C2	-2.22	105.23	110.35
13	r	505	CLA	C2D-C1D-ND	-2.22	108.47	110.10
17	H	1855	LHG	C11-C10-C9	-2.22	103.18	114.42
16	4	522	BCR	C23-C24-C25	-2.22	120.98	127.20
17	n	5218	LHG	C27-C26-C25	-2.22	103.18	114.42
16	G	4003	BCR	C10-C11-C12	-2.22	116.30	123.22
13	G	1113	CLA	C3B-C4B-NB	-2.22	108.46	110.52
13	H	1219	CLA	CHC-C4B-NB	2.22	126.60	124.26
13	b	503	CLA	C2D-C1D-ND	-2.21	108.47	110.10
13	f	1212	CLA	O2D-CGD-CBD	2.21	115.20	111.27
13	f	1012	CLA	CHB-C1B-NB	2.21	126.60	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4006	BCR	C21-C20-C19	-2.21	116.31	123.22
16	T	4012	BCR	C1-C6-C7	2.21	122.04	115.78
13	a	510	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
13	e	1124	CLA	CHD-C1D-ND	-2.21	122.42	124.45
16	b	523	BCR	C10-C11-C12	-2.21	116.31	123.22
13	2	502	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
13	G	1108	CLA	CHB-C4A-NA	2.21	127.57	124.51
16	s	524	BCR	C8-C7-C6	-2.21	120.99	127.20
13	Z	505	CLA	C2D-C1D-ND	-2.21	108.47	110.10
13	A	1138	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
13	s	506	CLA	CMB-C2B-C3B	2.21	131.94	126.59
13	3	509	CLA	C2A-C1A-CHA	2.21	127.72	123.86
13	s	509	CLA	C2A-C1A-CHA	2.21	127.72	123.86
13	B	1217	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
13	G	1108	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
13	H	1203	CLA	CHB-C1B-NB	2.21	126.60	124.26
16	A	4003	BCR	C10-C11-C12	-2.21	116.32	123.22
13	r	502	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
13	e	1138	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
13	e	1104	CLA	CMB-C2B-C3B	2.21	131.94	126.59
13	a	501	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
16	Y	521	BCR	C2-C1-C6	2.21	113.88	110.48
16	G	4008	BCR	C20-C19-C18	-2.21	120.21	126.42
16	t	522	BCR	C23-C24-C25	-2.21	121.00	127.20
13	H	1215	CLA	CMB-C2B-C3B	2.21	131.94	126.59
13	s	510	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
13	3	501	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
13	G	1107	CLA	CHC-C4B-NB	2.21	126.59	124.26
13	H	1221	CLA	CHB-C1B-NB	2.21	126.59	124.26
16	s	524	BCR	C1-C6-C5	-2.21	119.50	122.61
16	J	4012	BCR	C1-C6-C7	2.21	122.02	115.78
13	H	1212	CLA	O2D-CGD-CBD	2.21	115.19	111.27
13	B	1227	CLA	CHB-C1B-NB	2.21	126.59	124.26
16	W	4021	BCR	C30-C25-C24	2.21	122.02	115.78
13	G	1115	CLA	C4-C3-C5	2.21	118.98	115.27
13	G	1237	CLA	CHB-C1B-NB	2.21	126.59	124.26
13	H	1205	CLA	CHB-C1B-NB	2.21	126.59	124.26
13	r	510	CLA	CHB-C1B-NB	2.21	126.59	124.26
13	l	1302	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
13	v	509	CLA	CMB-C2B-C1B	-2.21	122.01	125.37
13	B	1215	CLA	CMB-C2B-C3B	2.21	131.93	126.59
16	A	4008	BCR	C20-C19-C18	-2.21	120.22	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	523	BCR	C11-C10-C9	-2.21	124.16	127.31
13	6	509	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
18	q	902	LMU	C1'-C2'-C3'	2.20	114.59	110.00
13	l	1303	CLA	C2A-C1A-CHA	2.20	127.71	123.86
16	M	4021	BCR	C30-C25-C24	2.20	122.01	115.78
13	T	1302	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
13	Z	502	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
13	A	1237	CLA	CHB-C1B-NB	2.20	126.59	124.26
13	B	1212	CLA	O2D-CGD-CBD	2.20	115.18	111.27
13	f	1217	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
13	s	508	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	B	1234	CLA	C3A-C2A-C1A	2.20	104.64	101.34
13	s	501	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
19	J	5104	LMG	O3-C3-C2	-2.20	105.26	110.35
13	f	1214	CLA	CHB-C1B-NB	2.20	126.59	124.26
13	f	1219	CLA	CHB-C4A-NA	2.20	127.56	124.51
16	3	524	BCR	C1-C6-C5	-2.20	119.51	122.61
13	a	508	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	T	1303	CLA	C2A-C1A-CHA	2.20	127.71	123.86
13	J	1302	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
13	f	1221	CLA	CHB-C1B-NB	2.20	126.59	124.26
13	G	1128	CLA	O2D-CGD-CBD	2.20	115.18	111.27
13	A	1109	CLA	C3B-C4B-NB	-2.20	108.47	110.52
13	c	503	CLA	C3B-C4B-NB	-2.20	108.47	110.52
13	H	1012	CLA	O2D-CGD-CBD	2.20	115.18	111.27
13	2	511	CLA	CHB-C1B-NB	2.20	126.59	124.26
13	e	1140	CLA	CHB-C4A-NA	2.20	127.56	124.51
16	n	4020	BCR	C33-C5-C6	-2.20	122.06	124.53
16	o	4021	BCR	C30-C25-C24	2.20	122.00	115.78
16	1	521	BCR	C2-C1-C6	2.20	113.87	110.48
13	f	1205	CLA	CHB-C1B-NB	2.20	126.59	124.26
13	f	1227	CLA	CHB-C1B-NB	2.20	126.59	124.26
16	A	4002	BCR	C23-C24-C25	-2.20	121.02	127.20
16	b	522	BCR	C23-C24-C25	-2.20	121.03	127.20
16	6	523	BCR	C34-C9-C8	2.20	121.54	118.08
13	e	1140	CLA	CHA-C1A-NA	-2.20	121.36	126.40
13	2	506	CLA	C3B-C4B-NB	-2.20	108.47	110.52
16	f	4006	BCR	C21-C20-C19	-2.20	116.36	123.22
16	e	4002	BCR	C38-C26-C25	-2.20	122.06	124.53
13	a	509	CLA	C2A-C1A-CHA	2.20	127.70	123.86
13	e	1104	CLA	O1D-CGD-CBD	2.20	128.98	124.48
13	c	519	CLA	CHB-C1B-NB	2.20	126.58	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1204	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	a	502	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
13	B	1012	CLA	C4-C3-C5	2.20	118.97	115.27
13	G	1138	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
13	c	509	CLA	C3B-C4B-NB	-2.20	108.48	110.52
13	s	507	CLA	C3B-C4B-NB	-2.20	108.48	110.52
16	l	4012	BCR	C1-C6-C7	2.20	121.99	115.78
16	c	522	BCR	C30-C25-C26	-2.20	119.52	122.61
16	f	4010	BCR	C20-C19-C18	-2.20	120.25	126.42
16	q	523	BCR	C37-C22-C23	2.20	121.54	118.08
16	f	4006	BCR	C28-C27-C26	-2.20	110.16	114.08
13	d	518	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
13	e	1123	CLA	O2D-CGD-CBD	2.20	115.17	111.27
13	f	1229	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
16	f	4014	BCR	C15-C14-C13	-2.20	124.18	127.31
13	1	511	CLA	CHB-C1B-NB	2.20	126.58	124.26
18	q	902	LMU	C4'-C3'-C2'	2.20	114.66	110.82
16	f	4010	BCR	C11-C12-C13	-2.19	120.25	126.42
13	G	1104	CLA	O1D-CGD-CBD	2.19	128.97	124.48
16	G	4002	BCR	C23-C24-C25	-2.19	121.04	127.20
13	1	509	CLA	C3B-C4B-NB	-2.19	108.48	110.52
16	q	521	BCR	C2-C1-C6	2.19	113.86	110.48
16	a	524	BCR	C1-C6-C5	-2.19	119.52	122.61
13	A	1140	CLA	CHB-C4A-NA	2.19	127.55	124.51
16	B	4010	BCR	C20-C19-C18	-2.19	120.25	126.42
16	e	4002	BCR	C23-C24-C25	-2.19	121.04	127.20
13	3	507	CLA	C3B-C4B-NB	-2.19	108.48	110.52
13	A	1104	CLA	CMB-C2B-C3B	2.19	131.90	126.59
13	H	1219	CLA	CHB-C4A-NA	2.19	127.54	124.51
16	A	4001	BCR	C8-C7-C6	-2.19	121.04	127.20
13	Y	509	CLA	C3B-C4B-NB	-2.19	108.48	110.52
13	3	510	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
13	d	509	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
17	G	5005	LHG	C27-C26-C25	-2.19	103.30	114.42
13	J	1303	CLA	O2D-CGD-CBD	2.19	115.16	111.27
16	G	4001	BCR	C8-C7-C6	-2.19	121.05	127.20
13	v	518	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
13	3	502	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
16	v	524	BCR	C21-C20-C19	-2.19	116.38	123.22
13	a	511	CLA	CHB-C1B-NB	2.19	126.58	124.26
13	q	511	CLA	CHB-C1B-NB	2.19	126.58	124.26
16	B	4014	BCR	C15-C14-C13	-2.19	124.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	508	CLA	C2D-C1D-ND	-2.19	108.49	110.10
13	G	1140	CLA	CHB-C4A-NA	2.19	127.54	124.51
13	r	511	CLA	CHB-C1B-NB	2.19	126.58	124.26
19	l	5104	LMG	O3-C3-C2	-2.19	105.29	110.35
13	e	1109	CLA	C3B-C4B-NB	-2.19	108.48	110.52
13	n	1501	CLA	C3B-C4B-NB	-2.19	108.48	110.52
13	H	1234	CLA	C3A-C2A-C1A	2.19	104.62	101.34
13	G	1104	CLA	CMB-C2B-C3B	2.19	131.89	126.59
16	1	523	BCR	C37-C22-C23	2.19	121.53	118.08
13	d	508	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
13	A	1237	CLA	CAC-C3C-C4C	2.19	127.65	124.81
13	4	511	CLA	C2D-C1D-ND	-2.19	108.49	110.10
13	f	1215	CLA	CMB-C2B-C3B	2.19	131.89	126.59
16	e	4008	BCR	C20-C19-C18	-2.19	120.27	126.42
17	e	5005	LHG	C27-C26-C25	-2.19	103.31	114.42
13	A	1113	CLA	C3B-C4B-NB	-2.19	108.48	110.52
13	b	502	CLA	C3B-C4B-NB	-2.19	108.48	110.52
13	s	502	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
20	H	1852	SQD	O48-C23-C24	2.19	118.77	111.91
20	B	1852	SQD	O48-C23-C24	2.19	118.77	111.91
13	H	1229	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
13	J	1303	CLA	C2A-C1A-CHA	2.19	127.68	123.86
13	H	1012	CLA	C4-C3-C5	2.19	118.95	115.27
17	A	5005	LHG	C27-C26-C25	-2.19	103.32	114.42
13	6	518	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
13	Y	509	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
13	b	511	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
13	T	1303	CLA	O2D-CGD-CBD	2.19	115.15	111.27
13	A	1104	CLA	O1D-CGD-CBD	2.19	128.96	124.48
16	a	524	BCR	C21-C20-C19	-2.19	116.40	123.22
13	A	1022	CLA	C4D-C3D-CAD	-2.18	105.52	108.10
16	3	524	BCR	C37-C22-C23	2.18	121.52	118.08
13	A	1106	CLA	CHC-C4B-NB	2.18	126.57	124.26
13	5	509	CLA	C3B-C4B-NB	-2.18	108.49	110.52
13	r	506	CLA	C3B-C4B-NB	-2.18	108.49	110.52
16	G	4002	BCR	C38-C26-C25	-2.18	122.08	124.53
13	3	508	CLA	CMB-C2B-C3B	2.18	131.88	126.59
16	H	4010	BCR	C20-C19-C18	-2.18	120.28	126.42
13	B	1217	CLA	CHC-C4B-NB	2.18	126.57	124.26
13	6	504	CLA	CHB-C1B-NB	2.18	126.57	124.26
13	s	508	CLA	CMB-C2B-C3B	2.18	131.88	126.59
16	v	523	BCR	C34-C9-C8	2.18	121.52	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4001	BCR	C8-C7-C6	-2.18	121.07	127.20
13	A	1135	CLA	O2D-CGD-CBD	2.18	115.14	111.27
13	H	1204	CLA	CHD-C1D-ND	-2.18	122.45	124.45
13	5	503	CLA	C3B-C4B-NB	-2.18	108.49	110.52
13	B	1229	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
16	d	523	BCR	C34-C9-C8	2.18	121.51	118.08
13	6	508	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
17	e	5001	LHG	C27-C26-C25	-2.18	103.35	114.42
13	e	1022	CLA	C4D-C3D-CAD	-2.18	105.53	108.10
13	d	504	CLA	CHB-C1B-NB	2.18	126.57	124.26
20	f	1852	SQD	O48-C23-C24	2.18	118.75	111.91
16	L	4020	BCR	C33-C5-C6	-2.18	122.08	124.53
13	f	1236	CLA	O2D-CGD-CBD	2.18	115.14	111.27
13	L	1501	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	v	504	CLA	CHB-C1B-NB	2.18	126.56	124.26
13	A	1118	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	b	503	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
13	f	1021	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	q	509	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
13	A	1108	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
16	3	524	BCR	C21-C20-C19	-2.18	116.42	123.22
16	6	524	BCR	C21-C20-C19	-2.18	116.42	123.22
16	d	524	BCR	C21-C20-C19	-2.18	116.42	123.22
13	A	1011	CLA	CHA-C1A-NA	-2.18	121.41	126.40
13	e	1108	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
16	B	4006	BCR	C28-C27-C26	-2.18	110.19	114.08
13	e	1011	CLA	CHA-C1A-NA	-2.18	121.41	126.40
16	H	4006	BCR	C28-C27-C26	-2.18	110.19	114.08
13	e	1118	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	e	1113	CLA	C3B-C4B-NB	-2.18	108.50	110.52
13	H	1222	CLA	CHD-C1D-ND	-2.18	122.45	124.45
16	H	4010	BCR	C11-C12-C13	-2.18	120.30	126.42
16	V	4019	BCR	C10-C11-C12	-2.18	116.42	123.22
17	G	5001	LHG	C27-C26-C25	-2.18	103.37	114.42
16	B	4010	BCR	C11-C12-C13	-2.18	120.30	126.42
13	e	1135	CLA	O2D-CGD-CBD	2.18	115.14	111.27
13	G	1123	CLA	CHA-C1A-NA	-2.18	121.41	126.40
13	H	1021	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	3	503	CLA	C2D-C1D-ND	-2.18	108.50	110.10
13	1	509	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
16	a	524	BCR	C37-C22-C23	2.18	121.51	118.08
16	Z	522	BCR	C23-C24-C25	-2.18	121.09	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1210	CLA	C3A-C2A-C1A	2.18	104.60	101.34
13	G	1117	CLA	C3C-C4C-NC	-2.18	108.13	110.57
13	H	1224	CLA	CMB-C2B-C3B	2.18	131.86	126.59
16	s	524	BCR	C21-C20-C19	-2.18	116.43	123.22
13	Y	518	CLA	CHC-C4B-NB	2.18	126.56	124.26
13	t	511	CLA	CMB-C2B-C1B	-2.18	122.06	125.37
17	A	5001	LHG	C27-C26-C25	-2.18	103.38	114.42
16	L	4019	BCR	C40-C30-C25	-2.18	106.77	110.30
13	B	1222	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
13	f	1222	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
13	f	1226	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
13	f	1203	CLA	CHB-C1B-NB	2.17	126.56	124.26
16	s	524	BCR	C37-C22-C23	2.17	121.50	118.08
13	B	1021	CLA	C2A-C1A-CHA	2.17	127.66	123.86
13	G	1237	CLA	CAC-C3C-C4C	2.17	127.63	124.81
16	n	4019	BCR	C40-C30-C25	-2.17	106.77	110.30
16	s	523	BCR	C3-C4-C5	-2.17	110.20	114.08
13	A	1123	CLA	CHA-C1A-NA	-2.17	121.42	126.40
13	b	503	CLA	CHD-C1D-ND	-2.17	122.46	124.45
16	L	4019	BCR	C10-C11-C12	-2.17	116.44	123.22
16	V	4020	BCR	C33-C5-C6	-2.17	122.09	124.53
16	H	4014	BCR	C15-C14-C13	-2.17	124.21	127.31
13	e	1123	CLA	CHA-C1A-NA	-2.17	121.42	126.40
13	4	502	CLA	C3B-C4B-NB	-2.17	108.50	110.52
13	a	507	CLA	C3B-C4B-NB	-2.17	108.50	110.52
13	3	508	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	v	508	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
13	B	1205	CLA	CHB-C1B-NB	2.17	126.56	124.26
16	1	521	BCR	C29-C30-C25	2.17	113.82	110.48
13	e	1115	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
17	A	5008	LHG	C27-C26-C25	-2.17	103.40	114.42
16	V	4019	BCR	C40-C30-C25	-2.17	106.78	110.30
13	B	1203	CLA	CMB-C2B-C3B	2.17	131.84	126.59
16	4	521	BCR	C20-C19-C18	-2.17	120.32	126.42
16	W	4021	BCR	C36-C18-C19	2.17	121.50	118.08
16	Y	521	BCR	C29-C30-C25	2.17	113.82	110.48
17	G	5008	LHG	C27-C26-C25	-2.17	103.41	114.42
18	1	902	LMU	C4'-C3'-C2'	2.17	114.61	110.82
13	e	1137	CLA	C2A-C1A-CHA	2.17	127.65	123.86
13	u	509	CLA	C3B-C4B-NB	-2.17	108.50	110.52
13	4	517	CLA	C2A-C1A-CHA	2.17	127.65	123.86
13	G	1130	CLA	C1-C2-C3	-2.17	122.29	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1226	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
13	f	1203	CLA	CMB-C2B-C3B	2.17	131.84	126.59
13	B	1226	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
13	e	1139	CLA	CHB-C4A-NA	2.17	127.51	124.51
13	a	508	CLA	CMB-C2B-C3B	2.17	131.84	126.59
13	l	1303	CLA	O2D-CGD-CBD	2.17	115.12	111.27
13	G	1022	CLA	C4D-C3D-CAD	-2.17	105.54	108.10
13	H	1217	CLA	CHC-C4B-NB	2.17	126.55	124.26
16	Y	523	BCR	C7-C8-C9	-2.17	122.96	126.23
13	m	1105	CLA	CAC-C3C-C2C	2.17	131.24	127.53
16	1	523	BCR	C11-C10-C9	-2.17	124.22	127.31
13	f	1222	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	G	1121	CLA	C1-C2-C3	-2.17	122.30	126.04
13	e	1237	CLA	CAC-C3C-C4C	2.17	127.62	124.81
17	e	5008	LHG	C27-C26-C25	-2.17	103.43	114.42
13	G	1118	CLA	C2A-C1A-CHA	2.17	127.65	123.86
13	G	1104	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
13	u	509	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
16	Y	523	BCR	C37-C22-C23	2.17	121.49	118.08
13	G	1135	CLA	O2D-CGD-CBD	2.17	115.12	111.27
16	2	522	BCR	C23-C24-C25	-2.16	121.12	127.20
13	A	1115	CLA	CMB-C2B-C1B	-2.16	122.07	125.37
16	a	524	BCR	C27-C26-C25	-2.16	119.59	122.73
13	H	1222	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
13	b	517	CLA	C2A-C1A-CHA	2.16	127.64	123.86
13	L	1501	CLA	C3B-C4B-NB	-2.16	108.51	110.52
13	q	509	CLA	C3B-C4B-NB	-2.16	108.51	110.52
16	r	522	BCR	C23-C24-C25	-2.16	121.12	127.20
16	3	524	BCR	C27-C26-C25	-2.16	119.59	122.73
13	1	510	CLA	CHB-C1B-NB	2.16	126.55	124.26
13	q	510	CLA	CHB-C1B-NB	2.16	126.55	124.26
16	n	4019	BCR	C10-C11-C12	-2.16	116.47	123.22
13	A	1121	CLA	C1-C2-C3	-2.16	122.30	126.04
13	G	1011	CLA	CHA-C1A-NA	-2.16	121.44	126.40
13	4	503	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
13	H	1224	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
13	f	1208	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	e	1130	CLA	C1-C2-C3	-2.16	122.30	126.04
13	5	509	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
16	Y	523	BCR	C36-C18-C19	2.16	121.48	118.08
13	A	1137	CLA	C2A-C1A-CHA	2.16	127.64	123.86
13	H	1239	CLA	C11-C10-C8	-2.16	108.93	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	t	521	BCR	C20-C19-C18	-2.16	120.34	126.42
16	Y	522	BCR	C27-C26-C25	-2.16	119.59	122.73
13	A	1130	CLA	C1-C2-C3	-2.16	122.30	126.04
13	B	1224	CLA	CMB-C2B-C3B	2.16	131.82	126.59
16	f	4009	BCR	C1-C6-C5	-2.16	119.57	122.61
13	4	511	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
13	H	1203	CLA	CMB-C2B-C3B	2.16	131.82	126.59
13	e	1022	CLA	C3B-C4B-NB	-2.16	108.51	110.52
16	a	523	BCR	C3-C4-C5	-2.16	110.22	114.08
16	Y	523	BCR	C11-C10-C9	-2.16	124.23	127.31
13	n	1501	CLA	C2A-C1A-CHA	2.16	127.64	123.86
13	e	1117	CLA	C3C-C4C-NC	-2.16	108.15	110.57
13	c	503	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	G	1130	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	f	1224	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	Y	511	CLA	CHB-C1B-NB	2.16	126.54	124.26
13	H	1023	CLA	CMD-C2D-C3D	2.16	132.58	127.61
13	G	1115	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
13	A	1104	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	B	1201	CLA	CHB-C1B-NB	2.16	126.54	124.26
13	1	518	CLA	CHC-C4B-NB	2.16	126.54	124.26
13	Y	510	CLA	CHB-C1B-NB	2.16	126.54	124.26
13	V	1501	CLA	C2A-C1A-CHA	2.16	127.63	123.86
13	e	1011	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	B	1236	CLA	O2D-CGD-CBD	2.16	115.10	111.27
16	H	4009	BCR	C1-C6-C5	-2.16	119.57	122.61
16	M	4021	BCR	C36-C18-C19	2.16	121.48	118.08
13	c	502	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
13	H	1213	CLA	CMB-C2B-C3B	2.16	131.81	126.59
13	K	1105	CLA	CAC-C3C-C2C	2.16	131.22	127.53
13	4	503	CLA	CHD-C1D-ND	-2.16	122.47	124.45
16	3	523	BCR	C3-C4-C5	-2.16	110.23	114.08
13	Z	511	CLA	CHB-C1B-NB	2.16	126.54	124.26
13	e	1111	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
13	B	1239	CLA	C11-C10-C8	-2.16	108.95	115.92
16	3	523	BCR	C36-C18-C19	2.16	121.47	118.08
16	f	4014	BCR	C31-C1-C6	-2.16	106.80	110.30
13	e	1103	CLA	C3B-C4B-NB	-2.16	108.52	110.52
16	b	521	BCR	C20-C19-C18	-2.16	120.36	126.42
17	B	1855	LHG	C27-C26-C25	-2.16	103.48	114.42
13	U	1401	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
16	1	523	BCR	C7-C8-C9	-2.16	122.98	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	822	SQD	O6-C1-C2	2.16	111.67	108.30
16	G	4003	BCR	C16-C15-C14	-2.15	119.06	123.47
13	e	1106	CLA	CHC-C4B-NB	2.15	126.54	124.26
13	e	1130	CLA	CHD-C1D-ND	-2.15	122.47	124.45
17	f	1855	LHG	C27-C26-C25	-2.15	103.49	114.42
13	f	1240	CLA	O1D-CGD-CBD	2.15	128.89	124.48
13	A	1011	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	f	1239	CLA	O2D-CGD-CBD	2.15	115.10	111.27
13	G	1101	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
13	Y	508	CLA	CHC-C1C-NC	2.15	127.47	124.20
13	B	1224	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
16	A	4003	BCR	C16-C15-C14	-2.15	119.06	123.47
16	t	522	BCR	C30-C25-C26	-2.15	119.58	122.61
13	t	502	CLA	C3B-C4B-NB	-2.15	108.52	110.52
13	b	508	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
13	t	508	CLA	C2D-C1D-ND	-2.15	108.52	110.10
13	f	1224	CLA	CMB-C2B-C3B	2.15	131.80	126.59
17	H	1855	LHG	C27-C26-C25	-2.15	103.49	114.42
16	J	4012	BCR	C10-C11-C12	-2.15	116.50	123.22
13	G	1106	CLA	CMB-C2B-C3B	2.15	131.80	126.59
16	b	524	BCR	C15-C16-C17	-2.15	119.06	123.47
13	G	1011	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	b	511	CLA	C2D-C1D-ND	-2.15	108.52	110.10
13	B	1023	CLA	CMD-C2D-C3D	2.15	132.56	127.61
13	G	1139	CLA	C11-C10-C8	-2.15	108.96	115.92
16	I	4018	BCR	C35-C13-C12	2.15	121.47	118.08
16	T	4012	BCR	C10-C11-C12	-2.15	116.50	123.22
13	A	1101	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
16	A	4008	BCR	C30-C25-C26	-2.15	119.58	122.61
13	B	1239	CLA	O2D-CGD-CBD	2.15	115.09	111.27
13	f	1234	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
13	c	509	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	a	502	CLA	C2A-C1A-CHA	2.15	127.62	123.86
13	B	1208	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	u	502	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
13	f	1239	CLA	C11-C10-C8	-2.15	108.97	115.92
16	l	4012	BCR	C10-C11-C12	-2.15	116.51	123.22
18	Y	902	LMU	C4'-C3'-C2'	2.15	114.58	110.82
13	e	1104	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	G	1140	CLA	CAA-C2A-C1A	2.15	119.02	111.97
13	B	1213	CLA	CMB-C2B-C3B	2.15	131.79	126.59
13	b	508	CLA	C2D-C1D-ND	-2.15	108.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1117	CLA	C2D-C1D-ND	-2.15	108.52	110.10
13	G	1137	CLA	C2A-C1A-CHA	2.15	127.62	123.86
13	e	1112	CLA	O2D-CGD-CBD	2.15	115.09	111.27
13	U	1103	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	Z	509	CLA	CMB-C2B-C3B	2.15	131.79	126.59
13	1	501	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	3	511	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	H	1201	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	e	1132	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	e	1101	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
13	a	509	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
20	c	822	SQD	O6-C1-C2	2.15	111.66	108.30
16	s	524	BCR	C27-C26-C25	-2.15	119.61	122.73
13	K	1401	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	5	502	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
16	t	522	BCR	C11-C10-C9	-2.15	124.25	127.31
13	H	1234	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
17	A	5002	LHG	C11-C10-C9	-2.15	103.52	114.42
13	H	1206	CLA	O1D-CGD-CBD	2.15	128.88	124.48
13	f	1023	CLA	CMD-C2D-C3D	2.15	132.55	127.61
13	Y	509	CLA	CMB-C2B-C3B	2.15	131.79	126.59
16	B	4014	BCR	C31-C1-C6	-2.15	106.82	110.30
13	B	1234	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
13	G	1111	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	e	1140	CLA	CAA-C2A-C1A	2.15	119.01	111.97
13	q	509	CLA	CMB-C2B-C3B	2.15	131.79	126.59
13	t	517	CLA	C2A-C1A-CHA	2.15	127.61	123.86
16	A	4011	BCR	C29-C30-C25	2.15	113.79	110.48
13	e	1139	CLA	C11-C10-C8	-2.15	108.98	115.92
17	G	5002	LHG	C11-C10-C9	-2.15	103.53	114.42
16	2	523	BCR	C16-C15-C14	-2.15	119.08	123.47
20	u	822	SQD	O6-C1-C2	2.15	111.65	108.30
13	a	504	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	s	511	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	1	508	CLA	CHC-C1C-NC	2.15	127.46	124.20
16	4	524	BCR	C15-C16-C17	-2.15	119.08	123.47
13	t	503	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	A	1139	CLA	C11-C10-C8	-2.15	108.98	115.92
13	s	502	CLA	C2A-C1A-CHA	2.15	127.61	123.86
16	r	523	BCR	C16-C15-C14	-2.15	119.08	123.47
13	G	1110	CLA	CAA-CBA-CGA	-2.15	106.98	113.25
16	S	4018	BCR	C35-C13-C12	2.15	121.46	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	523	BCR	C36-C18-C19	2.15	121.46	118.08
13	e	1130	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
13	t	503	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
13	v	502	CLA	C3B-C4B-NB	-2.15	108.53	110.52
13	f	1221	CLA	CHA-C1A-NA	-2.14	121.49	126.40
13	G	1130	CLA	CHD-C1D-ND	-2.14	122.48	124.45
13	A	1140	CLA	CAA-C2A-C1A	2.14	119.00	111.97
17	S	5001	LHG	C27-C26-C25	-2.14	103.54	114.42
16	q	523	BCR	C7-C8-C9	-2.14	123.00	126.23
16	e	4003	BCR	C16-C15-C14	-2.14	119.08	123.47
13	u	503	CLA	C3B-C4B-NB	-2.14	108.53	110.52
16	s	522	BCR	C23-C24-C25	-2.14	121.18	127.20
16	B	4009	BCR	C1-C6-C5	-2.14	119.59	122.61
16	S	4018	BCR	C10-C11-C12	-2.14	116.53	123.22
13	H	1239	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
13	4	508	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
16	c	523	BCR	C23-C24-C25	-2.14	121.18	127.20
16	t	524	BCR	C15-C16-C17	-2.14	119.08	123.47
13	A	1022	CLA	C3B-C4B-NB	-2.14	108.53	110.52
13	6	501	CLA	C1-C2-C3	-2.14	122.34	126.04
13	1	509	CLA	CMB-C2B-C3B	2.14	131.78	126.59
16	u	523	BCR	C23-C24-C25	-2.14	121.19	127.20
16	Z	523	BCR	C16-C15-C14	-2.14	119.09	123.47
13	c	507	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
17	e	5002	LHG	C11-C10-C9	-2.14	103.55	114.42
13	v	503	CLA	C2A-C1A-CHA	2.14	127.60	123.86
16	A	4002	BCR	C38-C26-C25	-2.14	122.12	124.53
13	t	508	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
13	e	1121	CLA	C1-C2-C3	-2.14	122.34	126.04
13	A	1110	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
13	B	1222	CLA	CHD-C1D-ND	-2.14	122.49	124.45
16	k	4018	BCR	C35-C13-C12	2.14	121.45	118.08
13	T	1302	CLA	O2D-CGD-CBD	2.14	115.07	111.27
13	A	1139	CLA	CHB-C4A-NA	2.14	127.47	124.51
13	Z	512	CLA	CHB-C4A-NA	2.14	127.47	124.51
13	2	509	CLA	CMB-C2B-C3B	2.14	131.77	126.59
13	3	502	CLA	C2A-C1A-CHA	2.14	127.60	123.86
13	f	1206	CLA	O1D-CGD-CBD	2.14	128.86	124.48
13	r	509	CLA	CMB-C2B-C3B	2.14	131.77	126.59
16	e	4011	BCR	C29-C30-C25	2.14	113.78	110.48
13	e	1110	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
13	A	1130	CLA	O2A-CGA-O1A	-2.14	118.19	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	5221	LHG	C18-C17-C16	-2.14	103.56	114.42
13	f	1213	CLA	CMB-C2B-C3B	2.14	131.77	126.59
13	A	1117	CLA	C2D-C1D-ND	-2.14	108.53	110.10
16	f	4004	BCR	C10-C11-C12	-2.14	116.54	123.22
16	k	4018	BCR	C10-C11-C12	-2.14	116.54	123.22
13	A	1133	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
13	e	1133	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
17	I	5001	LHG	C27-C26-C25	-2.14	103.56	114.42
16	q	521	BCR	C29-C30-C25	2.14	113.78	110.48
13	A	1111	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
13	f	1239	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
17	n	5221	LHG	C18-C17-C16	-2.14	103.57	114.42
16	s	523	BCR	C36-C18-C19	2.14	121.45	118.08
17	L	5221	LHG	C18-C17-C16	-2.14	103.57	114.42
13	d	501	CLA	C1-C2-C3	-2.14	122.34	126.04
16	I	4018	BCR	C10-C11-C12	-2.14	116.54	123.22
16	H	4004	BCR	C10-C11-C12	-2.14	116.54	123.22
13	A	1105	CLA	CHB-C1B-NB	2.14	126.52	124.26
13	H	1240	CLA	O1D-CGD-CBD	2.14	128.86	124.48
16	5	523	BCR	C23-C24-C25	-2.14	121.20	127.20
16	B	4004	BCR	C10-C11-C12	-2.14	116.55	123.22
16	q	522	BCR	C27-C26-C25	-2.14	119.63	122.73
16	3	524	BCR	C38-C26-C27	2.14	117.72	113.62
13	B	1221	CLA	CHA-C1A-NA	-2.14	121.50	126.40
13	G	1132	CLA	CHB-C1B-NB	2.14	126.52	124.26
16	1	523	BCR	C36-C18-C19	2.14	121.44	118.08
16	d	522	BCR	C36-C18-C19	2.14	121.44	118.08
16	o	4021	BCR	C36-C18-C19	2.14	121.44	118.08
13	A	1130	CLA	CHD-C1D-ND	-2.14	122.49	124.45
13	G	1119	CLA	CHD-C1D-ND	-2.14	122.49	124.45
16	b	522	BCR	C11-C10-C9	-2.14	124.26	127.31
13	U	1105	CLA	CAC-C3C-C2C	2.14	131.18	127.53
13	q	508	CLA	CHC-C1C-NC	2.14	127.44	124.20
13	m	1401	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
16	f	4009	BCR	C19-C18-C17	-2.14	115.66	118.94
13	H	1239	CLA	O2D-CGD-CBD	2.14	115.06	111.27
13	B	1206	CLA	O1D-CGD-CBD	2.14	128.86	124.48
13	q	501	CLA	CHB-C1B-NB	2.14	126.52	124.26
13	G	1133	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
16	Y	524	BCR	C3-C4-C5	-2.14	110.26	114.08
13	A	1117	CLA	C3C-C4C-NC	-2.14	108.17	110.57
13	J	1302	CLA	O2D-CGD-CBD	2.14	115.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	512	CLA	CHB-C4A-NA	2.14	127.47	124.51
13	U	1103	CLA	CHB-C1B-NB	2.14	126.52	124.26
16	B	4009	BCR	C19-C18-C17	-2.14	115.66	118.94
13	G	1129	CLA	CMB-C2B-C3B	2.14	131.76	126.59
16	e	4008	BCR	C30-C25-C26	-2.14	119.61	122.61
13	l	1302	CLA	O2D-CGD-CBD	2.14	115.06	111.27
17	A	5001	LHG	C18-C17-C16	-2.14	103.59	114.42
17	G	5001	LHG	C18-C17-C16	-2.14	103.59	114.42
13	f	1213	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
13	Y	503	CLA	C2A-C1A-CHA	2.13	127.59	123.86
13	G	1105	CLA	CHB-C1B-NB	2.13	126.52	124.26
13	G	1139	CLA	CHB-C4A-NA	2.13	127.46	124.51
16	a	523	BCR	C1-C6-C5	-2.13	119.61	122.61
16	B	4009	BCR	C28-C27-C26	-2.13	110.27	114.08
13	G	1104	CLA	CHD-C1D-ND	-2.13	122.49	124.45
13	v	516	CLA	CHD-C1D-ND	-2.13	122.49	124.45
16	d	524	BCR	C37-C22-C23	2.13	121.44	118.08
16	t	523	BCR	C16-C15-C14	-2.13	119.10	123.47
13	B	1240	CLA	O1D-CGD-CBD	2.13	128.85	124.48
13	H	1213	CLA	C2A-C1A-CHA	2.13	127.59	123.86
13	q	503	CLA	C2A-C1A-CHA	2.13	127.59	123.86
13	G	1107	CLA	O2D-CGD-CBD	2.13	115.06	111.27
13	A	1106	CLA	CMB-C2B-C3B	2.13	131.75	126.59
13	G	1127	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
13	u	503	CLA	CHD-C1D-ND	-2.13	122.49	124.45
17	H	1842	LHG	C27-C26-C25	-2.13	103.60	114.42
17	k	5001	LHG	C27-C26-C25	-2.13	103.60	114.42
13	6	502	CLA	C3B-C4B-NB	-2.13	108.54	110.52
17	e	5001	LHG	C18-C17-C16	-2.13	103.60	114.42
16	H	4006	BCR	C29-C30-C25	2.13	113.76	110.48
13	B	1210	CLA	C3A-C2A-C1A	2.13	104.53	101.34
16	s	524	BCR	C38-C26-C27	2.13	117.71	113.62
18	e	1849	LMU	O5'-C1'-C2'	2.13	114.86	110.35
16	4	522	BCR	C11-C10-C9	-2.13	124.27	127.31
16	H	4006	BCR	C20-C21-C22	-2.13	124.27	127.31
13	A	1237	CLA	C11-C12-C13	-2.13	109.03	115.92
13	B	1239	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
16	2	521	BCR	C20-C19-C18	-2.13	120.43	126.42
13	f	1210	CLA	C3A-C2A-C1A	2.13	104.53	101.34
13	e	1130	CLA	C16-C15-C13	-2.13	109.03	115.92
13	3	509	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
13	5	507	CLA	O2A-CGA-O1A	-2.13	117.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4006	BCR	C29-C30-C25	2.13	113.76	110.48
13	q	505	CLA	C3B-C4B-NB	-2.13	108.54	110.52
13	1	503	CLA	C2A-C1A-CHA	2.13	127.58	123.86
17	B	1842	LHG	C27-C26-C25	-2.13	103.61	114.42
13	A	1127	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
13	A	1112	CLA	O2D-CGD-CBD	2.13	115.05	111.27
13	G	1237	CLA	C11-C12-C13	-2.13	109.04	115.92
17	f	1842	LHG	C27-C26-C25	-2.13	103.61	114.42
16	r	523	BCR	C37-C22-C23	2.13	121.43	118.08
16	v	522	BCR	C36-C18-C19	2.13	121.43	118.08
16	3	523	BCR	C1-C6-C5	-2.13	119.61	122.61
13	e	1237	CLA	C11-C12-C13	-2.13	109.04	115.92
16	b	524	BCR	C28-C27-C26	-2.13	110.28	114.08
16	a	524	BCR	C38-C26-C27	2.13	117.70	113.62
13	A	1119	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	e	5009	LHG	C18-C17-C16	-2.13	103.62	114.42
13	G	1112	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
13	G	1103	CLA	C3B-C4B-NB	-2.13	108.54	110.52
17	G	5009	LHG	C18-C17-C16	-2.13	103.62	114.42
13	e	1107	CLA	O2D-CGD-CBD	2.13	115.05	111.27
13	v	501	CLA	C1-C2-C3	-2.13	122.36	126.04
13	B	1213	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
16	H	4014	BCR	C31-C1-C6	-2.13	106.85	110.30
16	c	522	BCR	C21-C20-C19	-2.13	116.58	123.22
16	B	4006	BCR	C29-C30-C25	2.13	113.76	110.48
17	A	5009	LHG	C18-C17-C16	-2.13	103.62	114.42
13	H	1221	CLA	CHA-C1A-NA	-2.13	121.53	126.40
13	3	507	CLA	CHC-C4B-NB	2.13	126.51	124.26
13	Y	501	CLA	CHB-C1B-NB	2.13	126.51	124.26
13	a	507	CLA	CHC-C4B-NB	2.13	126.51	124.26
13	q	518	CLA	CHC-C4B-NB	2.13	126.51	124.26
13	B	1240	CLA	C1-C2-C3	-2.13	122.36	126.04
16	Z	521	BCR	C20-C19-C18	-2.13	120.44	126.42
16	1	522	BCR	C27-C26-C25	-2.13	119.64	122.73
13	d	506	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
13	s	509	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
13	A	1237	CLA	C2D-C1D-ND	-2.13	108.54	110.10
13	2	502	CLA	CHB-C1B-NB	2.13	126.51	124.26
13	e	1104	CLA	CHD-C1D-ND	-2.13	122.50	124.45
13	H	1225	CLA	C1-C2-C3	-2.13	122.37	126.04
16	f	4009	BCR	C28-C27-C26	-2.13	110.28	114.08
13	A	1131	CLA	O2A-CGA-O1A	-2.13	118.23	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	6	524	BCR	C37-C22-C23	2.13	121.43	118.08
13	r	512	CLA	CHB-C4A-NA	2.13	127.45	124.51
13	e	1105	CLA	CHB-C1B-NB	2.13	126.51	124.26
13	G	1130	CLA	C16-C15-C13	-2.13	109.05	115.92
13	A	1107	CLA	O2D-CGD-CBD	2.12	115.04	111.27
13	n	1501	CLA	CMB-C2B-C1B	-2.12	122.13	125.37
16	G	4008	BCR	C30-C25-C26	-2.12	119.62	122.61
13	t	507	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
13	a	516	CLA	O2A-CGA-O1A	-2.12	118.00	123.30
13	B	1225	CLA	C1-C2-C3	-2.12	122.37	126.04
16	4	524	BCR	C28-C27-C26	-2.12	110.28	114.08
13	f	1203	CLA	O1D-CGD-CBD	2.12	128.83	124.48
16	b	522	BCR	C30-C25-C26	-2.12	119.62	122.61
16	B	4009	BCR	C20-C21-C22	-2.12	124.28	127.31
13	V	1501	CLA	C3B-C4B-NB	-2.12	108.55	110.52
13	e	1129	CLA	CMB-C2B-C3B	2.12	131.73	126.59
13	e	1127	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
13	s	513	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
13	H	1236	CLA	O2D-CGD-CBD	2.12	115.04	111.27
16	H	4009	BCR	C20-C21-C22	-2.12	124.28	127.31
13	6	516	CLA	CHD-C1D-ND	-2.12	122.50	124.45
16	G	4011	BCR	C29-C30-C25	2.12	113.75	110.48
13	e	1138	CLA	CHB-C1B-NB	2.12	126.50	124.26
13	A	1139	CLA	O2D-CGD-CBD	2.12	115.04	111.27
13	6	506	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
16	4	523	BCR	C16-C15-C14	-2.12	119.13	123.47
13	5	503	CLA	CHD-C1D-ND	-2.12	122.50	124.45
13	G	1131	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
16	u	523	BCR	C24-C23-C22	-2.12	123.03	126.23
13	A	1130	CLA	C16-C15-C13	-2.12	109.06	115.92
16	B	4006	BCR	C20-C21-C22	-2.12	124.28	127.31
13	4	507	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
13	A	1132	CLA	CHB-C1B-NB	2.12	126.50	124.26
13	1	505	CLA	C3B-C4B-NB	-2.12	108.55	110.52
17	G	5004	LHG	C27-C26-C25	-2.12	103.66	114.42
16	J	4012	BCR	C23-C24-C25	-2.12	121.25	127.20
13	H	1213	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
13	e	1131	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
13	G	1237	CLA	C2D-C1D-ND	-2.12	108.54	110.10
13	d	516	CLA	CHD-C1D-ND	-2.12	122.50	124.45
13	K	1103	CLA	CHB-C1B-NB	2.12	126.50	124.26
13	s	507	CLA	CHC-C4B-NB	2.12	126.50	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1235	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
13	A	1111	CLA	CMB-C2B-C3B	2.12	131.72	126.59
16	q	523	BCR	C36-C18-C19	2.12	121.42	118.08
16	c	523	BCR	C24-C23-C22	-2.12	123.03	126.23
16	4	522	BCR	C30-C25-C26	-2.12	119.63	122.61
13	H	1240	CLA	C1-C2-C3	-2.12	122.38	126.04
16	l	4013	BCR	C4-C5-C6	-2.12	119.65	122.73
16	1	524	BCR	C3-C4-C5	-2.12	110.29	114.08
13	3	504	CLA	CHB-C1B-NB	2.12	126.50	124.26
13	m	1103	CLA	CHB-C1B-NB	2.12	126.50	124.26
13	e	1106	CLA	CMB-C2B-C3B	2.12	131.72	126.59
13	f	1226	CLA	CHD-C1D-C2D	2.12	129.93	125.48
13	u	507	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
18	A	1849	LMU	O5'-C1'-C2'	2.12	114.83	110.35
13	H	1220	CLA	CHD-C1D-ND	-2.12	122.51	124.45
13	B	1203	CLA	O1D-CGD-CBD	2.12	128.82	124.48
13	A	1129	CLA	CMB-C2B-C3B	2.12	131.72	126.59
16	r	522	BCR	C30-C25-C26	-2.12	119.63	122.61
13	e	1139	CLA	O2D-CGD-CBD	2.12	115.03	111.27
13	f	1021	CLA	CHB-C4A-NA	2.12	127.44	124.51
13	G	1111	CLA	CMB-C2B-C3B	2.12	131.72	126.59
16	u	522	BCR	C21-C20-C19	-2.12	116.61	123.22
16	r	524	BCR	C1-C6-C5	-2.12	119.63	122.61
16	f	4009	BCR	C20-C21-C22	-2.12	124.29	127.31
16	5	522	BCR	C21-C20-C19	-2.12	116.61	123.22
13	B	1235	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
16	r	521	BCR	C20-C19-C18	-2.12	120.47	126.42
16	f	4004	BCR	C34-C9-C8	2.12	121.41	118.08
13	2	504	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
13	G	1112	CLA	O2D-CGD-CBD	2.12	115.03	111.27
16	R	4016	BCR	C20-C21-C22	-2.12	124.29	127.31
16	H	4009	BCR	C19-C18-C17	-2.12	115.69	118.94
13	Z	502	CLA	CHB-C1B-NB	2.12	126.50	124.26
16	q	524	BCR	C3-C4-C5	-2.12	110.30	114.08
13	B	1204	CLA	C11-C10-C8	-2.12	109.08	115.92
13	G	1136	CLA	O1D-CGD-CBD	2.12	128.81	124.48
13	H	1203	CLA	O1D-CGD-CBD	2.12	128.81	124.48
13	G	1112	CLA	CMB-C2B-C3B	2.12	131.71	126.59
13	e	1111	CLA	CMB-C2B-C3B	2.12	131.71	126.59
13	f	1219	CLA	C2D-C1D-ND	-2.12	108.55	110.10
16	3	522	BCR	C23-C24-C25	-2.12	121.26	127.20
16	T	4015	BCR	C10-C11-C12	-2.12	116.62	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	l	4012	BCR	C23-C24-C25	-2.11	121.26	127.20
13	A	1117	CLA	CMB-C2B-C3B	2.11	131.71	126.59
13	f	1021	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
13	f	1240	CLA	C1-C2-C3	-2.11	122.39	126.04
13	b	507	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
13	s	504	CLA	CHB-C1B-NB	2.11	126.50	124.26
16	t	522	BCR	C21-C20-C19	-2.11	116.62	123.22
13	G	1139	CLA	O2D-CGD-CBD	2.11	115.02	111.27
13	A	1118	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	A	1104	CLA	CHD-C1D-ND	-2.11	122.51	124.45
16	B	4004	BCR	C34-C9-C8	2.11	121.41	118.08
16	6	522	BCR	C36-C18-C19	2.11	121.41	118.08
13	H	1209	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	Z	504	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
16	j	4016	BCR	C20-C21-C22	-2.11	124.30	127.31
16	H	4009	BCR	C28-C27-C26	-2.11	110.31	114.08
13	f	1201	CLA	CHB-C1B-NB	2.11	126.49	124.26
17	A	5004	LHG	C27-C26-C25	-2.11	103.70	114.42
13	G	1117	CLA	CMB-C2B-C3B	2.11	131.70	126.59
13	e	1117	CLA	CMB-C2B-C3B	2.11	131.70	126.59
13	f	1220	CLA	C2D-C1D-ND	-2.11	108.55	110.10
13	6	503	CLA	C2A-C1A-CHA	2.11	127.55	123.86
16	a	522	BCR	C23-C24-C25	-2.11	121.27	127.20
16	b	523	BCR	C16-C15-C14	-2.11	119.15	123.47
13	A	1105	CLA	C3A-C2A-C1A	2.11	104.50	101.34
13	f	1225	CLA	C1-C2-C3	-2.11	122.39	126.04
13	B	1213	CLA	C2A-C1A-CHA	2.11	127.55	123.86
16	t	524	BCR	C28-C27-C26	-2.11	110.31	114.08
13	H	1235	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
13	d	502	CLA	C3B-C4B-NB	-2.11	108.56	110.52
13	f	1204	CLA	C11-C10-C8	-2.11	109.10	115.92
13	e	1118	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
16	b	522	BCR	C21-C20-C19	-2.11	116.63	123.22
16	2	523	BCR	C37-C22-C23	2.11	121.40	118.08
17	e	5004	LHG	C27-C26-C25	-2.11	103.72	114.42
13	Y	519	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
13	B	1231	CLA	C3B-C4B-NB	-2.11	108.56	110.52
13	B	1213	CLA	CHB-C1B-NB	2.11	126.49	124.26
13	A	1112	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
16	v	521	BCR	C16-C15-C14	-2.11	119.16	123.47
16	4	522	BCR	C21-C20-C19	-2.11	116.64	123.22
13	3	513	CLA	O2A-CGA-O1A	-2.11	118.27	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	r	518	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
16	q	523	BCR	C27-C26-C25	-2.11	119.67	122.73
20	Y	822	SQD	O48-C23-O10	-2.11	118.27	123.59
18	G	1849	LMU	O5'-C1'-C2'	2.11	114.81	110.35
13	A	1138	CLA	CHB-C1B-NB	2.11	126.49	124.26
13	G	1105	CLA	C3B-C4B-NB	-2.11	108.56	110.52
13	A	1116	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
16	2	524	BCR	C1-C6-C5	-2.11	119.65	122.61
13	e	1119	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	Z	523	BCR	C37-C22-C23	2.11	121.40	118.08
16	v	524	BCR	C37-C22-C23	2.11	121.40	118.08
16	5	523	BCR	C24-C23-C22	-2.11	123.05	126.23
13	L	1501	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
13	r	505	CLA	C3B-C4B-NB	-2.11	108.56	110.52
13	H	1204	CLA	C11-C10-C8	-2.11	109.11	115.92
13	B	1219	CLA	C2D-C1D-ND	-2.11	108.55	110.10
13	B	1023	CLA	CAA-CBA-CGA	-2.11	107.10	113.25
13	a	513	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
13	G	1105	CLA	C3A-C2A-C1A	2.11	104.49	101.34
16	v	524	BCR	C10-C11-C12	-2.10	116.65	123.22
13	Z	505	CLA	C3B-C4B-NB	-2.10	108.56	110.52
16	2	522	BCR	C30-C25-C26	-2.10	119.65	122.61
13	f	1234	CLA	C2A-C1A-CHA	2.10	127.54	123.86
16	n	4019	BCR	C21-C20-C19	-2.10	116.65	123.22
13	Z	518	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	1	822	SQD	O48-C23-O10	-2.10	118.28	123.59
16	s	523	BCR	C1-C6-C5	-2.10	119.65	122.61
16	H	4004	BCR	C39-C30-C25	-2.10	106.89	110.30
13	e	1116	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
16	H	4004	BCR	C29-C30-C25	2.10	113.72	110.48
13	B	1226	CLA	CHD-C1D-C2D	2.10	129.89	125.48
13	e	1105	CLA	C3A-C2A-C1A	2.10	104.49	101.34
13	2	518	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	e	1119	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	H	1224	CLA	C2A-C1A-CHA	2.10	127.53	123.86
16	J	4013	BCR	C4-C5-C6	-2.10	119.68	122.73
20	q	822	SQD	O48-C23-O10	-2.10	118.29	123.59
13	G	1022	CLA	C3B-C4B-NB	-2.10	108.56	110.52
13	H	1213	CLA	CHB-C1B-NB	2.10	126.48	124.26
13	s	507	CLA	C2A-C1A-CHA	2.10	127.53	123.86
20	a	822	SQD	O47-C7-O49	-2.10	118.62	123.70
20	s	822	SQD	O47-C7-O49	-2.10	118.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	516	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
13	B	1021	CLA	CHB-C4A-NA	2.10	127.42	124.51
16	T	4012	BCR	C23-C24-C25	-2.10	121.30	127.20
13	3	507	CLA	C2A-C1A-CHA	2.10	127.53	123.86
13	U	1105	CLA	C3B-C4B-NB	-2.10	108.57	110.52
13	m	1103	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	G	1115	CLA	CHC-C4B-NB	2.10	126.48	124.26
13	f	1213	CLA	C2A-C1A-CHA	2.10	127.53	123.86
16	Z	524	BCR	C1-C6-C5	-2.10	119.66	122.61
13	G	1118	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	r	502	CLA	CHB-C1B-NB	2.10	126.48	124.26
16	l	4015	BCR	C10-C11-C12	-2.10	116.66	123.22
13	V	1501	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
16	6	521	BCR	C16-C15-C14	-2.10	119.17	123.47
13	Y	508	CLA	CMB-C2B-C3B	2.10	131.67	126.59
16	f	4006	BCR	C20-C21-C22	-2.10	124.31	127.31
13	A	1119	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	G	1119	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	A	1112	CLA	CMB-C2B-C3B	2.10	131.67	126.59
13	Y	507	CLA	CHA-C1A-NA	-2.10	121.59	126.40
13	B	1209	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	e	1133	CLA	CHC-C4B-NB	2.10	126.48	124.26
13	B	1012	CLA	C11-C12-C13	-2.10	109.14	115.92
13	v	506	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
16	l	4015	BCR	C16-C15-C14	-2.10	119.18	123.47
13	e	1105	CLA	C3B-C4B-NB	-2.10	108.57	110.52
13	B	1021	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
16	L	4019	BCR	C21-C20-C19	-2.10	116.67	123.22
13	b	503	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
16	e	4007	BCR	C10-C11-C12	-2.10	116.67	123.22
13	f	1012	CLA	C11-C12-C13	-2.10	109.14	115.92
13	1	508	CLA	CMB-C2B-C3B	2.10	131.67	126.59
13	a	506	CLA	CHB-C1B-NB	2.10	126.48	124.26
13	4	503	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
16	T	4013	BCR	C4-C5-C6	-2.10	119.69	122.73
13	d	503	CLA	C2A-C1A-CHA	2.10	127.53	123.86
20	3	822	SQD	O47-C7-O49	-2.10	118.64	123.70
13	Y	513	CLA	CHB-C1B-NB	2.10	126.48	124.26
13	H	1023	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
16	d	521	BCR	C16-C15-C14	-2.10	119.18	123.47
16	c	524	BCR	C37-C22-C23	2.10	121.38	118.08
16	J	4015	BCR	C10-C11-C12	-2.10	116.68	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	522	BCR	C30-C25-C26	-2.10	119.66	122.61
13	A	1103	CLA	C3B-C4B-NB	-2.10	108.57	110.52
13	e	1119	CLA	CMB-C2B-C3B	2.10	131.66	126.59
16	d	524	BCR	C10-C11-C12	-2.10	116.68	123.22
13	t	503	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
13	e	1112	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
13	e	1122	CLA	C2D-C1D-ND	-2.10	108.56	110.10
13	A	1133	CLA	CHC-C4B-NB	2.10	126.47	124.26
13	G	1116	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
16	f	4004	BCR	C39-C30-C25	-2.09	106.90	110.30
13	s	516	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
16	J	4015	BCR	C16-C15-C14	-2.09	119.18	123.47
13	G	1138	CLA	CHB-C1B-NB	2.09	126.47	124.26
13	H	1012	CLA	C11-C12-C13	-2.09	109.15	115.92
16	V	4019	BCR	C21-C20-C19	-2.09	116.68	123.22
16	r	522	BCR	C36-C18-C19	2.09	121.38	118.08
16	F	4016	BCR	C20-C21-C22	-2.09	124.32	127.31
13	U	1103	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
13	A	1801	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
13	G	1801	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
13	f	1215	CLA	O2D-CGD-CBD	2.09	114.99	111.27
13	2	505	CLA	C3B-C4B-NB	-2.09	108.57	110.52
13	r	504	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
16	H	4004	BCR	C34-C9-C8	2.09	121.37	118.08
13	A	1136	CLA	O1D-CGD-CBD	2.09	128.76	124.48
13	B	1234	CLA	C2A-C1A-CHA	2.09	127.52	123.86
13	a	507	CLA	C2A-C1A-CHA	2.09	127.52	123.86
16	B	4004	BCR	C39-C30-C25	-2.09	106.91	110.30
13	d	507	CLA	C3B-C4B-NB	-2.09	108.58	110.52
13	H	1226	CLA	CHD-C1D-C2D	2.09	129.87	125.48
13	s	510	CLA	CHA-C1A-NA	-2.09	121.61	126.40
13	B	1220	CLA	C2D-C1D-ND	-2.09	108.56	110.10
13	G	1117	CLA	C2D-C1D-ND	-2.09	108.56	110.10
16	T	4015	BCR	C16-C15-C14	-2.09	119.19	123.47
13	2	504	CLA	CHB-C1B-NB	2.09	126.47	124.26
13	e	1801	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
13	q	505	CLA	C1-C2-C3	-2.09	122.43	126.04
13	f	1231	CLA	C3B-C4B-NB	-2.09	108.58	110.52
13	6	507	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
13	1	507	CLA	CHA-C1A-NA	-2.09	121.61	126.40
13	u	503	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
13	q	507	CLA	CHA-C1A-NA	-2.09	121.61	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1131	CLA	O1D-CGD-CBD	2.09	128.76	124.48
13	r	504	CLA	CHB-C1B-NB	2.09	126.47	124.26
13	G	1125	CLA	CMB-C2B-C3B	2.09	131.65	126.59
13	e	1103	CLA	CMB-C2B-C3B	2.09	131.65	126.59
20	H	1852	SQD	O47-C7-O49	-2.09	118.66	123.70
13	K	1103	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
13	q	519	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
13	d	505	CLA	C1-C2-C3	-2.09	122.43	126.04
16	G	4008	BCR	C28-C27-C26	-2.09	110.35	114.08
13	B	1224	CLA	C2A-C1A-CHA	2.09	127.51	123.86
13	Z	504	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
16	5	524	BCR	C37-C22-C23	2.09	121.36	118.08
13	r	504	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
16	6	524	BCR	C10-C11-C12	-2.09	116.71	123.22
13	H	1219	CLA	C2D-C1D-ND	-2.09	108.57	110.10
16	2	522	BCR	C36-C18-C19	2.09	121.36	118.08
16	J	4015	BCR	C15-C16-C17	-2.09	119.20	123.47
16	A	4007	BCR	C10-C11-C12	-2.09	116.71	123.22
13	e	1112	CLA	CMB-C2B-C3B	2.09	131.64	126.59
13	v	507	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
20	f	1852	SQD	O47-C7-O49	-2.09	118.66	123.70
13	1	519	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
13	f	1209	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
13	Y	505	CLA	C3B-C4B-NB	-2.08	108.58	110.52
13	c	503	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
16	G	4011	BCR	C36-C18-C17	-2.08	120.00	122.92
13	f	1023	CLA	C3A-C2A-C1A	2.08	104.46	101.34
13	f	1023	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
13	H	1208	CLA	CHD-C1D-ND	-2.08	122.54	124.45
13	Y	519	CLA	CHB-C1B-NB	2.08	126.46	124.26
13	5	503	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
13	Z	504	CLA	CHB-C1B-NB	2.08	126.46	124.26
13	f	1023	CLA	O2D-CGD-CBD	2.08	114.97	111.27
13	H	1021	CLA	CHB-C4A-NA	2.08	127.39	124.51
13	1	505	CLA	C1-C2-C3	-2.08	122.44	126.04
13	Y	505	CLA	C1-C2-C3	-2.08	122.44	126.04
13	e	1132	CLA	CBC-CAC-C3C	2.08	118.17	112.43
13	A	1136	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
13	A	1132	CLA	CBC-CAC-C3C	2.08	118.17	112.43
13	s	503	CLA	CHD-C1D-ND	-2.08	122.54	124.45
13	G	1136	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
13	d	507	CLA	CAA-C2A-C3A	-2.08	107.08	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1021	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
13	e	1136	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
13	e	1237	CLA	C2D-C1D-ND	-2.08	108.57	110.10
13	G	1133	CLA	CHC-C4B-NB	2.08	126.46	124.26
13	G	1103	CLA	CMB-C2B-C3B	2.08	131.62	126.59
13	Y	504	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
13	Y	518	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
16	T	4015	BCR	C15-C16-C17	-2.08	119.22	123.47
13	1	519	CLA	CHB-C1B-NB	2.08	126.46	124.26
16	l	4015	BCR	C15-C16-C17	-2.08	119.22	123.47
13	v	505	CLA	C1-C2-C3	-2.08	122.45	126.04
13	A	1103	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
16	d	523	BCR	C11-C10-C9	-2.08	124.34	127.31
16	1	523	BCR	C27-C26-C25	-2.08	119.71	122.73
16	G	4007	BCR	C10-C11-C12	-2.08	116.73	123.22
13	q	504	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
13	G	1132	CLA	CBC-CAC-C3C	2.08	118.16	112.43
13	6	505	CLA	C1-C2-C3	-2.08	122.45	126.04
13	G	1131	CLA	O1D-CGD-CBD	2.08	128.73	124.48
13	B	1023	CLA	C3A-C2A-C1A	2.08	104.45	101.34
13	H	1023	CLA	C3A-C2A-C1A	2.08	104.45	101.34
13	2	504	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
16	c	522	BCR	C27-C26-C25	-2.08	119.72	122.73
13	3	510	CLA	CHA-C1A-NA	-2.08	121.64	126.40
16	1	523	BCR	C23-C24-C25	-2.08	121.37	127.20
16	B	4004	BCR	C29-C30-C25	2.08	113.68	110.48
13	G	1103	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
13	q	507	CLA	CHC-C4B-NB	2.08	126.45	124.26
16	u	522	BCR	C27-C26-C25	-2.08	119.72	122.73
13	A	1101	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
17	B	1855	LHG	C18-C17-C16	-2.08	103.89	114.42
13	e	1103	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
13	e	1101	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
16	Y	523	BCR	C27-C26-C25	-2.07	119.72	122.73
13	q	508	CLA	CMB-C2B-C3B	2.07	131.61	126.59
13	v	506	CLA	CHB-C1B-NB	2.07	126.45	124.26
16	u	524	BCR	C37-C22-C23	2.07	121.34	118.08
16	A	4002	BCR	C27-C26-C25	-2.07	119.72	122.73
17	f	1855	LHG	C18-C17-C16	-2.07	103.90	114.42
13	G	1112	CLA	C2A-C1A-CHA	2.07	127.48	123.86
13	A	1103	CLA	CMB-C2B-C3B	2.07	131.61	126.59
16	G	4002	BCR	C27-C26-C25	-2.07	119.72	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1125	CLA	C3A-C2A-C1A	2.07	104.44	101.34
16	Y	523	BCR	C23-C24-C25	-2.07	121.38	127.20
16	B	4005	BCR	C3-C4-C5	-2.07	110.38	114.08
13	f	1215	CLA	CHC-C4B-NB	2.07	126.45	124.26
13	e	1136	CLA	O1D-CGD-CBD	2.07	128.72	124.48
16	A	4008	BCR	C28-C27-C26	-2.07	110.38	114.08
13	A	1127	CLA	C2A-C1A-CHA	2.07	127.48	123.86
13	G	1119	CLA	CMB-C2B-C3B	2.07	131.61	126.59
13	b	508	CLA	CHD-C1D-ND	-2.07	122.55	124.45
16	G	4008	BCR	C15-C16-C17	-2.07	119.23	123.47
13	H	1231	CLA	C3B-C4B-NB	-2.07	108.59	110.52
19	l	5104	LMG	O6-C1-O1	-2.07	105.07	109.97
13	1	504	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
16	f	4004	BCR	C29-C30-C25	2.07	113.67	110.48
13	B	1215	CLA	O2D-CGD-CBD	2.07	114.95	111.27
13	s	507	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
17	H	1855	LHG	C18-C17-C16	-2.07	103.91	114.42
13	f	1224	CLA	C2A-C1A-CHA	2.07	127.48	123.86
16	A	4008	BCR	C15-C16-C17	-2.07	119.23	123.47
13	G	1101	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
13	r	511	CLA	C2A-C1A-CHA	2.07	127.48	123.86
13	d	504	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	e	1117	CLA	C7-C6-C5	-2.07	107.73	113.36
13	1	518	CLA	C3B-C4B-NB	-2.07	108.59	110.52
13	6	507	CLA	C3B-C4B-NB	-2.07	108.59	110.52
13	f	1228	CLA	C3B-C4B-NB	-2.07	108.59	110.52
13	B	1215	CLA	CHC-C4B-NB	2.07	126.45	124.26
13	q	518	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
13	a	510	CLA	CHA-C1A-NA	-2.07	121.66	126.40
13	Y	502	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
13	A	1119	CLA	CMB-C2B-C3B	2.07	131.60	126.59
13	e	1120	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
13	q	503	CLA	C2D-C1D-ND	-2.07	108.58	110.10
16	f	4009	BCR	C4-C5-C6	-2.07	119.73	122.73
13	a	516	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	A	1123	CLA	C3B-C4B-NB	-2.07	108.60	110.52
13	H	1232	CLA	C3B-C4B-NB	-2.07	108.60	110.52
16	e	4008	BCR	C15-C16-C17	-2.07	119.24	123.47
13	e	1131	CLA	O1D-CGD-CBD	2.07	128.72	124.48
13	2	511	CLA	C2A-C1A-CHA	2.07	127.47	123.86
13	G	1022	CLA	C1D-ND-C4D	2.07	107.80	106.33
20	B	1852	SQD	O47-C7-O49	-2.07	118.70	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	K	1103	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	3	503	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	A	1105	CLA	C3B-C4B-NB	-2.07	108.60	110.52
13	e	1120	CLA	CMB-C2B-C3B	2.07	131.59	126.59
16	q	523	BCR	C23-C24-C25	-2.07	121.40	127.20
13	v	503	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
13	l	1303	CLA	C2D-C1D-ND	-2.07	108.58	110.10
13	c	505	CLA	C3B-C4B-NB	-2.07	108.60	110.52
13	u	505	CLA	C3B-C4B-NB	-2.07	108.60	110.52
13	H	1234	CLA	C2A-C1A-CHA	2.07	127.47	123.86
16	Z	522	BCR	C36-C18-C19	2.07	121.33	118.08
13	d	518	CLA	CHB-C1B-NB	2.07	126.44	124.26
13	u	511	CLA	CHB-C1B-NB	2.07	126.44	124.26
13	1	518	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
13	u	504	CLA	CHD-C1D-ND	-2.07	122.56	124.45
13	5	505	CLA	C3B-C4B-NB	-2.07	108.60	110.52
13	B	1023	CLA	CHC-C1C-NC	2.07	127.34	124.20
13	A	1115	CLA	CHC-C4B-NB	2.06	126.44	124.26
13	3	507	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
13	Z	519	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	t	504	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	v	510	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	3	506	CLA	CHB-C1B-NB	2.06	126.44	124.26
16	a	522	BCR	C2-C1-C6	2.06	113.66	110.48
13	Y	510	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
13	6	503	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
13	e	1124	CLA	CMB-C2B-C3B	2.06	131.59	126.59
13	K	1105	CLA	C3B-C4B-NB	-2.06	108.60	110.52
13	Y	518	CLA	C3B-C4B-NB	-2.06	108.60	110.52
13	6	510	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	H	1229	CLA	O2D-CGD-CBD	2.06	114.93	111.27
13	G	1125	CLA	C3A-C2A-C1A	2.06	104.43	101.34
13	t	518	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	G	1117	CLA	C7-C6-C5	-2.06	107.76	113.36
13	Y	502	CLA	CHC-C4B-NB	2.06	126.44	124.26
13	c	506	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
13	e	1125	CLA	CMB-C2B-C3B	2.06	131.58	126.59
13	H	1023	CLA	O2D-CGD-CBD	2.06	114.93	111.27
13	b	516	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
13	e	1128	CLA	C2D-C1D-ND	-2.06	108.58	110.10
13	K	1103	CLA	CHC-C4B-NB	2.06	126.44	124.26
13	G	1127	CLA	C2A-C1A-CHA	2.06	127.46	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	508	CLA	CHD-C1D-ND	-2.06	122.56	124.45
16	5	522	BCR	C27-C26-C25	-2.06	119.74	122.73
16	H	4017	BCR	C8-C7-C6	-2.06	121.42	127.20
13	f	1229	CLA	O2D-CGD-CBD	2.06	114.93	111.27
13	d	506	CLA	CHB-C1B-NB	2.06	126.44	124.26
13	e	1126	CLA	C16-C15-C13	-2.06	109.26	115.92
13	H	1228	CLA	C3B-C4B-NB	-2.06	108.60	110.52
13	t	509	CLA	C3B-C4B-NB	-2.06	108.60	110.52
13	v	507	CLA	C3B-C4B-NB	-2.06	108.60	110.52
13	A	1120	CLA	CMB-C2B-C3B	2.06	131.58	126.59
19	T	5104	LMG	O6-C1-O1	-2.06	105.10	109.97
13	e	1022	CLA	C1D-ND-C4D	2.06	107.80	106.33
13	1	507	CLA	CHC-C4B-NB	2.06	126.44	124.26
13	q	510	CLA	C4-C3-C5	2.06	118.73	115.27
13	A	1125	CLA	CMB-C2B-C3B	2.06	131.57	126.59
13	5	504	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	A	1124	CLA	CMB-C2B-C3B	2.06	131.57	126.59
13	m	1103	CLA	C2D-C1D-ND	-2.06	108.59	110.10
13	q	510	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
13	4	516	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
13	a	507	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
13	t	519	CLA	CHB-C1B-NB	2.06	126.44	124.26
19	J	5104	LMG	O6-C1-O1	-2.06	105.10	109.97
13	1	502	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
16	t	524	BCR	C11-C12-C13	-2.06	120.64	126.42
13	Y	507	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
13	n	1503	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	e	1115	CLA	CHC-C4B-NB	2.06	126.44	124.26
16	B	4017	BCR	C8-C7-C6	-2.06	121.42	127.20
16	e	4008	BCR	C28-C27-C26	-2.06	110.40	114.08
16	f	4005	BCR	C3-C4-C5	-2.06	110.40	114.08
13	m	1103	CLA	CHD-C1D-ND	-2.06	122.56	124.45
16	v	523	BCR	C11-C10-C9	-2.06	124.38	127.31
13	1	513	CLA	CHB-C1B-NB	2.06	126.43	124.26
13	2	501	CLA	CHB-C1B-NB	2.06	126.43	124.26
16	j	4016	BCR	C38-C26-C25	-2.06	122.22	124.53
16	H	4017	BCR	C15-C16-C17	-2.06	119.26	123.47
13	a	518	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
13	B	1239	CLA	C2A-C1A-CHA	2.06	127.45	123.86
17	A	5002	LHG	O10-C23-C24	-2.06	115.71	123.73
13	e	1112	CLA	C2A-C1A-CHA	2.06	127.45	123.86
13	A	1117	CLA	C7-C6-C5	-2.06	107.78	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	5	518	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
13	f	1023	CLA	CHC-C1C-NC	2.06	127.32	124.20
16	F	4016	BCR	C36-C18-C19	2.06	121.31	118.08
13	A	1125	CLA	C3A-C2A-C1A	2.05	104.42	101.34
16	B	4009	BCR	C4-C5-C6	-2.05	119.75	122.73
13	t	508	CLA	CHC-C1C-NC	2.05	127.32	124.20
13	H	1215	CLA	CHC-C4B-NB	2.05	126.43	124.26
16	v	522	BCR	C2-C3-C4	-2.05	106.79	111.38
13	b	508	CLA	CHC-C1C-NC	2.05	127.32	124.20
16	j	4016	BCR	C36-C18-C19	2.05	121.31	118.08
13	d	507	CLA	CHC-C4B-NB	2.05	126.43	124.26
13	q	519	CLA	CHB-C1B-NB	2.05	126.43	124.26
13	T	1303	CLA	CHA-C1A-NA	-2.05	121.69	126.40
19	B	5002	LMG	C3-C4-C5	-2.05	106.58	110.24
13	B	1220	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	G	1124	CLA	CMB-C2B-C3B	2.05	131.56	126.59
13	Y	501	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
16	b	522	BCR	C27-C26-C25	-2.05	119.75	122.73
13	J	1303	CLA	C2D-C1D-ND	-2.05	108.59	110.10
13	t	516	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
16	H	4006	BCR	C23-C22-C21	2.05	122.09	118.94
13	1	510	CLA	C4-C3-C5	2.05	118.72	115.27
17	G	5002	LHG	O10-C23-C24	-2.05	115.72	123.73
16	T	4015	BCR	C37-C22-C23	2.05	121.31	118.08
13	Z	502	CLA	C2A-C1A-CHA	2.05	127.45	123.86
13	m	1105	CLA	C3B-C4B-NB	-2.05	108.61	110.52
16	6	523	BCR	C11-C10-C9	-2.05	124.38	127.31
13	5	506	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
13	A	1112	CLA	C2A-C1A-CHA	2.05	127.45	123.86
13	q	501	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
16	H	4005	BCR	C3-C4-C5	-2.05	110.41	114.08
13	A	1120	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
13	d	503	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	s	518	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
16	H	4009	BCR	C16-C15-C14	-2.05	119.27	123.47
13	4	519	CLA	CHB-C1B-NB	2.05	126.43	124.26
13	u	506	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
13	1	507	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	4	518	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
16	d	524	BCR	C20-C19-C18	-2.05	120.66	126.42
13	K	1103	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
13	d	503	CLA	CAA-C2A-C3A	-2.05	107.16	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	4011	BCR	C36-C18-C17	-2.05	120.05	122.92
19	f	5002	LMG	C3-C4-C5	-2.05	106.58	110.24
16	3	522	BCR	C2-C1-C6	2.05	113.64	110.48
13	2	519	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	s	516	CLA	CHD-C1D-ND	-2.05	122.57	124.45
16	R	4016	BCR	C36-C18-C19	2.05	121.31	118.08
13	c	502	CLA	CHC-C4B-NB	2.05	126.43	124.26
13	v	507	CLA	CHC-C4B-NB	2.05	126.43	124.26
13	q	507	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	G	1120	CLA	CMB-C2B-C3B	2.05	131.55	126.59
13	4	508	CLA	CHC-C1C-NC	2.05	127.31	124.20
13	H	1215	CLA	O2D-CGD-CBD	2.05	114.91	111.27
13	1	501	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	q	502	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	b	507	CLA	CHC-C4B-NB	2.05	126.43	124.26
13	H	1230	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
13	Z	511	CLA	C2A-C1A-CHA	2.05	127.44	123.86
13	H	1215	CLA	C4-C3-C5	2.05	118.72	115.27
16	4	522	BCR	C27-C26-C25	-2.05	119.76	122.73
16	e	4002	BCR	C27-C26-C25	-2.05	119.76	122.73
16	V	4219	BCR	C16-C15-C14	-2.05	119.28	123.47
13	A	1022	CLA	C1D-ND-C4D	2.05	107.79	106.33
17	e	5002	LHG	O10-C23-C24	-2.05	115.74	123.73
13	3	516	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	s	506	CLA	CHB-C1B-NB	2.05	126.42	124.26
19	H	5002	LMG	C3-C4-C5	-2.05	106.59	110.24
17	G	5006	LHG	C11-C10-C9	-2.05	104.03	114.42
13	c	511	CLA	C2A-C1A-CHA	2.05	127.44	123.86
13	e	1127	CLA	C2A-C1A-CHA	2.05	127.44	123.86
16	6	522	BCR	C2-C3-C4	-2.05	106.80	111.38
13	B	1023	CLA	O2D-CGD-CBD	2.05	114.91	111.27
13	H	1023	CLA	CHC-C1C-NC	2.05	127.31	124.20
13	m	1103	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
13	q	518	CLA	C3B-C4B-NB	-2.05	108.62	110.52
16	f	4006	BCR	C23-C22-C21	2.05	122.08	118.94
16	4	524	BCR	C11-C12-C13	-2.05	120.67	126.42
13	G	1120	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
13	Y	508	CLA	C2D-C1D-ND	-2.05	108.60	110.10
13	f	1235	CLA	C2D-C1D-ND	-2.05	108.60	110.10
16	f	4017	BCR	C8-C7-C6	-2.05	121.45	127.20
13	1	502	CLA	CHC-C4B-NB	2.05	126.42	124.26
16	e	4011	BCR	C36-C18-C17	-2.05	120.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	506	CLA	C3B-C4B-NB	-2.05	108.62	110.52
13	q	511	CLA	C2A-C1A-CHA	2.05	127.44	123.86
13	u	509	CLA	C2A-C1A-CHA	2.05	127.44	123.86
13	G	1115	CLA	CMB-C2B-C3B	2.05	131.54	126.59
17	A	5006	LHG	C11-C10-C9	-2.05	104.04	114.42
16	b	524	BCR	C11-C12-C13	-2.05	120.67	126.42
13	B	1229	CLA	O2D-CGD-CBD	2.05	114.90	111.27
16	d	522	BCR	C2-C3-C4	-2.04	106.81	111.38
13	e	1115	CLA	CMB-C2B-C3B	2.04	131.54	126.59
13	U	1103	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
13	c	509	CLA	C2A-C1A-CHA	2.04	127.43	123.86
17	A	5002	LHG	C5-O7-C7	-2.04	112.76	117.79
16	s	522	BCR	C2-C1-C6	2.04	113.63	110.48
13	c	518	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	s	519	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	u	518	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	A	1122	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	Y	507	CLA	CHC-C4B-NB	2.04	126.42	124.26
13	H	1239	CLA	C2A-C1A-CHA	2.04	127.43	123.86
17	e	5002	LHG	C5-O7-C7	-2.04	112.76	117.79
13	v	503	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
13	Y	507	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	H	1235	CLA	C2D-C1D-ND	-2.04	108.60	110.10
13	1	510	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
13	Z	501	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	e	1122	CLA	CHC-C4B-NB	2.04	126.42	124.26
13	f	1213	CLA	CHB-C1B-NB	2.04	126.42	124.26
17	G	5002	LHG	C5-O7-C7	-2.04	112.76	117.79
16	l	4015	BCR	C37-C22-C23	2.04	121.30	118.08
13	B	1228	CLA	C3B-C4B-NB	-2.04	108.62	110.52
13	e	1123	CLA	C3B-C4B-NB	-2.04	108.62	110.52
13	3	518	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
13	A	1122	CLA	C2D-C1D-ND	-2.04	108.60	110.10
13	J	1303	CLA	CHA-C1A-NA	-2.04	121.72	126.40
16	L	4219	BCR	C16-C15-C14	-2.04	119.29	123.47
13	2	502	CLA	C2A-C1A-CHA	2.04	127.43	123.86
13	A	1126	CLA	C16-C15-C13	-2.04	109.32	115.92
16	B	4017	BCR	C15-C16-C17	-2.04	119.29	123.47
13	6	504	CLA	CHD-C1D-ND	-2.04	122.58	124.45
16	B	4006	BCR	C23-C22-C21	2.04	122.07	118.94
13	5	511	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
13	Z	508	CLA	CHC-C1C-NC	2.04	127.30	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	l	5104	LMG	O8-C28-O10	-2.04	118.44	123.59
13	B	1230	CLA	CAA-CBA-CGA	-2.04	107.29	113.25
13	6	503	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
16	J	4015	BCR	C37-C22-C23	2.04	121.29	118.08
13	6	518	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	G	1122	CLA	CHC-C4B-NB	2.04	126.42	124.26
13	l	1303	CLA	CHA-C1A-NA	-2.04	121.73	126.40
16	c	521	BCR	C2-C1-C6	2.04	113.62	110.48
13	u	507	CLA	C3B-C4B-NB	-2.04	108.62	110.52
13	A	1122	CLA	CHC-C4B-NB	2.04	126.42	124.26
13	G	1116	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	v	518	CLA	CHB-C1B-NB	2.04	126.42	124.26
16	v	524	BCR	C20-C19-C18	-2.04	120.69	126.42
14	G	2001	PQN	C2M-C2-C1	2.04	119.65	116.27
13	H	1235	CLA	CBA-CAA-C2A	2.04	119.88	113.86
16	5	523	BCR	C11-C10-C9	-2.04	124.40	127.31
16	t	522	BCR	C27-C26-C25	-2.04	119.77	122.73
13	H	1226	CLA	CHB-C4A-NA	2.04	127.33	124.51
17	e	5006	LHG	C11-C10-C9	-2.04	104.08	114.42
13	e	1122	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	v	513	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	G	1123	CLA	C3B-C4B-NB	-2.04	108.62	110.52
13	B	1214	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	V	1503	CLA	CHD-C1D-ND	-2.04	122.58	124.45
16	d	521	BCR	C2-C1-C6	2.04	113.62	110.48
16	F	4016	BCR	C38-C26-C25	-2.04	122.24	124.53
13	b	519	CLA	CHB-C1B-NB	2.04	126.41	124.26
13	q	513	CLA	CHB-C1B-NB	2.04	126.41	124.26
13	A	1126	CLA	C3B-C4B-NB	-2.04	108.62	110.52
13	f	1239	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	2	508	CLA	CHD-C1D-ND	-2.04	122.58	124.45
13	j	1301	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	f	1230	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
13	5	507	CLA	C3B-C4B-NB	-2.04	108.63	110.52
16	6	524	BCR	C20-C19-C18	-2.04	120.70	126.42
13	L	1503	CLA	CHD-C1D-ND	-2.04	122.58	124.45
16	1	522	BCR	C33-C5-C4	2.04	117.53	113.62
16	t	523	BCR	C15-C16-C17	-2.04	119.30	123.47
13	4	507	CLA	CHC-C4B-NB	2.04	126.41	124.26
13	G	1122	CLA	CHB-C1B-NB	2.04	126.41	124.26
13	c	512	CLA	CHB-C1B-NB	2.04	126.41	124.26
13	r	501	CLA	CHB-C1B-NB	2.04	126.41	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	c	523	BCR	C11-C10-C9	-2.04	124.41	127.31
13	B	1217	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	Y	511	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	H	1210	CLA	CAC-C3C-C4C	2.03	127.45	124.81
13	H	1212	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	q	507	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
13	f	1238	CLA	O2A-C1-C2	-2.03	103.29	108.64
16	f	4009	BCR	C16-C15-C14	-2.03	119.31	123.47
13	Y	504	CLA	C2A-C1A-CHA	2.03	127.42	123.86
17	A	5005	LHG	O8-C23-O10	-2.03	118.46	123.59
13	r	502	CLA	C2A-C1A-CHA	2.03	127.41	123.86
16	R	4016	BCR	C38-C26-C25	-2.03	122.25	124.53
13	H	1231	CLA	C1-C2-C3	-2.03	122.53	126.04
16	c	524	BCR	C34-C9-C8	2.03	121.28	118.08
16	n	4219	BCR	C16-C15-C14	-2.03	119.31	123.47
16	q	524	BCR	C1-C6-C7	2.03	121.53	115.78
16	2	523	BCR	C3-C4-C5	-2.03	110.45	114.08
17	G	5005	LHG	O8-C23-O10	-2.03	118.46	123.59
16	u	524	BCR	C34-C9-C8	2.03	121.28	118.08
16	H	4009	BCR	C4-C5-C6	-2.03	119.78	122.73
13	G	1126	CLA	C16-C15-C13	-2.03	109.35	115.92
13	c	504	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	c	511	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
13	b	517	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
13	G	1124	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
13	s	504	CLA	CMB-C2B-C3B	2.03	131.51	126.59
13	b	518	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
13	4	508	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	5	509	CLA	C2A-C1A-CHA	2.03	127.41	123.86
13	u	511	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
13	A	1128	CLA	C2D-C1D-ND	-2.03	108.61	110.10
13	1	502	CLA	CHB-C1B-NB	2.03	126.41	124.26
13	Z	519	CLA	CHC-C4B-NB	2.03	126.41	124.26
13	4	517	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
13	A	1124	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
13	t	508	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	A	1115	CLA	CMB-C2B-C3B	2.03	131.50	126.59
13	4	503	CLA	CAC-C3C-C4C	2.03	127.44	124.81
13	1	511	CLA	C2A-C1A-CHA	2.03	127.41	123.86
13	B	1235	CLA	CBA-CAA-C2A	2.03	119.85	113.86
13	H	1240	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
19	T	5104	LMG	O8-C28-O10	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1126	CLA	C3B-C4B-NB	-2.03	108.63	110.52
13	f	1232	CLA	C3B-C4B-NB	-2.03	108.63	110.52
13	B	1210	CLA	CAC-C3C-C4C	2.03	127.44	124.81
13	B	1226	CLA	CHB-C4A-NA	2.03	127.32	124.51
13	B	1238	CLA	O2A-C1-C2	-2.03	103.30	108.64
13	d	510	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	Y	510	CLA	C4-C3-C5	2.03	118.68	115.27
13	B	1210	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
13	2	513	CLA	CHB-C1B-NB	2.03	126.40	124.26
13	c	512	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
13	B	1232	CLA	C3B-C4B-NB	-2.03	108.63	110.52
13	5	511	CLA	C2A-C1A-CHA	2.03	127.40	123.86
13	b	502	CLA	C2A-C1A-CHA	2.03	127.40	123.86
13	5	510	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	c	510	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	4	511	CLA	CHB-C1B-NB	2.03	126.40	124.26
13	U	1103	CLA	CHC-C4B-NB	2.03	126.40	124.26
13	5	512	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
16	B	4009	BCR	C16-C15-C14	-2.03	119.32	123.47
16	b	524	BCR	C38-C26-C25	-2.03	122.25	124.53
13	f	1212	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	J	5104	LMG	O8-C28-O10	-2.03	118.48	123.59
13	e	1124	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
13	6	502	CLA	C1-C2-C3	-2.03	123.47	126.75
16	4	523	BCR	C15-C16-C17	-2.03	119.32	123.47
13	G	1129	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
13	f	1214	CLA	C2A-C1A-CHA	2.03	127.40	123.86
13	u	511	CLA	C2A-C1A-CHA	2.03	127.40	123.86
13	r	508	CLA	CHC-C1C-NC	2.03	127.28	124.20
13	A	1116	CLA	CHB-C1B-NB	2.03	126.40	124.26
13	c	513	CLA	CHB-C1B-NB	2.03	126.40	124.26
13	A	1112	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	4	504	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	r	518	CLA	CMB-C2B-C3B	2.03	131.50	126.59
20	u	822	SQD	C45-O47-C7	2.03	122.78	117.79
16	b	523	BCR	C15-C16-C17	-2.03	119.32	123.47
13	r	503	CLA	C2A-C1A-CHA	2.03	127.40	123.86
13	e	1124	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
16	1	524	BCR	C1-C6-C7	2.03	121.51	115.78
13	B	1215	CLA	C4-C3-C5	2.03	118.68	115.27
13	H	1240	CLA	CHB-C1B-NB	2.03	126.40	124.26
13	f	1217	CLA	C2A-C1A-CHA	2.03	127.40	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	4019	BCR	C38-C26-C27	2.02	117.51	113.62
13	d	504	CLA	CMB-C2B-C3B	2.02	131.49	126.59
13	B	1212	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
13	f	1210	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
13	t	511	CLA	CHB-C1B-NB	2.02	126.40	124.26
16	t	524	BCR	C38-C26-C25	-2.02	122.25	124.53
13	r	503	CLA	CMB-C2B-C3B	2.02	131.49	126.59
13	v	504	CLA	CHD-C1D-ND	-2.02	122.59	124.45
13	3	519	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
13	B	1240	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
20	c	822	SQD	C45-O47-C7	2.02	122.77	117.79
17	e	5005	LHG	O8-C23-O10	-2.02	118.48	123.59
16	v	521	BCR	C2-C1-C6	2.02	113.60	110.48
16	Z	523	BCR	C3-C4-C5	-2.02	110.46	114.08
13	1	506	CLA	C3B-C4B-NB	-2.02	108.64	110.52
13	H	1224	CLA	C3B-C4B-NB	-2.02	108.64	110.52
13	b	503	CLA	CAC-C3C-C4C	2.02	127.44	124.81
17	n	5220	LHG	C27-C26-C25	-2.02	104.16	114.42
13	r	508	CLA	CHD-C1D-ND	-2.02	122.59	124.45
20	c	822	SQD	O48-C23-O10	-2.02	118.49	123.59
13	t	517	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
16	V	4019	BCR	C38-C26-C27	2.02	117.50	113.62
13	H	1214	CLA	C2A-C1A-CHA	2.02	127.39	123.86
13	d	502	CLA	C1-C2-C3	-2.02	123.48	126.75
13	f	1224	CLA	C3B-C4B-NB	-2.02	108.64	110.52
16	Y	524	BCR	C1-C6-C7	2.02	121.50	115.78
13	1	507	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
13	H	1238	CLA	O2A-C1-C2	-2.02	103.32	108.64
16	5	521	BCR	C2-C1-C6	2.02	113.59	110.48
16	l	4012	BCR	C15-C16-C17	-2.02	119.33	123.47
16	u	523	BCR	C11-C10-C9	-2.02	124.42	127.31
16	5	524	BCR	C34-C9-C8	2.02	121.26	118.08
13	6	507	CLA	CHC-C4B-NB	2.02	126.40	124.26
13	q	502	CLA	CHC-C4B-NB	2.02	126.40	124.26
13	t	502	CLA	C2A-C1A-CHA	2.02	127.39	123.86
17	V	5220	LHG	C27-C26-C25	-2.02	104.17	114.42
13	B	1231	CLA	C1-C2-C3	-2.02	122.55	126.04
20	5	822	SQD	C45-O47-C7	2.02	122.77	117.79
13	1	511	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
16	1	522	BCR	C36-C18-C19	2.02	121.26	118.08
13	u	512	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
13	f	1210	CLA	CAC-C3C-C4C	2.02	127.43	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	t	503	CLA	CAC-C3C-C4C	2.02	127.43	124.81
16	f	4017	BCR	C15-C16-C17	-2.02	119.34	123.47
17	L	5220	LHG	C27-C26-C25	-2.02	104.17	114.42
13	1	504	CLA	C2A-C1A-CHA	2.02	127.39	123.86
13	s	516	CLA	C2A-C1A-CHA	2.02	127.39	123.86
14	A	2001	PQN	C2M-C2-C1	2.02	119.62	116.27
13	f	1220	CLA	CHD-C1D-ND	-2.02	122.60	124.45
16	6	521	BCR	C2-C1-C6	2.02	113.59	110.48
13	Z	518	CLA	CMB-C2B-C3B	2.02	131.48	126.59
13	f	1208	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	K	1103	CLA	C2D-C1D-ND	-2.02	108.62	110.10
13	e	1107	CLA	C2D-C1D-ND	-2.02	108.62	110.10
13	v	505	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
20	L	5216	SQD	C1-O5-C5	2.02	117.65	113.69
13	2	508	CLA	CHC-C1C-NC	2.02	127.27	124.20
13	F	1301	CLA	C2A-C1A-CHA	2.02	127.39	123.86
13	f	1226	CLA	CMC-C2C-C3C	2.02	131.60	126.12
13	A	1125	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
13	r	519	CLA	CHD-C1D-ND	-2.02	122.60	124.45
13	f	1235	CLA	CBA-CAA-C2A	2.02	119.82	113.86
13	2	503	CLA	CMB-C2B-C3B	2.02	131.48	126.59
16	T	4012	BCR	C15-C16-C17	-2.02	119.34	123.47
16	r	523	BCR	C3-C4-C5	-2.02	110.47	114.08
13	H	1220	CLA	C2D-C1D-ND	-2.02	108.62	110.10
16	L	4019	BCR	C38-C26-C27	2.02	117.49	113.62
13	q	504	CLA	C2A-C1A-CHA	2.02	127.39	123.86
13	f	1226	CLA	CHB-C4A-NA	2.02	127.30	124.51
13	H	1208	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
16	V	4020	BCR	C8-C9-C10	-2.02	115.84	118.94
13	a	503	CLA	CHD-C1D-ND	-2.02	122.60	124.45
16	G	4007	BCR	C8-C7-C6	-2.02	121.54	127.20
13	V	1503	CLA	CMB-C2B-C3B	2.02	131.47	126.59
13	a	510	CLA	CMB-C2B-C3B	2.02	131.47	126.59
14	e	2001	PQN	C2M-C2-C1	2.02	119.61	116.27
13	B	1226	CLA	CMC-C2C-C3C	2.02	131.59	126.12
13	6	506	CLA	CHB-C1B-NB	2.02	126.39	124.26
13	r	513	CLA	CHB-C1B-NB	2.02	126.39	124.26
13	3	504	CLA	CMB-C2B-C3B	2.02	131.47	126.59
13	s	510	CLA	CMB-C2B-C3B	2.02	131.47	126.59
13	H	1217	CLA	C2A-C1A-CHA	2.02	127.39	123.86
13	f	1240	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
13	3	508	CLA	O2A-CGA-O1A	-2.02	118.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	503	CLA	C2A-C1A-CHA	2.02	127.38	123.86
13	H	1239	CLA	CHC-C4B-NB	2.02	126.39	124.26
13	H	1210	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
13	B	1224	CLA	C3B-C4B-NB	-2.02	108.64	110.52
13	c	507	CLA	C3B-C4B-NB	-2.02	108.64	110.52
16	Y	522	BCR	C33-C5-C4	2.02	117.49	113.62
13	t	503	CLA	C2A-C1A-CHA	2.02	127.38	123.86
13	c	501	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
13	f	1231	CLA	C1-C2-C3	-2.02	122.56	126.04
13	2	518	CLA	CMB-C2B-C3B	2.01	131.47	126.59
13	J	1303	CLA	CHC-C4B-NB	2.01	126.39	124.26
13	u	502	CLA	CHC-C4B-NB	2.01	126.39	124.26
13	a	503	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
13	4	509	CLA	C3B-C4B-NB	-2.01	108.65	110.52
16	Z	522	BCR	C20-C21-C22	-2.01	124.44	127.31
16	Y	522	BCR	C36-C18-C19	2.01	121.25	118.08
13	Z	502	CLA	CHC-C4B-NB	2.01	126.39	124.26
13	c	511	CLA	CHB-C1B-NB	2.01	126.39	124.26
13	A	1129	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
13	B	1221	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
20	n	5216	SQD	C1-O5-C5	2.01	117.64	113.69
13	e	1121	CLA	CHA-C1A-NA	-2.01	121.79	126.40
13	5	501	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
13	u	510	CLA	CHD-C1D-ND	-2.01	122.60	124.45
13	q	519	CLA	O2D-CGD-CBD	2.01	114.84	111.27
13	f	1215	CLA	CHB-C1B-NB	2.01	126.39	124.26
13	G	1124	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
20	5	822	SQD	O48-C23-O10	-2.01	118.51	123.59
16	n	4022	BCR	C15-C16-C17	-2.01	119.35	123.47
16	e	4008	BCR	C30-C25-C24	2.01	121.47	115.78
13	a	519	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
16	n	4022	BCR	C21-C20-C19	-2.01	116.94	123.22
13	G	1121	CLA	CHA-C1A-NA	-2.01	121.79	126.40
13	A	1124	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
20	u	822	SQD	O48-C23-O10	-2.01	118.51	123.59
16	f	4006	BCR	C10-C11-C12	-2.01	116.94	123.22
13	2	519	CLA	CHC-C4B-NB	2.01	126.39	124.26
13	2	503	CLA	C2A-C1A-CHA	2.01	127.38	123.86
13	3	516	CLA	C2A-C1A-CHA	2.01	127.38	123.86
16	a	522	BCR	C21-C20-C19	-2.01	116.94	123.22
16	e	4007	BCR	C8-C7-C6	-2.01	121.55	127.20
16	f	4006	BCR	C8-C9-C10	2.01	122.03	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1208	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	U	1401	CLA	CHB-C1B-NB	2.01	126.39	124.26
16	u	521	BCR	C2-C1-C6	2.01	113.58	110.48
13	f	1221	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	3	510	CLA	CMB-C2B-C3B	2.01	131.46	126.59
16	Y	522	BCR	C1-C6-C5	-2.01	119.78	122.61
14	e	2001	PQN	C21-C20-C18	-2.01	109.42	115.92
13	H	1023	CLA	C2A-C1A-CHA	2.01	127.37	123.86
13	L	1503	CLA	CMB-C2B-C3B	2.01	131.46	126.59
13	b	509	CLA	CHA-C1A-NA	-2.01	121.80	126.40
13	G	1122	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	H	1217	CLA	C2D-C1D-ND	-2.01	108.62	110.10
13	Y	519	CLA	O2D-CGD-CBD	2.01	114.84	111.27
16	t	523	BCR	C34-C9-C8	2.01	121.24	118.08
13	e	1126	CLA	C3B-C4B-NB	-2.01	108.65	110.52
13	Z	513	CLA	CHB-C1B-NB	2.01	126.38	124.26
13	a	504	CLA	CMB-C2B-C3B	2.01	131.45	126.59
16	A	4007	BCR	C8-C7-C6	-2.01	121.56	127.20
13	e	1125	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
13	R	1301	CLA	C2A-C1A-CHA	2.01	127.37	123.86
13	Y	503	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	1	519	CLA	O2D-CGD-CBD	2.01	114.84	111.27
16	L	4020	BCR	C8-C9-C10	-2.01	115.86	118.94
18	e	1849	LMU	C6'-C5'-C4'	-2.01	108.30	113.00
13	Y	511	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
13	s	508	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
13	B	1240	CLA	CHB-C1B-NB	2.01	126.38	124.26
13	G	1125	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
14	A	2001	PQN	C21-C20-C18	-2.01	109.43	115.92
16	J	4012	BCR	C15-C16-C17	-2.01	119.36	123.47
13	A	1121	CLA	CHA-C1A-NA	-2.01	121.80	126.40
16	H	4006	BCR	C10-C11-C12	-2.01	116.95	123.22
13	e	1116	CLA	CHB-C1B-NB	2.01	126.38	124.26
13	a	516	CLA	C2A-C1A-CHA	2.01	127.37	123.86
13	u	513	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
16	3	522	BCR	C21-C20-C19	-2.01	116.96	123.22
13	q	511	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	G	2001	PQN	C21-C20-C18	-2.01	109.44	115.92
16	q	522	BCR	C36-C18-C19	2.01	121.24	118.08
13	B	1235	CLA	CHD-C1D-ND	-2.01	122.61	124.45
13	5	504	CLA	CHB-C1B-NB	2.01	126.38	124.26
13	Y	502	CLA	CHB-C1B-NB	2.01	126.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	t	507	CLA	CHC-C4B-NB	2.01	126.38	124.26
16	2	522	BCR	C20-C21-C22	-2.01	124.45	127.31
16	c	524	BCR	C24-C23-C22	-2.01	123.20	126.23
16	q	522	BCR	C33-C5-C4	2.01	117.47	113.62
13	H	1226	CLA	CMC-C2C-C3C	2.01	131.56	126.12
13	4	505	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
13	f	1202	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
13	s	503	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
16	4	524	BCR	C38-C26-C25	-2.00	122.28	124.53
13	H	1228	CLA	O2D-CGD-CBD	2.00	114.83	111.27
13	H	1221	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
13	q	502	CLA	CHB-C1B-NB	2.00	126.38	124.26
13	r	519	CLA	CHC-C4B-NB	2.00	126.38	124.26
13	b	504	CLA	CHD-C1D-ND	-2.00	122.61	124.45
16	L	4022	BCR	C21-C20-C19	-2.00	116.96	123.22
16	V	4022	BCR	C21-C20-C19	-2.00	116.96	123.22
13	u	508	CLA	C3B-C4B-NB	-2.00	108.66	110.52
13	Z	513	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
13	f	1226	CLA	CHA-C4D-ND	2.00	136.69	132.50
13	B	1218	CLA	C2A-C1A-CHA	2.00	127.36	123.86
13	3	503	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
16	A	4008	BCR	C30-C25-C24	2.00	121.44	115.78
13	v	504	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
13	u	513	CLA	CHB-C1B-NB	2.00	126.38	124.26
13	6	504	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
13	4	502	CLA	C2A-C1A-CHA	2.00	127.36	123.86
13	u	501	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
16	B	4006	BCR	C10-C11-C12	-2.00	116.97	123.22
13	n	1503	CLA	CMB-C2B-C3B	2.00	131.44	126.59
13	B	1226	CLA	CHA-C4D-ND	2.00	136.69	132.50
13	e	1129	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
18	G	1849	LMU	C6'-C5'-C4'	-2.00	108.31	113.00
13	Z	503	CLA	CMB-C2B-C3B	2.00	131.44	126.59
13	a	508	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
16	v	522	BCR	C23-C24-C25	-2.00	121.58	127.20
16	A	4002	BCR	C20-C19-C18	-2.00	120.80	126.42
13	6	513	CLA	CHB-C1B-NB	2.00	126.38	124.26
13	B	1216	CLA	C1-C2-C3	-2.00	122.58	126.04
13	H	1212	CLA	CMB-C2B-C3B	2.00	131.43	126.59
13	6	504	CLA	CMB-C2B-C3B	2.00	131.43	126.59
13	Y	511	CLA	CMB-C2B-C3B	2.00	131.43	126.59
13	G	1112	CLA	CHD-C1D-ND	-2.00	122.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	t	506	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

There are no chirality outliers.

All (8852) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CLA	CHA-CBD-CGD-O1D
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	C1A-C2A-CAA-CBA
13	A	1103	CLA	CHA-CBD-CGD-O1D
13	A	1103	CLA	CHA-CBD-CGD-O2D
13	A	1103	CLA	CAD-CBD-CGD-O1D
13	A	1104	CLA	C1A-C2A-CAA-CBA
13	A	1104	CLA	C4-C3-C5-C6
13	A	1106	CLA	C3A-C2A-CAA-CBA
13	A	1107	CLA	C2B-C3B-CAB-CBB
13	A	1107	CLA	C4B-C3B-CAB-CBB
13	A	1108	CLA	C1A-C2A-CAA-CBA
13	A	1108	CLA	C3A-C2A-CAA-CBA
13	A	1108	CLA	CHA-CBD-CGD-O2D
13	A	1110	CLA	C1A-C2A-CAA-CBA
13	A	1110	CLA	C3A-C2A-CAA-CBA
13	A	1110	CLA	C2-C3-C5-C6
13	A	1110	CLA	C4-C3-C5-C6
13	A	1116	CLA	C3A-C2A-CAA-CBA
13	A	1117	CLA	CBD-CGD-O2D-CED
13	A	1121	CLA	C2B-C3B-CAB-CBB
13	A	1121	CLA	C4B-C3B-CAB-CBB
13	A	1122	CLA	C2B-C3B-CAB-CBB
13	A	1122	CLA	C4B-C3B-CAB-CBB
13	A	1122	CLA	CHA-CBD-CGD-O1D
13	A	1122	CLA	CHA-CBD-CGD-O2D
13	A	1122	CLA	C2-C3-C5-C6
13	A	1122	CLA	C4-C3-C5-C6
13	A	1126	CLA	C1A-C2A-CAA-CBA
13	A	1126	CLA	C3A-C2A-CAA-CBA
13	A	1131	CLA	CBD-CGD-O2D-CED
13	A	1132	CLA	CHA-CBD-CGD-O2D
13	A	1134	CLA	C1A-C2A-CAA-CBA
13	A	1134	CLA	CHA-CBD-CGD-O1D
13	A	1134	CLA	CHA-CBD-CGD-O2D
13	A	1134	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	1134	CLA	C4-C3-C5-C6
13	A	1137	CLA	CHA-CBD-CGD-O1D
13	A	1137	CLA	CHA-CBD-CGD-O2D
13	A	1139	CLA	C1A-C2A-CAA-CBA
13	A	1139	CLA	C3A-C2A-CAA-CBA
13	A	1139	CLA	CBD-CGD-O2D-CED
13	A	1139	CLA	C2-C3-C5-C6
13	A	1139	CLA	C4-C3-C5-C6
13	A	1140	CLA	C1A-C2A-CAA-CBA
13	A	1140	CLA	C2-C3-C5-C6
13	A	1140	CLA	C4-C3-C5-C6
13	A	1237	CLA	C4-C3-C5-C6
13	A	1101	CLA	CHA-CBD-CGD-O1D
13	A	1101	CLA	CHA-CBD-CGD-O2D
13	B	1012	CLA	CHA-CBD-CGD-O1D
13	B	1012	CLA	CHA-CBD-CGD-O2D
13	B	1012	CLA	CAD-CBD-CGD-O1D
13	B	1012	CLA	C2-C3-C5-C6
13	B	1012	CLA	C4-C3-C5-C6
13	B	1021	CLA	CHA-CBD-CGD-O1D
13	B	1202	CLA	C1A-C2A-CAA-CBA
13	B	1202	CLA	C3A-C2A-CAA-CBA
13	B	1204	CLA	CHA-CBD-CGD-O1D
13	B	1204	CLA	CHA-CBD-CGD-O2D
13	B	1209	CLA	C1A-C2A-CAA-CBA
13	B	1209	CLA	C3A-C2A-CAA-CBA
13	B	1209	CLA	CHA-CBD-CGD-O1D
13	B	1209	CLA	CHA-CBD-CGD-O2D
13	B	1210	CLA	C1A-C2A-CAA-CBA
13	B	1210	CLA	C11-C12-C13-C15
13	B	1211	CLA	C11-C10-C8-C7
13	B	1212	CLA	C2-C3-C5-C6
13	B	1212	CLA	C4-C3-C5-C6
13	B	1214	CLA	C2A-CAA-CBA-CGA
13	B	1214	CLA	C2B-C3B-CAB-CBB
13	B	1214	CLA	C4B-C3B-CAB-CBB
13	B	1214	CLA	O2A-C1-C2-C3
13	B	1215	CLA	C1A-C2A-CAA-CBA
13	B	1215	CLA	C3A-C2A-CAA-CBA
13	B	1216	CLA	C2B-C3B-CAB-CBB
13	B	1216	CLA	C4B-C3B-CAB-CBB
13	B	1217	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	B	1217	CLA	C3A-C2A-CAA-CBA
13	B	1217	CLA	C2A-CAA-CBA-CGA
13	B	1219	CLA	C2B-C3B-CAB-CBB
13	B	1220	CLA	C2B-C3B-CAB-CBB
13	B	1220	CLA	C4B-C3B-CAB-CBB
13	B	1221	CLA	C1A-C2A-CAA-CBA
13	B	1223	CLA	CHA-CBD-CGD-O1D
13	B	1223	CLA	CHA-CBD-CGD-O2D
13	B	1224	CLA	C1A-C2A-CAA-CBA
13	B	1224	CLA	C3A-C2A-CAA-CBA
13	B	1239	CLA	C4B-C3B-CAB-CBB
13	B	1240	CLA	C1A-C2A-CAA-CBA
13	B	1240	CLA	CHA-CBD-CGD-O1D
13	B	1240	CLA	CHA-CBD-CGD-O2D
13	B	1230	CLA	C1A-C2A-CAA-CBA
13	B	1230	CLA	C3A-C2A-CAA-CBA
13	B	1230	CLA	C2B-C3B-CAB-CBB
13	B	1230	CLA	C4B-C3B-CAB-CBB
13	F	1302	CLA	C1A-C2A-CAA-CBA
13	F	1302	CLA	C3A-C2A-CAA-CBA
13	J	1302	CLA	CHA-CBD-CGD-O1D
13	J	1302	CLA	CHA-CBD-CGD-O2D
13	J	1302	CLA	CAD-CBD-CGD-O1D
13	J	1303	CLA	C1A-C2A-CAA-CBA
13	K	1401	CLA	C1A-C2A-CAA-CBA
13	K	1401	CLA	C4B-C3B-CAB-CBB
13	K	1401	CLA	CHA-CBD-CGD-O1D
13	K	1401	CLA	CHA-CBD-CGD-O2D
13	K	1103	CLA	C2B-C3B-CAB-CBB
13	K	1103	CLA	C4B-C3B-CAB-CBB
13	K	1105	CLA	C2B-C3B-CAB-CBB
13	K	1105	CLA	C4B-C3B-CAB-CBB
13	1	501	CLA	C4B-C3B-CAB-CBB
13	1	501	CLA	CHA-CBD-CGD-O1D
13	1	501	CLA	CHA-CBD-CGD-O2D
13	1	501	CLA	CAD-CBD-CGD-O1D
13	1	501	CLA	CBD-CGD-O2D-CED
13	1	504	CLA	C2B-C3B-CAB-CBB
13	1	504	CLA	C4B-C3B-CAB-CBB
13	1	506	CLA	CHA-CBD-CGD-O1D
13	1	506	CLA	CHA-CBD-CGD-O2D
13	1	507	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	1	507	CLA	C4-C3-C5-C6
13	1	508	CLA	C2-C3-C5-C6
13	1	508	CLA	C4-C3-C5-C6
13	1	510	CLA	CBD-CGD-O2D-CED
13	1	512	CLA	C4B-C3B-CAB-CBB
13	1	512	CLA	C3-C5-C6-C7
13	1	516	CLA	C1A-C2A-CAA-CBA
13	1	516	CLA	C3A-C2A-CAA-CBA
13	1	516	CLA	C2B-C3B-CAB-CBB
13	1	516	CLA	C4B-C3B-CAB-CBB
13	1	516	CLA	CHA-CBD-CGD-O1D
13	1	516	CLA	CHA-CBD-CGD-O2D
13	1	516	CLA	CAD-CBD-CGD-O1D
13	1	517	CLA	C2B-C3B-CAB-CBB
13	1	517	CLA	C4B-C3B-CAB-CBB
13	1	518	CLA	C2B-C3B-CAB-CBB
13	1	518	CLA	C4B-C3B-CAB-CBB
13	1	518	CLA	C2-C3-C5-C6
13	1	518	CLA	C4-C3-C5-C6
13	1	519	CLA	C2B-C3B-CAB-CBB
13	1	519	CLA	C4B-C3B-CAB-CBB
13	2	501	CLA	C4B-C3B-CAB-CBB
13	2	501	CLA	CBD-CGD-O2D-CED
13	2	501	CLA	C2-C3-C5-C6
13	2	501	CLA	C4-C3-C5-C6
13	2	502	CLA	C2B-C3B-CAB-CBB
13	2	502	CLA	CHA-CBD-CGD-O1D
13	2	506	CLA	C2-C3-C5-C6
13	2	506	CLA	C4-C3-C5-C6
13	2	507	CLA	C2-C3-C5-C6
13	2	507	CLA	C4-C3-C5-C6
13	2	513	CLA	CBD-CGD-O2D-CED
13	2	516	CLA	C2B-C3B-CAB-CBB
13	2	516	CLA	C4B-C3B-CAB-CBB
13	2	516	CLA	CHA-CBD-CGD-O1D
13	2	516	CLA	CHA-CBD-CGD-O2D
13	2	518	CLA	CHA-CBD-CGD-O1D
13	2	518	CLA	CHA-CBD-CGD-O2D
13	2	518	CLA	C2-C3-C5-C6
13	2	518	CLA	C4-C3-C5-C6
13	2	519	CLA	C2B-C3B-CAB-CBB
13	2	519	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	3	503	CLA	C2B-C3B-CAB-CBB
13	3	503	CLA	C4B-C3B-CAB-CBB
13	3	510	CLA	CHA-CBD-CGD-O1D
13	3	510	CLA	CHA-CBD-CGD-O2D
13	3	510	CLA	CAD-CBD-CGD-O1D
13	3	512	CLA	C4B-C3B-CAB-CBB
13	3	513	CLA	C1A-C2A-CAA-CBA
13	3	513	CLA	CBD-CGD-O2D-CED
13	3	516	CLA	C2A-CAA-CBA-CGA
13	3	516	CLA	CHA-CBD-CGD-O1D
13	3	516	CLA	CHA-CBD-CGD-O2D
13	3	516	CLA	CAD-CBD-CGD-O1D
13	3	517	CLA	C2B-C3B-CAB-CBB
13	3	517	CLA	C4B-C3B-CAB-CBB
13	3	517	CLA	CBD-CGD-O2D-CED
13	3	518	CLA	C2B-C3B-CAB-CBB
13	3	518	CLA	C4B-C3B-CAB-CBB
13	3	518	CLA	CHA-CBD-CGD-O1D
13	3	518	CLA	CHA-CBD-CGD-O2D
13	4	501	CLA	C4B-C3B-CAB-CBB
13	4	501	CLA	CHA-CBD-CGD-O1D
13	4	501	CLA	CBD-CGD-O2D-CED
13	4	501	CLA	O1D-CGD-O2D-CED
13	4	506	CLA	CBD-CGD-O2D-CED
13	4	510	CLA	CBD-CGD-O2D-CED
13	4	513	CLA	CHA-CBD-CGD-O1D
13	4	513	CLA	CHA-CBD-CGD-O2D
13	4	517	CLA	C1A-C2A-CAA-CBA
13	4	517	CLA	C3A-C2A-CAA-CBA
13	4	518	CLA	C2B-C3B-CAB-CBB
13	4	518	CLA	C4B-C3B-CAB-CBB
13	4	519	CLA	C2B-C3B-CAB-CBB
13	4	519	CLA	C4B-C3B-CAB-CBB
13	4	519	CLA	CHA-CBD-CGD-O1D
13	4	519	CLA	CHA-CBD-CGD-O2D
13	4	519	CLA	CAD-CBD-CGD-O1D
13	4	519	CLA	CAD-CBD-CGD-O2D
13	5	501	CLA	CBD-CGD-O2D-CED
13	5	501	CLA	C4-C3-C5-C6
13	5	502	CLA	C2B-C3B-CAB-CBB
13	5	504	CLA	CBD-CGD-O2D-CED
13	5	505	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	5	506	CLA	CHA-CBD-CGD-O1D
13	5	506	CLA	CHA-CBD-CGD-O2D
13	5	507	CLA	CBD-CGD-O2D-CED
13	5	511	CLA	CBD-CGD-O2D-CED
13	5	512	CLA	C4B-C3B-CAB-CBB
13	5	513	CLA	C2B-C3B-CAB-CBB
13	5	513	CLA	C4B-C3B-CAB-CBB
13	5	513	CLA	CBD-CGD-O2D-CED
13	5	516	CLA	C4B-C3B-CAB-CBB
13	5	517	CLA	C4B-C3B-CAB-CBB
13	5	517	CLA	CHA-CBD-CGD-O1D
13	5	517	CLA	CHA-CBD-CGD-O2D
13	5	518	CLA	C2B-C3B-CAB-CBB
13	5	518	CLA	C4B-C3B-CAB-CBB
13	5	519	CLA	CHA-CBD-CGD-O1D
13	5	519	CLA	CHA-CBD-CGD-O2D
13	5	519	CLA	CAD-CBD-CGD-O1D
13	5	519	CLA	CAD-CBD-CGD-O2D
13	6	501	CLA	CBD-CGD-O2D-CED
13	6	501	CLA	C2-C3-C5-C6
13	6	501	CLA	C4-C3-C5-C6
13	6	503	CLA	C2A-CAA-CBA-CGA
13	6	504	CLA	CHA-CBD-CGD-O1D
13	6	504	CLA	CHA-CBD-CGD-O2D
13	6	505	CLA	C6-C7-C8-C9
13	6	506	CLA	CHA-CBD-CGD-O1D
13	6	506	CLA	CHA-CBD-CGD-O2D
13	6	508	CLA	CHA-CBD-CGD-O1D
13	6	508	CLA	CHA-CBD-CGD-O2D
13	6	510	CLA	CHA-CBD-CGD-O1D
13	6	510	CLA	CHA-CBD-CGD-O2D
13	6	512	CLA	C4B-C3B-CAB-CBB
13	6	513	CLA	CBD-CGD-O2D-CED
13	6	516	CLA	CBD-CGD-O2D-CED
13	6	517	CLA	CHA-CBD-CGD-O1D
13	6	517	CLA	CHA-CBD-CGD-O2D
13	6	517	CLA	CAD-CBD-CGD-O1D
13	6	518	CLA	CHA-CBD-CGD-O1D
13	6	518	CLA	CHA-CBD-CGD-O2D
13	6	519	CLA	CBA-CGA-O2A-C1
13	G	1011	CLA	CHA-CBD-CGD-O1D
13	G	1102	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	G	1103	CLA	C1A-C2A-CAA-CBA
13	G	1103	CLA	CHA-CBD-CGD-O1D
13	G	1103	CLA	CHA-CBD-CGD-O2D
13	G	1103	CLA	CAD-CBD-CGD-O1D
13	G	1104	CLA	C1A-C2A-CAA-CBA
13	G	1104	CLA	C4-C3-C5-C6
13	G	1106	CLA	C3A-C2A-CAA-CBA
13	G	1107	CLA	C2B-C3B-CAB-CBB
13	G	1107	CLA	C4B-C3B-CAB-CBB
13	G	1108	CLA	C1A-C2A-CAA-CBA
13	G	1108	CLA	C3A-C2A-CAA-CBA
13	G	1110	CLA	C1A-C2A-CAA-CBA
13	G	1110	CLA	C3A-C2A-CAA-CBA
13	G	1110	CLA	C2-C3-C5-C6
13	G	1110	CLA	C4-C3-C5-C6
13	G	1116	CLA	C3A-C2A-CAA-CBA
13	G	1117	CLA	CBD-CGD-O2D-CED
13	G	1121	CLA	C2B-C3B-CAB-CBB
13	G	1121	CLA	C4B-C3B-CAB-CBB
13	G	1122	CLA	C2B-C3B-CAB-CBB
13	G	1122	CLA	C4B-C3B-CAB-CBB
13	G	1122	CLA	CHA-CBD-CGD-O1D
13	G	1122	CLA	CHA-CBD-CGD-O2D
13	G	1122	CLA	C2-C3-C5-C6
13	G	1122	CLA	C4-C3-C5-C6
13	G	1126	CLA	C1A-C2A-CAA-CBA
13	G	1126	CLA	C3A-C2A-CAA-CBA
13	G	1131	CLA	CBD-CGD-O2D-CED
13	G	1132	CLA	CHA-CBD-CGD-O2D
13	G	1134	CLA	C1A-C2A-CAA-CBA
13	G	1134	CLA	CHA-CBD-CGD-O1D
13	G	1134	CLA	CHA-CBD-CGD-O2D
13	G	1134	CLA	C2-C3-C5-C6
13	G	1134	CLA	C4-C3-C5-C6
13	G	1137	CLA	CHA-CBD-CGD-O1D
13	G	1137	CLA	CHA-CBD-CGD-O2D
13	G	1139	CLA	C1A-C2A-CAA-CBA
13	G	1139	CLA	C3A-C2A-CAA-CBA
13	G	1139	CLA	CBD-CGD-O2D-CED
13	G	1139	CLA	C2-C3-C5-C6
13	G	1139	CLA	C4-C3-C5-C6
13	G	1140	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	G	1140	CLA	C2-C3-C5-C6
13	G	1140	CLA	C4-C3-C5-C6
13	G	1237	CLA	C4-C3-C5-C6
13	G	1101	CLA	CHA-CBD-CGD-O1D
13	G	1101	CLA	CHA-CBD-CGD-O2D
13	H	1012	CLA	CHA-CBD-CGD-O1D
13	H	1012	CLA	CHA-CBD-CGD-O2D
13	H	1012	CLA	CAD-CBD-CGD-O1D
13	H	1012	CLA	C2-C3-C5-C6
13	H	1012	CLA	C4-C3-C5-C6
13	H	1021	CLA	CHA-CBD-CGD-O1D
13	H	1202	CLA	C1A-C2A-CAA-CBA
13	H	1202	CLA	C3A-C2A-CAA-CBA
13	H	1204	CLA	CHA-CBD-CGD-O1D
13	H	1204	CLA	CHA-CBD-CGD-O2D
13	H	1209	CLA	C1A-C2A-CAA-CBA
13	H	1209	CLA	C3A-C2A-CAA-CBA
13	H	1209	CLA	CHA-CBD-CGD-O1D
13	H	1209	CLA	CHA-CBD-CGD-O2D
13	H	1210	CLA	C1A-C2A-CAA-CBA
13	H	1210	CLA	C11-C12-C13-C15
13	H	1211	CLA	C11-C10-C8-C7
13	H	1212	CLA	C2-C3-C5-C6
13	H	1212	CLA	C4-C3-C5-C6
13	H	1214	CLA	C2A-CAA-CBA-CGA
13	H	1214	CLA	C2B-C3B-CAB-CBB
13	H	1214	CLA	C4B-C3B-CAB-CBB
13	H	1214	CLA	O2A-C1-C2-C3
13	H	1215	CLA	C1A-C2A-CAA-CBA
13	H	1215	CLA	C3A-C2A-CAA-CBA
13	H	1216	CLA	C2B-C3B-CAB-CBB
13	H	1216	CLA	C4B-C3B-CAB-CBB
13	H	1217	CLA	C1A-C2A-CAA-CBA
13	H	1217	CLA	C3A-C2A-CAA-CBA
13	H	1217	CLA	C2A-CAA-CBA-CGA
13	H	1219	CLA	C2B-C3B-CAB-CBB
13	H	1220	CLA	C2B-C3B-CAB-CBB
13	H	1220	CLA	C4B-C3B-CAB-CBB
13	H	1221	CLA	C1A-C2A-CAA-CBA
13	H	1223	CLA	CHA-CBD-CGD-O1D
13	H	1223	CLA	CHA-CBD-CGD-O2D
13	H	1224	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	H	1224	CLA	C3A-C2A-CAA-CBA
13	H	1239	CLA	C4B-C3B-CAB-CBB
13	H	1240	CLA	C1A-C2A-CAA-CBA
13	H	1240	CLA	CHA-CBD-CGD-O1D
13	H	1240	CLA	CHA-CBD-CGD-O2D
13	H	1230	CLA	C1A-C2A-CAA-CBA
13	H	1230	CLA	C3A-C2A-CAA-CBA
13	H	1230	CLA	C2B-C3B-CAB-CBB
13	H	1230	CLA	C4B-C3B-CAB-CBB
13	R	1302	CLA	C1A-C2A-CAA-CBA
13	R	1302	CLA	C3A-C2A-CAA-CBA
13	T	1302	CLA	CHA-CBD-CGD-O1D
13	T	1302	CLA	CHA-CBD-CGD-O2D
13	T	1302	CLA	CAD-CBD-CGD-O1D
13	T	1303	CLA	C1A-C2A-CAA-CBA
13	U	1401	CLA	C1A-C2A-CAA-CBA
13	U	1401	CLA	C4B-C3B-CAB-CBB
13	U	1401	CLA	CHA-CBD-CGD-O1D
13	U	1401	CLA	CHA-CBD-CGD-O2D
13	U	1103	CLA	C2B-C3B-CAB-CBB
13	U	1103	CLA	C4B-C3B-CAB-CBB
13	U	1105	CLA	C2B-C3B-CAB-CBB
13	U	1105	CLA	C4B-C3B-CAB-CBB
13	Y	501	CLA	C4B-C3B-CAB-CBB
13	Y	501	CLA	CHA-CBD-CGD-O1D
13	Y	501	CLA	CHA-CBD-CGD-O2D
13	Y	501	CLA	CAD-CBD-CGD-O1D
13	Y	501	CLA	CBD-CGD-O2D-CED
13	Y	504	CLA	C2B-C3B-CAB-CBB
13	Y	504	CLA	C4B-C3B-CAB-CBB
13	Y	506	CLA	CHA-CBD-CGD-O1D
13	Y	506	CLA	CHA-CBD-CGD-O2D
13	Y	507	CLA	C2-C3-C5-C6
13	Y	507	CLA	C4-C3-C5-C6
13	Y	508	CLA	C2-C3-C5-C6
13	Y	508	CLA	C4-C3-C5-C6
13	Y	510	CLA	CBD-CGD-O2D-CED
13	Y	512	CLA	C4B-C3B-CAB-CBB
13	Y	512	CLA	C3-C5-C6-C7
13	Y	516	CLA	C1A-C2A-CAA-CBA
13	Y	516	CLA	C3A-C2A-CAA-CBA
13	Y	516	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	Y	516	CLA	C4B-C3B-CAB-CBB
13	Y	516	CLA	CHA-CBD-CGD-O1D
13	Y	516	CLA	CHA-CBD-CGD-O2D
13	Y	516	CLA	CAD-CBD-CGD-O1D
13	Y	517	CLA	C2B-C3B-CAB-CBB
13	Y	517	CLA	C4B-C3B-CAB-CBB
13	Y	518	CLA	C2B-C3B-CAB-CBB
13	Y	518	CLA	C4B-C3B-CAB-CBB
13	Y	518	CLA	C2-C3-C5-C6
13	Y	518	CLA	C4-C3-C5-C6
13	Y	519	CLA	C2B-C3B-CAB-CBB
13	Y	519	CLA	C4B-C3B-CAB-CBB
13	Z	501	CLA	C4B-C3B-CAB-CBB
13	Z	501	CLA	CBD-CGD-O2D-CED
13	Z	501	CLA	C2-C3-C5-C6
13	Z	501	CLA	C4-C3-C5-C6
13	Z	502	CLA	C2B-C3B-CAB-CBB
13	Z	502	CLA	CHA-CBD-CGD-O1D
13	Z	506	CLA	C2-C3-C5-C6
13	Z	506	CLA	C4-C3-C5-C6
13	Z	507	CLA	C2-C3-C5-C6
13	Z	507	CLA	C4-C3-C5-C6
13	Z	513	CLA	CBD-CGD-O2D-CED
13	Z	516	CLA	C2B-C3B-CAB-CBB
13	Z	516	CLA	C4B-C3B-CAB-CBB
13	Z	516	CLA	CHA-CBD-CGD-O1D
13	Z	516	CLA	CHA-CBD-CGD-O2D
13	Z	518	CLA	CHA-CBD-CGD-O1D
13	Z	518	CLA	CHA-CBD-CGD-O2D
13	Z	518	CLA	C2-C3-C5-C6
13	Z	518	CLA	C4-C3-C5-C6
13	Z	519	CLA	C2B-C3B-CAB-CBB
13	Z	519	CLA	C4B-C3B-CAB-CBB
13	a	503	CLA	C2B-C3B-CAB-CBB
13	a	503	CLA	C4B-C3B-CAB-CBB
13	a	510	CLA	CHA-CBD-CGD-O1D
13	a	510	CLA	CHA-CBD-CGD-O2D
13	a	510	CLA	CAD-CBD-CGD-O1D
13	a	512	CLA	C4B-C3B-CAB-CBB
13	a	513	CLA	C1A-C2A-CAA-CBA
13	a	513	CLA	CBD-CGD-O2D-CED
13	a	516	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	a	516	CLA	CHA-CBD-CGD-O1D
13	a	516	CLA	CHA-CBD-CGD-O2D
13	a	517	CLA	C2B-C3B-CAB-CBB
13	a	517	CLA	C4B-C3B-CAB-CBB
13	a	517	CLA	CBD-CGD-O2D-CED
13	a	518	CLA	C2B-C3B-CAB-CBB
13	a	518	CLA	C4B-C3B-CAB-CBB
13	a	518	CLA	CHA-CBD-CGD-O1D
13	a	518	CLA	CHA-CBD-CGD-O2D
13	b	501	CLA	C4B-C3B-CAB-CBB
13	b	501	CLA	CBD-CGD-O2D-CED
13	b	501	CLA	O1D-CGD-O2D-CED
13	b	506	CLA	CBD-CGD-O2D-CED
13	b	510	CLA	CBD-CGD-O2D-CED
13	b	513	CLA	CHA-CBD-CGD-O1D
13	b	513	CLA	CHA-CBD-CGD-O2D
13	b	517	CLA	C1A-C2A-CAA-CBA
13	b	517	CLA	C3A-C2A-CAA-CBA
13	b	518	CLA	C2B-C3B-CAB-CBB
13	b	518	CLA	C4B-C3B-CAB-CBB
13	b	519	CLA	C2B-C3B-CAB-CBB
13	b	519	CLA	C4B-C3B-CAB-CBB
13	b	519	CLA	CHA-CBD-CGD-O1D
13	b	519	CLA	CHA-CBD-CGD-O2D
13	b	519	CLA	CAD-CBD-CGD-O1D
13	b	519	CLA	CAD-CBD-CGD-O2D
13	c	501	CLA	CBD-CGD-O2D-CED
13	c	501	CLA	C4-C3-C5-C6
13	c	502	CLA	C2B-C3B-CAB-CBB
13	c	504	CLA	CBD-CGD-O2D-CED
13	c	505	CLA	C2A-CAA-CBA-CGA
13	c	506	CLA	CHA-CBD-CGD-O1D
13	c	506	CLA	CHA-CBD-CGD-O2D
13	c	507	CLA	CBD-CGD-O2D-CED
13	c	511	CLA	CBD-CGD-O2D-CED
13	c	512	CLA	C4B-C3B-CAB-CBB
13	c	513	CLA	C2B-C3B-CAB-CBB
13	c	513	CLA	C4B-C3B-CAB-CBB
13	c	513	CLA	CBD-CGD-O2D-CED
13	c	516	CLA	C4B-C3B-CAB-CBB
13	c	517	CLA	C4B-C3B-CAB-CBB
13	c	517	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	c	517	CLA	CHA-CBD-CGD-O2D
13	c	518	CLA	C2B-C3B-CAB-CBB
13	c	518	CLA	C4B-C3B-CAB-CBB
13	c	519	CLA	CHA-CBD-CGD-O1D
13	c	519	CLA	CHA-CBD-CGD-O2D
13	c	519	CLA	CAD-CBD-CGD-O1D
13	c	519	CLA	CAD-CBD-CGD-O2D
13	d	501	CLA	CBD-CGD-O2D-CED
13	d	501	CLA	C2-C3-C5-C6
13	d	501	CLA	C4-C3-C5-C6
13	d	503	CLA	C2A-CAA-CBA-CGA
13	d	504	CLA	CHA-CBD-CGD-O1D
13	d	504	CLA	CHA-CBD-CGD-O2D
13	d	505	CLA	C6-C7-C8-C9
13	d	506	CLA	CHA-CBD-CGD-O1D
13	d	506	CLA	CHA-CBD-CGD-O2D
13	d	508	CLA	CHA-CBD-CGD-O1D
13	d	508	CLA	CHA-CBD-CGD-O2D
13	d	510	CLA	CHA-CBD-CGD-O1D
13	d	510	CLA	CHA-CBD-CGD-O2D
13	d	512	CLA	C4B-C3B-CAB-CBB
13	d	513	CLA	CBD-CGD-O2D-CED
13	d	516	CLA	CBD-CGD-O2D-CED
13	d	517	CLA	CHA-CBD-CGD-O1D
13	d	517	CLA	CHA-CBD-CGD-O2D
13	d	517	CLA	CAD-CBD-CGD-O1D
13	d	518	CLA	CHA-CBD-CGD-O1D
13	d	518	CLA	CHA-CBD-CGD-O2D
13	d	519	CLA	CBA-CGA-O2A-C1
13	e	1011	CLA	CHA-CBD-CGD-O1D
13	e	1102	CLA	C3A-C2A-CAA-CBA
13	e	1103	CLA	C1A-C2A-CAA-CBA
13	e	1103	CLA	CHA-CBD-CGD-O1D
13	e	1103	CLA	CHA-CBD-CGD-O2D
13	e	1103	CLA	CAD-CBD-CGD-O1D
13	e	1104	CLA	C1A-C2A-CAA-CBA
13	e	1104	CLA	C4-C3-C5-C6
13	e	1106	CLA	C3A-C2A-CAA-CBA
13	e	1107	CLA	C2B-C3B-CAB-CBB
13	e	1107	CLA	C4B-C3B-CAB-CBB
13	e	1108	CLA	C1A-C2A-CAA-CBA
13	e	1108	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	e	1108	CLA	CHA-CBD-CGD-O2D
13	e	1110	CLA	C1A-C2A-CAA-CBA
13	e	1110	CLA	C3A-C2A-CAA-CBA
13	e	1110	CLA	C2-C3-C5-C6
13	e	1110	CLA	C4-C3-C5-C6
13	e	1116	CLA	C3A-C2A-CAA-CBA
13	e	1117	CLA	CBD-CGD-O2D-CED
13	e	1121	CLA	C2B-C3B-CAB-CBB
13	e	1121	CLA	C4B-C3B-CAB-CBB
13	e	1122	CLA	C2B-C3B-CAB-CBB
13	e	1122	CLA	C4B-C3B-CAB-CBB
13	e	1122	CLA	CHA-CBD-CGD-O1D
13	e	1122	CLA	CHA-CBD-CGD-O2D
13	e	1122	CLA	C2-C3-C5-C6
13	e	1122	CLA	C4-C3-C5-C6
13	e	1126	CLA	C1A-C2A-CAA-CBA
13	e	1126	CLA	C3A-C2A-CAA-CBA
13	e	1131	CLA	CBD-CGD-O2D-CED
13	e	1132	CLA	CHA-CBD-CGD-O2D
13	e	1134	CLA	C1A-C2A-CAA-CBA
13	e	1134	CLA	CHA-CBD-CGD-O1D
13	e	1134	CLA	CHA-CBD-CGD-O2D
13	e	1134	CLA	C2-C3-C5-C6
13	e	1134	CLA	C4-C3-C5-C6
13	e	1137	CLA	CHA-CBD-CGD-O1D
13	e	1137	CLA	CHA-CBD-CGD-O2D
13	e	1139	CLA	C1A-C2A-CAA-CBA
13	e	1139	CLA	C3A-C2A-CAA-CBA
13	e	1139	CLA	CBD-CGD-O2D-CED
13	e	1139	CLA	C2-C3-C5-C6
13	e	1139	CLA	C4-C3-C5-C6
13	e	1140	CLA	C1A-C2A-CAA-CBA
13	e	1140	CLA	C2-C3-C5-C6
13	e	1140	CLA	C4-C3-C5-C6
13	e	1237	CLA	C4-C3-C5-C6
13	e	1101	CLA	CHA-CBD-CGD-O1D
13	e	1101	CLA	CHA-CBD-CGD-O2D
13	f	1012	CLA	CHA-CBD-CGD-O1D
13	f	1012	CLA	CHA-CBD-CGD-O2D
13	f	1012	CLA	CAD-CBD-CGD-O1D
13	f	1012	CLA	C2-C3-C5-C6
13	f	1012	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	f	1021	CLA	CHA-CBD-CGD-O1D
13	f	1202	CLA	C1A-C2A-CAA-CBA
13	f	1202	CLA	C3A-C2A-CAA-CBA
13	f	1204	CLA	CHA-CBD-CGD-O1D
13	f	1204	CLA	CHA-CBD-CGD-O2D
13	f	1209	CLA	C1A-C2A-CAA-CBA
13	f	1209	CLA	C3A-C2A-CAA-CBA
13	f	1209	CLA	CHA-CBD-CGD-O1D
13	f	1209	CLA	CHA-CBD-CGD-O2D
13	f	1210	CLA	C1A-C2A-CAA-CBA
13	f	1210	CLA	C11-C12-C13-C15
13	f	1211	CLA	C11-C10-C8-C7
13	f	1212	CLA	C2-C3-C5-C6
13	f	1212	CLA	C4-C3-C5-C6
13	f	1214	CLA	C2A-CAA-CBA-CGA
13	f	1214	CLA	C2B-C3B-CAB-CBB
13	f	1214	CLA	C4B-C3B-CAB-CBB
13	f	1214	CLA	O2A-C1-C2-C3
13	f	1215	CLA	C1A-C2A-CAA-CBA
13	f	1215	CLA	C3A-C2A-CAA-CBA
13	f	1216	CLA	C2B-C3B-CAB-CBB
13	f	1216	CLA	C4B-C3B-CAB-CBB
13	f	1217	CLA	C1A-C2A-CAA-CBA
13	f	1217	CLA	C3A-C2A-CAA-CBA
13	f	1217	CLA	C2A-CAA-CBA-CGA
13	f	1219	CLA	C2B-C3B-CAB-CBB
13	f	1220	CLA	C2B-C3B-CAB-CBB
13	f	1220	CLA	C4B-C3B-CAB-CBB
13	f	1221	CLA	C1A-C2A-CAA-CBA
13	f	1223	CLA	CHA-CBD-CGD-O1D
13	f	1223	CLA	CHA-CBD-CGD-O2D
13	f	1224	CLA	C1A-C2A-CAA-CBA
13	f	1224	CLA	C3A-C2A-CAA-CBA
13	f	1239	CLA	C4B-C3B-CAB-CBB
13	f	1240	CLA	C1A-C2A-CAA-CBA
13	f	1240	CLA	CHA-CBD-CGD-O1D
13	f	1240	CLA	CHA-CBD-CGD-O2D
13	f	1230	CLA	C1A-C2A-CAA-CBA
13	f	1230	CLA	C3A-C2A-CAA-CBA
13	f	1230	CLA	C2B-C3B-CAB-CBB
13	f	1230	CLA	C4B-C3B-CAB-CBB
13	j	1302	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	j	1302	CLA	C3A-C2A-CAA-CBA
13	l	1302	CLA	CHA-CBD-CGD-O1D
13	l	1302	CLA	CHA-CBD-CGD-O2D
13	l	1302	CLA	CAD-CBD-CGD-O1D
13	l	1303	CLA	C1A-C2A-CAA-CBA
13	m	1401	CLA	C1A-C2A-CAA-CBA
13	m	1401	CLA	C4B-C3B-CAB-CBB
13	m	1401	CLA	CHA-CBD-CGD-O1D
13	m	1401	CLA	CHA-CBD-CGD-O2D
13	m	1103	CLA	C2B-C3B-CAB-CBB
13	m	1103	CLA	C4B-C3B-CAB-CBB
13	m	1105	CLA	C2B-C3B-CAB-CBB
13	m	1105	CLA	C4B-C3B-CAB-CBB
13	q	501	CLA	C4B-C3B-CAB-CBB
13	q	501	CLA	CHA-CBD-CGD-O1D
13	q	501	CLA	CHA-CBD-CGD-O2D
13	q	501	CLA	CAD-CBD-CGD-O1D
13	q	501	CLA	CBD-CGD-O2D-CED
13	q	504	CLA	C2B-C3B-CAB-CBB
13	q	504	CLA	C4B-C3B-CAB-CBB
13	q	506	CLA	CHA-CBD-CGD-O1D
13	q	506	CLA	CHA-CBD-CGD-O2D
13	q	507	CLA	C2-C3-C5-C6
13	q	507	CLA	C4-C3-C5-C6
13	q	508	CLA	C2-C3-C5-C6
13	q	508	CLA	C4-C3-C5-C6
13	q	510	CLA	CBD-CGD-O2D-CED
13	q	512	CLA	C4B-C3B-CAB-CBB
13	q	512	CLA	C3-C5-C6-C7
13	q	516	CLA	C1A-C2A-CAA-CBA
13	q	516	CLA	C3A-C2A-CAA-CBA
13	q	516	CLA	C2B-C3B-CAB-CBB
13	q	516	CLA	C4B-C3B-CAB-CBB
13	q	516	CLA	CHA-CBD-CGD-O1D
13	q	516	CLA	CHA-CBD-CGD-O2D
13	q	516	CLA	CAD-CBD-CGD-O1D
13	q	517	CLA	C2B-C3B-CAB-CBB
13	q	517	CLA	C4B-C3B-CAB-CBB
13	q	518	CLA	C2B-C3B-CAB-CBB
13	q	518	CLA	C4B-C3B-CAB-CBB
13	q	518	CLA	C2-C3-C5-C6
13	q	518	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	q	519	CLA	C2B-C3B-CAB-CBB
13	q	519	CLA	C4B-C3B-CAB-CBB
13	r	501	CLA	C4B-C3B-CAB-CBB
13	r	501	CLA	CBD-CGD-O2D-CED
13	r	501	CLA	C2-C3-C5-C6
13	r	501	CLA	C4-C3-C5-C6
13	r	502	CLA	C2B-C3B-CAB-CBB
13	r	502	CLA	CHA-CBD-CGD-O1D
13	r	506	CLA	C2-C3-C5-C6
13	r	506	CLA	C4-C3-C5-C6
13	r	507	CLA	C2-C3-C5-C6
13	r	507	CLA	C4-C3-C5-C6
13	r	513	CLA	CBD-CGD-O2D-CED
13	r	516	CLA	C2B-C3B-CAB-CBB
13	r	516	CLA	C4B-C3B-CAB-CBB
13	r	516	CLA	CHA-CBD-CGD-O1D
13	r	516	CLA	CHA-CBD-CGD-O2D
13	r	518	CLA	CHA-CBD-CGD-O1D
13	r	518	CLA	CHA-CBD-CGD-O2D
13	r	518	CLA	C2-C3-C5-C6
13	r	518	CLA	C4-C3-C5-C6
13	r	519	CLA	C2B-C3B-CAB-CBB
13	r	519	CLA	C4B-C3B-CAB-CBB
13	s	503	CLA	C2B-C3B-CAB-CBB
13	s	503	CLA	C4B-C3B-CAB-CBB
13	s	510	CLA	CHA-CBD-CGD-O1D
13	s	510	CLA	CHA-CBD-CGD-O2D
13	s	510	CLA	CAD-CBD-CGD-O1D
13	s	512	CLA	C4B-C3B-CAB-CBB
13	s	513	CLA	C1A-C2A-CAA-CBA
13	s	513	CLA	CBD-CGD-O2D-CED
13	s	516	CLA	C2A-CAA-CBA-CGA
13	s	516	CLA	CHA-CBD-CGD-O1D
13	s	516	CLA	CHA-CBD-CGD-O2D
13	s	516	CLA	CAD-CBD-CGD-O1D
13	s	517	CLA	C2B-C3B-CAB-CBB
13	s	517	CLA	C4B-C3B-CAB-CBB
13	s	517	CLA	CBD-CGD-O2D-CED
13	s	518	CLA	C2B-C3B-CAB-CBB
13	s	518	CLA	C4B-C3B-CAB-CBB
13	s	518	CLA	CHA-CBD-CGD-O1D
13	s	518	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	t	501	CLA	C4B-C3B-CAB-CBB
13	t	501	CLA	CHA-CBD-CGD-O1D
13	t	501	CLA	CBD-CGD-O2D-CED
13	t	501	CLA	O1D-CGD-O2D-CED
13	t	506	CLA	CBD-CGD-O2D-CED
13	t	510	CLA	CBD-CGD-O2D-CED
13	t	513	CLA	CHA-CBD-CGD-O1D
13	t	513	CLA	CHA-CBD-CGD-O2D
13	t	517	CLA	C1A-C2A-CAA-CBA
13	t	517	CLA	C3A-C2A-CAA-CBA
13	t	518	CLA	C2B-C3B-CAB-CBB
13	t	518	CLA	C4B-C3B-CAB-CBB
13	t	519	CLA	C2B-C3B-CAB-CBB
13	t	519	CLA	C4B-C3B-CAB-CBB
13	t	519	CLA	CHA-CBD-CGD-O1D
13	t	519	CLA	CHA-CBD-CGD-O2D
13	t	519	CLA	CAD-CBD-CGD-O1D
13	t	519	CLA	CAD-CBD-CGD-O2D
13	u	501	CLA	CBD-CGD-O2D-CED
13	u	501	CLA	C4-C3-C5-C6
13	u	502	CLA	C2B-C3B-CAB-CBB
13	u	504	CLA	CBD-CGD-O2D-CED
13	u	505	CLA	C2A-CAA-CBA-CGA
13	u	506	CLA	CHA-CBD-CGD-O1D
13	u	506	CLA	CHA-CBD-CGD-O2D
13	u	507	CLA	CBD-CGD-O2D-CED
13	u	511	CLA	CBD-CGD-O2D-CED
13	u	512	CLA	C4B-C3B-CAB-CBB
13	u	513	CLA	C2B-C3B-CAB-CBB
13	u	513	CLA	C4B-C3B-CAB-CBB
13	u	513	CLA	CBD-CGD-O2D-CED
13	u	516	CLA	C4B-C3B-CAB-CBB
13	u	517	CLA	C4B-C3B-CAB-CBB
13	u	517	CLA	CHA-CBD-CGD-O1D
13	u	517	CLA	CHA-CBD-CGD-O2D
13	u	518	CLA	C2B-C3B-CAB-CBB
13	u	518	CLA	C4B-C3B-CAB-CBB
13	u	519	CLA	CHA-CBD-CGD-O1D
13	u	519	CLA	CHA-CBD-CGD-O2D
13	u	519	CLA	CAD-CBD-CGD-O1D
13	u	519	CLA	CAD-CBD-CGD-O2D
13	v	501	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	v	501	CLA	C2-C3-C5-C6
13	v	501	CLA	C4-C3-C5-C6
13	v	503	CLA	C2A-CAA-CBA-CGA
13	v	504	CLA	CHA-CBD-CGD-O1D
13	v	504	CLA	CHA-CBD-CGD-O2D
13	v	505	CLA	C6-C7-C8-C9
13	v	506	CLA	CHA-CBD-CGD-O1D
13	v	506	CLA	CHA-CBD-CGD-O2D
13	v	508	CLA	CHA-CBD-CGD-O1D
13	v	508	CLA	CHA-CBD-CGD-O2D
13	v	510	CLA	CHA-CBD-CGD-O1D
13	v	510	CLA	CHA-CBD-CGD-O2D
13	v	512	CLA	C4B-C3B-CAB-CBB
13	v	513	CLA	CBD-CGD-O2D-CED
13	v	516	CLA	CBD-CGD-O2D-CED
13	v	517	CLA	CHA-CBD-CGD-O1D
13	v	517	CLA	CHA-CBD-CGD-O2D
13	v	517	CLA	CAD-CBD-CGD-O1D
13	v	518	CLA	CHA-CBD-CGD-O1D
13	v	518	CLA	CHA-CBD-CGD-O2D
13	v	519	CLA	CBA-CGA-O2A-C1
16	A	4001	BCR	C11-C12-C13-C14
16	A	4001	BCR	C37-C22-C23-C24
16	A	4008	BCR	C21-C22-C23-C24
16	A	4008	BCR	C37-C22-C23-C24
16	A	4008	BCR	C23-C24-C25-C26
16	B	4004	BCR	C7-C8-C9-C10
16	B	4004	BCR	C7-C8-C9-C34
16	B	4004	BCR	C21-C22-C23-C24
16	B	4004	BCR	C37-C22-C23-C24
16	B	4004	BCR	C23-C24-C25-C30
16	B	4005	BCR	C7-C8-C9-C10
16	B	4005	BCR	C7-C8-C9-C34
16	B	4005	BCR	C21-C22-C23-C24
16	B	4005	BCR	C37-C22-C23-C24
16	B	4005	BCR	C23-C24-C25-C30
16	B	4010	BCR	C21-C22-C23-C24
16	B	4010	BCR	C37-C22-C23-C24
16	B	4017	BCR	C1-C6-C7-C8
16	B	4014	BCR	C17-C18-C19-C20
16	B	4014	BCR	C36-C18-C19-C20
16	B	4014	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	B	4014	BCR	C37-C22-C23-C24
16	J	4013	BCR	C17-C18-C19-C20
16	J	4013	BCR	C36-C18-C19-C20
16	J	4015	BCR	C23-C24-C25-C30
16	J	4012	BCR	C5-C6-C7-C8
16	J	4012	BCR	C11-C12-C13-C14
16	J	4012	BCR	C11-C12-C13-C35
16	K	4104	BCR	C21-C22-C23-C24
16	K	4104	BCR	C37-C22-C23-C24
16	L	4019	BCR	C7-C8-C9-C10
16	L	4019	BCR	C7-C8-C9-C34
16	L	4022	BCR	C7-C8-C9-C10
16	L	4022	BCR	C7-C8-C9-C34
16	M	4021	BCR	C5-C6-C7-C8
16	M	4021	BCR	C11-C12-C13-C35
16	M	4021	BCR	C17-C18-C19-C20
16	M	4021	BCR	C36-C18-C19-C20
16	1	521	BCR	C7-C8-C9-C10
16	1	521	BCR	C7-C8-C9-C34
16	1	522	BCR	C1-C6-C7-C8
16	1	522	BCR	C5-C6-C7-C8
16	1	522	BCR	C7-C8-C9-C10
16	1	522	BCR	C7-C8-C9-C34
16	1	523	BCR	C21-C22-C23-C24
16	1	523	BCR	C37-C22-C23-C24
16	2	521	BCR	C7-C8-C9-C10
16	2	521	BCR	C7-C8-C9-C34
16	2	522	BCR	C5-C6-C7-C8
16	2	522	BCR	C7-C8-C9-C10
16	2	522	BCR	C7-C8-C9-C34
16	2	523	BCR	C21-C22-C23-C24
16	2	523	BCR	C37-C22-C23-C24
16	3	521	BCR	C7-C8-C9-C34
16	3	522	BCR	C7-C8-C9-C10
16	3	522	BCR	C7-C8-C9-C34
16	3	523	BCR	C37-C22-C23-C24
16	4	521	BCR	C7-C8-C9-C10
16	4	521	BCR	C7-C8-C9-C34
16	4	523	BCR	C37-C22-C23-C24
16	5	521	BCR	C7-C8-C9-C10
16	5	521	BCR	C7-C8-C9-C34
16	5	521	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
16	5	521	BCR	C36-C18-C19-C20
16	5	522	BCR	C5-C6-C7-C8
16	5	522	BCR	C7-C8-C9-C10
16	5	522	BCR	C7-C8-C9-C34
16	5	523	BCR	C21-C22-C23-C24
16	5	523	BCR	C37-C22-C23-C24
16	6	522	BCR	C5-C6-C7-C8
16	6	523	BCR	C37-C22-C23-C24
16	6	524	BCR	C7-C8-C9-C10
16	6	524	BCR	C7-C8-C9-C34
16	G	4001	BCR	C11-C12-C13-C14
16	G	4001	BCR	C37-C22-C23-C24
16	G	4008	BCR	C21-C22-C23-C24
16	G	4008	BCR	C37-C22-C23-C24
16	G	4008	BCR	C23-C24-C25-C26
16	H	4004	BCR	C7-C8-C9-C10
16	H	4004	BCR	C7-C8-C9-C34
16	H	4004	BCR	C21-C22-C23-C24
16	H	4004	BCR	C37-C22-C23-C24
16	H	4004	BCR	C23-C24-C25-C30
16	H	4005	BCR	C7-C8-C9-C10
16	H	4005	BCR	C7-C8-C9-C34
16	H	4005	BCR	C21-C22-C23-C24
16	H	4005	BCR	C37-C22-C23-C24
16	H	4005	BCR	C23-C24-C25-C30
16	H	4010	BCR	C21-C22-C23-C24
16	H	4010	BCR	C37-C22-C23-C24
16	H	4017	BCR	C1-C6-C7-C8
16	H	4014	BCR	C17-C18-C19-C20
16	H	4014	BCR	C36-C18-C19-C20
16	H	4014	BCR	C21-C22-C23-C24
16	H	4014	BCR	C37-C22-C23-C24
16	T	4013	BCR	C17-C18-C19-C20
16	T	4013	BCR	C36-C18-C19-C20
16	T	4015	BCR	C23-C24-C25-C30
16	T	4012	BCR	C5-C6-C7-C8
16	T	4012	BCR	C11-C12-C13-C14
16	T	4012	BCR	C11-C12-C13-C35
16	U	4104	BCR	C21-C22-C23-C24
16	U	4104	BCR	C37-C22-C23-C24
16	V	4019	BCR	C7-C8-C9-C10
16	V	4019	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
16	V	4022	BCR	C7-C8-C9-C10
16	V	4022	BCR	C7-C8-C9-C34
16	W	4021	BCR	C5-C6-C7-C8
16	W	4021	BCR	C11-C12-C13-C35
16	W	4021	BCR	C17-C18-C19-C20
16	W	4021	BCR	C36-C18-C19-C20
16	Y	521	BCR	C7-C8-C9-C10
16	Y	521	BCR	C7-C8-C9-C34
16	Y	522	BCR	C1-C6-C7-C8
16	Y	522	BCR	C5-C6-C7-C8
16	Y	522	BCR	C7-C8-C9-C10
16	Y	522	BCR	C7-C8-C9-C34
16	Y	523	BCR	C21-C22-C23-C24
16	Y	523	BCR	C37-C22-C23-C24
16	Z	521	BCR	C7-C8-C9-C10
16	Z	521	BCR	C7-C8-C9-C34
16	Z	522	BCR	C5-C6-C7-C8
16	Z	522	BCR	C7-C8-C9-C10
16	Z	522	BCR	C7-C8-C9-C34
16	Z	523	BCR	C21-C22-C23-C24
16	Z	523	BCR	C37-C22-C23-C24
16	a	521	BCR	C7-C8-C9-C34
16	a	522	BCR	C7-C8-C9-C10
16	a	522	BCR	C7-C8-C9-C34
16	a	523	BCR	C37-C22-C23-C24
16	b	521	BCR	C7-C8-C9-C10
16	b	521	BCR	C7-C8-C9-C34
16	b	523	BCR	C37-C22-C23-C24
16	c	521	BCR	C7-C8-C9-C10
16	c	521	BCR	C7-C8-C9-C34
16	c	521	BCR	C17-C18-C19-C20
16	c	521	BCR	C36-C18-C19-C20
16	c	522	BCR	C5-C6-C7-C8
16	c	522	BCR	C7-C8-C9-C10
16	c	522	BCR	C7-C8-C9-C34
16	c	523	BCR	C21-C22-C23-C24
16	c	523	BCR	C37-C22-C23-C24
16	d	522	BCR	C5-C6-C7-C8
16	d	523	BCR	C37-C22-C23-C24
16	d	524	BCR	C7-C8-C9-C10
16	d	524	BCR	C7-C8-C9-C34
16	e	4001	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	e	4001	BCR	C37-C22-C23-C24
16	e	4008	BCR	C21-C22-C23-C24
16	e	4008	BCR	C37-C22-C23-C24
16	e	4008	BCR	C23-C24-C25-C26
16	f	4004	BCR	C7-C8-C9-C10
16	f	4004	BCR	C7-C8-C9-C34
16	f	4004	BCR	C21-C22-C23-C24
16	f	4004	BCR	C37-C22-C23-C24
16	f	4004	BCR	C23-C24-C25-C30
16	f	4005	BCR	C7-C8-C9-C10
16	f	4005	BCR	C7-C8-C9-C34
16	f	4005	BCR	C21-C22-C23-C24
16	f	4005	BCR	C37-C22-C23-C24
16	f	4005	BCR	C23-C24-C25-C30
16	f	4010	BCR	C21-C22-C23-C24
16	f	4010	BCR	C37-C22-C23-C24
16	f	4017	BCR	C1-C6-C7-C8
16	f	4014	BCR	C17-C18-C19-C20
16	f	4014	BCR	C36-C18-C19-C20
16	f	4014	BCR	C21-C22-C23-C24
16	f	4014	BCR	C37-C22-C23-C24
16	l	4013	BCR	C17-C18-C19-C20
16	l	4013	BCR	C36-C18-C19-C20
16	l	4015	BCR	C23-C24-C25-C30
16	l	4012	BCR	C5-C6-C7-C8
16	l	4012	BCR	C11-C12-C13-C14
16	l	4012	BCR	C11-C12-C13-C35
16	m	4104	BCR	C21-C22-C23-C24
16	m	4104	BCR	C37-C22-C23-C24
16	n	4019	BCR	C7-C8-C9-C10
16	n	4019	BCR	C7-C8-C9-C34
16	n	4022	BCR	C7-C8-C9-C10
16	n	4022	BCR	C7-C8-C9-C34
16	o	4021	BCR	C5-C6-C7-C8
16	o	4021	BCR	C11-C12-C13-C35
16	o	4021	BCR	C17-C18-C19-C20
16	o	4021	BCR	C36-C18-C19-C20
16	q	521	BCR	C7-C8-C9-C10
16	q	521	BCR	C7-C8-C9-C34
16	q	522	BCR	C1-C6-C7-C8
16	q	522	BCR	C5-C6-C7-C8
16	q	522	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	q	522	BCR	C7-C8-C9-C34
16	q	523	BCR	C21-C22-C23-C24
16	q	523	BCR	C37-C22-C23-C24
16	r	521	BCR	C7-C8-C9-C10
16	r	521	BCR	C7-C8-C9-C34
16	r	522	BCR	C5-C6-C7-C8
16	r	522	BCR	C7-C8-C9-C10
16	r	522	BCR	C7-C8-C9-C34
16	r	523	BCR	C21-C22-C23-C24
16	r	523	BCR	C37-C22-C23-C24
16	s	521	BCR	C7-C8-C9-C34
16	s	522	BCR	C7-C8-C9-C10
16	s	522	BCR	C7-C8-C9-C34
16	s	523	BCR	C37-C22-C23-C24
16	t	521	BCR	C7-C8-C9-C10
16	t	521	BCR	C7-C8-C9-C34
16	t	523	BCR	C37-C22-C23-C24
16	u	521	BCR	C7-C8-C9-C10
16	u	521	BCR	C7-C8-C9-C34
16	u	521	BCR	C17-C18-C19-C20
16	u	521	BCR	C36-C18-C19-C20
16	u	522	BCR	C5-C6-C7-C8
16	u	522	BCR	C7-C8-C9-C10
16	u	522	BCR	C7-C8-C9-C34
16	u	523	BCR	C21-C22-C23-C24
16	u	523	BCR	C37-C22-C23-C24
16	v	522	BCR	C5-C6-C7-C8
16	v	523	BCR	C37-C22-C23-C24
16	v	524	BCR	C7-C8-C9-C10
16	v	524	BCR	C7-C8-C9-C34
17	A	5002	LHG	C4-O6-P-O5
17	A	5002	LHG	C8-C7-O7-C5
17	A	5004	LHG	O1-C1-C2-C3
17	A	5004	LHG	C1-C2-C3-O3
17	A	5004	LHG	C3-O3-P-O4
17	A	5004	LHG	C3-O3-P-O6
17	A	5004	LHG	C8-C7-O7-C5
17	A	5005	LHG	O1-C1-C2-C3
17	A	5005	LHG	O2-C2-C3-O3
17	A	5005	LHG	C3-O3-P-O5
17	A	5006	LHG	O1-C1-C2-C3
17	A	5006	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
17	A	5006	LHG	C4-O6-P-O4
17	A	5007	LHG	O1-C1-C2-C3
17	A	5008	LHG	C4-O6-P-O3
17	A	5008	LHG	O7-C5-C6-O8
17	A	5009	LHG	O1-C1-C2-C3
17	A	5009	LHG	C3-O3-P-O4
17	A	5009	LHG	C3-O3-P-O5
17	A	5009	LHG	C3-O3-P-O6
17	A	5009	LHG	C4-O6-P-O4
17	A	5001	LHG	O1-C1-C2-C3
17	A	5003	LHG	C3-O3-P-O5
17	B	1842	LHG	O1-C1-C2-C3
17	B	1842	LHG	C3-O3-P-O5
17	B	1842	LHG	O9-C7-O7-C5
17	B	1842	LHG	C8-C7-O7-C5
17	B	1855	LHG	O1-C1-C2-C3
17	B	1855	LHG	C3-O3-P-O4
17	B	1855	LHG	C4-O6-P-O5
17	I	5001	LHG	C3-O3-P-O5
17	I	5001	LHG	C3-O3-P-O6
17	I	5001	LHG	C4-O6-P-O5
17	I	5001	LHG	O9-C7-O7-C5
17	I	5001	LHG	C8-C7-O7-C5
17	L	5218	LHG	O1-C1-C2-C3
17	L	5218	LHG	C3-O3-P-O4
17	L	5218	LHG	C3-O3-P-O5
17	L	5218	LHG	O7-C5-C6-O8
17	L	5218	LHG	O9-C7-O7-C5
17	L	5218	LHG	C8-C7-O7-C5
17	L	5220	LHG	O1-C1-C2-C3
17	L	5221	LHG	C3-O3-P-O5
17	L	5221	LHG	C4-O6-P-O3
17	L	5221	LHG	C4-O6-P-O4
17	L	5221	LHG	C4-O6-P-O5
17	G	5002	LHG	C4-O6-P-O5
17	G	5002	LHG	C8-C7-O7-C5
17	G	5004	LHG	O1-C1-C2-C3
17	G	5004	LHG	C1-C2-C3-O3
17	G	5004	LHG	C3-O3-P-O4
17	G	5004	LHG	C3-O3-P-O6
17	G	5004	LHG	C8-C7-O7-C5
17	G	5005	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
17	G	5005	LHG	O2-C2-C3-O3
17	G	5006	LHG	O1-C1-C2-C3
17	G	5006	LHG	C4-O6-P-O3
17	G	5006	LHG	C4-O6-P-O4
17	G	5007	LHG	O1-C1-C2-C3
17	G	5008	LHG	C4-O6-P-O3
17	G	5008	LHG	O7-C5-C6-O8
17	G	5009	LHG	O1-C1-C2-C3
17	G	5009	LHG	C3-O3-P-O4
17	G	5009	LHG	C3-O3-P-O5
17	G	5009	LHG	C3-O3-P-O6
17	G	5009	LHG	C4-O6-P-O4
17	G	5001	LHG	O1-C1-C2-C3
17	G	5003	LHG	C3-O3-P-O5
17	H	1842	LHG	O1-C1-C2-C3
17	H	1842	LHG	C3-O3-P-O5
17	H	1842	LHG	O9-C7-O7-C5
17	H	1842	LHG	C8-C7-O7-C5
17	H	1855	LHG	O1-C1-C2-C3
17	H	1855	LHG	C3-O3-P-O4
17	H	1855	LHG	C4-O6-P-O5
17	S	5001	LHG	C3-O3-P-O5
17	S	5001	LHG	C3-O3-P-O6
17	S	5001	LHG	C4-O6-P-O5
17	S	5001	LHG	O9-C7-O7-C5
17	S	5001	LHG	C8-C7-O7-C5
17	V	5218	LHG	O1-C1-C2-C3
17	V	5218	LHG	C3-O3-P-O4
17	V	5218	LHG	C3-O3-P-O5
17	V	5218	LHG	O7-C5-C6-O8
17	V	5218	LHG	O9-C7-O7-C5
17	V	5218	LHG	C8-C7-O7-C5
17	V	5220	LHG	O1-C1-C2-C3
17	V	5221	LHG	C3-O3-P-O5
17	V	5221	LHG	C4-O6-P-O3
17	V	5221	LHG	C4-O6-P-O4
17	V	5221	LHG	C4-O6-P-O5
17	e	5002	LHG	C4-O6-P-O5
17	e	5002	LHG	C8-C7-O7-C5
17	e	5004	LHG	O1-C1-C2-C3
17	e	5004	LHG	C1-C2-C3-O3
17	e	5004	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
17	e	5004	LHG	C3-O3-P-O6
17	e	5004	LHG	C8-C7-O7-C5
17	e	5005	LHG	O1-C1-C2-C3
17	e	5005	LHG	O2-C2-C3-O3
17	e	5005	LHG	C3-O3-P-O5
17	e	5006	LHG	O1-C1-C2-C3
17	e	5006	LHG	C4-O6-P-O3
17	e	5006	LHG	C4-O6-P-O4
17	e	5007	LHG	O1-C1-C2-C3
17	e	5008	LHG	C4-O6-P-O3
17	e	5008	LHG	O7-C5-C6-O8
17	e	5009	LHG	O1-C1-C2-C3
17	e	5009	LHG	C3-O3-P-O4
17	e	5009	LHG	C3-O3-P-O5
17	e	5009	LHG	C3-O3-P-O6
17	e	5009	LHG	C4-O6-P-O4
17	e	5001	LHG	O1-C1-C2-C3
17	e	5003	LHG	C3-O3-P-O5
17	f	1842	LHG	O1-C1-C2-C3
17	f	1842	LHG	C3-O3-P-O5
17	f	1842	LHG	O9-C7-O7-C5
17	f	1842	LHG	C8-C7-O7-C5
17	f	1855	LHG	O1-C1-C2-C3
17	f	1855	LHG	C3-O3-P-O4
17	f	1855	LHG	C4-O6-P-O5
17	k	5001	LHG	C3-O3-P-O5
17	k	5001	LHG	C3-O3-P-O6
17	k	5001	LHG	C4-O6-P-O5
17	k	5001	LHG	O9-C7-O7-C5
17	k	5001	LHG	C8-C7-O7-C5
17	n	5218	LHG	O1-C1-C2-C3
17	n	5218	LHG	C3-O3-P-O4
17	n	5218	LHG	C3-O3-P-O5
17	n	5218	LHG	O7-C5-C6-O8
17	n	5218	LHG	O9-C7-O7-C5
17	n	5218	LHG	C8-C7-O7-C5
17	n	5220	LHG	O1-C1-C2-C3
17	n	5221	LHG	C3-O3-P-O5
17	n	5221	LHG	C4-O6-P-O3
17	n	5221	LHG	C4-O6-P-O4
17	n	5221	LHG	C4-O6-P-O5
18	A	1849	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
18	B	1843	LMU	C2'-C1'-O1'-C1
18	B	1843	LMU	O5'-C1'-O1'-C1
18	J	5105	LMU	C2'-C1'-O1'-C1
18	J	5105	LMU	C2-C1-O1'-C1'
18	1	902	LMU	C2'-C1'-O1'-C1
18	1	902	LMU	O5'-C1'-O1'-C1
18	1	902	LMU	C2-C1-O1'-C1'
18	2	901	LMU	C2'-C1'-O1'-C1
18	G	1849	LMU	C2'-C1'-O1'-C1
18	H	1843	LMU	C2'-C1'-O1'-C1
18	H	1843	LMU	O5'-C1'-O1'-C1
18	T	5105	LMU	C2'-C1'-O1'-C1
18	T	5105	LMU	C2-C1-O1'-C1'
18	Y	902	LMU	C2'-C1'-O1'-C1
18	Y	902	LMU	O5'-C1'-O1'-C1
18	Y	902	LMU	C2-C1-O1'-C1'
18	Z	901	LMU	C2'-C1'-O1'-C1
18	Z	901	LMU	O5'-C1'-O1'-C1
18	e	1849	LMU	C2'-C1'-O1'-C1
18	f	1843	LMU	C2'-C1'-O1'-C1
18	f	1843	LMU	O5'-C1'-O1'-C1
18	l	5105	LMU	C2'-C1'-O1'-C1
18	l	5105	LMU	C2-C1-O1'-C1'
18	q	902	LMU	C2'-C1'-O1'-C1
18	q	902	LMU	O5'-C1'-O1'-C1
18	q	902	LMU	C2-C1-O1'-C1'
18	r	901	LMU	C2'-C1'-O1'-C1
18	r	901	LMU	O5'-C1'-O1'-C1
19	J	5104	LMG	O7-C8-C9-O8
19	T	5104	LMG	O7-C8-C9-O8
19	l	5104	LMG	O7-C8-C9-O8
20	L	5216	SQD	O47-C45-C46-O48
20	L	5216	SQD	C5-C6-S-O7
20	L	5216	SQD	C5-C6-S-O8
20	1	822	SQD	O49-C7-O47-C45
20	2	822	SQD	O49-C7-O47-C45
20	2	822	SQD	C8-C7-O47-C45
20	3	822	SQD	O47-C45-C46-O48
20	3	822	SQD	O49-C7-O47-C45
20	3	822	SQD	C8-C7-O47-C45
20	4	822	SQD	C8-C7-O47-C45
20	V	5216	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
20	V	5216	SQD	C5-C6-S-O7
20	V	5216	SQD	C5-C6-S-O8
20	Y	822	SQD	O49-C7-O47-C45
20	Z	822	SQD	O49-C7-O47-C45
20	Z	822	SQD	C8-C7-O47-C45
20	a	822	SQD	O47-C45-C46-O48
20	a	822	SQD	O49-C7-O47-C45
20	a	822	SQD	C8-C7-O47-C45
20	b	822	SQD	C8-C7-O47-C45
20	n	5216	SQD	O47-C45-C46-O48
20	n	5216	SQD	C5-C6-S-O7
20	n	5216	SQD	C5-C6-S-O8
20	q	822	SQD	O49-C7-O47-C45
20	r	822	SQD	O49-C7-O47-C45
20	r	822	SQD	C8-C7-O47-C45
20	s	822	SQD	O47-C45-C46-O48
20	s	822	SQD	O49-C7-O47-C45
20	s	822	SQD	C8-C7-O47-C45
20	t	822	SQD	C8-C7-O47-C45
20	4	822	SQD	O49-C7-O47-C45
20	6	822	SQD	C8-C7-O47-C45
20	b	822	SQD	O49-C7-O47-C45
20	d	822	SQD	C8-C7-O47-C45
20	t	822	SQD	O49-C7-O47-C45
20	v	822	SQD	C8-C7-O47-C45
13	B	1023	CLA	O1D-CGD-O2D-CED
13	1	503	CLA	O1D-CGD-O2D-CED
13	1	506	CLA	O1D-CGD-O2D-CED
13	3	503	CLA	O1D-CGD-O2D-CED
13	4	506	CLA	O1D-CGD-O2D-CED
13	5	506	CLA	O1D-CGD-O2D-CED
13	6	506	CLA	O1D-CGD-O2D-CED
13	H	1023	CLA	O1D-CGD-O2D-CED
13	Y	503	CLA	O1D-CGD-O2D-CED
13	Y	506	CLA	O1D-CGD-O2D-CED
13	a	503	CLA	O1D-CGD-O2D-CED
13	b	506	CLA	O1D-CGD-O2D-CED
13	c	506	CLA	O1D-CGD-O2D-CED
13	d	506	CLA	O1D-CGD-O2D-CED
13	f	1023	CLA	O1D-CGD-O2D-CED
13	q	503	CLA	O1D-CGD-O2D-CED
13	q	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	s	503	CLA	O1D-CGD-O2D-CED
13	t	506	CLA	O1D-CGD-O2D-CED
13	u	506	CLA	O1D-CGD-O2D-CED
13	v	506	CLA	O1D-CGD-O2D-CED
20	6	822	SQD	O49-C7-O47-C45
20	d	822	SQD	O49-C7-O47-C45
20	v	822	SQD	O49-C7-O47-C45
13	2	503	CLA	O1D-CGD-O2D-CED
13	3	510	CLA	O1D-CGD-O2D-CED
13	4	504	CLA	O1D-CGD-O2D-CED
13	5	503	CLA	O1D-CGD-O2D-CED
13	6	503	CLA	O1D-CGD-O2D-CED
13	Z	503	CLA	O1D-CGD-O2D-CED
13	a	510	CLA	O1D-CGD-O2D-CED
13	b	504	CLA	O1D-CGD-O2D-CED
13	c	503	CLA	O1D-CGD-O2D-CED
13	d	503	CLA	O1D-CGD-O2D-CED
13	r	503	CLA	O1D-CGD-O2D-CED
13	s	510	CLA	O1D-CGD-O2D-CED
13	t	504	CLA	O1D-CGD-O2D-CED
13	u	503	CLA	O1D-CGD-O2D-CED
13	v	503	CLA	O1D-CGD-O2D-CED
13	v	513	CLA	O1D-CGD-O2D-CED
13	A	1107	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	CBD-CGD-O2D-CED
13	A	1119	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	CBD-CGD-O2D-CED
13	A	1801	CLA	CBD-CGD-O2D-CED
13	B	1021	CLA	CBD-CGD-O2D-CED
13	B	1023	CLA	CBD-CGD-O2D-CED
13	B	1203	CLA	CBD-CGD-O2D-CED
13	B	1219	CLA	CBD-CGD-O2D-CED
13	B	1221	CLA	CBD-CGD-O2D-CED
13	B	1239	CLA	CBD-CGD-O2D-CED
13	B	1207	CLA	CBD-CGD-O2D-CED
13	F	1302	CLA	CBD-CGD-O2D-CED
13	J	1302	CLA	CBD-CGD-O2D-CED
13	K	1105	CLA	CBD-CGD-O2D-CED
13	1	503	CLA	CBD-CGD-O2D-CED
13	1	506	CLA	CBD-CGD-O2D-CED
13	1	516	CLA	CBD-CGD-O2D-CED
13	2	503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	2	506	CLA	CBD-CGD-O2D-CED
13	2	511	CLA	CBD-CGD-O2D-CED
13	3	503	CLA	CBD-CGD-O2D-CED
13	3	506	CLA	CBD-CGD-O2D-CED
13	3	510	CLA	CBD-CGD-O2D-CED
13	3	516	CLA	CBD-CGD-O2D-CED
13	3	518	CLA	CBD-CGD-O2D-CED
13	3	519	CLA	CBD-CGD-O2D-CED
13	4	504	CLA	CBD-CGD-O2D-CED
13	4	511	CLA	CBD-CGD-O2D-CED
13	4	517	CLA	CBD-CGD-O2D-CED
13	4	518	CLA	CBD-CGD-O2D-CED
13	5	503	CLA	CBD-CGD-O2D-CED
13	5	506	CLA	CBD-CGD-O2D-CED
13	5	508	CLA	CBD-CGD-O2D-CED
13	5	510	CLA	CBD-CGD-O2D-CED
13	5	517	CLA	CBD-CGD-O2D-CED
13	6	502	CLA	CBD-CGD-O2D-CED
13	6	503	CLA	CBD-CGD-O2D-CED
13	6	506	CLA	CBD-CGD-O2D-CED
13	6	509	CLA	CBD-CGD-O2D-CED
13	G	1107	CLA	CBD-CGD-O2D-CED
13	G	1108	CLA	CBD-CGD-O2D-CED
13	G	1119	CLA	CBD-CGD-O2D-CED
13	G	1120	CLA	CBD-CGD-O2D-CED
13	G	1801	CLA	CBD-CGD-O2D-CED
13	H	1021	CLA	CBD-CGD-O2D-CED
13	H	1023	CLA	CBD-CGD-O2D-CED
13	H	1203	CLA	CBD-CGD-O2D-CED
13	H	1219	CLA	CBD-CGD-O2D-CED
13	H	1221	CLA	CBD-CGD-O2D-CED
13	H	1239	CLA	CBD-CGD-O2D-CED
13	H	1207	CLA	CBD-CGD-O2D-CED
13	R	1302	CLA	CBD-CGD-O2D-CED
13	T	1302	CLA	CBD-CGD-O2D-CED
13	U	1105	CLA	CBD-CGD-O2D-CED
13	Y	503	CLA	CBD-CGD-O2D-CED
13	Y	506	CLA	CBD-CGD-O2D-CED
13	Y	516	CLA	CBD-CGD-O2D-CED
13	Z	503	CLA	CBD-CGD-O2D-CED
13	Z	506	CLA	CBD-CGD-O2D-CED
13	Z	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	503	CLA	CBD-CGD-O2D-CED
13	a	506	CLA	CBD-CGD-O2D-CED
13	a	510	CLA	CBD-CGD-O2D-CED
13	a	516	CLA	CBD-CGD-O2D-CED
13	a	518	CLA	CBD-CGD-O2D-CED
13	a	519	CLA	CBD-CGD-O2D-CED
13	b	504	CLA	CBD-CGD-O2D-CED
13	b	511	CLA	CBD-CGD-O2D-CED
13	b	517	CLA	CBD-CGD-O2D-CED
13	b	518	CLA	CBD-CGD-O2D-CED
13	c	503	CLA	CBD-CGD-O2D-CED
13	c	506	CLA	CBD-CGD-O2D-CED
13	c	508	CLA	CBD-CGD-O2D-CED
13	c	510	CLA	CBD-CGD-O2D-CED
13	c	517	CLA	CBD-CGD-O2D-CED
13	d	502	CLA	CBD-CGD-O2D-CED
13	d	503	CLA	CBD-CGD-O2D-CED
13	d	506	CLA	CBD-CGD-O2D-CED
13	d	509	CLA	CBD-CGD-O2D-CED
13	e	1107	CLA	CBD-CGD-O2D-CED
13	e	1108	CLA	CBD-CGD-O2D-CED
13	e	1119	CLA	CBD-CGD-O2D-CED
13	e	1120	CLA	CBD-CGD-O2D-CED
13	e	1801	CLA	CBD-CGD-O2D-CED
13	f	1021	CLA	CBD-CGD-O2D-CED
13	f	1023	CLA	CBD-CGD-O2D-CED
13	f	1203	CLA	CBD-CGD-O2D-CED
13	f	1219	CLA	CBD-CGD-O2D-CED
13	f	1221	CLA	CBD-CGD-O2D-CED
13	f	1239	CLA	CBD-CGD-O2D-CED
13	f	1207	CLA	CBD-CGD-O2D-CED
13	j	1302	CLA	CBD-CGD-O2D-CED
13	l	1302	CLA	CBD-CGD-O2D-CED
13	m	1105	CLA	CBD-CGD-O2D-CED
13	q	503	CLA	CBD-CGD-O2D-CED
13	q	506	CLA	CBD-CGD-O2D-CED
13	q	516	CLA	CBD-CGD-O2D-CED
13	r	503	CLA	CBD-CGD-O2D-CED
13	r	506	CLA	CBD-CGD-O2D-CED
13	r	511	CLA	CBD-CGD-O2D-CED
13	s	503	CLA	CBD-CGD-O2D-CED
13	s	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	s	510	CLA	CBD-CGD-O2D-CED
13	s	516	CLA	CBD-CGD-O2D-CED
13	s	518	CLA	CBD-CGD-O2D-CED
13	s	519	CLA	CBD-CGD-O2D-CED
13	t	504	CLA	CBD-CGD-O2D-CED
13	t	511	CLA	CBD-CGD-O2D-CED
13	t	517	CLA	CBD-CGD-O2D-CED
13	t	518	CLA	CBD-CGD-O2D-CED
13	u	503	CLA	CBD-CGD-O2D-CED
13	u	506	CLA	CBD-CGD-O2D-CED
13	u	508	CLA	CBD-CGD-O2D-CED
13	u	510	CLA	CBD-CGD-O2D-CED
13	u	517	CLA	CBD-CGD-O2D-CED
13	v	502	CLA	CBD-CGD-O2D-CED
13	v	503	CLA	CBD-CGD-O2D-CED
13	v	506	CLA	CBD-CGD-O2D-CED
13	v	509	CLA	CBD-CGD-O2D-CED
13	A	1109	CLA	O1A-CGA-O2A-C1
13	B	1209	CLA	O1A-CGA-O2A-C1
13	B	1217	CLA	O1A-CGA-O2A-C1
13	B	1219	CLA	O1A-CGA-O2A-C1
13	B	1227	CLA	O1A-CGA-O2A-C1
13	B	1207	CLA	O1A-CGA-O2A-C1
13	3	510	CLA	O1A-CGA-O2A-C1
13	6	505	CLA	O1A-CGA-O2A-C1
13	G	1109	CLA	O1A-CGA-O2A-C1
13	H	1209	CLA	O1A-CGA-O2A-C1
13	H	1217	CLA	O1A-CGA-O2A-C1
13	H	1219	CLA	O1A-CGA-O2A-C1
13	H	1227	CLA	O1A-CGA-O2A-C1
13	H	1207	CLA	O1A-CGA-O2A-C1
13	a	510	CLA	O1A-CGA-O2A-C1
13	d	505	CLA	O1A-CGA-O2A-C1
13	e	1109	CLA	O1A-CGA-O2A-C1
13	f	1209	CLA	O1A-CGA-O2A-C1
13	f	1217	CLA	O1A-CGA-O2A-C1
13	f	1219	CLA	O1A-CGA-O2A-C1
13	f	1227	CLA	O1A-CGA-O2A-C1
13	f	1207	CLA	O1A-CGA-O2A-C1
13	s	510	CLA	O1A-CGA-O2A-C1
13	v	505	CLA	O1A-CGA-O2A-C1
17	A	5006	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
17	I	5001	LHG	O10-C23-O8-C6
17	L	5221	LHG	O10-C23-O8-C6
17	G	5006	LHG	O10-C23-O8-C6
17	S	5001	LHG	O10-C23-O8-C6
17	V	5221	LHG	O10-C23-O8-C6
17	e	5006	LHG	O10-C23-O8-C6
17	k	5001	LHG	O10-C23-O8-C6
17	n	5221	LHG	O10-C23-O8-C6
13	A	1139	CLA	O1D-CGD-O2D-CED
13	B	1021	CLA	O1D-CGD-O2D-CED
13	3	506	CLA	O1D-CGD-O2D-CED
13	3	517	CLA	O1D-CGD-O2D-CED
13	6	513	CLA	O1D-CGD-O2D-CED
13	H	1021	CLA	O1D-CGD-O2D-CED
13	a	506	CLA	O1D-CGD-O2D-CED
13	a	517	CLA	O1D-CGD-O2D-CED
13	d	513	CLA	O1D-CGD-O2D-CED
13	e	1139	CLA	O1D-CGD-O2D-CED
13	f	1021	CLA	O1D-CGD-O2D-CED
13	s	506	CLA	O1D-CGD-O2D-CED
13	s	517	CLA	O1D-CGD-O2D-CED
13	K	1105	CLA	O1D-CGD-O2D-CED
13	1	510	CLA	O1D-CGD-O2D-CED
13	2	506	CLA	O1D-CGD-O2D-CED
13	2	513	CLA	O1D-CGD-O2D-CED
13	4	510	CLA	O1D-CGD-O2D-CED
13	5	504	CLA	O1D-CGD-O2D-CED
13	5	513	CLA	O1D-CGD-O2D-CED
13	6	501	CLA	O1D-CGD-O2D-CED
13	6	516	CLA	O1D-CGD-O2D-CED
13	G	1139	CLA	O1D-CGD-O2D-CED
13	U	1105	CLA	O1D-CGD-O2D-CED
13	Y	510	CLA	O1D-CGD-O2D-CED
13	Z	506	CLA	O1D-CGD-O2D-CED
13	Z	513	CLA	O1D-CGD-O2D-CED
13	b	510	CLA	O1D-CGD-O2D-CED
13	c	504	CLA	O1D-CGD-O2D-CED
13	c	513	CLA	O1D-CGD-O2D-CED
13	d	501	CLA	O1D-CGD-O2D-CED
13	d	516	CLA	O1D-CGD-O2D-CED
13	m	1105	CLA	O1D-CGD-O2D-CED
13	q	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	r	506	CLA	O1D-CGD-O2D-CED
13	r	513	CLA	O1D-CGD-O2D-CED
13	t	510	CLA	O1D-CGD-O2D-CED
13	u	504	CLA	O1D-CGD-O2D-CED
13	u	513	CLA	O1D-CGD-O2D-CED
13	v	501	CLA	O1D-CGD-O2D-CED
13	v	516	CLA	O1D-CGD-O2D-CED
13	A	1109	CLA	CBA-CGA-O2A-C1
13	A	1110	CLA	CBA-CGA-O2A-C1
13	B	1217	CLA	CBA-CGA-O2A-C1
13	B	1227	CLA	CBA-CGA-O2A-C1
13	6	505	CLA	CBA-CGA-O2A-C1
13	G	1109	CLA	CBA-CGA-O2A-C1
13	G	1110	CLA	CBA-CGA-O2A-C1
13	H	1217	CLA	CBA-CGA-O2A-C1
13	H	1227	CLA	CBA-CGA-O2A-C1
13	d	505	CLA	CBA-CGA-O2A-C1
13	e	1109	CLA	CBA-CGA-O2A-C1
13	e	1110	CLA	CBA-CGA-O2A-C1
13	f	1217	CLA	CBA-CGA-O2A-C1
13	f	1227	CLA	CBA-CGA-O2A-C1
13	v	505	CLA	CBA-CGA-O2A-C1
17	L	5221	LHG	C24-C23-O8-C6
17	V	5221	LHG	C24-C23-O8-C6
17	n	5221	LHG	C24-C23-O8-C6
20	4	822	SQD	C24-C23-O48-C46
20	b	822	SQD	C24-C23-O48-C46
20	t	822	SQD	C24-C23-O48-C46
13	A	1011	CLA	CBD-CGD-O2D-CED
13	A	1103	CLA	CBD-CGD-O2D-CED
13	A	1104	CLA	CBD-CGD-O2D-CED
13	A	1106	CLA	CBD-CGD-O2D-CED
13	A	1111	CLA	CBD-CGD-O2D-CED
13	A	1112	CLA	CBD-CGD-O2D-CED
13	A	1123	CLA	CBD-CGD-O2D-CED
13	A	1132	CLA	CBD-CGD-O2D-CED
13	B	1012	CLA	CBD-CGD-O2D-CED
13	B	1201	CLA	CBD-CGD-O2D-CED
13	B	1209	CLA	CBD-CGD-O2D-CED
13	B	1220	CLA	CBD-CGD-O2D-CED
13	B	1229	CLA	CBD-CGD-O2D-CED
13	B	1240	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	J	1303	CLA	CBD-CGD-O2D-CED
13	2	504	CLA	CBD-CGD-O2D-CED
13	2	507	CLA	CBD-CGD-O2D-CED
13	4	507	CLA	CBD-CGD-O2D-CED
13	4	508	CLA	CBD-CGD-O2D-CED
13	6	511	CLA	CBD-CGD-O2D-CED
13	6	512	CLA	CBD-CGD-O2D-CED
13	6	518	CLA	CBD-CGD-O2D-CED
13	6	519	CLA	CBD-CGD-O2D-CED
13	G	1011	CLA	CBD-CGD-O2D-CED
13	G	1103	CLA	CBD-CGD-O2D-CED
13	G	1104	CLA	CBD-CGD-O2D-CED
13	G	1106	CLA	CBD-CGD-O2D-CED
13	G	1111	CLA	CBD-CGD-O2D-CED
13	G	1112	CLA	CBD-CGD-O2D-CED
13	G	1123	CLA	CBD-CGD-O2D-CED
13	G	1132	CLA	CBD-CGD-O2D-CED
13	H	1012	CLA	CBD-CGD-O2D-CED
13	H	1201	CLA	CBD-CGD-O2D-CED
13	H	1209	CLA	CBD-CGD-O2D-CED
13	H	1220	CLA	CBD-CGD-O2D-CED
13	H	1229	CLA	CBD-CGD-O2D-CED
13	H	1240	CLA	CBD-CGD-O2D-CED
13	T	1303	CLA	CBD-CGD-O2D-CED
13	Z	504	CLA	CBD-CGD-O2D-CED
13	Z	507	CLA	CBD-CGD-O2D-CED
13	b	507	CLA	CBD-CGD-O2D-CED
13	b	508	CLA	CBD-CGD-O2D-CED
13	d	511	CLA	CBD-CGD-O2D-CED
13	d	512	CLA	CBD-CGD-O2D-CED
13	d	518	CLA	CBD-CGD-O2D-CED
13	d	519	CLA	CBD-CGD-O2D-CED
13	e	1011	CLA	CBD-CGD-O2D-CED
13	e	1103	CLA	CBD-CGD-O2D-CED
13	e	1104	CLA	CBD-CGD-O2D-CED
13	e	1106	CLA	CBD-CGD-O2D-CED
13	e	1111	CLA	CBD-CGD-O2D-CED
13	e	1112	CLA	CBD-CGD-O2D-CED
13	e	1123	CLA	CBD-CGD-O2D-CED
13	e	1132	CLA	CBD-CGD-O2D-CED
13	f	1012	CLA	CBD-CGD-O2D-CED
13	f	1201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	f	1209	CLA	CBD-CGD-O2D-CED
13	f	1220	CLA	CBD-CGD-O2D-CED
13	f	1229	CLA	CBD-CGD-O2D-CED
13	f	1240	CLA	CBD-CGD-O2D-CED
13	l	1303	CLA	CBD-CGD-O2D-CED
13	r	504	CLA	CBD-CGD-O2D-CED
13	r	507	CLA	CBD-CGD-O2D-CED
13	t	507	CLA	CBD-CGD-O2D-CED
13	t	508	CLA	CBD-CGD-O2D-CED
13	v	511	CLA	CBD-CGD-O2D-CED
13	v	512	CLA	CBD-CGD-O2D-CED
13	v	518	CLA	CBD-CGD-O2D-CED
13	v	519	CLA	CBD-CGD-O2D-CED
13	K	1105	CLA	C4C-C3C-CAC-CBC
13	A	1110	CLA	O1A-CGA-O2A-C1
13	A	1114	CLA	O1A-CGA-O2A-C1
13	A	1119	CLA	O1A-CGA-O2A-C1
13	A	1140	CLA	O1A-CGA-O2A-C1
13	A	1130	CLA	O1A-CGA-O2A-C1
13	B	1202	CLA	O1A-CGA-O2A-C1
13	B	1206	CLA	O1A-CGA-O2A-C1
13	B	1240	CLA	O1A-CGA-O2A-C1
13	1	505	CLA	O1A-CGA-O2A-C1
13	2	504	CLA	O1A-CGA-O2A-C1
13	2	505	CLA	O1A-CGA-O2A-C1
13	3	505	CLA	O1A-CGA-O2A-C1
13	4	505	CLA	O1A-CGA-O2A-C1
13	4	510	CLA	O1A-CGA-O2A-C1
13	5	505	CLA	O1A-CGA-O2A-C1
13	G	1110	CLA	O1A-CGA-O2A-C1
13	G	1114	CLA	O1A-CGA-O2A-C1
13	G	1119	CLA	O1A-CGA-O2A-C1
13	G	1140	CLA	O1A-CGA-O2A-C1
13	G	1130	CLA	O1A-CGA-O2A-C1
13	H	1202	CLA	O1A-CGA-O2A-C1
13	H	1206	CLA	O1A-CGA-O2A-C1
13	H	1240	CLA	O1A-CGA-O2A-C1
13	Y	505	CLA	O1A-CGA-O2A-C1
13	Z	504	CLA	O1A-CGA-O2A-C1
13	Z	505	CLA	O1A-CGA-O2A-C1
13	a	505	CLA	O1A-CGA-O2A-C1
13	b	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	510	CLA	O1A-CGA-O2A-C1
13	c	505	CLA	O1A-CGA-O2A-C1
13	e	1110	CLA	O1A-CGA-O2A-C1
13	e	1114	CLA	O1A-CGA-O2A-C1
13	e	1119	CLA	O1A-CGA-O2A-C1
13	e	1140	CLA	O1A-CGA-O2A-C1
13	e	1130	CLA	O1A-CGA-O2A-C1
13	f	1202	CLA	O1A-CGA-O2A-C1
13	f	1206	CLA	O1A-CGA-O2A-C1
13	f	1240	CLA	O1A-CGA-O2A-C1
13	q	505	CLA	O1A-CGA-O2A-C1
13	r	504	CLA	O1A-CGA-O2A-C1
13	r	505	CLA	O1A-CGA-O2A-C1
13	s	505	CLA	O1A-CGA-O2A-C1
13	t	505	CLA	O1A-CGA-O2A-C1
13	t	510	CLA	O1A-CGA-O2A-C1
13	u	505	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	O10-C23-O8-C6
17	A	5009	LHG	O10-C23-O8-C6
17	B	1842	LHG	O10-C23-O8-C6
17	L	5218	LHG	O10-C23-O8-C6
17	L	5220	LHG	O10-C23-O8-C6
17	G	5002	LHG	O10-C23-O8-C6
17	G	5009	LHG	O10-C23-O8-C6
17	H	1842	LHG	O10-C23-O8-C6
17	V	5218	LHG	O10-C23-O8-C6
17	V	5220	LHG	O10-C23-O8-C6
17	e	5002	LHG	O10-C23-O8-C6
17	e	5009	LHG	O10-C23-O8-C6
17	f	1842	LHG	O10-C23-O8-C6
17	n	5218	LHG	O10-C23-O8-C6
17	n	5220	LHG	O10-C23-O8-C6
19	J	5104	LMG	O10-C28-O8-C9
19	T	5104	LMG	O10-C28-O8-C9
19	l	5104	LMG	O10-C28-O8-C9
20	2	822	SQD	O10-C23-O48-C46
20	Z	822	SQD	O10-C23-O48-C46
20	r	822	SQD	O10-C23-O48-C46
13	A	1117	CLA	O1D-CGD-O2D-CED
13	5	501	CLA	O1D-CGD-O2D-CED
13	5	507	CLA	O1D-CGD-O2D-CED
13	5	511	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	G	1117	CLA	O1D-CGD-O2D-CED
13	c	501	CLA	O1D-CGD-O2D-CED
13	c	507	CLA	O1D-CGD-O2D-CED
13	c	511	CLA	O1D-CGD-O2D-CED
13	e	1117	CLA	O1D-CGD-O2D-CED
13	u	501	CLA	O1D-CGD-O2D-CED
13	u	507	CLA	O1D-CGD-O2D-CED
13	u	511	CLA	O1D-CGD-O2D-CED
13	U	1105	CLA	C4C-C3C-CAC-CBC
13	m	1105	CLA	C4C-C3C-CAC-CBC
13	1	501	CLA	O1D-CGD-O2D-CED
13	2	501	CLA	O1D-CGD-O2D-CED
13	3	513	CLA	O1D-CGD-O2D-CED
13	Y	501	CLA	O1D-CGD-O2D-CED
13	Z	501	CLA	O1D-CGD-O2D-CED
13	a	513	CLA	O1D-CGD-O2D-CED
13	q	501	CLA	O1D-CGD-O2D-CED
13	r	501	CLA	O1D-CGD-O2D-CED
13	s	513	CLA	O1D-CGD-O2D-CED
13	A	1113	CLA	CBD-CGD-O2D-CED
13	3	504	CLA	CBD-CGD-O2D-CED
13	6	507	CLA	CBD-CGD-O2D-CED
13	G	1113	CLA	CBD-CGD-O2D-CED
13	a	504	CLA	CBD-CGD-O2D-CED
13	d	507	CLA	CBD-CGD-O2D-CED
13	e	1113	CLA	CBD-CGD-O2D-CED
13	s	504	CLA	CBD-CGD-O2D-CED
13	v	507	CLA	CBD-CGD-O2D-CED
13	A	1131	CLA	O1D-CGD-O2D-CED
13	2	511	CLA	O1D-CGD-O2D-CED
13	3	518	CLA	O1D-CGD-O2D-CED
13	G	1131	CLA	O1D-CGD-O2D-CED
13	Z	511	CLA	O1D-CGD-O2D-CED
13	a	518	CLA	O1D-CGD-O2D-CED
13	e	1131	CLA	O1D-CGD-O2D-CED
13	r	511	CLA	O1D-CGD-O2D-CED
13	s	518	CLA	O1D-CGD-O2D-CED
17	A	5004	LHG	O9-C7-O7-C5
17	A	5007	LHG	O9-C7-O7-C5
17	A	5008	LHG	O9-C7-O7-C5
17	A	5009	LHG	O9-C7-O7-C5
17	B	1855	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
17	L	5220	LHG	O9-C7-O7-C5
17	G	5004	LHG	O9-C7-O7-C5
17	G	5007	LHG	O9-C7-O7-C5
17	G	5008	LHG	O9-C7-O7-C5
17	G	5009	LHG	O9-C7-O7-C5
17	H	1855	LHG	O9-C7-O7-C5
17	V	5220	LHG	O9-C7-O7-C5
17	e	5004	LHG	O9-C7-O7-C5
17	e	5007	LHG	O9-C7-O7-C5
17	e	5008	LHG	O9-C7-O7-C5
17	e	5009	LHG	O9-C7-O7-C5
17	f	1855	LHG	O9-C7-O7-C5
17	n	5220	LHG	O9-C7-O7-C5
13	K	1105	CLA	C2C-C3C-CAC-CBC
13	1	516	CLA	C2C-C3C-CAC-CBC
13	U	1105	CLA	C2C-C3C-CAC-CBC
13	m	1105	CLA	C2C-C3C-CAC-CBC
13	q	516	CLA	C2C-C3C-CAC-CBC
13	A	1102	CLA	C3-C5-C6-C7
13	A	1116	CLA	C3-C5-C6-C7
13	A	1118	CLA	C3-C5-C6-C7
13	A	1121	CLA	C3-C5-C6-C7
13	A	1122	CLA	C3-C5-C6-C7
13	A	1133	CLA	C3-C5-C6-C7
13	A	1136	CLA	C3-C5-C6-C7
13	A	1139	CLA	C3-C5-C6-C7
13	B	1216	CLA	C3-C5-C6-C7
13	B	1231	CLA	C3-C5-C6-C7
13	B	1239	CLA	C3-C5-C6-C7
13	J	1303	CLA	C3-C5-C6-C7
13	L	1503	CLA	C3-C5-C6-C7
13	1	502	CLA	C3-C5-C6-C7
13	1	505	CLA	C3-C5-C6-C7
13	1	510	CLA	C3-C5-C6-C7
13	1	511	CLA	C3-C5-C6-C7
13	1	518	CLA	C3-C5-C6-C7
13	2	505	CLA	C3-C5-C6-C7
13	2	511	CLA	C3-C5-C6-C7
13	3	508	CLA	C3-C5-C6-C7
13	3	513	CLA	C3-C5-C6-C7
13	5	501	CLA	C3-C5-C6-C7
13	6	501	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	6	505	CLA	C3-C5-C6-C7
13	G	1102	CLA	C3-C5-C6-C7
13	G	1116	CLA	C3-C5-C6-C7
13	G	1118	CLA	C3-C5-C6-C7
13	G	1121	CLA	C3-C5-C6-C7
13	G	1122	CLA	C3-C5-C6-C7
13	G	1133	CLA	C3-C5-C6-C7
13	G	1136	CLA	C3-C5-C6-C7
13	G	1139	CLA	C3-C5-C6-C7
13	H	1216	CLA	C3-C5-C6-C7
13	H	1231	CLA	C3-C5-C6-C7
13	H	1239	CLA	C3-C5-C6-C7
13	T	1303	CLA	C3-C5-C6-C7
13	V	1503	CLA	C3-C5-C6-C7
13	Y	502	CLA	C3-C5-C6-C7
13	Y	505	CLA	C3-C5-C6-C7
13	Y	510	CLA	C3-C5-C6-C7
13	Y	511	CLA	C3-C5-C6-C7
13	Y	518	CLA	C3-C5-C6-C7
13	Z	505	CLA	C3-C5-C6-C7
13	Z	511	CLA	C3-C5-C6-C7
13	a	508	CLA	C3-C5-C6-C7
13	a	513	CLA	C3-C5-C6-C7
13	c	501	CLA	C3-C5-C6-C7
13	d	501	CLA	C3-C5-C6-C7
13	d	505	CLA	C3-C5-C6-C7
13	e	1102	CLA	C3-C5-C6-C7
13	e	1116	CLA	C3-C5-C6-C7
13	e	1118	CLA	C3-C5-C6-C7
13	e	1121	CLA	C3-C5-C6-C7
13	e	1122	CLA	C3-C5-C6-C7
13	e	1133	CLA	C3-C5-C6-C7
13	e	1136	CLA	C3-C5-C6-C7
13	e	1139	CLA	C3-C5-C6-C7
13	f	1216	CLA	C3-C5-C6-C7
13	f	1231	CLA	C3-C5-C6-C7
13	f	1239	CLA	C3-C5-C6-C7
13	l	1303	CLA	C3-C5-C6-C7
13	n	1503	CLA	C3-C5-C6-C7
13	q	502	CLA	C3-C5-C6-C7
13	q	505	CLA	C3-C5-C6-C7
13	q	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	q	511	CLA	C3-C5-C6-C7
13	q	518	CLA	C3-C5-C6-C7
13	r	505	CLA	C3-C5-C6-C7
13	r	511	CLA	C3-C5-C6-C7
13	s	508	CLA	C3-C5-C6-C7
13	s	513	CLA	C3-C5-C6-C7
13	u	501	CLA	C3-C5-C6-C7
13	v	501	CLA	C3-C5-C6-C7
13	v	505	CLA	C3-C5-C6-C7
13	A	1114	CLA	CBA-CGA-O2A-C1
13	B	1209	CLA	CBA-CGA-O2A-C1
13	B	1219	CLA	CBA-CGA-O2A-C1
13	B	1207	CLA	CBA-CGA-O2A-C1
13	1	505	CLA	CBA-CGA-O2A-C1
13	2	505	CLA	CBA-CGA-O2A-C1
13	3	505	CLA	CBA-CGA-O2A-C1
13	3	510	CLA	CBA-CGA-O2A-C1
13	4	505	CLA	CBA-CGA-O2A-C1
13	4	510	CLA	CBA-CGA-O2A-C1
13	5	505	CLA	CBA-CGA-O2A-C1
13	G	1114	CLA	CBA-CGA-O2A-C1
13	H	1209	CLA	CBA-CGA-O2A-C1
13	H	1219	CLA	CBA-CGA-O2A-C1
13	H	1207	CLA	CBA-CGA-O2A-C1
13	Y	505	CLA	CBA-CGA-O2A-C1
13	Z	505	CLA	CBA-CGA-O2A-C1
13	a	505	CLA	CBA-CGA-O2A-C1
13	a	510	CLA	CBA-CGA-O2A-C1
13	b	505	CLA	CBA-CGA-O2A-C1
13	b	510	CLA	CBA-CGA-O2A-C1
13	c	502	CLA	CBA-CGA-O2A-C1
13	c	505	CLA	CBA-CGA-O2A-C1
13	e	1114	CLA	CBA-CGA-O2A-C1
13	f	1209	CLA	CBA-CGA-O2A-C1
13	f	1219	CLA	CBA-CGA-O2A-C1
13	f	1207	CLA	CBA-CGA-O2A-C1
13	q	505	CLA	CBA-CGA-O2A-C1
13	r	505	CLA	CBA-CGA-O2A-C1
13	s	505	CLA	CBA-CGA-O2A-C1
13	s	510	CLA	CBA-CGA-O2A-C1
13	t	505	CLA	CBA-CGA-O2A-C1
13	t	510	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	u	505	CLA	CBA-CGA-O2A-C1
17	A	5006	LHG	C24-C23-O8-C6
17	A	5009	LHG	C24-C23-O8-C6
17	I	5001	LHG	C24-C23-O8-C6
17	L	5218	LHG	C24-C23-O8-C6
17	L	5220	LHG	C24-C23-O8-C6
17	G	5006	LHG	C24-C23-O8-C6
17	G	5009	LHG	C24-C23-O8-C6
17	S	5001	LHG	C24-C23-O8-C6
17	V	5218	LHG	C24-C23-O8-C6
17	V	5220	LHG	C24-C23-O8-C6
17	e	5006	LHG	C24-C23-O8-C6
17	e	5009	LHG	C24-C23-O8-C6
17	k	5001	LHG	C24-C23-O8-C6
17	n	5218	LHG	C24-C23-O8-C6
17	n	5220	LHG	C24-C23-O8-C6
13	Y	516	CLA	C2C-C3C-CAC-CBC
20	4	822	SQD	O10-C23-O48-C46
20	b	822	SQD	O10-C23-O48-C46
20	t	822	SQD	O10-C23-O48-C46
17	A	5008	LHG	C8-C7-O7-C5
17	L	5220	LHG	C8-C7-O7-C5
17	G	5008	LHG	C8-C7-O7-C5
17	V	5220	LHG	C8-C7-O7-C5
17	e	5008	LHG	C8-C7-O7-C5
17	n	5220	LHG	C8-C7-O7-C5
20	1	822	SQD	C8-C7-O47-C45
20	5	822	SQD	C8-C7-O47-C45
20	Y	822	SQD	C8-C7-O47-C45
20	c	822	SQD	C8-C7-O47-C45
20	q	822	SQD	C8-C7-O47-C45
20	u	822	SQD	C8-C7-O47-C45
13	B	1219	CLA	O1D-CGD-O2D-CED
13	F	1302	CLA	O1D-CGD-O2D-CED
13	4	518	CLA	O1D-CGD-O2D-CED
13	H	1219	CLA	O1D-CGD-O2D-CED
13	R	1302	CLA	O1D-CGD-O2D-CED
13	b	518	CLA	O1D-CGD-O2D-CED
13	f	1219	CLA	O1D-CGD-O2D-CED
13	j	1302	CLA	O1D-CGD-O2D-CED
13	t	518	CLA	O1D-CGD-O2D-CED
13	A	1137	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	1227	CLA	CBD-CGD-O2D-CED
13	2	519	CLA	CBD-CGD-O2D-CED
13	4	505	CLA	CBD-CGD-O2D-CED
13	6	517	CLA	CBD-CGD-O2D-CED
13	G	1137	CLA	CBD-CGD-O2D-CED
13	H	1227	CLA	CBD-CGD-O2D-CED
13	Z	519	CLA	CBD-CGD-O2D-CED
13	b	505	CLA	CBD-CGD-O2D-CED
13	d	517	CLA	CBD-CGD-O2D-CED
13	e	1137	CLA	CBD-CGD-O2D-CED
13	f	1227	CLA	CBD-CGD-O2D-CED
13	r	519	CLA	CBD-CGD-O2D-CED
13	t	505	CLA	CBD-CGD-O2D-CED
13	v	517	CLA	CBD-CGD-O2D-CED
13	3	516	CLA	C2C-C3C-CAC-CBC
13	a	516	CLA	C2C-C3C-CAC-CBC
13	s	516	CLA	C2C-C3C-CAC-CBC
13	6	519	CLA	O1A-CGA-O2A-C1
13	d	519	CLA	O1A-CGA-O2A-C1
13	v	519	CLA	O1A-CGA-O2A-C1
13	A	1133	CLA	C4-C3-C5-C6
13	G	1133	CLA	C4-C3-C5-C6
13	e	1133	CLA	C4-C3-C5-C6
13	A	1104	CLA	C2-C3-C5-C6
13	A	1237	CLA	C2-C3-C5-C6
13	5	501	CLA	C2-C3-C5-C6
13	G	1104	CLA	C2-C3-C5-C6
13	G	1237	CLA	C2-C3-C5-C6
13	c	501	CLA	C2-C3-C5-C6
13	e	1104	CLA	C2-C3-C5-C6
13	e	1237	CLA	C2-C3-C5-C6
13	u	501	CLA	C2-C3-C5-C6
13	A	1013	CLA	CBD-CGD-O2D-CED
13	B	1226	CLA	CBD-CGD-O2D-CED
13	B	1232	CLA	CBD-CGD-O2D-CED
13	1	502	CLA	CBD-CGD-O2D-CED
13	4	513	CLA	CBD-CGD-O2D-CED
13	5	512	CLA	CBD-CGD-O2D-CED
13	G	1013	CLA	CBD-CGD-O2D-CED
13	H	1226	CLA	CBD-CGD-O2D-CED
13	H	1232	CLA	CBD-CGD-O2D-CED
13	Y	502	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	b	513	CLA	CBD-CGD-O2D-CED
13	c	512	CLA	CBD-CGD-O2D-CED
13	e	1013	CLA	CBD-CGD-O2D-CED
13	f	1226	CLA	CBD-CGD-O2D-CED
13	f	1232	CLA	CBD-CGD-O2D-CED
13	q	502	CLA	CBD-CGD-O2D-CED
13	t	513	CLA	CBD-CGD-O2D-CED
13	u	512	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	C2A-CAA-CBA-CGA
13	A	1119	CLA	C2A-CAA-CBA-CGA
13	A	1127	CLA	C2A-CAA-CBA-CGA
13	B	1012	CLA	C2A-CAA-CBA-CGA
13	B	1206	CLA	C2A-CAA-CBA-CGA
13	B	1221	CLA	C2A-CAA-CBA-CGA
13	B	1228	CLA	C2A-CAA-CBA-CGA
13	B	1232	CLA	C2A-CAA-CBA-CGA
13	B	1238	CLA	C2A-CAA-CBA-CGA
13	1	505	CLA	C2A-CAA-CBA-CGA
13	1	516	CLA	C2A-CAA-CBA-CGA
13	2	505	CLA	C2A-CAA-CBA-CGA
13	2	512	CLA	C2A-CAA-CBA-CGA
13	3	505	CLA	C2A-CAA-CBA-CGA
13	5	507	CLA	C2A-CAA-CBA-CGA
13	6	505	CLA	C2A-CAA-CBA-CGA
13	6	513	CLA	C2A-CAA-CBA-CGA
13	G	1108	CLA	C2A-CAA-CBA-CGA
13	G	1119	CLA	C2A-CAA-CBA-CGA
13	G	1127	CLA	C2A-CAA-CBA-CGA
13	H	1012	CLA	C2A-CAA-CBA-CGA
13	H	1206	CLA	C2A-CAA-CBA-CGA
13	H	1221	CLA	C2A-CAA-CBA-CGA
13	H	1228	CLA	C2A-CAA-CBA-CGA
13	H	1232	CLA	C2A-CAA-CBA-CGA
13	H	1238	CLA	C2A-CAA-CBA-CGA
13	Y	505	CLA	C2A-CAA-CBA-CGA
13	Y	516	CLA	C2A-CAA-CBA-CGA
13	Z	505	CLA	C2A-CAA-CBA-CGA
13	Z	512	CLA	C2A-CAA-CBA-CGA
13	a	505	CLA	C2A-CAA-CBA-CGA
13	c	507	CLA	C2A-CAA-CBA-CGA
13	d	505	CLA	C2A-CAA-CBA-CGA
13	d	513	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	e	1108	CLA	C2A-CAA-CBA-CGA
13	e	1119	CLA	C2A-CAA-CBA-CGA
13	e	1127	CLA	C2A-CAA-CBA-CGA
13	f	1012	CLA	C2A-CAA-CBA-CGA
13	f	1206	CLA	C2A-CAA-CBA-CGA
13	f	1221	CLA	C2A-CAA-CBA-CGA
13	f	1228	CLA	C2A-CAA-CBA-CGA
13	f	1232	CLA	C2A-CAA-CBA-CGA
13	f	1238	CLA	C2A-CAA-CBA-CGA
13	q	505	CLA	C2A-CAA-CBA-CGA
13	q	516	CLA	C2A-CAA-CBA-CGA
13	r	505	CLA	C2A-CAA-CBA-CGA
13	r	512	CLA	C2A-CAA-CBA-CGA
13	s	505	CLA	C2A-CAA-CBA-CGA
13	u	507	CLA	C2A-CAA-CBA-CGA
13	v	505	CLA	C2A-CAA-CBA-CGA
13	v	513	CLA	C2A-CAA-CBA-CGA
13	3	516	CLA	O1D-CGD-O2D-CED
13	a	516	CLA	O1D-CGD-O2D-CED
13	e	1107	CLA	O1D-CGD-O2D-CED
13	s	516	CLA	O1D-CGD-O2D-CED
13	A	1119	CLA	C3-C5-C6-C7
13	B	1206	CLA	C3-C5-C6-C7
13	2	501	CLA	C3-C5-C6-C7
13	3	505	CLA	C3-C5-C6-C7
13	3	507	CLA	C3-C5-C6-C7
13	4	505	CLA	C3-C5-C6-C7
13	5	505	CLA	C3-C5-C6-C7
13	5	511	CLA	C3-C5-C6-C7
13	5	518	CLA	C3-C5-C6-C7
13	G	1119	CLA	C3-C5-C6-C7
13	H	1206	CLA	C3-C5-C6-C7
13	Z	501	CLA	C3-C5-C6-C7
13	a	505	CLA	C3-C5-C6-C7
13	a	507	CLA	C3-C5-C6-C7
13	b	505	CLA	C3-C5-C6-C7
13	c	505	CLA	C3-C5-C6-C7
13	c	511	CLA	C3-C5-C6-C7
13	c	518	CLA	C3-C5-C6-C7
13	e	1119	CLA	C3-C5-C6-C7
13	f	1206	CLA	C3-C5-C6-C7
13	r	501	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	s	505	CLA	C3-C5-C6-C7
13	s	507	CLA	C3-C5-C6-C7
13	t	505	CLA	C3-C5-C6-C7
13	u	505	CLA	C3-C5-C6-C7
13	u	511	CLA	C3-C5-C6-C7
13	u	518	CLA	C3-C5-C6-C7
13	A	1119	CLA	CBA-CGA-O2A-C1
13	A	1122	CLA	CBA-CGA-O2A-C1
13	A	1129	CLA	CBA-CGA-O2A-C1
13	A	1135	CLA	CBA-CGA-O2A-C1
13	A	1140	CLA	CBA-CGA-O2A-C1
13	A	1130	CLA	CBA-CGA-O2A-C1
13	B	1202	CLA	CBA-CGA-O2A-C1
13	B	1206	CLA	CBA-CGA-O2A-C1
13	B	1240	CLA	CBA-CGA-O2A-C1
13	B	1230	CLA	CBA-CGA-O2A-C1
13	2	504	CLA	CBA-CGA-O2A-C1
13	4	502	CLA	CBA-CGA-O2A-C1
13	5	502	CLA	CBA-CGA-O2A-C1
13	G	1119	CLA	CBA-CGA-O2A-C1
13	G	1122	CLA	CBA-CGA-O2A-C1
13	G	1129	CLA	CBA-CGA-O2A-C1
13	G	1135	CLA	CBA-CGA-O2A-C1
13	G	1140	CLA	CBA-CGA-O2A-C1
13	G	1130	CLA	CBA-CGA-O2A-C1
13	H	1202	CLA	CBA-CGA-O2A-C1
13	H	1206	CLA	CBA-CGA-O2A-C1
13	H	1240	CLA	CBA-CGA-O2A-C1
13	H	1230	CLA	CBA-CGA-O2A-C1
13	Z	504	CLA	CBA-CGA-O2A-C1
13	b	502	CLA	CBA-CGA-O2A-C1
13	e	1119	CLA	CBA-CGA-O2A-C1
13	e	1122	CLA	CBA-CGA-O2A-C1
13	e	1129	CLA	CBA-CGA-O2A-C1
13	e	1135	CLA	CBA-CGA-O2A-C1
13	e	1140	CLA	CBA-CGA-O2A-C1
13	e	1130	CLA	CBA-CGA-O2A-C1
13	f	1202	CLA	CBA-CGA-O2A-C1
13	f	1206	CLA	CBA-CGA-O2A-C1
13	f	1240	CLA	CBA-CGA-O2A-C1
13	f	1230	CLA	CBA-CGA-O2A-C1
13	r	504	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	u	502	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C24-C23-O8-C6
17	G	5002	LHG	C24-C23-O8-C6
17	e	5002	LHG	C24-C23-O8-C6
19	J	5104	LMG	C29-C28-O8-C9
19	T	5104	LMG	C29-C28-O8-C9
19	l	5104	LMG	C29-C28-O8-C9
20	2	822	SQD	C24-C23-O48-C46
20	3	822	SQD	C24-C23-O48-C46
20	Z	822	SQD	C24-C23-O48-C46
20	a	822	SQD	C24-C23-O48-C46
20	r	822	SQD	C24-C23-O48-C46
20	s	822	SQD	C24-C23-O48-C46
19	B	5002	LMG	O6-C5-C6-O5
19	H	5002	LMG	O6-C5-C6-O5
19	f	5002	LMG	O6-C5-C6-O5
13	A	1107	CLA	O1D-CGD-O2D-CED
13	A	1119	CLA	O1D-CGD-O2D-CED
13	6	509	CLA	O1D-CGD-O2D-CED
13	G	1107	CLA	O1D-CGD-O2D-CED
13	G	1119	CLA	O1D-CGD-O2D-CED
13	d	509	CLA	O1D-CGD-O2D-CED
13	e	1119	CLA	O1D-CGD-O2D-CED
13	v	509	CLA	O1D-CGD-O2D-CED
14	A	2001	PQN	C11-C12-C13-C14
14	B	2002	PQN	C11-C12-C13-C14
14	G	2001	PQN	C11-C12-C13-C14
14	H	2002	PQN	C11-C12-C13-C14
14	e	2001	PQN	C11-C12-C13-C14
14	f	2002	PQN	C11-C12-C13-C14
13	B	1231	CLA	CBD-CGD-O2D-CED
13	3	511	CLA	CBD-CGD-O2D-CED
13	H	1231	CLA	CBD-CGD-O2D-CED
13	a	511	CLA	CBD-CGD-O2D-CED
13	f	1231	CLA	CBD-CGD-O2D-CED
13	s	511	CLA	CBD-CGD-O2D-CED
17	A	5006	LHG	C29-C30-C31-C32
17	G	5006	LHG	C29-C30-C31-C32
17	e	5006	LHG	C29-C30-C31-C32
13	A	1108	CLA	O1D-CGD-O2D-CED
13	A	1801	CLA	O1D-CGD-O2D-CED
13	1	516	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	4	517	CLA	O1D-CGD-O2D-CED
13	5	508	CLA	O1D-CGD-O2D-CED
13	5	510	CLA	O1D-CGD-O2D-CED
13	5	517	CLA	O1D-CGD-O2D-CED
13	G	1108	CLA	O1D-CGD-O2D-CED
13	G	1801	CLA	O1D-CGD-O2D-CED
13	H	1221	CLA	O1D-CGD-O2D-CED
13	Y	516	CLA	O1D-CGD-O2D-CED
13	b	517	CLA	O1D-CGD-O2D-CED
13	c	508	CLA	O1D-CGD-O2D-CED
13	c	510	CLA	O1D-CGD-O2D-CED
13	c	517	CLA	O1D-CGD-O2D-CED
13	e	1108	CLA	O1D-CGD-O2D-CED
13	e	1801	CLA	O1D-CGD-O2D-CED
13	f	1221	CLA	O1D-CGD-O2D-CED
13	q	516	CLA	O1D-CGD-O2D-CED
13	t	517	CLA	O1D-CGD-O2D-CED
13	u	508	CLA	O1D-CGD-O2D-CED
13	u	510	CLA	O1D-CGD-O2D-CED
13	u	517	CLA	O1D-CGD-O2D-CED
17	A	5002	LHG	O9-C7-O7-C5
17	G	5002	LHG	O9-C7-O7-C5
17	e	5002	LHG	O9-C7-O7-C5
20	5	822	SQD	O49-C7-O47-C45
20	c	822	SQD	O49-C7-O47-C45
20	u	822	SQD	O49-C7-O47-C45
13	A	1129	CLA	O1A-CGA-O2A-C1
13	B	1212	CLA	O1A-CGA-O2A-C1
13	B	1230	CLA	O1A-CGA-O2A-C1
13	G	1129	CLA	O1A-CGA-O2A-C1
13	H	1212	CLA	O1A-CGA-O2A-C1
13	H	1230	CLA	O1A-CGA-O2A-C1
13	e	1129	CLA	O1A-CGA-O2A-C1
13	f	1212	CLA	O1A-CGA-O2A-C1
13	f	1230	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	O10-C23-O8-C6
17	G	5001	LHG	O10-C23-O8-C6
17	e	5001	LHG	O10-C23-O8-C6
20	1	822	SQD	O10-C23-O48-C46
20	Y	822	SQD	O10-C23-O48-C46
20	q	822	SQD	O10-C23-O48-C46
13	B	1221	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	1843	LMU	O5B-C5B-C6B-O6B
18	H	1843	LMU	O5B-C5B-C6B-O6B
18	f	1843	LMU	O5B-C5B-C6B-O6B
13	A	1138	CLA	CBD-CGD-O2D-CED
13	B	1206	CLA	CBD-CGD-O2D-CED
13	B	1235	CLA	CBD-CGD-O2D-CED
13	K	1103	CLA	CBD-CGD-O2D-CED
13	1	507	CLA	CBD-CGD-O2D-CED
13	1	511	CLA	CBD-CGD-O2D-CED
13	1	512	CLA	CBD-CGD-O2D-CED
13	1	519	CLA	CBD-CGD-O2D-CED
13	6	510	CLA	CBD-CGD-O2D-CED
13	G	1138	CLA	CBD-CGD-O2D-CED
13	H	1206	CLA	CBD-CGD-O2D-CED
13	H	1235	CLA	CBD-CGD-O2D-CED
13	U	1103	CLA	CBD-CGD-O2D-CED
13	Y	507	CLA	CBD-CGD-O2D-CED
13	Y	511	CLA	CBD-CGD-O2D-CED
13	Y	512	CLA	CBD-CGD-O2D-CED
13	Y	519	CLA	CBD-CGD-O2D-CED
13	d	510	CLA	CBD-CGD-O2D-CED
13	e	1138	CLA	CBD-CGD-O2D-CED
13	f	1206	CLA	CBD-CGD-O2D-CED
13	f	1235	CLA	CBD-CGD-O2D-CED
13	m	1103	CLA	CBD-CGD-O2D-CED
13	q	507	CLA	CBD-CGD-O2D-CED
13	q	511	CLA	CBD-CGD-O2D-CED
13	q	512	CLA	CBD-CGD-O2D-CED
13	q	519	CLA	CBD-CGD-O2D-CED
13	v	510	CLA	CBD-CGD-O2D-CED
13	B	1203	CLA	O1D-CGD-O2D-CED
13	B	1207	CLA	O1D-CGD-O2D-CED
13	H	1203	CLA	O1D-CGD-O2D-CED
13	H	1207	CLA	O1D-CGD-O2D-CED
13	f	1203	CLA	O1D-CGD-O2D-CED
13	f	1207	CLA	O1D-CGD-O2D-CED
17	A	5004	LHG	O2-C2-C3-O3
17	G	5004	LHG	O2-C2-C3-O3
17	e	5004	LHG	O2-C2-C3-O3
13	A	1107	CLA	C3-C5-C6-C7
13	A	1108	CLA	C3-C5-C6-C7
13	B	1205	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	B	1215	CLA	C3-C5-C6-C7
13	2	507	CLA	C3-C5-C6-C7
13	3	510	CLA	C3-C5-C6-C7
13	G	1107	CLA	C3-C5-C6-C7
13	G	1108	CLA	C3-C5-C6-C7
13	H	1205	CLA	C3-C5-C6-C7
13	H	1215	CLA	C3-C5-C6-C7
13	Z	507	CLA	C3-C5-C6-C7
13	a	510	CLA	C3-C5-C6-C7
13	e	1107	CLA	C3-C5-C6-C7
13	e	1108	CLA	C3-C5-C6-C7
13	f	1205	CLA	C3-C5-C6-C7
13	f	1215	CLA	C3-C5-C6-C7
13	r	507	CLA	C3-C5-C6-C7
13	s	510	CLA	C3-C5-C6-C7
13	A	1108	CLA	CBA-CGA-O2A-C1
13	G	1108	CLA	CBA-CGA-O2A-C1
13	e	1108	CLA	CBA-CGA-O2A-C1
13	t	502	CLA	CBA-CGA-O2A-C1
17	B	1842	LHG	C24-C23-O8-C6
17	H	1842	LHG	C24-C23-O8-C6
17	f	1842	LHG	C24-C23-O8-C6
13	A	1135	CLA	O1A-CGA-O2A-C1
13	5	502	CLA	O1A-CGA-O2A-C1
13	G	1135	CLA	O1A-CGA-O2A-C1
13	c	502	CLA	O1A-CGA-O2A-C1
13	e	1135	CLA	O1A-CGA-O2A-C1
13	u	502	CLA	O1A-CGA-O2A-C1
18	A	1848	LMU	O5B-C5B-C6B-O6B
18	G	1848	LMU	O5B-C5B-C6B-O6B
18	e	1848	LMU	O5B-C5B-C6B-O6B
13	3	519	CLA	O1D-CGD-O2D-CED
13	6	502	CLA	O1D-CGD-O2D-CED
13	a	519	CLA	O1D-CGD-O2D-CED
13	d	502	CLA	O1D-CGD-O2D-CED
13	s	519	CLA	O1D-CGD-O2D-CED
13	v	502	CLA	O1D-CGD-O2D-CED
13	G	1120	CLA	O1D-CGD-O2D-CED
13	e	1120	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	CBD-CGD-O2D-CED
13	A	1134	CLA	CBD-CGD-O2D-CED
13	B	1230	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	1	518	CLA	CBD-CGD-O2D-CED
13	2	516	CLA	CBD-CGD-O2D-CED
13	5	502	CLA	CBD-CGD-O2D-CED
13	G	1126	CLA	CBD-CGD-O2D-CED
13	H	1230	CLA	CBD-CGD-O2D-CED
13	Y	518	CLA	CBD-CGD-O2D-CED
13	Z	516	CLA	CBD-CGD-O2D-CED
13	c	502	CLA	CBD-CGD-O2D-CED
13	e	1126	CLA	CBD-CGD-O2D-CED
13	e	1134	CLA	CBD-CGD-O2D-CED
13	f	1230	CLA	CBD-CGD-O2D-CED
13	q	518	CLA	CBD-CGD-O2D-CED
13	r	516	CLA	CBD-CGD-O2D-CED
13	u	502	CLA	CBD-CGD-O2D-CED
17	B	1855	LHG	C5-C6-O8-C23
17	H	1855	LHG	C5-C6-O8-C23
17	f	1855	LHG	C5-C6-O8-C23
13	A	1120	CLA	O1D-CGD-O2D-CED
13	G	1108	CLA	O1A-CGA-O2A-C1
13	e	1108	CLA	O1A-CGA-O2A-C1
19	B	5002	LMG	C4-C5-C6-O5
19	H	5002	LMG	C4-C5-C6-O5
19	f	5002	LMG	C4-C5-C6-O5
13	3	507	CLA	CBD-CGD-O2D-CED
13	G	1134	CLA	CBD-CGD-O2D-CED
13	a	507	CLA	CBD-CGD-O2D-CED
13	s	507	CLA	CBD-CGD-O2D-CED
13	A	1013	CLA	C3-C5-C6-C7
13	1	508	CLA	C3-C5-C6-C7
13	G	1013	CLA	C3-C5-C6-C7
13	Y	508	CLA	C3-C5-C6-C7
13	e	1013	CLA	C3-C5-C6-C7
13	q	508	CLA	C3-C5-C6-C7
13	B	1212	CLA	CBA-CGA-O2A-C1
13	H	1212	CLA	CBA-CGA-O2A-C1
13	f	1212	CLA	CBA-CGA-O2A-C1
13	4	511	CLA	O1D-CGD-O2D-CED
13	b	511	CLA	O1D-CGD-O2D-CED
18	B	1843	LMU	C4B-C5B-C6B-O6B
18	H	1843	LMU	C4B-C5B-C6B-O6B
18	f	1843	LMU	C4B-C5B-C6B-O6B
13	A	1108	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	1122	CLA	O1A-CGA-O2A-C1
13	4	502	CLA	O1A-CGA-O2A-C1
13	G	1122	CLA	O1A-CGA-O2A-C1
13	e	1122	CLA	O1A-CGA-O2A-C1
13	t	502	CLA	O1A-CGA-O2A-C1
17	A	5005	LHG	O10-C23-O8-C6
17	G	5005	LHG	O10-C23-O8-C6
17	e	5005	LHG	O10-C23-O8-C6
13	A	1115	CLA	C4-C3-C5-C6
13	1	510	CLA	C4-C3-C5-C6
13	G	1115	CLA	C4-C3-C5-C6
13	Y	510	CLA	C4-C3-C5-C6
13	e	1115	CLA	C4-C3-C5-C6
13	q	510	CLA	C4-C3-C5-C6
18	A	1848	LMU	C4B-C5B-C6B-O6B
18	G	1848	LMU	C4B-C5B-C6B-O6B
18	e	1848	LMU	C4B-C5B-C6B-O6B
13	A	1115	CLA	C2-C3-C5-C6
13	1	510	CLA	C2-C3-C5-C6
13	G	1115	CLA	C2-C3-C5-C6
13	Y	510	CLA	C2-C3-C5-C6
13	e	1115	CLA	C2-C3-C5-C6
13	q	510	CLA	C2-C3-C5-C6
13	A	1134	CLA	C2A-CAA-CBA-CGA
13	B	1218	CLA	C2A-CAA-CBA-CGA
13	1	517	CLA	C2A-CAA-CBA-CGA
13	G	1134	CLA	C2A-CAA-CBA-CGA
13	H	1218	CLA	C2A-CAA-CBA-CGA
13	Y	517	CLA	C2A-CAA-CBA-CGA
13	e	1134	CLA	C2A-CAA-CBA-CGA
13	f	1218	CLA	C2A-CAA-CBA-CGA
13	q	517	CLA	C2A-CAA-CBA-CGA
13	B	1239	CLA	O1D-CGD-O2D-CED
13	H	1239	CLA	O1D-CGD-O2D-CED
13	f	1239	CLA	O1D-CGD-O2D-CED
13	t	511	CLA	O1D-CGD-O2D-CED
18	B	1843	LMU	O5'-C5'-C6'-O6'
18	H	1843	LMU	O5'-C5'-C6'-O6'
18	f	1843	LMU	O5'-C5'-C6'-O6'
13	3	502	CLA	O1A-CGA-O2A-C1
13	a	502	CLA	O1A-CGA-O2A-C1
13	b	502	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	s	502	CLA	O1A-CGA-O2A-C1
18	A	1849	LMU	O5'-C1'-O1'-C1
18	J	5105	LMU	O5'-C1'-O1'-C1
18	2	901	LMU	O5'-C1'-O1'-C1
18	G	1849	LMU	O5'-C1'-O1'-C1
18	T	5105	LMU	O5'-C1'-O1'-C1
18	e	1849	LMU	O5'-C1'-O1'-C1
18	l	5105	LMU	O5'-C1'-O1'-C1
13	B	1234	CLA	CBA-CGA-O2A-C1
13	J	1303	CLA	CBA-CGA-O2A-C1
13	3	502	CLA	CBA-CGA-O2A-C1
13	H	1234	CLA	CBA-CGA-O2A-C1
13	T	1303	CLA	CBA-CGA-O2A-C1
13	a	502	CLA	CBA-CGA-O2A-C1
13	f	1234	CLA	CBA-CGA-O2A-C1
13	l	1303	CLA	CBA-CGA-O2A-C1
13	s	502	CLA	CBA-CGA-O2A-C1
13	e	1124	CLA	CBD-CGD-O2D-CED
19	J	5104	LMG	C4-C5-C6-O5
19	T	5104	LMG	C4-C5-C6-O5
19	l	5104	LMG	C4-C5-C6-O5
13	J	1302	CLA	O1D-CGD-O2D-CED
13	T	1302	CLA	O1D-CGD-O2D-CED
13	l	1302	CLA	O1D-CGD-O2D-CED
13	1	516	CLA	C4C-C3C-CAC-CBC
13	Y	516	CLA	C4C-C3C-CAC-CBC
13	q	516	CLA	C4C-C3C-CAC-CBC
13	A	1103	CLA	O1D-CGD-O2D-CED
13	A	1132	CLA	O1D-CGD-O2D-CED
13	B	1012	CLA	O1D-CGD-O2D-CED
13	B	1229	CLA	O1D-CGD-O2D-CED
13	B	1240	CLA	O1D-CGD-O2D-CED
13	6	519	CLA	O1D-CGD-O2D-CED
13	G	1103	CLA	O1D-CGD-O2D-CED
13	G	1111	CLA	O1D-CGD-O2D-CED
13	G	1132	CLA	O1D-CGD-O2D-CED
13	H	1012	CLA	O1D-CGD-O2D-CED
13	H	1229	CLA	O1D-CGD-O2D-CED
13	H	1240	CLA	O1D-CGD-O2D-CED
13	d	519	CLA	O1D-CGD-O2D-CED
13	e	1103	CLA	O1D-CGD-O2D-CED
13	e	1132	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	f	1012	CLA	O1D-CGD-O2D-CED
13	f	1229	CLA	O1D-CGD-O2D-CED
13	f	1240	CLA	O1D-CGD-O2D-CED
13	v	519	CLA	O1D-CGD-O2D-CED
13	A	1124	CLA	CBD-CGD-O2D-CED
13	G	1124	CLA	CBD-CGD-O2D-CED
13	A	1111	CLA	O1D-CGD-O2D-CED
13	6	511	CLA	O1D-CGD-O2D-CED
13	6	518	CLA	O1D-CGD-O2D-CED
13	d	511	CLA	O1D-CGD-O2D-CED
13	d	518	CLA	O1D-CGD-O2D-CED
13	e	1111	CLA	O1D-CGD-O2D-CED
13	v	511	CLA	O1D-CGD-O2D-CED
13	v	518	CLA	O1D-CGD-O2D-CED
17	A	5005	LHG	C1-C2-C3-O3
17	G	5005	LHG	C1-C2-C3-O3
17	e	5005	LHG	C1-C2-C3-O3
13	B	1234	CLA	O1A-CGA-O2A-C1
13	H	1234	CLA	O1A-CGA-O2A-C1
13	f	1234	CLA	O1A-CGA-O2A-C1
20	3	822	SQD	O10-C23-O48-C46
20	a	822	SQD	O10-C23-O48-C46
20	s	822	SQD	O10-C23-O48-C46
13	A	1130	CLA	C3-C5-C6-C7
13	4	503	CLA	C3-C5-C6-C7
13	G	1130	CLA	C3-C5-C6-C7
13	b	503	CLA	C3-C5-C6-C7
13	e	1130	CLA	C3-C5-C6-C7
13	t	503	CLA	C3-C5-C6-C7
13	J	1303	CLA	O1D-CGD-O2D-CED
13	2	504	CLA	O1D-CGD-O2D-CED
13	T	1303	CLA	O1D-CGD-O2D-CED
13	Z	504	CLA	O1D-CGD-O2D-CED
13	l	1303	CLA	O1D-CGD-O2D-CED
13	r	504	CLA	O1D-CGD-O2D-CED
13	A	1104	CLA	CBA-CGA-O2A-C1
13	A	1106	CLA	CBA-CGA-O2A-C1
13	A	1118	CLA	CBA-CGA-O2A-C1
13	A	1133	CLA	CBA-CGA-O2A-C1
13	A	1237	CLA	CBA-CGA-O2A-C1
13	B	1214	CLA	CBA-CGA-O2A-C1
13	B	1225	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	B	1239	CLA	CBA-CGA-O2A-C1
13	K	1401	CLA	CBA-CGA-O2A-C1
13	2	502	CLA	CBA-CGA-O2A-C1
13	2	512	CLA	CBA-CGA-O2A-C1
13	6	518	CLA	CBA-CGA-O2A-C1
13	G	1104	CLA	CBA-CGA-O2A-C1
13	G	1106	CLA	CBA-CGA-O2A-C1
13	G	1118	CLA	CBA-CGA-O2A-C1
13	G	1133	CLA	CBA-CGA-O2A-C1
13	G	1237	CLA	CBA-CGA-O2A-C1
13	H	1214	CLA	CBA-CGA-O2A-C1
13	H	1225	CLA	CBA-CGA-O2A-C1
13	H	1239	CLA	CBA-CGA-O2A-C1
13	U	1401	CLA	CBA-CGA-O2A-C1
13	Z	502	CLA	CBA-CGA-O2A-C1
13	Z	512	CLA	CBA-CGA-O2A-C1
13	d	518	CLA	CBA-CGA-O2A-C1
13	e	1104	CLA	CBA-CGA-O2A-C1
13	e	1106	CLA	CBA-CGA-O2A-C1
13	e	1118	CLA	CBA-CGA-O2A-C1
13	e	1133	CLA	CBA-CGA-O2A-C1
13	e	1237	CLA	CBA-CGA-O2A-C1
13	f	1214	CLA	CBA-CGA-O2A-C1
13	f	1225	CLA	CBA-CGA-O2A-C1
13	f	1239	CLA	CBA-CGA-O2A-C1
13	m	1401	CLA	CBA-CGA-O2A-C1
13	r	502	CLA	CBA-CGA-O2A-C1
13	r	512	CLA	CBA-CGA-O2A-C1
13	v	518	CLA	CBA-CGA-O2A-C1
17	A	5001	LHG	C24-C23-O8-C6
17	G	5001	LHG	C24-C23-O8-C6
17	e	5001	LHG	C24-C23-O8-C6
20	L	5216	SQD	C24-C23-O48-C46
20	1	822	SQD	C24-C23-O48-C46
20	V	5216	SQD	C24-C23-O48-C46
20	Y	822	SQD	C24-C23-O48-C46
20	n	5216	SQD	C24-C23-O48-C46
20	q	822	SQD	C24-C23-O48-C46
13	2	510	CLA	CBD-CGD-O2D-CED
13	3	505	CLA	CBD-CGD-O2D-CED
13	4	509	CLA	CBD-CGD-O2D-CED
13	Z	510	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	b	509	CLA	CBD-CGD-O2D-CED
13	r	510	CLA	CBD-CGD-O2D-CED
13	s	505	CLA	CBD-CGD-O2D-CED
13	t	509	CLA	CBD-CGD-O2D-CED
13	A	1106	CLA	O1D-CGD-O2D-CED
18	B	1843	LMU	C4'-C5'-C6'-O6'
18	H	1843	LMU	C4'-C5'-C6'-O6'
18	f	1843	LMU	C4'-C5'-C6'-O6'
13	a	505	CLA	CBD-CGD-O2D-CED
13	G	1106	CLA	O1D-CGD-O2D-CED
13	e	1106	CLA	O1D-CGD-O2D-CED
13	A	1115	CLA	C10-C11-C12-C13
13	B	1215	CLA	C10-C11-C12-C13
13	B	1220	CLA	C5-C6-C7-C8
13	B	1223	CLA	C8-C10-C11-C12
13	B	1225	CLA	C15-C16-C17-C18
13	L	1503	CLA	C5-C6-C7-C8
13	L	1503	CLA	C8-C10-C11-C12
13	2	510	CLA	C8-C10-C11-C12
13	G	1115	CLA	C10-C11-C12-C13
13	H	1215	CLA	C10-C11-C12-C13
13	H	1220	CLA	C5-C6-C7-C8
13	H	1223	CLA	C8-C10-C11-C12
13	H	1225	CLA	C15-C16-C17-C18
13	V	1503	CLA	C5-C6-C7-C8
13	V	1503	CLA	C8-C10-C11-C12
13	Z	510	CLA	C8-C10-C11-C12
13	e	1115	CLA	C10-C11-C12-C13
13	f	1215	CLA	C10-C11-C12-C13
13	f	1220	CLA	C5-C6-C7-C8
13	f	1223	CLA	C8-C10-C11-C12
13	f	1225	CLA	C15-C16-C17-C18
13	n	1503	CLA	C5-C6-C7-C8
13	n	1503	CLA	C8-C10-C11-C12
13	r	510	CLA	C8-C10-C11-C12
13	B	1204	CLA	C3-C5-C6-C7
13	H	1204	CLA	C3-C5-C6-C7
13	f	1204	CLA	C3-C5-C6-C7
13	A	1135	CLA	C3-C5-C6-C7
13	G	1135	CLA	C3-C5-C6-C7
13	e	1135	CLA	C3-C5-C6-C7
13	4	507	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	1118	CLA	O1A-CGA-O2A-C1
13	A	1133	CLA	O1A-CGA-O2A-C1
13	G	1118	CLA	O1A-CGA-O2A-C1
13	G	1133	CLA	O1A-CGA-O2A-C1
13	e	1118	CLA	O1A-CGA-O2A-C1
13	e	1133	CLA	O1A-CGA-O2A-C1
13	B	1217	CLA	C4-C3-C5-C6
13	L	1503	CLA	C4-C3-C5-C6
13	H	1217	CLA	C4-C3-C5-C6
13	V	1503	CLA	C4-C3-C5-C6
13	f	1217	CLA	C4-C3-C5-C6
13	n	1503	CLA	C4-C3-C5-C6
13	A	1133	CLA	C2-C3-C5-C6
13	G	1133	CLA	C2-C3-C5-C6
13	e	1133	CLA	C2-C3-C5-C6
13	A	1116	CLA	C6-C7-C8-C9
13	A	1137	CLA	C6-C7-C8-C9
13	A	1139	CLA	C6-C7-C8-C9
13	B	1215	CLA	C6-C7-C8-C9
13	B	1215	CLA	C11-C12-C13-C14
13	B	1226	CLA	C14-C13-C15-C16
13	J	1303	CLA	C14-C13-C15-C16
13	3	505	CLA	C6-C7-C8-C9
13	G	1116	CLA	C6-C7-C8-C9
13	G	1137	CLA	C6-C7-C8-C9
13	G	1139	CLA	C6-C7-C8-C9
13	H	1215	CLA	C6-C7-C8-C9
13	H	1215	CLA	C11-C12-C13-C14
13	H	1226	CLA	C14-C13-C15-C16
13	T	1303	CLA	C14-C13-C15-C16
13	a	505	CLA	C6-C7-C8-C9
13	e	1116	CLA	C6-C7-C8-C9
13	e	1137	CLA	C6-C7-C8-C9
13	e	1139	CLA	C6-C7-C8-C9
13	f	1215	CLA	C6-C7-C8-C9
13	f	1215	CLA	C11-C12-C13-C14
13	f	1226	CLA	C14-C13-C15-C16
13	l	1303	CLA	C14-C13-C15-C16
13	s	505	CLA	C6-C7-C8-C9
14	A	2001	PQN	C21-C22-C23-C24
14	G	2001	PQN	C21-C22-C23-C24
14	e	2001	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	A	1112	CLA	O1D-CGD-O2D-CED
13	B	1201	CLA	O1D-CGD-O2D-CED
13	B	1209	CLA	O1D-CGD-O2D-CED
13	2	507	CLA	O1D-CGD-O2D-CED
13	G	1112	CLA	O1D-CGD-O2D-CED
13	H	1201	CLA	O1D-CGD-O2D-CED
13	H	1209	CLA	O1D-CGD-O2D-CED
13	Z	507	CLA	O1D-CGD-O2D-CED
13	b	507	CLA	O1D-CGD-O2D-CED
13	e	1112	CLA	O1D-CGD-O2D-CED
13	f	1201	CLA	O1D-CGD-O2D-CED
13	f	1209	CLA	O1D-CGD-O2D-CED
13	r	507	CLA	O1D-CGD-O2D-CED
13	t	507	CLA	O1D-CGD-O2D-CED
13	v	512	CLA	O1D-CGD-O2D-CED
13	L	1503	CLA	CBD-CGD-O2D-CED
13	V	1503	CLA	CBD-CGD-O2D-CED
13	n	1503	CLA	CBD-CGD-O2D-CED
13	A	1106	CLA	C8-C10-C11-C12
13	A	1133	CLA	C8-C10-C11-C12
13	1	509	CLA	C10-C11-C12-C13
13	G	1106	CLA	C8-C10-C11-C12
13	G	1133	CLA	C8-C10-C11-C12
13	Y	509	CLA	C10-C11-C12-C13
13	e	1106	CLA	C8-C10-C11-C12
13	e	1133	CLA	C8-C10-C11-C12
13	q	509	CLA	C10-C11-C12-C13
13	B	1224	CLA	C2A-CAA-CBA-CGA
13	B	1207	CLA	C2A-CAA-CBA-CGA
13	3	512	CLA	C2A-CAA-CBA-CGA
13	4	505	CLA	C2A-CAA-CBA-CGA
13	H	1224	CLA	C2A-CAA-CBA-CGA
13	H	1207	CLA	C2A-CAA-CBA-CGA
13	a	512	CLA	C2A-CAA-CBA-CGA
13	b	505	CLA	C2A-CAA-CBA-CGA
13	f	1224	CLA	C2A-CAA-CBA-CGA
13	f	1207	CLA	C2A-CAA-CBA-CGA
13	s	512	CLA	C2A-CAA-CBA-CGA
13	t	505	CLA	C2A-CAA-CBA-CGA
16	A	4001	BCR	C7-C8-C9-C34
16	A	4001	BCR	C11-C12-C13-C35
16	A	4011	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
16	A	4011	BCR	C37-C22-C23-C24
16	B	4010	BCR	C11-C12-C13-C35
16	B	4014	BCR	C7-C8-C9-C34
16	J	4013	BCR	C37-C22-C23-C24
16	J	4012	BCR	C37-C22-C23-C24
16	3	524	BCR	C7-C8-C9-C34
16	4	521	BCR	C36-C18-C19-C20
16	4	524	BCR	C7-C8-C9-C34
16	6	522	BCR	C7-C8-C9-C34
16	G	4001	BCR	C7-C8-C9-C34
16	G	4001	BCR	C11-C12-C13-C35
16	G	4011	BCR	C36-C18-C19-C20
16	G	4011	BCR	C37-C22-C23-C24
16	H	4010	BCR	C11-C12-C13-C35
16	H	4014	BCR	C7-C8-C9-C34
16	T	4013	BCR	C37-C22-C23-C24
16	T	4012	BCR	C37-C22-C23-C24
16	a	524	BCR	C7-C8-C9-C34
16	b	521	BCR	C36-C18-C19-C20
16	b	524	BCR	C7-C8-C9-C34
16	d	522	BCR	C7-C8-C9-C34
16	e	4001	BCR	C7-C8-C9-C34
16	e	4001	BCR	C11-C12-C13-C35
16	e	4011	BCR	C36-C18-C19-C20
16	e	4011	BCR	C37-C22-C23-C24
16	f	4010	BCR	C11-C12-C13-C35
16	f	4014	BCR	C7-C8-C9-C34
16	l	4013	BCR	C37-C22-C23-C24
16	l	4012	BCR	C37-C22-C23-C24
16	s	524	BCR	C7-C8-C9-C34
16	t	521	BCR	C36-C18-C19-C20
16	t	524	BCR	C7-C8-C9-C34
16	v	522	BCR	C7-C8-C9-C34
16	A	4011	BCR	C21-C22-C23-C24
16	J	4013	BCR	C21-C22-C23-C24
16	J	4012	BCR	C21-C22-C23-C24
16	3	521	BCR	C7-C8-C9-C10
16	G	4011	BCR	C21-C22-C23-C24
16	T	4013	BCR	C21-C22-C23-C24
16	T	4012	BCR	C21-C22-C23-C24
16	a	521	BCR	C7-C8-C9-C10
16	e	4011	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	l	4013	BCR	C21-C22-C23-C24
16	l	4012	BCR	C21-C22-C23-C24
16	s	521	BCR	C7-C8-C9-C10
13	6	512	CLA	O1D-CGD-O2D-CED
13	d	512	CLA	O1D-CGD-O2D-CED
13	B	1023	CLA	C2C-C3C-CAC-CBC
13	H	1023	CLA	C2C-C3C-CAC-CBC
13	f	1023	CLA	C2C-C3C-CAC-CBC
13	B	1214	CLA	O1A-CGA-O2A-C1
13	B	1239	CLA	O1A-CGA-O2A-C1
13	2	502	CLA	O1A-CGA-O2A-C1
13	H	1214	CLA	O1A-CGA-O2A-C1
13	H	1239	CLA	O1A-CGA-O2A-C1
13	Z	502	CLA	O1A-CGA-O2A-C1
13	f	1214	CLA	O1A-CGA-O2A-C1
13	f	1239	CLA	O1A-CGA-O2A-C1
13	r	502	CLA	O1A-CGA-O2A-C1
13	A	1102	CLA	C13-C15-C16-C17
13	B	1203	CLA	C8-C10-C11-C12
13	B	1214	CLA	C13-C15-C16-C17
13	3	510	CLA	C8-C10-C11-C12
13	G	1102	CLA	C13-C15-C16-C17
13	H	1203	CLA	C8-C10-C11-C12
13	H	1214	CLA	C13-C15-C16-C17
13	a	510	CLA	C8-C10-C11-C12
13	e	1102	CLA	C13-C15-C16-C17
13	f	1203	CLA	C8-C10-C11-C12
13	f	1214	CLA	C13-C15-C16-C17
13	s	510	CLA	C8-C10-C11-C12
13	4	508	CLA	O1D-CGD-O2D-CED
13	b	508	CLA	O1D-CGD-O2D-CED
13	t	508	CLA	O1D-CGD-O2D-CED
13	2	502	CLA	CBD-CGD-O2D-CED
13	Z	502	CLA	CBD-CGD-O2D-CED
13	r	502	CLA	CBD-CGD-O2D-CED
13	B	1210	CLA	C3-C5-C6-C7
13	H	1210	CLA	C3-C5-C6-C7
13	f	1210	CLA	C3-C5-C6-C7
13	J	1302	CLA	CBA-CGA-O2A-C1
13	1	502	CLA	CBA-CGA-O2A-C1
13	T	1302	CLA	CBA-CGA-O2A-C1
13	Y	502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	l	1302	CLA	CBA-CGA-O2A-C1
13	q	502	CLA	CBA-CGA-O2A-C1
19	B	5002	LMG	C29-C28-O8-C9
19	H	5002	LMG	C29-C28-O8-C9
19	f	5002	LMG	C29-C28-O8-C9
13	A	1013	CLA	C13-C15-C16-C17
13	A	1116	CLA	C5-C6-C7-C8
13	A	1126	CLA	C15-C16-C17-C18
13	A	1137	CLA	C5-C6-C7-C8
13	A	1137	CLA	C10-C11-C12-C13
13	B	1227	CLA	C13-C15-C16-C17
13	L	1501	CLA	C8-C10-C11-C12
13	3	519	CLA	C5-C6-C7-C8
13	4	505	CLA	C15-C16-C17-C18
13	5	503	CLA	C5-C6-C7-C8
13	G	1013	CLA	C13-C15-C16-C17
13	G	1116	CLA	C5-C6-C7-C8
13	G	1126	CLA	C15-C16-C17-C18
13	G	1137	CLA	C5-C6-C7-C8
13	G	1137	CLA	C10-C11-C12-C13
13	H	1227	CLA	C13-C15-C16-C17
13	V	1501	CLA	C8-C10-C11-C12
13	a	519	CLA	C5-C6-C7-C8
13	b	505	CLA	C15-C16-C17-C18
13	c	503	CLA	C5-C6-C7-C8
13	e	1116	CLA	C5-C6-C7-C8
13	e	1126	CLA	C15-C16-C17-C18
13	e	1137	CLA	C5-C6-C7-C8
13	e	1137	CLA	C10-C11-C12-C13
13	f	1227	CLA	C13-C15-C16-C17
13	n	1501	CLA	C8-C10-C11-C12
13	s	519	CLA	C5-C6-C7-C8
13	t	505	CLA	C15-C16-C17-C18
13	u	503	CLA	C5-C6-C7-C8
17	B	1842	LHG	C23-C24-C25-C26
17	L	5220	LHG	C23-C24-C25-C26
17	V	5218	LHG	C23-C24-C25-C26
17	V	5220	LHG	C23-C24-C25-C26
17	f	1842	LHG	C23-C24-C25-C26
17	n	5218	LHG	C23-C24-C25-C26
17	n	5220	LHG	C23-C24-C25-C26
13	A	1123	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	G	1123	CLA	O1D-CGD-O2D-CED
13	e	1123	CLA	O1D-CGD-O2D-CED
13	3	516	CLA	C4C-C3C-CAC-CBC
13	a	516	CLA	C4C-C3C-CAC-CBC
13	s	516	CLA	C4C-C3C-CAC-CBC
13	A	1106	CLA	C5-C6-C7-C8
13	A	1115	CLA	C5-C6-C7-C8
13	A	1125	CLA	C10-C11-C12-C13
13	A	1101	CLA	C10-C11-C12-C13
13	A	1101	CLA	C13-C15-C16-C17
13	B	1012	CLA	C5-C6-C7-C8
13	B	1204	CLA	C5-C6-C7-C8
13	B	1213	CLA	C5-C6-C7-C8
13	B	1219	CLA	C15-C16-C17-C18
13	B	1223	CLA	C13-C15-C16-C17
13	B	1239	CLA	C15-C16-C17-C18
13	B	1240	CLA	C10-C11-C12-C13
13	L	1503	CLA	C10-C11-C12-C13
13	1	509	CLA	C15-C16-C17-C18
13	1	510	CLA	C5-C6-C7-C8
13	2	502	CLA	C10-C11-C12-C13
13	3	513	CLA	C13-C15-C16-C17
13	5	501	CLA	C13-C15-C16-C17
13	5	505	CLA	C8-C10-C11-C12
13	G	1106	CLA	C5-C6-C7-C8
13	G	1115	CLA	C5-C6-C7-C8
13	G	1125	CLA	C10-C11-C12-C13
13	G	1101	CLA	C10-C11-C12-C13
13	G	1101	CLA	C13-C15-C16-C17
13	H	1012	CLA	C5-C6-C7-C8
13	H	1204	CLA	C5-C6-C7-C8
13	H	1213	CLA	C5-C6-C7-C8
13	H	1219	CLA	C15-C16-C17-C18
13	H	1223	CLA	C13-C15-C16-C17
13	H	1239	CLA	C15-C16-C17-C18
13	H	1240	CLA	C10-C11-C12-C13
13	V	1503	CLA	C10-C11-C12-C13
13	Y	509	CLA	C15-C16-C17-C18
13	Y	510	CLA	C5-C6-C7-C8
13	Z	502	CLA	C10-C11-C12-C13
13	a	513	CLA	C13-C15-C16-C17
13	c	501	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	c	505	CLA	C8-C10-C11-C12
13	e	1013	CLA	C13-C15-C16-C17
13	e	1106	CLA	C5-C6-C7-C8
13	e	1115	CLA	C5-C6-C7-C8
13	e	1125	CLA	C10-C11-C12-C13
13	e	1101	CLA	C10-C11-C12-C13
13	e	1101	CLA	C13-C15-C16-C17
13	f	1012	CLA	C5-C6-C7-C8
13	f	1204	CLA	C5-C6-C7-C8
13	f	1213	CLA	C5-C6-C7-C8
13	f	1219	CLA	C15-C16-C17-C18
13	f	1223	CLA	C13-C15-C16-C17
13	f	1239	CLA	C15-C16-C17-C18
13	f	1240	CLA	C10-C11-C12-C13
13	n	1503	CLA	C10-C11-C12-C13
13	q	509	CLA	C15-C16-C17-C18
13	q	510	CLA	C5-C6-C7-C8
13	r	502	CLA	C10-C11-C12-C13
13	s	513	CLA	C13-C15-C16-C17
13	u	501	CLA	C13-C15-C16-C17
13	u	505	CLA	C8-C10-C11-C12
13	B	1220	CLA	O1D-CGD-O2D-CED
13	H	1220	CLA	O1D-CGD-O2D-CED
13	e	1104	CLA	O1D-CGD-O2D-CED
13	f	1220	CLA	O1D-CGD-O2D-CED
17	A	5004	LHG	O1-C1-C2-O2
17	A	5007	LHG	O1-C1-C2-O2
17	G	5004	LHG	O1-C1-C2-O2
17	G	5007	LHG	O1-C1-C2-O2
17	e	5004	LHG	O1-C1-C2-O2
17	e	5007	LHG	O1-C1-C2-O2
17	A	5006	LHG	C23-C24-C25-C26
17	A	5008	LHG	C23-C24-C25-C26
17	A	5009	LHG	C23-C24-C25-C26
17	A	5001	LHG	C23-C24-C25-C26
17	L	5218	LHG	C23-C24-C25-C26
17	L	5220	LHG	C7-C8-C9-C10
17	G	5006	LHG	C23-C24-C25-C26
17	G	5008	LHG	C23-C24-C25-C26
17	G	5009	LHG	C23-C24-C25-C26
17	G	5001	LHG	C23-C24-C25-C26
17	H	1842	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
17	V	5220	LHG	C7-C8-C9-C10
17	e	5006	LHG	C23-C24-C25-C26
17	e	5008	LHG	C23-C24-C25-C26
17	e	5009	LHG	C23-C24-C25-C26
17	e	5001	LHG	C23-C24-C25-C26
17	n	5220	LHG	C7-C8-C9-C10
20	L	5216	SQD	C7-C8-C9-C10
20	V	5216	SQD	C7-C8-C9-C10
20	n	5216	SQD	C7-C8-C9-C10
19	J	5104	LMG	O6-C5-C6-O5
19	T	5104	LMG	O6-C5-C6-O5
19	l	5104	LMG	O6-C5-C6-O5
13	A	1128	CLA	CBD-CGD-O2D-CED
13	G	1128	CLA	CBD-CGD-O2D-CED
13	e	1128	CLA	CBD-CGD-O2D-CED
13	A	1104	CLA	O1D-CGD-O2D-CED
13	G	1104	CLA	O1D-CGD-O2D-CED
13	A	1106	CLA	C10-C11-C12-C13
13	B	1205	CLA	C13-C15-C16-C17
13	B	1210	CLA	C8-C10-C11-C12
13	B	1207	CLA	C13-C15-C16-C17
13	L	1501	CLA	C10-C11-C12-C13
13	1	505	CLA	C8-C10-C11-C12
13	2	505	CLA	C8-C10-C11-C12
13	3	505	CLA	C8-C10-C11-C12
13	3	513	CLA	C8-C10-C11-C12
13	5	509	CLA	C8-C10-C11-C12
13	G	1106	CLA	C10-C11-C12-C13
13	H	1205	CLA	C13-C15-C16-C17
13	H	1210	CLA	C8-C10-C11-C12
13	H	1207	CLA	C13-C15-C16-C17
13	V	1501	CLA	C10-C11-C12-C13
13	Y	505	CLA	C8-C10-C11-C12
13	Z	505	CLA	C8-C10-C11-C12
13	a	505	CLA	C8-C10-C11-C12
13	a	513	CLA	C8-C10-C11-C12
13	c	509	CLA	C8-C10-C11-C12
13	e	1106	CLA	C10-C11-C12-C13
13	f	1205	CLA	C13-C15-C16-C17
13	f	1210	CLA	C8-C10-C11-C12
13	f	1207	CLA	C13-C15-C16-C17
13	n	1501	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	q	505	CLA	C8-C10-C11-C12
13	r	505	CLA	C8-C10-C11-C12
13	s	505	CLA	C8-C10-C11-C12
13	s	513	CLA	C8-C10-C11-C12
13	u	509	CLA	C8-C10-C11-C12
14	A	2001	PQN	C15-C16-C17-C18
14	G	2001	PQN	C15-C16-C17-C18
14	e	2001	PQN	C15-C16-C17-C18
18	A	1849	LMU	O1'-C1-C2-C3
18	G	1849	LMU	O1'-C1-C2-C3
18	e	1849	LMU	O1'-C1-C2-C3
13	A	1104	CLA	C15-C16-C17-C18
13	B	1023	CLA	C10-C11-C12-C13
13	B	1214	CLA	C5-C6-C7-C8
13	3	509	CLA	C15-C16-C17-C18
13	G	1104	CLA	C15-C16-C17-C18
13	H	1023	CLA	C10-C11-C12-C13
13	H	1214	CLA	C5-C6-C7-C8
13	e	1104	CLA	C15-C16-C17-C18
13	f	1023	CLA	C10-C11-C12-C13
13	f	1214	CLA	C5-C6-C7-C8
17	A	5008	LHG	C7-C8-C9-C10
17	G	5008	LHG	C7-C8-C9-C10
17	e	5008	LHG	C7-C8-C9-C10
20	1	822	SQD	C23-C24-C25-C26
20	Y	822	SQD	C23-C24-C25-C26
20	q	822	SQD	C23-C24-C25-C26
13	B	1224	CLA	CBD-CGD-O2D-CED
13	H	1224	CLA	CBD-CGD-O2D-CED
13	f	1224	CLA	CBD-CGD-O2D-CED
13	B	1217	CLA	C8-C10-C11-C12
13	H	1217	CLA	C8-C10-C11-C12
13	f	1217	CLA	C8-C10-C11-C12
13	A	1126	CLA	C10-C11-C12-C13
13	A	1137	CLA	C15-C16-C17-C18
13	6	505	CLA	C8-C10-C11-C12
13	G	1126	CLA	C10-C11-C12-C13
13	G	1137	CLA	C15-C16-C17-C18
13	a	509	CLA	C15-C16-C17-C18
13	d	505	CLA	C8-C10-C11-C12
13	e	1126	CLA	C10-C11-C12-C13
13	e	1137	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	s	509	CLA	C15-C16-C17-C18
13	v	505	CLA	C8-C10-C11-C12
13	A	1113	CLA	O1D-CGD-O2D-CED
13	6	507	CLA	O1D-CGD-O2D-CED
13	G	1113	CLA	O1D-CGD-O2D-CED
13	e	1113	CLA	O1D-CGD-O2D-CED
13	B	1221	CLA	C11-C10-C8-C7
13	B	1230	CLA	C6-C7-C8-C10
13	F	1301	CLA	C11-C10-C8-C7
13	L	1501	CLA	C6-C7-C8-C10
13	3	513	CLA	C6-C7-C8-C10
13	H	1221	CLA	C11-C10-C8-C7
13	H	1230	CLA	C6-C7-C8-C10
13	R	1301	CLA	C11-C10-C8-C7
13	V	1501	CLA	C6-C7-C8-C10
13	a	513	CLA	C6-C7-C8-C10
13	f	1221	CLA	C11-C10-C8-C7
13	f	1230	CLA	C6-C7-C8-C10
13	j	1301	CLA	C11-C10-C8-C7
13	n	1501	CLA	C6-C7-C8-C10
13	s	513	CLA	C6-C7-C8-C10
14	A	2001	PQN	C21-C22-C23-C25
14	G	2001	PQN	C21-C22-C23-C25
14	e	2001	PQN	C21-C22-C23-C25
13	A	1115	CLA	C3-C5-C6-C7
13	B	1219	CLA	C3-C5-C6-C7
13	2	518	CLA	C3-C5-C6-C7
13	4	509	CLA	C3-C5-C6-C7
13	G	1115	CLA	C3-C5-C6-C7
13	H	1219	CLA	C3-C5-C6-C7
13	Z	518	CLA	C3-C5-C6-C7
13	e	1115	CLA	C3-C5-C6-C7
13	f	1219	CLA	C3-C5-C6-C7
13	r	518	CLA	C3-C5-C6-C7
13	t	509	CLA	C3-C5-C6-C7
13	B	1225	CLA	O1A-CGA-O2A-C1
13	K	1401	CLA	O1A-CGA-O2A-C1
13	6	518	CLA	O1A-CGA-O2A-C1
13	H	1225	CLA	O1A-CGA-O2A-C1
13	U	1401	CLA	O1A-CGA-O2A-C1
13	d	518	CLA	O1A-CGA-O2A-C1
13	f	1225	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	m	1401	CLA	O1A-CGA-O2A-C1
13	v	518	CLA	O1A-CGA-O2A-C1
17	B	1855	LHG	O10-C23-O8-C6
17	H	1855	LHG	O10-C23-O8-C6
17	f	1855	LHG	O10-C23-O8-C6
16	6	522	BCR	C9-C10-C11-C12
16	d	522	BCR	C9-C10-C11-C12
16	v	522	BCR	C9-C10-C11-C12
13	A	1107	CLA	C2A-CAA-CBA-CGA
13	B	1201	CLA	C2A-CAA-CBA-CGA
13	F	1302	CLA	C2A-CAA-CBA-CGA
13	6	516	CLA	C2A-CAA-CBA-CGA
13	G	1107	CLA	C2A-CAA-CBA-CGA
13	H	1201	CLA	C2A-CAA-CBA-CGA
13	R	1302	CLA	C2A-CAA-CBA-CGA
13	d	516	CLA	C2A-CAA-CBA-CGA
13	e	1107	CLA	C2A-CAA-CBA-CGA
13	f	1201	CLA	C2A-CAA-CBA-CGA
13	j	1302	CLA	C2A-CAA-CBA-CGA
13	a	504	CLA	O1D-CGD-O2D-CED
13	d	507	CLA	O1D-CGD-O2D-CED
13	v	507	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C8-C10-C11-C12
13	1	510	CLA	C8-C10-C11-C12
13	2	509	CLA	C15-C16-C17-C18
13	4	505	CLA	C8-C10-C11-C12
13	6	505	CLA	C5-C6-C7-C8
13	G	1126	CLA	C8-C10-C11-C12
13	Y	510	CLA	C8-C10-C11-C12
13	Z	509	CLA	C15-C16-C17-C18
13	b	505	CLA	C8-C10-C11-C12
13	d	505	CLA	C5-C6-C7-C8
13	e	1126	CLA	C8-C10-C11-C12
13	q	510	CLA	C8-C10-C11-C12
13	r	509	CLA	C15-C16-C17-C18
13	t	505	CLA	C8-C10-C11-C12
13	v	505	CLA	C5-C6-C7-C8
14	A	2001	PQN	C18-C20-C21-C22
14	G	2001	PQN	C18-C20-C21-C22
14	e	2001	PQN	C18-C20-C21-C22
13	A	1106	CLA	O1A-CGA-O2A-C1
13	2	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	G	1106	CLA	O1A-CGA-O2A-C1
13	Z	512	CLA	O1A-CGA-O2A-C1
13	e	1106	CLA	O1A-CGA-O2A-C1
13	r	512	CLA	O1A-CGA-O2A-C1
13	A	1136	CLA	C8-C10-C11-C12
13	B	1203	CLA	C5-C6-C7-C8
13	B	1208	CLA	C10-C11-C12-C13
13	B	1210	CLA	C10-C11-C12-C13
13	G	1136	CLA	C8-C10-C11-C12
13	H	1203	CLA	C5-C6-C7-C8
13	H	1208	CLA	C10-C11-C12-C13
13	H	1210	CLA	C10-C11-C12-C13
13	f	1210	CLA	C10-C11-C12-C13
13	A	1013	CLA	O1D-CGD-O2D-CED
13	A	1137	CLA	O1D-CGD-O2D-CED
13	3	504	CLA	O1D-CGD-O2D-CED
13	G	1013	CLA	O1D-CGD-O2D-CED
13	G	1137	CLA	O1D-CGD-O2D-CED
13	e	1013	CLA	O1D-CGD-O2D-CED
13	e	1137	CLA	O1D-CGD-O2D-CED
13	s	504	CLA	O1D-CGD-O2D-CED
17	A	5002	LHG	C7-C8-C9-C10
17	L	5218	LHG	C7-C8-C9-C10
17	G	5002	LHG	C7-C8-C9-C10
17	V	5218	LHG	C7-C8-C9-C10
17	e	5002	LHG	C7-C8-C9-C10
17	n	5218	LHG	C7-C8-C9-C10
17	A	5009	LHG	O2-C2-C3-O3
17	A	5003	LHG	O2-C2-C3-O3
17	B	1842	LHG	O2-C2-C3-O3
17	L	5220	LHG	O2-C2-C3-O3
17	G	5009	LHG	O2-C2-C3-O3
17	G	5003	LHG	O2-C2-C3-O3
17	H	1842	LHG	O2-C2-C3-O3
17	S	5001	LHG	O2-C2-C3-O3
17	V	5220	LHG	O2-C2-C3-O3
17	e	5009	LHG	O2-C2-C3-O3
17	e	5003	LHG	O2-C2-C3-O3
17	f	1842	LHG	O2-C2-C3-O3
17	n	5220	LHG	O2-C2-C3-O3
13	b	509	CLA	C3-C5-C6-C7
13	A	1013	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	A	1122	CLA	C8-C10-C11-C12
13	1	501	CLA	C15-C16-C17-C18
13	1	502	CLA	C8-C10-C11-C12
13	1	509	CLA	C8-C10-C11-C12
13	G	1013	CLA	C15-C16-C17-C18
13	G	1122	CLA	C8-C10-C11-C12
13	Y	501	CLA	C15-C16-C17-C18
13	Y	502	CLA	C8-C10-C11-C12
13	Y	509	CLA	C8-C10-C11-C12
13	e	1013	CLA	C15-C16-C17-C18
13	e	1122	CLA	C8-C10-C11-C12
13	e	1136	CLA	C8-C10-C11-C12
13	f	1203	CLA	C5-C6-C7-C8
13	f	1208	CLA	C10-C11-C12-C13
13	q	501	CLA	C15-C16-C17-C18
13	q	502	CLA	C8-C10-C11-C12
13	q	509	CLA	C8-C10-C11-C12
13	6	517	CLA	O1D-CGD-O2D-CED
13	b	505	CLA	O1D-CGD-O2D-CED
13	d	517	CLA	O1D-CGD-O2D-CED
13	v	517	CLA	O1D-CGD-O2D-CED
13	J	1302	CLA	O1A-CGA-O2A-C1
13	J	1303	CLA	O1A-CGA-O2A-C1
13	1	502	CLA	O1A-CGA-O2A-C1
13	T	1302	CLA	O1A-CGA-O2A-C1
13	T	1303	CLA	O1A-CGA-O2A-C1
13	Y	502	CLA	O1A-CGA-O2A-C1
13	e	1237	CLA	O1A-CGA-O2A-C1
13	l	1302	CLA	O1A-CGA-O2A-C1
13	l	1303	CLA	O1A-CGA-O2A-C1
13	q	502	CLA	O1A-CGA-O2A-C1
18	2	901	LMU	O1'-C1-C2-C3
18	Z	901	LMU	O1'-C1-C2-C3
13	B	1221	CLA	C8-C10-C11-C12
13	B	1225	CLA	C13-C15-C16-C17
13	F	1301	CLA	C13-C15-C16-C17
13	6	501	CLA	C8-C10-C11-C12
13	H	1221	CLA	C8-C10-C11-C12
13	H	1225	CLA	C13-C15-C16-C17
13	R	1301	CLA	C13-C15-C16-C17
13	d	501	CLA	C8-C10-C11-C12
13	f	1225	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	j	1301	CLA	C13-C15-C16-C17
13	v	501	CLA	C8-C10-C11-C12
18	r	901	LMU	O1'-C1-C2-C3
13	A	1011	CLA	O1D-CGD-O2D-CED
13	B	1226	CLA	O1D-CGD-O2D-CED
13	4	505	CLA	O1D-CGD-O2D-CED
13	H	1226	CLA	O1D-CGD-O2D-CED
13	f	1226	CLA	O1D-CGD-O2D-CED
13	t	505	CLA	O1D-CGD-O2D-CED
13	A	1104	CLA	O1A-CGA-O2A-C1
13	A	1237	CLA	O1A-CGA-O2A-C1
13	G	1104	CLA	O1A-CGA-O2A-C1
13	G	1237	CLA	O1A-CGA-O2A-C1
13	e	1104	CLA	O1A-CGA-O2A-C1
17	B	1855	LHG	C8-C7-O7-C5
17	H	1855	LHG	C8-C7-O7-C5
17	f	1855	LHG	C8-C7-O7-C5
17	G	5002	LHG	C28-C29-C30-C31
13	G	1011	CLA	O1D-CGD-O2D-CED
13	e	1011	CLA	O1D-CGD-O2D-CED
13	A	1102	CLA	C15-C16-C17-C18
13	A	1109	CLA	C13-C15-C16-C17
13	A	1126	CLA	C5-C6-C7-C8
13	A	1133	CLA	C10-C11-C12-C13
13	A	1137	CLA	C13-C15-C16-C17
13	A	1139	CLA	C15-C16-C17-C18
13	B	1234	CLA	C10-C11-C12-C13
13	B	1235	CLA	C8-C10-C11-C12
13	2	507	CLA	C5-C6-C7-C8
13	3	505	CLA	C5-C6-C7-C8
13	G	1102	CLA	C15-C16-C17-C18
13	G	1109	CLA	C13-C15-C16-C17
13	G	1126	CLA	C5-C6-C7-C8
13	G	1133	CLA	C10-C11-C12-C13
13	G	1137	CLA	C13-C15-C16-C17
13	G	1139	CLA	C15-C16-C17-C18
13	H	1234	CLA	C10-C11-C12-C13
13	H	1235	CLA	C8-C10-C11-C12
13	Z	507	CLA	C5-C6-C7-C8
13	a	505	CLA	C5-C6-C7-C8
13	e	1102	CLA	C15-C16-C17-C18
13	e	1109	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	e	1126	CLA	C5-C6-C7-C8
13	e	1133	CLA	C10-C11-C12-C13
13	e	1137	CLA	C13-C15-C16-C17
13	e	1139	CLA	C15-C16-C17-C18
13	f	1221	CLA	C8-C10-C11-C12
13	f	1234	CLA	C10-C11-C12-C13
13	f	1235	CLA	C8-C10-C11-C12
13	r	507	CLA	C5-C6-C7-C8
13	s	505	CLA	C5-C6-C7-C8
17	A	5002	LHG	C3-O3-P-O6
17	A	5002	LHG	C4-O6-P-O3
17	A	5005	LHG	C3-O3-P-O6
17	A	5009	LHG	C4-O6-P-O3
17	B	1842	LHG	C3-O3-P-O6
17	B	1855	LHG	C3-O3-P-O6
17	B	1855	LHG	C4-O6-P-O3
17	I	5001	LHG	C4-O6-P-O3
17	L	5218	LHG	C3-O3-P-O6
17	L	5221	LHG	C3-O3-P-O6
17	G	5002	LHG	C3-O3-P-O6
17	G	5002	LHG	C4-O6-P-O3
17	G	5005	LHG	C3-O3-P-O6
17	G	5009	LHG	C4-O6-P-O3
17	H	1842	LHG	C3-O3-P-O6
17	H	1855	LHG	C3-O3-P-O6
17	H	1855	LHG	C4-O6-P-O3
17	S	5001	LHG	C4-O6-P-O3
17	V	5218	LHG	C3-O3-P-O6
17	V	5221	LHG	C3-O3-P-O6
17	e	5002	LHG	C3-O3-P-O6
17	e	5002	LHG	C4-O6-P-O3
17	e	5005	LHG	C3-O3-P-O6
17	e	5009	LHG	C4-O6-P-O3
17	f	1842	LHG	C3-O3-P-O6
17	f	1855	LHG	C3-O3-P-O6
17	f	1855	LHG	C4-O6-P-O3
17	k	5001	LHG	C4-O6-P-O3
17	n	5218	LHG	C3-O3-P-O6
17	n	5221	LHG	C3-O3-P-O6
13	A	1011	CLA	C3-C5-C6-C7
13	A	1128	CLA	C3-C5-C6-C7
13	G	1011	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	G	1128	CLA	C3-C5-C6-C7
13	e	1128	CLA	C3-C5-C6-C7
17	A	5002	LHG	C28-C29-C30-C31
17	e	5002	LHG	C28-C29-C30-C31
13	A	1134	CLA	CBA-CGA-O2A-C1
13	B	1215	CLA	CBA-CGA-O2A-C1
13	G	1134	CLA	CBA-CGA-O2A-C1
13	H	1215	CLA	CBA-CGA-O2A-C1
13	e	1134	CLA	CBA-CGA-O2A-C1
13	f	1215	CLA	CBA-CGA-O2A-C1
13	B	1208	CLA	C15-C16-C17-C18
13	B	1214	CLA	C10-C11-C12-C13
13	H	1208	CLA	C15-C16-C17-C18
13	H	1214	CLA	C10-C11-C12-C13
13	c	509	CLA	C15-C16-C17-C18
13	f	1208	CLA	C15-C16-C17-C18
13	f	1214	CLA	C10-C11-C12-C13
13	1	502	CLA	O1D-CGD-O2D-CED
13	2	519	CLA	O1D-CGD-O2D-CED
13	4	513	CLA	O1D-CGD-O2D-CED
13	Y	502	CLA	O1D-CGD-O2D-CED
13	Z	519	CLA	O1D-CGD-O2D-CED
13	b	513	CLA	O1D-CGD-O2D-CED
13	q	502	CLA	O1D-CGD-O2D-CED
13	r	519	CLA	O1D-CGD-O2D-CED
13	t	513	CLA	O1D-CGD-O2D-CED
17	A	5009	LHG	C1-C2-C3-O3
17	A	5003	LHG	C1-C2-C3-O3
17	B	1842	LHG	C1-C2-C3-O3
17	L	5220	LHG	C1-C2-C3-O3
17	G	5009	LHG	C1-C2-C3-O3
17	G	5003	LHG	C1-C2-C3-O3
17	H	1842	LHG	C1-C2-C3-O3
17	V	5220	LHG	C1-C2-C3-O3
17	e	5009	LHG	C1-C2-C3-O3
17	e	5003	LHG	C1-C2-C3-O3
17	f	1842	LHG	C1-C2-C3-O3
17	n	5220	LHG	C1-C2-C3-O3
18	A	1848	LMU	O5'-C5'-C6'-O6'
18	G	1848	LMU	O5'-C5'-C6'-O6'
18	e	1848	LMU	O5'-C5'-C6'-O6'
17	A	5001	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
17	G	5001	LHG	O9-C7-O7-C5
17	e	5001	LHG	O9-C7-O7-C5
13	1	507	CLA	C10-C11-C12-C13
13	2	518	CLA	C10-C11-C12-C13
13	5	509	CLA	C15-C16-C17-C18
13	Y	507	CLA	C10-C11-C12-C13
13	Z	518	CLA	C10-C11-C12-C13
13	q	507	CLA	C10-C11-C12-C13
13	r	518	CLA	C10-C11-C12-C13
13	u	509	CLA	C15-C16-C17-C18
14	B	2002	PQN	C15-C16-C17-C18
14	H	2002	PQN	C15-C16-C17-C18
14	f	2002	PQN	C15-C16-C17-C18
13	q	504	CLA	CBD-CGD-O2D-CED
13	5	512	CLA	O1D-CGD-O2D-CED
13	u	512	CLA	O1D-CGD-O2D-CED
13	B	1239	CLA	C2C-C3C-CAC-CBC
13	H	1239	CLA	C2C-C3C-CAC-CBC
13	f	1239	CLA	C2C-C3C-CAC-CBC
13	A	1116	CLA	C2A-CAA-CBA-CGA
13	A	1125	CLA	C2A-CAA-CBA-CGA
13	A	1022	CLA	C2A-CAA-CBA-CGA
13	B	1203	CLA	C2A-CAA-CBA-CGA
13	K	1103	CLA	C2A-CAA-CBA-CGA
13	1	518	CLA	C2A-CAA-CBA-CGA
13	5	518	CLA	C2A-CAA-CBA-CGA
13	G	1116	CLA	C2A-CAA-CBA-CGA
13	G	1125	CLA	C2A-CAA-CBA-CGA
13	G	1022	CLA	C2A-CAA-CBA-CGA
13	H	1203	CLA	C2A-CAA-CBA-CGA
13	U	1103	CLA	C2A-CAA-CBA-CGA
13	Y	518	CLA	C2A-CAA-CBA-CGA
13	c	518	CLA	C2A-CAA-CBA-CGA
13	e	1116	CLA	C2A-CAA-CBA-CGA
13	e	1125	CLA	C2A-CAA-CBA-CGA
13	e	1022	CLA	C2A-CAA-CBA-CGA
13	f	1203	CLA	C2A-CAA-CBA-CGA
13	m	1103	CLA	C2A-CAA-CBA-CGA
13	q	518	CLA	C2A-CAA-CBA-CGA
13	u	518	CLA	C2A-CAA-CBA-CGA
13	v	516	CLA	C2A-CAA-CBA-CGA
13	A	1126	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	G	1126	CLA	C16-C17-C18-C20
13	e	1126	CLA	C16-C17-C18-C20
13	F	1301	CLA	C3-C5-C6-C7
13	R	1301	CLA	C3-C5-C6-C7
13	e	1011	CLA	C3-C5-C6-C7
13	j	1301	CLA	C3-C5-C6-C7
13	c	512	CLA	O1D-CGD-O2D-CED
13	A	1137	CLA	CBA-CGA-O2A-C1
13	G	1137	CLA	CBA-CGA-O2A-C1
13	e	1137	CLA	CBA-CGA-O2A-C1
17	A	5005	LHG	C24-C23-O8-C6
17	G	5005	LHG	C24-C23-O8-C6
17	e	5005	LHG	C24-C23-O8-C6
13	1	504	CLA	CBD-CGD-O2D-CED
16	4	522	BCR	C9-C10-C11-C12
16	4	522	BCR	C13-C14-C15-C16
16	b	522	BCR	C9-C10-C11-C12
16	b	522	BCR	C13-C14-C15-C16
16	t	522	BCR	C9-C10-C11-C12
16	t	522	BCR	C13-C14-C15-C16
17	A	5002	LHG	C30-C31-C32-C33
17	e	5002	LHG	C30-C31-C32-C33
20	3	822	SQD	C25-C26-C27-C28
20	a	822	SQD	C25-C26-C27-C28
20	s	822	SQD	C25-C26-C27-C28
13	H	1232	CLA	O1D-CGD-O2D-CED
13	Y	504	CLA	CBD-CGD-O2D-CED
17	A	5009	LHG	C8-C7-O7-C5
17	G	5009	LHG	C8-C7-O7-C5
17	e	5009	LHG	C8-C7-O7-C5
13	5	509	CLA	C13-C15-C16-C17
13	c	509	CLA	C13-C15-C16-C17
13	u	509	CLA	C13-C15-C16-C17
13	3	509	CLA	C3-C5-C6-C7
13	a	509	CLA	C3-C5-C6-C7
13	s	509	CLA	C3-C5-C6-C7
17	A	5002	LHG	C24-C25-C26-C27
17	A	5005	LHG	C10-C11-C12-C13
17	A	5005	LHG	C14-C15-C16-C17
17	A	5007	LHG	C32-C33-C34-C35
17	A	5009	LHG	C16-C17-C18-C19
17	A	5001	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	C25-C26-C27-C28
17	A	5003	LHG	C10-C11-C12-C13
17	G	5002	LHG	C24-C25-C26-C27
17	G	5002	LHG	C30-C31-C32-C33
17	G	5005	LHG	C14-C15-C16-C17
17	G	5007	LHG	C32-C33-C34-C35
17	G	5009	LHG	C16-C17-C18-C19
17	G	5001	LHG	C15-C16-C17-C18
17	G	5001	LHG	C25-C26-C27-C28
17	G	5003	LHG	C10-C11-C12-C13
17	V	5221	LHG	C29-C30-C31-C32
17	e	5002	LHG	C24-C25-C26-C27
17	e	5005	LHG	C10-C11-C12-C13
17	e	5005	LHG	C14-C15-C16-C17
17	e	5007	LHG	C32-C33-C34-C35
17	e	5009	LHG	C16-C17-C18-C19
17	e	5001	LHG	C15-C16-C17-C18
17	e	5001	LHG	C25-C26-C27-C28
17	e	5003	LHG	C10-C11-C12-C13
19	B	5002	LMG	C29-C30-C31-C32
19	H	5002	LMG	C29-C30-C31-C32
19	f	5002	LMG	C29-C30-C31-C32
20	B	1852	SQD	C28-C29-C30-C31
20	H	1852	SQD	C28-C29-C30-C31
13	B	1227	CLA	O1D-CGD-O2D-CED
13	B	1232	CLA	O1D-CGD-O2D-CED
13	H	1227	CLA	O1D-CGD-O2D-CED
13	f	1227	CLA	O1D-CGD-O2D-CED
13	f	1232	CLA	O1D-CGD-O2D-CED
13	A	1105	CLA	C6-C7-C8-C9
13	B	1218	CLA	C11-C12-C13-C15
13	B	1239	CLA	C16-C17-C18-C20
13	B	1207	CLA	C16-C17-C18-C19
13	G	1105	CLA	C6-C7-C8-C9
13	H	1218	CLA	C11-C12-C13-C15
13	H	1239	CLA	C16-C17-C18-C20
13	Z	508	CLA	C6-C7-C8-C10
13	f	1218	CLA	C11-C12-C13-C15
13	f	1239	CLA	C16-C17-C18-C20
13	f	1207	CLA	C16-C17-C18-C19
17	B	1855	LHG	C12-C13-C14-C15
17	L	5221	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
17	G	5005	LHG	C10-C11-C12-C13
17	H	1855	LHG	C12-C13-C14-C15
17	f	1855	LHG	C12-C13-C14-C15
17	n	5221	LHG	C29-C30-C31-C32
20	f	1852	SQD	C28-C29-C30-C31
20	5	822	SQD	C46-C45-O47-C7
20	6	822	SQD	C46-C45-O47-C7
20	c	822	SQD	C46-C45-O47-C7
20	d	822	SQD	C46-C45-O47-C7
20	u	822	SQD	C46-C45-O47-C7
20	v	822	SQD	C46-C45-O47-C7
13	3	511	CLA	O1D-CGD-O2D-CED
13	a	511	CLA	O1D-CGD-O2D-CED
13	s	511	CLA	O1D-CGD-O2D-CED
13	B	1218	CLA	C8-C10-C11-C12
13	f	1218	CLA	C8-C10-C11-C12
13	A	1122	CLA	CBD-CGD-O2D-CED
13	G	1122	CLA	CBD-CGD-O2D-CED
13	e	1122	CLA	CBD-CGD-O2D-CED
17	L	5218	LHG	C28-C29-C30-C31
17	V	5218	LHG	C28-C29-C30-C31
17	n	5218	LHG	C28-C29-C30-C31
17	n	5220	LHG	C27-C28-C29-C30
19	J	5104	LMG	C11-C12-C13-C14
19	T	5104	LMG	C11-C12-C13-C14
19	l	5104	LMG	C11-C12-C13-C14
20	B	1852	SQD	C11-C10-C9-C8
20	H	1852	SQD	C11-C10-C9-C8
20	f	1852	SQD	C11-C10-C9-C8
17	L	5221	LHG	C5-C4-O6-P
17	V	5221	LHG	C5-C4-O6-P
17	n	5221	LHG	C5-C4-O6-P
17	L	5220	LHG	C27-C28-C29-C30
17	V	5220	LHG	C27-C28-C29-C30
13	H	1235	CLA	O1D-CGD-O2D-CED
13	H	1218	CLA	C8-C10-C11-C12
17	I	5001	LHG	O2-C2-C3-O3
17	k	5001	LHG	O2-C2-C3-O3
18	A	1849	LMU	C4-C5-C6-C7
18	G	1849	LMU	C4-C5-C6-C7
18	e	1849	LMU	C4-C5-C6-C7
13	B	1231	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	6	510	CLA	O1D-CGD-O2D-CED
13	H	1231	CLA	O1D-CGD-O2D-CED
13	d	510	CLA	O1D-CGD-O2D-CED
13	f	1231	CLA	O1D-CGD-O2D-CED
13	v	510	CLA	O1D-CGD-O2D-CED
20	B	1852	SQD	C2-C1-O6-C44
20	H	1852	SQD	C2-C1-O6-C44
20	f	1852	SQD	C2-C1-O6-C44
17	A	5002	LHG	C32-C33-C34-C35
17	B	1855	LHG	C11-C12-C13-C14
17	G	5002	LHG	C32-C33-C34-C35
17	H	1855	LHG	C11-C12-C13-C14
17	e	5002	LHG	C32-C33-C34-C35
17	f	1855	LHG	C11-C12-C13-C14
18	B	1843	LMU	C5-C6-C7-C8
18	2	901	LMU	C2-C3-C4-C5
18	H	1843	LMU	C5-C6-C7-C8
18	Z	901	LMU	C2-C3-C4-C5
18	f	1843	LMU	C5-C6-C7-C8
18	r	901	LMU	C2-C3-C4-C5
19	B	5002	LMG	C22-C23-C24-C25
19	H	5002	LMG	C22-C23-C24-C25
19	f	5002	LMG	C22-C23-C24-C25
20	L	5216	SQD	C12-C13-C14-C15
20	V	5216	SQD	C12-C13-C14-C15
20	n	5216	SQD	C12-C13-C14-C15
13	A	1103	CLA	C10-C11-C12-C13
13	A	1103	CLA	C15-C16-C17-C18
13	G	1103	CLA	C10-C11-C12-C13
13	G	1103	CLA	C15-C16-C17-C18
13	e	1103	CLA	C10-C11-C12-C13
13	e	1103	CLA	C15-C16-C17-C18
13	A	1137	CLA	O1A-CGA-O2A-C1
13	G	1137	CLA	O1A-CGA-O2A-C1
13	e	1137	CLA	O1A-CGA-O2A-C1
13	A	1116	CLA	C11-C12-C13-C15
13	A	1140	CLA	C16-C17-C18-C20
13	B	1222	CLA	C11-C12-C13-C15
13	2	508	CLA	C6-C7-C8-C10
13	G	1116	CLA	C11-C12-C13-C15
13	G	1140	CLA	C16-C17-C18-C20
13	H	1222	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	H	1207	CLA	C16-C17-C18-C19
13	e	1105	CLA	C6-C7-C8-C9
13	e	1116	CLA	C11-C12-C13-C15
13	e	1140	CLA	C16-C17-C18-C20
13	f	1222	CLA	C11-C12-C13-C15
13	r	508	CLA	C6-C7-C8-C10
14	B	2002	PQN	C26-C27-C28-C30
14	H	2002	PQN	C26-C27-C28-C30
14	f	2002	PQN	C26-C27-C28-C30
13	B	1235	CLA	O1D-CGD-O2D-CED
13	1	507	CLA	O1D-CGD-O2D-CED
13	1	519	CLA	O1D-CGD-O2D-CED
13	G	1138	CLA	O1D-CGD-O2D-CED
13	Y	507	CLA	O1D-CGD-O2D-CED
13	Y	519	CLA	O1D-CGD-O2D-CED
13	f	1235	CLA	O1D-CGD-O2D-CED
13	q	507	CLA	O1D-CGD-O2D-CED
13	q	519	CLA	O1D-CGD-O2D-CED
13	A	1117	CLA	C4-C3-C5-C6
13	B	1208	CLA	C4-C3-C5-C6
13	B	1229	CLA	C4-C3-C5-C6
13	G	1117	CLA	C4-C3-C5-C6
13	H	1208	CLA	C4-C3-C5-C6
13	H	1229	CLA	C4-C3-C5-C6
13	e	1117	CLA	C4-C3-C5-C6
13	f	1208	CLA	C4-C3-C5-C6
13	f	1229	CLA	C4-C3-C5-C6
17	A	5004	LHG	C24-C25-C26-C27
17	A	5003	LHG	C12-C13-C14-C15
17	B	1842	LHG	C27-C28-C29-C30
17	G	5004	LHG	C24-C25-C26-C27
17	G	5003	LHG	C12-C13-C14-C15
17	H	1842	LHG	C27-C28-C29-C30
17	e	5004	LHG	C24-C25-C26-C27
17	e	5003	LHG	C12-C13-C14-C15
17	f	1842	LHG	C27-C28-C29-C30
18	A	1848	LMU	C2-C3-C4-C5
18	G	1848	LMU	C2-C3-C4-C5
18	e	1848	LMU	C2-C3-C4-C5
20	2	822	SQD	C10-C11-C12-C13
20	Z	822	SQD	C10-C11-C12-C13
20	r	822	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	B	1229	CLA	C2-C3-C5-C6
13	H	1229	CLA	C2-C3-C5-C6
13	f	1229	CLA	C2-C3-C5-C6
13	A	1106	CLA	C6-C7-C8-C9
13	A	1111	CLA	C11-C12-C13-C14
13	A	1119	CLA	C6-C7-C8-C9
13	A	1122	CLA	C6-C7-C8-C9
13	A	1133	CLA	C11-C12-C13-C14
13	A	1237	CLA	C14-C13-C15-C16
13	B	1213	CLA	C6-C7-C8-C9
13	B	1216	CLA	C6-C7-C8-C9
13	B	1229	CLA	C6-C7-C8-C9
13	6	501	CLA	C6-C7-C8-C9
13	G	1106	CLA	C6-C7-C8-C9
13	G	1111	CLA	C11-C12-C13-C14
13	G	1119	CLA	C6-C7-C8-C9
13	G	1122	CLA	C6-C7-C8-C9
13	G	1133	CLA	C11-C12-C13-C14
13	G	1237	CLA	C14-C13-C15-C16
13	H	1213	CLA	C6-C7-C8-C9
13	H	1216	CLA	C6-C7-C8-C9
13	H	1229	CLA	C6-C7-C8-C9
13	d	501	CLA	C6-C7-C8-C9
13	e	1106	CLA	C6-C7-C8-C9
13	e	1111	CLA	C11-C12-C13-C14
13	e	1119	CLA	C6-C7-C8-C9
13	e	1122	CLA	C6-C7-C8-C9
13	e	1133	CLA	C11-C12-C13-C14
13	e	1237	CLA	C14-C13-C15-C16
13	f	1213	CLA	C6-C7-C8-C9
13	f	1216	CLA	C6-C7-C8-C9
13	f	1229	CLA	C6-C7-C8-C9
13	v	501	CLA	C6-C7-C8-C9
13	A	1138	CLA	O1D-CGD-O2D-CED
13	1	511	CLA	O1D-CGD-O2D-CED
13	Y	511	CLA	O1D-CGD-O2D-CED
13	e	1138	CLA	O1D-CGD-O2D-CED
13	q	511	CLA	O1D-CGD-O2D-CED
19	J	5104	LMG	C28-C29-C30-C31
19	T	5104	LMG	C28-C29-C30-C31
19	l	5104	LMG	C28-C29-C30-C31
17	A	5007	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	B	1842	LHG	C32-C33-C34-C35
17	L	5220	LHG	C10-C11-C12-C13
17	G	5007	LHG	C11-C10-C9-C8
17	H	1842	LHG	C32-C33-C34-C35
17	V	5220	LHG	C10-C11-C12-C13
17	e	5007	LHG	C11-C10-C9-C8
17	f	1842	LHG	C32-C33-C34-C35
17	n	5220	LHG	C10-C11-C12-C13
19	B	5002	LMG	C32-C33-C34-C35
19	H	5002	LMG	C32-C33-C34-C35
19	f	5002	LMG	C32-C33-C34-C35
20	1	822	SQD	C11-C10-C9-C8
20	3	822	SQD	C27-C28-C29-C30
20	Y	822	SQD	C11-C10-C9-C8
20	a	822	SQD	C27-C28-C29-C30
20	q	822	SQD	C11-C10-C9-C8
20	s	822	SQD	C27-C28-C29-C30
13	B	1208	CLA	C8-C10-C11-C12
13	5	509	CLA	C10-C11-C12-C13
13	H	1208	CLA	C8-C10-C11-C12
13	c	509	CLA	C10-C11-C12-C13
13	f	1208	CLA	C8-C10-C11-C12
13	u	509	CLA	C10-C11-C12-C13
16	L	4019	BCR	C37-C22-C23-C24
16	V	4019	BCR	C37-C22-C23-C24
16	n	4019	BCR	C37-C22-C23-C24
17	A	5005	LHG	C24-C25-C26-C27
17	G	5005	LHG	C24-C25-C26-C27
17	e	5005	LHG	C24-C25-C26-C27
20	s	822	SQD	C9-C10-C11-C12
17	A	5002	LHG	O1-C1-C2-C3
17	A	5008	LHG	O1-C1-C2-C3
17	L	5221	LHG	O1-C1-C2-C3
17	G	5002	LHG	O1-C1-C2-C3
17	G	5008	LHG	O1-C1-C2-C3
17	V	5221	LHG	O1-C1-C2-C3
17	e	5002	LHG	O1-C1-C2-C3
17	e	5008	LHG	O1-C1-C2-C3
17	n	5221	LHG	O1-C1-C2-C3
16	L	4019	BCR	C21-C22-C23-C24
16	3	523	BCR	C21-C22-C23-C24
16	4	523	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	6	523	BCR	C21-C22-C23-C24
16	V	4019	BCR	C21-C22-C23-C24
16	a	523	BCR	C21-C22-C23-C24
16	b	523	BCR	C21-C22-C23-C24
16	d	523	BCR	C21-C22-C23-C24
16	n	4019	BCR	C21-C22-C23-C24
16	s	523	BCR	C21-C22-C23-C24
16	t	523	BCR	C21-C22-C23-C24
16	v	523	BCR	C21-C22-C23-C24
13	B	1203	CLA	C3-C5-C6-C7
13	B	1218	CLA	C3-C5-C6-C7
13	H	1203	CLA	C3-C5-C6-C7
13	H	1218	CLA	C3-C5-C6-C7
13	f	1203	CLA	C3-C5-C6-C7
13	f	1218	CLA	C3-C5-C6-C7
13	4	509	CLA	C15-C16-C17-C18
13	b	509	CLA	C15-C16-C17-C18
13	t	509	CLA	C15-C16-C17-C18
17	A	5007	LHG	C28-C29-C30-C31
17	G	5007	LHG	C28-C29-C30-C31
17	e	5007	LHG	C28-C29-C30-C31
20	1	822	SQD	C12-C13-C14-C15
20	3	822	SQD	C9-C10-C11-C12
20	Y	822	SQD	C12-C13-C14-C15
20	a	822	SQD	C9-C10-C11-C12
20	q	822	SQD	C12-C13-C14-C15
13	B	1205	CLA	CBD-CGD-O2D-CED
13	H	1205	CLA	CBD-CGD-O2D-CED
13	f	1205	CLA	CBD-CGD-O2D-CED
17	A	5002	LHG	C23-C24-C25-C26
17	G	5002	LHG	C23-C24-C25-C26
17	e	5002	LHG	C23-C24-C25-C26
20	B	1852	SQD	C23-C24-C25-C26
20	H	1852	SQD	C23-C24-C25-C26
20	f	1852	SQD	C23-C24-C25-C26
17	A	5008	LHG	C10-C11-C12-C13
17	A	5001	LHG	C27-C28-C29-C30
17	I	5001	LHG	C10-C11-C12-C13
17	L	5220	LHG	C9-C10-C11-C12
17	L	5220	LHG	C13-C14-C15-C16
17	L	5221	LHG	C11-C12-C13-C14
17	L	5221	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
17	L	5221	LHG	C25-C26-C27-C28
17	G	5001	LHG	C27-C28-C29-C30
17	S	5001	LHG	C10-C11-C12-C13
17	V	5220	LHG	C9-C10-C11-C12
17	V	5220	LHG	C13-C14-C15-C16
17	V	5221	LHG	C11-C12-C13-C14
17	V	5221	LHG	C17-C18-C19-C20
17	V	5221	LHG	C25-C26-C27-C28
17	e	5001	LHG	C27-C28-C29-C30
17	k	5001	LHG	C10-C11-C12-C13
17	n	5220	LHG	C9-C10-C11-C12
17	n	5220	LHG	C13-C14-C15-C16
17	n	5221	LHG	C11-C12-C13-C14
17	n	5221	LHG	C17-C18-C19-C20
17	n	5221	LHG	C25-C26-C27-C28
18	B	1843	LMU	C4-C5-C6-C7
18	H	1843	LMU	C4-C5-C6-C7
18	f	1843	LMU	C4-C5-C6-C7
13	A	1118	CLA	C4B-C3B-CAB-CBB
13	A	1129	CLA	C4B-C3B-CAB-CBB
13	A	1131	CLA	C4B-C3B-CAB-CBB
13	A	1132	CLA	C4B-C3B-CAB-CBB
13	A	1134	CLA	C4B-C3B-CAB-CBB
13	A	1138	CLA	C4B-C3B-CAB-CBB
13	A	1139	CLA	C4B-C3B-CAB-CBB
13	A	1237	CLA	C4B-C3B-CAB-CBB
13	B	1021	CLA	C4B-C3B-CAB-CBB
13	B	1219	CLA	C4B-C3B-CAB-CBB
13	B	1227	CLA	C4B-C3B-CAB-CBB
13	B	1235	CLA	C4B-C3B-CAB-CBB
13	B	1207	CLA	C4B-C3B-CAB-CBB
13	F	1302	CLA	C4B-C3B-CAB-CBB
13	J	1302	CLA	C4B-C3B-CAB-CBB
13	2	502	CLA	C4B-C3B-CAB-CBB
13	3	502	CLA	C4B-C3B-CAB-CBB
13	3	519	CLA	C4B-C3B-CAB-CBB
13	4	505	CLA	C4B-C3B-CAB-CBB
13	5	502	CLA	C4B-C3B-CAB-CBB
13	5	519	CLA	C4B-C3B-CAB-CBB
13	6	501	CLA	C4B-C3B-CAB-CBB
13	6	507	CLA	C4B-C3B-CAB-CBB
13	6	518	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	6	519	CLA	C4B-C3B-CAB-CBB
13	G	1118	CLA	C4B-C3B-CAB-CBB
13	G	1129	CLA	C4B-C3B-CAB-CBB
13	G	1131	CLA	C4B-C3B-CAB-CBB
13	G	1132	CLA	C4B-C3B-CAB-CBB
13	G	1134	CLA	C4B-C3B-CAB-CBB
13	G	1138	CLA	C4B-C3B-CAB-CBB
13	G	1139	CLA	C4B-C3B-CAB-CBB
13	G	1237	CLA	C4B-C3B-CAB-CBB
13	H	1021	CLA	C4B-C3B-CAB-CBB
13	H	1219	CLA	C4B-C3B-CAB-CBB
13	H	1227	CLA	C4B-C3B-CAB-CBB
13	H	1235	CLA	C4B-C3B-CAB-CBB
13	H	1207	CLA	C4B-C3B-CAB-CBB
13	R	1302	CLA	C4B-C3B-CAB-CBB
13	T	1302	CLA	C4B-C3B-CAB-CBB
13	Z	502	CLA	C4B-C3B-CAB-CBB
13	a	502	CLA	C4B-C3B-CAB-CBB
13	a	519	CLA	C4B-C3B-CAB-CBB
13	b	505	CLA	C4B-C3B-CAB-CBB
13	c	502	CLA	C4B-C3B-CAB-CBB
13	c	519	CLA	C4B-C3B-CAB-CBB
13	d	501	CLA	C4B-C3B-CAB-CBB
13	d	507	CLA	C4B-C3B-CAB-CBB
13	d	518	CLA	C4B-C3B-CAB-CBB
13	d	519	CLA	C4B-C3B-CAB-CBB
13	e	1118	CLA	C4B-C3B-CAB-CBB
13	e	1129	CLA	C4B-C3B-CAB-CBB
13	e	1131	CLA	C4B-C3B-CAB-CBB
13	e	1132	CLA	C4B-C3B-CAB-CBB
13	e	1134	CLA	C4B-C3B-CAB-CBB
13	e	1138	CLA	C4B-C3B-CAB-CBB
13	e	1139	CLA	C4B-C3B-CAB-CBB
13	e	1237	CLA	C4B-C3B-CAB-CBB
13	f	1021	CLA	C4B-C3B-CAB-CBB
13	f	1219	CLA	C4B-C3B-CAB-CBB
13	f	1227	CLA	C4B-C3B-CAB-CBB
13	f	1235	CLA	C4B-C3B-CAB-CBB
13	f	1207	CLA	C4B-C3B-CAB-CBB
13	j	1302	CLA	C4B-C3B-CAB-CBB
13	l	1302	CLA	C4B-C3B-CAB-CBB
13	r	502	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	s	502	CLA	C4B-C3B-CAB-CBB
13	s	519	CLA	C4B-C3B-CAB-CBB
13	t	505	CLA	C4B-C3B-CAB-CBB
13	u	502	CLA	C4B-C3B-CAB-CBB
13	u	519	CLA	C4B-C3B-CAB-CBB
13	v	501	CLA	C4B-C3B-CAB-CBB
13	v	507	CLA	C4B-C3B-CAB-CBB
13	v	518	CLA	C4B-C3B-CAB-CBB
13	v	519	CLA	C4B-C3B-CAB-CBB
13	A	1101	CLA	C16-C17-C18-C19
13	B	1213	CLA	C16-C17-C18-C19
13	B	1213	CLA	C16-C17-C18-C20
13	B	1224	CLA	C11-C12-C13-C14
13	B	1224	CLA	C11-C12-C13-C15
13	B	1238	CLA	C16-C17-C18-C19
13	1	505	CLA	C16-C17-C18-C20
13	6	501	CLA	C11-C12-C13-C14
13	6	505	CLA	C16-C17-C18-C20
13	G	1101	CLA	C16-C17-C18-C19
13	H	1213	CLA	C16-C17-C18-C19
13	H	1213	CLA	C16-C17-C18-C20
13	H	1224	CLA	C11-C12-C13-C14
13	H	1224	CLA	C11-C12-C13-C15
13	H	1238	CLA	C16-C17-C18-C19
13	Y	505	CLA	C16-C17-C18-C20
13	d	501	CLA	C11-C12-C13-C14
13	d	505	CLA	C16-C17-C18-C20
13	e	1101	CLA	C16-C17-C18-C19
13	f	1213	CLA	C16-C17-C18-C19
13	f	1213	CLA	C16-C17-C18-C20
13	f	1224	CLA	C11-C12-C13-C14
13	f	1224	CLA	C11-C12-C13-C15
13	f	1238	CLA	C16-C17-C18-C19
13	q	505	CLA	C16-C17-C18-C20
13	v	501	CLA	C11-C12-C13-C14
13	v	505	CLA	C16-C17-C18-C20
14	A	2001	PQN	C26-C27-C28-C29
14	G	2001	PQN	C26-C27-C28-C29
14	e	2001	PQN	C26-C27-C28-C29
13	A	1127	CLA	C15-C16-C17-C18
13	G	1127	CLA	C15-C16-C17-C18
13	H	1206	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B	1855	LHG	C26-C27-C28-C29
17	I	5001	LHG	C29-C30-C31-C32
17	G	5008	LHG	C10-C11-C12-C13
17	H	1855	LHG	C26-C27-C28-C29
17	S	5001	LHG	C29-C30-C31-C32
17	e	5008	LHG	C10-C11-C12-C13
17	f	1855	LHG	C26-C27-C28-C29
17	k	5001	LHG	C29-C30-C31-C32
13	1	508	CLA	CBD-CGD-O2D-CED
13	Y	508	CLA	CBD-CGD-O2D-CED
13	q	508	CLA	CBD-CGD-O2D-CED
13	B	1206	CLA	O1D-CGD-O2D-CED
13	f	1206	CLA	O1D-CGD-O2D-CED
17	A	5005	LHG	C13-C14-C15-C16
17	A	5007	LHG	C25-C26-C27-C28
17	B	1842	LHG	C28-C29-C30-C31
17	L	5218	LHG	C11-C10-C9-C8
17	G	5007	LHG	C25-C26-C27-C28
17	H	1842	LHG	C28-C29-C30-C31
17	V	5218	LHG	C11-C10-C9-C8
17	V	5221	LHG	C32-C33-C34-C35
17	e	5005	LHG	C13-C14-C15-C16
17	e	5007	LHG	C25-C26-C27-C28
17	e	5007	LHG	C33-C34-C35-C36
17	f	1842	LHG	C28-C29-C30-C31
17	n	5218	LHG	C11-C10-C9-C8
20	2	822	SQD	C9-C10-C11-C12
20	Z	822	SQD	C9-C10-C11-C12
20	r	822	SQD	C9-C10-C11-C12
13	B	1229	CLA	C15-C16-C17-C18
13	H	1229	CLA	C15-C16-C17-C18
13	e	1127	CLA	C15-C16-C17-C18
13	f	1229	CLA	C15-C16-C17-C18
17	A	5007	LHG	C33-C34-C35-C36
17	L	5221	LHG	C32-C33-C34-C35
17	G	5005	LHG	C13-C14-C15-C16
17	G	5007	LHG	C33-C34-C35-C36
17	n	5221	LHG	C32-C33-C34-C35
20	1	822	SQD	C30-C31-C32-C33
20	Y	822	SQD	C30-C31-C32-C33
20	q	822	SQD	C30-C31-C32-C33
13	4	501	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	b	501	CLA	C3-C5-C6-C7
13	t	501	CLA	C3-C5-C6-C7
13	B	1232	CLA	CBA-CGA-O2A-C1
13	1	512	CLA	CBA-CGA-O2A-C1
13	H	1232	CLA	CBA-CGA-O2A-C1
13	Y	512	CLA	CBA-CGA-O2A-C1
13	f	1232	CLA	CBA-CGA-O2A-C1
13	q	512	CLA	CBA-CGA-O2A-C1
17	A	5001	LHG	C32-C33-C34-C35
17	I	5001	LHG	C26-C27-C28-C29
17	G	5001	LHG	C32-C33-C34-C35
17	S	5001	LHG	C26-C27-C28-C29
17	e	5001	LHG	C32-C33-C34-C35
17	k	5001	LHG	C26-C27-C28-C29
13	1	512	CLA	O1D-CGD-O2D-CED
13	U	1103	CLA	O1D-CGD-O2D-CED
13	Y	512	CLA	O1D-CGD-O2D-CED
13	q	512	CLA	O1D-CGD-O2D-CED
13	A	1103	CLA	C3A-C2A-CAA-CBA
13	A	1125	CLA	C3A-C2A-CAA-CBA
13	A	1134	CLA	C3A-C2A-CAA-CBA
13	A	1135	CLA	C3A-C2A-CAA-CBA
13	A	1140	CLA	C3A-C2A-CAA-CBA
13	A	1022	CLA	C3A-C2A-CAA-CBA
13	A	1101	CLA	C3A-C2A-CAA-CBA
13	B	1210	CLA	C3A-C2A-CAA-CBA
13	B	1219	CLA	C3A-C2A-CAA-CBA
13	B	1221	CLA	C3A-C2A-CAA-CBA
13	K	1105	CLA	C3A-C2A-CAA-CBA
13	2	516	CLA	C3A-C2A-CAA-CBA
13	2	519	CLA	C3A-C2A-CAA-CBA
13	3	513	CLA	C3A-C2A-CAA-CBA
13	4	516	CLA	C3A-C2A-CAA-CBA
13	5	516	CLA	C3A-C2A-CAA-CBA
13	6	512	CLA	C3A-C2A-CAA-CBA
13	6	516	CLA	C3A-C2A-CAA-CBA
13	G	1103	CLA	C3A-C2A-CAA-CBA
13	G	1125	CLA	C3A-C2A-CAA-CBA
13	G	1134	CLA	C3A-C2A-CAA-CBA
13	G	1135	CLA	C3A-C2A-CAA-CBA
13	G	1140	CLA	C3A-C2A-CAA-CBA
13	G	1022	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	G	1101	CLA	C3A-C2A-CAA-CBA
13	H	1210	CLA	C3A-C2A-CAA-CBA
13	H	1219	CLA	C3A-C2A-CAA-CBA
13	H	1221	CLA	C3A-C2A-CAA-CBA
13	U	1105	CLA	C3A-C2A-CAA-CBA
13	Z	516	CLA	C3A-C2A-CAA-CBA
13	Z	519	CLA	C3A-C2A-CAA-CBA
13	a	513	CLA	C3A-C2A-CAA-CBA
13	b	516	CLA	C3A-C2A-CAA-CBA
13	c	516	CLA	C3A-C2A-CAA-CBA
13	d	512	CLA	C3A-C2A-CAA-CBA
13	d	516	CLA	C3A-C2A-CAA-CBA
13	e	1103	CLA	C3A-C2A-CAA-CBA
13	e	1125	CLA	C3A-C2A-CAA-CBA
13	e	1134	CLA	C3A-C2A-CAA-CBA
13	e	1135	CLA	C3A-C2A-CAA-CBA
13	e	1140	CLA	C3A-C2A-CAA-CBA
13	e	1022	CLA	C3A-C2A-CAA-CBA
13	e	1101	CLA	C3A-C2A-CAA-CBA
13	f	1210	CLA	C3A-C2A-CAA-CBA
13	f	1219	CLA	C3A-C2A-CAA-CBA
13	f	1221	CLA	C3A-C2A-CAA-CBA
13	m	1105	CLA	C3A-C2A-CAA-CBA
13	r	516	CLA	C3A-C2A-CAA-CBA
13	r	519	CLA	C3A-C2A-CAA-CBA
13	s	513	CLA	C3A-C2A-CAA-CBA
13	t	516	CLA	C3A-C2A-CAA-CBA
13	u	516	CLA	C3A-C2A-CAA-CBA
13	v	512	CLA	C3A-C2A-CAA-CBA
13	v	516	CLA	C3A-C2A-CAA-CBA
13	A	1101	CLA	C15-C16-C17-C18
13	2	502	CLA	C8-C10-C11-C12
13	2	503	CLA	C8-C10-C11-C12
13	G	1101	CLA	C15-C16-C17-C18
13	Z	502	CLA	C8-C10-C11-C12
13	e	1101	CLA	C15-C16-C17-C18
13	r	502	CLA	C8-C10-C11-C12
13	r	503	CLA	C8-C10-C11-C12
18	B	1843	LMU	C2-C1-O1'-C1'
18	H	1843	LMU	C2-C1-O1'-C1'
18	f	1843	LMU	C2-C1-O1'-C1'
20	L	5216	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	V	5216	SQD	C18-C19-C20-C21
20	n	5216	SQD	C18-C19-C20-C21
13	K	1103	CLA	O1D-CGD-O2D-CED
13	1	518	CLA	O1D-CGD-O2D-CED
13	Y	518	CLA	O1D-CGD-O2D-CED
13	m	1103	CLA	O1D-CGD-O2D-CED
13	q	518	CLA	O1D-CGD-O2D-CED
13	A	1134	CLA	O1A-CGA-O2A-C1
13	G	1134	CLA	O1A-CGA-O2A-C1
13	e	1134	CLA	O1A-CGA-O2A-C1
13	A	1140	CLA	C16-C17-C18-C19
13	B	1210	CLA	C16-C17-C18-C19
13	B	1218	CLA	C11-C12-C13-C14
13	B	1207	CLA	C16-C17-C18-C20
13	6	505	CLA	C16-C17-C18-C19
13	G	1140	CLA	C16-C17-C18-C19
13	H	1210	CLA	C16-C17-C18-C19
13	H	1218	CLA	C11-C12-C13-C14
13	H	1207	CLA	C16-C17-C18-C20
13	d	505	CLA	C16-C17-C18-C19
13	e	1140	CLA	C16-C17-C18-C19
13	f	1210	CLA	C16-C17-C18-C19
13	f	1218	CLA	C11-C12-C13-C14
13	f	1207	CLA	C16-C17-C18-C20
13	v	505	CLA	C16-C17-C18-C19
17	A	5001	LHG	C29-C30-C31-C32
17	L	5221	LHG	C26-C27-C28-C29
17	L	5221	LHG	C28-C29-C30-C31
17	G	5001	LHG	C29-C30-C31-C32
17	V	5221	LHG	C26-C27-C28-C29
17	e	5001	LHG	C29-C30-C31-C32
17	n	5221	LHG	C26-C27-C28-C29
17	n	5221	LHG	C28-C29-C30-C31
20	Y	822	SQD	C27-C28-C29-C30
17	A	5002	LHG	C25-C26-C27-C28
17	A	5003	LHG	C11-C10-C9-C8
17	L	5221	LHG	C18-C19-C20-C21
17	G	5002	LHG	C25-C26-C27-C28
17	G	5003	LHG	C11-C10-C9-C8
17	V	5221	LHG	C18-C19-C20-C21
17	V	5221	LHG	C28-C29-C30-C31
17	e	5002	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
17	e	5003	LHG	C11-C10-C9-C8
17	n	5221	LHG	C18-C19-C20-C21
19	B	5002	LMG	C21-C22-C23-C24
19	H	5002	LMG	C21-C22-C23-C24
19	f	5002	LMG	C21-C22-C23-C24
20	1	822	SQD	C27-C28-C29-C30
20	q	822	SQD	C27-C28-C29-C30
13	2	512	CLA	C3-C5-C6-C7
13	Z	512	CLA	C3-C5-C6-C7
13	r	512	CLA	C3-C5-C6-C7
20	3	822	SQD	C7-C8-C9-C10
20	s	822	SQD	C7-C8-C9-C10
17	A	5004	LHG	C27-C28-C29-C30
17	e	5004	LHG	C27-C28-C29-C30
13	Z	503	CLA	C8-C10-C11-C12
13	A	1124	CLA	C4-C3-C5-C6
13	J	1302	CLA	C4-C3-C5-C6
13	G	1124	CLA	C4-C3-C5-C6
13	T	1302	CLA	C4-C3-C5-C6
13	e	1124	CLA	C4-C3-C5-C6
13	l	1302	CLA	C4-C3-C5-C6
14	B	2002	PQN	C14-C13-C15-C16
14	H	2002	PQN	C14-C13-C15-C16
14	f	2002	PQN	C14-C13-C15-C16
13	1	508	CLA	CBA-CGA-O2A-C1
13	Y	508	CLA	CBA-CGA-O2A-C1
13	q	508	CLA	CBA-CGA-O2A-C1
13	A	1124	CLA	C2-C3-C5-C6
13	B	1227	CLA	C2-C3-C5-C6
13	J	1302	CLA	C2-C3-C5-C6
13	L	1503	CLA	C2-C3-C5-C6
13	4	519	CLA	C2-C3-C5-C6
13	G	1124	CLA	C2-C3-C5-C6
13	H	1227	CLA	C2-C3-C5-C6
13	T	1302	CLA	C2-C3-C5-C6
13	V	1503	CLA	C2-C3-C5-C6
13	b	519	CLA	C2-C3-C5-C6
13	e	1124	CLA	C2-C3-C5-C6
13	f	1227	CLA	C2-C3-C5-C6
13	l	1302	CLA	C2-C3-C5-C6
13	n	1503	CLA	C2-C3-C5-C6
13	t	519	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	A	5007	LHG	C8-C7-O7-C5
17	G	5007	LHG	C8-C7-O7-C5
17	e	5007	LHG	C8-C7-O7-C5
19	J	5104	LMG	C11-C10-O7-C8
19	T	5104	LMG	C11-C10-O7-C8
19	l	5104	LMG	C11-C10-O7-C8
17	A	5005	LHG	C9-C10-C11-C12
17	A	5009	LHG	C24-C25-C26-C27
17	G	5004	LHG	C27-C28-C29-C30
17	G	5005	LHG	C9-C10-C11-C12
17	G	5009	LHG	C24-C25-C26-C27
17	e	5005	LHG	C9-C10-C11-C12
17	e	5009	LHG	C24-C25-C26-C27
17	A	5002	LHG	O1-C1-C2-O2
17	A	5005	LHG	O1-C1-C2-O2
17	A	5008	LHG	O1-C1-C2-O2
17	A	5009	LHG	O1-C1-C2-O2
17	B	1842	LHG	O1-C1-C2-O2
17	B	1855	LHG	O1-C1-C2-O2
17	L	5218	LHG	O1-C1-C2-O2
17	L	5220	LHG	O1-C1-C2-O2
17	G	5002	LHG	O1-C1-C2-O2
17	G	5005	LHG	O1-C1-C2-O2
17	G	5008	LHG	O1-C1-C2-O2
17	G	5009	LHG	O1-C1-C2-O2
17	H	1842	LHG	O1-C1-C2-O2
17	H	1855	LHG	O1-C1-C2-O2
17	V	5218	LHG	O1-C1-C2-O2
17	V	5220	LHG	O1-C1-C2-O2
17	e	5002	LHG	O1-C1-C2-O2
17	e	5005	LHG	O1-C1-C2-O2
17	e	5008	LHG	O1-C1-C2-O2
17	e	5009	LHG	O1-C1-C2-O2
17	f	1842	LHG	O1-C1-C2-O2
17	f	1855	LHG	O1-C1-C2-O2
17	n	5218	LHG	O1-C1-C2-O2
17	n	5220	LHG	O1-C1-C2-O2
13	H	1235	CLA	C5-C6-C7-C8
20	a	822	SQD	C7-C8-C9-C10
13	A	1105	CLA	C6-C7-C8-C10
13	A	1115	CLA	C11-C12-C13-C15
13	B	1238	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	G	1105	CLA	C6-C7-C8-C10
13	H	1238	CLA	C16-C17-C18-C20
13	e	1105	CLA	C6-C7-C8-C10
13	e	1115	CLA	C11-C12-C13-C15
13	f	1238	CLA	C16-C17-C18-C20
13	A	1118	CLA	C2B-C3B-CAB-CBB
13	A	1131	CLA	C2B-C3B-CAB-CBB
13	A	1132	CLA	C2B-C3B-CAB-CBB
13	A	1134	CLA	C2B-C3B-CAB-CBB
13	A	1138	CLA	C2B-C3B-CAB-CBB
13	A	1139	CLA	C2B-C3B-CAB-CBB
13	A	1237	CLA	C2B-C3B-CAB-CBB
13	B	1227	CLA	C2B-C3B-CAB-CBB
13	B	1235	CLA	C2B-C3B-CAB-CBB
13	B	1239	CLA	C2B-C3B-CAB-CBB
13	B	1207	CLA	C2B-C3B-CAB-CBB
13	F	1302	CLA	C2B-C3B-CAB-CBB
13	J	1302	CLA	C2B-C3B-CAB-CBB
13	K	1401	CLA	C2B-C3B-CAB-CBB
13	1	501	CLA	C2B-C3B-CAB-CBB
13	1	512	CLA	C2B-C3B-CAB-CBB
13	2	501	CLA	C2B-C3B-CAB-CBB
13	2	513	CLA	C2B-C3B-CAB-CBB
13	3	502	CLA	C2B-C3B-CAB-CBB
13	3	512	CLA	C2B-C3B-CAB-CBB
13	3	519	CLA	C2B-C3B-CAB-CBB
13	4	501	CLA	C2B-C3B-CAB-CBB
13	4	502	CLA	C2B-C3B-CAB-CBB
13	4	505	CLA	C2B-C3B-CAB-CBB
13	4	508	CLA	C2B-C3B-CAB-CBB
13	5	512	CLA	C2B-C3B-CAB-CBB
13	5	516	CLA	C2B-C3B-CAB-CBB
13	5	517	CLA	C2B-C3B-CAB-CBB
13	5	519	CLA	C2B-C3B-CAB-CBB
13	6	501	CLA	C2B-C3B-CAB-CBB
13	6	503	CLA	C2B-C3B-CAB-CBB
13	6	512	CLA	C2B-C3B-CAB-CBB
13	6	518	CLA	C2B-C3B-CAB-CBB
13	6	519	CLA	C2B-C3B-CAB-CBB
13	G	1118	CLA	C2B-C3B-CAB-CBB
13	G	1131	CLA	C2B-C3B-CAB-CBB
13	G	1132	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	G	1134	CLA	C2B-C3B-CAB-CBB
13	G	1138	CLA	C2B-C3B-CAB-CBB
13	G	1139	CLA	C2B-C3B-CAB-CBB
13	G	1237	CLA	C2B-C3B-CAB-CBB
13	H	1227	CLA	C2B-C3B-CAB-CBB
13	H	1235	CLA	C2B-C3B-CAB-CBB
13	H	1239	CLA	C2B-C3B-CAB-CBB
13	H	1207	CLA	C2B-C3B-CAB-CBB
13	R	1302	CLA	C2B-C3B-CAB-CBB
13	T	1302	CLA	C2B-C3B-CAB-CBB
13	U	1401	CLA	C2B-C3B-CAB-CBB
13	Y	501	CLA	C2B-C3B-CAB-CBB
13	Y	512	CLA	C2B-C3B-CAB-CBB
13	Z	501	CLA	C2B-C3B-CAB-CBB
13	Z	513	CLA	C2B-C3B-CAB-CBB
13	a	502	CLA	C2B-C3B-CAB-CBB
13	a	512	CLA	C2B-C3B-CAB-CBB
13	a	519	CLA	C2B-C3B-CAB-CBB
13	b	501	CLA	C2B-C3B-CAB-CBB
13	b	502	CLA	C2B-C3B-CAB-CBB
13	b	505	CLA	C2B-C3B-CAB-CBB
13	b	508	CLA	C2B-C3B-CAB-CBB
13	c	512	CLA	C2B-C3B-CAB-CBB
13	c	516	CLA	C2B-C3B-CAB-CBB
13	c	517	CLA	C2B-C3B-CAB-CBB
13	c	519	CLA	C2B-C3B-CAB-CBB
13	d	501	CLA	C2B-C3B-CAB-CBB
13	d	512	CLA	C2B-C3B-CAB-CBB
13	d	518	CLA	C2B-C3B-CAB-CBB
13	d	519	CLA	C2B-C3B-CAB-CBB
13	e	1118	CLA	C2B-C3B-CAB-CBB
13	e	1131	CLA	C2B-C3B-CAB-CBB
13	e	1132	CLA	C2B-C3B-CAB-CBB
13	e	1134	CLA	C2B-C3B-CAB-CBB
13	e	1138	CLA	C2B-C3B-CAB-CBB
13	e	1139	CLA	C2B-C3B-CAB-CBB
13	e	1237	CLA	C2B-C3B-CAB-CBB
13	f	1227	CLA	C2B-C3B-CAB-CBB
13	f	1235	CLA	C2B-C3B-CAB-CBB
13	f	1239	CLA	C2B-C3B-CAB-CBB
13	f	1207	CLA	C2B-C3B-CAB-CBB
13	j	1302	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	l	1302	CLA	C2B-C3B-CAB-CBB
13	m	1401	CLA	C2B-C3B-CAB-CBB
13	q	501	CLA	C2B-C3B-CAB-CBB
13	q	512	CLA	C2B-C3B-CAB-CBB
13	r	501	CLA	C2B-C3B-CAB-CBB
13	r	513	CLA	C2B-C3B-CAB-CBB
13	s	502	CLA	C2B-C3B-CAB-CBB
13	s	512	CLA	C2B-C3B-CAB-CBB
13	s	519	CLA	C2B-C3B-CAB-CBB
13	t	501	CLA	C2B-C3B-CAB-CBB
13	t	502	CLA	C2B-C3B-CAB-CBB
13	t	505	CLA	C2B-C3B-CAB-CBB
13	t	508	CLA	C2B-C3B-CAB-CBB
13	u	512	CLA	C2B-C3B-CAB-CBB
13	u	516	CLA	C2B-C3B-CAB-CBB
13	u	517	CLA	C2B-C3B-CAB-CBB
13	u	519	CLA	C2B-C3B-CAB-CBB
13	v	501	CLA	C2B-C3B-CAB-CBB
13	v	503	CLA	C2B-C3B-CAB-CBB
13	v	512	CLA	C2B-C3B-CAB-CBB
13	v	518	CLA	C2B-C3B-CAB-CBB
13	v	519	CLA	C2B-C3B-CAB-CBB
13	2	516	CLA	O1D-CGD-O2D-CED
13	r	516	CLA	O1D-CGD-O2D-CED
13	A	1127	CLA	C8-C10-C11-C12
13	B	1210	CLA	C5-C6-C7-C8
13	B	1235	CLA	C5-C6-C7-C8
13	G	1127	CLA	C8-C10-C11-C12
13	H	1210	CLA	C5-C6-C7-C8
13	e	1127	CLA	C8-C10-C11-C12
13	f	1210	CLA	C5-C6-C7-C8
13	f	1235	CLA	C5-C6-C7-C8
14	f	2002	PQN	C25-C26-C27-C28
17	A	5008	LHG	C13-C14-C15-C16
17	G	5008	LHG	C13-C14-C15-C16
17	e	5008	LHG	C13-C14-C15-C16
20	B	1852	SQD	C11-C12-C13-C14
20	H	1852	SQD	C11-C12-C13-C14
20	f	1852	SQD	C11-C12-C13-C14
18	1	902	LMU	C1-C2-C3-C4
18	Y	902	LMU	C1-C2-C3-C4
18	q	902	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
17	A	5006	LHG	C25-C26-C27-C28
17	G	5006	LHG	C25-C26-C27-C28
17	A	5005	LHG	C23-C24-C25-C26
17	G	5005	LHG	C23-C24-C25-C26
17	e	5005	LHG	C23-C24-C25-C26
14	B	2002	PQN	C25-C26-C27-C28
14	H	2002	PQN	C25-C26-C27-C28
17	e	5006	LHG	C25-C26-C27-C28
19	B	5002	LMG	C16-C17-C18-C19
19	H	5002	LMG	C16-C17-C18-C19
19	f	5002	LMG	C16-C17-C18-C19
13	A	1118	CLA	C2-C1-O2A-CGA
13	J	1302	CLA	C2-C1-O2A-CGA
13	3	510	CLA	C2-C1-O2A-CGA
13	T	1302	CLA	C2-C1-O2A-CGA
13	a	510	CLA	C2-C1-O2A-CGA
13	e	1118	CLA	C2-C1-O2A-CGA
13	l	1302	CLA	C2-C1-O2A-CGA
13	s	510	CLA	C2-C1-O2A-CGA
17	A	5009	LHG	C9-C10-C11-C12
17	e	5009	LHG	C9-C10-C11-C12
18	1	902	LMU	C2-C3-C4-C5
18	Y	902	LMU	C2-C3-C4-C5
18	q	902	LMU	C2-C3-C4-C5
20	L	5216	SQD	C11-C12-C13-C14
20	V	5216	SQD	C11-C12-C13-C14
20	n	5216	SQD	C11-C12-C13-C14
20	6	822	SQD	C24-C23-O48-C46
20	d	822	SQD	C24-C23-O48-C46
20	v	822	SQD	C24-C23-O48-C46
13	B	1219	CLA	C5-C6-C7-C8
13	f	1219	CLA	C5-C6-C7-C8
13	B	1215	CLA	O1A-CGA-O2A-C1
13	H	1215	CLA	O1A-CGA-O2A-C1
13	f	1215	CLA	O1A-CGA-O2A-C1
20	L	5216	SQD	O10-C23-O48-C46
20	V	5216	SQD	O10-C23-O48-C46
20	n	5216	SQD	O10-C23-O48-C46
18	J	5105	LMU	C1-C2-C3-C4
18	T	5105	LMU	C1-C2-C3-C4
18	l	5105	LMU	C1-C2-C3-C4
17	G	5009	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	G	1115	CLA	C11-C12-C13-C15
16	A	4008	BCR	C23-C24-C25-C30
16	A	4011	BCR	C23-C24-C25-C26
16	A	4011	BCR	C23-C24-C25-C30
16	B	4004	BCR	C1-C6-C7-C8
16	B	4004	BCR	C5-C6-C7-C8
16	B	4004	BCR	C23-C24-C25-C26
16	B	4005	BCR	C23-C24-C25-C26
16	B	4017	BCR	C5-C6-C7-C8
16	J	4015	BCR	C23-C24-C25-C26
16	J	4012	BCR	C1-C6-C7-C8
16	J	4012	BCR	C23-C24-C25-C26
16	J	4012	BCR	C23-C24-C25-C30
16	L	4019	BCR	C23-C24-C25-C26
16	L	4019	BCR	C23-C24-C25-C30
16	L	4020	BCR	C23-C24-C25-C26
16	M	4021	BCR	C1-C6-C7-C8
16	1	521	BCR	C1-C6-C7-C8
16	1	521	BCR	C5-C6-C7-C8
16	1	521	BCR	C23-C24-C25-C26
16	1	521	BCR	C23-C24-C25-C30
16	1	523	BCR	C1-C6-C7-C8
16	1	523	BCR	C5-C6-C7-C8
16	1	523	BCR	C23-C24-C25-C26
16	1	523	BCR	C23-C24-C25-C30
16	2	521	BCR	C1-C6-C7-C8
16	2	521	BCR	C5-C6-C7-C8
16	2	522	BCR	C1-C6-C7-C8
16	2	523	BCR	C23-C24-C25-C26
16	2	523	BCR	C23-C24-C25-C30
16	2	524	BCR	C23-C24-C25-C26
16	2	524	BCR	C23-C24-C25-C30
16	3	521	BCR	C1-C6-C7-C8
16	3	521	BCR	C5-C6-C7-C8
16	3	521	BCR	C23-C24-C25-C26
16	3	523	BCR	C23-C24-C25-C26
16	3	523	BCR	C23-C24-C25-C30
16	4	521	BCR	C1-C6-C7-C8
16	4	521	BCR	C5-C6-C7-C8
16	4	521	BCR	C23-C24-C25-C26
16	4	521	BCR	C23-C24-C25-C30
16	4	522	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	4	522	BCR	C5-C6-C7-C8
16	4	523	BCR	C23-C24-C25-C26
16	4	523	BCR	C23-C24-C25-C30
16	4	524	BCR	C23-C24-C25-C26
16	4	524	BCR	C23-C24-C25-C30
16	5	522	BCR	C1-C6-C7-C8
16	5	523	BCR	C23-C24-C25-C26
16	5	523	BCR	C23-C24-C25-C30
16	5	524	BCR	C23-C24-C25-C26
16	5	524	BCR	C23-C24-C25-C30
16	6	521	BCR	C1-C6-C7-C8
16	6	521	BCR	C5-C6-C7-C8
16	6	522	BCR	C1-C6-C7-C8
16	6	523	BCR	C23-C24-C25-C26
16	6	523	BCR	C23-C24-C25-C30
16	G	4008	BCR	C23-C24-C25-C30
16	G	4011	BCR	C23-C24-C25-C26
16	G	4011	BCR	C23-C24-C25-C30
16	H	4004	BCR	C1-C6-C7-C8
16	H	4004	BCR	C5-C6-C7-C8
16	H	4004	BCR	C23-C24-C25-C26
16	H	4005	BCR	C23-C24-C25-C26
16	H	4017	BCR	C5-C6-C7-C8
16	T	4015	BCR	C23-C24-C25-C26
16	T	4012	BCR	C1-C6-C7-C8
16	T	4012	BCR	C23-C24-C25-C26
16	T	4012	BCR	C23-C24-C25-C30
16	V	4019	BCR	C23-C24-C25-C26
16	V	4019	BCR	C23-C24-C25-C30
16	V	4020	BCR	C23-C24-C25-C26
16	W	4021	BCR	C1-C6-C7-C8
16	Y	521	BCR	C1-C6-C7-C8
16	Y	521	BCR	C5-C6-C7-C8
16	Y	521	BCR	C23-C24-C25-C26
16	Y	521	BCR	C23-C24-C25-C30
16	Y	523	BCR	C1-C6-C7-C8
16	Y	523	BCR	C5-C6-C7-C8
16	Y	523	BCR	C23-C24-C25-C26
16	Y	523	BCR	C23-C24-C25-C30
16	Z	521	BCR	C1-C6-C7-C8
16	Z	521	BCR	C5-C6-C7-C8
16	Z	522	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	Z	523	BCR	C23-C24-C25-C26
16	Z	523	BCR	C23-C24-C25-C30
16	Z	524	BCR	C23-C24-C25-C26
16	Z	524	BCR	C23-C24-C25-C30
16	a	521	BCR	C1-C6-C7-C8
16	a	521	BCR	C5-C6-C7-C8
16	a	521	BCR	C23-C24-C25-C26
16	a	523	BCR	C23-C24-C25-C26
16	a	523	BCR	C23-C24-C25-C30
16	b	521	BCR	C1-C6-C7-C8
16	b	521	BCR	C5-C6-C7-C8
16	b	521	BCR	C23-C24-C25-C26
16	b	521	BCR	C23-C24-C25-C30
16	b	522	BCR	C1-C6-C7-C8
16	b	522	BCR	C5-C6-C7-C8
16	b	523	BCR	C23-C24-C25-C26
16	b	523	BCR	C23-C24-C25-C30
16	b	524	BCR	C23-C24-C25-C26
16	b	524	BCR	C23-C24-C25-C30
16	c	522	BCR	C1-C6-C7-C8
16	c	523	BCR	C23-C24-C25-C26
16	c	523	BCR	C23-C24-C25-C30
16	c	524	BCR	C23-C24-C25-C26
16	c	524	BCR	C23-C24-C25-C30
16	d	521	BCR	C1-C6-C7-C8
16	d	521	BCR	C5-C6-C7-C8
16	d	522	BCR	C1-C6-C7-C8
16	d	523	BCR	C23-C24-C25-C26
16	d	523	BCR	C23-C24-C25-C30
16	e	4008	BCR	C23-C24-C25-C30
16	e	4011	BCR	C23-C24-C25-C26
16	e	4011	BCR	C23-C24-C25-C30
16	f	4004	BCR	C1-C6-C7-C8
16	f	4004	BCR	C5-C6-C7-C8
16	f	4004	BCR	C23-C24-C25-C26
16	f	4005	BCR	C23-C24-C25-C26
16	f	4017	BCR	C5-C6-C7-C8
16	l	4015	BCR	C23-C24-C25-C26
16	l	4012	BCR	C1-C6-C7-C8
16	l	4012	BCR	C23-C24-C25-C26
16	l	4012	BCR	C23-C24-C25-C30
16	n	4019	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	n	4019	BCR	C23-C24-C25-C30
16	n	4020	BCR	C23-C24-C25-C26
16	o	4021	BCR	C1-C6-C7-C8
16	q	521	BCR	C1-C6-C7-C8
16	q	521	BCR	C5-C6-C7-C8
16	q	521	BCR	C23-C24-C25-C26
16	q	521	BCR	C23-C24-C25-C30
16	q	523	BCR	C1-C6-C7-C8
16	q	523	BCR	C5-C6-C7-C8
16	q	523	BCR	C23-C24-C25-C26
16	q	523	BCR	C23-C24-C25-C30
16	r	521	BCR	C1-C6-C7-C8
16	r	521	BCR	C5-C6-C7-C8
16	r	522	BCR	C1-C6-C7-C8
16	r	523	BCR	C23-C24-C25-C26
16	r	523	BCR	C23-C24-C25-C30
16	r	524	BCR	C23-C24-C25-C26
16	r	524	BCR	C23-C24-C25-C30
16	s	521	BCR	C1-C6-C7-C8
16	s	521	BCR	C5-C6-C7-C8
16	s	521	BCR	C23-C24-C25-C26
16	s	523	BCR	C23-C24-C25-C26
16	s	523	BCR	C23-C24-C25-C30
16	t	521	BCR	C1-C6-C7-C8
16	t	521	BCR	C5-C6-C7-C8
16	t	521	BCR	C23-C24-C25-C26
16	t	521	BCR	C23-C24-C25-C30
16	t	522	BCR	C1-C6-C7-C8
16	t	522	BCR	C5-C6-C7-C8
16	t	523	BCR	C23-C24-C25-C26
16	t	523	BCR	C23-C24-C25-C30
16	t	524	BCR	C23-C24-C25-C26
16	t	524	BCR	C23-C24-C25-C30
16	u	522	BCR	C1-C6-C7-C8
16	u	523	BCR	C23-C24-C25-C26
16	u	523	BCR	C23-C24-C25-C30
16	u	524	BCR	C23-C24-C25-C26
16	u	524	BCR	C23-C24-C25-C30
16	v	521	BCR	C1-C6-C7-C8
16	v	521	BCR	C5-C6-C7-C8
16	v	522	BCR	C1-C6-C7-C8
16	v	523	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	v	523	BCR	C23-C24-C25-C30
13	Z	516	CLA	O1D-CGD-O2D-CED
13	A	1132	CLA	CBA-CGA-O2A-C1
13	3	513	CLA	CBA-CGA-O2A-C1
13	6	502	CLA	CBA-CGA-O2A-C1
13	G	1132	CLA	CBA-CGA-O2A-C1
13	a	513	CLA	CBA-CGA-O2A-C1
13	d	502	CLA	CBA-CGA-O2A-C1
13	e	1132	CLA	CBA-CGA-O2A-C1
13	s	513	CLA	CBA-CGA-O2A-C1
13	v	502	CLA	CBA-CGA-O2A-C1
13	A	1117	CLA	C13-C15-C16-C17
13	A	1133	CLA	C13-C15-C16-C17
13	B	1221	CLA	C5-C6-C7-C8
13	1	501	CLA	C13-C15-C16-C17
13	1	508	CLA	C5-C6-C7-C8
13	2	501	CLA	C10-C11-C12-C13
13	2	513	CLA	C8-C10-C11-C12
13	G	1117	CLA	C13-C15-C16-C17
13	G	1133	CLA	C13-C15-C16-C17
13	H	1221	CLA	C5-C6-C7-C8
13	Y	501	CLA	C13-C15-C16-C17
13	Y	508	CLA	C5-C6-C7-C8
13	Z	501	CLA	C10-C11-C12-C13
13	Z	513	CLA	C8-C10-C11-C12
13	e	1117	CLA	C13-C15-C16-C17
13	e	1133	CLA	C13-C15-C16-C17
13	f	1221	CLA	C5-C6-C7-C8
13	q	501	CLA	C13-C15-C16-C17
13	q	508	CLA	C5-C6-C7-C8
13	r	501	CLA	C10-C11-C12-C13
13	r	513	CLA	C8-C10-C11-C12
19	J	5104	LMG	C31-C32-C33-C34
19	T	5104	LMG	C31-C32-C33-C34
13	B	1215	CLA	CBD-CGD-O2D-CED
13	f	1215	CLA	CBD-CGD-O2D-CED
13	A	1124	CLA	C11-C10-C8-C9
13	G	1124	CLA	C11-C10-C8-C9
13	e	1124	CLA	C11-C10-C8-C9
17	A	5006	LHG	C7-C8-C9-C10
17	G	5006	LHG	C7-C8-C9-C10
17	e	5006	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
19	B	5002	LMG	C28-C29-C30-C31
19	H	5002	LMG	C28-C29-C30-C31
17	e	5009	LHG	C11-C12-C13-C14
19	l	5104	LMG	C31-C32-C33-C34
20	3	822	SQD	C10-C11-C12-C13
20	a	822	SQD	C10-C11-C12-C13
20	s	822	SQD	C10-C11-C12-C13
13	B	1218	CLA	C5-C6-C7-C8
13	1	518	CLA	C10-C11-C12-C13
13	H	1218	CLA	C5-C6-C7-C8
13	H	1219	CLA	C5-C6-C7-C8
13	Y	518	CLA	C10-C11-C12-C13
13	f	1218	CLA	C5-C6-C7-C8
13	q	518	CLA	C10-C11-C12-C13
17	A	5009	LHG	C11-C12-C13-C14
17	G	5009	LHG	C11-C12-C13-C14
20	L	5216	SQD	C15-C16-C17-C18
20	V	5216	SQD	C15-C16-C17-C18
20	n	5216	SQD	C15-C16-C17-C18
13	A	1132	CLA	C4-C3-C5-C6
13	A	1130	CLA	C4-C3-C5-C6
13	L	1501	CLA	C4-C3-C5-C6
13	4	519	CLA	C4-C3-C5-C6
13	G	1132	CLA	C4-C3-C5-C6
13	G	1137	CLA	C4-C3-C5-C6
13	G	1130	CLA	C4-C3-C5-C6
13	V	1501	CLA	C4-C3-C5-C6
13	b	519	CLA	C4-C3-C5-C6
13	e	1132	CLA	C4-C3-C5-C6
13	e	1137	CLA	C4-C3-C5-C6
13	e	1130	CLA	C4-C3-C5-C6
13	n	1501	CLA	C4-C3-C5-C6
13	t	519	CLA	C4-C3-C5-C6
13	5	502	CLA	O1D-CGD-O2D-CED
13	c	502	CLA	O1D-CGD-O2D-CED
13	A	1119	CLA	C6-C7-C8-C10
13	A	1133	CLA	C11-C12-C13-C15
13	A	1138	CLA	C11-C10-C8-C7
13	A	1237	CLA	C12-C13-C15-C16
13	B	1208	CLA	C2-C3-C5-C6
13	B	1213	CLA	C6-C7-C8-C10
13	B	1214	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	B	1217	CLA	C2-C3-C5-C6
13	B	1223	CLA	C12-C13-C15-C16
13	B	1229	CLA	C6-C7-C8-C10
13	B	1231	CLA	C2-C3-C5-C6
13	B	1239	CLA	C6-C7-C8-C10
13	2	501	CLA	C6-C7-C8-C10
13	2	518	CLA	C11-C10-C8-C7
13	5	501	CLA	C11-C12-C13-C15
13	6	501	CLA	C6-C7-C8-C10
13	G	1119	CLA	C6-C7-C8-C10
13	G	1133	CLA	C11-C12-C13-C15
13	G	1138	CLA	C11-C10-C8-C7
13	G	1237	CLA	C12-C13-C15-C16
13	H	1208	CLA	C2-C3-C5-C6
13	H	1213	CLA	C6-C7-C8-C10
13	H	1214	CLA	C12-C13-C15-C16
13	H	1217	CLA	C2-C3-C5-C6
13	H	1223	CLA	C12-C13-C15-C16
13	H	1229	CLA	C6-C7-C8-C10
13	H	1231	CLA	C2-C3-C5-C6
13	H	1239	CLA	C6-C7-C8-C10
13	Z	501	CLA	C6-C7-C8-C10
13	Z	518	CLA	C11-C10-C8-C7
13	c	501	CLA	C11-C12-C13-C15
13	d	501	CLA	C6-C7-C8-C10
13	e	1119	CLA	C6-C7-C8-C10
13	e	1133	CLA	C11-C12-C13-C15
13	e	1138	CLA	C11-C10-C8-C7
13	e	1237	CLA	C12-C13-C15-C16
13	f	1208	CLA	C2-C3-C5-C6
13	f	1213	CLA	C6-C7-C8-C10
13	f	1214	CLA	C12-C13-C15-C16
13	f	1217	CLA	C2-C3-C5-C6
13	f	1223	CLA	C12-C13-C15-C16
13	f	1229	CLA	C6-C7-C8-C10
13	f	1231	CLA	C2-C3-C5-C6
13	f	1239	CLA	C6-C7-C8-C10
13	r	501	CLA	C6-C7-C8-C10
13	r	518	CLA	C11-C10-C8-C7
13	u	501	CLA	C11-C12-C13-C15
13	v	501	CLA	C6-C7-C8-C10
13	A	1124	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	G	1124	CLA	C3-C5-C6-C7
13	e	1124	CLA	C3-C5-C6-C7
13	B	1232	CLA	O1A-CGA-O2A-C1
13	1	512	CLA	O1A-CGA-O2A-C1
13	H	1232	CLA	O1A-CGA-O2A-C1
13	Y	512	CLA	O1A-CGA-O2A-C1
13	f	1232	CLA	O1A-CGA-O2A-C1
13	q	512	CLA	O1A-CGA-O2A-C1
13	v	502	CLA	O1A-CGA-O2A-C1
17	L	5221	LHG	C31-C32-C33-C34
17	V	5221	LHG	C31-C32-C33-C34
17	n	5221	LHG	C31-C32-C33-C34
19	B	5002	LMG	C23-C24-C25-C26
19	H	5002	LMG	C23-C24-C25-C26
19	f	5002	LMG	C23-C24-C25-C26
13	A	1138	CLA	C8-C10-C11-C12
13	B	1216	CLA	C8-C10-C11-C12
13	G	1117	CLA	C8-C10-C11-C12
13	G	1138	CLA	C8-C10-C11-C12
13	H	1216	CLA	C8-C10-C11-C12
13	H	1207	CLA	C10-C11-C12-C13
13	e	1138	CLA	C8-C10-C11-C12
13	f	1216	CLA	C8-C10-C11-C12
16	B	4010	BCR	C9-C10-C11-C12
16	2	522	BCR	C9-C10-C11-C12
16	H	4010	BCR	C9-C10-C11-C12
16	Z	522	BCR	C9-C10-C11-C12
16	f	4010	BCR	C9-C10-C11-C12
16	r	522	BCR	C9-C10-C11-C12
13	H	1215	CLA	CBD-CGD-O2D-CED
13	u	502	CLA	O1D-CGD-O2D-CED
19	f	5002	LMG	C28-C29-C30-C31
13	A	1105	CLA	CBA-CGA-O2A-C1
13	A	1116	CLA	CBA-CGA-O2A-C1
13	B	1201	CLA	CBA-CGA-O2A-C1
13	L	1502	CLA	CBA-CGA-O2A-C1
13	3	507	CLA	CBA-CGA-O2A-C1
13	G	1105	CLA	CBA-CGA-O2A-C1
13	G	1116	CLA	CBA-CGA-O2A-C1
13	H	1201	CLA	CBA-CGA-O2A-C1
13	V	1502	CLA	CBA-CGA-O2A-C1
13	a	507	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	e	1105	CLA	CBA-CGA-O2A-C1
13	e	1116	CLA	CBA-CGA-O2A-C1
13	f	1201	CLA	CBA-CGA-O2A-C1
13	n	1502	CLA	CBA-CGA-O2A-C1
13	s	507	CLA	CBA-CGA-O2A-C1
17	A	5003	LHG	C24-C23-O8-C6
17	G	5003	LHG	C24-C23-O8-C6
17	e	5003	LHG	C24-C23-O8-C6
17	A	5009	LHG	C27-C28-C29-C30
17	G	5009	LHG	C27-C28-C29-C30
17	e	5009	LHG	C27-C28-C29-C30
13	A	1135	CLA	C2A-CAA-CBA-CGA
13	B	1023	CLA	C2A-CAA-CBA-CGA
13	1	501	CLA	C2A-CAA-CBA-CGA
13	3	501	CLA	C2A-CAA-CBA-CGA
13	4	501	CLA	C2A-CAA-CBA-CGA
13	6	518	CLA	C2A-CAA-CBA-CGA
13	G	1135	CLA	C2A-CAA-CBA-CGA
13	H	1023	CLA	C2A-CAA-CBA-CGA
13	Y	501	CLA	C2A-CAA-CBA-CGA
13	a	501	CLA	C2A-CAA-CBA-CGA
13	b	501	CLA	C2A-CAA-CBA-CGA
13	d	518	CLA	C2A-CAA-CBA-CGA
13	e	1135	CLA	C2A-CAA-CBA-CGA
13	f	1023	CLA	C2A-CAA-CBA-CGA
13	q	501	CLA	C2A-CAA-CBA-CGA
13	s	501	CLA	C2A-CAA-CBA-CGA
13	t	501	CLA	C2A-CAA-CBA-CGA
13	v	518	CLA	C2A-CAA-CBA-CGA
13	s	507	CLA	O1D-CGD-O2D-CED
13	A	1117	CLA	C8-C10-C11-C12
13	A	1136	CLA	C10-C11-C12-C13
13	A	1137	CLA	C8-C10-C11-C12
13	B	1202	CLA	C13-C15-C16-C17
13	B	1210	CLA	C13-C15-C16-C17
13	B	1207	CLA	C10-C11-C12-C13
13	G	1136	CLA	C10-C11-C12-C13
13	G	1137	CLA	C8-C10-C11-C12
13	H	1202	CLA	C13-C15-C16-C17
13	H	1210	CLA	C13-C15-C16-C17
13	e	1117	CLA	C8-C10-C11-C12
13	e	1136	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	e	1137	CLA	C8-C10-C11-C12
13	f	1202	CLA	C13-C15-C16-C17
13	f	1207	CLA	C10-C11-C12-C13
17	A	5005	LHG	C16-C17-C18-C19
17	G	5005	LHG	C16-C17-C18-C19
17	V	5220	LHG	C29-C30-C31-C32
17	V	5221	LHG	C14-C15-C16-C17
17	e	5005	LHG	C16-C17-C18-C19
17	n	5220	LHG	C29-C30-C31-C32
20	2	822	SQD	C16-C17-C18-C19
20	r	822	SQD	C16-C17-C18-C19
13	d	502	CLA	O1A-CGA-O2A-C1
13	3	507	CLA	O1D-CGD-O2D-CED
13	a	507	CLA	O1D-CGD-O2D-CED
17	L	5220	LHG	C29-C30-C31-C32
17	L	5221	LHG	C14-C15-C16-C17
17	n	5221	LHG	C14-C15-C16-C17
20	1	822	SQD	C10-C11-C12-C13
20	Y	822	SQD	C10-C11-C12-C13
20	Z	822	SQD	C16-C17-C18-C19
20	q	822	SQD	C10-C11-C12-C13
13	A	1124	CLA	C11-C10-C8-C7
13	G	1124	CLA	C11-C10-C8-C7
13	e	1124	CLA	C11-C10-C8-C7
13	f	1210	CLA	C13-C15-C16-C17
13	B	1239	CLA	C4C-C3C-CAC-CBC
19	B	5002	LMG	C37-C38-C39-C40
19	H	5002	LMG	C37-C38-C39-C40
19	f	5002	LMG	C37-C38-C39-C40
13	H	1239	CLA	C4C-C3C-CAC-CBC
13	f	1239	CLA	C4C-C3C-CAC-CBC
20	f	1852	SQD	C25-C26-C27-C28
13	6	502	CLA	O1A-CGA-O2A-C1
13	A	1103	CLA	C16-C17-C18-C20
13	A	1121	CLA	C6-C7-C8-C9
13	5	518	CLA	C6-C7-C8-C10
13	G	1103	CLA	C16-C17-C18-C20
13	G	1121	CLA	C6-C7-C8-C9
13	c	518	CLA	C6-C7-C8-C10
13	e	1103	CLA	C16-C17-C18-C20
13	e	1121	CLA	C6-C7-C8-C9
13	u	518	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	B	1852	SQD	O5-C1-O6-C44
20	H	1852	SQD	O5-C1-O6-C44
20	f	1852	SQD	O5-C1-O6-C44
13	A	1134	CLA	O1D-CGD-O2D-CED
13	B	1230	CLA	O1D-CGD-O2D-CED
13	G	1134	CLA	O1D-CGD-O2D-CED
13	H	1230	CLA	O1D-CGD-O2D-CED
13	e	1126	CLA	O1D-CGD-O2D-CED
13	e	1134	CLA	O1D-CGD-O2D-CED
13	f	1230	CLA	O1D-CGD-O2D-CED
17	A	5003	LHG	C9-C10-C11-C12
17	G	5003	LHG	C9-C10-C11-C12
17	e	5003	LHG	C9-C10-C11-C12
20	B	1852	SQD	C25-C26-C27-C28
20	H	1852	SQD	C25-C26-C27-C28
17	A	5005	LHG	C8-C7-O7-C5
17	A	5001	LHG	C8-C7-O7-C5
17	G	5005	LHG	C8-C7-O7-C5
17	G	5001	LHG	C8-C7-O7-C5
17	e	5005	LHG	C8-C7-O7-C5
17	e	5001	LHG	C8-C7-O7-C5
20	a	822	SQD	C26-C27-C28-C29
20	s	822	SQD	C26-C27-C28-C29
13	A	1125	CLA	C13-C15-C16-C17
13	2	509	CLA	C5-C6-C7-C8
13	G	1125	CLA	C13-C15-C16-C17
13	Z	509	CLA	C5-C6-C7-C8
13	e	1125	CLA	C13-C15-C16-C17
13	r	509	CLA	C5-C6-C7-C8
13	5	518	CLA	CBD-CGD-O2D-CED
13	c	518	CLA	CBD-CGD-O2D-CED
13	u	518	CLA	CBD-CGD-O2D-CED
17	A	5007	LHG	C30-C31-C32-C33
17	e	5007	LHG	C30-C31-C32-C33
20	3	822	SQD	C26-C27-C28-C29
17	A	5006	LHG	O9-C7-O7-C5
17	G	5006	LHG	O9-C7-O7-C5
17	e	5006	LHG	O9-C7-O7-C5
17	G	5007	LHG	C30-C31-C32-C33
17	H	1842	LHG	C29-C30-C31-C32
17	A	5001	LHG	O7-C5-C6-O8
17	I	5001	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
17	G	5001	LHG	O7-C5-C6-O8
17	S	5001	LHG	O7-C5-C6-O8
17	e	5001	LHG	O7-C5-C6-O8
17	k	5001	LHG	O7-C5-C6-O8
19	B	5002	LMG	O7-C8-C9-O8
19	J	5104	LMG	O1-C7-C8-O7
19	H	5002	LMG	O7-C8-C9-O8
19	T	5104	LMG	O1-C7-C8-O7
19	f	5002	LMG	O7-C8-C9-O8
19	l	5104	LMG	O1-C7-C8-O7
20	1	822	SQD	O47-C45-C46-O48
20	Y	822	SQD	O47-C45-C46-O48
20	q	822	SQD	O47-C45-C46-O48
13	B	1220	CLA	CBA-CGA-O2A-C1
13	1	518	CLA	CBA-CGA-O2A-C1
13	Y	518	CLA	CBA-CGA-O2A-C1
13	f	1220	CLA	CBA-CGA-O2A-C1
17	B	1842	LHG	C29-C30-C31-C32
17	G	5009	LHG	C28-C29-C30-C31
17	f	1842	LHG	C29-C30-C31-C32
13	A	1126	CLA	O1D-CGD-O2D-CED
13	e	1128	CLA	O1D-CGD-O2D-CED
13	3	513	CLA	O1A-CGA-O2A-C1
13	s	513	CLA	O1A-CGA-O2A-C1
13	B	1239	CLA	C16-C17-C18-C19
13	H	1239	CLA	C16-C17-C18-C19
13	f	1239	CLA	C16-C17-C18-C19
17	A	5009	LHG	C28-C29-C30-C31
17	e	5009	LHG	C28-C29-C30-C31
13	B	1222	CLA	C5-C6-C7-C8
13	H	1222	CLA	C5-C6-C7-C8
13	f	1222	CLA	C5-C6-C7-C8
13	A	1137	CLA	C4-C3-C5-C6
13	B	1227	CLA	C4-C3-C5-C6
13	H	1227	CLA	C4-C3-C5-C6
13	f	1227	CLA	C4-C3-C5-C6
14	A	2001	PQN	C14-C13-C15-C16
14	G	2001	PQN	C14-C13-C15-C16
14	e	2001	PQN	C14-C13-C15-C16
13	A	1117	CLA	C2-C3-C5-C6
13	A	1132	CLA	C2-C3-C5-C6
13	G	1117	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	G	1132	CLA	C2-C3-C5-C6
13	e	1117	CLA	C2-C3-C5-C6
13	e	1132	CLA	C2-C3-C5-C6
13	A	1102	CLA	C14-C13-C15-C16
13	A	1103	CLA	C11-C10-C8-C9
13	A	1103	CLA	C14-C13-C15-C16
13	A	1127	CLA	C14-C13-C15-C16
13	A	1138	CLA	C11-C10-C8-C9
13	A	1101	CLA	C11-C10-C8-C9
13	B	1214	CLA	C14-C13-C15-C16
13	B	1221	CLA	C11-C10-C8-C9
13	B	1223	CLA	C14-C13-C15-C16
13	B	1231	CLA	C6-C7-C8-C9
13	B	1239	CLA	C6-C7-C8-C9
13	F	1301	CLA	C14-C13-C15-C16
13	L	1501	CLA	C6-C7-C8-C9
13	2	501	CLA	C6-C7-C8-C9
13	2	518	CLA	C11-C10-C8-C9
13	3	513	CLA	C6-C7-C8-C9
13	5	501	CLA	C6-C7-C8-C9
13	5	501	CLA	C11-C12-C13-C14
13	5	509	CLA	C11-C10-C8-C9
13	G	1102	CLA	C14-C13-C15-C16
13	G	1103	CLA	C11-C10-C8-C9
13	G	1103	CLA	C14-C13-C15-C16
13	G	1127	CLA	C14-C13-C15-C16
13	G	1138	CLA	C11-C10-C8-C9
13	G	1101	CLA	C11-C10-C8-C9
13	H	1214	CLA	C14-C13-C15-C16
13	H	1221	CLA	C11-C10-C8-C9
13	H	1223	CLA	C14-C13-C15-C16
13	H	1231	CLA	C6-C7-C8-C9
13	H	1239	CLA	C6-C7-C8-C9
13	R	1301	CLA	C14-C13-C15-C16
13	V	1501	CLA	C6-C7-C8-C9
13	Z	501	CLA	C6-C7-C8-C9
13	Z	518	CLA	C11-C10-C8-C9
13	a	513	CLA	C6-C7-C8-C9
13	c	501	CLA	C6-C7-C8-C9
13	c	501	CLA	C11-C12-C13-C14
13	c	509	CLA	C11-C10-C8-C9
13	e	1102	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	e	1103	CLA	C11-C10-C8-C9
13	e	1103	CLA	C14-C13-C15-C16
13	e	1127	CLA	C14-C13-C15-C16
13	e	1138	CLA	C11-C10-C8-C9
13	e	1101	CLA	C11-C10-C8-C9
13	f	1214	CLA	C14-C13-C15-C16
13	f	1221	CLA	C11-C10-C8-C9
13	f	1223	CLA	C14-C13-C15-C16
13	f	1231	CLA	C6-C7-C8-C9
13	f	1239	CLA	C6-C7-C8-C9
13	j	1301	CLA	C14-C13-C15-C16
13	n	1501	CLA	C6-C7-C8-C9
13	r	501	CLA	C6-C7-C8-C9
13	r	518	CLA	C11-C10-C8-C9
13	s	513	CLA	C6-C7-C8-C9
13	u	501	CLA	C6-C7-C8-C9
13	u	501	CLA	C11-C12-C13-C14
13	u	509	CLA	C11-C10-C8-C9
13	A	1128	CLA	O1D-CGD-O2D-CED
13	G	1126	CLA	O1D-CGD-O2D-CED
13	G	1128	CLA	O1D-CGD-O2D-CED
13	Z	508	CLA	CBD-CGD-O2D-CED
17	A	5001	LHG	C10-C11-C12-C13
17	G	5001	LHG	C10-C11-C12-C13
17	e	5001	LHG	C10-C11-C12-C13
13	B	1213	CLA	C3-C5-C6-C7
13	H	1213	CLA	C3-C5-C6-C7
13	f	1213	CLA	C3-C5-C6-C7
13	A	1118	CLA	C2A-CAA-CBA-CGA
13	A	1121	CLA	C2A-CAA-CBA-CGA
13	L	1501	CLA	C2A-CAA-CBA-CGA
13	1	512	CLA	C2A-CAA-CBA-CGA
13	5	501	CLA	C2A-CAA-CBA-CGA
13	5	503	CLA	C2A-CAA-CBA-CGA
13	5	517	CLA	C2A-CAA-CBA-CGA
13	G	1118	CLA	C2A-CAA-CBA-CGA
13	G	1121	CLA	C2A-CAA-CBA-CGA
13	V	1501	CLA	C2A-CAA-CBA-CGA
13	Y	512	CLA	C2A-CAA-CBA-CGA
13	c	501	CLA	C2A-CAA-CBA-CGA
13	c	503	CLA	C2A-CAA-CBA-CGA
13	c	517	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	e	1118	CLA	C2A-CAA-CBA-CGA
13	e	1121	CLA	C2A-CAA-CBA-CGA
13	n	1501	CLA	C2A-CAA-CBA-CGA
13	q	512	CLA	C2A-CAA-CBA-CGA
13	u	501	CLA	C2A-CAA-CBA-CGA
13	u	503	CLA	C2A-CAA-CBA-CGA
13	u	517	CLA	C2A-CAA-CBA-CGA
17	A	5005	LHG	C31-C32-C33-C34
17	G	5005	LHG	C31-C32-C33-C34
17	e	5005	LHG	C31-C32-C33-C34
13	H	1220	CLA	CBA-CGA-O2A-C1
13	q	518	CLA	CBA-CGA-O2A-C1
20	5	822	SQD	C24-C23-O48-C46
20	u	822	SQD	C24-C23-O48-C46
16	3	524	BCR	C37-C22-C23-C24
16	T	4015	BCR	C7-C8-C9-C34
16	a	524	BCR	C37-C22-C23-C24
16	s	524	BCR	C37-C22-C23-C24
13	A	1131	CLA	C13-C15-C16-C17
13	B	1203	CLA	C13-C15-C16-C17
13	G	1125	CLA	C8-C10-C11-C12
13	G	1131	CLA	C13-C15-C16-C17
13	H	1203	CLA	C13-C15-C16-C17
13	e	1131	CLA	C13-C15-C16-C17
13	f	1203	CLA	C13-C15-C16-C17
13	2	508	CLA	CBD-CGD-O2D-CED
17	A	5006	LHG	C24-C25-C26-C27
17	G	5006	LHG	C24-C25-C26-C27
17	e	5006	LHG	C24-C25-C26-C27
18	B	1843	LMU	C7-C8-C9-C10
18	H	1843	LMU	C7-C8-C9-C10
18	f	1843	LMU	C7-C8-C9-C10
16	A	4001	BCR	C21-C22-C23-C24
16	G	4001	BCR	C21-C22-C23-C24
16	e	4001	BCR	C21-C22-C23-C24
13	A	1132	CLA	O1A-CGA-O2A-C1
13	1	508	CLA	O1A-CGA-O2A-C1
13	G	1132	CLA	O1A-CGA-O2A-C1
13	Y	508	CLA	O1A-CGA-O2A-C1
13	a	513	CLA	O1A-CGA-O2A-C1
13	e	1132	CLA	O1A-CGA-O2A-C1
13	q	508	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	1102	CLA	C1A-C2A-CAA-CBA
13	A	1106	CLA	C1A-C2A-CAA-CBA
13	A	1107	CLA	C1A-C2A-CAA-CBA
13	A	1113	CLA	C1A-C2A-CAA-CBA
13	A	1116	CLA	C1A-C2A-CAA-CBA
13	A	1118	CLA	C1A-C2A-CAA-CBA
13	A	1120	CLA	C1A-C2A-CAA-CBA
13	A	1122	CLA	C1A-C2A-CAA-CBA
13	A	1125	CLA	C1A-C2A-CAA-CBA
13	A	1128	CLA	C1A-C2A-CAA-CBA
13	A	1132	CLA	C1A-C2A-CAA-CBA
13	A	1135	CLA	C1A-C2A-CAA-CBA
13	A	1101	CLA	C1A-C2A-CAA-CBA
13	A	1130	CLA	C1A-C2A-CAA-CBA
13	B	1219	CLA	C1A-C2A-CAA-CBA
13	B	1225	CLA	C1A-C2A-CAA-CBA
13	B	1226	CLA	C1A-C2A-CAA-CBA
13	B	1227	CLA	C1A-C2A-CAA-CBA
13	B	1236	CLA	C1A-C2A-CAA-CBA
13	B	1239	CLA	C1A-C2A-CAA-CBA
13	K	1103	CLA	C1A-C2A-CAA-CBA
13	K	1105	CLA	C1A-C2A-CAA-CBA
13	L	1501	CLA	C1A-C2A-CAA-CBA
13	1	501	CLA	C1A-C2A-CAA-CBA
13	1	505	CLA	C1A-C2A-CAA-CBA
13	1	519	CLA	C1A-C2A-CAA-CBA
13	2	501	CLA	C1A-C2A-CAA-CBA
13	2	505	CLA	C1A-C2A-CAA-CBA
13	2	508	CLA	C1A-C2A-CAA-CBA
13	2	516	CLA	C1A-C2A-CAA-CBA
13	2	518	CLA	C1A-C2A-CAA-CBA
13	3	503	CLA	C1A-C2A-CAA-CBA
13	3	517	CLA	C1A-C2A-CAA-CBA
13	4	511	CLA	C1A-C2A-CAA-CBA
13	4	516	CLA	C1A-C2A-CAA-CBA
13	4	518	CLA	C1A-C2A-CAA-CBA
13	5	501	CLA	C1A-C2A-CAA-CBA
13	5	516	CLA	C1A-C2A-CAA-CBA
13	5	518	CLA	C1A-C2A-CAA-CBA
13	6	501	CLA	C1A-C2A-CAA-CBA
13	6	505	CLA	C1A-C2A-CAA-CBA
13	6	508	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	6	512	CLA	C1A-C2A-CAA-CBA
13	6	516	CLA	C1A-C2A-CAA-CBA
13	6	517	CLA	C1A-C2A-CAA-CBA
13	6	518	CLA	C1A-C2A-CAA-CBA
13	6	519	CLA	C1A-C2A-CAA-CBA
13	G	1102	CLA	C1A-C2A-CAA-CBA
13	G	1106	CLA	C1A-C2A-CAA-CBA
13	G	1107	CLA	C1A-C2A-CAA-CBA
13	G	1113	CLA	C1A-C2A-CAA-CBA
13	G	1116	CLA	C1A-C2A-CAA-CBA
13	G	1118	CLA	C1A-C2A-CAA-CBA
13	G	1120	CLA	C1A-C2A-CAA-CBA
13	G	1122	CLA	C1A-C2A-CAA-CBA
13	G	1125	CLA	C1A-C2A-CAA-CBA
13	G	1128	CLA	C1A-C2A-CAA-CBA
13	G	1132	CLA	C1A-C2A-CAA-CBA
13	G	1135	CLA	C1A-C2A-CAA-CBA
13	G	1101	CLA	C1A-C2A-CAA-CBA
13	G	1130	CLA	C1A-C2A-CAA-CBA
13	H	1219	CLA	C1A-C2A-CAA-CBA
13	H	1225	CLA	C1A-C2A-CAA-CBA
13	H	1226	CLA	C1A-C2A-CAA-CBA
13	H	1227	CLA	C1A-C2A-CAA-CBA
13	H	1236	CLA	C1A-C2A-CAA-CBA
13	H	1239	CLA	C1A-C2A-CAA-CBA
13	U	1103	CLA	C1A-C2A-CAA-CBA
13	U	1105	CLA	C1A-C2A-CAA-CBA
13	V	1501	CLA	C1A-C2A-CAA-CBA
13	Y	501	CLA	C1A-C2A-CAA-CBA
13	Y	505	CLA	C1A-C2A-CAA-CBA
13	Y	519	CLA	C1A-C2A-CAA-CBA
13	Z	501	CLA	C1A-C2A-CAA-CBA
13	Z	505	CLA	C1A-C2A-CAA-CBA
13	Z	508	CLA	C1A-C2A-CAA-CBA
13	Z	516	CLA	C1A-C2A-CAA-CBA
13	Z	518	CLA	C1A-C2A-CAA-CBA
13	a	503	CLA	C1A-C2A-CAA-CBA
13	a	517	CLA	C1A-C2A-CAA-CBA
13	b	511	CLA	C1A-C2A-CAA-CBA
13	b	516	CLA	C1A-C2A-CAA-CBA
13	b	518	CLA	C1A-C2A-CAA-CBA
13	c	501	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	c	516	CLA	C1A-C2A-CAA-CBA
13	c	518	CLA	C1A-C2A-CAA-CBA
13	d	501	CLA	C1A-C2A-CAA-CBA
13	d	505	CLA	C1A-C2A-CAA-CBA
13	d	508	CLA	C1A-C2A-CAA-CBA
13	d	512	CLA	C1A-C2A-CAA-CBA
13	d	516	CLA	C1A-C2A-CAA-CBA
13	d	517	CLA	C1A-C2A-CAA-CBA
13	d	518	CLA	C1A-C2A-CAA-CBA
13	d	519	CLA	C1A-C2A-CAA-CBA
13	e	1102	CLA	C1A-C2A-CAA-CBA
13	e	1106	CLA	C1A-C2A-CAA-CBA
13	e	1107	CLA	C1A-C2A-CAA-CBA
13	e	1113	CLA	C1A-C2A-CAA-CBA
13	e	1116	CLA	C1A-C2A-CAA-CBA
13	e	1118	CLA	C1A-C2A-CAA-CBA
13	e	1120	CLA	C1A-C2A-CAA-CBA
13	e	1122	CLA	C1A-C2A-CAA-CBA
13	e	1125	CLA	C1A-C2A-CAA-CBA
13	e	1128	CLA	C1A-C2A-CAA-CBA
13	e	1132	CLA	C1A-C2A-CAA-CBA
13	e	1135	CLA	C1A-C2A-CAA-CBA
13	e	1101	CLA	C1A-C2A-CAA-CBA
13	e	1130	CLA	C1A-C2A-CAA-CBA
13	f	1219	CLA	C1A-C2A-CAA-CBA
13	f	1225	CLA	C1A-C2A-CAA-CBA
13	f	1226	CLA	C1A-C2A-CAA-CBA
13	f	1227	CLA	C1A-C2A-CAA-CBA
13	f	1236	CLA	C1A-C2A-CAA-CBA
13	f	1239	CLA	C1A-C2A-CAA-CBA
13	m	1103	CLA	C1A-C2A-CAA-CBA
13	m	1105	CLA	C1A-C2A-CAA-CBA
13	n	1501	CLA	C1A-C2A-CAA-CBA
13	q	501	CLA	C1A-C2A-CAA-CBA
13	q	505	CLA	C1A-C2A-CAA-CBA
13	q	519	CLA	C1A-C2A-CAA-CBA
13	r	501	CLA	C1A-C2A-CAA-CBA
13	r	505	CLA	C1A-C2A-CAA-CBA
13	r	508	CLA	C1A-C2A-CAA-CBA
13	r	516	CLA	C1A-C2A-CAA-CBA
13	r	518	CLA	C1A-C2A-CAA-CBA
13	s	503	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	s	517	CLA	C1A-C2A-CAA-CBA
13	t	511	CLA	C1A-C2A-CAA-CBA
13	t	516	CLA	C1A-C2A-CAA-CBA
13	t	518	CLA	C1A-C2A-CAA-CBA
13	u	501	CLA	C1A-C2A-CAA-CBA
13	u	516	CLA	C1A-C2A-CAA-CBA
13	u	518	CLA	C1A-C2A-CAA-CBA
13	v	501	CLA	C1A-C2A-CAA-CBA
13	v	505	CLA	C1A-C2A-CAA-CBA
13	v	508	CLA	C1A-C2A-CAA-CBA
13	v	512	CLA	C1A-C2A-CAA-CBA
13	v	516	CLA	C1A-C2A-CAA-CBA
13	v	517	CLA	C1A-C2A-CAA-CBA
13	v	518	CLA	C1A-C2A-CAA-CBA
13	v	519	CLA	C1A-C2A-CAA-CBA
13	A	1116	CLA	C11-C12-C13-C14
13	A	1121	CLA	C6-C7-C8-C10
13	A	1127	CLA	C16-C17-C18-C20
13	A	1136	CLA	C11-C12-C13-C15
13	A	1101	CLA	C16-C17-C18-C20
13	B	1219	CLA	C16-C17-C18-C20
13	B	1222	CLA	C11-C12-C13-C14
13	L	1502	CLA	C16-C17-C18-C19
13	1	502	CLA	C11-C12-C13-C14
13	2	508	CLA	C6-C7-C8-C9
13	5	518	CLA	C6-C7-C8-C9
13	G	1116	CLA	C11-C12-C13-C14
13	G	1121	CLA	C6-C7-C8-C10
13	G	1127	CLA	C16-C17-C18-C20
13	G	1136	CLA	C11-C12-C13-C15
13	G	1101	CLA	C16-C17-C18-C20
13	H	1219	CLA	C16-C17-C18-C20
13	H	1222	CLA	C11-C12-C13-C14
13	V	1502	CLA	C16-C17-C18-C19
13	Y	502	CLA	C11-C12-C13-C14
13	Z	508	CLA	C6-C7-C8-C9
13	c	518	CLA	C6-C7-C8-C9
13	d	501	CLA	C11-C12-C13-C15
13	e	1116	CLA	C11-C12-C13-C14
13	e	1121	CLA	C6-C7-C8-C10
13	e	1127	CLA	C16-C17-C18-C20
13	e	1136	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	e	1101	CLA	C16-C17-C18-C20
13	f	1219	CLA	C16-C17-C18-C20
13	f	1222	CLA	C11-C12-C13-C14
13	n	1502	CLA	C16-C17-C18-C19
13	q	502	CLA	C11-C12-C13-C14
13	r	508	CLA	C6-C7-C8-C9
13	u	518	CLA	C6-C7-C8-C9
14	B	2002	PQN	C26-C27-C28-C29
14	H	2002	PQN	C26-C27-C28-C29
14	f	2002	PQN	C26-C27-C28-C29
17	A	5005	LHG	O9-C7-O7-C5
17	G	5005	LHG	O9-C7-O7-C5
17	e	5005	LHG	O9-C7-O7-C5
20	3	822	SQD	C12-C13-C14-C15
20	a	822	SQD	C12-C13-C14-C15
20	s	822	SQD	C12-C13-C14-C15
16	1	522	BCR	C9-C10-C11-C12
16	Y	522	BCR	C9-C10-C11-C12
16	q	522	BCR	C9-C10-C11-C12
13	2	510	CLA	O1D-CGD-O2D-CED
13	Z	510	CLA	O1D-CGD-O2D-CED
13	A	1125	CLA	C8-C10-C11-C12
13	B	1223	CLA	C10-C11-C12-C13
13	B	1224	CLA	C10-C11-C12-C13
13	3	505	CLA	C15-C16-C17-C18
13	H	1223	CLA	C10-C11-C12-C13
13	H	1224	CLA	C10-C11-C12-C13
13	a	505	CLA	C15-C16-C17-C18
13	e	1125	CLA	C8-C10-C11-C12
13	f	1223	CLA	C10-C11-C12-C13
13	f	1224	CLA	C10-C11-C12-C13
13	s	505	CLA	C15-C16-C17-C18
17	A	5008	LHG	C25-C26-C27-C28
17	G	5008	LHG	C25-C26-C27-C28
17	e	5008	LHG	C25-C26-C27-C28
20	B	1852	SQD	C7-C8-C9-C10
20	H	1852	SQD	C7-C8-C9-C10
20	f	1852	SQD	C7-C8-C9-C10
13	r	508	CLA	CBD-CGD-O2D-CED
13	r	510	CLA	O1D-CGD-O2D-CED
14	A	2001	PQN	C25-C26-C27-C28
14	G	2001	PQN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
14	e	2001	PQN	C25-C26-C27-C28
20	c	822	SQD	C24-C23-O48-C46
17	A	5005	LHG	O6-C4-C5-C6
17	G	5005	LHG	O6-C4-C5-C6
17	e	5005	LHG	O6-C4-C5-C6
17	A	5008	LHG	C12-C13-C14-C15
17	G	5008	LHG	C12-C13-C14-C15
17	e	5008	LHG	C12-C13-C14-C15
13	4	509	CLA	O1D-CGD-O2D-CED
13	b	509	CLA	O1D-CGD-O2D-CED
13	t	509	CLA	O1D-CGD-O2D-CED
13	6	501	CLA	C11-C12-C13-C15
13	v	501	CLA	C11-C12-C13-C15
20	1	822	SQD	C25-C26-C27-C28
20	Y	822	SQD	C25-C26-C27-C28
20	q	822	SQD	C25-C26-C27-C28
17	A	5004	LHG	C26-C27-C28-C29
17	G	5004	LHG	C26-C27-C28-C29
13	3	511	CLA	CBA-CGA-O2A-C1
13	a	511	CLA	CBA-CGA-O2A-C1
13	s	511	CLA	CBA-CGA-O2A-C1
17	I	5001	LHG	C1-C2-C3-O3
17	S	5001	LHG	C1-C2-C3-O3
17	k	5001	LHG	C1-C2-C3-O3
13	A	1108	CLA	C4-C3-C5-C6
13	B	1231	CLA	C4-C3-C5-C6
13	J	1303	CLA	C4-C3-C5-C6
13	G	1108	CLA	C4-C3-C5-C6
13	H	1231	CLA	C4-C3-C5-C6
13	T	1303	CLA	C4-C3-C5-C6
13	e	1108	CLA	C4-C3-C5-C6
13	f	1231	CLA	C4-C3-C5-C6
13	l	1303	CLA	C4-C3-C5-C6
17	A	5006	LHG	C16-C17-C18-C19
17	G	5006	LHG	C16-C17-C18-C19
17	e	5004	LHG	C26-C27-C28-C29
17	e	5006	LHG	C16-C17-C18-C19
13	A	1105	CLA	O1A-CGA-O2A-C1
13	3	507	CLA	O1A-CGA-O2A-C1
13	G	1105	CLA	O1A-CGA-O2A-C1
13	G	1116	CLA	O1A-CGA-O2A-C1
13	a	507	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	e	1105	CLA	O1A-CGA-O2A-C1
13	e	1116	CLA	O1A-CGA-O2A-C1
13	s	507	CLA	O1A-CGA-O2A-C1
19	B	5002	LMG	O10-C28-O8-C9
19	f	5002	LMG	O10-C28-O8-C9
17	B	1855	LHG	C27-C28-C29-C30
17	H	1855	LHG	C27-C28-C29-C30
17	f	1855	LHG	C27-C28-C29-C30
13	A	1127	CLA	C16-C17-C18-C19
13	1	505	CLA	C16-C17-C18-C19
13	G	1127	CLA	C16-C17-C18-C19
13	Y	505	CLA	C16-C17-C18-C19
13	e	1127	CLA	C16-C17-C18-C19
13	q	505	CLA	C16-C17-C18-C19
17	A	5002	LHG	C4-C5-C6-O8
17	A	5004	LHG	C4-C5-C6-O8
17	A	5005	LHG	C11-C10-C9-C8
17	A	5001	LHG	C4-C5-C6-O8
17	L	5218	LHG	C4-C5-C6-O8
17	G	5002	LHG	C4-C5-C6-O8
17	G	5004	LHG	C4-C5-C6-O8
17	G	5005	LHG	C11-C10-C9-C8
17	G	5001	LHG	C4-C5-C6-O8
17	V	5218	LHG	C4-C5-C6-O8
17	e	5002	LHG	C4-C5-C6-O8
17	e	5004	LHG	C4-C5-C6-O8
17	e	5005	LHG	C11-C10-C9-C8
17	e	5001	LHG	C4-C5-C6-O8
17	f	1855	LHG	C19-C20-C21-C22
17	n	5218	LHG	C4-C5-C6-O8
20	1	822	SQD	C44-C45-C46-O48
20	Y	822	SQD	C44-C45-C46-O48
20	q	822	SQD	C44-C45-C46-O48
17	B	1855	LHG	C19-C20-C21-C22
17	I	5001	LHG	C31-C32-C33-C34
17	H	1855	LHG	C19-C20-C21-C22
17	S	5001	LHG	C31-C32-C33-C34
17	k	5001	LHG	C31-C32-C33-C34
13	A	1116	CLA	O1A-CGA-O2A-C1
19	H	5002	LMG	O10-C28-O8-C9
13	A	1108	CLA	C5-C6-C7-C8
13	2	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	Z	502	CLA	O1D-CGD-O2D-CED
13	e	1124	CLA	O1D-CGD-O2D-CED
13	5	501	CLA	C8-C10-C11-C12
13	c	501	CLA	C8-C10-C11-C12
13	u	501	CLA	C8-C10-C11-C12
13	G	1108	CLA	C5-C6-C7-C8
13	e	1108	CLA	C5-C6-C7-C8
13	A	1124	CLA	O1D-CGD-O2D-CED
13	3	505	CLA	O1D-CGD-O2D-CED
13	G	1124	CLA	O1D-CGD-O2D-CED
13	r	502	CLA	O1D-CGD-O2D-CED
13	s	505	CLA	O1D-CGD-O2D-CED
13	f	1201	CLA	O1A-CGA-O2A-C1
17	B	1855	LHG	C30-C31-C32-C33
17	H	1855	LHG	C30-C31-C32-C33
17	f	1855	LHG	C30-C31-C32-C33
17	e	5005	LHG	C25-C26-C27-C28
17	A	5006	LHG	O1-C1-C2-O2
17	G	5006	LHG	O1-C1-C2-O2
17	e	5006	LHG	O1-C1-C2-O2
17	A	5005	LHG	C25-C26-C27-C28
17	G	5005	LHG	C25-C26-C27-C28
13	B	1201	CLA	O1A-CGA-O2A-C1
13	H	1201	CLA	O1A-CGA-O2A-C1
17	G	5001	LHG	C9-C10-C11-C12
17	A	5004	LHG	C9-C10-C11-C12
17	A	5001	LHG	C9-C10-C11-C12
17	e	5004	LHG	C9-C10-C11-C12
17	e	5001	LHG	C9-C10-C11-C12
13	a	505	CLA	O1D-CGD-O2D-CED
13	B	1204	CLA	C13-C15-C16-C17
13	B	1215	CLA	C13-C15-C16-C17
13	F	1301	CLA	C15-C16-C17-C18
13	6	505	CLA	C13-C15-C16-C17
13	H	1204	CLA	C13-C15-C16-C17
13	H	1215	CLA	C13-C15-C16-C17
13	d	505	CLA	C13-C15-C16-C17
13	e	1126	CLA	C13-C15-C16-C17
13	f	1204	CLA	C13-C15-C16-C17
13	f	1215	CLA	C13-C15-C16-C17
13	j	1301	CLA	C15-C16-C17-C18
13	v	505	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	A	1102	CLA	C4-C3-C5-C6
13	A	1119	CLA	C4-C3-C5-C6
13	G	1102	CLA	C4-C3-C5-C6
13	G	1119	CLA	C4-C3-C5-C6
13	e	1102	CLA	C4-C3-C5-C6
13	e	1119	CLA	C4-C3-C5-C6
17	G	5004	LHG	C9-C10-C11-C12
18	A	1849	LMU	O5'-C5'-C6'-O6'
18	G	1849	LMU	O5'-C5'-C6'-O6'
18	e	1849	LMU	O5'-C5'-C6'-O6'
18	B	1843	LMU	C11-C10-C9-C8
18	H	1843	LMU	C11-C10-C9-C8
18	f	1843	LMU	C11-C10-C9-C8
13	A	1121	CLA	C5-C6-C7-C8
13	A	1126	CLA	C13-C15-C16-C17
13	1	502	CLA	C10-C11-C12-C13
13	G	1121	CLA	C5-C6-C7-C8
13	G	1126	CLA	C13-C15-C16-C17
13	R	1301	CLA	C15-C16-C17-C18
13	Y	502	CLA	C10-C11-C12-C13
13	e	1121	CLA	C5-C6-C7-C8
13	q	502	CLA	C10-C11-C12-C13
20	2	822	SQD	C46-C45-O47-C7
20	4	822	SQD	C46-C45-O47-C7
20	Z	822	SQD	C46-C45-O47-C7
20	b	822	SQD	C46-C45-O47-C7
20	r	822	SQD	C46-C45-O47-C7
20	t	822	SQD	C46-C45-O47-C7
13	A	1129	CLA	C2A-CAA-CBA-CGA
13	G	1129	CLA	C2A-CAA-CBA-CGA
13	e	1129	CLA	C2A-CAA-CBA-CGA
13	A	1138	CLA	C13-C15-C16-C17
13	G	1138	CLA	C13-C15-C16-C17
13	e	1138	CLA	C13-C15-C16-C17
13	G	1118	CLA	C2-C1-O2A-CGA
17	L	5218	LHG	C9-C10-C11-C12
17	V	5218	LHG	C9-C10-C11-C12
17	n	5218	LHG	C9-C10-C11-C12
13	L	1503	CLA	O1D-CGD-O2D-CED
13	V	1503	CLA	O1D-CGD-O2D-CED
13	n	1503	CLA	O1D-CGD-O2D-CED
13	r	505	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	f	5002	LMG	C41-C42-C43-C44
13	1	509	CLA	C5-C6-C7-C8
13	2	502	CLA	C5-C6-C7-C8
13	Y	509	CLA	C5-C6-C7-C8
13	Z	502	CLA	C5-C6-C7-C8
13	f	1240	CLA	C8-C10-C11-C12
13	q	509	CLA	C5-C6-C7-C8
13	r	502	CLA	C5-C6-C7-C8
19	B	5002	LMG	C41-C42-C43-C44
19	H	5002	LMG	C41-C42-C43-C44
13	B	1210	CLA	CBA-CGA-O2A-C1
13	4	519	CLA	CBA-CGA-O2A-C1
13	5	518	CLA	CBA-CGA-O2A-C1
13	H	1210	CLA	CBA-CGA-O2A-C1
13	b	519	CLA	CBA-CGA-O2A-C1
13	c	518	CLA	CBA-CGA-O2A-C1
13	f	1210	CLA	CBA-CGA-O2A-C1
13	t	519	CLA	CBA-CGA-O2A-C1
13	u	518	CLA	CBA-CGA-O2A-C1
13	L	1502	CLA	O1A-CGA-O2A-C1
13	V	1502	CLA	O1A-CGA-O2A-C1
13	n	1502	CLA	O1A-CGA-O2A-C1
13	A	1136	CLA	C11-C12-C13-C14
13	G	1136	CLA	C11-C12-C13-C14
13	e	1136	CLA	C11-C12-C13-C14
13	r	505	CLA	C16-C17-C18-C20
13	A	1132	CLA	C5-C6-C7-C8
13	G	1132	CLA	C5-C6-C7-C8
13	e	1132	CLA	C5-C6-C7-C8
13	2	505	CLA	CBD-CGD-O2D-CED
13	Z	505	CLA	CBD-CGD-O2D-CED
17	A	5006	LHG	C8-C7-O7-C5
17	G	5006	LHG	C8-C7-O7-C5
17	e	5006	LHG	C8-C7-O7-C5
13	A	1103	CLA	C13-C15-C16-C17
13	A	1140	CLA	C15-C16-C17-C18
13	B	1240	CLA	C8-C10-C11-C12
13	G	1140	CLA	C15-C16-C17-C18
13	H	1240	CLA	C8-C10-C11-C12
13	e	1140	CLA	C15-C16-C17-C18
20	6	822	SQD	C2-C1-O6-C44
20	d	822	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
20	v	822	SQD	C2-C1-O6-C44
17	A	5006	LHG	O7-C5-C6-O8
17	G	5006	LHG	O7-C5-C6-O8
17	e	5006	LHG	O7-C5-C6-O8
13	e	1111	CLA	CBA-CGA-O2A-C1
13	G	1103	CLA	C13-C15-C16-C17
13	e	1103	CLA	C13-C15-C16-C17
13	B	1220	CLA	O1A-CGA-O2A-C1
13	1	518	CLA	O1A-CGA-O2A-C1
13	3	511	CLA	O1A-CGA-O2A-C1
13	H	1220	CLA	O1A-CGA-O2A-C1
13	Y	518	CLA	O1A-CGA-O2A-C1
13	a	511	CLA	O1A-CGA-O2A-C1
13	f	1220	CLA	O1A-CGA-O2A-C1
13	q	518	CLA	O1A-CGA-O2A-C1
13	s	511	CLA	O1A-CGA-O2A-C1
13	2	505	CLA	C16-C17-C18-C19
13	2	505	CLA	C16-C17-C18-C20
13	Z	505	CLA	C16-C17-C18-C19
13	Z	505	CLA	C16-C17-C18-C20
13	r	505	CLA	C16-C17-C18-C19
17	A	5008	LHG	C26-C27-C28-C29
17	G	5008	LHG	C26-C27-C28-C29
17	e	5008	LHG	C26-C27-C28-C29
13	A	1103	CLA	C11-C10-C8-C7
13	A	1103	CLA	C12-C13-C15-C16
13	A	1106	CLA	C12-C13-C15-C16
13	A	1116	CLA	C6-C7-C8-C10
13	A	1119	CLA	C2-C3-C5-C6
13	A	1123	CLA	C11-C10-C8-C7
13	A	1127	CLA	C11-C12-C13-C15
13	A	1127	CLA	C12-C13-C15-C16
13	A	1132	CLA	C12-C13-C15-C16
13	A	1137	CLA	C6-C7-C8-C10
13	A	1137	CLA	C12-C13-C15-C16
13	A	1138	CLA	C12-C13-C15-C16
13	A	1237	CLA	C11-C10-C8-C7
13	A	1101	CLA	C11-C10-C8-C7
13	A	1101	CLA	C11-C12-C13-C15
13	B	1203	CLA	C11-C10-C8-C7
13	B	1206	CLA	C6-C7-C8-C10
13	B	1210	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	B	1217	CLA	C11-C10-C8-C7
13	B	1231	CLA	C6-C7-C8-C10
13	B	1234	CLA	C11-C12-C13-C15
13	F	1301	CLA	C12-C13-C15-C16
13	1	509	CLA	C11-C12-C13-C15
13	5	501	CLA	C6-C7-C8-C10
13	5	509	CLA	C11-C10-C8-C7
13	6	501	CLA	C11-C10-C8-C7
13	G	1103	CLA	C11-C10-C8-C7
13	G	1103	CLA	C12-C13-C15-C16
13	G	1106	CLA	C12-C13-C15-C16
13	G	1116	CLA	C6-C7-C8-C10
13	G	1119	CLA	C2-C3-C5-C6
13	G	1123	CLA	C11-C10-C8-C7
13	G	1127	CLA	C11-C12-C13-C15
13	G	1127	CLA	C12-C13-C15-C16
13	G	1132	CLA	C12-C13-C15-C16
13	G	1137	CLA	C6-C7-C8-C10
13	G	1137	CLA	C12-C13-C15-C16
13	G	1138	CLA	C12-C13-C15-C16
13	G	1237	CLA	C11-C10-C8-C7
13	G	1101	CLA	C11-C10-C8-C7
13	G	1101	CLA	C11-C12-C13-C15
13	H	1203	CLA	C11-C10-C8-C7
13	H	1206	CLA	C6-C7-C8-C10
13	H	1210	CLA	C6-C7-C8-C10
13	H	1217	CLA	C11-C10-C8-C7
13	H	1231	CLA	C6-C7-C8-C10
13	H	1234	CLA	C11-C12-C13-C15
13	R	1301	CLA	C12-C13-C15-C16
13	Y	509	CLA	C11-C12-C13-C15
13	c	501	CLA	C6-C7-C8-C10
13	c	509	CLA	C11-C10-C8-C7
13	d	501	CLA	C11-C10-C8-C7
13	e	1103	CLA	C11-C10-C8-C7
13	e	1103	CLA	C12-C13-C15-C16
13	e	1106	CLA	C12-C13-C15-C16
13	e	1116	CLA	C6-C7-C8-C10
13	e	1119	CLA	C2-C3-C5-C6
13	e	1123	CLA	C11-C10-C8-C7
13	e	1127	CLA	C11-C12-C13-C15
13	e	1127	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	e	1132	CLA	C12-C13-C15-C16
13	e	1137	CLA	C6-C7-C8-C10
13	e	1137	CLA	C12-C13-C15-C16
13	e	1138	CLA	C12-C13-C15-C16
13	e	1237	CLA	C11-C10-C8-C7
13	e	1101	CLA	C11-C10-C8-C7
13	e	1101	CLA	C11-C12-C13-C15
13	f	1203	CLA	C11-C10-C8-C7
13	f	1206	CLA	C6-C7-C8-C10
13	f	1210	CLA	C6-C7-C8-C10
13	f	1217	CLA	C11-C10-C8-C7
13	f	1231	CLA	C6-C7-C8-C10
13	f	1234	CLA	C11-C12-C13-C15
13	j	1301	CLA	C12-C13-C15-C16
13	q	509	CLA	C11-C12-C13-C15
13	u	501	CLA	C6-C7-C8-C10
13	u	509	CLA	C11-C10-C8-C7
13	v	501	CLA	C11-C10-C8-C7
14	A	2001	PQN	C22-C23-C25-C26
14	G	2001	PQN	C22-C23-C25-C26
14	e	2001	PQN	C22-C23-C25-C26
17	A	5004	LHG	C30-C31-C32-C33
17	G	5004	LHG	C30-C31-C32-C33
13	A	1107	CLA	C11-C12-C13-C14
13	A	1109	CLA	C11-C12-C13-C14
13	A	1123	CLA	C11-C10-C8-C9
13	A	1127	CLA	C11-C12-C13-C14
13	A	1138	CLA	C14-C13-C15-C16
13	A	1237	CLA	C11-C10-C8-C9
13	B	1206	CLA	C6-C7-C8-C9
13	B	1215	CLA	C11-C10-C8-C9
13	B	1225	CLA	C14-C13-C15-C16
13	B	1235	CLA	C6-C7-C8-C9
13	F	1301	CLA	C11-C10-C8-C9
13	L	1501	CLA	C14-C13-C15-C16
13	L	1503	CLA	C6-C7-C8-C9
13	1	507	CLA	C11-C10-C8-C9
13	1	509	CLA	C11-C12-C13-C14
13	2	510	CLA	C14-C13-C15-C16
13	3	507	CLA	C11-C10-C8-C9
13	4	505	CLA	C14-C13-C15-C16
13	G	1107	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	G	1109	CLA	C11-C12-C13-C14
13	G	1123	CLA	C11-C10-C8-C9
13	G	1127	CLA	C11-C12-C13-C14
13	G	1137	CLA	C14-C13-C15-C16
13	G	1138	CLA	C14-C13-C15-C16
13	G	1237	CLA	C11-C10-C8-C9
13	H	1206	CLA	C6-C7-C8-C9
13	H	1215	CLA	C11-C10-C8-C9
13	H	1225	CLA	C14-C13-C15-C16
13	H	1235	CLA	C6-C7-C8-C9
13	R	1301	CLA	C11-C10-C8-C9
13	V	1501	CLA	C14-C13-C15-C16
13	V	1503	CLA	C6-C7-C8-C9
13	Y	507	CLA	C11-C10-C8-C9
13	Y	509	CLA	C11-C12-C13-C14
13	Z	510	CLA	C14-C13-C15-C16
13	a	507	CLA	C11-C10-C8-C9
13	b	505	CLA	C14-C13-C15-C16
13	e	1107	CLA	C11-C12-C13-C14
13	e	1109	CLA	C11-C12-C13-C14
13	e	1117	CLA	C11-C12-C13-C14
13	e	1123	CLA	C11-C10-C8-C9
13	e	1127	CLA	C11-C12-C13-C14
13	e	1138	CLA	C14-C13-C15-C16
13	e	1237	CLA	C11-C10-C8-C9
13	f	1206	CLA	C6-C7-C8-C9
13	f	1215	CLA	C11-C10-C8-C9
13	f	1225	CLA	C14-C13-C15-C16
13	f	1235	CLA	C6-C7-C8-C9
13	j	1301	CLA	C11-C10-C8-C9
13	n	1501	CLA	C14-C13-C15-C16
13	n	1503	CLA	C6-C7-C8-C9
13	q	507	CLA	C11-C10-C8-C9
13	q	509	CLA	C11-C12-C13-C14
13	r	510	CLA	C14-C13-C15-C16
13	s	507	CLA	C11-C10-C8-C9
13	t	505	CLA	C14-C13-C15-C16
17	e	5004	LHG	C30-C31-C32-C33
20	B	1852	SQD	C12-C13-C14-C15
20	H	1852	SQD	C12-C13-C14-C15
20	f	1852	SQD	C12-C13-C14-C15
13	A	1111	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	B	1208	CLA	CBA-CGA-O2A-C1
13	2	518	CLA	CBA-CGA-O2A-C1
13	G	1111	CLA	CBA-CGA-O2A-C1
13	H	1208	CLA	CBA-CGA-O2A-C1
13	Z	518	CLA	CBA-CGA-O2A-C1
13	f	1208	CLA	CBA-CGA-O2A-C1
13	r	518	CLA	CBA-CGA-O2A-C1
13	2	507	CLA	C10-C11-C12-C13
13	Z	507	CLA	C10-C11-C12-C13
13	r	507	CLA	C10-C11-C12-C13
13	2	519	CLA	C2A-CAA-CBA-CGA
13	4	518	CLA	C2A-CAA-CBA-CGA
13	Z	519	CLA	C2A-CAA-CBA-CGA
13	b	518	CLA	C2A-CAA-CBA-CGA
13	r	519	CLA	C2A-CAA-CBA-CGA
13	t	518	CLA	C2A-CAA-CBA-CGA
19	B	5002	LMG	C35-C36-C37-C38
19	H	5002	LMG	C35-C36-C37-C38
13	Y	504	CLA	O1D-CGD-O2D-CED
13	q	504	CLA	O1D-CGD-O2D-CED
16	J	4015	BCR	C7-C8-C9-C34
16	1	524	BCR	C11-C12-C13-C35
16	Y	524	BCR	C11-C12-C13-C35
16	Z	523	BCR	C7-C8-C9-C34
16	l	4015	BCR	C7-C8-C9-C34
16	q	524	BCR	C11-C12-C13-C35
17	A	5004	LHG	C31-C32-C33-C34
17	G	5004	LHG	C31-C32-C33-C34
17	e	5004	LHG	C31-C32-C33-C34
17	e	5005	LHG	C17-C18-C19-C20
19	f	5002	LMG	C35-C36-C37-C38
17	A	5005	LHG	C17-C18-C19-C20
17	B	1855	LHG	C13-C14-C15-C16
17	G	5005	LHG	C17-C18-C19-C20
17	f	1855	LHG	C13-C14-C15-C16
13	1	504	CLA	O1D-CGD-O2D-CED
13	A	1117	CLA	C15-C16-C17-C18
13	J	1303	CLA	C13-C15-C16-C17
13	3	507	CLA	C5-C6-C7-C8
13	G	1117	CLA	C15-C16-C17-C18
13	T	1303	CLA	C13-C15-C16-C17
13	a	507	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	e	1117	CLA	C15-C16-C17-C18
13	l	1303	CLA	C13-C15-C16-C17
13	s	507	CLA	C5-C6-C7-C8
17	I	5001	LHG	C33-C34-C35-C36
17	H	1855	LHG	C13-C14-C15-C16
17	S	5001	LHG	C33-C34-C35-C36
17	k	5001	LHG	C33-C34-C35-C36
17	n	5218	LHG	C24-C25-C26-C27
13	1	501	CLA	CBA-CGA-O2A-C1
13	2	513	CLA	CBA-CGA-O2A-C1
13	Y	501	CLA	CBA-CGA-O2A-C1
13	Z	513	CLA	CBA-CGA-O2A-C1
13	r	513	CLA	CBA-CGA-O2A-C1
13	J	1302	CLA	C10-C11-C12-C13
13	T	1302	CLA	C10-C11-C12-C13
13	l	1302	CLA	C10-C11-C12-C13
17	L	5218	LHG	C24-C25-C26-C27
17	V	5218	LHG	C24-C25-C26-C27
17	e	5003	LHG	C15-C16-C17-C18
19	B	5002	LMG	C30-C31-C32-C33
19	f	5002	LMG	C30-C31-C32-C33
13	B	1231	CLA	C5-C6-C7-C8
13	H	1231	CLA	C5-C6-C7-C8
13	H	1230	CLA	C5-C6-C7-C8
13	f	1231	CLA	C5-C6-C7-C8
17	A	5006	LHG	C14-C15-C16-C17
17	A	5003	LHG	C15-C16-C17-C18
17	L	5220	LHG	C28-C29-C30-C31
17	G	5006	LHG	C14-C15-C16-C17
17	G	5003	LHG	C15-C16-C17-C18
17	V	5220	LHG	C28-C29-C30-C31
17	e	5006	LHG	C14-C15-C16-C17
17	n	5220	LHG	C28-C29-C30-C31
19	H	5002	LMG	C30-C31-C32-C33
13	1	518	CLA	CAA-CBA-CGA-O2A
13	Y	518	CLA	CAA-CBA-CGA-O2A
13	q	518	CLA	CAA-CBA-CGA-O2A
13	A	1011	CLA	C4B-C3B-CAB-CBB
13	A	1112	CLA	C4B-C3B-CAB-CBB
13	A	1115	CLA	C4B-C3B-CAB-CBB
13	A	1140	CLA	C4B-C3B-CAB-CBB
13	B	1208	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	1217	CLA	C4B-C3B-CAB-CBB
13	B	1240	CLA	C4B-C3B-CAB-CBB
13	1	503	CLA	C4B-C3B-CAB-CBB
13	1	513	CLA	C4B-C3B-CAB-CBB
13	2	504	CLA	C4B-C3B-CAB-CBB
13	2	507	CLA	C4B-C3B-CAB-CBB
13	2	513	CLA	C4B-C3B-CAB-CBB
13	2	517	CLA	C4B-C3B-CAB-CBB
13	3	507	CLA	C4B-C3B-CAB-CBB
13	3	513	CLA	C4B-C3B-CAB-CBB
13	3	516	CLA	C4B-C3B-CAB-CBB
13	4	502	CLA	C4B-C3B-CAB-CBB
13	4	503	CLA	C4B-C3B-CAB-CBB
13	4	506	CLA	C4B-C3B-CAB-CBB
13	4	507	CLA	C4B-C3B-CAB-CBB
13	4	508	CLA	C4B-C3B-CAB-CBB
13	4	510	CLA	C4B-C3B-CAB-CBB
13	4	512	CLA	C4B-C3B-CAB-CBB
13	4	513	CLA	C4B-C3B-CAB-CBB
13	4	516	CLA	C4B-C3B-CAB-CBB
13	4	517	CLA	C4B-C3B-CAB-CBB
13	5	501	CLA	C4B-C3B-CAB-CBB
13	5	503	CLA	C4B-C3B-CAB-CBB
13	5	504	CLA	C4B-C3B-CAB-CBB
13	5	507	CLA	C4B-C3B-CAB-CBB
13	5	510	CLA	C4B-C3B-CAB-CBB
13	6	502	CLA	C4B-C3B-CAB-CBB
13	6	503	CLA	C4B-C3B-CAB-CBB
13	6	510	CLA	C4B-C3B-CAB-CBB
13	6	511	CLA	C4B-C3B-CAB-CBB
13	6	516	CLA	C4B-C3B-CAB-CBB
13	6	517	CLA	C4B-C3B-CAB-CBB
13	G	1011	CLA	C4B-C3B-CAB-CBB
13	G	1112	CLA	C4B-C3B-CAB-CBB
13	G	1115	CLA	C4B-C3B-CAB-CBB
13	G	1140	CLA	C4B-C3B-CAB-CBB
13	H	1208	CLA	C4B-C3B-CAB-CBB
13	H	1217	CLA	C4B-C3B-CAB-CBB
13	H	1240	CLA	C4B-C3B-CAB-CBB
13	Y	503	CLA	C4B-C3B-CAB-CBB
13	Y	513	CLA	C4B-C3B-CAB-CBB
13	Z	504	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	Z	507	CLA	C4B-C3B-CAB-CBB
13	Z	513	CLA	C4B-C3B-CAB-CBB
13	Z	517	CLA	C4B-C3B-CAB-CBB
13	a	507	CLA	C4B-C3B-CAB-CBB
13	a	513	CLA	C4B-C3B-CAB-CBB
13	a	516	CLA	C4B-C3B-CAB-CBB
13	b	502	CLA	C4B-C3B-CAB-CBB
13	b	503	CLA	C4B-C3B-CAB-CBB
13	b	506	CLA	C4B-C3B-CAB-CBB
13	b	507	CLA	C4B-C3B-CAB-CBB
13	b	508	CLA	C4B-C3B-CAB-CBB
13	b	510	CLA	C4B-C3B-CAB-CBB
13	b	512	CLA	C4B-C3B-CAB-CBB
13	b	513	CLA	C4B-C3B-CAB-CBB
13	b	516	CLA	C4B-C3B-CAB-CBB
13	b	517	CLA	C4B-C3B-CAB-CBB
13	c	501	CLA	C4B-C3B-CAB-CBB
13	c	503	CLA	C4B-C3B-CAB-CBB
13	c	504	CLA	C4B-C3B-CAB-CBB
13	c	507	CLA	C4B-C3B-CAB-CBB
13	c	510	CLA	C4B-C3B-CAB-CBB
13	d	502	CLA	C4B-C3B-CAB-CBB
13	d	503	CLA	C4B-C3B-CAB-CBB
13	d	510	CLA	C4B-C3B-CAB-CBB
13	d	511	CLA	C4B-C3B-CAB-CBB
13	d	516	CLA	C4B-C3B-CAB-CBB
13	d	517	CLA	C4B-C3B-CAB-CBB
13	e	1011	CLA	C4B-C3B-CAB-CBB
13	e	1112	CLA	C4B-C3B-CAB-CBB
13	e	1115	CLA	C4B-C3B-CAB-CBB
13	e	1140	CLA	C4B-C3B-CAB-CBB
13	f	1208	CLA	C4B-C3B-CAB-CBB
13	f	1217	CLA	C4B-C3B-CAB-CBB
13	f	1240	CLA	C4B-C3B-CAB-CBB
13	q	503	CLA	C4B-C3B-CAB-CBB
13	q	513	CLA	C4B-C3B-CAB-CBB
13	r	504	CLA	C4B-C3B-CAB-CBB
13	r	507	CLA	C4B-C3B-CAB-CBB
13	r	513	CLA	C4B-C3B-CAB-CBB
13	r	517	CLA	C4B-C3B-CAB-CBB
13	s	507	CLA	C4B-C3B-CAB-CBB
13	s	513	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	s	516	CLA	C4B-C3B-CAB-CBB
13	t	502	CLA	C4B-C3B-CAB-CBB
13	t	503	CLA	C4B-C3B-CAB-CBB
13	t	506	CLA	C4B-C3B-CAB-CBB
13	t	507	CLA	C4B-C3B-CAB-CBB
13	t	508	CLA	C4B-C3B-CAB-CBB
13	t	510	CLA	C4B-C3B-CAB-CBB
13	t	512	CLA	C4B-C3B-CAB-CBB
13	t	513	CLA	C4B-C3B-CAB-CBB
13	t	516	CLA	C4B-C3B-CAB-CBB
13	t	517	CLA	C4B-C3B-CAB-CBB
13	u	501	CLA	C4B-C3B-CAB-CBB
13	u	503	CLA	C4B-C3B-CAB-CBB
13	u	504	CLA	C4B-C3B-CAB-CBB
13	u	507	CLA	C4B-C3B-CAB-CBB
13	u	510	CLA	C4B-C3B-CAB-CBB
13	v	502	CLA	C4B-C3B-CAB-CBB
13	v	503	CLA	C4B-C3B-CAB-CBB
13	v	510	CLA	C4B-C3B-CAB-CBB
13	v	511	CLA	C4B-C3B-CAB-CBB
13	v	516	CLA	C4B-C3B-CAB-CBB
13	v	517	CLA	C4B-C3B-CAB-CBB
13	A	1126	CLA	C16-C17-C18-C19
13	G	1126	CLA	C16-C17-C18-C19
13	e	1126	CLA	C16-C17-C18-C19
13	B	1230	CLA	C5-C6-C7-C8
13	f	1230	CLA	C5-C6-C7-C8
17	e	5007	LHG	O6-C4-C5-C6
17	f	1842	LHG	C31-C32-C33-C34
17	A	5004	LHG	C11-C10-C9-C8
17	B	1842	LHG	C31-C32-C33-C34
17	G	5004	LHG	C11-C10-C9-C8
17	H	1842	LHG	C31-C32-C33-C34
17	e	5004	LHG	C11-C10-C9-C8
13	q	501	CLA	CBA-CGA-O2A-C1
13	f	1224	CLA	O1D-CGD-O2D-CED
18	J	5105	LMU	C3-C4-C5-C6
18	T	5105	LMU	C3-C4-C5-C6
18	l	5105	LMU	C3-C4-C5-C6
13	A	1102	CLA	C2-C3-C5-C6
13	A	1130	CLA	C2-C3-C5-C6
13	G	1102	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	G	1130	CLA	C2-C3-C5-C6
13	e	1102	CLA	C2-C3-C5-C6
13	e	1130	CLA	C2-C3-C5-C6
19	J	5104	LMG	C10-C11-C12-C13
19	T	5104	LMG	C10-C11-C12-C13
19	l	5104	LMG	C10-C11-C12-C13
13	B	1224	CLA	O1D-CGD-O2D-CED
13	H	1224	CLA	O1D-CGD-O2D-CED
13	1	507	CLA	C8-C10-C11-C12
13	Y	507	CLA	C8-C10-C11-C12
13	q	507	CLA	C8-C10-C11-C12
13	B	1211	CLA	C11-C10-C8-C9
13	H	1211	CLA	C11-C10-C8-C9
13	f	1211	CLA	C11-C10-C8-C9
17	A	5001	LHG	C31-C32-C33-C34
17	G	5001	LHG	C31-C32-C33-C34
17	e	5001	LHG	C31-C32-C33-C34
13	B	1220	CLA	C6-C7-C8-C10
13	B	1227	CLA	C16-C17-C18-C20
13	H	1220	CLA	C6-C7-C8-C10
13	H	1227	CLA	C16-C17-C18-C20
13	f	1220	CLA	C6-C7-C8-C10
13	f	1227	CLA	C16-C17-C18-C20
13	A	1103	CLA	CBA-CGA-O2A-C1
13	1	507	CLA	CBA-CGA-O2A-C1
13	3	508	CLA	CBA-CGA-O2A-C1
13	G	1103	CLA	CBA-CGA-O2A-C1
13	Y	507	CLA	CBA-CGA-O2A-C1
13	a	508	CLA	CBA-CGA-O2A-C1
13	e	1103	CLA	CBA-CGA-O2A-C1
13	q	507	CLA	CBA-CGA-O2A-C1
13	s	508	CLA	CBA-CGA-O2A-C1
17	L	5221	LHG	C2-C3-O3-P
17	V	5221	LHG	C2-C3-O3-P
17	n	5221	LHG	C2-C3-O3-P
13	A	1104	CLA	C3A-C2A-CAA-CBA
13	B	1206	CLA	C3A-C2A-CAA-CBA
13	B	1227	CLA	C3A-C2A-CAA-CBA
13	B	1240	CLA	C3A-C2A-CAA-CBA
13	J	1303	CLA	C3A-C2A-CAA-CBA
13	3	517	CLA	C3A-C2A-CAA-CBA
13	6	517	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	G	1104	CLA	C3A-C2A-CAA-CBA
13	H	1206	CLA	C3A-C2A-CAA-CBA
13	H	1227	CLA	C3A-C2A-CAA-CBA
13	H	1240	CLA	C3A-C2A-CAA-CBA
13	T	1303	CLA	C3A-C2A-CAA-CBA
13	a	517	CLA	C3A-C2A-CAA-CBA
13	d	517	CLA	C3A-C2A-CAA-CBA
13	e	1104	CLA	C3A-C2A-CAA-CBA
13	f	1206	CLA	C3A-C2A-CAA-CBA
13	f	1227	CLA	C3A-C2A-CAA-CBA
13	f	1240	CLA	C3A-C2A-CAA-CBA
13	l	1303	CLA	C3A-C2A-CAA-CBA
13	s	517	CLA	C3A-C2A-CAA-CBA
13	v	517	CLA	C3A-C2A-CAA-CBA
17	A	5007	LHG	C35-C36-C37-C38
17	A	5003	LHG	C25-C26-C27-C28
17	G	5007	LHG	C35-C36-C37-C38
17	G	5003	LHG	C25-C26-C27-C28
17	e	5007	LHG	C35-C36-C37-C38
17	e	5003	LHG	C25-C26-C27-C28
13	B	1201	CLA	C11-C12-C13-C15
13	H	1201	CLA	C11-C12-C13-C15
13	H	1205	CLA	O1D-CGD-O2D-CED
13	B	1206	CLA	C13-C15-C16-C17
13	2	518	CLA	C8-C10-C11-C12
13	H	1206	CLA	C13-C15-C16-C17
13	Z	518	CLA	C8-C10-C11-C12
13	f	1206	CLA	C13-C15-C16-C17
13	r	518	CLA	C8-C10-C11-C12
13	B	1205	CLA	O1D-CGD-O2D-CED
13	f	1205	CLA	O1D-CGD-O2D-CED
17	A	5005	LHG	C4-C5-C6-O8
17	A	5007	LHG	C4-C5-C6-O8
17	A	5009	LHG	C4-C5-C6-O8
17	I	5001	LHG	C4-C5-C6-O8
17	L	5220	LHG	C4-C5-C6-O8
17	G	5005	LHG	C4-C5-C6-O8
17	G	5007	LHG	C4-C5-C6-O8
17	G	5009	LHG	C4-C5-C6-O8
17	S	5001	LHG	C4-C5-C6-O8
17	V	5220	LHG	C4-C5-C6-O8
17	e	5005	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
17	e	5007	LHG	C4-C5-C6-O8
17	e	5009	LHG	C4-C5-C6-O8
17	k	5001	LHG	C4-C5-C6-O8
17	n	5220	LHG	C4-C5-C6-O8
20	B	1852	SQD	O6-C44-C45-C46
20	4	822	SQD	C44-C45-C46-O48
20	6	822	SQD	C44-C45-C46-O48
20	H	1852	SQD	O6-C44-C45-C46
20	b	822	SQD	C44-C45-C46-O48
20	d	822	SQD	C44-C45-C46-O48
20	f	1852	SQD	O6-C44-C45-C46
20	t	822	SQD	C44-C45-C46-O48
20	v	822	SQD	C44-C45-C46-O48
17	L	5221	LHG	C24-C25-C26-C27
17	V	5221	LHG	C24-C25-C26-C27
17	n	5221	LHG	C24-C25-C26-C27
17	A	5009	LHG	C32-C33-C34-C35
17	G	5009	LHG	C32-C33-C34-C35
17	e	5009	LHG	C32-C33-C34-C35
13	A	1104	CLA	C3-C5-C6-C7
13	A	1125	CLA	C3-C5-C6-C7
13	G	1104	CLA	C3-C5-C6-C7
13	e	1104	CLA	C3-C5-C6-C7
13	Y	508	CLA	O1D-CGD-O2D-CED
17	A	5007	LHG	C15-C16-C17-C18
17	L	5220	LHG	C11-C10-C9-C8
17	G	5007	LHG	C15-C16-C17-C18
17	V	5220	LHG	C11-C10-C9-C8
17	n	5220	LHG	C11-C10-C9-C8
13	B	1210	CLA	C4-C3-C5-C6
13	H	1210	CLA	C4-C3-C5-C6
13	f	1210	CLA	C4-C3-C5-C6
13	f	1201	CLA	C11-C12-C13-C15
13	r	513	CLA	C16-C17-C18-C19
13	1	508	CLA	O1D-CGD-O2D-CED
13	q	508	CLA	O1D-CGD-O2D-CED
17	e	5007	LHG	C15-C16-C17-C18
17	B	1855	LHG	C24-C25-C26-C27
17	L	5221	LHG	C19-C20-C21-C22
17	H	1855	LHG	C24-C25-C26-C27
17	V	5221	LHG	C19-C20-C21-C22
17	f	1855	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
17	n	5221	LHG	C19-C20-C21-C22
13	B	1208	CLA	C13-C15-C16-C17
13	H	1208	CLA	C13-C15-C16-C17
13	f	1208	CLA	C13-C15-C16-C17
13	5	518	CLA	O1A-CGA-O2A-C1
13	b	519	CLA	O1A-CGA-O2A-C1
13	c	518	CLA	O1A-CGA-O2A-C1
17	A	5006	LHG	C30-C31-C32-C33
17	e	5006	LHG	C30-C31-C32-C33
18	2	901	LMU	C1-C2-C3-C4
18	Z	901	LMU	C1-C2-C3-C4
18	r	901	LMU	C1-C2-C3-C4
13	B	1012	CLA	C3-C5-C6-C7
13	B	1227	CLA	C3-C5-C6-C7
13	G	1125	CLA	C3-C5-C6-C7
13	H	1012	CLA	C3-C5-C6-C7
13	H	1227	CLA	C3-C5-C6-C7
13	e	1125	CLA	C3-C5-C6-C7
13	f	1012	CLA	C3-C5-C6-C7
13	f	1227	CLA	C3-C5-C6-C7
13	A	1111	CLA	C2A-CAA-CBA-CGA
13	3	518	CLA	C2A-CAA-CBA-CGA
13	G	1111	CLA	C2A-CAA-CBA-CGA
13	a	518	CLA	C2A-CAA-CBA-CGA
13	e	1106	CLA	C2A-CAA-CBA-CGA
13	e	1111	CLA	C2A-CAA-CBA-CGA
17	G	5006	LHG	C30-C31-C32-C33
19	f	5002	LMG	C34-C35-C36-C37
17	B	1855	LHG	O6-C4-C5-O7
17	H	1855	LHG	O6-C4-C5-O7
17	f	1855	LHG	O6-C4-C5-O7
19	B	5002	LMG	C34-C35-C36-C37
19	H	5002	LMG	C34-C35-C36-C37
13	B	1210	CLA	O1A-CGA-O2A-C1
13	4	519	CLA	O1A-CGA-O2A-C1
13	H	1210	CLA	O1A-CGA-O2A-C1
13	f	1210	CLA	O1A-CGA-O2A-C1
13	t	519	CLA	O1A-CGA-O2A-C1
13	u	518	CLA	O1A-CGA-O2A-C1
13	B	1219	CLA	C16-C17-C18-C19
13	2	513	CLA	C16-C17-C18-C19
13	H	1219	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	Z	513	CLA	C16-C17-C18-C19
13	f	1219	CLA	C16-C17-C18-C19
13	G	1237	CLA	C10-C11-C12-C13
13	e	1237	CLA	C10-C11-C12-C13
17	G	5004	LHG	C25-C26-C27-C28
13	A	1112	CLA	C2B-C3B-CAB-CBB
13	A	1129	CLA	C2B-C3B-CAB-CBB
13	B	1021	CLA	C2B-C3B-CAB-CBB
13	2	504	CLA	C2B-C3B-CAB-CBB
13	2	507	CLA	C2B-C3B-CAB-CBB
13	2	517	CLA	C2B-C3B-CAB-CBB
13	4	503	CLA	C2B-C3B-CAB-CBB
13	4	507	CLA	C2B-C3B-CAB-CBB
13	4	510	CLA	C2B-C3B-CAB-CBB
13	4	516	CLA	C2B-C3B-CAB-CBB
13	4	517	CLA	C2B-C3B-CAB-CBB
13	5	503	CLA	C2B-C3B-CAB-CBB
13	5	504	CLA	C2B-C3B-CAB-CBB
13	5	507	CLA	C2B-C3B-CAB-CBB
13	5	510	CLA	C2B-C3B-CAB-CBB
13	6	502	CLA	C2B-C3B-CAB-CBB
13	6	507	CLA	C2B-C3B-CAB-CBB
13	6	510	CLA	C2B-C3B-CAB-CBB
13	6	516	CLA	C2B-C3B-CAB-CBB
13	6	517	CLA	C2B-C3B-CAB-CBB
13	G	1112	CLA	C2B-C3B-CAB-CBB
13	G	1129	CLA	C2B-C3B-CAB-CBB
13	H	1021	CLA	C2B-C3B-CAB-CBB
13	Z	504	CLA	C2B-C3B-CAB-CBB
13	Z	507	CLA	C2B-C3B-CAB-CBB
13	Z	517	CLA	C2B-C3B-CAB-CBB
13	a	513	CLA	C2B-C3B-CAB-CBB
13	b	503	CLA	C2B-C3B-CAB-CBB
13	b	507	CLA	C2B-C3B-CAB-CBB
13	b	510	CLA	C2B-C3B-CAB-CBB
13	b	516	CLA	C2B-C3B-CAB-CBB
13	b	517	CLA	C2B-C3B-CAB-CBB
13	c	503	CLA	C2B-C3B-CAB-CBB
13	c	504	CLA	C2B-C3B-CAB-CBB
13	c	507	CLA	C2B-C3B-CAB-CBB
13	d	502	CLA	C2B-C3B-CAB-CBB
13	d	503	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	d	507	CLA	C2B-C3B-CAB-CBB
13	d	510	CLA	C2B-C3B-CAB-CBB
13	d	516	CLA	C2B-C3B-CAB-CBB
13	d	517	CLA	C2B-C3B-CAB-CBB
13	e	1112	CLA	C2B-C3B-CAB-CBB
13	e	1129	CLA	C2B-C3B-CAB-CBB
13	f	1021	CLA	C2B-C3B-CAB-CBB
13	r	504	CLA	C2B-C3B-CAB-CBB
13	r	507	CLA	C2B-C3B-CAB-CBB
13	r	517	CLA	C2B-C3B-CAB-CBB
13	t	503	CLA	C2B-C3B-CAB-CBB
13	t	507	CLA	C2B-C3B-CAB-CBB
13	t	510	CLA	C2B-C3B-CAB-CBB
13	t	513	CLA	C2B-C3B-CAB-CBB
13	t	516	CLA	C2B-C3B-CAB-CBB
13	t	517	CLA	C2B-C3B-CAB-CBB
13	u	503	CLA	C2B-C3B-CAB-CBB
13	u	504	CLA	C2B-C3B-CAB-CBB
13	u	507	CLA	C2B-C3B-CAB-CBB
13	u	510	CLA	C2B-C3B-CAB-CBB
13	v	502	CLA	C2B-C3B-CAB-CBB
13	v	507	CLA	C2B-C3B-CAB-CBB
13	v	510	CLA	C2B-C3B-CAB-CBB
13	v	516	CLA	C2B-C3B-CAB-CBB
13	v	517	CLA	C2B-C3B-CAB-CBB
17	B	1842	LHG	C34-C35-C36-C37
20	B	1852	SQD	C32-C33-C34-C35
20	3	822	SQD	C28-C29-C30-C31
20	H	1852	SQD	C32-C33-C34-C35
20	f	1852	SQD	C32-C33-C34-C35
13	A	1111	CLA	O1A-CGA-O2A-C1
13	G	1111	CLA	O1A-CGA-O2A-C1
13	e	1111	CLA	O1A-CGA-O2A-C1
17	A	5004	LHG	C25-C26-C27-C28
17	H	1842	LHG	C34-C35-C36-C37
17	e	5004	LHG	C25-C26-C27-C28
17	f	1842	LHG	C34-C35-C36-C37
20	a	822	SQD	C28-C29-C30-C31
20	s	822	SQD	C28-C29-C30-C31
17	A	5009	LHG	O7-C5-C6-O8
17	G	5009	LHG	O7-C5-C6-O8
17	e	5009	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
20	1	822	SQD	O6-C44-C45-O47
20	Y	822	SQD	O6-C44-C45-O47
20	q	822	SQD	O6-C44-C45-O47
13	A	1122	CLA	C10-C11-C12-C13
13	A	1132	CLA	C13-C15-C16-C17
13	A	1237	CLA	C10-C11-C12-C13
13	B	1221	CLA	C13-C15-C16-C17
13	G	1122	CLA	C10-C11-C12-C13
13	G	1132	CLA	C13-C15-C16-C17
13	H	1221	CLA	C13-C15-C16-C17
13	e	1132	CLA	C13-C15-C16-C17
13	f	1221	CLA	C13-C15-C16-C17
13	B	1224	CLA	CAA-CBA-CGA-O2A
13	H	1224	CLA	CAA-CBA-CGA-O2A
13	f	1224	CLA	CAA-CBA-CGA-O2A
13	B	1210	CLA	C16-C17-C18-C20
13	2	513	CLA	C16-C17-C18-C20
13	H	1210	CLA	C16-C17-C18-C20
13	Z	513	CLA	C16-C17-C18-C20
13	f	1210	CLA	C16-C17-C18-C20
13	r	513	CLA	C16-C17-C18-C20
13	A	1128	CLA	C5-C6-C7-C8
13	G	1128	CLA	C5-C6-C7-C8
13	e	1122	CLA	C10-C11-C12-C13
13	e	1128	CLA	C5-C6-C7-C8
17	H	1855	LHG	C14-C15-C16-C17
17	f	1855	LHG	C14-C15-C16-C17
19	J	5104	LMG	O9-C10-O7-C8
19	T	5104	LMG	O9-C10-O7-C8
19	l	5104	LMG	O9-C10-O7-C8
13	A	1105	CLA	C2-C1-O2A-CGA
13	B	1223	CLA	C2-C1-O2A-CGA
13	2	502	CLA	C2-C1-O2A-CGA
13	5	505	CLA	C2-C1-O2A-CGA
13	G	1105	CLA	C2-C1-O2A-CGA
13	H	1223	CLA	C2-C1-O2A-CGA
13	Z	502	CLA	C2-C1-O2A-CGA
13	c	505	CLA	C2-C1-O2A-CGA
13	e	1105	CLA	C2-C1-O2A-CGA
13	f	1223	CLA	C2-C1-O2A-CGA
13	r	502	CLA	C2-C1-O2A-CGA
13	u	505	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
17	B	1855	LHG	C14-C15-C16-C17
13	A	1106	CLA	C14-C13-C15-C16
13	A	1109	CLA	C14-C13-C15-C16
13	A	1117	CLA	C11-C12-C13-C14
13	A	1125	CLA	C11-C12-C13-C14
13	A	1128	CLA	C6-C7-C8-C9
13	A	1132	CLA	C14-C13-C15-C16
13	A	1137	CLA	C14-C13-C15-C16
13	A	1140	CLA	C6-C7-C8-C9
13	B	1201	CLA	C6-C7-C8-C9
13	B	1204	CLA	C11-C10-C8-C9
13	B	1205	CLA	C14-C13-C15-C16
13	B	1214	CLA	C11-C10-C8-C9
13	B	1234	CLA	C6-C7-C8-C9
13	B	1239	CLA	C14-C13-C15-C16
13	5	501	CLA	C11-C10-C8-C9
13	5	509	CLA	C11-C12-C13-C14
13	5	509	CLA	C14-C13-C15-C16
13	G	1106	CLA	C14-C13-C15-C16
13	G	1109	CLA	C14-C13-C15-C16
13	G	1117	CLA	C11-C12-C13-C14
13	G	1125	CLA	C11-C12-C13-C14
13	G	1128	CLA	C6-C7-C8-C9
13	G	1132	CLA	C14-C13-C15-C16
13	G	1140	CLA	C6-C7-C8-C9
13	H	1201	CLA	C6-C7-C8-C9
13	H	1204	CLA	C11-C10-C8-C9
13	H	1205	CLA	C14-C13-C15-C16
13	H	1214	CLA	C11-C10-C8-C9
13	H	1234	CLA	C6-C7-C8-C9
13	H	1239	CLA	C14-C13-C15-C16
13	c	501	CLA	C11-C10-C8-C9
13	c	509	CLA	C11-C12-C13-C14
13	c	509	CLA	C14-C13-C15-C16
13	e	1106	CLA	C14-C13-C15-C16
13	e	1109	CLA	C14-C13-C15-C16
13	e	1125	CLA	C11-C12-C13-C14
13	e	1128	CLA	C6-C7-C8-C9
13	e	1132	CLA	C14-C13-C15-C16
13	e	1137	CLA	C14-C13-C15-C16
13	e	1140	CLA	C6-C7-C8-C9
13	f	1201	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	f	1204	CLA	C11-C10-C8-C9
13	f	1205	CLA	C14-C13-C15-C16
13	f	1214	CLA	C11-C10-C8-C9
13	f	1234	CLA	C6-C7-C8-C9
13	f	1239	CLA	C14-C13-C15-C16
13	u	501	CLA	C11-C10-C8-C9
13	u	509	CLA	C11-C12-C13-C14
13	u	509	CLA	C14-C13-C15-C16
14	A	2001	PQN	C19-C18-C20-C21
14	G	2001	PQN	C19-C18-C20-C21
14	e	2001	PQN	C19-C18-C20-C21
17	L	5220	LHG	C30-C31-C32-C33
17	V	5220	LHG	C30-C31-C32-C33
17	n	5220	LHG	C30-C31-C32-C33
20	B	1852	SQD	C10-C11-C12-C13
20	f	1852	SQD	C10-C11-C12-C13
17	A	5004	LHG	C2-C3-O3-P
17	A	5005	LHG	C2-C3-O3-P
17	G	5004	LHG	C2-C3-O3-P
17	G	5005	LHG	C2-C3-O3-P
17	e	5004	LHG	C2-C3-O3-P
17	e	5005	LHG	C2-C3-O3-P
20	H	1852	SQD	C10-C11-C12-C13
13	A	1106	CLA	C2A-CAA-CBA-CGA
13	A	1115	CLA	C2A-CAA-CBA-CGA
13	2	501	CLA	C2A-CAA-CBA-CGA
13	2	518	CLA	C2A-CAA-CBA-CGA
13	G	1106	CLA	C2A-CAA-CBA-CGA
13	G	1115	CLA	C2A-CAA-CBA-CGA
13	Z	501	CLA	C2A-CAA-CBA-CGA
13	Z	518	CLA	C2A-CAA-CBA-CGA
13	e	1115	CLA	C2A-CAA-CBA-CGA
13	r	501	CLA	C2A-CAA-CBA-CGA
13	r	518	CLA	C2A-CAA-CBA-CGA
13	s	518	CLA	C2A-CAA-CBA-CGA
13	A	1103	CLA	C16-C17-C18-C19
13	B	1220	CLA	C6-C7-C8-C9
13	1	501	CLA	C16-C17-C18-C19
13	1	502	CLA	C11-C12-C13-C15
13	G	1103	CLA	C16-C17-C18-C19
13	H	1220	CLA	C6-C7-C8-C9
13	Y	501	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	Y	502	CLA	C11-C12-C13-C15
13	e	1103	CLA	C16-C17-C18-C19
13	f	1220	CLA	C6-C7-C8-C9
13	n	1502	CLA	C16-C17-C18-C20
13	q	501	CLA	C16-C17-C18-C19
13	q	502	CLA	C11-C12-C13-C15
16	L	4020	BCR	C23-C24-C25-C30
16	L	4219	BCR	C1-C6-C7-C8
16	L	4219	BCR	C5-C6-C7-C8
16	3	521	BCR	C23-C24-C25-C30
16	3	522	BCR	C5-C6-C7-C8
16	5	521	BCR	C5-C6-C7-C8
16	6	524	BCR	C5-C6-C7-C8
16	V	4020	BCR	C23-C24-C25-C30
16	V	4219	BCR	C1-C6-C7-C8
16	V	4219	BCR	C5-C6-C7-C8
16	a	521	BCR	C23-C24-C25-C30
16	a	522	BCR	C5-C6-C7-C8
16	c	521	BCR	C5-C6-C7-C8
16	d	524	BCR	C5-C6-C7-C8
16	n	4020	BCR	C23-C24-C25-C30
16	n	4219	BCR	C1-C6-C7-C8
16	n	4219	BCR	C5-C6-C7-C8
16	s	521	BCR	C23-C24-C25-C30
16	s	522	BCR	C5-C6-C7-C8
16	u	521	BCR	C5-C6-C7-C8
16	v	524	BCR	C5-C6-C7-C8
13	B	1224	CLA	C5-C6-C7-C8
13	H	1224	CLA	C5-C6-C7-C8
13	f	1224	CLA	C5-C6-C7-C8
16	2	523	BCR	C7-C8-C9-C34
16	r	523	BCR	C7-C8-C9-C34
13	B	1208	CLA	O1A-CGA-O2A-C1
13	2	518	CLA	O1A-CGA-O2A-C1
13	H	1208	CLA	O1A-CGA-O2A-C1
13	Z	518	CLA	O1A-CGA-O2A-C1
13	f	1208	CLA	O1A-CGA-O2A-C1
13	r	518	CLA	O1A-CGA-O2A-C1
13	B	1215	CLA	O1D-CGD-O2D-CED
16	A	4001	BCR	C7-C8-C9-C10
16	A	4011	BCR	C17-C18-C19-C20
16	B	4014	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	M	4021	BCR	C11-C12-C13-C14
16	3	524	BCR	C7-C8-C9-C10
16	4	524	BCR	C7-C8-C9-C10
16	6	522	BCR	C7-C8-C9-C10
16	G	4001	BCR	C7-C8-C9-C10
16	G	4011	BCR	C17-C18-C19-C20
16	H	4014	BCR	C7-C8-C9-C10
16	W	4021	BCR	C11-C12-C13-C14
16	a	524	BCR	C7-C8-C9-C10
16	b	524	BCR	C7-C8-C9-C10
16	d	522	BCR	C7-C8-C9-C10
16	e	4001	BCR	C7-C8-C9-C10
16	e	4011	BCR	C17-C18-C19-C20
16	f	4014	BCR	C7-C8-C9-C10
16	o	4021	BCR	C11-C12-C13-C14
16	s	524	BCR	C7-C8-C9-C10
16	t	524	BCR	C7-C8-C9-C10
16	v	522	BCR	C7-C8-C9-C10
13	H	1215	CLA	O1D-CGD-O2D-CED
13	f	1215	CLA	O1D-CGD-O2D-CED
20	B	1852	SQD	C8-C7-O47-C45
20	H	1852	SQD	C8-C7-O47-C45
20	f	1852	SQD	C8-C7-O47-C45
17	A	5009	LHG	C10-C11-C12-C13
17	G	5009	LHG	C10-C11-C12-C13
17	e	5009	LHG	C10-C11-C12-C13
20	s	822	SQD	C11-C10-C9-C8
13	A	1115	CLA	C11-C12-C13-C14
13	L	1502	CLA	C16-C17-C18-C20
13	1	501	CLA	C16-C17-C18-C20
13	G	1115	CLA	C11-C12-C13-C14
13	V	1502	CLA	C16-C17-C18-C20
13	Y	501	CLA	C16-C17-C18-C20
13	e	1115	CLA	C11-C12-C13-C14
13	q	501	CLA	C16-C17-C18-C20
14	A	2001	PQN	C26-C27-C28-C30
14	G	2001	PQN	C26-C27-C28-C30
14	e	2001	PQN	C26-C27-C28-C30
13	A	1237	CLA	C3-C5-C6-C7
13	5	505	CLA	C14-C13-C15-C16
13	c	505	CLA	C14-C13-C15-C16
13	u	505	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	3	822	SQD	C11-C10-C9-C8
13	2	507	CLA	C13-C15-C16-C17
13	Z	507	CLA	C13-C15-C16-C17
13	r	507	CLA	C13-C15-C16-C17
20	a	822	SQD	C11-C10-C9-C8
20	V	5216	SQD	C31-C32-C33-C34
20	n	5216	SQD	C31-C32-C33-C34
17	A	5002	LHG	O6-C4-C5-C6
17	A	5007	LHG	O6-C4-C5-C6
17	L	5218	LHG	O6-C4-C5-C6
17	G	5002	LHG	O6-C4-C5-C6
17	G	5007	LHG	O6-C4-C5-C6
17	V	5218	LHG	O6-C4-C5-C6
17	e	5002	LHG	O6-C4-C5-C6
17	n	5218	LHG	O6-C4-C5-C6
20	L	5216	SQD	C31-C32-C33-C34
13	A	1106	CLA	C11-C12-C13-C15
13	A	1107	CLA	C11-C12-C13-C15
13	A	1109	CLA	C11-C12-C13-C15
13	A	1117	CLA	C11-C12-C13-C15
13	A	1122	CLA	C6-C7-C8-C10
13	A	1125	CLA	C11-C12-C13-C15
13	A	1128	CLA	C6-C7-C8-C10
13	A	1131	CLA	C12-C13-C15-C16
13	A	1139	CLA	C6-C7-C8-C10
13	B	1012	CLA	C11-C10-C8-C7
13	B	1201	CLA	C6-C7-C8-C10
13	B	1203	CLA	C6-C7-C8-C10
13	B	1203	CLA	C11-C12-C13-C15
13	B	1206	CLA	C11-C10-C8-C7
13	B	1208	CLA	C6-C7-C8-C10
13	B	1214	CLA	C11-C12-C13-C15
13	B	1215	CLA	C11-C10-C8-C7
13	B	1225	CLA	C12-C13-C15-C16
13	B	1226	CLA	C11-C12-C13-C15
13	B	1234	CLA	C6-C7-C8-C10
13	B	1235	CLA	C6-C7-C8-C10
13	B	1239	CLA	C12-C13-C15-C16
13	B	1240	CLA	C11-C12-C13-C15
13	L	1501	CLA	C12-C13-C15-C16
13	1	507	CLA	C11-C10-C8-C7
13	1	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	2	507	CLA	C11-C10-C8-C7
13	2	510	CLA	C12-C13-C15-C16
13	3	507	CLA	C11-C10-C8-C7
13	4	501	CLA	C6-C7-C8-C10
13	4	505	CLA	C12-C13-C15-C16
13	5	501	CLA	C11-C10-C8-C7
13	5	509	CLA	C11-C12-C13-C15
13	5	509	CLA	C12-C13-C15-C16
13	6	505	CLA	C6-C7-C8-C10
13	G	1106	CLA	C11-C12-C13-C15
13	G	1107	CLA	C11-C12-C13-C15
13	G	1109	CLA	C11-C12-C13-C15
13	G	1117	CLA	C11-C12-C13-C15
13	G	1122	CLA	C6-C7-C8-C10
13	G	1125	CLA	C11-C12-C13-C15
13	G	1128	CLA	C6-C7-C8-C10
13	G	1131	CLA	C12-C13-C15-C16
13	G	1139	CLA	C6-C7-C8-C10
13	H	1012	CLA	C11-C10-C8-C7
13	H	1201	CLA	C6-C7-C8-C10
13	H	1203	CLA	C6-C7-C8-C10
13	H	1203	CLA	C11-C12-C13-C15
13	H	1206	CLA	C11-C10-C8-C7
13	H	1208	CLA	C6-C7-C8-C10
13	H	1214	CLA	C11-C12-C13-C15
13	H	1215	CLA	C11-C10-C8-C7
13	H	1225	CLA	C12-C13-C15-C16
13	H	1226	CLA	C11-C12-C13-C15
13	H	1234	CLA	C6-C7-C8-C10
13	H	1235	CLA	C6-C7-C8-C10
13	H	1239	CLA	C12-C13-C15-C16
13	H	1240	CLA	C11-C12-C13-C15
13	V	1501	CLA	C12-C13-C15-C16
13	Y	507	CLA	C11-C10-C8-C7
13	Y	510	CLA	C6-C7-C8-C10
13	Z	507	CLA	C11-C10-C8-C7
13	Z	510	CLA	C12-C13-C15-C16
13	a	507	CLA	C11-C10-C8-C7
13	b	501	CLA	C6-C7-C8-C10
13	b	505	CLA	C12-C13-C15-C16
13	c	501	CLA	C11-C10-C8-C7
13	c	509	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	c	509	CLA	C12-C13-C15-C16
13	d	505	CLA	C6-C7-C8-C10
13	e	1106	CLA	C11-C12-C13-C15
13	e	1107	CLA	C11-C12-C13-C15
13	e	1109	CLA	C11-C12-C13-C15
13	e	1117	CLA	C11-C12-C13-C15
13	e	1122	CLA	C6-C7-C8-C10
13	e	1125	CLA	C11-C12-C13-C15
13	e	1128	CLA	C6-C7-C8-C10
13	e	1131	CLA	C12-C13-C15-C16
13	e	1139	CLA	C6-C7-C8-C10
13	f	1012	CLA	C11-C10-C8-C7
13	f	1201	CLA	C6-C7-C8-C10
13	f	1203	CLA	C6-C7-C8-C10
13	f	1203	CLA	C11-C12-C13-C15
13	f	1206	CLA	C11-C10-C8-C7
13	f	1208	CLA	C6-C7-C8-C10
13	f	1214	CLA	C11-C12-C13-C15
13	f	1215	CLA	C11-C10-C8-C7
13	f	1225	CLA	C12-C13-C15-C16
13	f	1226	CLA	C11-C12-C13-C15
13	f	1234	CLA	C6-C7-C8-C10
13	f	1235	CLA	C6-C7-C8-C10
13	f	1239	CLA	C12-C13-C15-C16
13	f	1240	CLA	C11-C12-C13-C15
13	n	1501	CLA	C12-C13-C15-C16
13	q	507	CLA	C11-C10-C8-C7
13	q	510	CLA	C6-C7-C8-C10
13	r	507	CLA	C11-C10-C8-C7
13	r	510	CLA	C12-C13-C15-C16
13	s	507	CLA	C11-C10-C8-C7
13	t	501	CLA	C6-C7-C8-C10
13	t	505	CLA	C12-C13-C15-C16
13	u	501	CLA	C11-C10-C8-C7
13	u	509	CLA	C12-C13-C15-C16
13	v	505	CLA	C6-C7-C8-C10
14	A	2001	PQN	C17-C18-C20-C21
14	G	2001	PQN	C17-C18-C20-C21
14	e	2001	PQN	C17-C18-C20-C21
13	G	1237	CLA	C3-C5-C6-C7
13	e	1237	CLA	C3-C5-C6-C7
16	5	522	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	c	522	BCR	C9-C10-C11-C12
16	u	522	BCR	C9-C10-C11-C12
13	B	1227	CLA	C16-C17-C18-C19
13	H	1227	CLA	C16-C17-C18-C19
13	f	1227	CLA	C16-C17-C18-C19
17	G	5008	LHG	C11-C12-C13-C14
13	R	1301	CLA	CBA-CGA-O2A-C1
17	A	5008	LHG	C11-C12-C13-C14
17	e	5008	LHG	C11-C12-C13-C14
13	T	1303	CLA	C5-C6-C7-C8
13	f	1223	CLA	CBD-CGD-O2D-CED
17	A	5007	LHG	C10-C11-C12-C13
17	G	5007	LHG	C10-C11-C12-C13
17	e	5007	LHG	C10-C11-C12-C13
13	J	1303	CLA	C5-C6-C7-C8
17	A	5003	LHG	C13-C14-C15-C16
17	G	5003	LHG	C13-C14-C15-C16
17	e	5003	LHG	C13-C14-C15-C16
13	A	1103	CLA	C3-C5-C6-C7
13	G	1103	CLA	C3-C5-C6-C7
13	e	1103	CLA	C3-C5-C6-C7
13	B	1023	CLA	C4C-C3C-CAC-CBC
13	B	1223	CLA	CBD-CGD-O2D-CED
13	2	518	CLA	C13-C15-C16-C17
13	Z	518	CLA	C13-C15-C16-C17
13	f	1219	CLA	C8-C10-C11-C12
13	l	1303	CLA	C5-C6-C7-C8
13	r	518	CLA	C13-C15-C16-C17
13	B	1236	CLA	CBA-CGA-O2A-C1
13	F	1301	CLA	CBA-CGA-O2A-C1
13	4	518	CLA	CBA-CGA-O2A-C1
13	H	1236	CLA	CBA-CGA-O2A-C1
13	b	518	CLA	CBA-CGA-O2A-C1
13	f	1236	CLA	CBA-CGA-O2A-C1
13	j	1301	CLA	CBA-CGA-O2A-C1
13	t	518	CLA	CBA-CGA-O2A-C1
13	5	518	CLA	O1D-CGD-O2D-CED
17	A	5003	LHG	C23-C24-C25-C26
17	G	5003	LHG	C23-C24-C25-C26
17	e	5003	LHG	C23-C24-C25-C26
13	f	1023	CLA	C4C-C3C-CAC-CBC
13	B	1219	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	G	1130	CLA	C5-C6-C7-C8
13	H	1219	CLA	C8-C10-C11-C12
13	r	513	CLA	O1A-CGA-O2A-C1
13	H	1223	CLA	CBD-CGD-O2D-CED
17	B	1842	LHG	C30-C31-C32-C33
17	G	5009	LHG	C34-C35-C36-C37
17	H	1842	LHG	C30-C31-C32-C33
17	e	5009	LHG	C34-C35-C36-C37
13	A	1102	CLA	CAD-CBD-CGD-O2D
13	A	1110	CLA	CAD-CBD-CGD-O2D
13	A	1116	CLA	CAD-CBD-CGD-O2D
13	B	1012	CLA	CAD-CBD-CGD-O2D
13	B	1201	CLA	CAD-CBD-CGD-O2D
13	B	1208	CLA	CAD-CBD-CGD-O2D
13	B	1214	CLA	CAD-CBD-CGD-O2D
13	B	1217	CLA	CAD-CBD-CGD-O2D
13	B	1218	CLA	CAD-CBD-CGD-O2D
13	B	1238	CLA	CAD-CBD-CGD-O2D
13	B	1230	CLA	CAD-CBD-CGD-O2D
13	J	1302	CLA	CAD-CBD-CGD-O2D
13	K	1105	CLA	CAD-CBD-CGD-O2D
13	1	505	CLA	CAD-CBD-CGD-O2D
13	1	516	CLA	CAD-CBD-CGD-O2D
13	1	519	CLA	CAD-CBD-CGD-O2D
13	2	513	CLA	CAD-CBD-CGD-O2D
13	2	519	CLA	CAD-CBD-CGD-O2D
13	3	505	CLA	CAD-CBD-CGD-O2D
13	3	510	CLA	CAD-CBD-CGD-O2D
13	4	509	CLA	CAD-CBD-CGD-O2D
13	5	501	CLA	CAD-CBD-CGD-O2D
13	5	504	CLA	CAD-CBD-CGD-O2D
13	G	1102	CLA	CAD-CBD-CGD-O2D
13	G	1110	CLA	CAD-CBD-CGD-O2D
13	G	1116	CLA	CAD-CBD-CGD-O2D
13	H	1012	CLA	CAD-CBD-CGD-O2D
13	H	1201	CLA	CAD-CBD-CGD-O2D
13	H	1208	CLA	CAD-CBD-CGD-O2D
13	H	1214	CLA	CAD-CBD-CGD-O2D
13	H	1217	CLA	CAD-CBD-CGD-O2D
13	H	1218	CLA	CAD-CBD-CGD-O2D
13	H	1238	CLA	CAD-CBD-CGD-O2D
13	H	1230	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	T	1302	CLA	CAD-CBD-CGD-O2D
13	U	1105	CLA	CAD-CBD-CGD-O2D
13	Y	505	CLA	CAD-CBD-CGD-O2D
13	Y	516	CLA	CAD-CBD-CGD-O2D
13	Y	519	CLA	CAD-CBD-CGD-O2D
13	Z	513	CLA	CAD-CBD-CGD-O2D
13	Z	519	CLA	CAD-CBD-CGD-O2D
13	a	505	CLA	CAD-CBD-CGD-O2D
13	a	510	CLA	CAD-CBD-CGD-O2D
13	b	509	CLA	CAD-CBD-CGD-O2D
13	c	501	CLA	CAD-CBD-CGD-O2D
13	c	504	CLA	CAD-CBD-CGD-O2D
13	e	1102	CLA	CAD-CBD-CGD-O2D
13	e	1110	CLA	CAD-CBD-CGD-O2D
13	e	1116	CLA	CAD-CBD-CGD-O2D
13	f	1012	CLA	CAD-CBD-CGD-O2D
13	f	1201	CLA	CAD-CBD-CGD-O2D
13	f	1208	CLA	CAD-CBD-CGD-O2D
13	f	1214	CLA	CAD-CBD-CGD-O2D
13	f	1217	CLA	CAD-CBD-CGD-O2D
13	f	1218	CLA	CAD-CBD-CGD-O2D
13	f	1238	CLA	CAD-CBD-CGD-O2D
13	f	1230	CLA	CAD-CBD-CGD-O2D
13	l	1302	CLA	CAD-CBD-CGD-O2D
13	m	1105	CLA	CAD-CBD-CGD-O2D
13	q	505	CLA	CAD-CBD-CGD-O2D
13	q	516	CLA	CAD-CBD-CGD-O2D
13	q	519	CLA	CAD-CBD-CGD-O2D
13	r	513	CLA	CAD-CBD-CGD-O2D
13	r	519	CLA	CAD-CBD-CGD-O2D
13	s	505	CLA	CAD-CBD-CGD-O2D
13	s	510	CLA	CAD-CBD-CGD-O2D
13	t	509	CLA	CAD-CBD-CGD-O2D
13	u	501	CLA	CAD-CBD-CGD-O2D
13	u	504	CLA	CAD-CBD-CGD-O2D
17	B	1855	LHG	C6-C5-O7-C7
17	H	1855	LHG	C6-C5-O7-C7
17	f	1855	LHG	C6-C5-O7-C7
13	c	518	CLA	O1D-CGD-O2D-CED
13	u	518	CLA	O1D-CGD-O2D-CED
13	H	1023	CLA	C4C-C3C-CAC-CBC
17	A	5009	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
17	f	1842	LHG	C30-C31-C32-C33
13	A	1130	CLA	C5-C6-C7-C8
13	e	1130	CLA	C5-C6-C7-C8
13	2	513	CLA	O1A-CGA-O2A-C1
13	Z	513	CLA	O1A-CGA-O2A-C1
13	6	503	CLA	CBA-CGA-O2A-C1
13	d	503	CLA	CBA-CGA-O2A-C1
13	v	503	CLA	CBA-CGA-O2A-C1
13	5	505	CLA	C4-C3-C5-C6
13	c	505	CLA	C4-C3-C5-C6
13	u	505	CLA	C4-C3-C5-C6
18	A	1848	LMU	O5'-C1'-O1'-C1
18	G	1848	LMU	O5'-C1'-O1'-C1
18	e	1848	LMU	O5'-C1'-O1'-C1
19	J	5104	LMG	O6-C1-O1-C7
19	T	5104	LMG	O6-C1-O1-C7
19	l	5104	LMG	O6-C1-O1-C7
20	5	822	SQD	O5-C1-O6-C44
20	c	822	SQD	O5-C1-O6-C44
20	u	822	SQD	O5-C1-O6-C44
17	A	5007	LHG	C34-C35-C36-C37
17	e	5007	LHG	C34-C35-C36-C37
20	1	822	SQD	C28-C29-C30-C31
20	Y	822	SQD	C28-C29-C30-C31
20	q	822	SQD	C28-C29-C30-C31
17	A	5008	LHG	C4-C5-C6-O8
17	A	5009	LHG	C5-C4-O6-P
17	L	5221	LHG	C4-C5-C6-O8
17	G	5008	LHG	C4-C5-C6-O8
17	G	5009	LHG	C5-C4-O6-P
17	V	5221	LHG	C4-C5-C6-O8
17	e	5008	LHG	C4-C5-C6-O8
17	e	5009	LHG	C5-C4-O6-P
17	k	5001	LHG	C2-C3-O3-P
17	n	5221	LHG	C4-C5-C6-O8
19	J	5104	LMG	C7-C8-C9-O8
19	T	5104	LMG	C7-C8-C9-O8
19	l	5104	LMG	C7-C8-C9-O8
20	L	5216	SQD	C44-C45-C46-O48
20	1	822	SQD	O6-C44-C45-C46
20	V	5216	SQD	C44-C45-C46-O48
20	Y	822	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
20	n	5216	SQD	C44-C45-C46-O48
20	q	822	SQD	O6-C44-C45-C46
13	1	501	CLA	O1A-CGA-O2A-C1
13	3	508	CLA	O1A-CGA-O2A-C1
13	e	1103	CLA	O1A-CGA-O2A-C1
13	s	508	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	O6-C4-C5-O7
17	L	5218	LHG	O6-C4-C5-O7
17	G	5002	LHG	O6-C4-C5-O7
17	V	5218	LHG	O6-C4-C5-O7
17	e	5002	LHG	O6-C4-C5-O7
17	n	5218	LHG	O6-C4-C5-O7
13	B	1215	CLA	C5-C6-C7-C8
17	G	5007	LHG	C34-C35-C36-C37
13	H	1215	CLA	C5-C6-C7-C8
13	u	509	CLA	C5-C6-C7-C8
17	A	5002	LHG	C33-C34-C35-C36
17	G	5002	LHG	C33-C34-C35-C36
17	e	5002	LHG	C33-C34-C35-C36
13	a	508	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	C14-C15-C16-C17
20	B	1852	SQD	O49-C7-O47-C45
20	H	1852	SQD	O49-C7-O47-C45
20	f	1852	SQD	O49-C7-O47-C45
13	A	1106	CLA	CHA-CBD-CGD-O1D
13	A	1106	CLA	CHA-CBD-CGD-O2D
13	A	1108	CLA	CHA-CBD-CGD-O1D
13	A	1111	CLA	CHA-CBD-CGD-O1D
13	A	1118	CLA	CHA-CBD-CGD-O1D
13	A	1128	CLA	CHA-CBD-CGD-O1D
13	A	1128	CLA	CHA-CBD-CGD-O2D
13	A	1132	CLA	CHA-CBD-CGD-O1D
13	A	1801	CLA	CHA-CBD-CGD-O1D
13	B	1021	CLA	CHA-CBD-CGD-O2D
13	B	1202	CLA	CHA-CBD-CGD-O1D
13	B	1205	CLA	CHA-CBD-CGD-O1D
13	B	1205	CLA	CHA-CBD-CGD-O2D
13	B	1222	CLA	CHA-CBD-CGD-O1D
13	B	1222	CLA	CHA-CBD-CGD-O2D
13	B	1207	CLA	CHA-CBD-CGD-O1D
13	B	1207	CLA	CHA-CBD-CGD-O2D
13	J	1303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	J	1303	CLA	CHA-CBD-CGD-O2D
13	K	1103	CLA	CHA-CBD-CGD-O1D
13	K	1103	CLA	CHA-CBD-CGD-O2D
13	1	502	CLA	CHA-CBD-CGD-O1D
13	1	503	CLA	CHA-CBD-CGD-O1D
13	1	503	CLA	CHA-CBD-CGD-O2D
13	1	504	CLA	CHA-CBD-CGD-O1D
13	1	504	CLA	CHA-CBD-CGD-O2D
13	2	502	CLA	CHA-CBD-CGD-O2D
13	2	503	CLA	CHA-CBD-CGD-O1D
13	2	503	CLA	CHA-CBD-CGD-O2D
13	2	506	CLA	CHA-CBD-CGD-O1D
13	2	506	CLA	CHA-CBD-CGD-O2D
13	2	507	CLA	CHA-CBD-CGD-O1D
13	2	507	CLA	CHA-CBD-CGD-O2D
13	2	517	CLA	CHA-CBD-CGD-O1D
13	3	503	CLA	CHA-CBD-CGD-O1D
13	3	503	CLA	CHA-CBD-CGD-O2D
13	3	504	CLA	CHA-CBD-CGD-O1D
13	3	504	CLA	CHA-CBD-CGD-O2D
13	3	506	CLA	CHA-CBD-CGD-O1D
13	3	506	CLA	CHA-CBD-CGD-O2D
13	3	507	CLA	CHA-CBD-CGD-O1D
13	3	517	CLA	CHA-CBD-CGD-O1D
13	3	517	CLA	CHA-CBD-CGD-O2D
13	4	501	CLA	CHA-CBD-CGD-O2D
13	4	502	CLA	CHA-CBD-CGD-O1D
13	4	502	CLA	CHA-CBD-CGD-O2D
13	4	504	CLA	CHA-CBD-CGD-O1D
13	4	504	CLA	CHA-CBD-CGD-O2D
13	4	507	CLA	CHA-CBD-CGD-O1D
13	4	507	CLA	CHA-CBD-CGD-O2D
13	4	516	CLA	CHA-CBD-CGD-O1D
13	5	503	CLA	CHA-CBD-CGD-O1D
13	5	503	CLA	CHA-CBD-CGD-O2D
13	5	510	CLA	CHA-CBD-CGD-O1D
13	5	510	CLA	CHA-CBD-CGD-O2D
13	6	503	CLA	CHA-CBD-CGD-O1D
13	6	503	CLA	CHA-CBD-CGD-O2D
13	G	1106	CLA	CHA-CBD-CGD-O1D
13	G	1106	CLA	CHA-CBD-CGD-O2D
13	G	1108	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	G	1108	CLA	CHA-CBD-CGD-O2D
13	G	1111	CLA	CHA-CBD-CGD-O1D
13	G	1118	CLA	CHA-CBD-CGD-O1D
13	G	1128	CLA	CHA-CBD-CGD-O1D
13	G	1128	CLA	CHA-CBD-CGD-O2D
13	G	1132	CLA	CHA-CBD-CGD-O1D
13	G	1801	CLA	CHA-CBD-CGD-O1D
13	H	1021	CLA	CHA-CBD-CGD-O2D
13	H	1202	CLA	CHA-CBD-CGD-O1D
13	H	1205	CLA	CHA-CBD-CGD-O1D
13	H	1205	CLA	CHA-CBD-CGD-O2D
13	H	1222	CLA	CHA-CBD-CGD-O1D
13	H	1222	CLA	CHA-CBD-CGD-O2D
13	H	1207	CLA	CHA-CBD-CGD-O1D
13	H	1207	CLA	CHA-CBD-CGD-O2D
13	T	1303	CLA	CHA-CBD-CGD-O1D
13	T	1303	CLA	CHA-CBD-CGD-O2D
13	U	1103	CLA	CHA-CBD-CGD-O1D
13	U	1103	CLA	CHA-CBD-CGD-O2D
13	Y	502	CLA	CHA-CBD-CGD-O1D
13	Y	503	CLA	CHA-CBD-CGD-O1D
13	Y	503	CLA	CHA-CBD-CGD-O2D
13	Y	504	CLA	CHA-CBD-CGD-O1D
13	Y	504	CLA	CHA-CBD-CGD-O2D
13	Z	502	CLA	CHA-CBD-CGD-O2D
13	Z	503	CLA	CHA-CBD-CGD-O1D
13	Z	503	CLA	CHA-CBD-CGD-O2D
13	Z	506	CLA	CHA-CBD-CGD-O1D
13	Z	506	CLA	CHA-CBD-CGD-O2D
13	Z	507	CLA	CHA-CBD-CGD-O1D
13	Z	507	CLA	CHA-CBD-CGD-O2D
13	Z	517	CLA	CHA-CBD-CGD-O1D
13	a	503	CLA	CHA-CBD-CGD-O1D
13	a	503	CLA	CHA-CBD-CGD-O2D
13	a	504	CLA	CHA-CBD-CGD-O1D
13	a	504	CLA	CHA-CBD-CGD-O2D
13	a	506	CLA	CHA-CBD-CGD-O1D
13	a	506	CLA	CHA-CBD-CGD-O2D
13	a	507	CLA	CHA-CBD-CGD-O1D
13	a	517	CLA	CHA-CBD-CGD-O1D
13	a	517	CLA	CHA-CBD-CGD-O2D
13	b	501	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	b	501	CLA	CHA-CBD-CGD-O2D
13	b	502	CLA	CHA-CBD-CGD-O1D
13	b	502	CLA	CHA-CBD-CGD-O2D
13	b	504	CLA	CHA-CBD-CGD-O1D
13	b	504	CLA	CHA-CBD-CGD-O2D
13	b	507	CLA	CHA-CBD-CGD-O1D
13	b	507	CLA	CHA-CBD-CGD-O2D
13	b	516	CLA	CHA-CBD-CGD-O1D
13	c	503	CLA	CHA-CBD-CGD-O1D
13	c	503	CLA	CHA-CBD-CGD-O2D
13	c	510	CLA	CHA-CBD-CGD-O1D
13	c	510	CLA	CHA-CBD-CGD-O2D
13	d	503	CLA	CHA-CBD-CGD-O1D
13	d	503	CLA	CHA-CBD-CGD-O2D
13	e	1106	CLA	CHA-CBD-CGD-O1D
13	e	1106	CLA	CHA-CBD-CGD-O2D
13	e	1108	CLA	CHA-CBD-CGD-O1D
13	e	1111	CLA	CHA-CBD-CGD-O1D
13	e	1118	CLA	CHA-CBD-CGD-O1D
13	e	1128	CLA	CHA-CBD-CGD-O1D
13	e	1128	CLA	CHA-CBD-CGD-O2D
13	e	1132	CLA	CHA-CBD-CGD-O1D
13	e	1801	CLA	CHA-CBD-CGD-O1D
13	f	1021	CLA	CHA-CBD-CGD-O2D
13	f	1202	CLA	CHA-CBD-CGD-O1D
13	f	1205	CLA	CHA-CBD-CGD-O1D
13	f	1205	CLA	CHA-CBD-CGD-O2D
13	f	1222	CLA	CHA-CBD-CGD-O1D
13	f	1222	CLA	CHA-CBD-CGD-O2D
13	f	1207	CLA	CHA-CBD-CGD-O1D
13	f	1207	CLA	CHA-CBD-CGD-O2D
13	l	1303	CLA	CHA-CBD-CGD-O1D
13	l	1303	CLA	CHA-CBD-CGD-O2D
13	m	1103	CLA	CHA-CBD-CGD-O1D
13	m	1103	CLA	CHA-CBD-CGD-O2D
13	q	502	CLA	CHA-CBD-CGD-O1D
13	q	503	CLA	CHA-CBD-CGD-O1D
13	q	503	CLA	CHA-CBD-CGD-O2D
13	q	504	CLA	CHA-CBD-CGD-O1D
13	q	504	CLA	CHA-CBD-CGD-O2D
13	r	502	CLA	CHA-CBD-CGD-O2D
13	r	503	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	r	503	CLA	CHA-CBD-CGD-O2D
13	r	506	CLA	CHA-CBD-CGD-O1D
13	r	506	CLA	CHA-CBD-CGD-O2D
13	r	507	CLA	CHA-CBD-CGD-O1D
13	r	507	CLA	CHA-CBD-CGD-O2D
13	r	517	CLA	CHA-CBD-CGD-O1D
13	s	503	CLA	CHA-CBD-CGD-O1D
13	s	503	CLA	CHA-CBD-CGD-O2D
13	s	504	CLA	CHA-CBD-CGD-O1D
13	s	504	CLA	CHA-CBD-CGD-O2D
13	s	506	CLA	CHA-CBD-CGD-O1D
13	s	506	CLA	CHA-CBD-CGD-O2D
13	s	507	CLA	CHA-CBD-CGD-O1D
13	s	517	CLA	CHA-CBD-CGD-O1D
13	s	517	CLA	CHA-CBD-CGD-O2D
13	t	501	CLA	CHA-CBD-CGD-O2D
13	t	502	CLA	CHA-CBD-CGD-O1D
13	t	502	CLA	CHA-CBD-CGD-O2D
13	t	504	CLA	CHA-CBD-CGD-O1D
13	t	504	CLA	CHA-CBD-CGD-O2D
13	t	507	CLA	CHA-CBD-CGD-O1D
13	t	507	CLA	CHA-CBD-CGD-O2D
13	t	516	CLA	CHA-CBD-CGD-O1D
13	u	503	CLA	CHA-CBD-CGD-O1D
13	u	503	CLA	CHA-CBD-CGD-O2D
13	u	510	CLA	CHA-CBD-CGD-O1D
13	u	510	CLA	CHA-CBD-CGD-O2D
13	v	503	CLA	CHA-CBD-CGD-O1D
13	v	503	CLA	CHA-CBD-CGD-O2D
13	5	509	CLA	C5-C6-C7-C8
13	c	509	CLA	C5-C6-C7-C8
17	e	5001	LHG	C14-C15-C16-C17
13	2	508	CLA	O1D-CGD-O2D-CED
13	r	508	CLA	O1D-CGD-O2D-CED
13	B	1217	CLA	C3-C5-C6-C7
13	2	506	CLA	C3-C5-C6-C7
13	H	1217	CLA	C3-C5-C6-C7
13	Z	506	CLA	C3-C5-C6-C7
13	f	1217	CLA	C3-C5-C6-C7
13	r	506	CLA	C3-C5-C6-C7
13	A	1103	CLA	O1A-CGA-O2A-C1
13	G	1103	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	Y	501	CLA	O1A-CGA-O2A-C1
13	q	501	CLA	O1A-CGA-O2A-C1
17	G	5001	LHG	C14-C15-C16-C17
18	2	901	LMU	C5-C6-C7-C8
18	r	901	LMU	C5-C6-C7-C8
13	A	1122	CLA	O1D-CGD-O2D-CED
13	G	1122	CLA	O1D-CGD-O2D-CED
13	Z	508	CLA	O1D-CGD-O2D-CED
13	e	1122	CLA	O1D-CGD-O2D-CED
13	f	1215	CLA	C5-C6-C7-C8
18	Z	901	LMU	C5-C6-C7-C8
17	A	5007	LHG	O7-C5-C6-O8
17	L	5220	LHG	O7-C5-C6-O8
17	G	5007	LHG	O7-C5-C6-O8
17	V	5220	LHG	O7-C5-C6-O8
17	e	5007	LHG	O7-C5-C6-O8
17	n	5220	LHG	O7-C5-C6-O8
20	B	1852	SQD	O6-C44-C45-O47
20	2	822	SQD	O47-C45-C46-O48
20	4	822	SQD	O47-C45-C46-O48
20	H	1852	SQD	O6-C44-C45-O47
20	Z	822	SQD	O47-C45-C46-O48
20	b	822	SQD	O47-C45-C46-O48
20	f	1852	SQD	O6-C44-C45-O47
20	r	822	SQD	O47-C45-C46-O48
20	t	822	SQD	O47-C45-C46-O48
13	B	1212	CLA	C5-C6-C7-C8
13	H	1212	CLA	C5-C6-C7-C8
13	H	1223	CLA	C5-C6-C7-C8
13	f	1212	CLA	C5-C6-C7-C8
13	1	507	CLA	O1A-CGA-O2A-C1
13	Y	507	CLA	O1A-CGA-O2A-C1
17	B	1855	LHG	C18-C19-C20-C21
17	f	1855	LHG	C18-C19-C20-C21
17	A	5001	LHG	O1-C1-C2-O2
17	L	5221	LHG	O1-C1-C2-O2
17	G	5001	LHG	O1-C1-C2-O2
17	V	5221	LHG	O1-C1-C2-O2
17	e	5001	LHG	O1-C1-C2-O2
17	n	5221	LHG	O1-C1-C2-O2
17	H	1855	LHG	C18-C19-C20-C21
13	B	1204	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	H	1204	CLA	C4-C3-C5-C6
13	f	1204	CLA	C4-C3-C5-C6
13	A	1108	CLA	C6-C7-C8-C9
13	G	1108	CLA	C6-C7-C8-C9
13	4	518	CLA	O1A-CGA-O2A-C1
13	q	507	CLA	O1A-CGA-O2A-C1
13	L	1501	CLA	C2-C3-C5-C6
13	V	1501	CLA	C2-C3-C5-C6
13	e	1108	CLA	C6-C7-C8-C9
13	B	1202	CLA	C15-C16-C17-C18
13	B	1223	CLA	C5-C6-C7-C8
13	f	1202	CLA	C15-C16-C17-C18
13	f	1223	CLA	C5-C6-C7-C8
13	A	1104	CLA	C14-C13-C15-C16
13	A	1106	CLA	C11-C12-C13-C14
13	B	1210	CLA	C11-C12-C13-C14
13	B	1214	CLA	C11-C12-C13-C14
13	G	1104	CLA	C14-C13-C15-C16
13	G	1106	CLA	C11-C12-C13-C14
13	H	1210	CLA	C11-C12-C13-C14
13	H	1214	CLA	C11-C12-C13-C14
13	R	1301	CLA	C6-C7-C8-C9
13	e	1104	CLA	C14-C13-C15-C16
13	e	1106	CLA	C11-C12-C13-C14
13	f	1210	CLA	C11-C12-C13-C14
13	f	1214	CLA	C11-C12-C13-C14
13	j	1301	CLA	C6-C7-C8-C9
13	2	505	CLA	O1D-CGD-O2D-CED
13	B	1236	CLA	O1A-CGA-O2A-C1
13	G	1125	CLA	O1A-CGA-O2A-C1
13	H	1236	CLA	O1A-CGA-O2A-C1
13	b	518	CLA	O1A-CGA-O2A-C1
13	e	1125	CLA	O1A-CGA-O2A-C1
13	f	1236	CLA	O1A-CGA-O2A-C1
13	t	518	CLA	O1A-CGA-O2A-C1
13	H	1202	CLA	C15-C16-C17-C18
20	4	822	SQD	C5-C6-S-O8
20	b	822	SQD	C5-C6-S-O8
20	t	822	SQD	C5-C6-S-O8
13	r	505	CLA	O1D-CGD-O2D-CED
13	A	1121	CLA	CAA-CBA-CGA-O2A
13	G	1121	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	e	1121	CLA	CAA-CBA-CGA-O2A
13	A	1125	CLA	O1A-CGA-O2A-C1
13	F	1301	CLA	O1A-CGA-O2A-C1
13	R	1301	CLA	O1A-CGA-O2A-C1
13	j	1301	CLA	O1A-CGA-O2A-C1
16	6	521	BCR	C7-C8-C9-C34
16	d	521	BCR	C7-C8-C9-C34
16	v	521	BCR	C7-C8-C9-C34
13	B	1234	CLA	C15-C16-C17-C18
13	H	1234	CLA	C15-C16-C17-C18
13	f	1234	CLA	C15-C16-C17-C18
16	3	524	BCR	C21-C22-C23-C24
16	4	521	BCR	C17-C18-C19-C20
16	a	524	BCR	C21-C22-C23-C24
16	b	521	BCR	C17-C18-C19-C20
16	s	524	BCR	C21-C22-C23-C24
16	t	521	BCR	C17-C18-C19-C20
13	Z	505	CLA	O1D-CGD-O2D-CED
13	A	1129	CLA	C1A-C2A-CAA-CBA
13	A	1022	CLA	C1A-C2A-CAA-CBA
13	1	508	CLA	C1A-C2A-CAA-CBA
13	3	501	CLA	C1A-C2A-CAA-CBA
13	3	516	CLA	C1A-C2A-CAA-CBA
13	4	501	CLA	C1A-C2A-CAA-CBA
13	5	503	CLA	C1A-C2A-CAA-CBA
13	G	1129	CLA	C1A-C2A-CAA-CBA
13	G	1022	CLA	C1A-C2A-CAA-CBA
13	Y	508	CLA	C1A-C2A-CAA-CBA
13	Z	503	CLA	C1A-C2A-CAA-CBA
13	a	501	CLA	C1A-C2A-CAA-CBA
13	a	516	CLA	C1A-C2A-CAA-CBA
13	b	501	CLA	C1A-C2A-CAA-CBA
13	c	503	CLA	C1A-C2A-CAA-CBA
13	e	1129	CLA	C1A-C2A-CAA-CBA
13	e	1022	CLA	C1A-C2A-CAA-CBA
13	q	508	CLA	C1A-C2A-CAA-CBA
13	s	501	CLA	C1A-C2A-CAA-CBA
13	s	516	CLA	C1A-C2A-CAA-CBA
13	t	501	CLA	C1A-C2A-CAA-CBA
13	u	503	CLA	C1A-C2A-CAA-CBA
13	B	1201	CLA	C11-C12-C13-C14
13	f	1201	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	A	1125	CLA	CBA-CGA-O2A-C1
13	B	1021	CLA	CBA-CGA-O2A-C1
13	4	509	CLA	CBA-CGA-O2A-C1
13	G	1125	CLA	CBA-CGA-O2A-C1
13	H	1021	CLA	CBA-CGA-O2A-C1
13	b	509	CLA	CBA-CGA-O2A-C1
13	e	1125	CLA	CBA-CGA-O2A-C1
13	f	1021	CLA	CBA-CGA-O2A-C1
13	t	509	CLA	CBA-CGA-O2A-C1
16	J	4015	BCR	C15-C16-C17-C18
16	3	522	BCR	C9-C10-C11-C12
16	T	4015	BCR	C15-C16-C17-C18
16	a	522	BCR	C9-C10-C11-C12
16	l	4015	BCR	C15-C16-C17-C18
16	s	522	BCR	C9-C10-C11-C12
13	B	1223	CLA	O1D-CGD-O2D-CED
13	f	1223	CLA	O1D-CGD-O2D-CED
17	A	5007	LHG	C3-O3-P-O6
17	G	5007	LHG	C3-O3-P-O6
17	e	5007	LHG	C3-O3-P-O6
17	A	5005	LHG	C12-C13-C14-C15
17	G	5005	LHG	C12-C13-C14-C15
17	e	5005	LHG	C12-C13-C14-C15
13	H	1223	CLA	O1D-CGD-O2D-CED
13	5	503	CLA	C4-C3-C5-C6
13	c	503	CLA	C4-C3-C5-C6
13	u	503	CLA	C4-C3-C5-C6
13	A	1123	CLA	C15-C16-C17-C18
13	e	1123	CLA	C15-C16-C17-C18
17	I	5001	LHG	C2-C3-O3-P
17	S	5001	LHG	C2-C3-O3-P
13	A	1108	CLA	C2-C3-C5-C6
13	A	1137	CLA	C2-C3-C5-C6
13	J	1303	CLA	C2-C3-C5-C6
13	G	1108	CLA	C2-C3-C5-C6
13	G	1137	CLA	C2-C3-C5-C6
13	e	1108	CLA	C2-C3-C5-C6
13	e	1137	CLA	C2-C3-C5-C6
13	l	1303	CLA	C2-C3-C5-C6
13	n	1501	CLA	C2-C3-C5-C6
13	4	509	CLA	O1A-CGA-O2A-C1
13	b	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	1110	CLA	C4B-C3B-CAB-CBB
13	B	1205	CLA	C4B-C3B-CAB-CBB
13	B	1236	CLA	C4B-C3B-CAB-CBB
13	2	512	CLA	C4B-C3B-CAB-CBB
13	6	513	CLA	C4B-C3B-CAB-CBB
13	G	1110	CLA	C4B-C3B-CAB-CBB
13	H	1205	CLA	C4B-C3B-CAB-CBB
13	H	1236	CLA	C4B-C3B-CAB-CBB
13	Z	512	CLA	C4B-C3B-CAB-CBB
13	d	513	CLA	C4B-C3B-CAB-CBB
13	e	1110	CLA	C4B-C3B-CAB-CBB
13	f	1205	CLA	C4B-C3B-CAB-CBB
13	f	1236	CLA	C4B-C3B-CAB-CBB
13	r	512	CLA	C4B-C3B-CAB-CBB
13	v	513	CLA	C4B-C3B-CAB-CBB
17	A	5002	LHG	C3-O3-P-O5
17	A	5002	LHG	C4-O6-P-O4
17	A	5007	LHG	C3-O3-P-O4
17	A	5008	LHG	C4-O6-P-O4
17	B	1855	LHG	C3-O3-P-O5
17	B	1855	LHG	C4-O6-P-O4
17	I	5001	LHG	C4-O6-P-O4
17	L	5221	LHG	C3-O3-P-O4
17	G	5002	LHG	C3-O3-P-O5
17	G	5002	LHG	C4-O6-P-O4
17	G	5005	LHG	C3-O3-P-O5
17	G	5007	LHG	C3-O3-P-O4
17	G	5008	LHG	C4-O6-P-O4
17	H	1855	LHG	C3-O3-P-O5
17	H	1855	LHG	C4-O6-P-O4
17	S	5001	LHG	C4-O6-P-O4
17	V	5221	LHG	C3-O3-P-O4
17	e	5002	LHG	C3-O3-P-O5
17	e	5002	LHG	C4-O6-P-O4
17	e	5007	LHG	C3-O3-P-O4
17	e	5008	LHG	C4-O6-P-O4
17	f	1855	LHG	C3-O3-P-O5
17	f	1855	LHG	C4-O6-P-O4
17	k	5001	LHG	C4-O6-P-O4
17	n	5221	LHG	C3-O3-P-O4
13	H	1201	CLA	C11-C12-C13-C14
13	2	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	5	501	CLA	C15-C16-C17-C18
13	G	1123	CLA	C15-C16-C17-C18
13	Z	508	CLA	C5-C6-C7-C8
13	a	501	CLA	C15-C16-C17-C18
13	c	501	CLA	C15-C16-C17-C18
13	r	508	CLA	C5-C6-C7-C8
13	u	501	CLA	C15-C16-C17-C18
13	L	1501	CLA	CBA-CGA-O2A-C1
13	V	1501	CLA	CBA-CGA-O2A-C1
17	B	1855	LHG	O6-C4-C5-C6
17	H	1855	LHG	O6-C4-C5-C6
17	f	1855	LHG	O6-C4-C5-C6
13	t	509	CLA	O1A-CGA-O2A-C1
13	3	501	CLA	C15-C16-C17-C18
13	s	501	CLA	C15-C16-C17-C18
13	B	1213	CLA	C2A-CAA-CBA-CGA
13	2	517	CLA	C2A-CAA-CBA-CGA
13	H	1213	CLA	C2A-CAA-CBA-CGA
13	Y	513	CLA	C2A-CAA-CBA-CGA
13	Z	517	CLA	C2A-CAA-CBA-CGA
13	f	1213	CLA	C2A-CAA-CBA-CGA
13	r	517	CLA	C2A-CAA-CBA-CGA
13	L	1502	CLA	C3-C5-C6-C7
13	V	1502	CLA	C3-C5-C6-C7
13	n	1502	CLA	C3-C5-C6-C7
13	A	1013	CLA	C16-C17-C18-C19
13	G	1013	CLA	C16-C17-C18-C19
13	e	1013	CLA	C16-C17-C18-C19
13	A	1011	CLA	CAD-CBD-CGD-O1D
13	A	1801	CLA	CAD-CBD-CGD-O1D
13	B	1202	CLA	CAD-CBD-CGD-O1D
13	B	1207	CLA	CAD-CBD-CGD-O1D
13	K	1103	CLA	CAD-CBD-CGD-O1D
13	1	502	CLA	CAD-CBD-CGD-O1D
13	1	503	CLA	CAD-CBD-CGD-O1D
13	1	504	CLA	CAD-CBD-CGD-O1D
13	1	506	CLA	CAD-CBD-CGD-O1D
13	2	502	CLA	CAD-CBD-CGD-O1D
13	2	503	CLA	CAD-CBD-CGD-O1D
13	2	506	CLA	CAD-CBD-CGD-O1D
13	2	518	CLA	CAD-CBD-CGD-O1D
13	3	503	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	3	504	CLA	CAD-CBD-CGD-O1D
13	3	506	CLA	CAD-CBD-CGD-O1D
13	3	507	CLA	CAD-CBD-CGD-O1D
13	3	517	CLA	CAD-CBD-CGD-O1D
13	3	518	CLA	CAD-CBD-CGD-O1D
13	4	504	CLA	CAD-CBD-CGD-O1D
13	5	503	CLA	CAD-CBD-CGD-O1D
13	5	506	CLA	CAD-CBD-CGD-O1D
13	5	510	CLA	CAD-CBD-CGD-O1D
13	5	517	CLA	CAD-CBD-CGD-O1D
13	6	503	CLA	CAD-CBD-CGD-O1D
13	6	504	CLA	CAD-CBD-CGD-O1D
13	6	506	CLA	CAD-CBD-CGD-O1D
13	6	510	CLA	CAD-CBD-CGD-O1D
13	6	518	CLA	CAD-CBD-CGD-O1D
13	G	1011	CLA	CAD-CBD-CGD-O1D
13	G	1801	CLA	CAD-CBD-CGD-O1D
13	H	1202	CLA	CAD-CBD-CGD-O1D
13	H	1207	CLA	CAD-CBD-CGD-O1D
13	U	1103	CLA	CAD-CBD-CGD-O1D
13	Y	502	CLA	CAD-CBD-CGD-O1D
13	Y	503	CLA	CAD-CBD-CGD-O1D
13	Y	504	CLA	CAD-CBD-CGD-O1D
13	Y	506	CLA	CAD-CBD-CGD-O1D
13	Z	502	CLA	CAD-CBD-CGD-O1D
13	Z	503	CLA	CAD-CBD-CGD-O1D
13	Z	506	CLA	CAD-CBD-CGD-O1D
13	Z	518	CLA	CAD-CBD-CGD-O1D
13	a	503	CLA	CAD-CBD-CGD-O1D
13	a	504	CLA	CAD-CBD-CGD-O1D
13	a	506	CLA	CAD-CBD-CGD-O1D
13	a	507	CLA	CAD-CBD-CGD-O1D
13	a	516	CLA	CAD-CBD-CGD-O1D
13	a	517	CLA	CAD-CBD-CGD-O1D
13	a	518	CLA	CAD-CBD-CGD-O1D
13	b	504	CLA	CAD-CBD-CGD-O1D
13	c	503	CLA	CAD-CBD-CGD-O1D
13	c	506	CLA	CAD-CBD-CGD-O1D
13	c	510	CLA	CAD-CBD-CGD-O1D
13	c	517	CLA	CAD-CBD-CGD-O1D
13	d	503	CLA	CAD-CBD-CGD-O1D
13	d	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	d	506	CLA	CAD-CBD-CGD-O1D
13	d	510	CLA	CAD-CBD-CGD-O1D
13	d	518	CLA	CAD-CBD-CGD-O1D
13	e	1011	CLA	CAD-CBD-CGD-O1D
13	e	1801	CLA	CAD-CBD-CGD-O1D
13	f	1202	CLA	CAD-CBD-CGD-O1D
13	f	1207	CLA	CAD-CBD-CGD-O1D
13	m	1103	CLA	CAD-CBD-CGD-O1D
13	q	502	CLA	CAD-CBD-CGD-O1D
13	q	503	CLA	CAD-CBD-CGD-O1D
13	q	504	CLA	CAD-CBD-CGD-O1D
13	q	506	CLA	CAD-CBD-CGD-O1D
13	r	502	CLA	CAD-CBD-CGD-O1D
13	r	503	CLA	CAD-CBD-CGD-O1D
13	r	506	CLA	CAD-CBD-CGD-O1D
13	r	518	CLA	CAD-CBD-CGD-O1D
13	s	503	CLA	CAD-CBD-CGD-O1D
13	s	504	CLA	CAD-CBD-CGD-O1D
13	s	506	CLA	CAD-CBD-CGD-O1D
13	s	507	CLA	CAD-CBD-CGD-O1D
13	s	517	CLA	CAD-CBD-CGD-O1D
13	s	518	CLA	CAD-CBD-CGD-O1D
13	t	504	CLA	CAD-CBD-CGD-O1D
13	u	503	CLA	CAD-CBD-CGD-O1D
13	u	506	CLA	CAD-CBD-CGD-O1D
13	u	510	CLA	CAD-CBD-CGD-O1D
13	u	517	CLA	CAD-CBD-CGD-O1D
13	v	503	CLA	CAD-CBD-CGD-O1D
13	v	504	CLA	CAD-CBD-CGD-O1D
13	v	506	CLA	CAD-CBD-CGD-O1D
13	v	510	CLA	CAD-CBD-CGD-O1D
13	v	518	CLA	CAD-CBD-CGD-O1D
13	6	503	CLA	O1A-CGA-O2A-C1
13	d	503	CLA	O1A-CGA-O2A-C1
13	e	1237	CLA	C5-C6-C7-C8
13	B	1213	CLA	CBA-CGA-O2A-C1
13	n	1501	CLA	CBA-CGA-O2A-C1
13	v	503	CLA	O1A-CGA-O2A-C1
17	n	5218	LHG	C30-C31-C32-C33
13	A	1102	CLA	C16-C17-C18-C20
13	G	1102	CLA	C16-C17-C18-C20
13	e	1102	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	A	1104	CLA	C12-C13-C15-C16
13	B	1012	CLA	C12-C13-C15-C16
13	B	1208	CLA	C11-C12-C13-C15
13	B	1208	CLA	C12-C13-C15-C16
13	B	1210	CLA	C2-C3-C5-C6
13	B	1234	CLA	C12-C13-C15-C16
13	F	1301	CLA	C6-C7-C8-C10
13	J	1303	CLA	C6-C7-C8-C10
13	K	1401	CLA	C3A-C2A-CAA-CBA
13	1	502	CLA	C11-C10-C8-C7
13	2	513	CLA	C11-C10-C8-C7
13	3	505	CLA	C6-C7-C8-C10
13	3	505	CLA	C12-C13-C15-C16
13	3	513	CLA	C12-C13-C15-C16
13	6	505	CLA	C11-C12-C13-C15
13	G	1104	CLA	C12-C13-C15-C16
13	H	1012	CLA	C12-C13-C15-C16
13	H	1208	CLA	C11-C12-C13-C15
13	H	1208	CLA	C12-C13-C15-C16
13	H	1210	CLA	C2-C3-C5-C6
13	H	1234	CLA	C12-C13-C15-C16
13	R	1301	CLA	C6-C7-C8-C10
13	T	1303	CLA	C2-C3-C5-C6
13	T	1303	CLA	C6-C7-C8-C10
13	U	1401	CLA	C3A-C2A-CAA-CBA
13	Y	502	CLA	C11-C10-C8-C7
13	Z	513	CLA	C11-C10-C8-C7
13	a	505	CLA	C6-C7-C8-C10
13	a	505	CLA	C12-C13-C15-C16
13	a	513	CLA	C12-C13-C15-C16
13	d	505	CLA	C11-C12-C13-C15
13	e	1104	CLA	C12-C13-C15-C16
13	f	1012	CLA	C12-C13-C15-C16
13	f	1208	CLA	C11-C12-C13-C15
13	f	1208	CLA	C12-C13-C15-C16
13	f	1210	CLA	C2-C3-C5-C6
13	f	1234	CLA	C12-C13-C15-C16
13	j	1301	CLA	C6-C7-C8-C10
13	l	1303	CLA	C6-C7-C8-C10
13	m	1401	CLA	C3A-C2A-CAA-CBA
13	q	502	CLA	C11-C10-C8-C7
13	r	513	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	s	505	CLA	C6-C7-C8-C10
13	s	505	CLA	C12-C13-C15-C16
13	s	513	CLA	C12-C13-C15-C16
13	u	509	CLA	C11-C12-C13-C15
13	v	505	CLA	C11-C12-C13-C15
14	B	2002	PQN	C21-C22-C23-C25
14	H	2002	PQN	C21-C22-C23-C25
14	f	2002	PQN	C21-C22-C23-C25
17	A	5005	LHG	O6-C4-C5-O7
17	A	5007	LHG	O6-C4-C5-O7
17	G	5005	LHG	O6-C4-C5-O7
17	G	5007	LHG	O6-C4-C5-O7
17	e	5005	LHG	O6-C4-C5-O7
17	e	5007	LHG	O6-C4-C5-O7
17	L	5218	LHG	C30-C31-C32-C33
17	V	5218	LHG	C30-C31-C32-C33
13	A	1237	CLA	C5-C6-C7-C8
13	G	1237	CLA	C5-C6-C7-C8
18	2	901	LMU	C2-C1-O1'-C1'
18	r	901	LMU	C2-C1-O1'-C1'
13	B	1228	CLA	CAA-CBA-CGA-O2A
13	H	1228	CLA	CAA-CBA-CGA-O2A
13	f	1228	CLA	CAA-CBA-CGA-O2A
18	1	902	LMU	C3-C4-C5-C6
18	Y	902	LMU	C3-C4-C5-C6
18	q	902	LMU	C3-C4-C5-C6
13	f	1213	CLA	CBA-CGA-O2A-C1
13	H	1211	CLA	O1A-CGA-O2A-C1
13	B	1234	CLA	C5-C6-C7-C8
13	2	519	CLA	C5-C6-C7-C8
13	H	1234	CLA	C5-C6-C7-C8
13	Z	519	CLA	C5-C6-C7-C8
13	f	1234	CLA	C5-C6-C7-C8
13	r	505	CLA	C5-C6-C7-C8
13	r	519	CLA	C5-C6-C7-C8
13	1	513	CLA	C2A-CAA-CBA-CGA
13	q	513	CLA	C2A-CAA-CBA-CGA
13	B	1229	CLA	CAA-CBA-CGA-O2A
13	H	1229	CLA	CAA-CBA-CGA-O2A
13	f	1229	CLA	CAA-CBA-CGA-O2A
17	A	5006	LHG	C4-C5-C6-O8
17	G	5006	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
17	e	5006	LHG	C4-C5-C6-O8
20	L	5216	SQD	O6-C44-C45-C46
20	2	822	SQD	C44-C45-C46-O48
20	3	822	SQD	O6-C44-C45-C46
20	3	822	SQD	C44-C45-C46-O48
20	V	5216	SQD	O6-C44-C45-C46
20	Z	822	SQD	C44-C45-C46-O48
20	a	822	SQD	O6-C44-C45-C46
20	a	822	SQD	C44-C45-C46-O48
20	n	5216	SQD	O6-C44-C45-C46
20	r	822	SQD	C44-C45-C46-O48
20	s	822	SQD	O6-C44-C45-C46
20	s	822	SQD	C44-C45-C46-O48
13	B	1211	CLA	O1A-CGA-O2A-C1
13	f	1211	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	O7-C5-C6-O8
17	A	5004	LHG	O7-C5-C6-O8
17	A	5005	LHG	O7-C5-C6-O8
17	L	5221	LHG	O7-C5-C6-O8
17	G	5002	LHG	O7-C5-C6-O8
17	G	5004	LHG	O7-C5-C6-O8
17	G	5005	LHG	O7-C5-C6-O8
17	V	5221	LHG	O7-C5-C6-O8
17	e	5002	LHG	O7-C5-C6-O8
17	e	5004	LHG	O7-C5-C6-O8
17	e	5005	LHG	O7-C5-C6-O8
17	n	5221	LHG	O7-C5-C6-O8
20	3	822	SQD	O6-C44-C45-O47
20	6	822	SQD	O47-C45-C46-O48
20	a	822	SQD	O6-C44-C45-O47
20	d	822	SQD	O47-C45-C46-O48
20	s	822	SQD	O6-C44-C45-O47
20	v	822	SQD	O47-C45-C46-O48
13	H	1213	CLA	CBA-CGA-O2A-C1
13	2	505	CLA	C5-C6-C7-C8
13	Z	505	CLA	C5-C6-C7-C8
19	B	5002	LMG	C39-C40-C41-C42
19	H	5002	LMG	C39-C40-C41-C42
19	f	5002	LMG	C39-C40-C41-C42
13	3	510	CLA	C16-C17-C18-C19
13	a	510	CLA	C16-C17-C18-C19
13	s	510	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	f	1234	CLA	C2C-C3C-CAC-CBC
13	B	1234	CLA	C2C-C3C-CAC-CBC
13	H	1234	CLA	C2C-C3C-CAC-CBC
13	A	1107	CLA	C4-C3-C5-C6
13	B	1202	CLA	C4-C3-C5-C6
13	G	1107	CLA	C4-C3-C5-C6
13	H	1202	CLA	C4-C3-C5-C6
13	f	1202	CLA	C4-C3-C5-C6
13	B	1211	CLA	CBA-CGA-O2A-C1
13	2	509	CLA	CBA-CGA-O2A-C1
13	H	1211	CLA	CBA-CGA-O2A-C1
13	Z	509	CLA	CBA-CGA-O2A-C1
13	f	1211	CLA	CBA-CGA-O2A-C1
13	r	509	CLA	CBA-CGA-O2A-C1
13	A	1128	CLA	C10-C11-C12-C13
13	G	1128	CLA	C10-C11-C12-C13
13	e	1128	CLA	C10-C11-C12-C13
13	A	1237	CLA	C6-C7-C8-C9
13	B	1012	CLA	C11-C10-C8-C9
13	B	1012	CLA	C14-C13-C15-C16
13	B	1203	CLA	C6-C7-C8-C9
13	B	1203	CLA	C11-C12-C13-C14
13	B	1206	CLA	C11-C10-C8-C9
13	B	1208	CLA	C6-C7-C8-C9
13	B	1210	CLA	C6-C7-C8-C9
13	B	1215	CLA	C14-C13-C15-C16
13	B	1217	CLA	C11-C10-C8-C9
13	B	1219	CLA	C11-C12-C13-C14
13	B	1223	CLA	C11-C12-C13-C14
13	B	1226	CLA	C11-C12-C13-C14
13	B	1240	CLA	C11-C12-C13-C14
13	F	1301	CLA	C6-C7-C8-C9
13	1	510	CLA	C6-C7-C8-C9
13	2	507	CLA	C11-C10-C8-C9
13	3	513	CLA	C14-C13-C15-C16
13	4	501	CLA	C6-C7-C8-C9
13	5	505	CLA	C6-C7-C8-C9
13	G	1237	CLA	C6-C7-C8-C9
13	H	1012	CLA	C11-C10-C8-C9
13	H	1012	CLA	C14-C13-C15-C16
13	H	1203	CLA	C6-C7-C8-C9
13	H	1203	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	H	1206	CLA	C11-C10-C8-C9
13	H	1208	CLA	C6-C7-C8-C9
13	H	1210	CLA	C6-C7-C8-C9
13	H	1215	CLA	C14-C13-C15-C16
13	H	1219	CLA	C11-C12-C13-C14
13	H	1223	CLA	C11-C12-C13-C14
13	H	1226	CLA	C11-C12-C13-C14
13	H	1240	CLA	C11-C12-C13-C14
13	Y	510	CLA	C6-C7-C8-C9
13	Z	507	CLA	C11-C10-C8-C9
13	a	513	CLA	C14-C13-C15-C16
13	b	501	CLA	C6-C7-C8-C9
13	c	505	CLA	C6-C7-C8-C9
13	d	501	CLA	C11-C10-C8-C9
13	e	1237	CLA	C6-C7-C8-C9
13	f	1012	CLA	C11-C10-C8-C9
13	f	1012	CLA	C14-C13-C15-C16
13	f	1203	CLA	C6-C7-C8-C9
13	f	1203	CLA	C11-C12-C13-C14
13	f	1206	CLA	C11-C10-C8-C9
13	f	1208	CLA	C6-C7-C8-C9
13	f	1210	CLA	C6-C7-C8-C9
13	f	1215	CLA	C14-C13-C15-C16
13	f	1217	CLA	C11-C10-C8-C9
13	f	1219	CLA	C11-C12-C13-C14
13	f	1223	CLA	C11-C12-C13-C14
13	f	1226	CLA	C11-C12-C13-C14
13	f	1240	CLA	C11-C12-C13-C14
13	q	510	CLA	C6-C7-C8-C9
13	r	507	CLA	C11-C10-C8-C9
13	s	513	CLA	C14-C13-C15-C16
13	t	501	CLA	C6-C7-C8-C9
13	u	505	CLA	C6-C7-C8-C9
13	3	508	CLA	CBD-CGD-O2D-CED
13	a	508	CLA	CBD-CGD-O2D-CED
13	s	508	CLA	CBD-CGD-O2D-CED
13	A	1102	CLA	C16-C17-C18-C19
13	G	1102	CLA	C16-C17-C18-C19
13	e	1013	CLA	C16-C17-C18-C20
13	e	1102	CLA	C16-C17-C18-C19
17	A	5006	LHG	C32-C33-C34-C35
17	G	5006	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
17	e	5006	LHG	C32-C33-C34-C35
17	n	5221	LHG	C13-C14-C15-C16
13	B	1021	CLA	O1A-CGA-O2A-C1
13	L	1501	CLA	O1A-CGA-O2A-C1
13	V	1501	CLA	O1A-CGA-O2A-C1
13	n	1501	CLA	O1A-CGA-O2A-C1
13	6	518	CLA	CAA-CBA-CGA-O2A
13	d	518	CLA	CAA-CBA-CGA-O2A
13	v	518	CLA	CAA-CBA-CGA-O2A
17	L	5221	LHG	C13-C14-C15-C16
17	V	5221	LHG	C13-C14-C15-C16
16	J	4012	BCR	C9-C10-C11-C12
16	T	4012	BCR	C9-C10-C11-C12
13	5	505	CLA	C5-C6-C7-C8
13	c	505	CLA	C5-C6-C7-C8
13	u	505	CLA	C5-C6-C7-C8
17	V	5218	LHG	C27-C28-C29-C30
13	A	1013	CLA	C16-C17-C18-C20
13	G	1013	CLA	C16-C17-C18-C20
13	e	1117	CLA	C16-C17-C18-C20
17	L	5218	LHG	C27-C28-C29-C30
17	n	5218	LHG	C27-C28-C29-C30
16	f	4010	BCR	C11-C12-C13-C14
17	V	5221	LHG	C15-C16-C17-C18
13	A	1106	CLA	C2B-C3B-CAB-CBB
13	A	1109	CLA	C2B-C3B-CAB-CBB
13	A	1111	CLA	C2B-C3B-CAB-CBB
13	A	1115	CLA	C2B-C3B-CAB-CBB
13	A	1140	CLA	C2B-C3B-CAB-CBB
13	B	1203	CLA	C2B-C3B-CAB-CBB
13	B	1205	CLA	C2B-C3B-CAB-CBB
13	B	1208	CLA	C2B-C3B-CAB-CBB
13	B	1210	CLA	C2B-C3B-CAB-CBB
13	B	1217	CLA	C2B-C3B-CAB-CBB
13	B	1240	CLA	C2B-C3B-CAB-CBB
13	L	1501	CLA	C2B-C3B-CAB-CBB
13	L	1502	CLA	C2B-C3B-CAB-CBB
13	1	502	CLA	C2B-C3B-CAB-CBB
13	1	503	CLA	C2B-C3B-CAB-CBB
13	1	510	CLA	C2B-C3B-CAB-CBB
13	1	513	CLA	C2B-C3B-CAB-CBB
13	2	508	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	2	511	CLA	C2B-C3B-CAB-CBB
13	3	507	CLA	C2B-C3B-CAB-CBB
13	3	511	CLA	C2B-C3B-CAB-CBB
13	3	513	CLA	C2B-C3B-CAB-CBB
13	3	516	CLA	C2B-C3B-CAB-CBB
13	4	504	CLA	C2B-C3B-CAB-CBB
13	4	506	CLA	C2B-C3B-CAB-CBB
13	4	511	CLA	C2B-C3B-CAB-CBB
13	4	512	CLA	C2B-C3B-CAB-CBB
13	4	513	CLA	C2B-C3B-CAB-CBB
13	5	501	CLA	C2B-C3B-CAB-CBB
13	5	508	CLA	C2B-C3B-CAB-CBB
13	5	511	CLA	C2B-C3B-CAB-CBB
13	6	508	CLA	C2B-C3B-CAB-CBB
13	6	511	CLA	C2B-C3B-CAB-CBB
13	6	513	CLA	C2B-C3B-CAB-CBB
13	G	1106	CLA	C2B-C3B-CAB-CBB
13	G	1109	CLA	C2B-C3B-CAB-CBB
13	G	1111	CLA	C2B-C3B-CAB-CBB
13	G	1115	CLA	C2B-C3B-CAB-CBB
13	G	1140	CLA	C2B-C3B-CAB-CBB
13	H	1203	CLA	C2B-C3B-CAB-CBB
13	H	1205	CLA	C2B-C3B-CAB-CBB
13	H	1208	CLA	C2B-C3B-CAB-CBB
13	H	1210	CLA	C2B-C3B-CAB-CBB
13	H	1217	CLA	C2B-C3B-CAB-CBB
13	H	1240	CLA	C2B-C3B-CAB-CBB
13	V	1501	CLA	C2B-C3B-CAB-CBB
13	V	1502	CLA	C2B-C3B-CAB-CBB
13	Y	502	CLA	C2B-C3B-CAB-CBB
13	Y	503	CLA	C2B-C3B-CAB-CBB
13	Y	510	CLA	C2B-C3B-CAB-CBB
13	Y	513	CLA	C2B-C3B-CAB-CBB
13	Z	508	CLA	C2B-C3B-CAB-CBB
13	Z	511	CLA	C2B-C3B-CAB-CBB
13	Z	512	CLA	C2B-C3B-CAB-CBB
13	a	507	CLA	C2B-C3B-CAB-CBB
13	a	511	CLA	C2B-C3B-CAB-CBB
13	a	516	CLA	C2B-C3B-CAB-CBB
13	b	504	CLA	C2B-C3B-CAB-CBB
13	b	506	CLA	C2B-C3B-CAB-CBB
13	b	511	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	b	512	CLA	C2B-C3B-CAB-CBB
13	b	513	CLA	C2B-C3B-CAB-CBB
13	c	501	CLA	C2B-C3B-CAB-CBB
13	c	508	CLA	C2B-C3B-CAB-CBB
13	c	510	CLA	C2B-C3B-CAB-CBB
13	c	511	CLA	C2B-C3B-CAB-CBB
13	d	508	CLA	C2B-C3B-CAB-CBB
13	d	511	CLA	C2B-C3B-CAB-CBB
13	d	513	CLA	C2B-C3B-CAB-CBB
13	e	1106	CLA	C2B-C3B-CAB-CBB
13	e	1109	CLA	C2B-C3B-CAB-CBB
13	e	1111	CLA	C2B-C3B-CAB-CBB
13	e	1115	CLA	C2B-C3B-CAB-CBB
13	e	1140	CLA	C2B-C3B-CAB-CBB
13	f	1203	CLA	C2B-C3B-CAB-CBB
13	f	1205	CLA	C2B-C3B-CAB-CBB
13	f	1208	CLA	C2B-C3B-CAB-CBB
13	f	1210	CLA	C2B-C3B-CAB-CBB
13	f	1217	CLA	C2B-C3B-CAB-CBB
13	f	1240	CLA	C2B-C3B-CAB-CBB
13	n	1501	CLA	C2B-C3B-CAB-CBB
13	n	1502	CLA	C2B-C3B-CAB-CBB
13	q	502	CLA	C2B-C3B-CAB-CBB
13	q	503	CLA	C2B-C3B-CAB-CBB
13	q	510	CLA	C2B-C3B-CAB-CBB
13	q	513	CLA	C2B-C3B-CAB-CBB
13	r	508	CLA	C2B-C3B-CAB-CBB
13	r	511	CLA	C2B-C3B-CAB-CBB
13	s	507	CLA	C2B-C3B-CAB-CBB
13	s	511	CLA	C2B-C3B-CAB-CBB
13	s	513	CLA	C2B-C3B-CAB-CBB
13	s	516	CLA	C2B-C3B-CAB-CBB
13	t	504	CLA	C2B-C3B-CAB-CBB
13	t	506	CLA	C2B-C3B-CAB-CBB
13	t	511	CLA	C2B-C3B-CAB-CBB
13	t	512	CLA	C2B-C3B-CAB-CBB
13	u	501	CLA	C2B-C3B-CAB-CBB
13	u	508	CLA	C2B-C3B-CAB-CBB
13	u	511	CLA	C2B-C3B-CAB-CBB
13	v	508	CLA	C2B-C3B-CAB-CBB
13	v	511	CLA	C2B-C3B-CAB-CBB
13	v	513	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	H	1021	CLA	O1A-CGA-O2A-C1
13	f	1021	CLA	O1A-CGA-O2A-C1
17	L	5221	LHG	C15-C16-C17-C18
17	G	5002	LHG	C31-C32-C33-C34
17	A	5002	LHG	C31-C32-C33-C34
17	n	5221	LHG	C15-C16-C17-C18
20	2	822	SQD	C14-C15-C16-C17
13	e	1107	CLA	C4-C3-C5-C6
17	e	5002	LHG	C31-C32-C33-C34
20	r	822	SQD	C14-C15-C16-C17
13	B	1204	CLA	C2-C3-C5-C6
13	H	1204	CLA	C2-C3-C5-C6
13	f	1204	CLA	C2-C3-C5-C6
13	A	1117	CLA	C16-C17-C18-C20
13	G	1117	CLA	C16-C17-C18-C20
20	Z	822	SQD	C14-C15-C16-C17
13	G	1133	CLA	O1D-CGD-O2D-CED
13	B	1213	CLA	O1A-CGA-O2A-C1
13	f	1213	CLA	O1A-CGA-O2A-C1
13	A	1133	CLA	O1D-CGD-O2D-CED
13	3	518	CLA	CAA-CBA-CGA-O2A
13	4	518	CLA	CAA-CBA-CGA-O2A
13	a	518	CLA	CAA-CBA-CGA-O2A
13	b	518	CLA	CAA-CBA-CGA-O2A
13	s	518	CLA	CAA-CBA-CGA-O2A
13	t	518	CLA	CAA-CBA-CGA-O2A
13	H	1213	CLA	O1A-CGA-O2A-C1
13	A	1106	CLA	C2-C1-O2A-CGA
13	A	1138	CLA	C2-C1-O2A-CGA
13	A	1237	CLA	C2-C1-O2A-CGA
13	B	1219	CLA	C2-C1-O2A-CGA
13	1	511	CLA	C2-C1-O2A-CGA
13	5	511	CLA	C2-C1-O2A-CGA
13	6	505	CLA	C2-C1-O2A-CGA
13	G	1106	CLA	C2-C1-O2A-CGA
13	G	1138	CLA	C2-C1-O2A-CGA
13	G	1237	CLA	C2-C1-O2A-CGA
13	H	1219	CLA	C2-C1-O2A-CGA
13	Y	511	CLA	C2-C1-O2A-CGA
13	c	511	CLA	C2-C1-O2A-CGA
13	d	505	CLA	C2-C1-O2A-CGA
13	e	1106	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
13	e	1138	CLA	C2-C1-O2A-CGA
13	e	1237	CLA	C2-C1-O2A-CGA
13	f	1219	CLA	C2-C1-O2A-CGA
13	q	511	CLA	C2-C1-O2A-CGA
13	u	511	CLA	C2-C1-O2A-CGA
13	v	505	CLA	C2-C1-O2A-CGA
13	A	1116	CLA	C8-C10-C11-C12
13	A	1132	CLA	C8-C10-C11-C12
13	H	1212	CLA	O1D-CGD-O2D-CED
13	e	1133	CLA	O1D-CGD-O2D-CED
13	L	1501	CLA	C3-C5-C6-C7
13	V	1501	CLA	C3-C5-C6-C7
13	n	1501	CLA	C3-C5-C6-C7
13	G	1116	CLA	C8-C10-C11-C12
13	G	1132	CLA	C8-C10-C11-C12
13	e	1116	CLA	C8-C10-C11-C12
13	e	1132	CLA	C8-C10-C11-C12
16	l	4012	BCR	C9-C10-C11-C12
13	2	509	CLA	O1A-CGA-O2A-C1
13	Z	509	CLA	O1A-CGA-O2A-C1
13	r	509	CLA	O1A-CGA-O2A-C1
13	B	1212	CLA	O1D-CGD-O2D-CED
16	3	522	BCR	C1-C6-C7-C8
16	a	522	BCR	C1-C6-C7-C8
16	s	522	BCR	C1-C6-C7-C8
13	5	505	CLA	C2-C3-C5-C6
13	u	505	CLA	C2-C3-C5-C6
13	f	1212	CLA	O1D-CGD-O2D-CED
13	B	1207	CLA	C15-C16-C17-C18
13	B	1205	CLA	CBA-CGA-O2A-C1
13	H	1205	CLA	CBA-CGA-O2A-C1
13	f	1205	CLA	CBA-CGA-O2A-C1
13	A	1126	CLA	CAA-CBA-CGA-O2A
13	G	1126	CLA	CAA-CBA-CGA-O2A
13	e	1126	CLA	CAA-CBA-CGA-O2A
13	H	1207	CLA	C15-C16-C17-C18
13	f	1207	CLA	C15-C16-C17-C18
13	B	1212	CLA	C2A-CAA-CBA-CGA
13	H	1212	CLA	C2A-CAA-CBA-CGA
13	f	1212	CLA	C2A-CAA-CBA-CGA
17	A	5006	LHG	C3-O3-P-O6
17	A	5001	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
17	A	5003	LHG	C3-O3-P-O6
17	G	5006	LHG	C3-O3-P-O6
17	G	5001	LHG	C3-O3-P-O6
17	G	5003	LHG	C3-O3-P-O6
17	e	5006	LHG	C3-O3-P-O6
17	e	5001	LHG	C3-O3-P-O6
17	e	5003	LHG	C3-O3-P-O6
13	2	503	CLA	C13-C15-C16-C17
13	r	503	CLA	C13-C15-C16-C17
17	A	5006	LHG	C28-C29-C30-C31
20	3	822	SQD	C11-C12-C13-C14
20	a	822	SQD	C11-C12-C13-C14
19	B	5002	LMG	C7-C8-C9-O8
19	J	5104	LMG	O1-C7-C8-C9
19	H	5002	LMG	C7-C8-C9-O8
19	T	5104	LMG	O1-C7-C8-C9
19	f	5002	LMG	C7-C8-C9-O8
19	l	5104	LMG	O1-C7-C8-C9
13	B	1224	CLA	C4-C3-C5-C6
13	H	1224	CLA	C4-C3-C5-C6
13	e	1022	CLA	C4-C3-C5-C6
13	f	1224	CLA	C4-C3-C5-C6
17	G	5006	LHG	C28-C29-C30-C31
17	e	5006	LHG	C28-C29-C30-C31
20	s	822	SQD	C11-C12-C13-C14
13	Z	503	CLA	C13-C15-C16-C17
13	A	1111	CLA	C11-C12-C13-C15
13	B	1204	CLA	C11-C10-C8-C7
13	B	1205	CLA	C12-C13-C15-C16
13	B	1215	CLA	C11-C12-C13-C15
13	B	1216	CLA	C6-C7-C8-C10
13	B	1219	CLA	C11-C12-C13-C15
13	L	1503	CLA	C6-C7-C8-C10
13	1	501	CLA	C11-C10-C8-C7
13	G	1111	CLA	C11-C12-C13-C15
13	H	1204	CLA	C11-C10-C8-C7
13	H	1205	CLA	C12-C13-C15-C16
13	H	1215	CLA	C11-C12-C13-C15
13	H	1216	CLA	C6-C7-C8-C10
13	H	1219	CLA	C11-C12-C13-C15
13	V	1503	CLA	C6-C7-C8-C10
13	Y	501	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	c	505	CLA	C2-C3-C5-C6
13	e	1111	CLA	C11-C12-C13-C15
13	f	1204	CLA	C11-C10-C8-C7
13	f	1205	CLA	C12-C13-C15-C16
13	f	1215	CLA	C11-C12-C13-C15
13	f	1216	CLA	C6-C7-C8-C10
13	f	1219	CLA	C11-C12-C13-C15
13	n	1503	CLA	C6-C7-C8-C10
13	q	501	CLA	C11-C10-C8-C7
17	A	5002	LHG	C9-C10-C11-C12
17	G	5002	LHG	C9-C10-C11-C12
17	e	5002	LHG	C9-C10-C11-C12
13	A	1131	CLA	C14-C13-C15-C16
13	A	1101	CLA	C11-C12-C13-C14
13	B	1023	CLA	C11-C10-C8-C9
13	B	1208	CLA	C11-C12-C13-C14
13	B	1234	CLA	C11-C12-C13-C14
13	B	1230	CLA	C6-C7-C8-C9
13	1	501	CLA	C11-C10-C8-C9
13	1	502	CLA	C11-C10-C8-C9
13	2	505	CLA	C6-C7-C8-C9
13	2	513	CLA	C11-C10-C8-C9
13	3	505	CLA	C14-C13-C15-C16
13	5	509	CLA	C6-C7-C8-C9
13	6	501	CLA	C11-C10-C8-C9
13	6	505	CLA	C11-C12-C13-C14
13	G	1131	CLA	C14-C13-C15-C16
13	G	1101	CLA	C11-C12-C13-C14
13	H	1023	CLA	C11-C10-C8-C9
13	H	1208	CLA	C11-C12-C13-C14
13	H	1217	CLA	C11-C10-C8-C9
13	H	1234	CLA	C11-C12-C13-C14
13	H	1230	CLA	C6-C7-C8-C9
13	Y	501	CLA	C11-C10-C8-C9
13	Y	502	CLA	C11-C10-C8-C9
13	Z	505	CLA	C6-C7-C8-C9
13	Z	513	CLA	C11-C10-C8-C9
13	a	505	CLA	C14-C13-C15-C16
13	c	509	CLA	C6-C7-C8-C9
13	d	505	CLA	C11-C12-C13-C14
13	e	1131	CLA	C14-C13-C15-C16
13	e	1101	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	f	1023	CLA	C11-C10-C8-C9
13	f	1208	CLA	C11-C12-C13-C14
13	f	1234	CLA	C11-C12-C13-C14
13	f	1230	CLA	C6-C7-C8-C9
13	q	501	CLA	C11-C10-C8-C9
13	q	502	CLA	C11-C10-C8-C9
13	r	505	CLA	C6-C7-C8-C9
13	r	513	CLA	C11-C10-C8-C9
13	s	505	CLA	C14-C13-C15-C16
13	u	509	CLA	C6-C7-C8-C9
13	v	501	CLA	C11-C10-C8-C9
13	v	505	CLA	C11-C12-C13-C14
14	A	2001	PQN	C24-C23-C25-C26
14	B	2002	PQN	C21-C22-C23-C24
14	G	2001	PQN	C24-C23-C25-C26
14	H	2002	PQN	C21-C22-C23-C24
14	e	2001	PQN	C24-C23-C25-C26
14	f	2002	PQN	C21-C22-C23-C24
13	e	1109	CLA	C15-C16-C17-C18
13	A	1128	CLA	O1A-CGA-O2A-C1
13	G	1128	CLA	O1A-CGA-O2A-C1
17	L	5220	LHG	C25-C26-C27-C28
17	V	5220	LHG	C25-C26-C27-C28
17	n	5220	LHG	C25-C26-C27-C28
13	e	1128	CLA	O1A-CGA-O2A-C1
13	B	1021	CLA	C16-C17-C18-C20
13	H	1021	CLA	C16-C17-C18-C20
13	f	1021	CLA	C16-C17-C18-C20
20	L	5216	SQD	C10-C11-C12-C13
13	A	1109	CLA	C15-C16-C17-C18
13	G	1109	CLA	C15-C16-C17-C18
13	s	508	CLA	O1D-CGD-O2D-CED
16	B	4010	BCR	C11-C12-C13-C14
16	H	4010	BCR	C11-C12-C13-C14
20	V	5216	SQD	C10-C11-C12-C13
20	n	5216	SQD	C10-C11-C12-C13
13	5	505	CLA	C12-C13-C15-C16
13	c	505	CLA	C12-C13-C15-C16
13	u	505	CLA	C12-C13-C15-C16
13	3	510	CLA	C5-C6-C7-C8
13	s	510	CLA	C5-C6-C7-C8
17	G	5003	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	e	5003	LHG	C11-C12-C13-C14
13	A	1022	CLA	C4-C3-C5-C6
13	G	1022	CLA	C4-C3-C5-C6
17	A	5003	LHG	C11-C12-C13-C14
13	B	1021	CLA	C16-C17-C18-C19
13	H	1021	CLA	C16-C17-C18-C19
13	f	1021	CLA	C16-C17-C18-C19
13	A	1128	CLA	CBA-CGA-O2A-C1
13	B	1228	CLA	CBA-CGA-O2A-C1
13	G	1128	CLA	CBA-CGA-O2A-C1
13	H	1228	CLA	CBA-CGA-O2A-C1
13	e	1128	CLA	CBA-CGA-O2A-C1
13	f	1228	CLA	CBA-CGA-O2A-C1
17	B	1855	LHG	C24-C23-O8-C6
17	H	1855	LHG	C24-C23-O8-C6
17	f	1855	LHG	C24-C23-O8-C6
13	G	1118	CLA	O1D-CGD-O2D-CED
13	a	510	CLA	C5-C6-C7-C8
13	3	508	CLA	O1D-CGD-O2D-CED
20	Y	822	SQD	O10-C23-C24-C25
20	q	822	SQD	O10-C23-C24-C25
13	G	1118	CLA	CBD-CGD-O2D-CED
13	A	1118	CLA	O1D-CGD-O2D-CED
13	A	1106	CLA	C4B-C3B-CAB-CBB
13	A	1109	CLA	C4B-C3B-CAB-CBB
13	A	1124	CLA	C4B-C3B-CAB-CBB
13	B	1203	CLA	C4B-C3B-CAB-CBB
13	B	1210	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	C4B-C3B-CAB-CBB
13	L	1502	CLA	C4B-C3B-CAB-CBB
13	1	502	CLA	C4B-C3B-CAB-CBB
13	1	508	CLA	C4B-C3B-CAB-CBB
13	1	510	CLA	C4B-C3B-CAB-CBB
13	2	508	CLA	C4B-C3B-CAB-CBB
13	2	511	CLA	C4B-C3B-CAB-CBB
13	3	511	CLA	C4B-C3B-CAB-CBB
13	4	504	CLA	C4B-C3B-CAB-CBB
13	5	508	CLA	C4B-C3B-CAB-CBB
13	5	511	CLA	C4B-C3B-CAB-CBB
13	6	504	CLA	C4B-C3B-CAB-CBB
13	6	508	CLA	C4B-C3B-CAB-CBB
13	G	1106	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	G	1109	CLA	C4B-C3B-CAB-CBB
13	G	1124	CLA	C4B-C3B-CAB-CBB
13	H	1203	CLA	C4B-C3B-CAB-CBB
13	H	1210	CLA	C4B-C3B-CAB-CBB
13	R	1301	CLA	C4B-C3B-CAB-CBB
13	V	1502	CLA	C4B-C3B-CAB-CBB
13	Y	502	CLA	C4B-C3B-CAB-CBB
13	Y	508	CLA	C4B-C3B-CAB-CBB
13	Y	510	CLA	C4B-C3B-CAB-CBB
13	Z	508	CLA	C4B-C3B-CAB-CBB
13	Z	511	CLA	C4B-C3B-CAB-CBB
13	a	511	CLA	C4B-C3B-CAB-CBB
13	b	504	CLA	C4B-C3B-CAB-CBB
13	c	508	CLA	C4B-C3B-CAB-CBB
13	c	511	CLA	C4B-C3B-CAB-CBB
13	d	504	CLA	C4B-C3B-CAB-CBB
13	d	508	CLA	C4B-C3B-CAB-CBB
13	e	1106	CLA	C4B-C3B-CAB-CBB
13	e	1109	CLA	C4B-C3B-CAB-CBB
13	e	1124	CLA	C4B-C3B-CAB-CBB
13	f	1203	CLA	C4B-C3B-CAB-CBB
13	f	1210	CLA	C4B-C3B-CAB-CBB
13	j	1301	CLA	C4B-C3B-CAB-CBB
13	n	1502	CLA	C4B-C3B-CAB-CBB
13	q	502	CLA	C4B-C3B-CAB-CBB
13	q	508	CLA	C4B-C3B-CAB-CBB
13	q	510	CLA	C4B-C3B-CAB-CBB
13	r	508	CLA	C4B-C3B-CAB-CBB
13	r	511	CLA	C4B-C3B-CAB-CBB
13	s	511	CLA	C4B-C3B-CAB-CBB
13	t	504	CLA	C4B-C3B-CAB-CBB
13	u	508	CLA	C4B-C3B-CAB-CBB
13	u	511	CLA	C4B-C3B-CAB-CBB
13	v	504	CLA	C4B-C3B-CAB-CBB
13	v	508	CLA	C4B-C3B-CAB-CBB
13	3	510	CLA	C16-C17-C18-C20
13	a	510	CLA	C16-C17-C18-C20
13	s	510	CLA	C16-C17-C18-C20
20	1	822	SQD	O10-C23-C24-C25
16	A	4001	BCR	C13-C14-C15-C16
16	3	521	BCR	C9-C10-C11-C12
16	3	524	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	4	521	BCR	C13-C14-C15-C16
16	G	4001	BCR	C13-C14-C15-C16
16	a	521	BCR	C9-C10-C11-C12
16	a	524	BCR	C9-C10-C11-C12
16	b	521	BCR	C13-C14-C15-C16
16	e	4001	BCR	C13-C14-C15-C16
16	s	521	BCR	C9-C10-C11-C12
16	s	524	BCR	C9-C10-C11-C12
16	t	521	BCR	C13-C14-C15-C16
13	a	508	CLA	O1D-CGD-O2D-CED
13	f	1212	CLA	CBD-CGD-O2D-CED
18	A	1848	LMU	O1'-C1-C2-C3
18	G	1848	LMU	O1'-C1-C2-C3
18	e	1848	LMU	O1'-C1-C2-C3
13	l	1303	CLA	C15-C16-C17-C18
17	n	5220	LHG	C26-C27-C28-C29
13	A	1132	CLA	C2C-C3C-CAC-CBC
13	G	1132	CLA	C2C-C3C-CAC-CBC
13	e	1132	CLA	C2C-C3C-CAC-CBC
17	L	5220	LHG	C26-C27-C28-C29
17	V	5220	LHG	C26-C27-C28-C29
13	A	1118	CLA	CBD-CGD-O2D-CED
13	B	1212	CLA	CBD-CGD-O2D-CED
13	H	1212	CLA	CBD-CGD-O2D-CED
13	J	1303	CLA	C15-C16-C17-C18
20	1	822	SQD	C9-C10-C11-C12
20	Y	822	SQD	C9-C10-C11-C12
20	q	822	SQD	C9-C10-C11-C12
13	2	507	CLA	C16-C17-C18-C19
13	Z	507	CLA	C16-C17-C18-C19
13	r	507	CLA	C16-C17-C18-C19
13	2	518	CLA	CAA-CBA-CGA-O2A
13	Z	518	CLA	CAA-CBA-CGA-O2A
13	r	518	CLA	CAA-CBA-CGA-O2A
13	e	1118	CLA	CBD-CGD-O2D-CED
13	e	1118	CLA	O1D-CGD-O2D-CED
18	l	5105	LMU	C5-C6-C7-C8
13	T	1303	CLA	C15-C16-C17-C18
18	J	5105	LMU	C5-C6-C7-C8
18	T	5105	LMU	C5-C6-C7-C8
13	A	1107	CLA	C2-C1-O2A-CGA
13	B	1212	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
13	L	1502	CLA	C2-C1-O2A-CGA
13	3	505	CLA	C2-C1-O2A-CGA
13	G	1107	CLA	C2-C1-O2A-CGA
13	H	1212	CLA	C2-C1-O2A-CGA
13	V	1502	CLA	C2-C1-O2A-CGA
13	a	505	CLA	C2-C1-O2A-CGA
13	e	1107	CLA	C2-C1-O2A-CGA
13	f	1212	CLA	C2-C1-O2A-CGA
13	n	1502	CLA	C2-C1-O2A-CGA
13	s	505	CLA	C2-C1-O2A-CGA
13	A	1237	CLA	C2A-CAA-CBA-CGA
13	B	1204	CLA	C2A-CAA-CBA-CGA
13	B	1210	CLA	C2A-CAA-CBA-CGA
13	4	513	CLA	C2A-CAA-CBA-CGA
13	G	1237	CLA	C2A-CAA-CBA-CGA
13	H	1204	CLA	C2A-CAA-CBA-CGA
13	H	1210	CLA	C2A-CAA-CBA-CGA
13	b	513	CLA	C2A-CAA-CBA-CGA
13	e	1237	CLA	C2A-CAA-CBA-CGA
13	f	1204	CLA	C2A-CAA-CBA-CGA
13	f	1210	CLA	C2A-CAA-CBA-CGA
13	t	513	CLA	C2A-CAA-CBA-CGA
13	1	503	CLA	C16-C17-C18-C19
13	Y	503	CLA	C16-C17-C18-C19
13	q	503	CLA	C16-C17-C18-C19
13	B	1228	CLA	C3A-C2A-CAA-CBA
13	H	1228	CLA	C3A-C2A-CAA-CBA
13	f	1228	CLA	C3A-C2A-CAA-CBA
13	K	1105	CLA	CAA-CBA-CGA-O1A
13	K	1105	CLA	CAA-CBA-CGA-O2A
13	U	1105	CLA	CAA-CBA-CGA-O1A
13	U	1105	CLA	CAA-CBA-CGA-O2A
13	m	1105	CLA	CAA-CBA-CGA-O1A
13	m	1105	CLA	CAA-CBA-CGA-O2A
13	A	1011	CLA	CAA-CBA-CGA-O2A
13	G	1011	CLA	CAA-CBA-CGA-O2A
13	e	1011	CLA	CAA-CBA-CGA-O2A
18	Z	901	LMU	C2-C1-O1'-C1'
17	G	5009	LHG	C12-C13-C14-C15
17	A	5009	LHG	C12-C13-C14-C15
17	e	5009	LHG	C12-C13-C14-C15
17	L	5220	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
17	V	5220	LHG	C31-C32-C33-C34
13	A	1116	CLA	C11-C10-C8-C9
13	A	1124	CLA	C6-C7-C8-C9
13	J	1303	CLA	C6-C7-C8-C9
13	1	505	CLA	C6-C7-C8-C9
13	1	510	CLA	C11-C12-C13-C14
13	G	1116	CLA	C11-C10-C8-C9
13	G	1124	CLA	C6-C7-C8-C9
13	T	1303	CLA	C6-C7-C8-C9
13	Y	505	CLA	C6-C7-C8-C9
13	Y	510	CLA	C11-C12-C13-C14
13	e	1116	CLA	C11-C10-C8-C9
13	e	1124	CLA	C6-C7-C8-C9
13	l	1303	CLA	C6-C7-C8-C9
13	q	505	CLA	C6-C7-C8-C9
13	q	510	CLA	C11-C12-C13-C14
17	n	5220	LHG	C31-C32-C33-C34
13	4	508	CLA	CAA-CBA-CGA-O2A
13	b	508	CLA	CAA-CBA-CGA-O2A
13	t	508	CLA	CAA-CBA-CGA-O1A
13	t	508	CLA	CAA-CBA-CGA-O2A
17	I	5001	LHG	C24-C25-C26-C27
17	S	5001	LHG	C24-C25-C26-C27
17	k	5001	LHG	C24-C25-C26-C27
19	B	5002	LMG	C40-C41-C42-C43
19	f	5002	LMG	C40-C41-C42-C43
19	H	5002	LMG	C40-C41-C42-C43
16	A	4011	BCR	C11-C10-C9-C34
16	A	4011	BCR	C16-C17-C18-C36
16	B	4006	BCR	C11-C10-C9-C34
16	B	4006	BCR	C20-C21-C22-C37
16	F	4016	BCR	C35-C13-C14-C15
16	L	4020	BCR	C20-C21-C22-C37
16	G	4011	BCR	C11-C10-C9-C34
16	G	4011	BCR	C16-C17-C18-C36
16	H	4006	BCR	C11-C10-C9-C34
16	H	4006	BCR	C20-C21-C22-C37
16	R	4016	BCR	C35-C13-C14-C15
16	V	4020	BCR	C20-C21-C22-C37
16	e	4011	BCR	C11-C10-C9-C34
16	e	4011	BCR	C16-C17-C18-C36
16	f	4006	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
16	f	4006	BCR	C20-C21-C22-C37
16	j	4016	BCR	C35-C13-C14-C15
16	n	4020	BCR	C20-C21-C22-C37
13	4	508	CLA	CAA-CBA-CGA-O1A
13	J	1302	CLA	C2A-CAA-CBA-CGA
13	1	507	CLA	C2A-CAA-CBA-CGA
13	3	503	CLA	C2A-CAA-CBA-CGA
13	T	1302	CLA	C2A-CAA-CBA-CGA
13	a	503	CLA	C2A-CAA-CBA-CGA
13	l	1302	CLA	C2A-CAA-CBA-CGA
13	s	503	CLA	C2A-CAA-CBA-CGA
13	H	1228	CLA	O1A-CGA-O2A-C1
13	A	1117	CLA	C16-C17-C18-C19
13	B	1229	CLA	C16-C17-C18-C19
13	G	1117	CLA	C16-C17-C18-C19
13	H	1229	CLA	C16-C17-C18-C19
13	e	1117	CLA	C16-C17-C18-C19
13	f	1229	CLA	C16-C17-C18-C19
13	A	1126	CLA	O2A-C1-C2-C3
13	G	1126	CLA	O2A-C1-C2-C3
13	e	1126	CLA	O2A-C1-C2-C3
13	3	518	CLA	CBA-CGA-O2A-C1
13	a	518	CLA	CBA-CGA-O2A-C1
13	s	518	CLA	CBA-CGA-O2A-C1
20	6	822	SQD	O5-C1-O6-C44
20	d	822	SQD	O5-C1-O6-C44
20	v	822	SQD	O5-C1-O6-C44
13	b	508	CLA	CAA-CBA-CGA-O1A
13	v	517	CLA	CAA-CBA-CGA-O1A
17	e	5004	LHG	C28-C29-C30-C31
17	A	5004	LHG	C28-C29-C30-C31
17	G	5004	LHG	C28-C29-C30-C31
17	S	5001	LHG	C28-C29-C30-C31
17	k	5001	LHG	C28-C29-C30-C31
20	2	822	SQD	C26-C27-C28-C29
20	Z	822	SQD	C26-C27-C28-C29
20	r	822	SQD	C26-C27-C28-C29
13	6	517	CLA	CAA-CBA-CGA-O1A
13	d	517	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	C13-C15-C16-C17
13	A	1237	CLA	C8-C10-C11-C12
13	A	1022	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	G	1237	CLA	C8-C10-C11-C12
13	G	1022	CLA	C15-C16-C17-C18
13	e	1123	CLA	C13-C15-C16-C17
13	A	1135	CLA	C4-C3-C5-C6
13	G	1135	CLA	C4-C3-C5-C6
13	e	1135	CLA	C4-C3-C5-C6
13	A	1111	CLA	C1A-C2A-CAA-CBA
13	B	1206	CLA	C1A-C2A-CAA-CBA
13	B	1212	CLA	C1A-C2A-CAA-CBA
13	B	1223	CLA	C1A-C2A-CAA-CBA
13	B	1228	CLA	C1A-C2A-CAA-CBA
13	B	1229	CLA	C1A-C2A-CAA-CBA
13	1	503	CLA	C1A-C2A-CAA-CBA
13	1	506	CLA	C1A-C2A-CAA-CBA
13	2	503	CLA	C1A-C2A-CAA-CBA
13	2	513	CLA	C1A-C2A-CAA-CBA
13	2	519	CLA	C1A-C2A-CAA-CBA
13	3	504	CLA	C1A-C2A-CAA-CBA
13	3	508	CLA	C1A-C2A-CAA-CBA
13	3	518	CLA	C1A-C2A-CAA-CBA
13	5	511	CLA	C1A-C2A-CAA-CBA
13	5	519	CLA	C1A-C2A-CAA-CBA
13	G	1111	CLA	C1A-C2A-CAA-CBA
13	H	1206	CLA	C1A-C2A-CAA-CBA
13	H	1212	CLA	C1A-C2A-CAA-CBA
13	H	1223	CLA	C1A-C2A-CAA-CBA
13	H	1228	CLA	C1A-C2A-CAA-CBA
13	H	1229	CLA	C1A-C2A-CAA-CBA
13	Y	503	CLA	C1A-C2A-CAA-CBA
13	Y	506	CLA	C1A-C2A-CAA-CBA
13	Z	513	CLA	C1A-C2A-CAA-CBA
13	Z	519	CLA	C1A-C2A-CAA-CBA
13	a	504	CLA	C1A-C2A-CAA-CBA
13	a	508	CLA	C1A-C2A-CAA-CBA
13	a	518	CLA	C1A-C2A-CAA-CBA
13	c	511	CLA	C1A-C2A-CAA-CBA
13	c	519	CLA	C1A-C2A-CAA-CBA
13	e	1111	CLA	C1A-C2A-CAA-CBA
13	f	1206	CLA	C1A-C2A-CAA-CBA
13	f	1212	CLA	C1A-C2A-CAA-CBA
13	f	1223	CLA	C1A-C2A-CAA-CBA
13	f	1228	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	f	1229	CLA	C1A-C2A-CAA-CBA
13	q	506	CLA	C1A-C2A-CAA-CBA
13	r	503	CLA	C1A-C2A-CAA-CBA
13	r	513	CLA	C1A-C2A-CAA-CBA
13	r	519	CLA	C1A-C2A-CAA-CBA
13	s	504	CLA	C1A-C2A-CAA-CBA
13	s	508	CLA	C1A-C2A-CAA-CBA
13	s	518	CLA	C1A-C2A-CAA-CBA
13	u	511	CLA	C1A-C2A-CAA-CBA
13	u	519	CLA	C1A-C2A-CAA-CBA
17	I	5001	LHG	C28-C29-C30-C31
13	A	1107	CLA	C11-C10-C8-C7
13	A	1131	CLA	C11-C12-C13-C15
13	B	1023	CLA	C11-C10-C8-C7
13	B	1215	CLA	C6-C7-C8-C10
13	B	1226	CLA	C11-C10-C8-C7
13	B	1229	CLA	C11-C10-C8-C7
13	J	1303	CLA	C12-C13-C15-C16
13	2	513	CLA	C12-C13-C15-C16
13	G	1107	CLA	C11-C10-C8-C7
13	G	1131	CLA	C11-C12-C13-C15
13	H	1023	CLA	C11-C10-C8-C7
13	H	1215	CLA	C6-C7-C8-C10
13	H	1226	CLA	C11-C10-C8-C7
13	H	1229	CLA	C11-C10-C8-C7
13	T	1303	CLA	C12-C13-C15-C16
13	Z	513	CLA	C12-C13-C15-C16
13	e	1107	CLA	C11-C10-C8-C7
13	e	1131	CLA	C11-C12-C13-C15
13	f	1023	CLA	C11-C10-C8-C7
13	f	1215	CLA	C6-C7-C8-C10
13	f	1226	CLA	C11-C10-C8-C7
13	f	1229	CLA	C11-C10-C8-C7
13	l	1303	CLA	C12-C13-C15-C16
13	r	513	CLA	C12-C13-C15-C16
14	B	2002	PQN	C17-C18-C20-C21
14	H	2002	PQN	C17-C18-C20-C21
14	f	2002	PQN	C17-C18-C20-C21
18	l	5105	LMU	C2-C3-C4-C5
13	1	505	CLA	C13-C15-C16-C17
13	G	1123	CLA	C13-C15-C16-C17
13	Y	505	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	e	1237	CLA	C8-C10-C11-C12
13	e	1022	CLA	C15-C16-C17-C18
13	q	505	CLA	C13-C15-C16-C17
13	q	518	CLA	C8-C10-C11-C12
13	B	1228	CLA	O1A-CGA-O2A-C1
13	f	1228	CLA	O1A-CGA-O2A-C1
18	J	5105	LMU	C2-C3-C4-C5
18	T	5105	LMU	C2-C3-C4-C5
13	1	518	CLA	C8-C10-C11-C12
13	6	510	CLA	CAA-CBA-CGA-O2A
13	d	510	CLA	CAA-CBA-CGA-O2A
13	v	510	CLA	CAA-CBA-CGA-O2A
13	A	1022	CLA	C16-C17-C18-C20
13	G	1022	CLA	C16-C17-C18-C20
13	e	1022	CLA	C16-C17-C18-C20
17	L	5221	LHG	C16-C17-C18-C19
17	n	5221	LHG	C16-C17-C18-C19
13	B	1222	CLA	C3-C5-C6-C7
13	H	1222	CLA	C3-C5-C6-C7
13	f	1222	CLA	C3-C5-C6-C7
17	L	5218	LHG	C5-C4-O6-P
17	V	5218	LHG	C5-C4-O6-P
17	n	5218	LHG	C5-C4-O6-P
13	A	1137	CLA	C2A-CAA-CBA-CGA
13	B	1216	CLA	C2A-CAA-CBA-CGA
13	1	503	CLA	C2A-CAA-CBA-CGA
13	2	503	CLA	C2A-CAA-CBA-CGA
13	G	1137	CLA	C2A-CAA-CBA-CGA
13	H	1216	CLA	C2A-CAA-CBA-CGA
13	Y	503	CLA	C2A-CAA-CBA-CGA
13	Y	507	CLA	C2A-CAA-CBA-CGA
13	Z	503	CLA	C2A-CAA-CBA-CGA
13	e	1137	CLA	C2A-CAA-CBA-CGA
13	f	1216	CLA	C2A-CAA-CBA-CGA
13	q	503	CLA	C2A-CAA-CBA-CGA
13	q	507	CLA	C2A-CAA-CBA-CGA
13	r	503	CLA	C2A-CAA-CBA-CGA
13	Y	518	CLA	C8-C10-C11-C12
14	A	2001	PQN	C23-C25-C26-C27
14	G	2001	PQN	C23-C25-C26-C27
14	e	2001	PQN	C23-C25-C26-C27
17	B	1842	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	H	1842	LHG	C11-C10-C9-C8
17	V	5221	LHG	C16-C17-C18-C19
17	f	1842	LHG	C11-C10-C9-C8
13	3	510	CLA	C13-C15-C16-C17
13	s	510	CLA	C13-C15-C16-C17
13	a	510	CLA	C13-C15-C16-C17
13	3	512	CLA	CAA-CBA-CGA-O2A
13	a	512	CLA	CAA-CBA-CGA-O2A
13	d	510	CLA	CAA-CBA-CGA-O1A
13	s	512	CLA	CAA-CBA-CGA-O2A
13	G	1022	CLA	C2-C3-C5-C6
13	A	1108	CLA	C2B-C3B-CAB-CBB
13	A	1110	CLA	C2B-C3B-CAB-CBB
13	A	1124	CLA	C2B-C3B-CAB-CBB
13	A	1133	CLA	C2B-C3B-CAB-CBB
13	A	1130	CLA	C2B-C3B-CAB-CBB
13	B	1236	CLA	C2B-C3B-CAB-CBB
13	1	508	CLA	C2B-C3B-CAB-CBB
13	2	512	CLA	C2B-C3B-CAB-CBB
13	3	505	CLA	C2B-C3B-CAB-CBB
13	3	510	CLA	C2B-C3B-CAB-CBB
13	5	506	CLA	C2B-C3B-CAB-CBB
13	6	504	CLA	C2B-C3B-CAB-CBB
13	G	1108	CLA	C2B-C3B-CAB-CBB
13	G	1110	CLA	C2B-C3B-CAB-CBB
13	G	1124	CLA	C2B-C3B-CAB-CBB
13	G	1133	CLA	C2B-C3B-CAB-CBB
13	G	1130	CLA	C2B-C3B-CAB-CBB
13	H	1236	CLA	C2B-C3B-CAB-CBB
13	Y	508	CLA	C2B-C3B-CAB-CBB
13	a	505	CLA	C2B-C3B-CAB-CBB
13	a	510	CLA	C2B-C3B-CAB-CBB
13	c	506	CLA	C2B-C3B-CAB-CBB
13	d	504	CLA	C2B-C3B-CAB-CBB
13	e	1108	CLA	C2B-C3B-CAB-CBB
13	e	1110	CLA	C2B-C3B-CAB-CBB
13	e	1124	CLA	C2B-C3B-CAB-CBB
13	e	1133	CLA	C2B-C3B-CAB-CBB
13	e	1130	CLA	C2B-C3B-CAB-CBB
13	f	1236	CLA	C2B-C3B-CAB-CBB
13	q	508	CLA	C2B-C3B-CAB-CBB
13	r	512	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	s	505	CLA	C2B-C3B-CAB-CBB
13	s	510	CLA	C2B-C3B-CAB-CBB
13	u	506	CLA	C2B-C3B-CAB-CBB
13	v	504	CLA	C2B-C3B-CAB-CBB
13	6	510	CLA	CAA-CBA-CGA-O1A
13	v	510	CLA	CAA-CBA-CGA-O1A
13	a	518	CLA	O1A-CGA-O2A-C1
13	a	519	CLA	O1A-CGA-O2A-C1
16	A	4011	BCR	C11-C10-C9-C8
16	A	4011	BCR	C16-C17-C18-C19
16	B	4006	BCR	C11-C10-C9-C8
16	B	4006	BCR	C20-C21-C22-C23
16	F	4016	BCR	C12-C13-C14-C15
16	L	4020	BCR	C20-C21-C22-C23
16	G	4011	BCR	C11-C10-C9-C8
16	G	4011	BCR	C16-C17-C18-C19
16	H	4006	BCR	C11-C10-C9-C8
16	H	4006	BCR	C20-C21-C22-C23
16	R	4016	BCR	C12-C13-C14-C15
16	V	4020	BCR	C20-C21-C22-C23
16	e	4011	BCR	C11-C10-C9-C8
16	e	4011	BCR	C16-C17-C18-C19
16	f	4006	BCR	C11-C10-C9-C8
16	f	4006	BCR	C20-C21-C22-C23
16	j	4016	BCR	C12-C13-C14-C15
16	n	4020	BCR	C20-C21-C22-C23
13	a	512	CLA	CAA-CBA-CGA-O1A
13	s	518	CLA	O1A-CGA-O2A-C1
17	A	5004	LHG	C24-C23-O8-C6
17	G	5004	LHG	C24-C23-O8-C6
16	A	4008	BCR	C19-C20-C21-C22
16	G	4008	BCR	C19-C20-C21-C22
16	e	4008	BCR	C19-C20-C21-C22
13	G	1109	CLA	C3-C5-C6-C7
13	3	512	CLA	CAA-CBA-CGA-O1A
13	4	512	CLA	CAA-CBA-CGA-O1A
13	b	512	CLA	CAA-CBA-CGA-O1A
13	s	512	CLA	CAA-CBA-CGA-O1A
13	t	512	CLA	CAA-CBA-CGA-O1A
13	L	1501	CLA	C13-C15-C16-C17
13	V	1501	CLA	C13-C15-C16-C17
13	n	1501	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	3	519	CLA	O1A-CGA-O2A-C1
13	s	519	CLA	O1A-CGA-O2A-C1
17	e	5007	LHG	O10-C23-O8-C6
13	2	507	CLA	C16-C17-C18-C20
13	Z	507	CLA	C16-C17-C18-C20
13	r	507	CLA	C16-C17-C18-C20
17	I	5001	LHG	C30-C31-C32-C33
17	S	5001	LHG	C30-C31-C32-C33
17	k	5001	LHG	C30-C31-C32-C33
13	H	1226	CLA	C8-C10-C11-C12
13	3	518	CLA	O1A-CGA-O2A-C1
17	A	5007	LHG	O10-C23-O8-C6
17	G	5007	LHG	O10-C23-O8-C6
13	d	517	CLA	CAA-CBA-CGA-O2A
13	t	512	CLA	CAA-CBA-CGA-O2A
17	A	5008	LHG	C9-C10-C11-C12
17	G	5008	LHG	C9-C10-C11-C12
17	e	5008	LHG	C9-C10-C11-C12
13	B	1207	CLA	C2-C1-O2A-CGA
13	3	511	CLA	C2-C1-O2A-CGA
13	4	519	CLA	C2-C1-O2A-CGA
13	H	1207	CLA	C2-C1-O2A-CGA
13	a	511	CLA	C2-C1-O2A-CGA
13	b	519	CLA	C2-C1-O2A-CGA
13	f	1207	CLA	C2-C1-O2A-CGA
13	s	511	CLA	C2-C1-O2A-CGA
13	t	519	CLA	C2-C1-O2A-CGA
13	A	1022	CLA	C2-C3-C5-C6
13	B	1224	CLA	C2-C3-C5-C6
13	H	1224	CLA	C2-C3-C5-C6
13	e	1022	CLA	C2-C3-C5-C6
13	f	1224	CLA	C2-C3-C5-C6
13	H	1228	CLA	CBD-CGD-O2D-CED
13	B	1226	CLA	C8-C10-C11-C12
13	4	512	CLA	CAA-CBA-CGA-O2A
13	6	517	CLA	CAA-CBA-CGA-O2A
13	b	512	CLA	CAA-CBA-CGA-O2A
13	v	517	CLA	CAA-CBA-CGA-O2A
13	u	518	CLA	CAA-CBA-CGA-O2A
13	f	1226	CLA	C8-C10-C11-C12
18	B	1843	LMU	C6-C7-C8-C9
18	H	1843	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	1	822	SQD	O48-C23-C24-C25
20	Y	822	SQD	O48-C23-C24-C25
20	q	822	SQD	O48-C23-C24-C25
13	A	1133	CLA	CBD-CGD-O2D-CED
13	G	1133	CLA	CBD-CGD-O2D-CED
18	f	1843	LMU	C6-C7-C8-C9
13	3	501	CLA	C10-C11-C12-C13
13	a	501	CLA	C10-C11-C12-C13
13	s	501	CLA	C10-C11-C12-C13
13	A	1013	CLA	C2A-CAA-CBA-CGA
13	G	1013	CLA	C2A-CAA-CBA-CGA
13	e	1013	CLA	C2A-CAA-CBA-CGA
13	e	1120	CLA	C2A-CAA-CBA-CGA
13	f	1202	CLA	C16-C17-C18-C20
17	e	5004	LHG	C24-C23-O8-C6
17	e	5001	LHG	C24-C25-C26-C27
13	A	1109	CLA	C3-C5-C6-C7
13	e	1109	CLA	C3-C5-C6-C7
16	A	4001	BCR	C1-C6-C7-C8
16	A	4008	BCR	C1-C6-C7-C8
16	B	4014	BCR	C1-C6-C7-C8
16	4	523	BCR	C1-C6-C7-C8
16	5	521	BCR	C1-C6-C7-C8
16	6	524	BCR	C1-C6-C7-C8
16	6	524	BCR	C23-C24-C25-C30
16	G	4001	BCR	C1-C6-C7-C8
16	G	4008	BCR	C1-C6-C7-C8
16	H	4014	BCR	C1-C6-C7-C8
16	b	523	BCR	C1-C6-C7-C8
16	c	521	BCR	C1-C6-C7-C8
16	d	524	BCR	C1-C6-C7-C8
16	d	524	BCR	C23-C24-C25-C30
16	e	4001	BCR	C1-C6-C7-C8
16	e	4008	BCR	C1-C6-C7-C8
16	f	4014	BCR	C1-C6-C7-C8
16	t	523	BCR	C1-C6-C7-C8
16	u	521	BCR	C1-C6-C7-C8
16	v	524	BCR	C1-C6-C7-C8
16	v	524	BCR	C23-C24-C25-C30
13	5	518	CLA	CAA-CBA-CGA-O2A
13	c	518	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
17	G	5001	LHG	C24-C25-C26-C27
16	A	4011	BCR	C19-C20-C21-C22
16	1	522	BCR	C15-C16-C17-C18
16	4	521	BCR	C15-C16-C17-C18
16	6	521	BCR	C9-C10-C11-C12
16	G	4011	BCR	C19-C20-C21-C22
16	Y	522	BCR	C15-C16-C17-C18
16	b	521	BCR	C15-C16-C17-C18
16	d	521	BCR	C9-C10-C11-C12
16	e	4011	BCR	C19-C20-C21-C22
16	q	522	BCR	C15-C16-C17-C18
16	v	521	BCR	C9-C10-C11-C12
13	A	1106	CLA	C4-C3-C5-C6
13	A	1127	CLA	C4-C3-C5-C6
13	G	1106	CLA	C4-C3-C5-C6
13	e	1106	CLA	C4-C3-C5-C6
13	e	1127	CLA	C4-C3-C5-C6
16	J	4015	BCR	C7-C8-C9-C10
16	2	523	BCR	C7-C8-C9-C10
16	6	521	BCR	C7-C8-C9-C10
16	T	4015	BCR	C7-C8-C9-C10
16	Z	523	BCR	C7-C8-C9-C10
16	d	521	BCR	C7-C8-C9-C10
16	l	4015	BCR	C7-C8-C9-C10
16	r	523	BCR	C7-C8-C9-C10
16	v	521	BCR	C7-C8-C9-C10
13	B	1202	CLA	C16-C17-C18-C20
13	a	509	CLA	C5-C6-C7-C8
13	s	509	CLA	C5-C6-C7-C8
13	A	1107	CLA	C2-C3-C5-C6
13	B	1202	CLA	C2-C3-C5-C6
13	G	1107	CLA	C2-C3-C5-C6
13	H	1202	CLA	C2-C3-C5-C6
13	e	1107	CLA	C2-C3-C5-C6
13	f	1202	CLA	C2-C3-C5-C6
13	B	1228	CLA	CBD-CGD-O2D-CED
13	5	507	CLA	CAA-CBA-CGA-O2A
13	c	507	CLA	CAA-CBA-CGA-O2A
13	u	507	CLA	CAA-CBA-CGA-O2A
13	3	509	CLA	C5-C6-C7-C8
19	J	5104	LMG	C8-C7-O1-C1
19	T	5104	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
19	l	5104	LMG	C8-C7-O1-C1
13	a	519	CLA	CBA-CGA-O2A-C1
13	1	516	CLA	CAA-CBA-CGA-O2A
13	6	509	CLA	CAA-CBA-CGA-O2A
13	d	509	CLA	CAA-CBA-CGA-O2A
13	v	509	CLA	CAA-CBA-CGA-O2A
20	L	5216	SQD	C17-C18-C19-C20
20	n	5216	SQD	C17-C18-C19-C20
13	H	1202	CLA	C16-C17-C18-C20
13	H	1212	CLA	C3-C5-C6-C7
17	A	5001	LHG	C19-C20-C21-C22
17	G	5001	LHG	C19-C20-C21-C22
20	V	5216	SQD	C17-C18-C19-C20
13	B	1201	CLA	C8-C10-C11-C12
13	H	1201	CLA	C8-C10-C11-C12
13	f	1201	CLA	C8-C10-C11-C12
13	Y	516	CLA	CAA-CBA-CGA-O2A
13	q	516	CLA	CAA-CBA-CGA-O2A
13	A	1120	CLA	C2A-CAA-CBA-CGA
13	G	1120	CLA	C2A-CAA-CBA-CGA
17	e	5001	LHG	C19-C20-C21-C22
13	f	1228	CLA	CBD-CGD-O2D-CED
13	A	1011	CLA	CBA-CGA-O2A-C1
13	3	519	CLA	CBA-CGA-O2A-C1
13	G	1011	CLA	CBA-CGA-O2A-C1
13	e	1011	CLA	CBA-CGA-O2A-C1
13	s	519	CLA	CBA-CGA-O2A-C1
13	B	1228	CLA	O1D-CGD-O2D-CED
13	B	1212	CLA	C3-C5-C6-C7
13	f	1212	CLA	C3-C5-C6-C7
13	5	510	CLA	CAA-CBA-CGA-O2A
13	5	512	CLA	CAA-CBA-CGA-O2A
13	c	510	CLA	CAA-CBA-CGA-O2A
13	c	512	CLA	CAA-CBA-CGA-O2A
13	u	510	CLA	CAA-CBA-CGA-O2A
13	u	512	CLA	CAA-CBA-CGA-O2A
13	A	1108	CLA	C4B-C3B-CAB-CBB
13	A	1111	CLA	C4B-C3B-CAB-CBB
13	A	1117	CLA	C4B-C3B-CAB-CBB
13	A	1133	CLA	C4B-C3B-CAB-CBB
13	A	1130	CLA	C4B-C3B-CAB-CBB
13	B	1204	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	L	1501	CLA	C4B-C3B-CAB-CBB
13	1	507	CLA	C4B-C3B-CAB-CBB
13	3	505	CLA	C4B-C3B-CAB-CBB
13	3	510	CLA	C4B-C3B-CAB-CBB
13	4	511	CLA	C4B-C3B-CAB-CBB
13	5	506	CLA	C4B-C3B-CAB-CBB
13	6	506	CLA	C4B-C3B-CAB-CBB
13	G	1108	CLA	C4B-C3B-CAB-CBB
13	G	1111	CLA	C4B-C3B-CAB-CBB
13	G	1117	CLA	C4B-C3B-CAB-CBB
13	G	1133	CLA	C4B-C3B-CAB-CBB
13	G	1130	CLA	C4B-C3B-CAB-CBB
13	H	1204	CLA	C4B-C3B-CAB-CBB
13	V	1501	CLA	C4B-C3B-CAB-CBB
13	Y	507	CLA	C4B-C3B-CAB-CBB
13	a	505	CLA	C4B-C3B-CAB-CBB
13	a	510	CLA	C4B-C3B-CAB-CBB
13	b	511	CLA	C4B-C3B-CAB-CBB
13	c	506	CLA	C4B-C3B-CAB-CBB
13	d	506	CLA	C4B-C3B-CAB-CBB
13	e	1108	CLA	C4B-C3B-CAB-CBB
13	e	1111	CLA	C4B-C3B-CAB-CBB
13	e	1117	CLA	C4B-C3B-CAB-CBB
13	e	1133	CLA	C4B-C3B-CAB-CBB
13	e	1130	CLA	C4B-C3B-CAB-CBB
13	f	1204	CLA	C4B-C3B-CAB-CBB
13	n	1501	CLA	C4B-C3B-CAB-CBB
13	q	507	CLA	C4B-C3B-CAB-CBB
13	s	505	CLA	C4B-C3B-CAB-CBB
13	s	510	CLA	C4B-C3B-CAB-CBB
13	t	511	CLA	C4B-C3B-CAB-CBB
13	u	506	CLA	C4B-C3B-CAB-CBB
13	v	506	CLA	C4B-C3B-CAB-CBB
13	B	1240	CLA	C4-C3-C5-C6
13	G	1127	CLA	C4-C3-C5-C6
13	H	1240	CLA	C4-C3-C5-C6
13	H	1228	CLA	O1D-CGD-O2D-CED
13	3	510	CLA	C12-C13-C15-C16
13	a	510	CLA	C12-C13-C15-C16
13	f	1226	CLA	C12-C13-C15-C16
13	s	510	CLA	C12-C13-C15-C16
13	6	511	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	d	511	CLA	CAA-CBA-CGA-O2A
13	v	511	CLA	CAA-CBA-CGA-O2A
13	L	1501	CLA	C15-C16-C17-C18
13	n	1501	CLA	C15-C16-C17-C18
13	f	1228	CLA	O1D-CGD-O2D-CED
18	T	5105	LMU	O1'-C1-C2-C3
13	V	1501	CLA	C15-C16-C17-C18
16	t	521	BCR	C15-C16-C17-C18
20	B	1852	SQD	O47-C7-C8-C9
20	H	1852	SQD	O47-C7-C8-C9
13	e	1133	CLA	CBD-CGD-O2D-CED
18	l	5105	LMU	O1'-C1-C2-C3
13	4	513	CLA	CAA-CBA-CGA-O2A
13	b	513	CLA	CAA-CBA-CGA-O2A
13	t	513	CLA	CAA-CBA-CGA-O2A
20	L	5216	SQD	O6-C44-C45-O47
20	V	5216	SQD	O6-C44-C45-O47
20	n	5216	SQD	O6-C44-C45-O47
13	A	1124	CLA	CBA-CGA-O2A-C1
13	G	1124	CLA	CBA-CGA-O2A-C1
13	H	1204	CLA	CBA-CGA-O2A-C1
18	J	5105	LMU	O1'-C1-C2-C3
13	1	518	CLA	CAA-CBA-CGA-O1A
13	q	518	CLA	CAA-CBA-CGA-O1A
13	d	507	CLA	CAA-CBA-CGA-O2A
13	v	509	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	CAA-CBA-CGA-O2A
13	3	519	CLA	CAA-CBA-CGA-O2A
13	G	1123	CLA	CAA-CBA-CGA-O2A
13	a	519	CLA	CAA-CBA-CGA-O2A
13	e	1123	CLA	CAA-CBA-CGA-O2A
13	s	519	CLA	CAA-CBA-CGA-O2A
17	H	1842	LHG	O7-C7-C8-C9
17	f	1842	LHG	O7-C7-C8-C9
13	G	1126	CLA	O1A-CGA-O2A-C1
13	u	505	CLA	O1D-CGD-O2D-CED
13	Y	518	CLA	CAA-CBA-CGA-O1A
13	5	510	CLA	CAA-CBA-CGA-O1A
13	6	507	CLA	CAA-CBA-CGA-O2A
13	6	509	CLA	CAA-CBA-CGA-O1A
13	6	512	CLA	CAA-CBA-CGA-O2A
13	c	510	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	d	509	CLA	CAA-CBA-CGA-O1A
13	u	510	CLA	CAA-CBA-CGA-O1A
13	v	507	CLA	CAA-CBA-CGA-O2A
13	A	1140	CLA	O1D-CGD-O2D-CED
13	B	1204	CLA	CBA-CGA-O2A-C1
13	e	1124	CLA	CBA-CGA-O2A-C1
13	f	1204	CLA	CBA-CGA-O2A-C1
17	e	5003	LHG	C26-C27-C28-C29
17	B	1842	LHG	O7-C7-C8-C9
20	3	822	SQD	O48-C23-C24-C25
20	a	822	SQD	O48-C23-C24-C25
20	f	1852	SQD	O47-C7-C8-C9
20	s	822	SQD	O48-C23-C24-C25
13	A	1013	CLA	C4-C3-C5-C6
13	A	1126	CLA	C4-C3-C5-C6
13	2	513	CLA	C4-C3-C5-C6
13	G	1013	CLA	C4-C3-C5-C6
13	G	1126	CLA	C4-C3-C5-C6
13	Z	513	CLA	C4-C3-C5-C6
13	e	1013	CLA	C4-C3-C5-C6
13	e	1126	CLA	C4-C3-C5-C6
13	f	1240	CLA	C4-C3-C5-C6
13	r	513	CLA	C4-C3-C5-C6
13	2	510	CLA	C13-C15-C16-C17
13	Z	510	CLA	C13-C15-C16-C17
13	r	510	CLA	C13-C15-C16-C17
17	A	5003	LHG	C26-C27-C28-C29
13	4	507	CLA	CAA-CBA-CGA-O2A
13	b	507	CLA	CAA-CBA-CGA-O2A
13	d	512	CLA	CAA-CBA-CGA-O2A
13	q	517	CLA	CAA-CBA-CGA-O2A
13	t	507	CLA	CAA-CBA-CGA-O2A
13	v	512	CLA	CAA-CBA-CGA-O2A
13	e	1126	CLA	O1A-CGA-O2A-C1
13	B	1213	CLA	C2-C3-C5-C6
13	5	503	CLA	C2-C3-C5-C6
13	H	1213	CLA	C2-C3-C5-C6
13	c	503	CLA	C2-C3-C5-C6
13	u	503	CLA	C2-C3-C5-C6
13	A	1022	CLA	C16-C17-C18-C19
13	G	1022	CLA	C16-C17-C18-C19
13	3	507	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	a	507	CLA	CAA-CBA-CGA-O2A
17	G	5003	LHG	C26-C27-C28-C29
13	A	1123	CLA	C11-C12-C13-C14
13	B	1208	CLA	C14-C13-C15-C16
13	B	1234	CLA	C14-C13-C15-C16
13	G	1123	CLA	C11-C12-C13-C14
13	H	1208	CLA	C14-C13-C15-C16
13	H	1234	CLA	C14-C13-C15-C16
13	e	1123	CLA	C11-C12-C13-C14
13	f	1208	CLA	C14-C13-C15-C16
13	f	1234	CLA	C14-C13-C15-C16
13	A	1011	CLA	O1A-CGA-O2A-C1
13	e	1011	CLA	O1A-CGA-O2A-C1
13	1	517	CLA	CAA-CBA-CGA-O2A
13	Y	517	CLA	CAA-CBA-CGA-O2A
13	A	1111	CLA	C3A-C2A-CAA-CBA
13	A	1118	CLA	C3A-C2A-CAA-CBA
13	G	1111	CLA	C3A-C2A-CAA-CBA
13	G	1118	CLA	C3A-C2A-CAA-CBA
13	e	1111	CLA	C3A-C2A-CAA-CBA
13	e	1118	CLA	C3A-C2A-CAA-CBA
13	q	512	CLA	C3A-C2A-CAA-CBA
13	A	1126	CLA	O1A-CGA-O2A-C1
13	B	1205	CLA	O1A-CGA-O2A-C1
13	G	1011	CLA	O1A-CGA-O2A-C1
13	H	1205	CLA	O1A-CGA-O2A-C1
13	f	1205	CLA	O1A-CGA-O2A-C1
13	B	1203	CLA	CAA-CBA-CGA-O2A
13	L	1501	CLA	CAA-CBA-CGA-O2A
13	H	1203	CLA	CAA-CBA-CGA-O2A
13	V	1501	CLA	CAA-CBA-CGA-O2A
13	f	1203	CLA	CAA-CBA-CGA-O2A
13	n	1501	CLA	CAA-CBA-CGA-O2A
13	s	507	CLA	CAA-CBA-CGA-O2A
13	2	516	CLA	CAA-CBA-CGA-O2A
13	Z	516	CLA	CAA-CBA-CGA-O2A
13	c	512	CLA	CAA-CBA-CGA-O1A
13	r	516	CLA	CAA-CBA-CGA-O2A
13	A	1103	CLA	CAD-CBD-CGD-O2D
13	A	1105	CLA	CAD-CBD-CGD-O2D
13	A	1109	CLA	CAD-CBD-CGD-O2D
13	A	1112	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	A	1115	CLA	CAD-CBD-CGD-O2D
13	A	1124	CLA	CAD-CBD-CGD-O2D
13	A	1129	CLA	CAD-CBD-CGD-O2D
13	B	1203	CLA	CAD-CBD-CGD-O2D
13	B	1210	CLA	CAD-CBD-CGD-O2D
13	B	1234	CLA	CAD-CBD-CGD-O2D
13	F	1302	CLA	CAD-CBD-CGD-O2D
13	L	1501	CLA	CAD-CBD-CGD-O2D
13	1	501	CLA	CAD-CBD-CGD-O2D
13	1	512	CLA	CAD-CBD-CGD-O2D
13	1	513	CLA	CAD-CBD-CGD-O2D
13	1	517	CLA	CAD-CBD-CGD-O2D
13	2	501	CLA	CAD-CBD-CGD-O2D
13	2	504	CLA	CAD-CBD-CGD-O2D
13	2	509	CLA	CAD-CBD-CGD-O2D
13	2	510	CLA	CAD-CBD-CGD-O2D
13	2	512	CLA	CAD-CBD-CGD-O2D
13	3	508	CLA	CAD-CBD-CGD-O2D
13	3	509	CLA	CAD-CBD-CGD-O2D
13	4	505	CLA	CAD-CBD-CGD-O2D
13	5	502	CLA	CAD-CBD-CGD-O2D
13	6	502	CLA	CAD-CBD-CGD-O2D
13	6	516	CLA	CAD-CBD-CGD-O2D
13	G	1103	CLA	CAD-CBD-CGD-O2D
13	G	1105	CLA	CAD-CBD-CGD-O2D
13	G	1109	CLA	CAD-CBD-CGD-O2D
13	G	1112	CLA	CAD-CBD-CGD-O2D
13	G	1115	CLA	CAD-CBD-CGD-O2D
13	G	1124	CLA	CAD-CBD-CGD-O2D
13	G	1129	CLA	CAD-CBD-CGD-O2D
13	H	1203	CLA	CAD-CBD-CGD-O2D
13	H	1210	CLA	CAD-CBD-CGD-O2D
13	H	1234	CLA	CAD-CBD-CGD-O2D
13	R	1302	CLA	CAD-CBD-CGD-O2D
13	V	1501	CLA	CAD-CBD-CGD-O2D
13	Y	501	CLA	CAD-CBD-CGD-O2D
13	Y	512	CLA	CAD-CBD-CGD-O2D
13	Y	513	CLA	CAD-CBD-CGD-O2D
13	Y	517	CLA	CAD-CBD-CGD-O2D
13	Z	501	CLA	CAD-CBD-CGD-O2D
13	Z	504	CLA	CAD-CBD-CGD-O2D
13	Z	509	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	Z	510	CLA	CAD-CBD-CGD-O2D
13	Z	512	CLA	CAD-CBD-CGD-O2D
13	a	508	CLA	CAD-CBD-CGD-O2D
13	a	509	CLA	CAD-CBD-CGD-O2D
13	b	505	CLA	CAD-CBD-CGD-O2D
13	c	502	CLA	CAD-CBD-CGD-O2D
13	d	502	CLA	CAD-CBD-CGD-O2D
13	d	516	CLA	CAD-CBD-CGD-O2D
13	e	1103	CLA	CAD-CBD-CGD-O2D
13	e	1105	CLA	CAD-CBD-CGD-O2D
13	e	1109	CLA	CAD-CBD-CGD-O2D
13	e	1112	CLA	CAD-CBD-CGD-O2D
13	e	1115	CLA	CAD-CBD-CGD-O2D
13	e	1124	CLA	CAD-CBD-CGD-O2D
13	e	1129	CLA	CAD-CBD-CGD-O2D
13	f	1203	CLA	CAD-CBD-CGD-O2D
13	f	1210	CLA	CAD-CBD-CGD-O2D
13	f	1234	CLA	CAD-CBD-CGD-O2D
13	j	1302	CLA	CAD-CBD-CGD-O2D
13	n	1501	CLA	CAD-CBD-CGD-O2D
13	q	501	CLA	CAD-CBD-CGD-O2D
13	q	512	CLA	CAD-CBD-CGD-O2D
13	q	513	CLA	CAD-CBD-CGD-O2D
13	q	517	CLA	CAD-CBD-CGD-O2D
13	r	501	CLA	CAD-CBD-CGD-O2D
13	r	504	CLA	CAD-CBD-CGD-O2D
13	r	509	CLA	CAD-CBD-CGD-O2D
13	r	510	CLA	CAD-CBD-CGD-O2D
13	r	512	CLA	CAD-CBD-CGD-O2D
13	s	508	CLA	CAD-CBD-CGD-O2D
13	s	509	CLA	CAD-CBD-CGD-O2D
13	t	505	CLA	CAD-CBD-CGD-O2D
13	u	502	CLA	CAD-CBD-CGD-O2D
13	v	502	CLA	CAD-CBD-CGD-O2D
13	v	516	CLA	CAD-CBD-CGD-O2D
13	e	1022	CLA	C16-C17-C18-C19
19	f	5002	LMG	C38-C39-C40-C41
13	5	505	CLA	O1D-CGD-O2D-CED
13	e	1140	CLA	O1D-CGD-O2D-CED
13	e	1127	CLA	O1A-CGA-O2A-C1
13	q	503	CLA	C15-C16-C17-C18
19	B	5002	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
13	5	513	CLA	CAA-CBA-CGA-O2A
13	6	504	CLA	CAA-CBA-CGA-O2A
13	6	516	CLA	CAA-CBA-CGA-O2A
13	c	513	CLA	CAA-CBA-CGA-O2A
13	d	504	CLA	CAA-CBA-CGA-O2A
13	d	516	CLA	CAA-CBA-CGA-O2A
13	u	513	CLA	CAA-CBA-CGA-O2A
13	v	504	CLA	CAA-CBA-CGA-O2A
13	1	503	CLA	C15-C16-C17-C18
19	H	5002	LMG	C38-C39-C40-C41
17	A	5003	LHG	O7-C7-C8-C9
17	G	5003	LHG	O7-C7-C8-C9
17	e	5003	LHG	O7-C7-C8-C9
13	Y	503	CLA	C15-C16-C17-C18
13	A	1127	CLA	O1A-CGA-O2A-C1
13	G	1127	CLA	O1A-CGA-O2A-C1
13	5	512	CLA	CAA-CBA-CGA-O1A
13	c	507	CLA	CAA-CBA-CGA-O1A
13	u	512	CLA	CAA-CBA-CGA-O1A
13	v	516	CLA	CAA-CBA-CGA-O2A
13	G	1140	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C2-C3-C5-C6
13	G	1126	CLA	C2-C3-C5-C6
13	e	1126	CLA	C2-C3-C5-C6
13	f	1213	CLA	C2-C3-C5-C6
13	A	1237	CLA	CAA-CBA-CGA-O2A
13	5	501	CLA	CAA-CBA-CGA-O2A
13	G	1237	CLA	CAA-CBA-CGA-O2A
13	c	501	CLA	CAA-CBA-CGA-O2A
13	e	1237	CLA	CAA-CBA-CGA-O2A
13	u	501	CLA	CAA-CBA-CGA-O2A
19	B	5002	LMG	O7-C10-C11-C12
19	f	5002	LMG	O7-C10-C11-C12
16	Y	524	BCR	C11-C12-C13-C14
13	4	513	CLA	CAA-CBA-CGA-O1A
13	5	507	CLA	CAA-CBA-CGA-O1A
13	5	505	CLA	CBD-CGD-O2D-CED
13	u	505	CLA	CBD-CGD-O2D-CED
13	c	505	CLA	O1D-CGD-O2D-CED
13	B	1206	CLA	CAA-CBA-CGA-O2A
13	H	1206	CLA	CAA-CBA-CGA-O2A
13	U	1401	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	a	501	CLA	CAA-CBA-CGA-O2A
13	f	1206	CLA	CAA-CBA-CGA-O2A
13	m	1401	CLA	CAA-CBA-CGA-O2A
19	H	5002	LMG	O7-C10-C11-C12
20	H	1852	SQD	C30-C31-C32-C33
20	f	1852	SQD	C30-C31-C32-C33
13	5	517	CLA	CAA-CBA-CGA-O2A
13	6	511	CLA	CAA-CBA-CGA-O1A
13	b	513	CLA	CAA-CBA-CGA-O1A
13	c	517	CLA	CAA-CBA-CGA-O2A
13	d	511	CLA	CAA-CBA-CGA-O1A
13	t	513	CLA	CAA-CBA-CGA-O1A
13	u	507	CLA	CAA-CBA-CGA-O1A
13	u	517	CLA	CAA-CBA-CGA-O2A
13	v	511	CLA	CAA-CBA-CGA-O1A
13	c	505	CLA	CBD-CGD-O2D-CED
20	B	1852	SQD	C30-C31-C32-C33
13	G	1123	CLA	C8-C10-C11-C12
13	A	1125	CLA	O2A-C1-C2-C3
13	G	1125	CLA	O2A-C1-C2-C3
13	e	1125	CLA	O2A-C1-C2-C3
17	e	5007	LHG	C27-C28-C29-C30
13	A	1106	CLA	CAA-CBA-CGA-O2A
13	K	1401	CLA	CAA-CBA-CGA-O2A
13	3	501	CLA	CAA-CBA-CGA-O2A
13	4	519	CLA	CAA-CBA-CGA-O2A
13	G	1106	CLA	CAA-CBA-CGA-O2A
13	b	519	CLA	CAA-CBA-CGA-O2A
13	e	1106	CLA	CAA-CBA-CGA-O2A
13	s	501	CLA	CAA-CBA-CGA-O2A
13	t	519	CLA	CAA-CBA-CGA-O2A
17	L	5220	LHG	O8-C23-C24-C25
17	n	5220	LHG	O8-C23-C24-C25
13	B	1224	CLA	CAA-CBA-CGA-O1A
13	H	1224	CLA	CAA-CBA-CGA-O1A
13	f	1224	CLA	CAA-CBA-CGA-O1A
13	1	516	CLA	CAA-CBA-CGA-O1A
13	5	513	CLA	CAA-CBA-CGA-O1A
13	6	507	CLA	CAA-CBA-CGA-O1A
13	Y	516	CLA	CAA-CBA-CGA-O1A
13	c	513	CLA	CAA-CBA-CGA-O1A
13	d	504	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	q	516	CLA	CAA-CBA-CGA-O1A
13	t	507	CLA	CAA-CBA-CGA-O1A
13	u	513	CLA	CAA-CBA-CGA-O1A
13	v	507	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	C8-C10-C11-C12
13	e	1123	CLA	C8-C10-C11-C12
17	A	5007	LHG	C27-C28-C29-C30
17	L	5221	LHG	C7-C8-C9-C10
17	V	5221	LHG	C7-C8-C9-C10
17	G	5007	LHG	C27-C28-C29-C30
13	A	1011	CLA	CHA-CBD-CGD-O2D
13	A	1111	CLA	CHA-CBD-CGD-O2D
13	A	1113	CLA	CHA-CBD-CGD-O1D
13	A	1118	CLA	CHA-CBD-CGD-O2D
13	A	1119	CLA	CHA-CBD-CGD-O1D
13	A	1119	CLA	CHA-CBD-CGD-O2D
13	A	1138	CLA	CHA-CBD-CGD-O1D
13	A	1138	CLA	CHA-CBD-CGD-O2D
13	A	1139	CLA	CHA-CBD-CGD-O1D
13	A	1139	CLA	CHA-CBD-CGD-O2D
13	A	1801	CLA	CHA-CBD-CGD-O2D
13	B	1202	CLA	CHA-CBD-CGD-O2D
13	B	1213	CLA	CHA-CBD-CGD-O1D
13	B	1213	CLA	CHA-CBD-CGD-O2D
13	B	1220	CLA	CHA-CBD-CGD-O1D
13	B	1220	CLA	CHA-CBD-CGD-O2D
13	B	1221	CLA	CHA-CBD-CGD-O1D
13	B	1221	CLA	CHA-CBD-CGD-O2D
13	B	1226	CLA	CHA-CBD-CGD-O1D
13	B	1226	CLA	CHA-CBD-CGD-O2D
13	B	1232	CLA	CHA-CBD-CGD-O2D
13	1	502	CLA	CHA-CBD-CGD-O2D
13	1	507	CLA	CHA-CBD-CGD-O1D
13	1	507	CLA	CHA-CBD-CGD-O2D
13	1	518	CLA	CHA-CBD-CGD-O1D
13	1	518	CLA	CHA-CBD-CGD-O2D
13	2	517	CLA	CHA-CBD-CGD-O2D
13	3	502	CLA	CHA-CBD-CGD-O1D
13	3	502	CLA	CHA-CBD-CGD-O2D
13	3	507	CLA	CHA-CBD-CGD-O2D
13	3	519	CLA	CHA-CBD-CGD-O1D
13	4	510	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	4	512	CLA	CHA-CBD-CGD-O1D
13	4	516	CLA	CHA-CBD-CGD-O2D
13	4	517	CLA	CHA-CBD-CGD-O2D
13	4	518	CLA	CHA-CBD-CGD-O1D
13	5	505	CLA	CHA-CBD-CGD-O2D
13	5	512	CLA	CHA-CBD-CGD-O1D
13	5	518	CLA	CHA-CBD-CGD-O1D
13	6	519	CLA	CHA-CBD-CGD-O2D
13	G	1011	CLA	CHA-CBD-CGD-O2D
13	G	1111	CLA	CHA-CBD-CGD-O2D
13	G	1113	CLA	CHA-CBD-CGD-O1D
13	G	1118	CLA	CHA-CBD-CGD-O2D
13	G	1119	CLA	CHA-CBD-CGD-O1D
13	G	1119	CLA	CHA-CBD-CGD-O2D
13	G	1138	CLA	CHA-CBD-CGD-O1D
13	G	1138	CLA	CHA-CBD-CGD-O2D
13	G	1139	CLA	CHA-CBD-CGD-O1D
13	G	1139	CLA	CHA-CBD-CGD-O2D
13	G	1801	CLA	CHA-CBD-CGD-O2D
13	H	1202	CLA	CHA-CBD-CGD-O2D
13	H	1213	CLA	CHA-CBD-CGD-O1D
13	H	1213	CLA	CHA-CBD-CGD-O2D
13	H	1220	CLA	CHA-CBD-CGD-O1D
13	H	1220	CLA	CHA-CBD-CGD-O2D
13	H	1221	CLA	CHA-CBD-CGD-O1D
13	H	1221	CLA	CHA-CBD-CGD-O2D
13	H	1226	CLA	CHA-CBD-CGD-O1D
13	H	1226	CLA	CHA-CBD-CGD-O2D
13	H	1232	CLA	CHA-CBD-CGD-O2D
13	Y	502	CLA	CHA-CBD-CGD-O2D
13	Y	507	CLA	CHA-CBD-CGD-O1D
13	Y	507	CLA	CHA-CBD-CGD-O2D
13	Y	518	CLA	CHA-CBD-CGD-O1D
13	Y	518	CLA	CHA-CBD-CGD-O2D
13	Z	517	CLA	CHA-CBD-CGD-O2D
13	a	502	CLA	CHA-CBD-CGD-O1D
13	a	502	CLA	CHA-CBD-CGD-O2D
13	a	507	CLA	CHA-CBD-CGD-O2D
13	a	519	CLA	CHA-CBD-CGD-O1D
13	b	510	CLA	CHA-CBD-CGD-O1D
13	b	512	CLA	CHA-CBD-CGD-O1D
13	b	516	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	b	517	CLA	CHA-CBD-CGD-O2D
13	b	518	CLA	CHA-CBD-CGD-O1D
13	c	505	CLA	CHA-CBD-CGD-O2D
13	c	512	CLA	CHA-CBD-CGD-O1D
13	c	518	CLA	CHA-CBD-CGD-O1D
13	d	509	CLA	CHA-CBD-CGD-O1D
13	d	519	CLA	CHA-CBD-CGD-O2D
13	e	1011	CLA	CHA-CBD-CGD-O2D
13	e	1111	CLA	CHA-CBD-CGD-O2D
13	e	1113	CLA	CHA-CBD-CGD-O1D
13	e	1118	CLA	CHA-CBD-CGD-O2D
13	e	1119	CLA	CHA-CBD-CGD-O1D
13	e	1119	CLA	CHA-CBD-CGD-O2D
13	e	1138	CLA	CHA-CBD-CGD-O1D
13	e	1138	CLA	CHA-CBD-CGD-O2D
13	e	1139	CLA	CHA-CBD-CGD-O1D
13	e	1139	CLA	CHA-CBD-CGD-O2D
13	e	1801	CLA	CHA-CBD-CGD-O2D
13	f	1202	CLA	CHA-CBD-CGD-O2D
13	f	1213	CLA	CHA-CBD-CGD-O1D
13	f	1213	CLA	CHA-CBD-CGD-O2D
13	f	1220	CLA	CHA-CBD-CGD-O1D
13	f	1220	CLA	CHA-CBD-CGD-O2D
13	f	1221	CLA	CHA-CBD-CGD-O1D
13	f	1221	CLA	CHA-CBD-CGD-O2D
13	f	1226	CLA	CHA-CBD-CGD-O1D
13	f	1226	CLA	CHA-CBD-CGD-O2D
13	f	1232	CLA	CHA-CBD-CGD-O2D
13	q	502	CLA	CHA-CBD-CGD-O2D
13	q	507	CLA	CHA-CBD-CGD-O1D
13	q	507	CLA	CHA-CBD-CGD-O2D
13	q	518	CLA	CHA-CBD-CGD-O1D
13	q	518	CLA	CHA-CBD-CGD-O2D
13	r	517	CLA	CHA-CBD-CGD-O2D
13	s	502	CLA	CHA-CBD-CGD-O1D
13	s	502	CLA	CHA-CBD-CGD-O2D
13	s	505	CLA	CHA-CBD-CGD-O2D
13	s	507	CLA	CHA-CBD-CGD-O2D
13	s	519	CLA	CHA-CBD-CGD-O1D
13	t	510	CLA	CHA-CBD-CGD-O1D
13	t	512	CLA	CHA-CBD-CGD-O1D
13	t	516	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	t	517	CLA	CHA-CBD-CGD-O2D
13	t	518	CLA	CHA-CBD-CGD-O1D
13	u	505	CLA	CHA-CBD-CGD-O2D
13	u	512	CLA	CHA-CBD-CGD-O1D
13	u	518	CLA	CHA-CBD-CGD-O1D
13	v	509	CLA	CHA-CBD-CGD-O1D
13	v	519	CLA	CHA-CBD-CGD-O2D
16	B	4009	BCR	C19-C20-C21-C22
16	f	4009	BCR	C19-C20-C21-C22
13	4	507	CLA	CAA-CBA-CGA-O1A
13	5	517	CLA	CAA-CBA-CGA-O1A
13	b	507	CLA	CAA-CBA-CGA-O1A
13	c	517	CLA	CAA-CBA-CGA-O1A
13	d	507	CLA	CAA-CBA-CGA-O1A
13	u	517	CLA	CAA-CBA-CGA-O1A
13	1	501	CLA	CAA-CBA-CGA-O2A
13	Y	501	CLA	CAA-CBA-CGA-O2A
13	q	501	CLA	CAA-CBA-CGA-O2A
13	1	507	CLA	C3-C5-C6-C7
13	Y	507	CLA	C3-C5-C6-C7
13	q	507	CLA	C3-C5-C6-C7
13	2	516	CLA	CAA-CBA-CGA-O1A
13	6	504	CLA	CAA-CBA-CGA-O1A
13	r	516	CLA	CAA-CBA-CGA-O1A
13	v	504	CLA	CAA-CBA-CGA-O1A
13	Z	505	CLA	C13-C15-C16-C17
13	A	1135	CLA	CAA-CBA-CGA-O2A
13	B	1221	CLA	CAA-CBA-CGA-O2A
13	G	1135	CLA	CAA-CBA-CGA-O2A
13	e	1135	CLA	CAA-CBA-CGA-O2A
13	f	1221	CLA	CAA-CBA-CGA-O2A
17	V	5220	LHG	O8-C23-C24-C25
17	H	1855	LHG	C16-C17-C18-C19
17	f	1855	LHG	C16-C17-C18-C19
18	A	1848	LMU	C7-C8-C9-C10
18	G	1848	LMU	C7-C8-C9-C10
20	5	822	SQD	O10-C23-C24-C25
20	c	822	SQD	O10-C23-C24-C25
20	u	822	SQD	O10-C23-C24-C25
17	n	5221	LHG	C7-C8-C9-C10
17	B	1855	LHG	C16-C17-C18-C19
17	n	5218	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
18	e	1848	LMU	C7-C8-C9-C10
13	2	505	CLA	C13-C15-C16-C17
13	r	505	CLA	C13-C15-C16-C17
13	5	508	CLA	CAA-CBA-CGA-O2A
13	Z	516	CLA	CAA-CBA-CGA-O1A
13	c	508	CLA	CAA-CBA-CGA-O2A
13	d	512	CLA	CAA-CBA-CGA-O1A
13	u	508	CLA	CAA-CBA-CGA-O2A
13	v	512	CLA	CAA-CBA-CGA-O1A
13	v	516	CLA	CAA-CBA-CGA-O1A
17	V	5218	LHG	C25-C26-C27-C28
13	f	1215	CLA	C15-C16-C17-C18
13	A	1107	CLA	CAA-CBA-CGA-O2A
13	G	1107	CLA	CAA-CBA-CGA-O2A
13	H	1221	CLA	CAA-CBA-CGA-O2A
13	e	1107	CLA	CAA-CBA-CGA-O2A
17	L	5218	LHG	C25-C26-C27-C28
13	v	501	CLA	C2A-CAA-CBA-CGA
13	F	1302	CLA	CAA-CBA-CGA-O1A
13	6	512	CLA	CAA-CBA-CGA-O1A
13	6	516	CLA	CAA-CBA-CGA-O1A
13	b	516	CLA	CAA-CBA-CGA-O1A
13	d	516	CLA	CAA-CBA-CGA-O1A
13	A	1107	CLA	C8-C10-C11-C12
13	B	1215	CLA	C15-C16-C17-C18
13	G	1107	CLA	C8-C10-C11-C12
13	H	1215	CLA	C15-C16-C17-C18
13	e	1107	CLA	C8-C10-C11-C12
13	A	1127	CLA	CBA-CGA-O2A-C1
13	G	1127	CLA	CBA-CGA-O2A-C1
13	e	1127	CLA	CBA-CGA-O2A-C1
13	6	501	CLA	CAA-CBA-CGA-O2A
13	d	501	CLA	CAA-CBA-CGA-O2A
13	v	501	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	O8-C23-C24-C25
17	G	5001	LHG	O8-C23-C24-C25
17	e	5001	LHG	O8-C23-C24-C25
13	4	516	CLA	CAA-CBA-CGA-O1A
13	j	1302	CLA	CAA-CBA-CGA-O1A
13	t	516	CLA	CAA-CBA-CGA-O1A
13	H	1023	CLA	C8-C10-C11-C12
17	G	5005	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
13	B	1226	CLA	C12-C13-C15-C16
13	2	505	CLA	C12-C13-C15-C16
13	2	513	CLA	C2-C3-C5-C6
13	H	1226	CLA	C12-C13-C15-C16
13	Z	505	CLA	C12-C13-C15-C16
13	Z	513	CLA	C2-C3-C5-C6
13	r	505	CLA	C12-C13-C15-C16
13	r	513	CLA	C2-C3-C5-C6
17	A	5005	LHG	C33-C34-C35-C36
13	A	1108	CLA	CAA-CBA-CGA-O2A
13	B	1219	CLA	CAA-CBA-CGA-O2A
13	4	501	CLA	CAA-CBA-CGA-O2A
13	G	1108	CLA	CAA-CBA-CGA-O2A
13	H	1219	CLA	CAA-CBA-CGA-O2A
13	b	501	CLA	CAA-CBA-CGA-O2A
13	e	1108	CLA	CAA-CBA-CGA-O2A
13	f	1219	CLA	CAA-CBA-CGA-O2A
13	t	501	CLA	CAA-CBA-CGA-O2A
13	R	1302	CLA	CAA-CBA-CGA-O1A
17	e	5005	LHG	C33-C34-C35-C36
19	J	5104	LMG	C29-C30-C31-C32
19	l	5104	LMG	C29-C30-C31-C32
13	A	1119	CLA	C14-C13-C15-C16
13	A	1126	CLA	C14-C13-C15-C16
13	B	1203	CLA	C11-C10-C8-C9
13	B	1229	CLA	C11-C10-C8-C9
13	G	1119	CLA	C14-C13-C15-C16
13	G	1126	CLA	C14-C13-C15-C16
13	H	1203	CLA	C11-C10-C8-C9
13	H	1229	CLA	C11-C10-C8-C9
13	e	1119	CLA	C14-C13-C15-C16
13	e	1126	CLA	C14-C13-C15-C16
13	f	1203	CLA	C11-C10-C8-C9
13	f	1229	CLA	C11-C10-C8-C9
16	5	521	BCR	C9-C10-C11-C12
16	H	4009	BCR	C19-C20-C21-C22
16	c	521	BCR	C9-C10-C11-C12
16	u	521	BCR	C9-C10-C11-C12
19	T	5104	LMG	C29-C30-C31-C32
20	1	822	SQD	C11-C12-C13-C14
20	Y	822	SQD	C11-C12-C13-C14
13	6	506	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	G	1011	CLA	C2B-C3B-CAB-CBB
13	G	1125	CLA	C2B-C3B-CAB-CBB
13	d	506	CLA	C2B-C3B-CAB-CBB
13	v	506	CLA	C2B-C3B-CAB-CBB
13	f	1023	CLA	C8-C10-C11-C12
20	B	1852	SQD	C5-C6-S-O8
20	3	822	SQD	C5-C6-S-O8
20	H	1852	SQD	C5-C6-S-O8
20	a	822	SQD	C5-C6-S-O8
20	f	1852	SQD	C5-C6-S-O8
20	s	822	SQD	C5-C6-S-O8
20	q	822	SQD	C11-C12-C13-C14
13	B	1023	CLA	C8-C10-C11-C12
13	1	517	CLA	CAA-CBA-CGA-O1A
13	A	1110	CLA	C2A-CAA-CBA-CGA
13	A	1117	CLA	C2A-CAA-CBA-CGA
13	6	501	CLA	C2A-CAA-CBA-CGA
13	G	1117	CLA	C2A-CAA-CBA-CGA
13	d	501	CLA	C2A-CAA-CBA-CGA
13	e	1110	CLA	C2A-CAA-CBA-CGA
13	e	1117	CLA	C2A-CAA-CBA-CGA
13	4	519	CLA	CAA-CBA-CGA-O1A
13	b	519	CLA	CAA-CBA-CGA-O1A
13	t	519	CLA	CAA-CBA-CGA-O1A
17	A	5005	LHG	C32-C33-C34-C35
17	G	5005	LHG	C32-C33-C34-C35
18	Z	901	LMU	C3-C4-C5-C6
17	e	5005	LHG	C32-C33-C34-C35
18	2	901	LMU	C3-C4-C5-C6
18	r	901	LMU	C3-C4-C5-C6
13	Y	517	CLA	CAA-CBA-CGA-O1A
13	q	517	CLA	CAA-CBA-CGA-O1A
16	1	521	BCR	C36-C18-C19-C20
16	q	521	BCR	C36-C18-C19-C20
13	B	1206	CLA	CAA-CBA-CGA-O1A
13	3	519	CLA	CAA-CBA-CGA-O1A
13	H	1206	CLA	CAA-CBA-CGA-O1A
13	a	519	CLA	CAA-CBA-CGA-O1A
13	s	519	CLA	CAA-CBA-CGA-O1A
13	Z	511	CLA	C4-C3-C5-C6
20	Z	822	SQD	C25-C26-C27-C28
17	G	5006	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	2	822	SQD	C25-C26-C27-C28
20	r	822	SQD	C25-C26-C27-C28
13	f	1206	CLA	CAA-CBA-CGA-O1A
16	1	524	BCR	C11-C12-C13-C14
16	q	524	BCR	C11-C12-C13-C14
13	e	1126	CLA	CBA-CGA-O2A-C1
13	B	1012	CLA	C1A-C2A-CAA-CBA
13	L	1502	CLA	C1A-C2A-CAA-CBA
13	1	512	CLA	C1A-C2A-CAA-CBA
13	1	518	CLA	C1A-C2A-CAA-CBA
13	4	502	CLA	C1A-C2A-CAA-CBA
13	5	505	CLA	C1A-C2A-CAA-CBA
13	5	517	CLA	C1A-C2A-CAA-CBA
13	H	1012	CLA	C1A-C2A-CAA-CBA
13	V	1502	CLA	C1A-C2A-CAA-CBA
13	Y	512	CLA	C1A-C2A-CAA-CBA
13	Y	518	CLA	C1A-C2A-CAA-CBA
13	b	502	CLA	C1A-C2A-CAA-CBA
13	c	505	CLA	C1A-C2A-CAA-CBA
13	c	517	CLA	C1A-C2A-CAA-CBA
13	f	1012	CLA	C1A-C2A-CAA-CBA
13	n	1502	CLA	C1A-C2A-CAA-CBA
13	q	503	CLA	C1A-C2A-CAA-CBA
13	q	512	CLA	C1A-C2A-CAA-CBA
13	q	518	CLA	C1A-C2A-CAA-CBA
13	t	502	CLA	C1A-C2A-CAA-CBA
13	u	505	CLA	C1A-C2A-CAA-CBA
13	u	517	CLA	C1A-C2A-CAA-CBA
13	A	1123	CLA	CAA-CBA-CGA-O1A
13	3	501	CLA	CAA-CBA-CGA-O1A
13	e	1123	CLA	CAA-CBA-CGA-O1A
13	s	507	CLA	CAA-CBA-CGA-O1A
17	A	5006	LHG	O8-C23-C24-C25
13	H	1023	CLA	C13-C15-C16-C17
13	A	1124	CLA	O1A-CGA-O2A-C1
13	B	1204	CLA	O1A-CGA-O2A-C1
13	H	1204	CLA	O1A-CGA-O2A-C1
13	e	1124	CLA	O1A-CGA-O2A-C1
13	f	1204	CLA	O1A-CGA-O2A-C1
13	A	1126	CLA	CBA-CGA-O2A-C1
13	G	1126	CLA	CBA-CGA-O2A-C1
13	3	507	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	G	1123	CLA	CAA-CBA-CGA-O1A
13	s	501	CLA	CAA-CBA-CGA-O1A
17	A	5007	LHG	O9-C7-C8-C9
20	f	1852	SQD	O49-C7-C8-C9
13	B	1023	CLA	C13-C15-C16-C17
13	f	1023	CLA	C13-C15-C16-C17
13	G	1110	CLA	C2A-CAA-CBA-CGA
13	a	501	CLA	CAA-CBA-CGA-O1A
13	a	507	CLA	CAA-CBA-CGA-O1A
13	f	1203	CLA	CAA-CBA-CGA-O1A
17	e	5007	LHG	O9-C7-C8-C9
20	B	1852	SQD	O49-C7-C8-C9
20	H	1852	SQD	O49-C7-C8-C9
13	G	1124	CLA	O1A-CGA-O2A-C1
13	B	1213	CLA	C4-C3-C5-C6
13	H	1213	CLA	C4-C3-C5-C6
13	f	1213	CLA	C4-C3-C5-C6
17	G	5008	LHG	O7-C7-C8-C9
17	e	5006	LHG	O8-C23-C24-C25
13	A	1011	CLA	C8-C10-C11-C12
13	e	1011	CLA	C8-C10-C11-C12
13	B	1203	CLA	CAA-CBA-CGA-O1A
13	H	1203	CLA	CAA-CBA-CGA-O1A
13	Y	501	CLA	CAA-CBA-CGA-O1A
17	G	5007	LHG	O9-C7-C8-C9
20	s	822	SQD	O10-C23-C24-C25
13	5	508	CLA	CAA-CBA-CGA-O1A
13	c	508	CLA	CAA-CBA-CGA-O1A
13	u	508	CLA	CAA-CBA-CGA-O1A
13	A	1133	CLA	C15-C16-C17-C18
13	4	519	CLA	C5-C6-C7-C8
13	G	1011	CLA	C8-C10-C11-C12
13	b	519	CLA	C5-C6-C7-C8
13	t	519	CLA	C5-C6-C7-C8
17	e	5001	LHG	C28-C29-C30-C31
17	A	5006	LHG	C3-O3-P-O5
17	A	5009	LHG	C4-O6-P-O5
17	A	5001	LHG	C3-O3-P-O5
17	B	1842	LHG	C3-O3-P-O4
17	G	5006	LHG	C3-O3-P-O5
17	G	5009	LHG	C4-O6-P-O5
17	G	5001	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
17	H	1842	LHG	C3-O3-P-O4
17	e	5006	LHG	C3-O3-P-O5
17	e	5009	LHG	C4-O6-P-O5
17	e	5001	LHG	C3-O3-P-O5
17	f	1842	LHG	C3-O3-P-O4
13	A	1106	CLA	CAA-CBA-CGA-O1A
13	B	1221	CLA	CAA-CBA-CGA-O1A
13	K	1401	CLA	CAA-CBA-CGA-O1A
13	1	501	CLA	CAA-CBA-CGA-O1A
13	H	1221	CLA	CAA-CBA-CGA-O1A
13	U	1401	CLA	CAA-CBA-CGA-O1A
13	f	1221	CLA	CAA-CBA-CGA-O1A
13	m	1401	CLA	CAA-CBA-CGA-O1A
13	q	501	CLA	CAA-CBA-CGA-O1A
17	B	1842	LHG	O9-C7-C8-C9
17	f	1842	LHG	O9-C7-C8-C9
20	3	822	SQD	O10-C23-C24-C25
20	a	822	SQD	O10-C23-C24-C25
13	A	1137	CLA	CAA-CBA-CGA-O2A
13	G	1137	CLA	CAA-CBA-CGA-O2A
13	e	1137	CLA	CAA-CBA-CGA-O2A
17	A	5008	LHG	O7-C7-C8-C9
17	e	5008	LHG	O7-C7-C8-C9
13	G	1133	CLA	C15-C16-C17-C18
17	A	5001	LHG	C28-C29-C30-C31
16	A	4008	BCR	C5-C6-C7-C8
16	B	4014	BCR	C5-C6-C7-C8
16	B	4014	BCR	C23-C24-C25-C26
16	G	4008	BCR	C5-C6-C7-C8
16	H	4014	BCR	C5-C6-C7-C8
16	H	4014	BCR	C23-C24-C25-C26
16	e	4008	BCR	C5-C6-C7-C8
16	f	4014	BCR	C5-C6-C7-C8
16	f	4014	BCR	C23-C24-C25-C26
13	H	1222	CLA	O1D-CGD-O2D-CED
13	A	1123	CLA	C10-C11-C12-C13
13	A	1138	CLA	C15-C16-C17-C18
13	B	1021	CLA	C13-C15-C16-C17
13	L	1502	CLA	C8-C10-C11-C12
13	G	1123	CLA	C10-C11-C12-C13
13	G	1138	CLA	C15-C16-C17-C18
13	H	1021	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	V	1502	CLA	C8-C10-C11-C12
13	e	1123	CLA	C10-C11-C12-C13
13	e	1133	CLA	C15-C16-C17-C18
13	e	1138	CLA	C15-C16-C17-C18
13	f	1021	CLA	C13-C15-C16-C17
13	n	1502	CLA	C8-C10-C11-C12
13	L	1501	CLA	CAA-CBA-CGA-O1A
13	5	501	CLA	CAA-CBA-CGA-O1A
13	G	1106	CLA	CAA-CBA-CGA-O1A
13	V	1501	CLA	CAA-CBA-CGA-O1A
13	e	1106	CLA	CAA-CBA-CGA-O1A
17	H	1842	LHG	O9-C7-C8-C9
19	B	5002	LMG	O10-C28-C29-C30
19	H	5002	LMG	O10-C28-C29-C30
19	f	5002	LMG	O10-C28-C29-C30
17	G	5001	LHG	C28-C29-C30-C31
17	G	5007	LHG	O7-C7-C8-C9
13	A	1108	CLA	CAA-CBA-CGA-O1A
13	A	1237	CLA	CAA-CBA-CGA-O1A
13	B	1219	CLA	CAA-CBA-CGA-O1A
13	G	1108	CLA	CAA-CBA-CGA-O1A
13	G	1237	CLA	CAA-CBA-CGA-O1A
13	H	1219	CLA	CAA-CBA-CGA-O1A
13	e	1108	CLA	CAA-CBA-CGA-O1A
13	e	1237	CLA	CAA-CBA-CGA-O1A
13	f	1219	CLA	CAA-CBA-CGA-O1A
13	u	501	CLA	CAA-CBA-CGA-O1A
17	A	5008	LHG	O9-C7-C8-C9
17	G	5008	LHG	O9-C7-C8-C9
17	e	5008	LHG	O9-C7-C8-C9
13	5	519	CLA	CAA-CBA-CGA-O2A
13	c	519	CLA	CAA-CBA-CGA-O2A
17	A	5007	LHG	O7-C7-C8-C9
13	H	1229	CLA	C10-C11-C12-C13
13	B	1222	CLA	O1D-CGD-O2D-CED
13	c	501	CLA	CAA-CBA-CGA-O1A
13	n	1501	CLA	CAA-CBA-CGA-O1A
13	2	511	CLA	C4-C3-C5-C6
13	r	511	CLA	C4-C3-C5-C6
13	4	516	CLA	CAA-CBA-CGA-O2A
13	b	516	CLA	CAA-CBA-CGA-O2A
13	t	516	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	1111	CLA	CAD-CBD-CGD-O1D
13	A	1113	CLA	CAD-CBD-CGD-O1D
13	A	1118	CLA	CAD-CBD-CGD-O1D
13	A	1119	CLA	CAD-CBD-CGD-O1D
13	B	1021	CLA	CAD-CBD-CGD-O1D
13	B	1225	CLA	CAD-CBD-CGD-O1D
13	2	517	CLA	CAD-CBD-CGD-O1D
13	4	501	CLA	CAD-CBD-CGD-O1D
13	4	516	CLA	CAD-CBD-CGD-O1D
13	6	509	CLA	CAD-CBD-CGD-O1D
13	G	1111	CLA	CAD-CBD-CGD-O1D
13	G	1113	CLA	CAD-CBD-CGD-O1D
13	G	1118	CLA	CAD-CBD-CGD-O1D
13	G	1119	CLA	CAD-CBD-CGD-O1D
13	H	1021	CLA	CAD-CBD-CGD-O1D
13	Z	517	CLA	CAD-CBD-CGD-O1D
13	b	501	CLA	CAD-CBD-CGD-O1D
13	b	516	CLA	CAD-CBD-CGD-O1D
13	d	509	CLA	CAD-CBD-CGD-O1D
13	e	1111	CLA	CAD-CBD-CGD-O1D
13	e	1113	CLA	CAD-CBD-CGD-O1D
13	e	1118	CLA	CAD-CBD-CGD-O1D
13	e	1119	CLA	CAD-CBD-CGD-O1D
13	f	1021	CLA	CAD-CBD-CGD-O1D
13	r	517	CLA	CAD-CBD-CGD-O1D
13	t	501	CLA	CAD-CBD-CGD-O1D
13	t	516	CLA	CAD-CBD-CGD-O1D
13	v	509	CLA	CAD-CBD-CGD-O1D
20	L	5216	SQD	O5-C5-C6-S
20	5	822	SQD	O5-C5-C6-S
20	6	822	SQD	O5-C5-C6-S
20	V	5216	SQD	O5-C5-C6-S
20	c	822	SQD	O5-C5-C6-S
20	d	822	SQD	O5-C5-C6-S
20	n	5216	SQD	O5-C5-C6-S
20	u	822	SQD	O5-C5-C6-S
20	v	822	SQD	O5-C5-C6-S
13	A	1135	CLA	CAA-CBA-CGA-O1A
13	4	501	CLA	CAA-CBA-CGA-O1A
13	G	1135	CLA	CAA-CBA-CGA-O1A
13	e	1135	CLA	CAA-CBA-CGA-O1A
13	q	512	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	u	519	CLA	CAA-CBA-CGA-O2A
17	e	5007	LHG	O7-C7-C8-C9
13	B	1229	CLA	C10-C11-C12-C13
13	f	1229	CLA	C10-C11-C12-C13
13	A	1133	CLA	C14-C13-C15-C16
13	B	1226	CLA	C11-C10-C8-C9
13	2	513	CLA	C14-C13-C15-C16
13	3	505	CLA	C11-C12-C13-C14
13	3	510	CLA	C14-C13-C15-C16
13	G	1133	CLA	C14-C13-C15-C16
13	H	1226	CLA	C11-C10-C8-C9
13	Z	513	CLA	C14-C13-C15-C16
13	a	505	CLA	C11-C12-C13-C14
13	a	510	CLA	C14-C13-C15-C16
13	e	1133	CLA	C14-C13-C15-C16
13	f	1226	CLA	C11-C10-C8-C9
13	r	513	CLA	C14-C13-C15-C16
13	s	505	CLA	C11-C12-C13-C14
13	s	510	CLA	C14-C13-C15-C16
13	F	1302	CLA	CAA-CBA-CGA-O2A
13	R	1302	CLA	CAA-CBA-CGA-O2A
13	j	1302	CLA	CAA-CBA-CGA-O2A
13	b	501	CLA	CAA-CBA-CGA-O1A
13	t	501	CLA	CAA-CBA-CGA-O1A
13	A	1013	CLA	CAA-CBA-CGA-O2A
13	A	1115	CLA	CAA-CBA-CGA-O2A
13	1	510	CLA	CAA-CBA-CGA-O2A
13	1	512	CLA	CAA-CBA-CGA-O2A
13	2	509	CLA	CAA-CBA-CGA-O2A
13	2	510	CLA	CAA-CBA-CGA-O2A
13	G	1013	CLA	CAA-CBA-CGA-O2A
13	G	1115	CLA	CAA-CBA-CGA-O2A
13	Y	512	CLA	CAA-CBA-CGA-O2A
13	Z	509	CLA	CAA-CBA-CGA-O2A
13	Z	510	CLA	CAA-CBA-CGA-O2A
13	e	1115	CLA	CAA-CBA-CGA-O2A
13	q	510	CLA	CAA-CBA-CGA-O2A
13	r	509	CLA	CAA-CBA-CGA-O2A
13	r	510	CLA	CAA-CBA-CGA-O2A
19	B	5002	LMG	O8-C28-C29-C30
19	H	5002	LMG	O8-C28-C29-C30
19	f	5002	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
13	A	1110	CLA	CAA-CBA-CGA-O2A
13	A	1125	CLA	CAA-CBA-CGA-O2A
13	B	1213	CLA	CAA-CBA-CGA-O2A
13	2	501	CLA	CAA-CBA-CGA-O2A
13	G	1125	CLA	CAA-CBA-CGA-O2A
13	H	1213	CLA	CAA-CBA-CGA-O2A
13	Z	501	CLA	CAA-CBA-CGA-O2A
13	e	1013	CLA	CAA-CBA-CGA-O2A
13	e	1110	CLA	CAA-CBA-CGA-O2A
13	e	1125	CLA	CAA-CBA-CGA-O2A
13	f	1213	CLA	CAA-CBA-CGA-O2A
13	r	501	CLA	CAA-CBA-CGA-O2A
17	B	1855	LHG	O7-C7-C8-C9
17	H	1855	LHG	O7-C7-C8-C9
17	f	1855	LHG	O7-C7-C8-C9
13	d	501	CLA	CAA-CBA-CGA-O1A
17	A	5002	LHG	C5-C4-O6-P
17	G	5002	LHG	C5-C4-O6-P
17	e	5002	LHG	C5-C4-O6-P
16	e	4011	BCR	C7-C8-C9-C34
13	A	1119	CLA	C12-C13-C15-C16
13	A	1133	CLA	C12-C13-C15-C16
13	A	1135	CLA	C2-C3-C5-C6
13	A	1237	CLA	C6-C7-C8-C10
13	B	1215	CLA	C12-C13-C15-C16
13	B	1223	CLA	C3A-C2A-CAA-CBA
13	1	512	CLA	C3A-C2A-CAA-CBA
13	3	505	CLA	C11-C12-C13-C15
13	G	1119	CLA	C12-C13-C15-C16
13	G	1133	CLA	C12-C13-C15-C16
13	G	1135	CLA	C2-C3-C5-C6
13	G	1237	CLA	C6-C7-C8-C10
13	H	1215	CLA	C12-C13-C15-C16
13	H	1223	CLA	C3A-C2A-CAA-CBA
13	a	505	CLA	C11-C12-C13-C15
13	e	1119	CLA	C12-C13-C15-C16
13	e	1133	CLA	C12-C13-C15-C16
13	e	1135	CLA	C2-C3-C5-C6
13	e	1237	CLA	C6-C7-C8-C10
13	f	1215	CLA	C12-C13-C15-C16
13	f	1223	CLA	C3A-C2A-CAA-CBA
13	s	505	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	O6-C4-C5-O7
17	G	5001	LHG	O6-C4-C5-O7
17	e	5001	LHG	O6-C4-C5-O7
13	A	1107	CLA	CAA-CBA-CGA-O1A
13	6	501	CLA	CAA-CBA-CGA-O1A
13	G	1107	CLA	CAA-CBA-CGA-O1A
13	v	501	CLA	CAA-CBA-CGA-O1A
13	A	1111	CLA	CAA-CBA-CGA-O2A
13	1	519	CLA	CAA-CBA-CGA-O2A
13	2	519	CLA	CAA-CBA-CGA-O2A
13	G	1110	CLA	CAA-CBA-CGA-O2A
13	G	1111	CLA	CAA-CBA-CGA-O2A
13	Y	510	CLA	CAA-CBA-CGA-O2A
13	Y	519	CLA	CAA-CBA-CGA-O2A
13	Z	519	CLA	CAA-CBA-CGA-O2A
13	e	1111	CLA	CAA-CBA-CGA-O2A
13	f	1202	CLA	CAA-CBA-CGA-O2A
13	q	519	CLA	CAA-CBA-CGA-O2A
13	r	519	CLA	CAA-CBA-CGA-O2A
16	A	4011	BCR	C7-C8-C9-C10
16	I	4018	BCR	C21-C22-C23-C24
16	G	4011	BCR	C7-C8-C9-C10
16	S	4018	BCR	C21-C22-C23-C24
16	e	4011	BCR	C7-C8-C9-C10
16	k	4018	BCR	C21-C22-C23-C24
13	A	1111	CLA	CAA-CBA-CGA-O1A
13	G	1111	CLA	CAA-CBA-CGA-O1A
13	e	1107	CLA	CAA-CBA-CGA-O1A
13	e	1111	CLA	CAA-CBA-CGA-O1A
16	M	4021	BCR	C9-C10-C11-C12
16	2	522	BCR	C15-C16-C17-C18
16	W	4021	BCR	C9-C10-C11-C12
16	Z	522	BCR	C15-C16-C17-C18
16	o	4021	BCR	C9-C10-C11-C12
16	r	522	BCR	C15-C16-C17-C18
18	A	1849	LMU	C2-C1-O1'-C1'
18	G	1849	LMU	C2-C1-O1'-C1'
18	e	1849	LMU	C2-C1-O1'-C1'
13	B	1202	CLA	CAA-CBA-CGA-O2A
13	1	507	CLA	CAA-CBA-CGA-O2A
13	H	1202	CLA	CAA-CBA-CGA-O2A
13	Y	507	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	q	507	CLA	CAA-CBA-CGA-O2A
13	f	1222	CLA	O1D-CGD-O2D-CED
13	A	1125	CLA	CAA-CBA-CGA-O1A
13	G	1125	CLA	CAA-CBA-CGA-O1A
13	e	1125	CLA	CAA-CBA-CGA-O1A
13	1	519	CLA	CAA-CBA-CGA-O1A
13	2	519	CLA	CAA-CBA-CGA-O1A
13	Y	519	CLA	CAA-CBA-CGA-O1A
13	Z	510	CLA	CAA-CBA-CGA-O1A
13	Z	519	CLA	CAA-CBA-CGA-O1A
13	q	519	CLA	CAA-CBA-CGA-O1A
13	r	519	CLA	CAA-CBA-CGA-O1A
17	A	5006	LHG	O10-C23-C24-C25
17	G	5006	LHG	O10-C23-C24-C25
17	e	5006	LHG	O10-C23-C24-C25
17	e	5003	LHG	O9-C7-C8-C9
13	5	519	CLA	C2A-CAA-CBA-CGA
13	6	504	CLA	C2A-CAA-CBA-CGA
13	c	519	CLA	C2A-CAA-CBA-CGA
13	d	504	CLA	C2A-CAA-CBA-CGA
13	u	519	CLA	C2A-CAA-CBA-CGA
13	v	504	CLA	C2A-CAA-CBA-CGA
13	A	1237	CLA	C13-C15-C16-C17
13	e	1237	CLA	C13-C15-C16-C17
13	A	1013	CLA	CAA-CBA-CGA-O1A
13	2	510	CLA	CAA-CBA-CGA-O1A
13	5	519	CLA	CAA-CBA-CGA-O1A
13	G	1013	CLA	CAA-CBA-CGA-O1A
13	c	519	CLA	CAA-CBA-CGA-O1A
13	e	1013	CLA	CAA-CBA-CGA-O1A
13	r	510	CLA	CAA-CBA-CGA-O1A
13	u	519	CLA	CAA-CBA-CGA-O1A
17	A	5003	LHG	O9-C7-C8-C9
13	A	1116	CLA	CAA-CBA-CGA-O2A
13	G	1116	CLA	CAA-CBA-CGA-O2A
13	H	1021	CLA	CAA-CBA-CGA-O2A
13	e	1116	CLA	CAA-CBA-CGA-O2A
13	f	1021	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

704 monomers are involved in 1558 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	505	CLA	3	0
13	3	519	CLA	1	0
13	5	503	CLA	3	0
16	c	524	BCR	3	0
13	A	1123	CLA	2	0
13	A	1115	CLA	1	0
13	V	1501	CLA	8	0
13	5	511	CLA	1	0
13	G	1108	CLA	1	0
13	f	1207	CLA	8	0
13	e	1126	CLA	9	0
13	a	510	CLA	3	0
13	4	511	CLA	1	0
13	e	1138	CLA	2	0
20	2	822	SQD	1	0
19	B	5002	LMG	7	0
13	c	502	CLA	3	0
16	3	522	BCR	5	0
13	d	511	CLA	1	0
18	T	5105	LMU	2	0
13	1	513	CLA	1	0
13	B	1225	CLA	3	0
13	f	1227	CLA	3	0
13	G	1106	CLA	2	0
13	G	1139	CLA	2	0
13	a	501	CLA	2	0
20	6	822	SQD	1	0
17	G	5007	LHG	1	0
16	F	4016	BCR	5	0
16	d	523	BCR	2	0
16	H	4014	BCR	4	0
16	v	521	BCR	2	0
16	B	4005	BCR	3	0
13	H	1201	CLA	3	0
13	q	519	CLA	1	0
16	e	4002	BCR	3	0
13	B	1023	CLA	3	0
13	1	501	CLA	4	0
13	s	503	CLA	3	0
13	H	1238	CLA	1	0
20	L	5216	SQD	4	0
20	r	822	SQD	1	0
20	f	1852	SQD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	c	505	CLA	1	0
13	B	1205	CLA	1	0
13	3	513	CLA	3	0
13	t	513	CLA	1	0
13	A	1109	CLA	3	0
16	u	523	BCR	2	0
13	e	1022	CLA	4	0
16	c	522	BCR	2	0
13	e	1135	CLA	3	0
13	l	1302	CLA	1	0
13	f	1201	CLA	3	0
13	d	501	CLA	3	0
13	L	1501	CLA	8	0
13	R	1302	CLA	2	0
13	d	512	CLA	4	0
13	e	1013	CLA	8	0
16	V	4020	BCR	3	0
17	A	5003	LHG	2	0
13	B	1220	CLA	4	0
13	q	513	CLA	1	0
13	s	512	CLA	2	0
13	A	1135	CLA	2	0
13	L	1502	CLA	2	0
13	f	1213	CLA	1	0
13	H	1217	CLA	4	0
13	G	1135	CLA	3	0
13	u	506	CLA	3	0
13	2	517	CLA	1	0
13	q	508	CLA	2	0
16	u	521	BCR	4	0
13	t	501	CLA	2	0
13	q	502	CLA	7	0
13	H	1227	CLA	3	0
13	H	1239	CLA	2	0
13	A	1116	CLA	2	0
13	H	1226	CLA	7	0
13	A	1106	CLA	2	0
13	s	509	CLA	1	0
13	A	1105	CLA	2	0
13	t	510	CLA	1	0
13	Z	518	CLA	2	0
14	H	2002	PQN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	c	509	CLA	1	0
13	f	1222	CLA	4	0
13	f	1235	CLA	4	0
13	4	518	CLA	1	0
16	v	524	BCR	6	0
13	A	1124	CLA	1	0
13	H	1223	CLA	1	0
13	G	1111	CLA	1	0
13	r	519	CLA	1	0
16	L	4022	BCR	5	0
16	G	4002	BCR	3	0
13	u	503	CLA	3	0
13	B	1231	CLA	3	0
13	c	503	CLA	3	0
13	Z	507	CLA	2	0
13	F	1301	CLA	2	0
13	s	507	CLA	2	0
13	u	513	CLA	1	0
16	e	4001	BCR	2	0
13	G	1133	CLA	1	0
13	2	512	CLA	5	0
16	A	4011	BCR	4	0
13	u	507	CLA	1	0
13	K	1103	CLA	2	0
13	A	1128	CLA	5	0
13	a	518	CLA	1	0
16	H	4017	BCR	3	0
13	s	519	CLA	1	0
13	c	511	CLA	1	0
13	G	1138	CLA	2	0
16	K	4104	BCR	7	0
16	G	4003	BCR	3	0
20	Y	822	SQD	5	0
13	A	1122	CLA	2	0
16	s	524	BCR	4	0
13	A	1139	CLA	3	0
13	q	501	CLA	4	0
13	1	512	CLA	6	0
13	H	1234	CLA	4	0
13	6	511	CLA	1	0
16	l	4015	BCR	4	0
13	c	506	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	522	BCR	2	0
13	R	1301	CLA	1	0
20	H	1852	SQD	10	0
13	f	1236	CLA	4	0
13	6	505	CLA	4	0
13	e	1124	CLA	1	0
13	4	503	CLA	1	0
13	A	1140	CLA	6	0
13	H	1212	CLA	1	0
13	s	501	CLA	2	0
13	B	1209	CLA	1	0
13	f	1217	CLA	4	0
13	u	501	CLA	4	0
13	A	1133	CLA	1	0
13	e	1121	CLA	3	0
13	s	506	CLA	1	0
13	B	1239	CLA	2	0
13	e	1131	CLA	1	0
17	A	5002	LHG	3	0
13	q	516	CLA	2	0
17	V	5220	LHG	2	0
13	s	513	CLA	2	0
13	A	1138	CLA	2	0
13	u	505	CLA	2	0
13	H	1207	CLA	6	0
13	l	1303	CLA	3	0
13	f	1214	CLA	2	0
13	f	1216	CLA	1	0
13	H	1202	CLA	2	0
13	2	511	CLA	3	0
16	V	4219	BCR	5	0
13	F	1302	CLA	2	0
16	Y	522	BCR	5	0
20	Z	822	SQD	1	0
16	f	4004	BCR	3	0
13	2	507	CLA	3	0
13	e	1801	CLA	4	0
16	l	4012	BCR	5	0
14	f	2002	PQN	3	0
13	A	1107	CLA	1	0
13	s	502	CLA	2	0
13	Z	501	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	5221	LHG	9	0
13	H	1023	CLA	2	0
13	e	1130	CLA	4	0
20	1	822	SQD	4	0
13	b	510	CLA	1	0
13	2	506	CLA	5	0
13	2	519	CLA	1	0
16	u	522	BCR	3	0
16	M	4021	BCR	2	0
13	H	1231	CLA	3	0
13	b	506	CLA	1	0
13	4	501	CLA	2	0
17	n	5220	LHG	2	0
16	W	4021	BCR	4	0
13	Z	510	CLA	2	0
13	b	517	CLA	2	0
13	a	517	CLA	1	0
13	e	1136	CLA	2	0
13	r	518	CLA	2	0
13	v	511	CLA	1	0
13	a	505	CLA	3	0
16	Z	524	BCR	5	0
13	V	1502	CLA	2	0
13	Z	511	CLA	4	0
16	H	4006	BCR	1	0
17	e	5002	LHG	4	0
13	A	1129	CLA	2	0
13	4	510	CLA	1	0
17	e	5006	LHG	1	0
16	b	521	BCR	2	0
13	q	503	CLA	4	0
16	1	524	BCR	5	0
13	G	1134	CLA	1	0
20	a	822	SQD	1	0
13	u	511	CLA	1	0
13	5	501	CLA	4	0
13	H	1224	CLA	6	0
13	f	1209	CLA	2	0
16	S	4018	BCR	5	0
16	f	4009	BCR	5	0
13	3	511	CLA	2	0
16	4	523	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	5003	LHG	1	0
13	f	1204	CLA	2	0
13	t	512	CLA	2	0
17	B	1855	LHG	2	0
13	f	1208	CLA	1	0
13	G	1105	CLA	2	0
13	B	1212	CLA	1	0
13	f	1219	CLA	4	0
16	n	4022	BCR	6	0
16	a	524	BCR	6	0
13	G	1011	CLA	3	0
14	G	2001	PQN	3	0
20	q	822	SQD	4	0
16	G	4001	BCR	2	0
13	a	512	CLA	2	0
13	b	518	CLA	1	0
13	B	1012	CLA	3	0
13	H	1205	CLA	1	0
17	G	5004	LHG	1	0
13	e	1137	CLA	4	0
13	2	509	CLA	1	0
13	A	1118	CLA	2	0
16	4	524	BCR	4	0
13	A	1117	CLA	2	0
13	4	506	CLA	1	0
13	T	1303	CLA	3	0
13	Y	511	CLA	3	0
13	B	1202	CLA	2	0
16	6	521	BCR	2	0
13	B	1226	CLA	5	0
13	A	1136	CLA	1	0
13	a	513	CLA	3	0
13	q	504	CLA	1	0
16	1	521	BCR	1	0
16	d	521	BCR	2	0
17	A	5001	LHG	4	0
13	A	1121	CLA	3	0
16	T	4012	BCR	6	0
18	J	5105	LMU	2	0
13	m	1401	CLA	1	0
16	q	524	BCR	5	0
13	u	512	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1111	CLA	1	0
13	Y	509	CLA	4	0
13	1	508	CLA	2	0
16	e	4008	BCR	1	0
13	G	1126	CLA	8	0
13	U	1401	CLA	1	0
17	e	5008	LHG	2	0
13	Y	518	CLA	2	0
13	A	1102	CLA	4	0
16	T	4013	BCR	6	0
16	U	4104	BCR	6	0
13	6	512	CLA	4	0
13	B	1228	CLA	4	0
16	G	4007	BCR	5	0
16	a	521	BCR	3	0
16	f	4005	BCR	1	0
13	e	1104	CLA	7	0
16	n	4020	BCR	3	0
19	H	5002	LMG	7	0
13	3	506	CLA	1	0
13	e	1103	CLA	4	0
13	f	1221	CLA	6	0
16	t	521	BCR	1	0
13	t	517	CLA	2	0
13	1	503	CLA	4	0
16	t	524	BCR	5	0
17	L	5221	LHG	11	0
13	f	1239	CLA	3	0
13	6	513	CLA	1	0
13	L	1503	CLA	1	0
13	B	1217	CLA	3	0
16	e	4007	BCR	4	0
17	G	5001	LHG	4	0
16	V	4019	BCR	1	0
13	3	502	CLA	2	0
16	a	523	BCR	2	0
13	1	505	CLA	8	0
16	Z	523	BCR	1	0
13	m	1103	CLA	2	0
19	f	5002	LMG	7	0
17	A	5009	LHG	4	0
13	H	1221	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1229	CLA	5	0
13	c	510	CLA	1	0
13	s	516	CLA	1	0
13	H	1225	CLA	3	0
13	d	513	CLA	1	0
14	B	2002	PQN	2	0
16	L	4219	BCR	4	0
16	G	4008	BCR	1	0
16	q	522	BCR	4	0
13	e	1123	CLA	2	0
15	C	3002	SF4	1	0
13	H	1213	CLA	1	0
13	G	1131	CLA	1	0
13	v	505	CLA	4	0
13	6	501	CLA	4	0
13	A	1130	CLA	4	0
13	r	510	CLA	3	0
13	5	512	CLA	4	0
13	G	1119	CLA	4	0
13	G	1013	CLA	8	0
20	s	822	SQD	1	0
13	B	1206	CLA	2	0
13	e	1119	CLA	5	0
13	t	505	CLA	1	0
16	e	4011	BCR	3	0
13	A	1137	CLA	3	0
13	a	519	CLA	1	0
13	6	519	CLA	2	0
13	U	1105	CLA	1	0
13	4	505	CLA	1	0
14	e	2001	PQN	2	0
13	e	1128	CLA	5	0
16	H	4005	BCR	2	0
20	n	5216	SQD	4	0
13	4	516	CLA	1	0
13	a	516	CLA	1	0
13	e	1120	CLA	2	0
16	Z	521	BCR	2	0
16	t	523	BCR	3	0
16	r	522	BCR	2	0
13	A	1011	CLA	4	0
13	Z	502	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	f	1215	CLA	2	0
13	t	516	CLA	1	0
13	f	1220	CLA	4	0
13	2	510	CLA	2	0
13	J	1302	CLA	1	0
13	3	518	CLA	1	0
13	b	509	CLA	2	0
17	A	5004	LHG	1	0
16	6	522	BCR	4	0
16	k	4018	BCR	4	0
20	v	822	SQD	1	0
13	B	1238	CLA	1	0
16	1	522	BCR	4	0
13	A	1108	CLA	2	0
13	H	1210	CLA	4	0
16	d	522	BCR	9	0
13	3	507	CLA	2	0
13	H	1220	CLA	3	0
16	u	524	BCR	3	0
16	s	522	BCR	1	0
13	e	1118	CLA	2	0
13	5	510	CLA	1	0
13	Y	510	CLA	1	0
13	f	1012	CLA	2	0
18	A	1849	LMU	1	0
13	H	1021	CLA	2	0
13	a	507	CLA	2	0
13	B	1221	CLA	7	0
13	Z	505	CLA	2	0
16	6	524	BCR	8	0
13	e	1102	CLA	2	0
13	a	502	CLA	2	0
13	b	512	CLA	2	0
17	A	5007	LHG	1	0
13	e	1107	CLA	2	0
16	5	522	BCR	2	0
13	2	501	CLA	4	0
16	o	4021	BCR	4	0
16	A	4007	BCR	5	0
13	B	1227	CLA	4	0
13	B	1214	CLA	2	0
13	r	509	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	4	521	BCR	1	0
13	H	1236	CLA	4	0
13	f	1203	CLA	3	0
13	Z	517	CLA	2	0
13	e	1101	CLA	3	0
13	e	1237	CLA	3	0
13	n	1501	CLA	9	0
13	Y	508	CLA	1	0
13	2	518	CLA	2	0
13	e	1140	CLA	6	0
13	f	1228	CLA	3	0
13	f	1234	CLA	4	0
14	A	2001	PQN	3	0
17	L	5220	LHG	2	0
13	5	506	CLA	3	0
13	G	1124	CLA	1	0
13	n	1502	CLA	2	0
16	J	4013	BCR	6	0
13	H	1214	CLA	2	0
16	j	4016	BCR	3	0
13	H	1228	CLA	4	0
13	b	503	CLA	1	0
13	e	1109	CLA	3	0
13	Z	512	CLA	5	0
13	G	1114	CLA	1	0
15	N	3002	SF4	1	0
13	G	1122	CLA	3	0
13	5	513	CLA	1	0
13	r	511	CLA	3	0
16	2	522	BCR	2	0
13	f	1223	CLA	2	0
13	q	518	CLA	4	0
13	r	507	CLA	3	0
13	u	502	CLA	3	0
17	e	5005	LHG	1	0
13	e	1114	CLA	1	0
13	v	517	CLA	2	0
16	b	524	BCR	4	0
17	f	1842	LHG	2	0
16	A	4008	BCR	2	0
13	Z	506	CLA	5	0
13	v	513	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	3	523	BCR	1	0
20	3	822	SQD	1	0
13	H	1012	CLA	2	0
16	l	4013	BCR	6	0
13	1	504	CLA	1	0
13	B	1215	CLA	3	0
13	B	1201	CLA	2	0
13	A	1104	CLA	6	0
13	Y	505	CLA	5	0
16	B	4017	BCR	6	0
13	G	1801	CLA	2	0
13	e	1122	CLA	3	0
16	Y	521	BCR	2	0
13	1	509	CLA	4	0
13	4	509	CLA	3	0
13	b	502	CLA	2	0
13	a	509	CLA	1	0
13	A	1119	CLA	4	0
13	A	1013	CLA	7	0
13	G	1101	CLA	4	0
13	s	511	CLA	1	0
13	1	519	CLA	1	0
13	b	519	CLA	2	0
13	q	507	CLA	3	0
13	B	1222	CLA	4	0
13	B	1208	CLA	2	0
13	K	1401	CLA	1	0
13	3	510	CLA	3	0
13	H	1215	CLA	4	0
13	B	1234	CLA	2	0
16	A	4001	BCR	1	0
13	Z	519	CLA	1	0
16	B	4010	BCR	6	0
13	A	1120	CLA	2	0
13	v	512	CLA	3	0
20	B	1852	SQD	7	0
13	A	1022	CLA	4	0
16	3	524	BCR	6	0
13	c	507	CLA	1	0
13	G	1136	CLA	2	0
13	e	1106	CLA	2	0
13	e	1139	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	1120	CLA	2	0
13	G	1022	CLA	3	0
13	B	1218	CLA	1	0
13	H	1204	CLA	1	0
13	f	1206	CLA	1	0
16	c	521	BCR	5	0
13	r	505	CLA	4	0
13	Y	501	CLA	4	0
17	G	5002	LHG	2	0
17	G	5006	LHG	1	0
13	6	517	CLA	3	0
16	V	4022	BCR	6	0
13	B	1207	CLA	6	0
13	q	510	CLA	2	0
13	H	1208	CLA	2	0
13	Z	503	CLA	4	0
13	f	1218	CLA	2	0
13	1	518	CLA	1	0
13	e	1133	CLA	1	0
16	f	4014	BCR	4	0
13	1	507	CLA	3	0
13	r	502	CLA	5	0
13	Z	513	CLA	1	0
16	B	4004	BCR	4	0
13	Y	516	CLA	2	0
16	A	4003	BCR	2	0
13	B	1235	CLA	3	0
13	6	502	CLA	2	0
16	I	4018	BCR	3	0
13	A	1101	CLA	3	0
13	B	1219	CLA	5	0
13	G	1109	CLA	3	0
13	t	509	CLA	3	0
13	b	501	CLA	2	0
16	J	4015	BCR	3	0
17	G	5008	LHG	2	0
13	v	501	CLA	3	0
17	I	5001	LHG	1	0
13	e	1117	CLA	3	0
13	u	510	CLA	1	0
13	G	1104	CLA	7	0
16	2	524	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	d	822	SQD	1	0
13	1	511	CLA	3	0
13	b	511	CLA	1	0
16	n	4019	BCR	2	0
16	m	4104	BCR	5	0
16	B	4014	BCR	4	0
16	A	4002	BCR	4	0
13	G	1129	CLA	1	0
13	t	519	CLA	2	0
13	B	1216	CLA	1	0
13	G	1112	CLA	1	0
16	r	523	BCR	2	0
13	j	1301	CLA	3	0
13	4	517	CLA	2	0
13	v	519	CLA	2	0
13	n	1503	CLA	2	0
16	r	521	BCR	2	0
13	B	1203	CLA	2	0
13	2	503	CLA	4	0
13	r	517	CLA	1	0
13	v	506	CLA	1	0
13	4	513	CLA	1	0
13	H	1218	CLA	2	0
13	A	1114	CLA	1	0
17	G	5005	LHG	1	0
13	B	1213	CLA	1	0
13	a	511	CLA	1	0
13	e	1129	CLA	2	0
16	v	522	BCR	4	0
13	4	502	CLA	2	0
16	s	523	BCR	3	0
13	G	1103	CLA	4	0
13	G	1117	CLA	3	0
13	H	1216	CLA	2	0
13	3	505	CLA	2	0
13	G	1107	CLA	2	0
13	e	1110	CLA	1	0
13	3	516	CLA	1	0
16	2	521	BCR	4	0
13	r	512	CLA	5	0
13	G	1116	CLA	3	0
13	j	1302	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1236	CLA	5	0
13	U	1103	CLA	2	0
17	e	5007	LHG	1	0
13	r	503	CLA	4	0
13	t	503	CLA	1	0
16	e	4003	BCR	4	0
16	J	4012	BCR	4	0
13	r	506	CLA	5	0
13	f	1210	CLA	4	0
13	Y	512	CLA	6	0
13	s	510	CLA	4	0
13	B	1240	CLA	1	0
13	Y	504	CLA	1	0
13	r	513	CLA	1	0
13	u	509	CLA	2	0
13	Y	517	CLA	1	0
13	6	506	CLA	1	0
13	e	1116	CLA	4	0
13	A	1801	CLA	3	0
13	d	506	CLA	1	0
13	e	1111	CLA	1	0
17	A	5006	LHG	1	0
16	Z	522	BCR	2	0
16	q	523	BCR	1	0
16	Y	523	BCR	1	0
13	q	509	CLA	3	0
13	G	1118	CLA	2	0
17	f	1855	LHG	2	0
16	B	4006	BCR	1	0
13	e	1108	CLA	2	0
13	H	1222	CLA	4	0
13	3	517	CLA	1	0
13	G	1125	CLA	1	0
13	c	512	CLA	4	0
13	H	1235	CLA	4	0
13	e	1115	CLA	1	0
13	f	1229	CLA	4	0
16	B	4009	BCR	5	0
13	t	511	CLA	1	0
13	f	1238	CLA	1	0
16	f	4010	BCR	5	0
13	G	1110	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	1121	CLA	2	0
13	1	502	CLA	7	0
13	A	1237	CLA	3	0
13	d	502	CLA	2	0
13	f	1212	CLA	1	0
13	B	1223	CLA	1	0
16	G	4011	BCR	3	0
16	H	4009	BCR	4	0
13	f	1021	CLA	1	0
16	f	4006	BCR	3	0
17	B	1842	LHG	2	0
16	3	521	BCR	2	0
13	H	1203	CLA	3	0
13	H	1229	CLA	4	0
13	a	506	CLA	1	0
13	J	1303	CLA	4	0
13	c	513	CLA	1	0
13	r	501	CLA	4	0
13	G	1128	CLA	3	0
16	H	4010	BCR	6	0
13	t	506	CLA	1	0
17	n	5221	LHG	10	0
13	B	1210	CLA	4	0
13	H	1219	CLA	5	0
13	t	518	CLA	1	0
13	A	1103	CLA	4	0
16	5	524	BCR	3	0
13	B	1224	CLA	6	0
15	g	3002	SF4	1	0
16	2	523	BCR	1	0
13	q	511	CLA	3	0
13	G	1130	CLA	4	0
13	5	507	CLA	1	0
13	Y	507	CLA	3	0
13	f	1202	CLA	3	0
16	1	523	BCR	1	0
16	R	4016	BCR	4	0
16	b	523	BCR	2	0
13	4	512	CLA	2	0
16	d	524	BCR	8	0
13	s	518	CLA	1	0
13	b	516	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	v	523	BCR	3	0
13	Z	509	CLA	1	0
13	A	1126	CLA	8	0
13	c	501	CLA	4	0
13	f	1225	CLA	3	0
13	Y	519	CLA	1	0
13	d	505	CLA	4	0
17	k	5001	LHG	1	0
13	4	519	CLA	2	0
16	Y	524	BCR	5	0
16	f	4017	BCR	5	0
13	3	503	CLA	4	0
13	s	505	CLA	2	0
16	L	4020	BCR	3	0
16	s	521	BCR	3	0
13	d	519	CLA	2	0
13	f	1226	CLA	6	0
16	H	4004	BCR	3	0
13	H	1209	CLA	2	0
17	G	5009	LHG	4	0
16	c	523	BCR	1	0
13	f	1023	CLA	4	0
13	G	1102	CLA	3	0
13	3	512	CLA	2	0
17	H	1855	LHG	3	0
13	V	1503	CLA	3	0
16	T	4015	BCR	5	0
13	3	509	CLA	1	0
17	A	5008	LHG	2	0
17	e	5001	LHG	5	0
17	A	5005	LHG	1	0
17	e	5003	LHG	1	0
16	n	4219	BCR	4	0
13	Y	503	CLA	4	0
13	e	1105	CLA	2	0
13	5	505	CLA	1	0
13	2	502	CLA	5	0
13	q	505	CLA	24	0
16	5	521	BCR	4	0
13	f	1224	CLA	6	0
13	1	510	CLA	2	0
16	r	524	BCR	7	0

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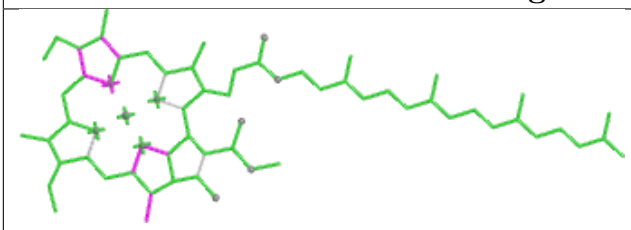
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	e	5009	LHG	4	0
13	1	516	CLA	2	0
13	Y	513	CLA	1	0
13	b	513	CLA	1	0
13	G	1123	CLA	2	0
13	e	1011	CLA	3	0
13	G	1237	CLA	4	0
16	6	523	BCR	2	0
18	e	1849	LMU	1	0
13	q	512	CLA	6	0
17	e	5004	LHG	1	0
13	G	1140	CLA	6	0
13	H	1206	CLA	2	0
16	q	521	BCR	1	0
13	K	1105	CLA	1	0
13	f	1231	CLA	3	0
17	H	1842	LHG	2	0
13	5	502	CLA	3	0
13	Y	502	CLA	7	0
13	s	517	CLA	1	0
13	m	1105	CLA	1	0
13	t	502	CLA	2	0
13	3	501	CLA	2	0
13	G	1137	CLA	2	0
13	a	503	CLA	3	0
13	B	1021	CLA	1	0
18	l	5105	LMU	2	0
13	v	502	CLA	2	0
13	d	517	CLA	3	0
13	B	1204	CLA	1	0
20	V	5216	SQD	3	0

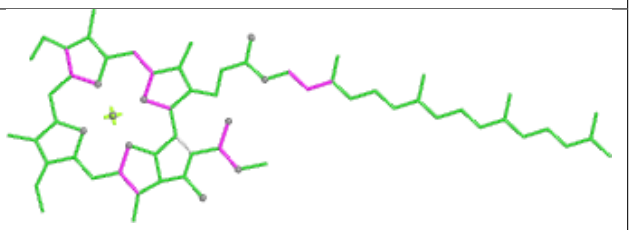
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

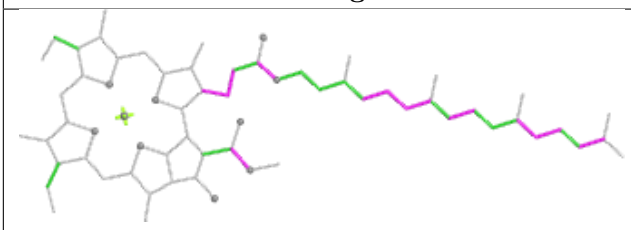
Ligand CLA 2 505



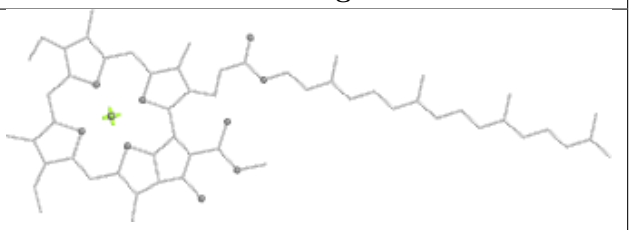
Bond lengths



Bond angles

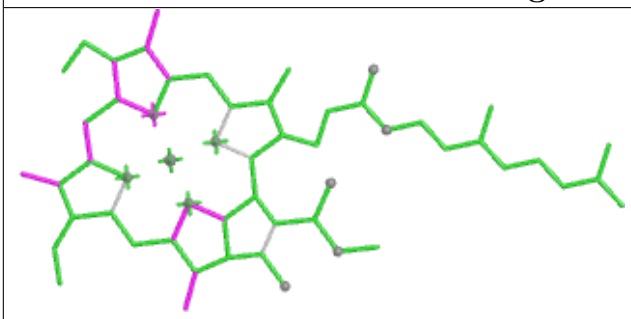


Torsions

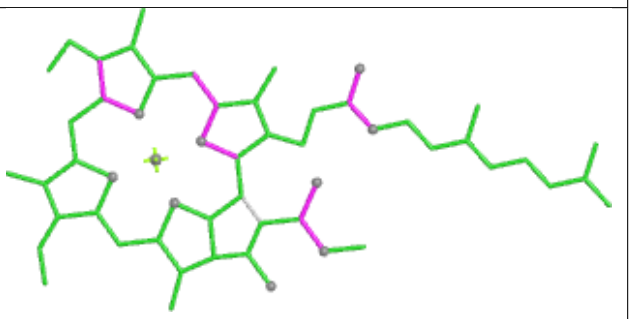


Rings

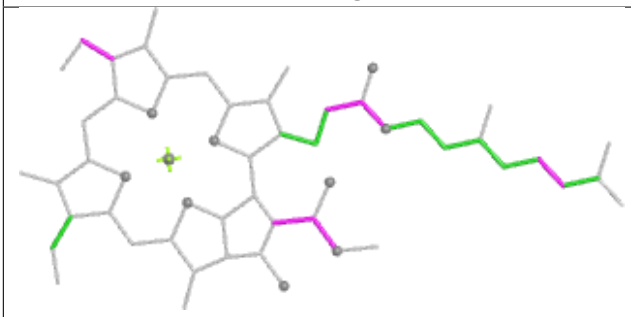
Ligand CLA 3 519



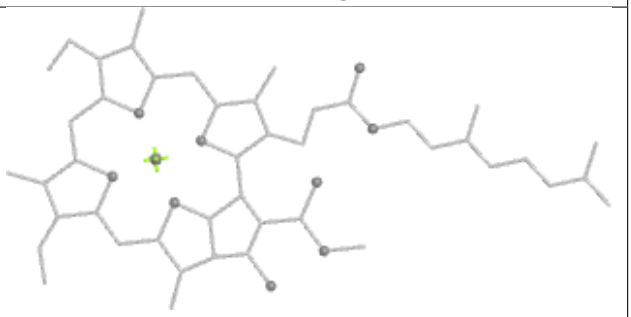
Bond lengths



Bond angles

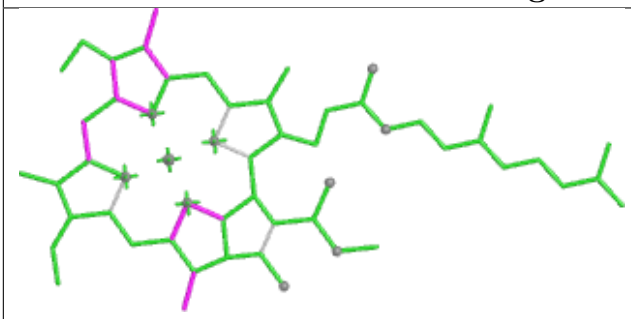


Torsions



Rings

Ligand CLA 5 503



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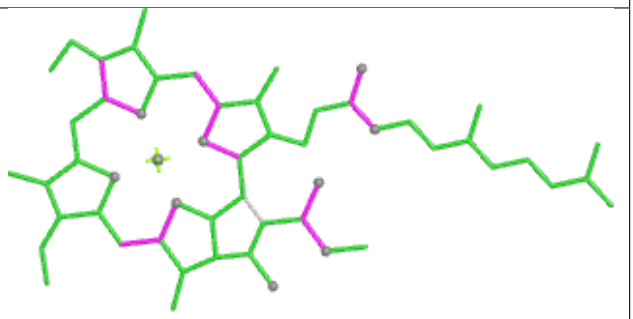
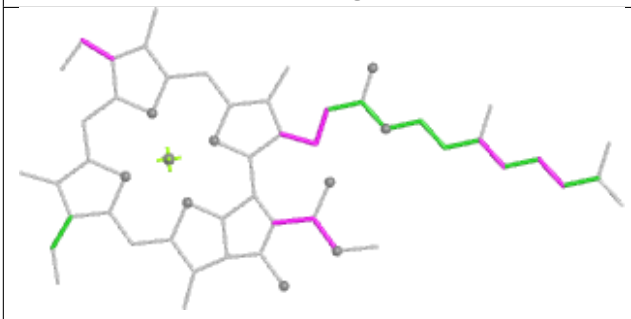
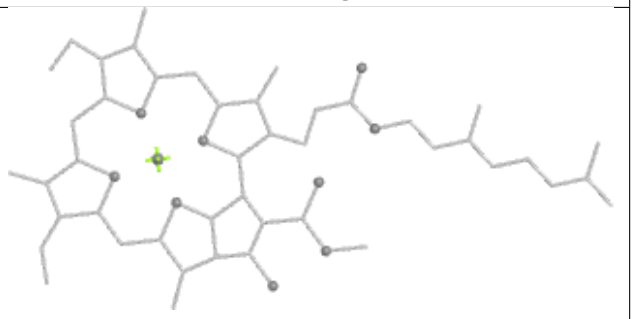


Bond angles

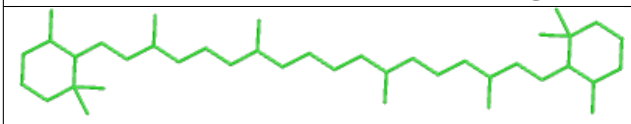


Torsions

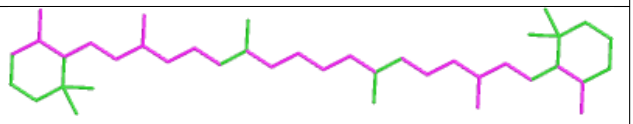


Rings

Ligand BCR c 524



Bond lengths



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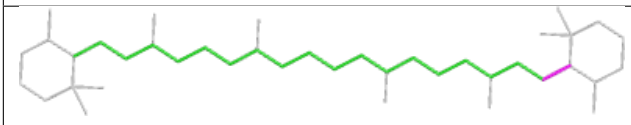
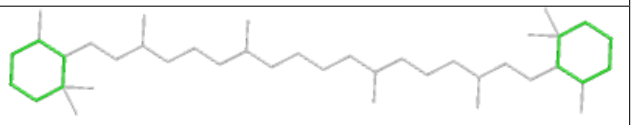


Torsions



Rings

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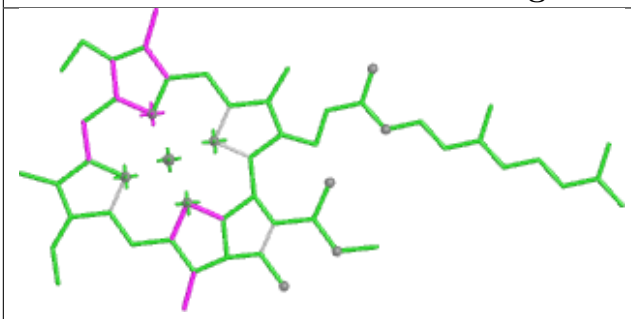
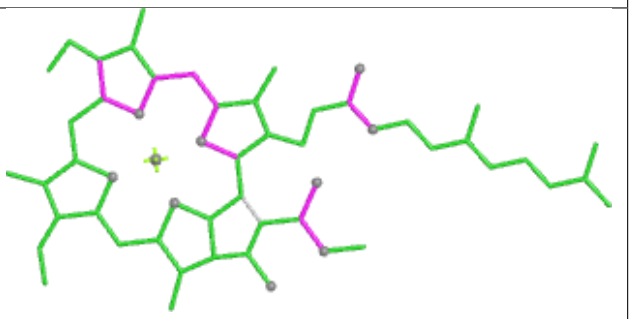
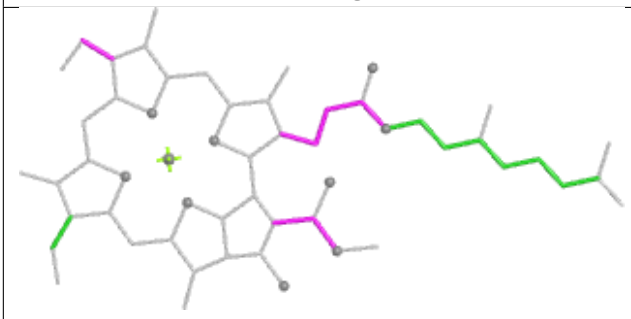
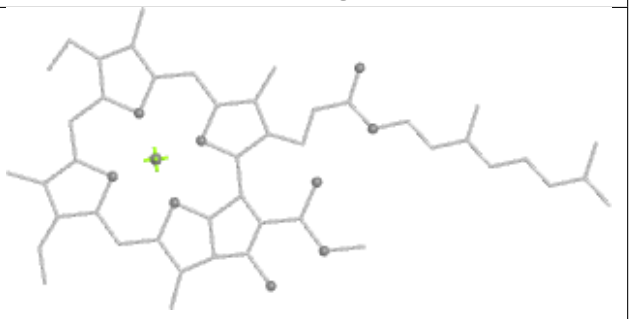
 Bond lengths	 Bond angles
 Torsions	 Rings

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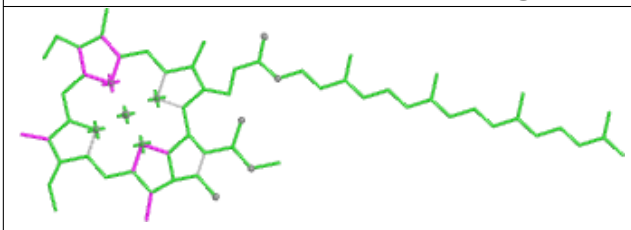
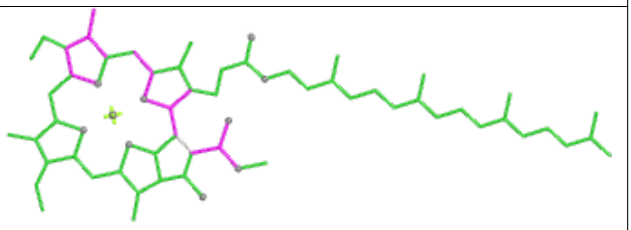
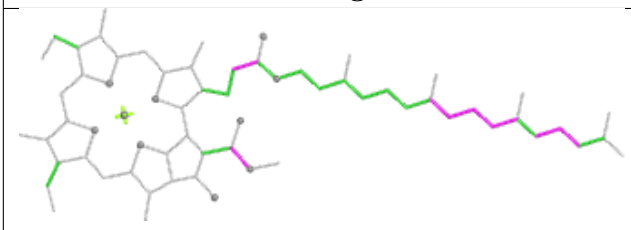
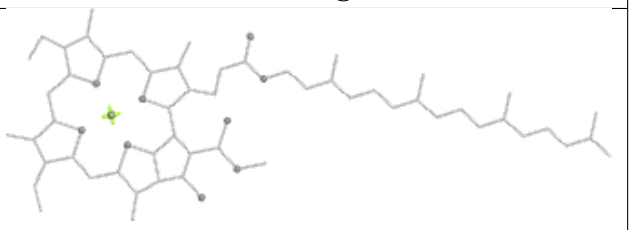
 Bond lengths	 Bond angles
 Torsions	 Rings

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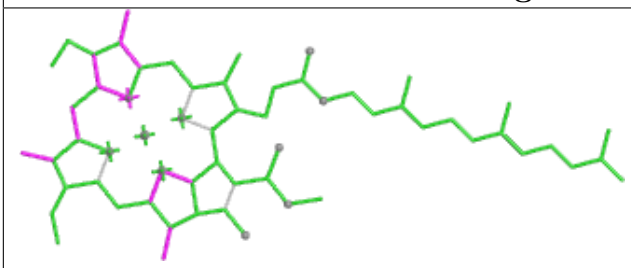
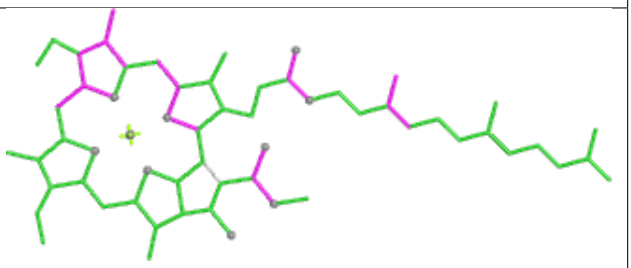
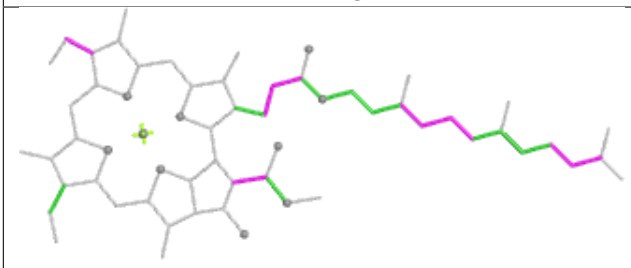
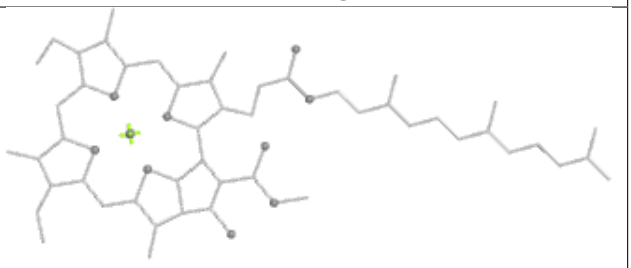
	
Bond lengths	Bond angles
	
Torsions	Rings

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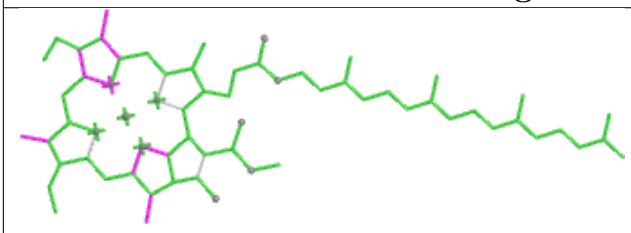
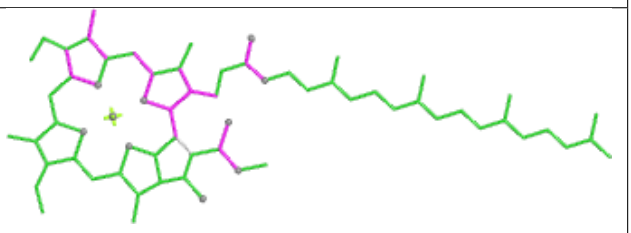
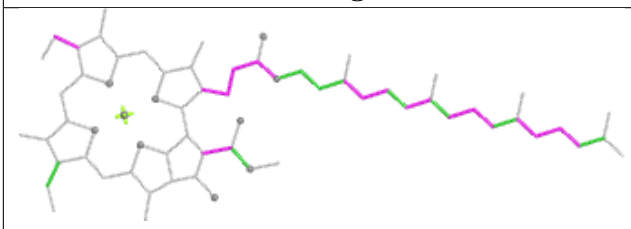
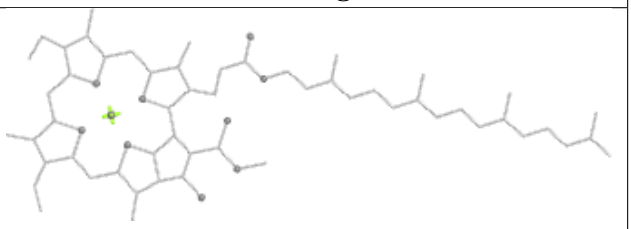
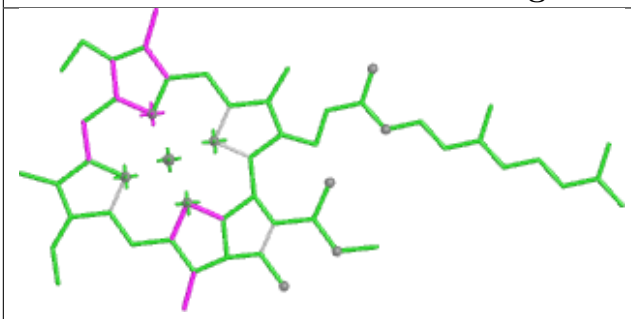
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 511



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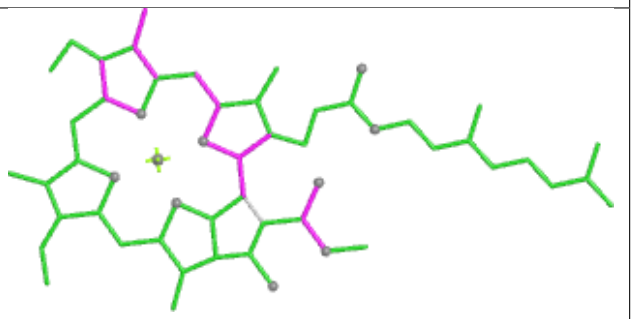
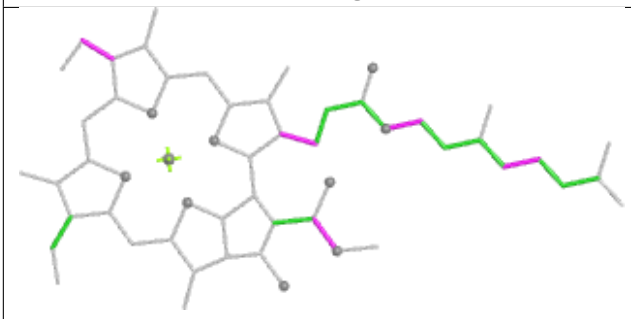
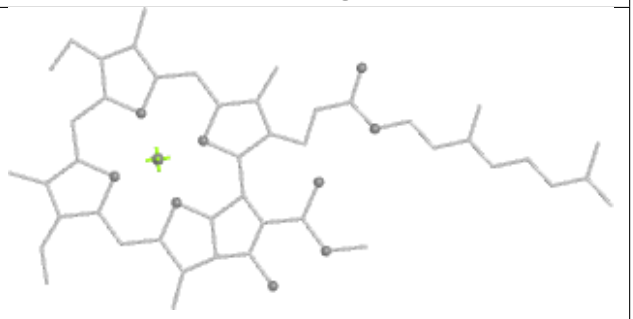


Bond angles

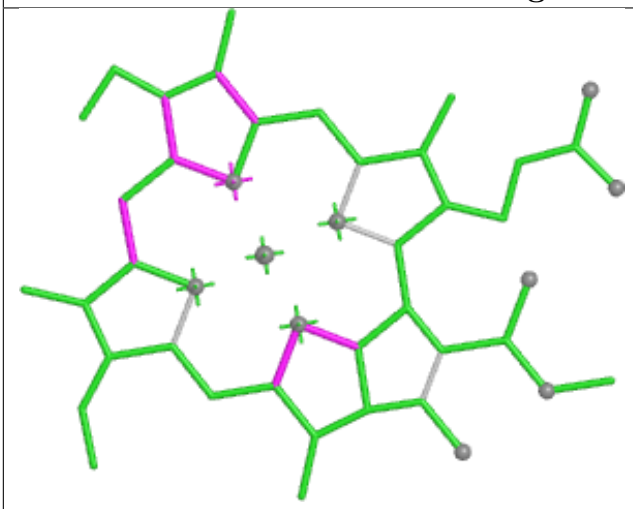


Torsions

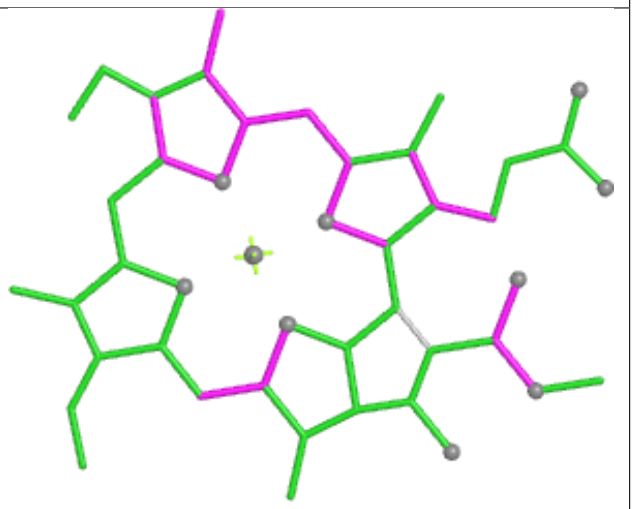


Rings

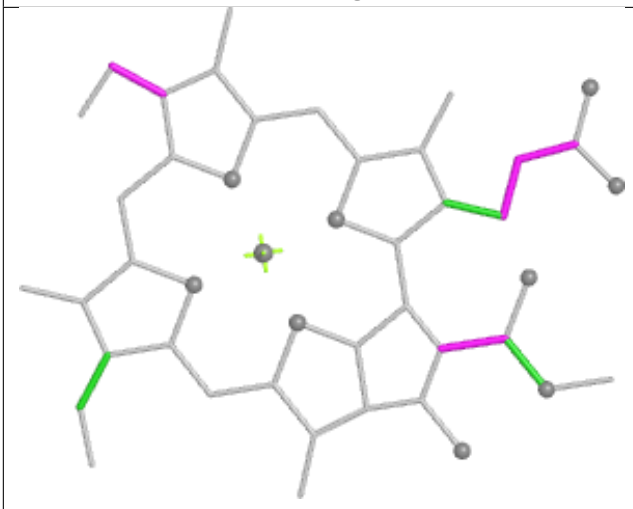
Ligand CLA v 504



Bond lengths

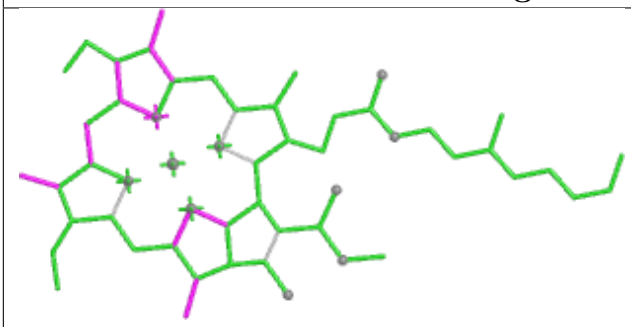
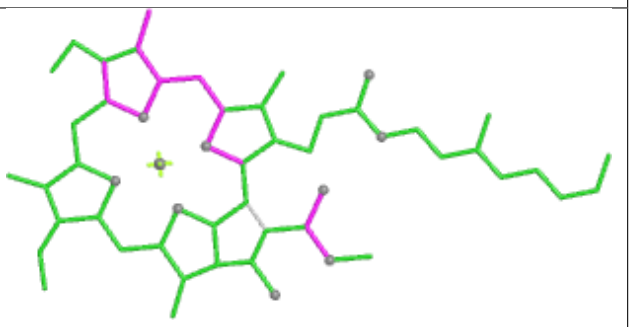
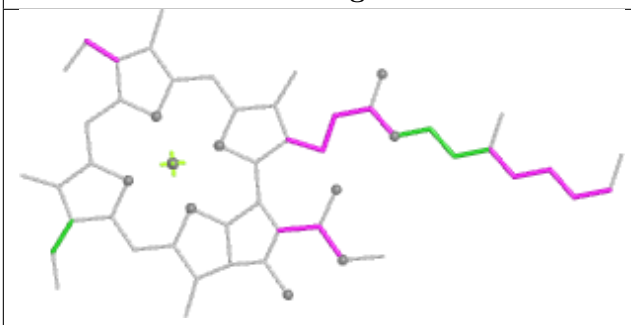
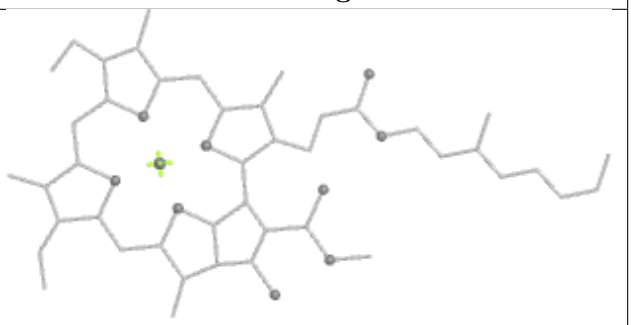


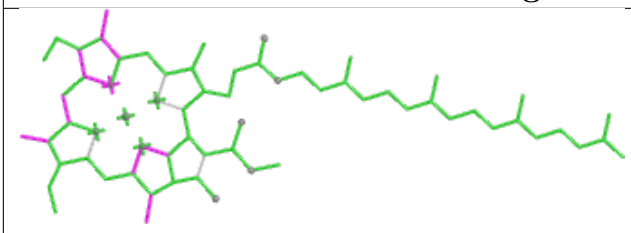
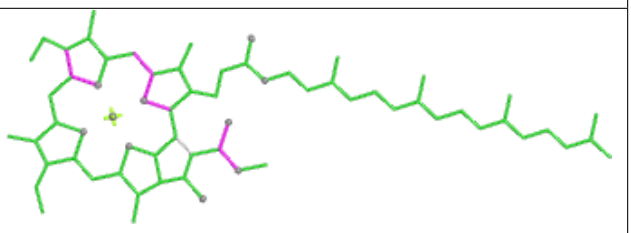
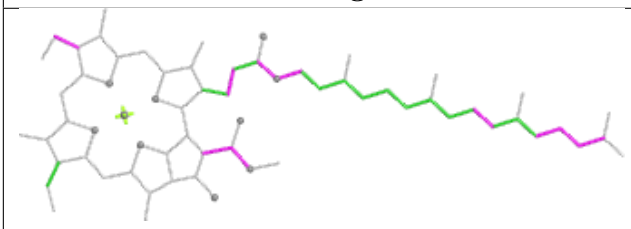
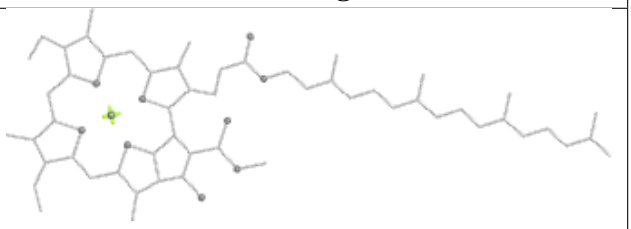
Bond angles



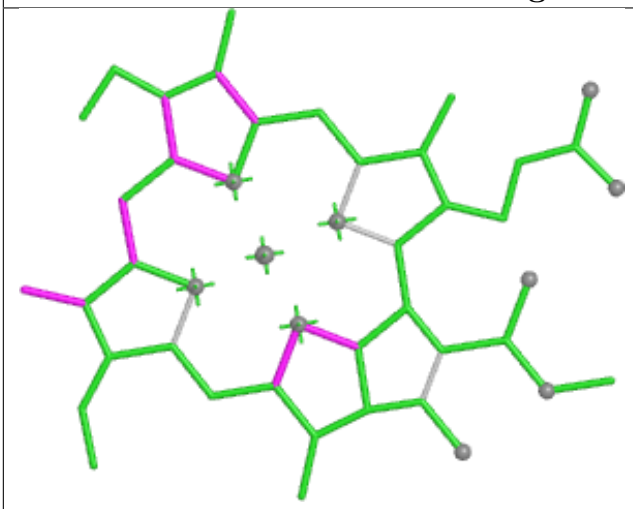
Torsions

Rings

Ligand CLA G 1108	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 1207	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 506



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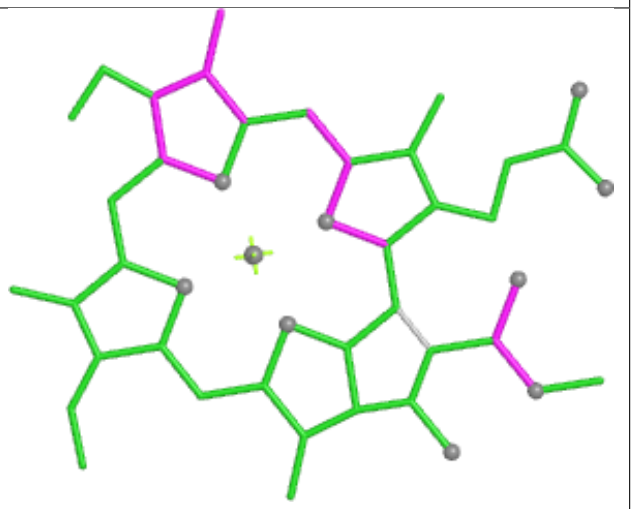
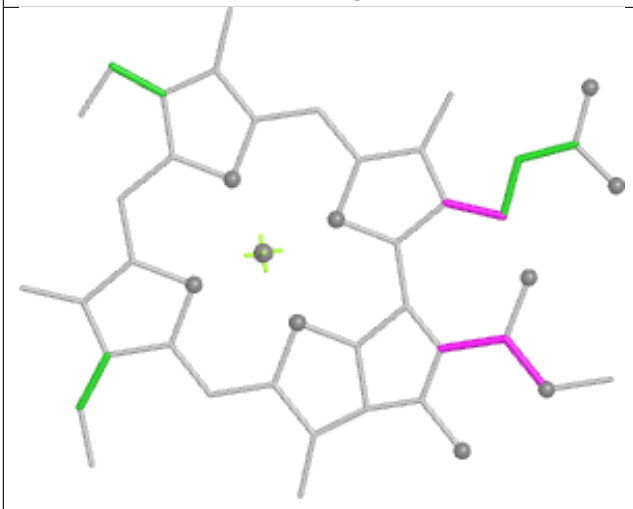


Bond angles



Torsions

Rings

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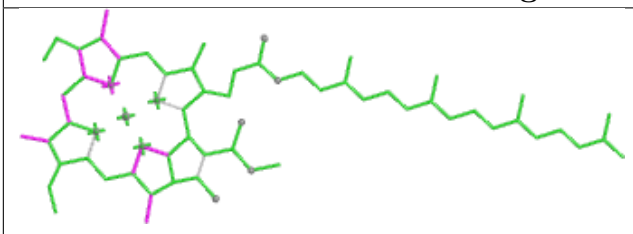

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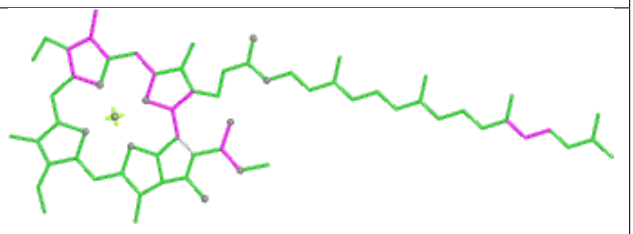

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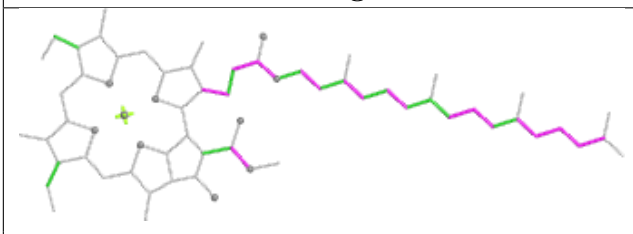

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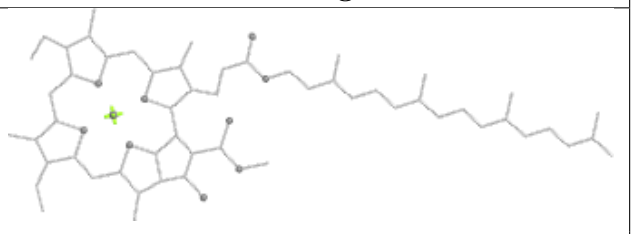
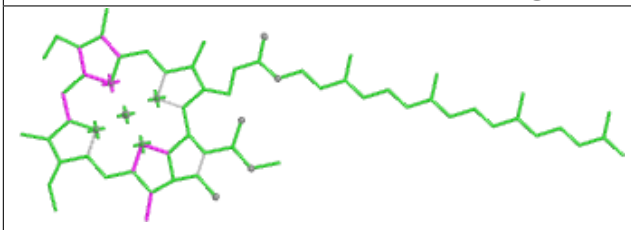


Rings

Ligand CLA a 510



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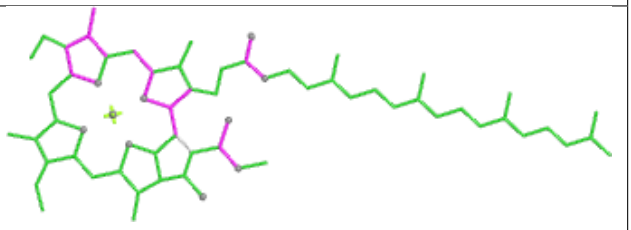
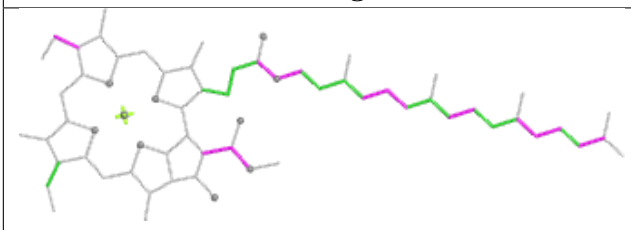


Bond angles



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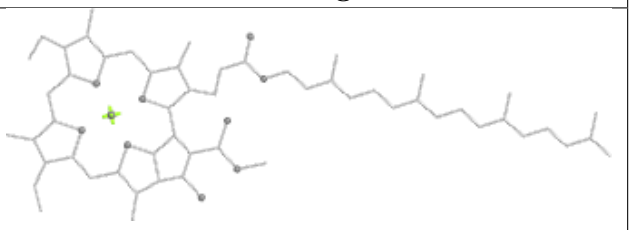

Rings

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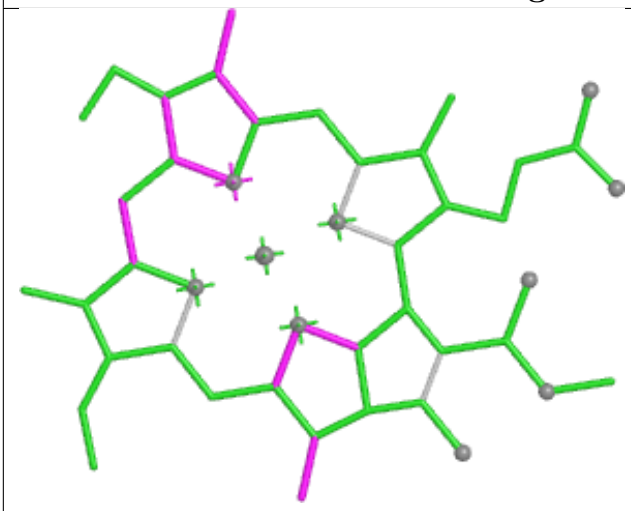

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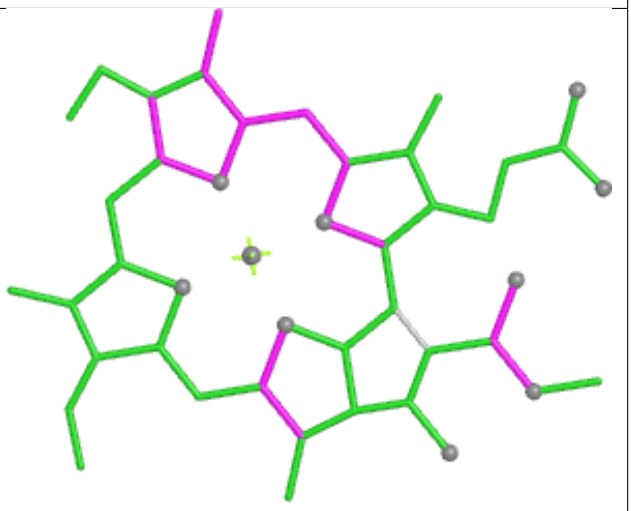

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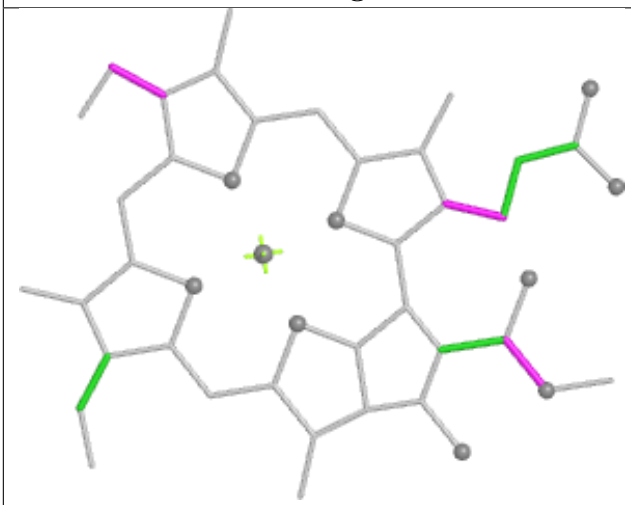

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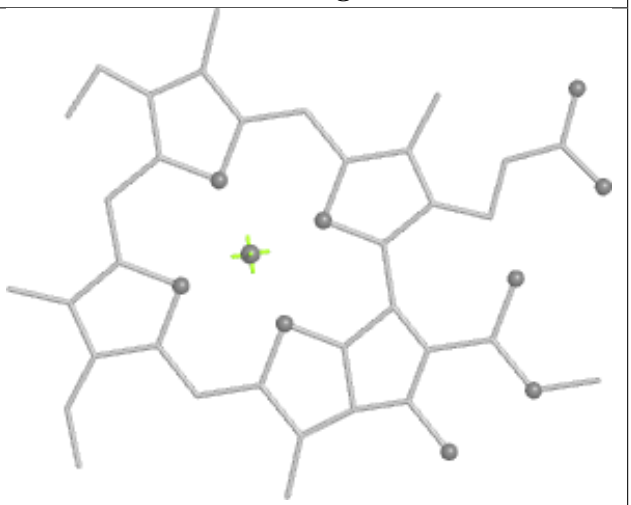

Rings

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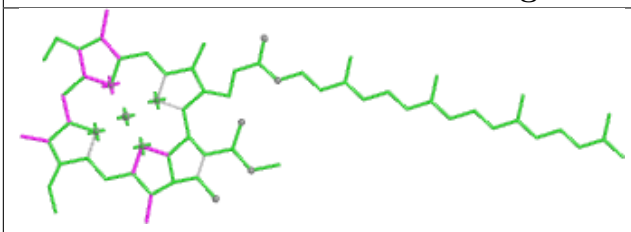

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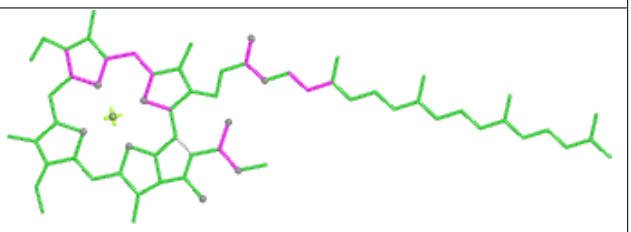

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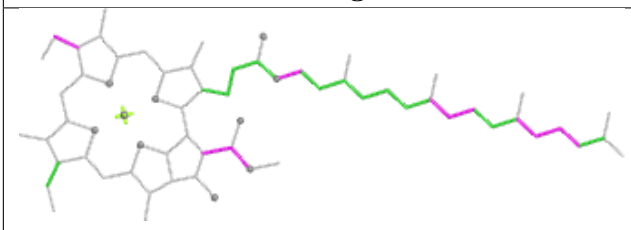

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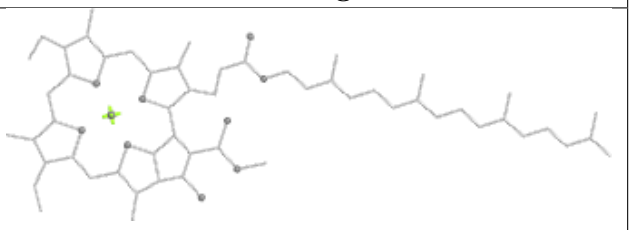
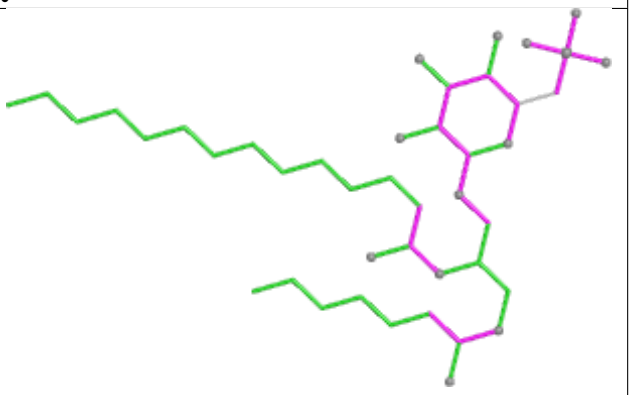


Rings

Ligand SQD 2 822

Bond lengths



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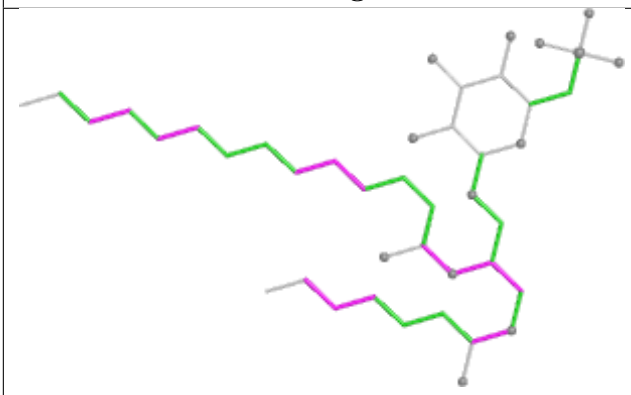

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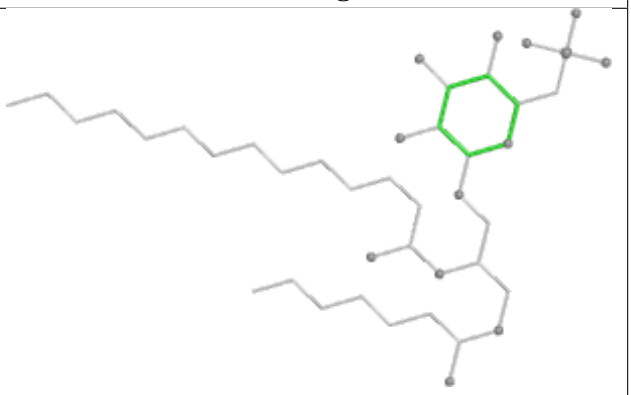
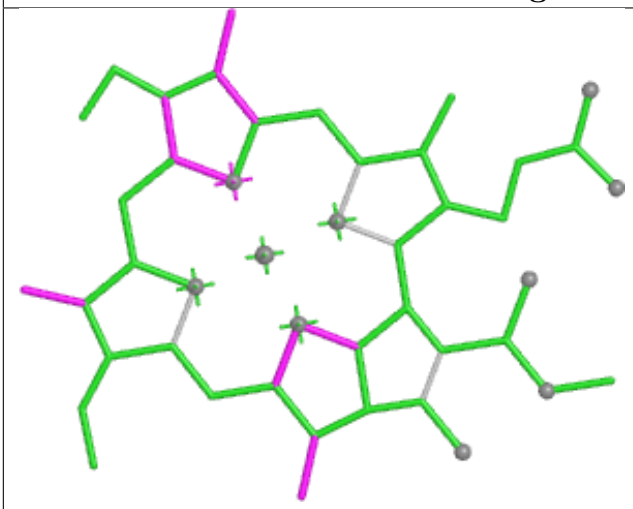


Rings

Ligand CLA c 508



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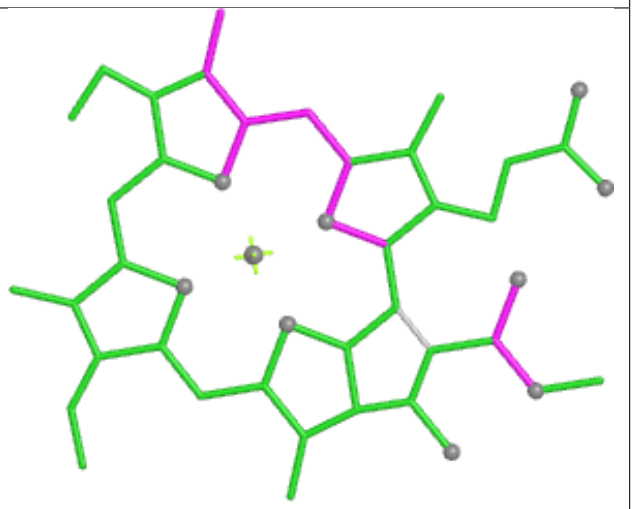
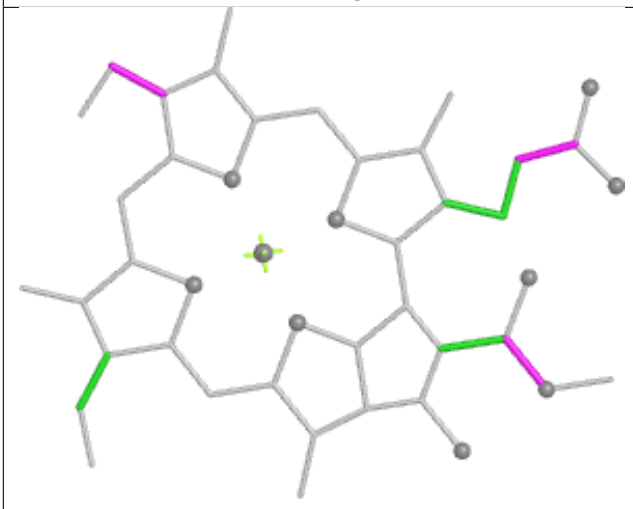


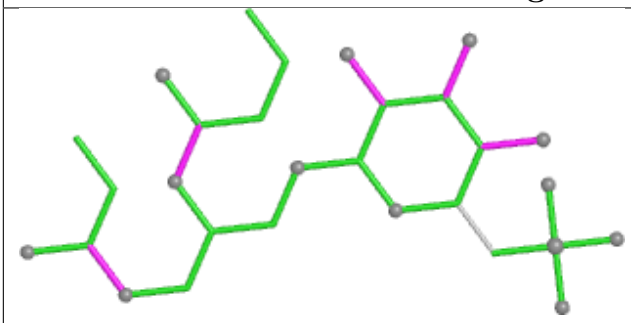
Bond angles



Torsions

Rings

Ligand SQD u 822



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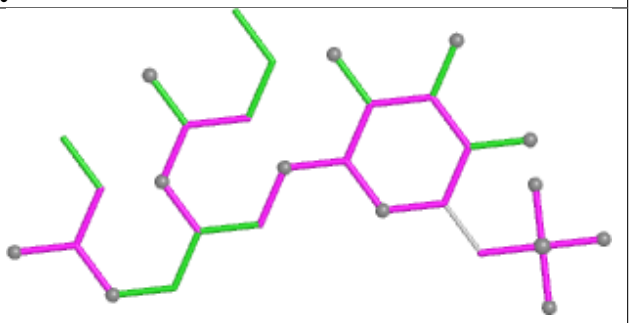

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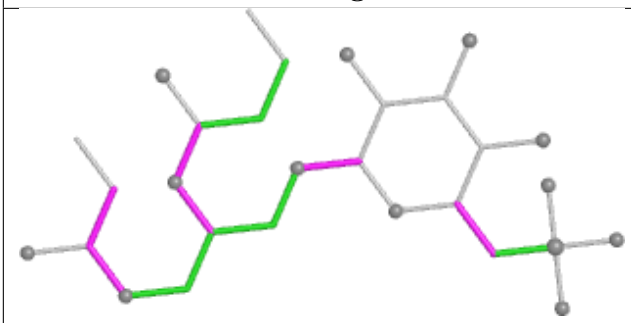

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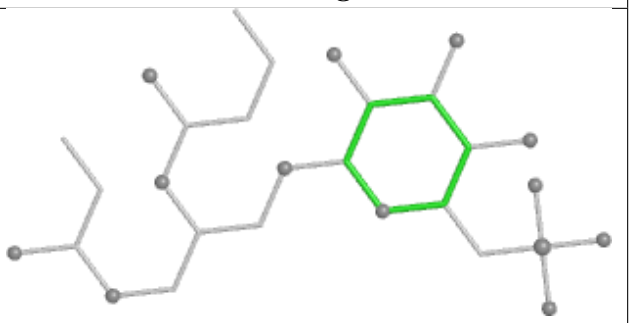
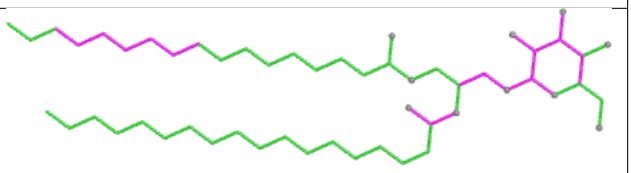


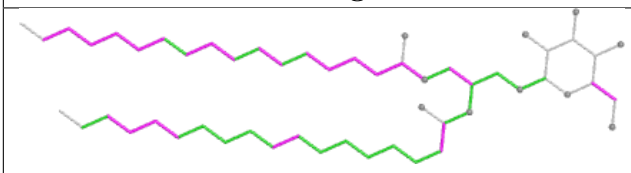
Rings

Ligand LMG B 5002

Bond lengths



Bond angles



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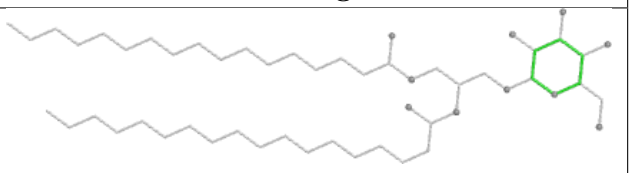
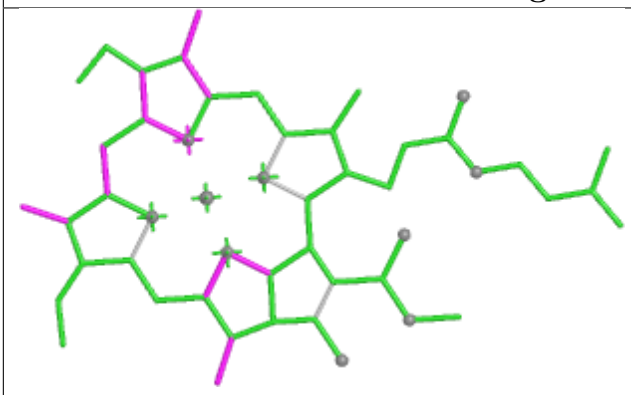


Rings

Ligand CLA c 502



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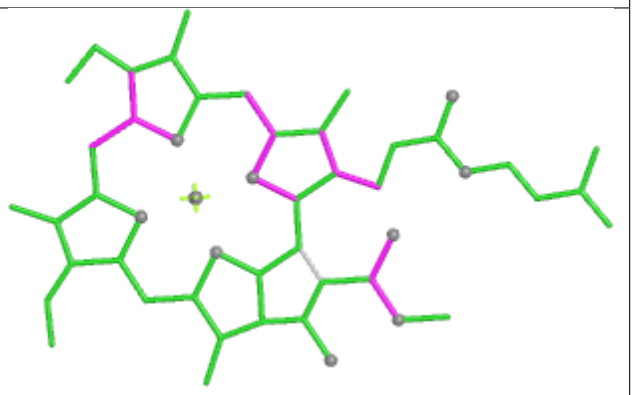
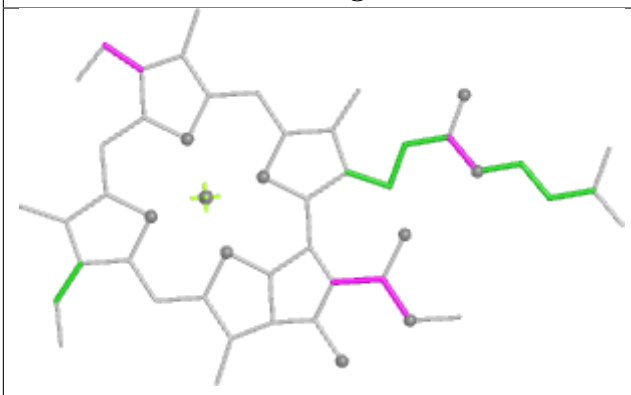


Bond angles



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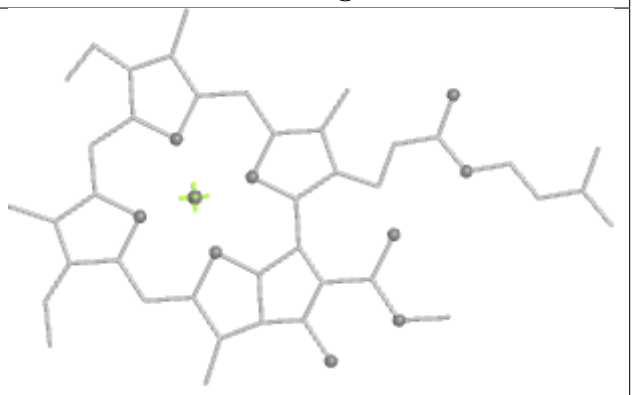
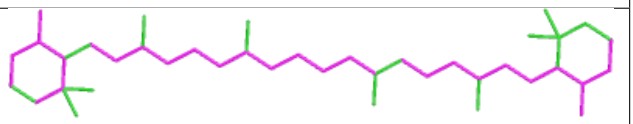


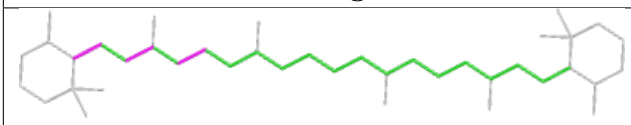
Rings

Ligand BCR 3 522

Bond lengths



Bond angles



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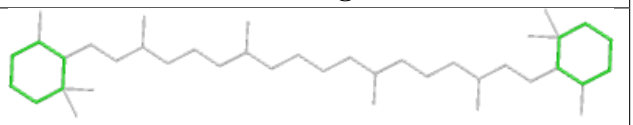
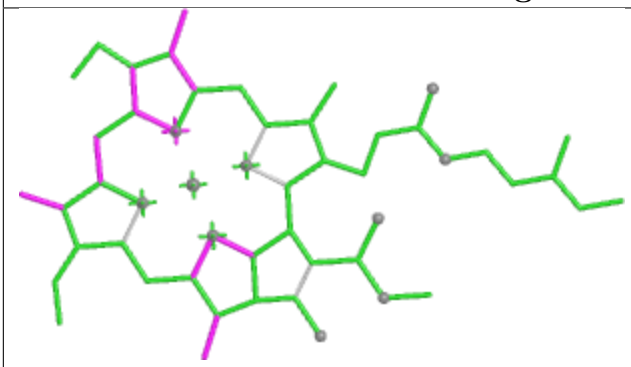
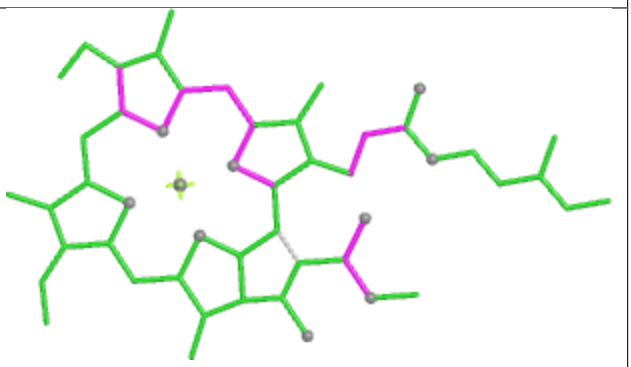


Rings

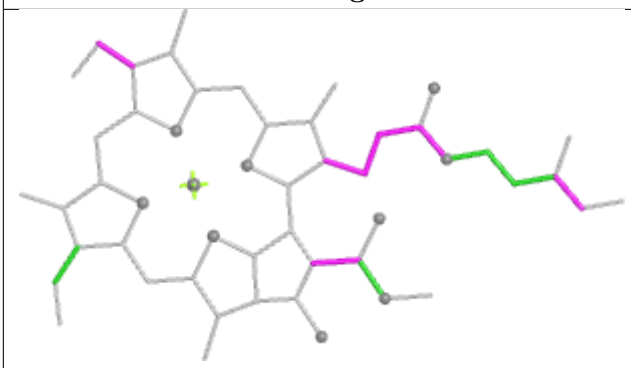
Ligand CLA A 1110



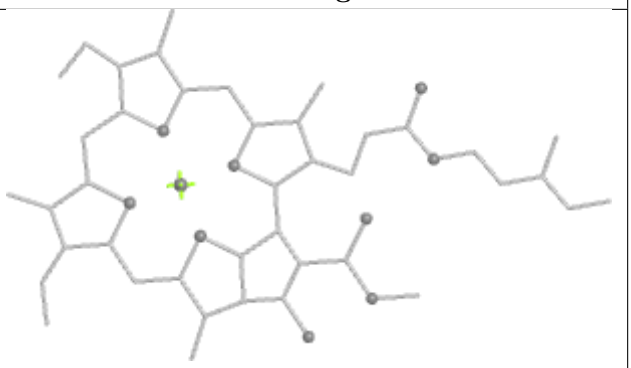
Bond lengths



Bond angles

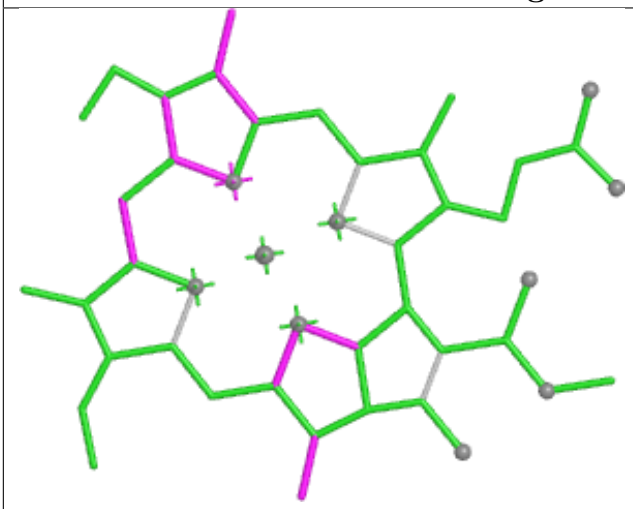


Torsions

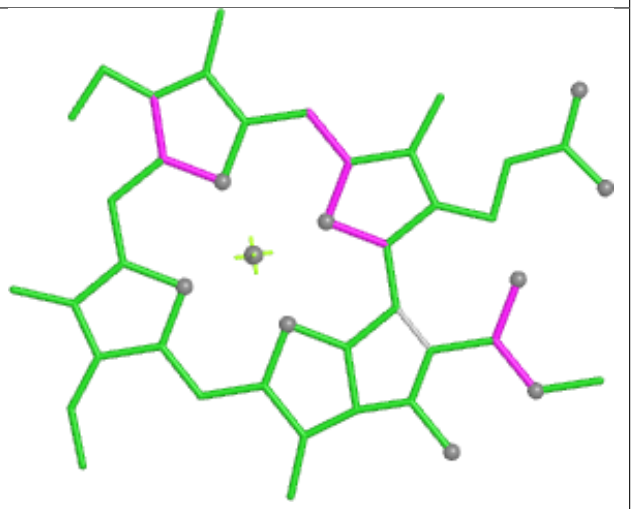


Rings

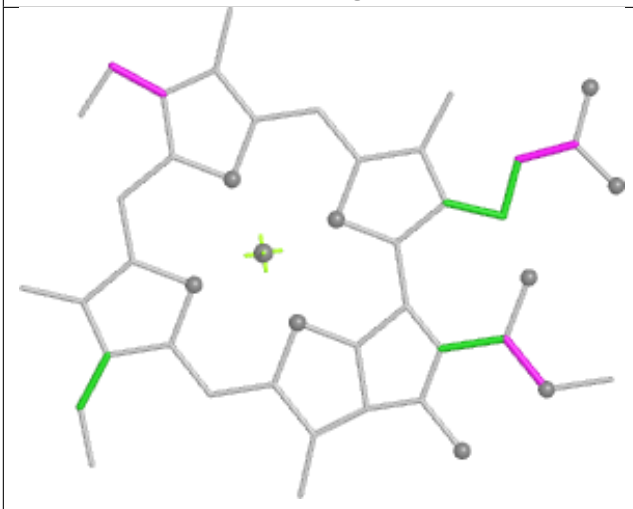
Ligand CLA d 511



Bond lengths



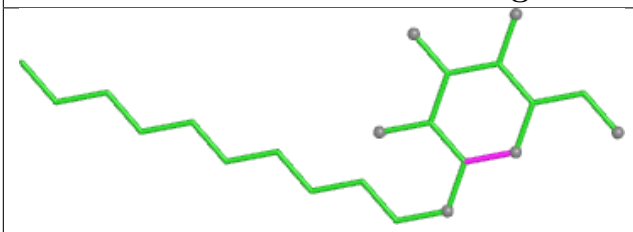
Bond angles



Torsions

Rings

Ligand LMU T 5105



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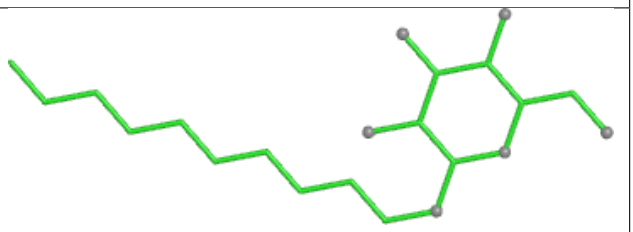

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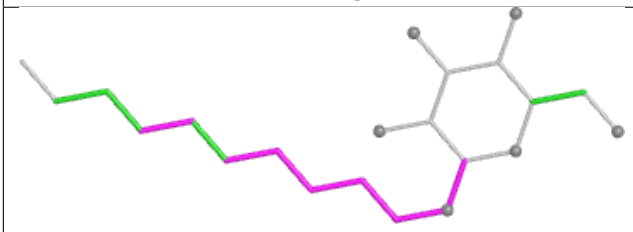
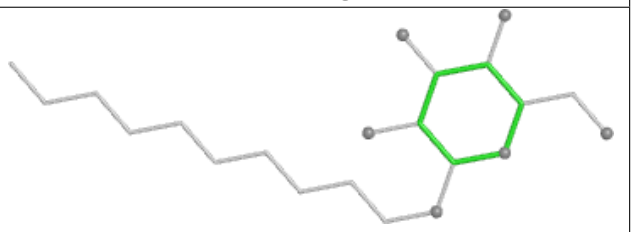


Torsions



Rings

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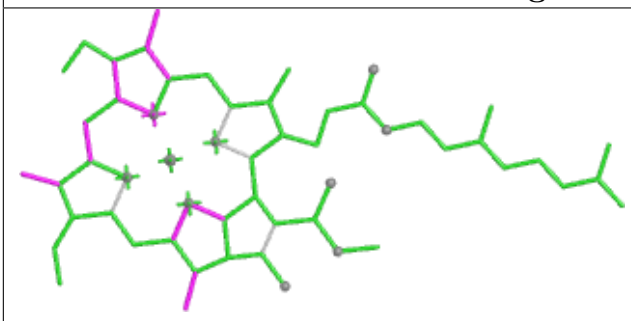
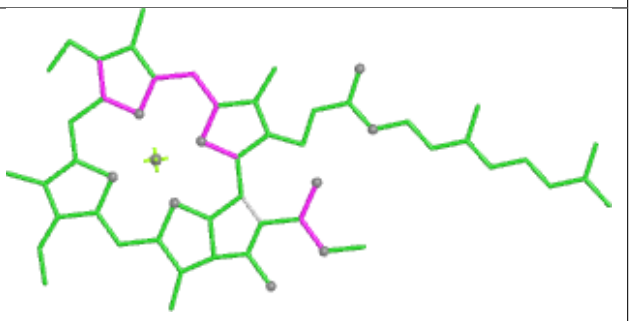
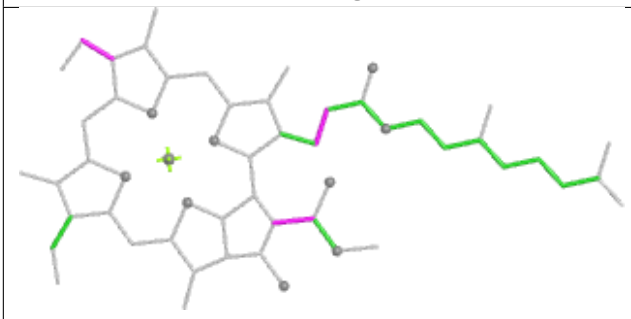
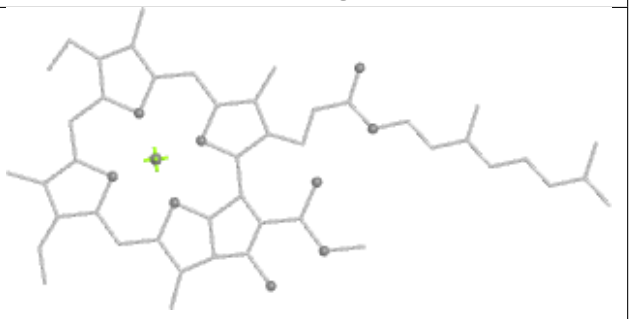
	
Bond lengths	Bond angles
	
Torsions	Rings

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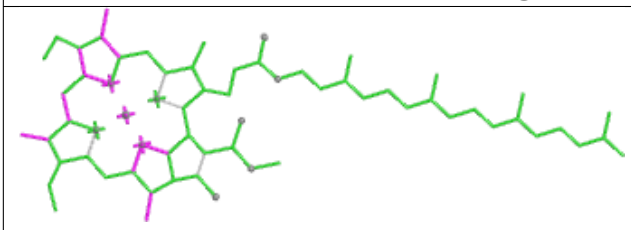
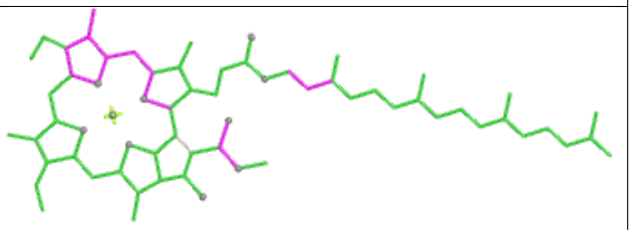
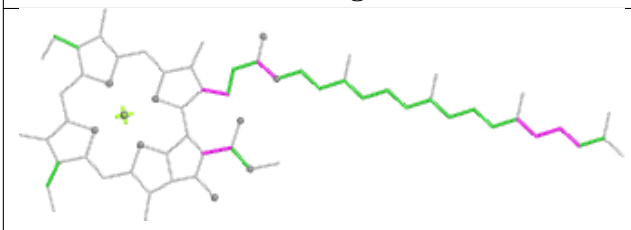
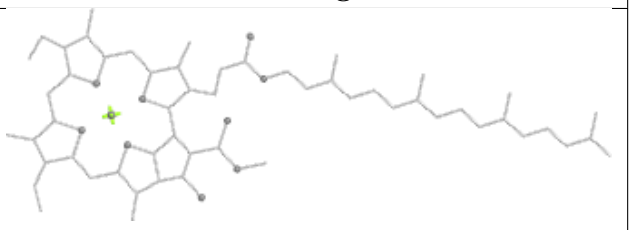
	
Bond lengths	Bond angles
	
Torsions	Rings

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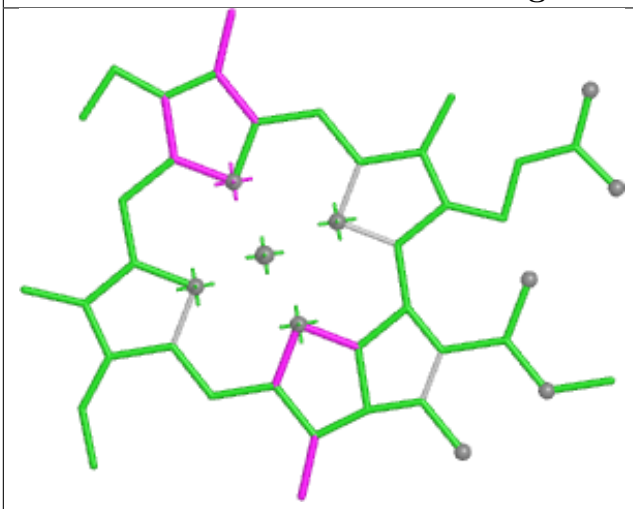

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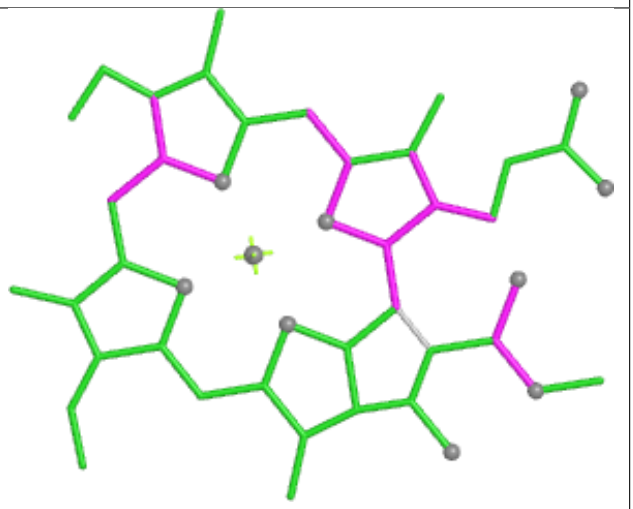
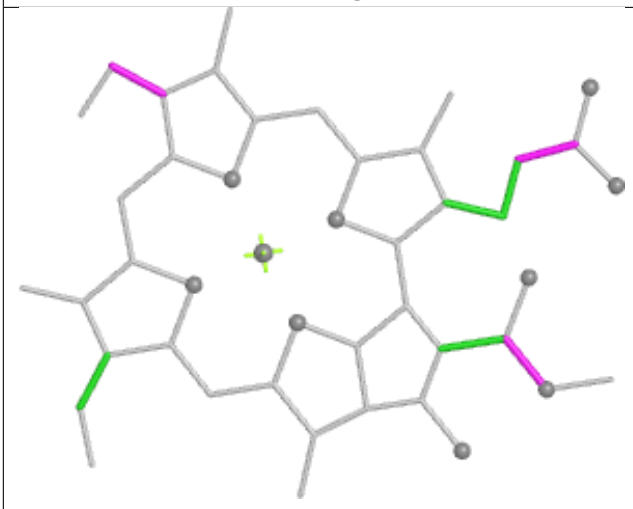


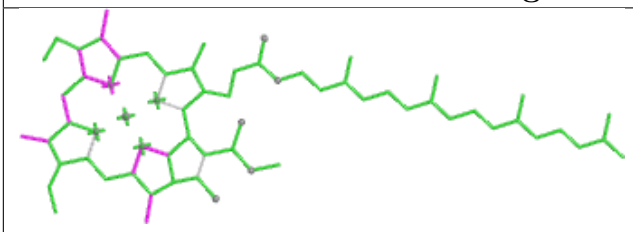
Bond angles



Torsions

Rings

Ligand CLA f 1227



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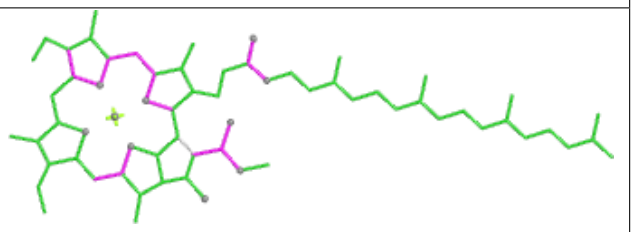

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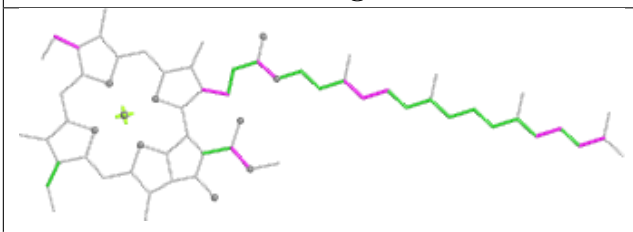

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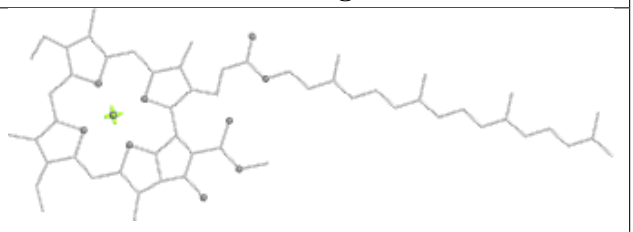

Rings

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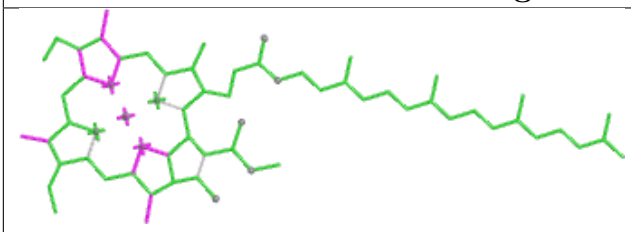

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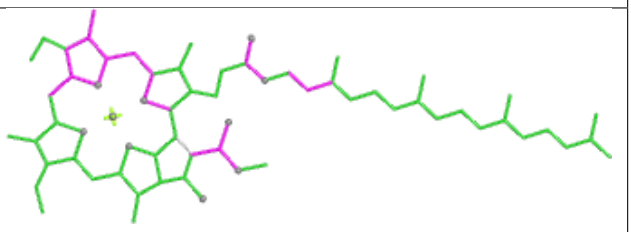

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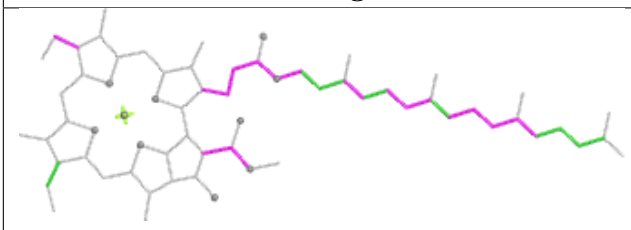

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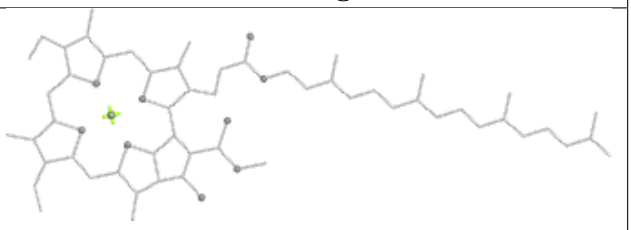

Rings

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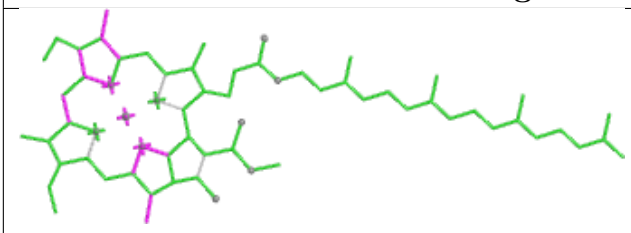

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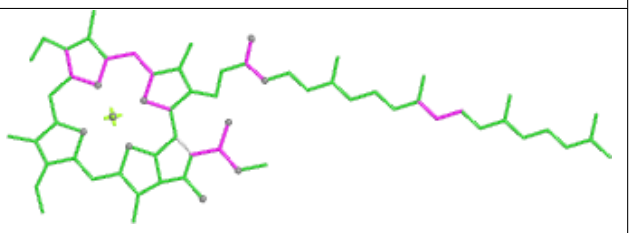

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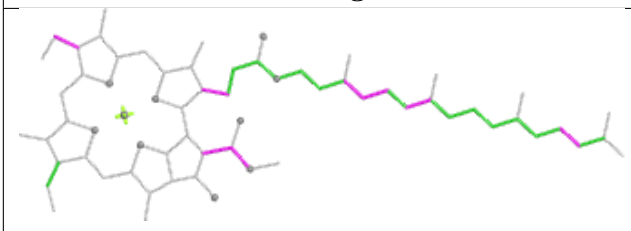

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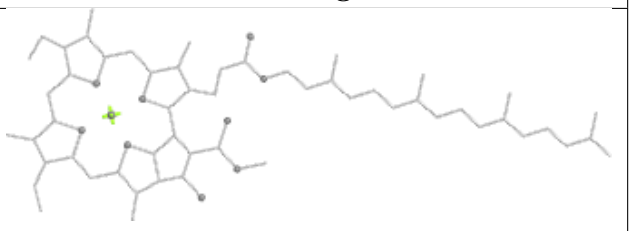
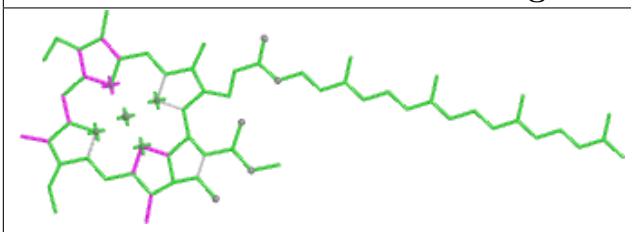


Rings

Ligand CLA a 501



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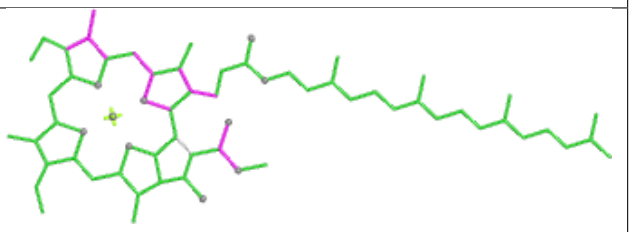

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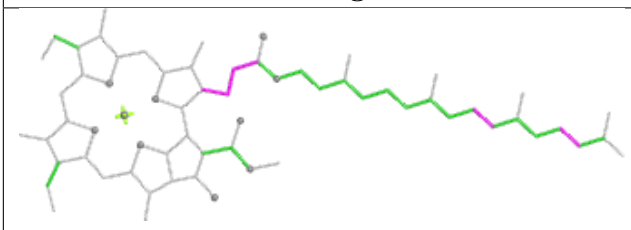

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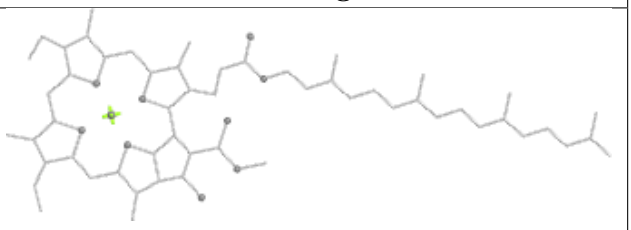
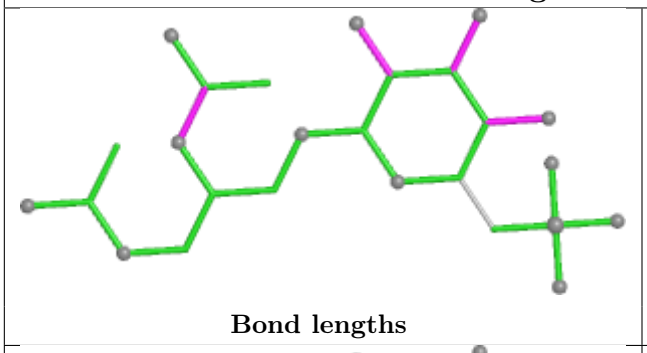


Rings

Ligand SQD 6 822



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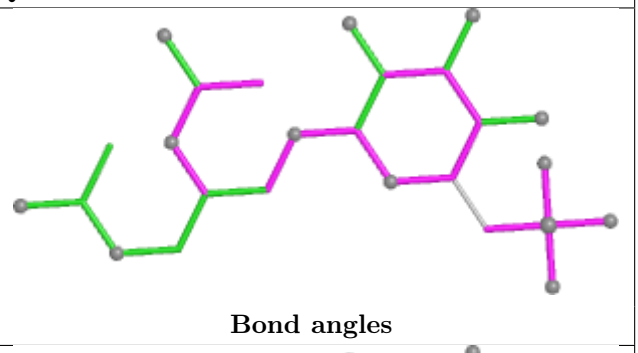

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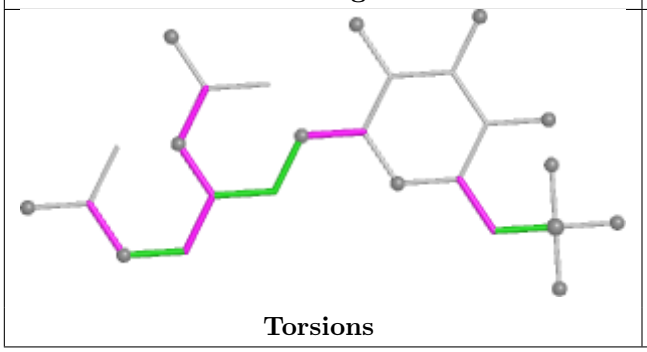

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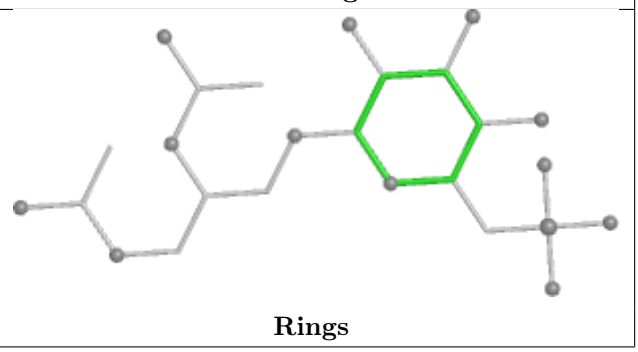
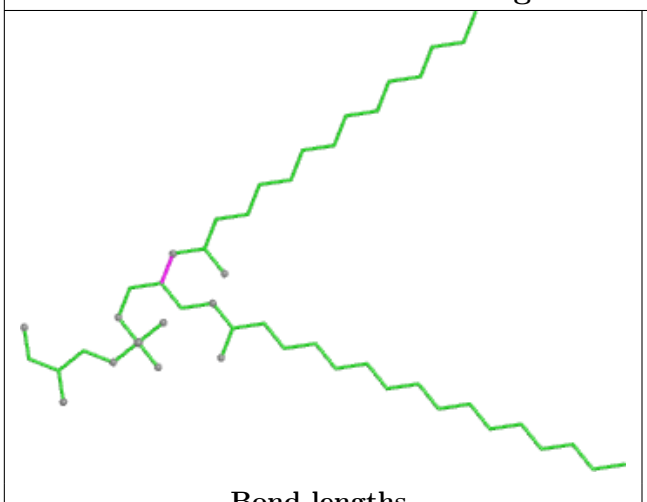


Rings

Ligand LHG G 5007



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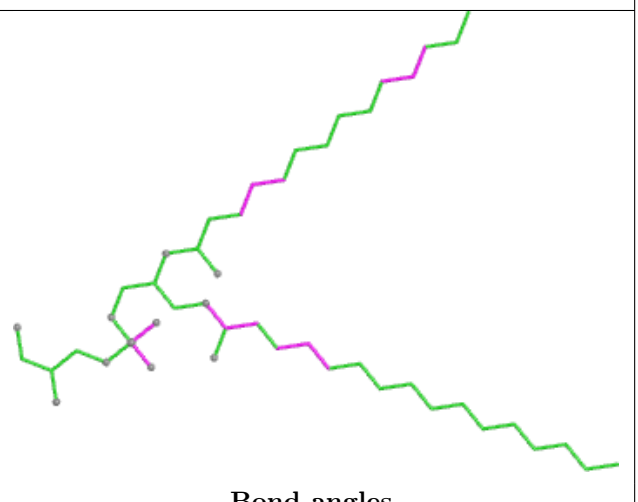

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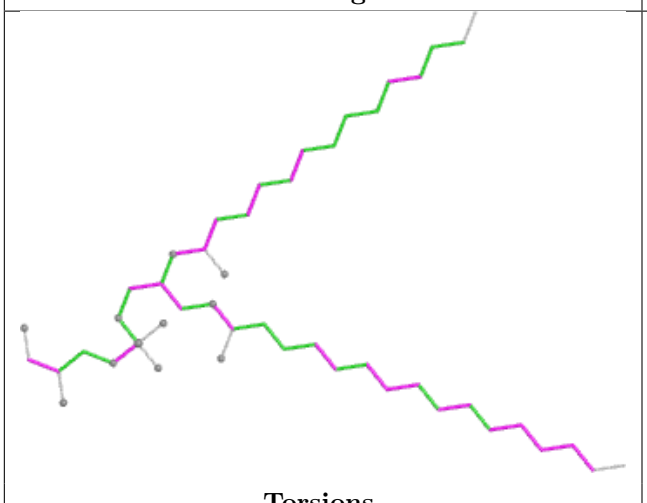

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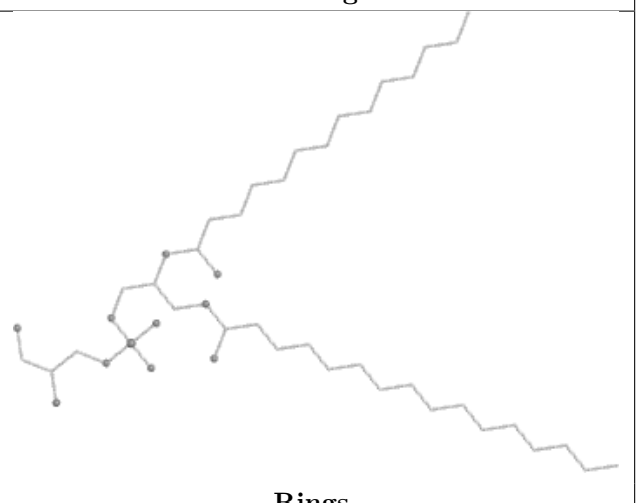
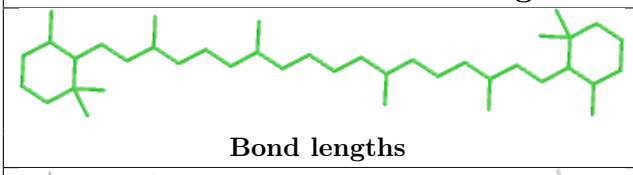


Rings

Ligand BCR F 4016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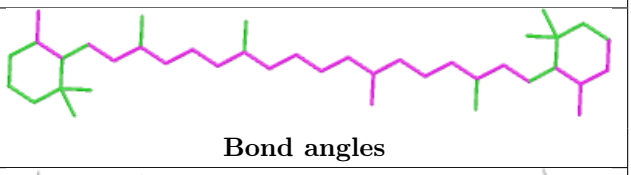
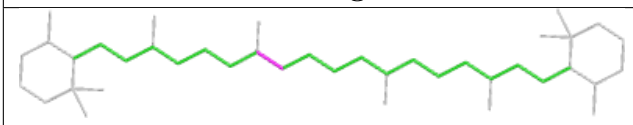

Bond angles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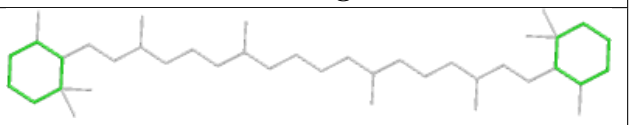
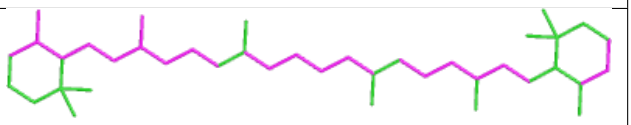
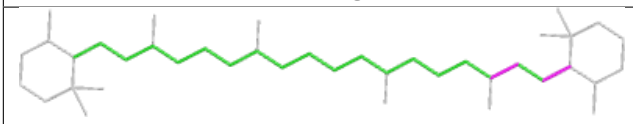
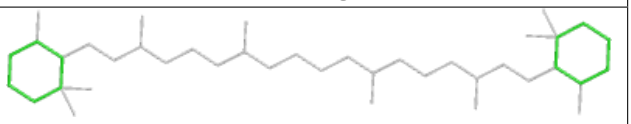

Rings

Ligand BCR d 523

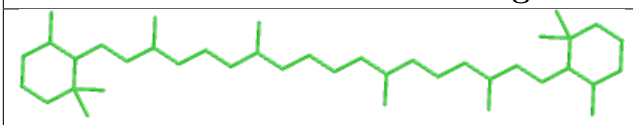
Bond lengths


Bond angles


Torsions


Rings

Ligand BCR H 4014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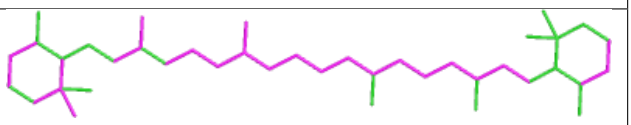
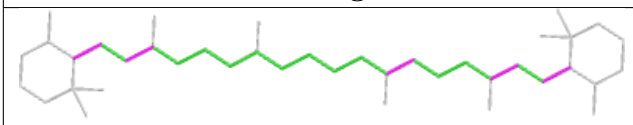

Bond angles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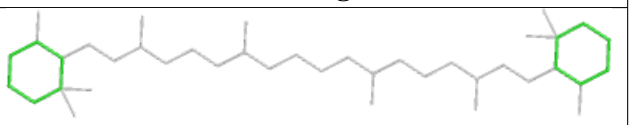
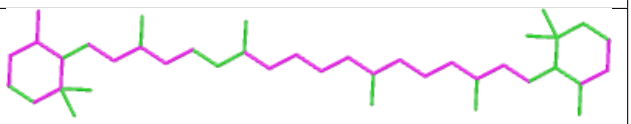
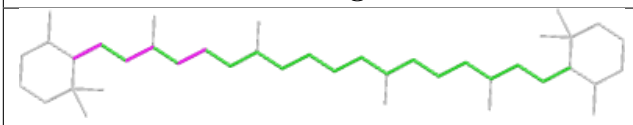
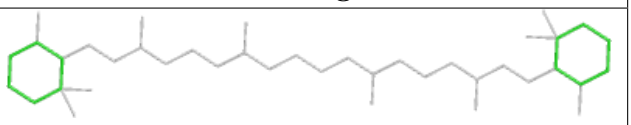

Rings

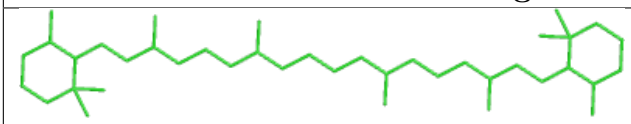
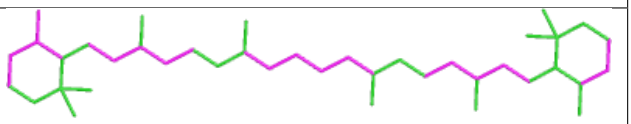
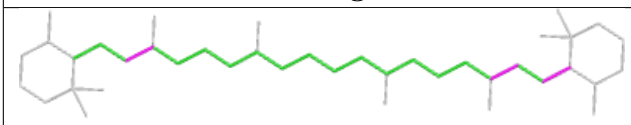
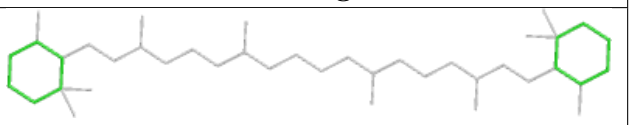
Ligand BCR v 521

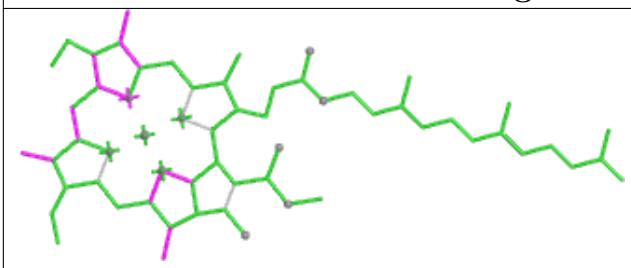
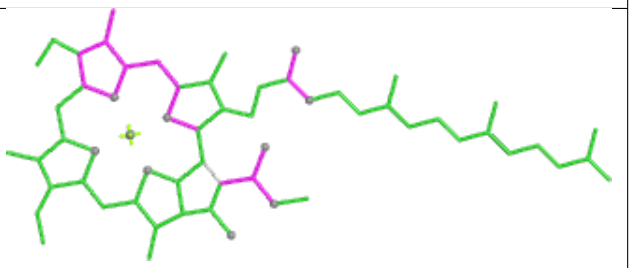
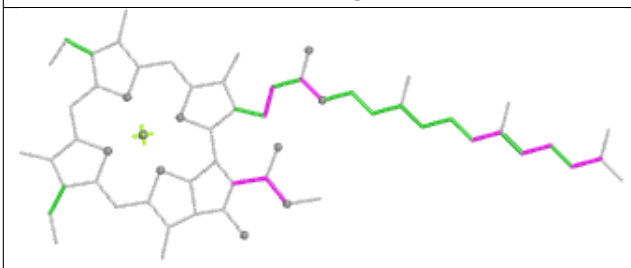
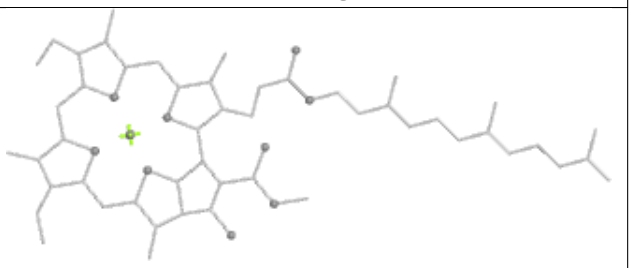
Bond lengths


Bond angles

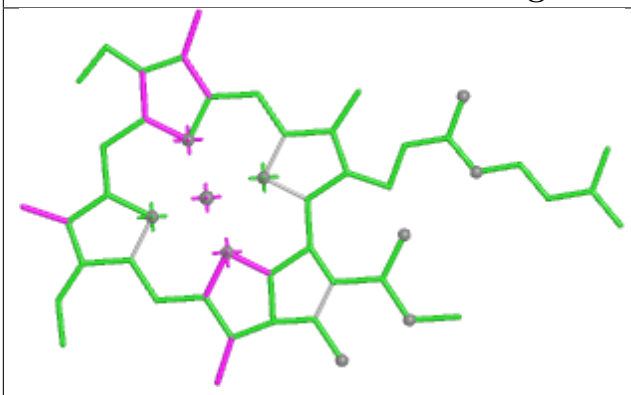

Torsions


Rings

Ligand BCR B 4005	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 519



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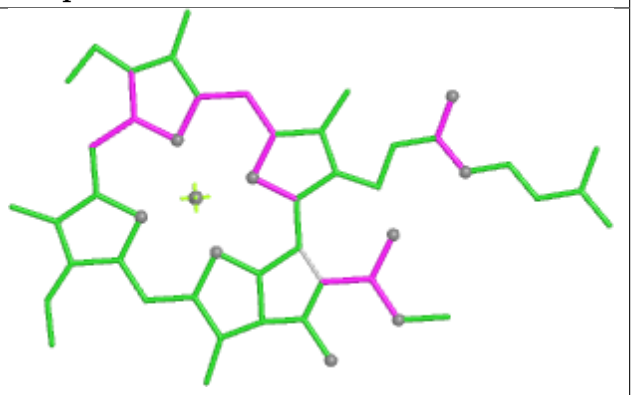
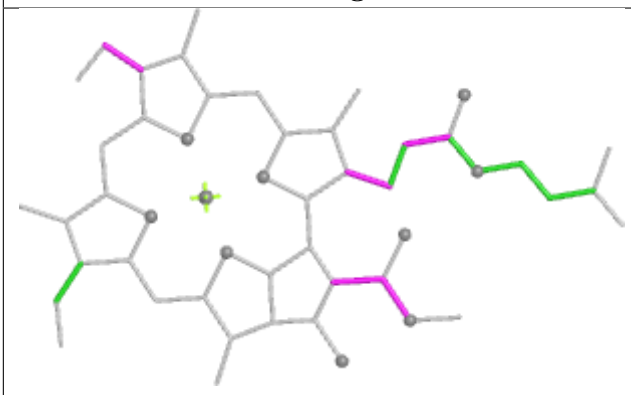


Bond angles



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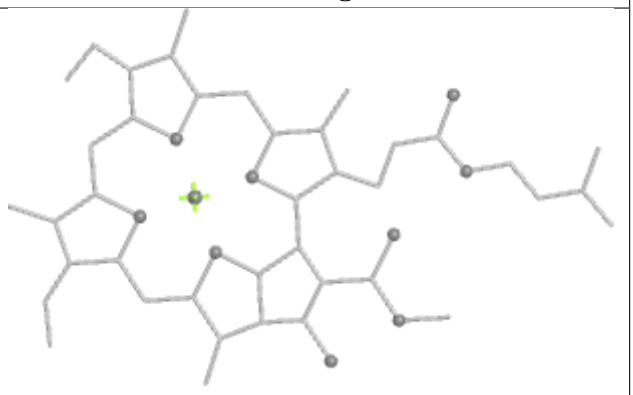
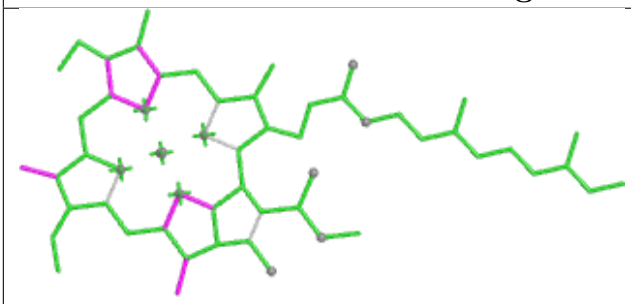


Rings

Ligand CLA B 1211



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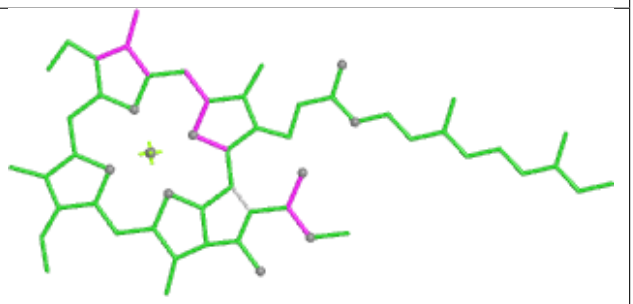

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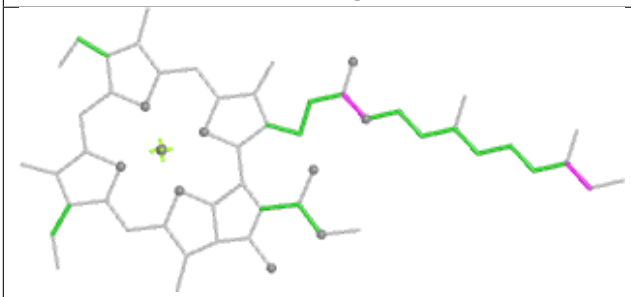

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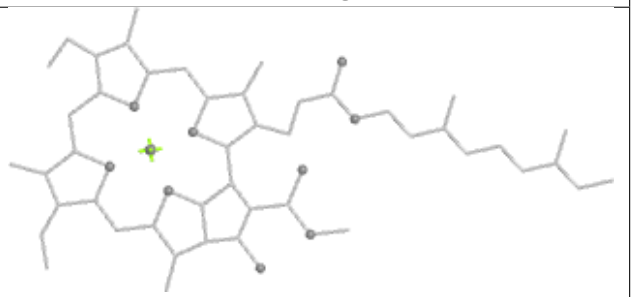
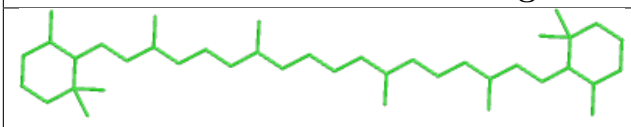


Rings

Ligand BCR e 4002



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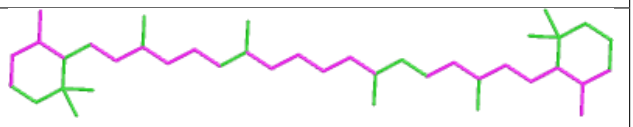
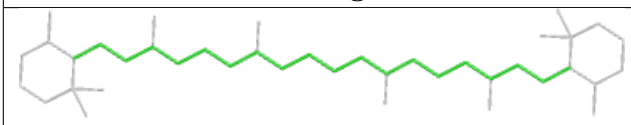


Bond angles



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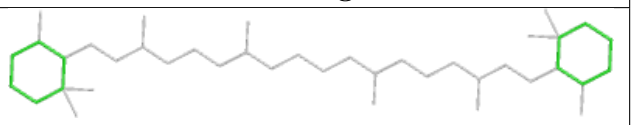

Rings

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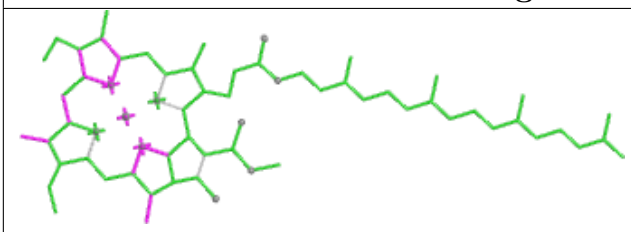

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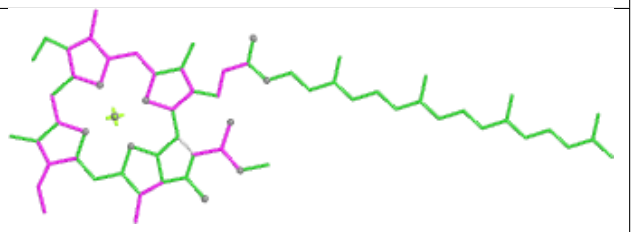
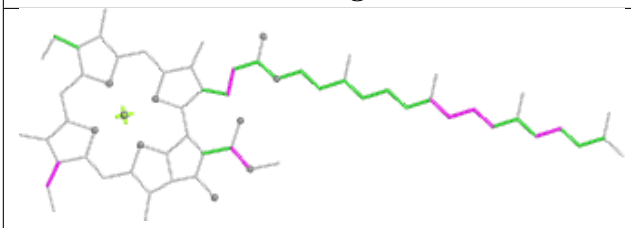


Bond angles



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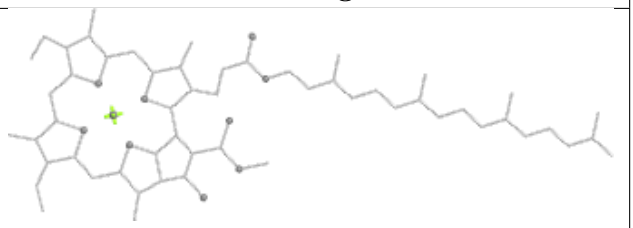

Rings

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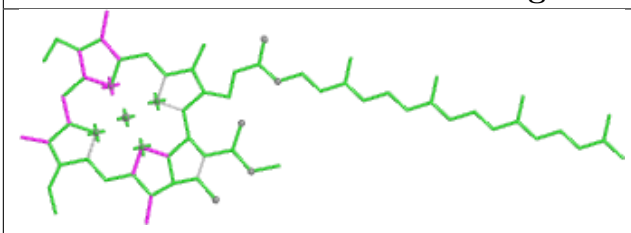

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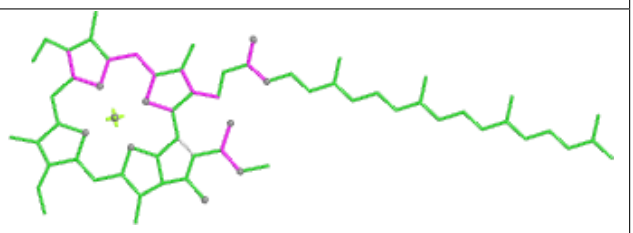

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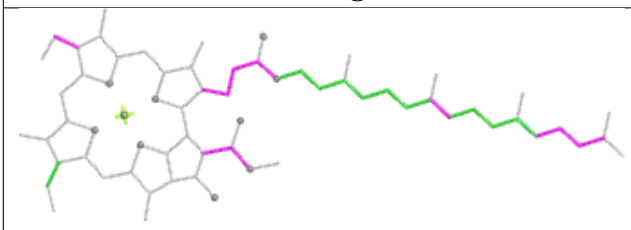

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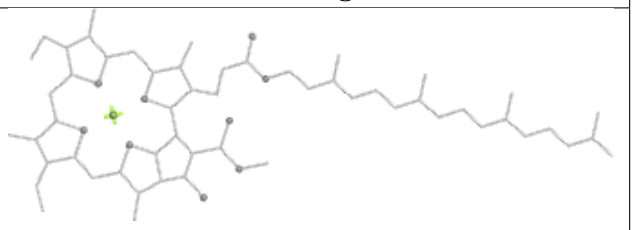
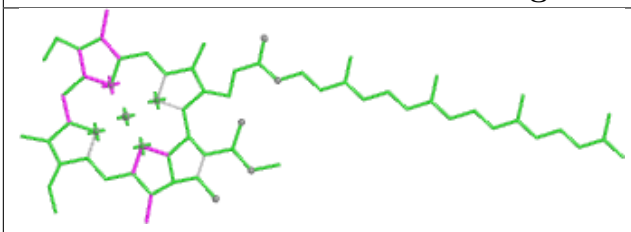


Rings

Ligand CLA s 503



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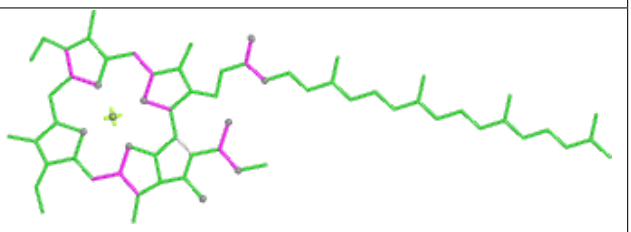
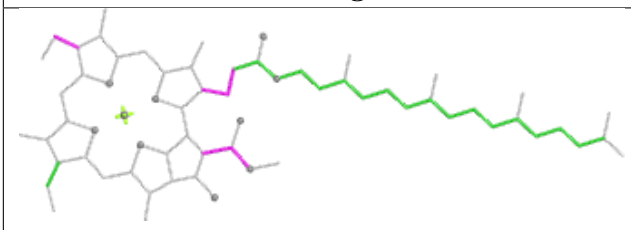


Bond angles



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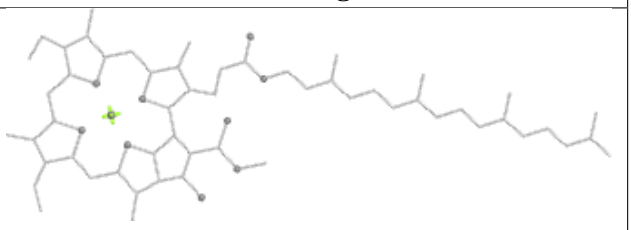
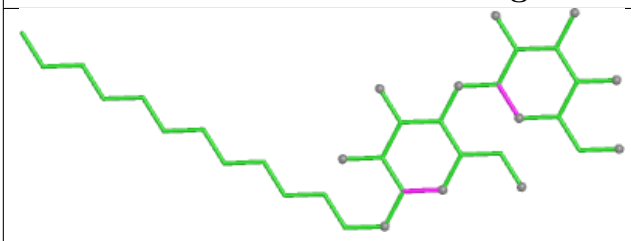


Rings

Ligand LMU A 1848



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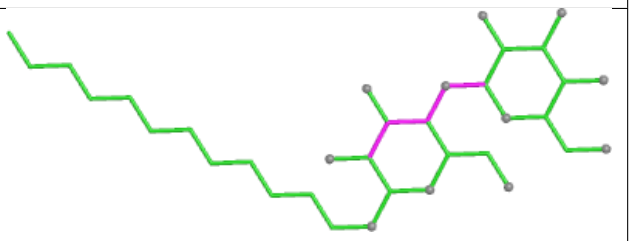

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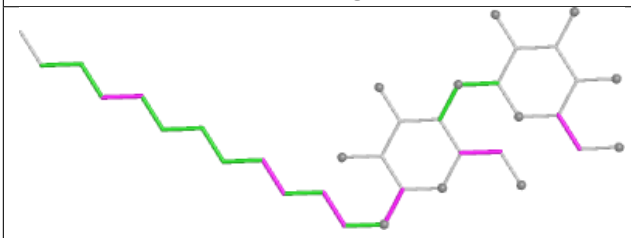

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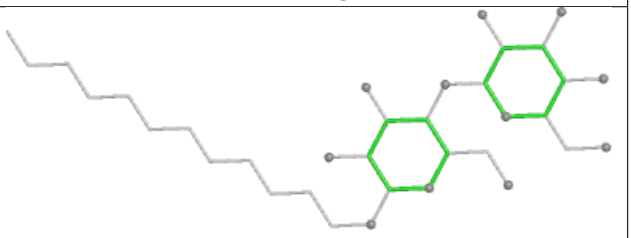

Rings

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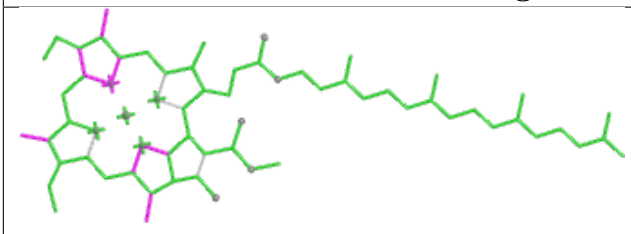

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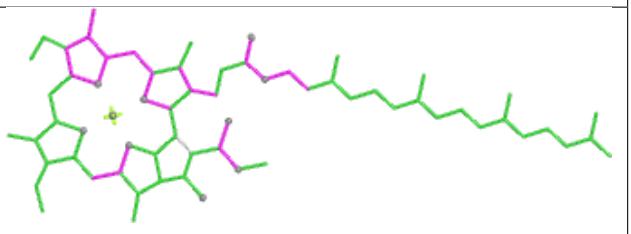

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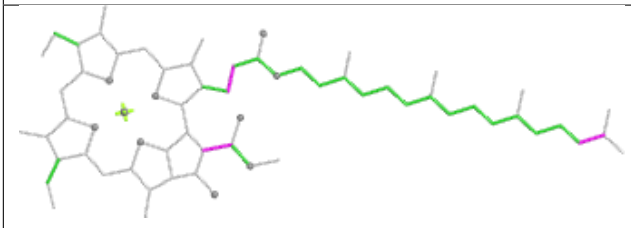

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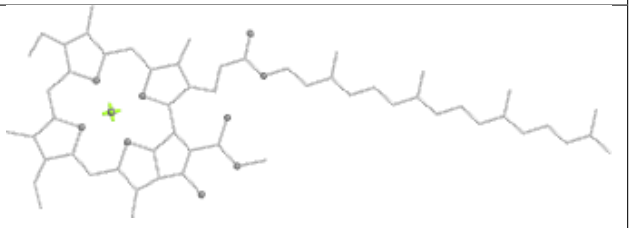
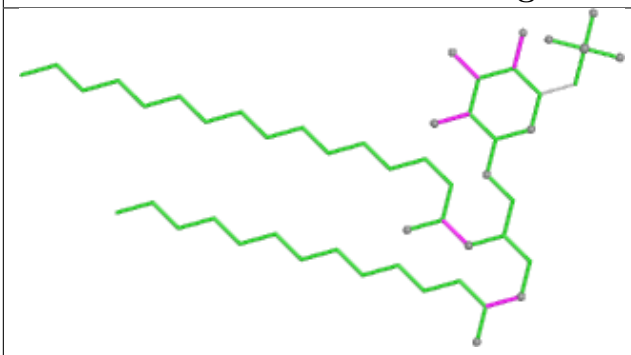


Rings

Ligand SQD L 5216



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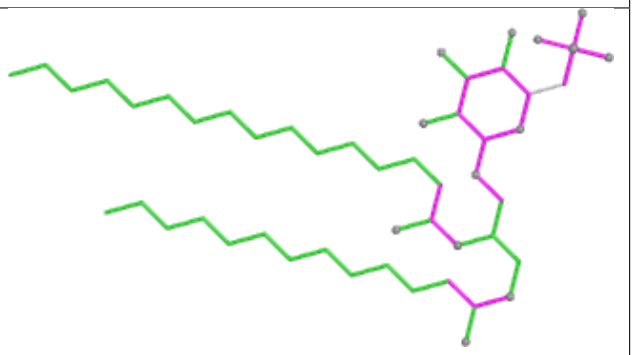

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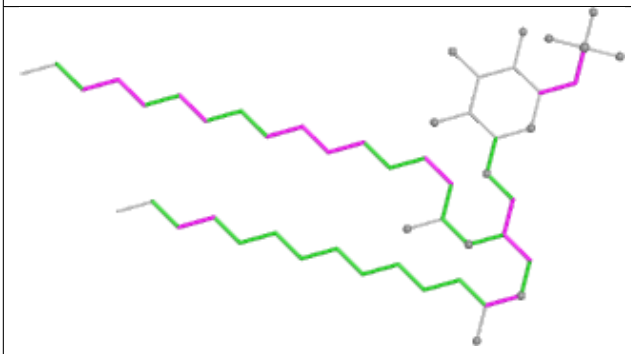

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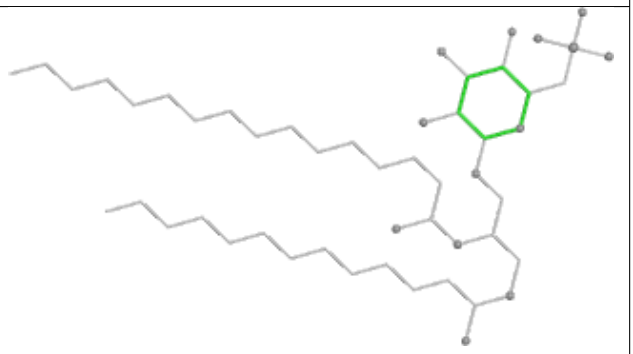
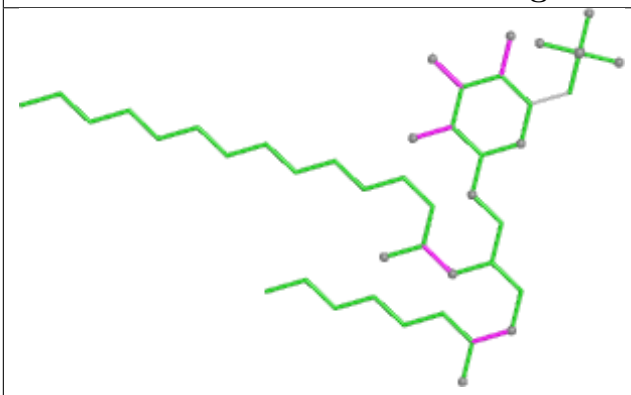


Rings

Ligand SQD r 822



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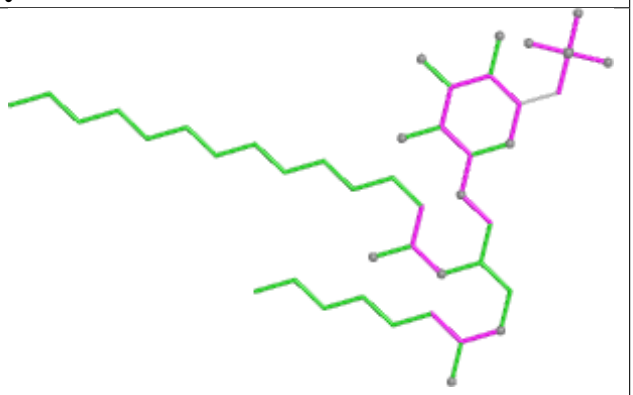
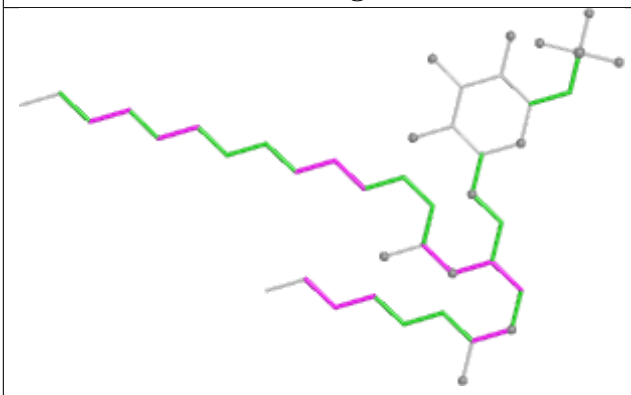


Bond angles



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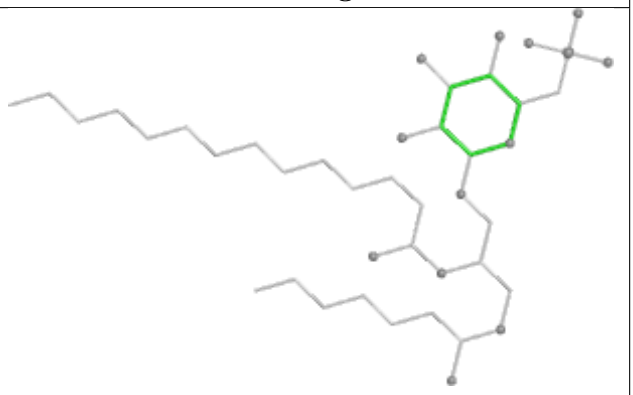
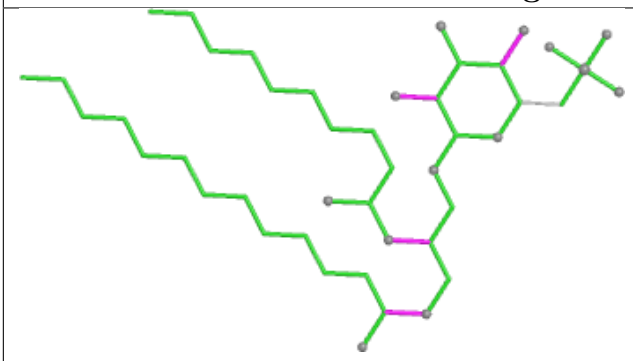
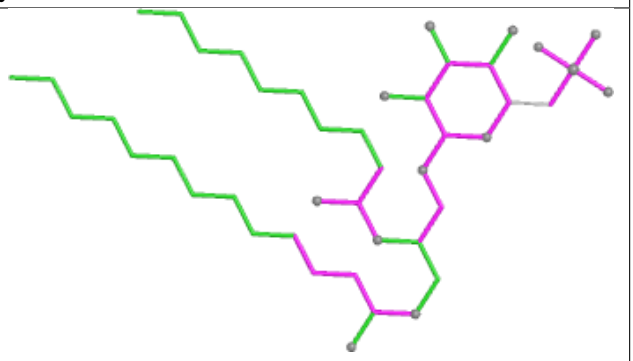


Rings

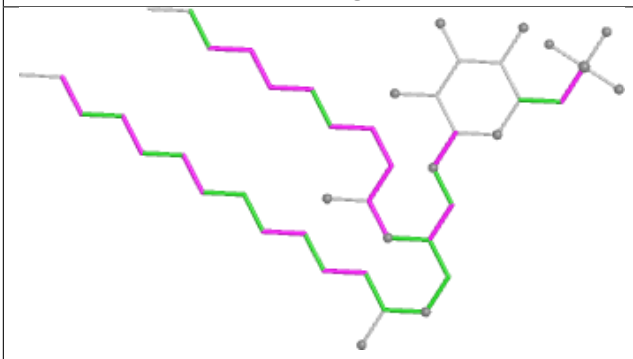
Ligand SQD f 1852



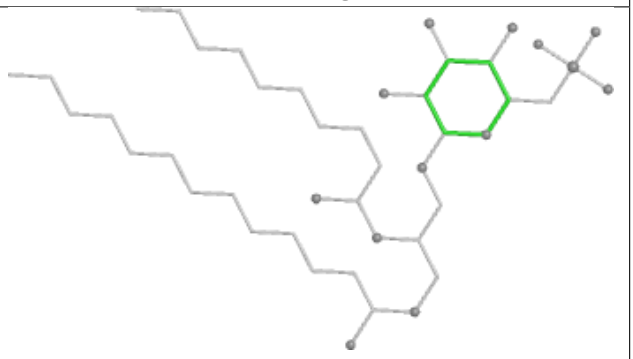
Bond lengths



Bond angles

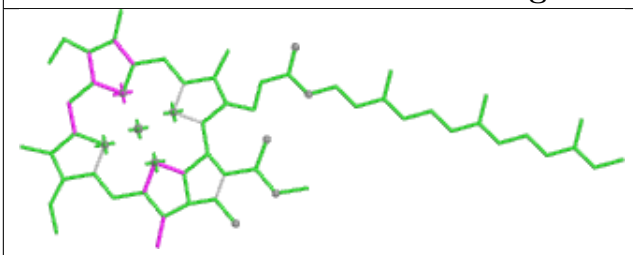


Torsions

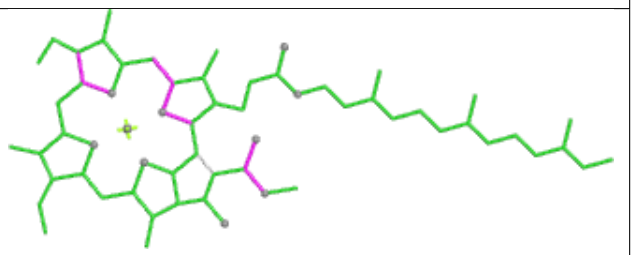


Rings

Ligand CLA c 505



Bond lengths



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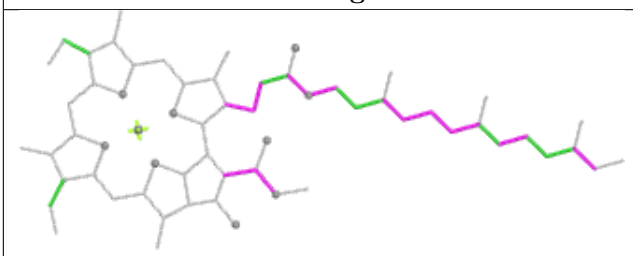
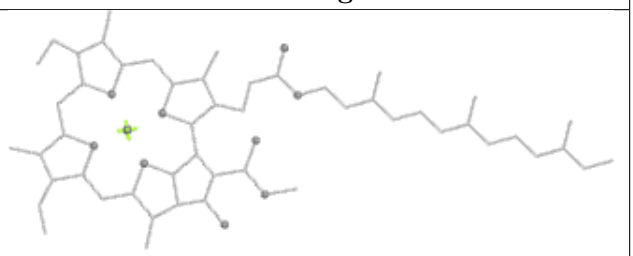
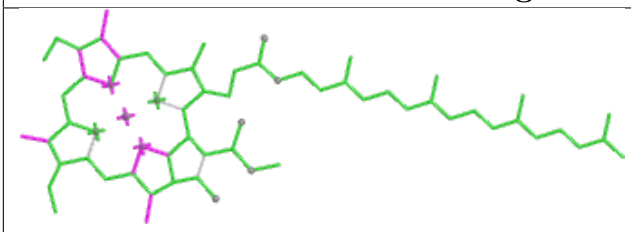
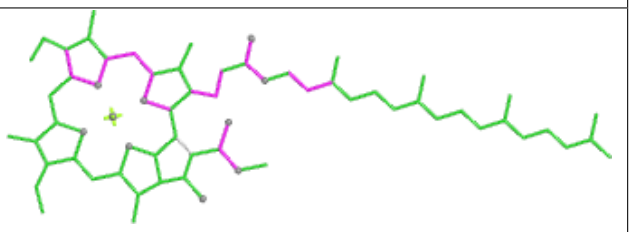
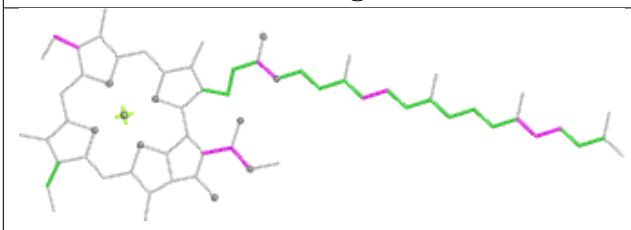
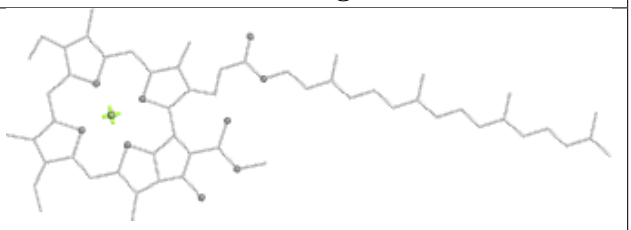
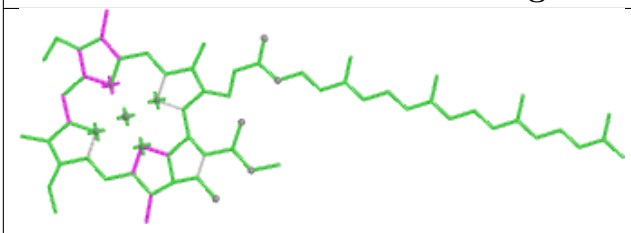
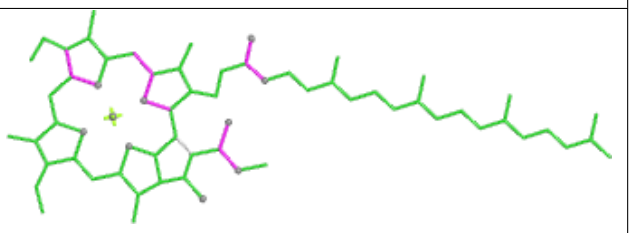
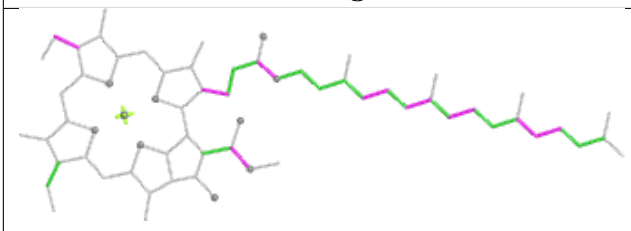
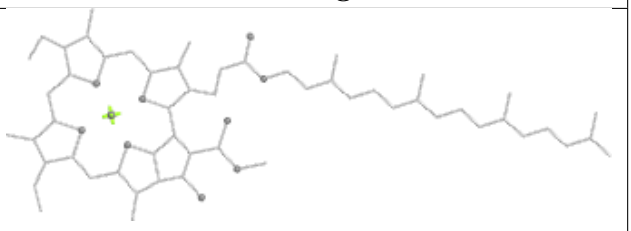


Torsions

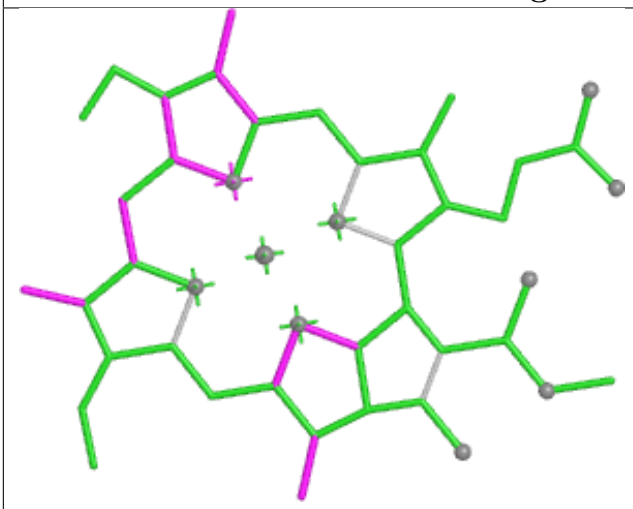


Rings

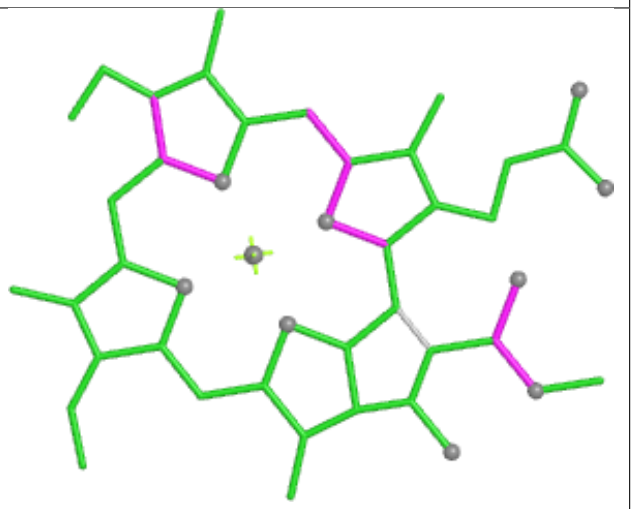
Ligand CLA B 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

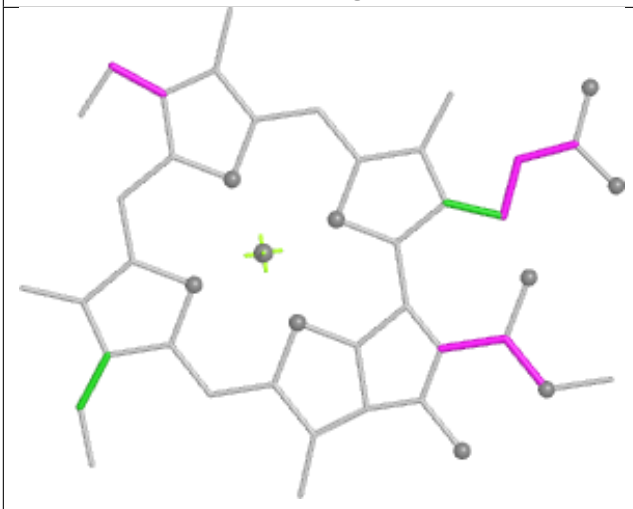
Ligand CLA t 513



Bond lengths



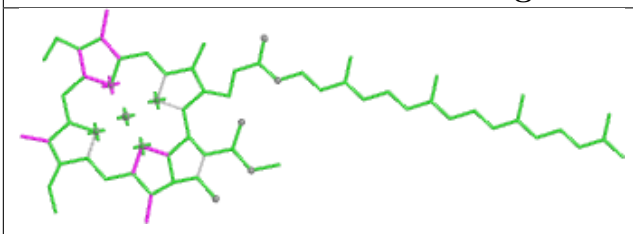
Bond angles



Torsions

Rings

Ligand CLA A 1109



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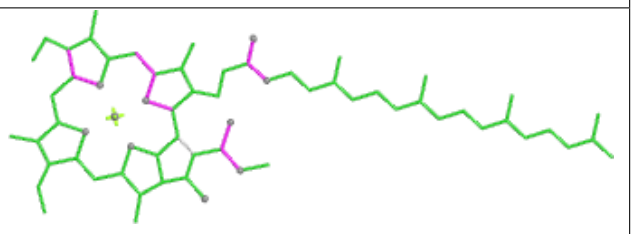
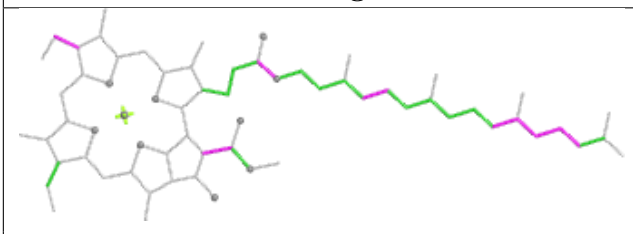


Bond angles



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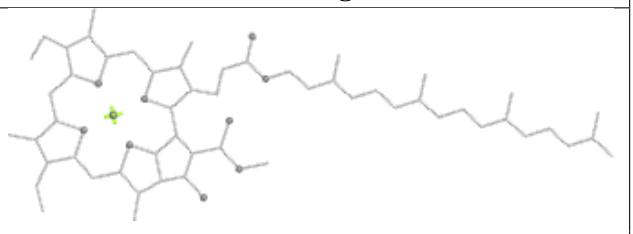
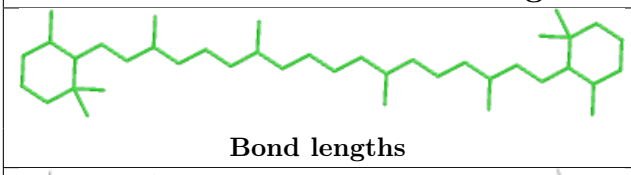


Rings

Ligand BCR u 523



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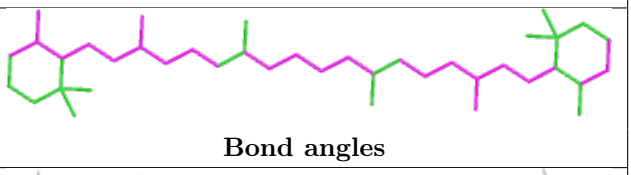

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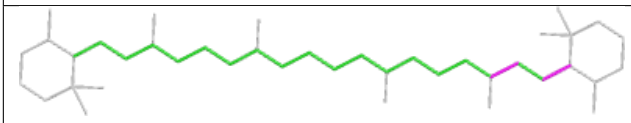

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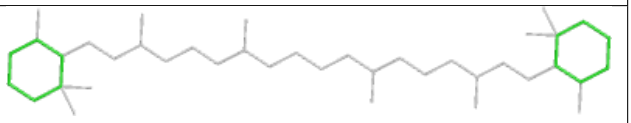
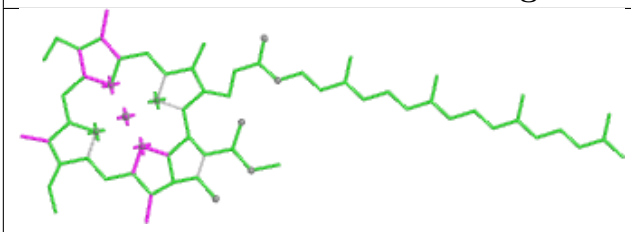


Rings

Ligand CLA e 1022



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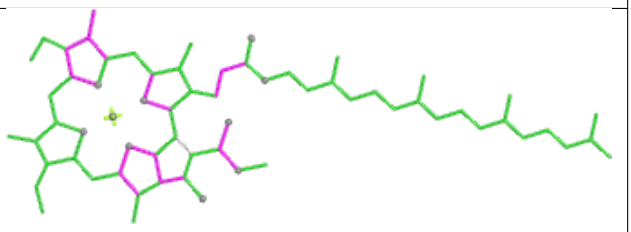

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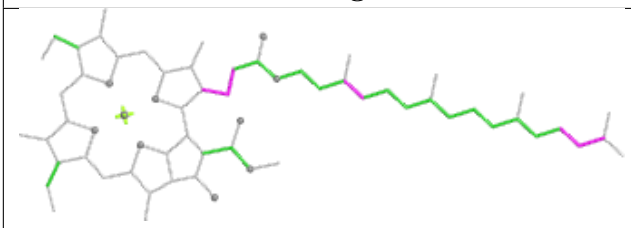

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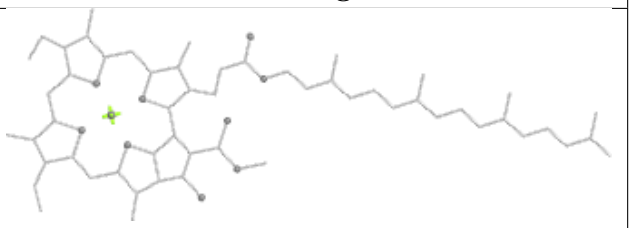
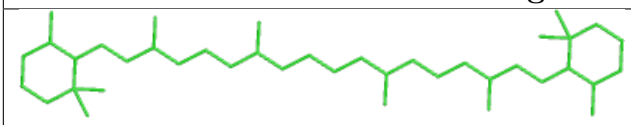


Rings

Ligand BCR c 522



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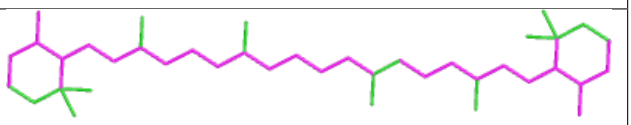
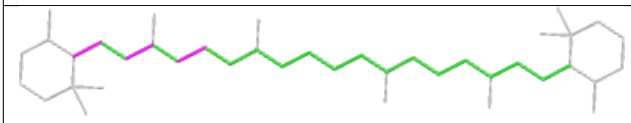


Bond angles



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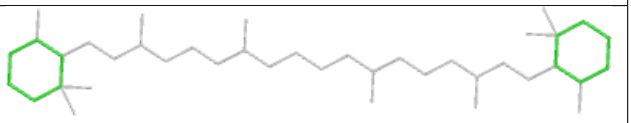
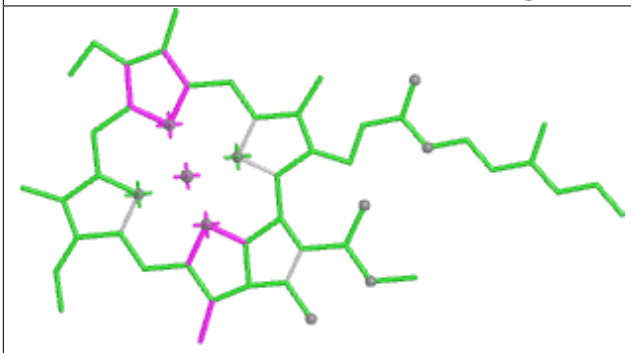


Rings

Ligand CLA e 1135



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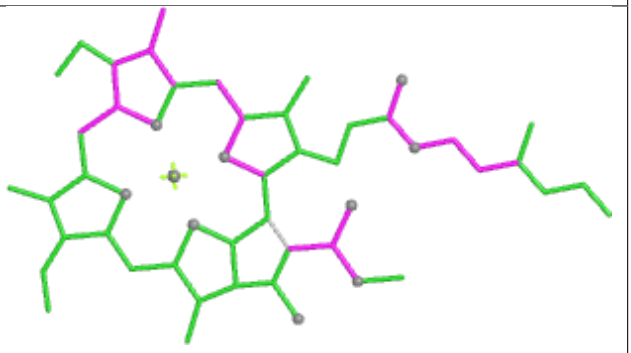

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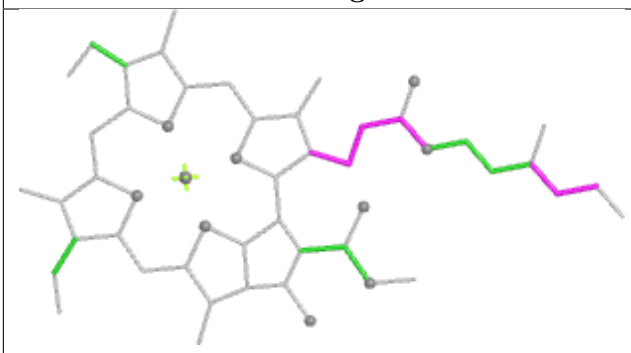

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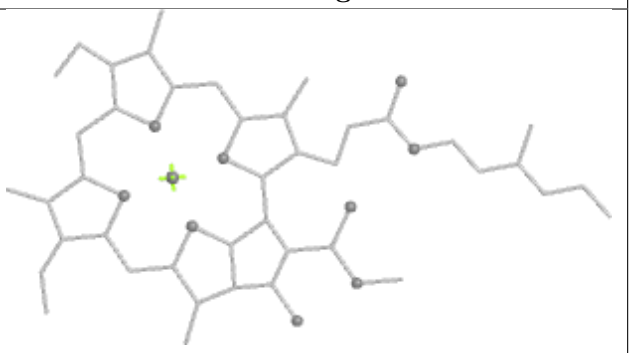
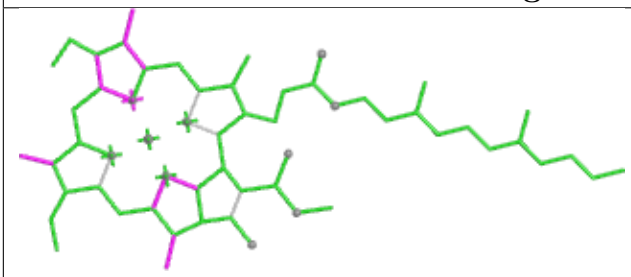


Rings

Ligand CLA l 1302



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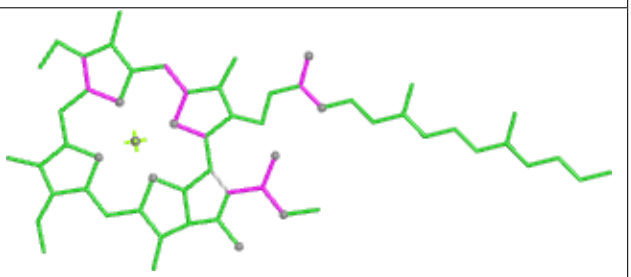
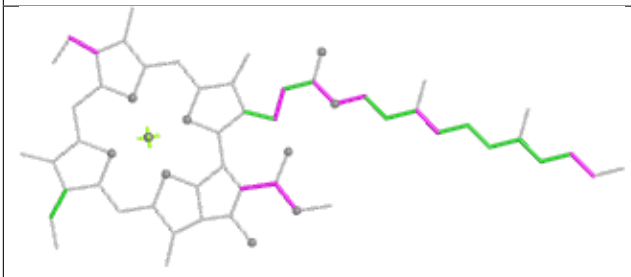


Bond angles



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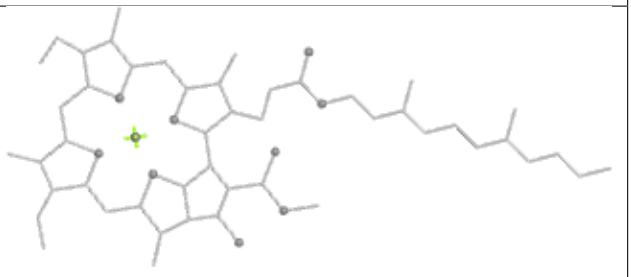
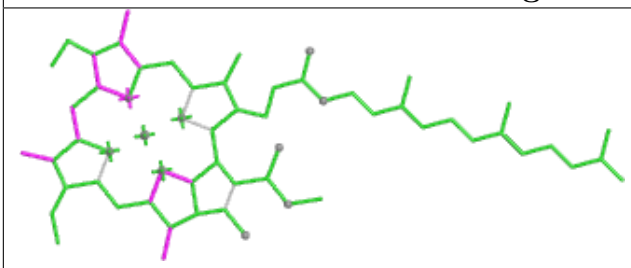
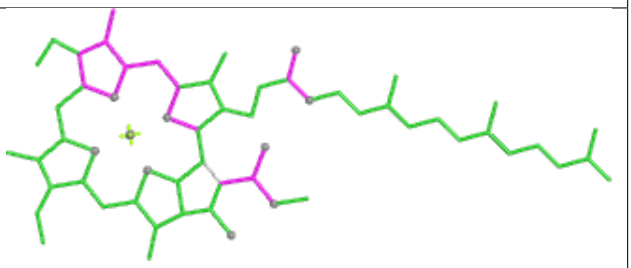
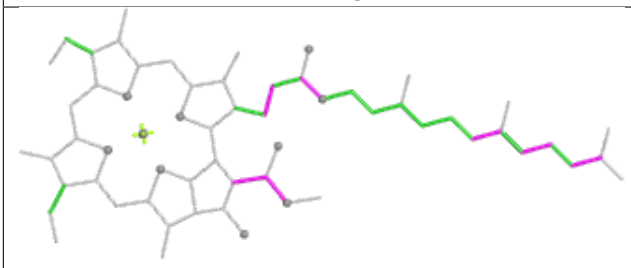
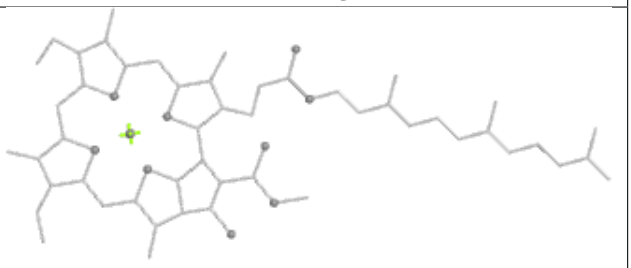
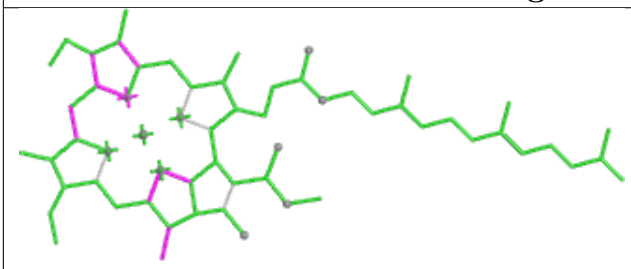
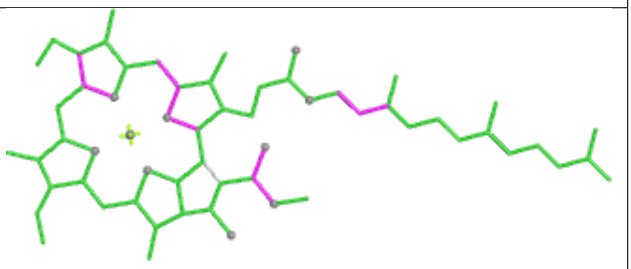
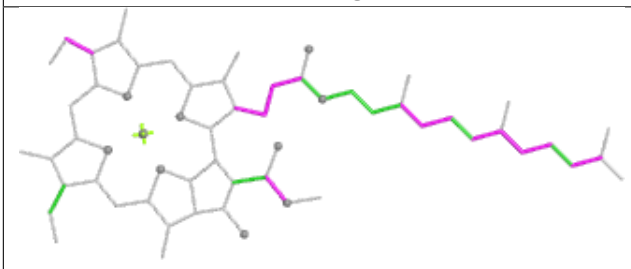
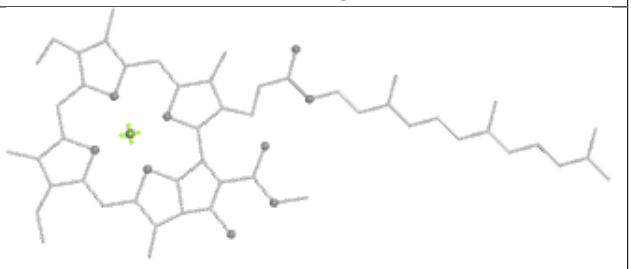
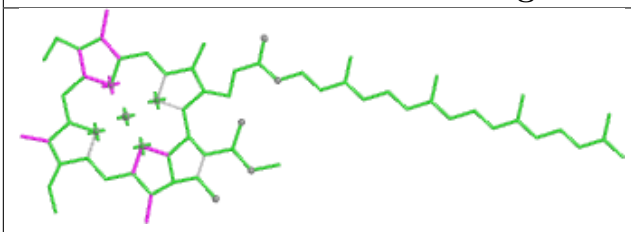


Rings

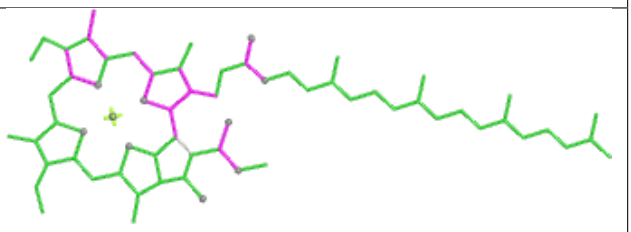
Ligand CLA f 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

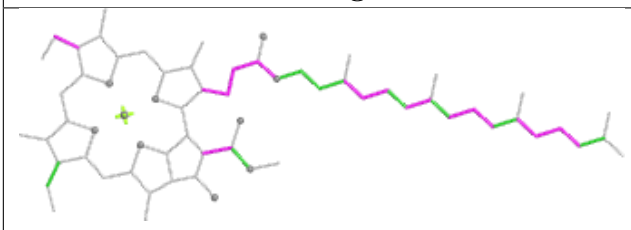
Ligand CLA L 1501



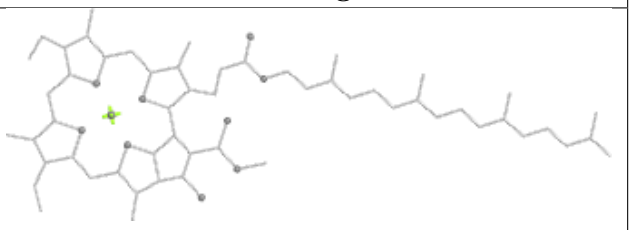
Bond lengths



Bond angles

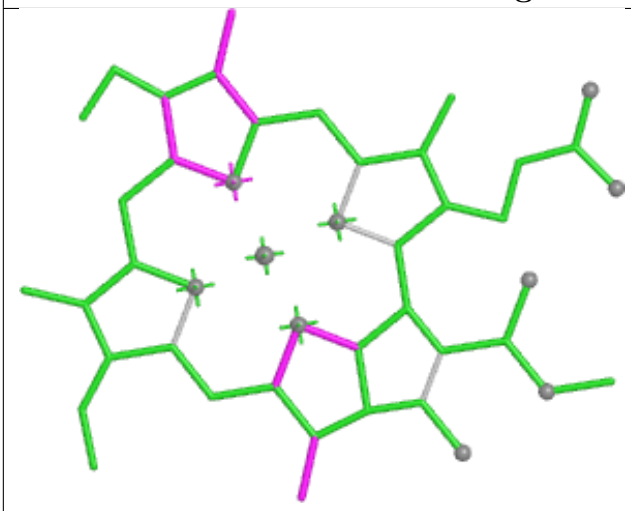


Torsions

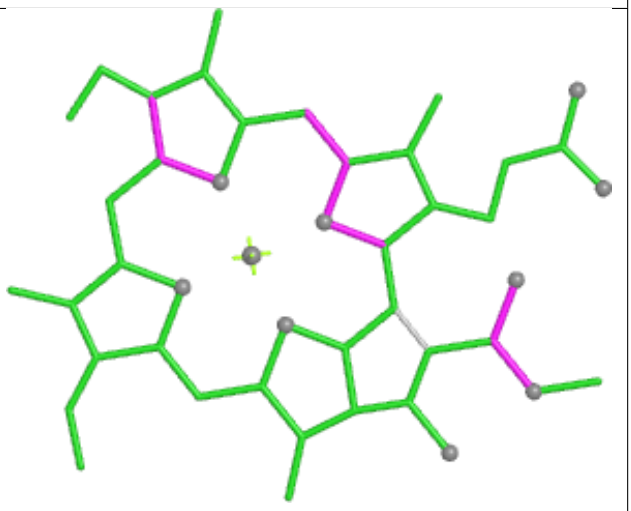


Rings

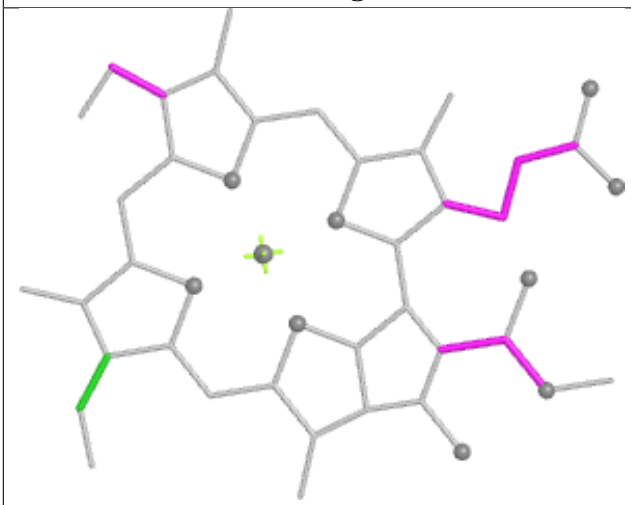
Ligand CLA R 1302



Bond lengths



Bond angles



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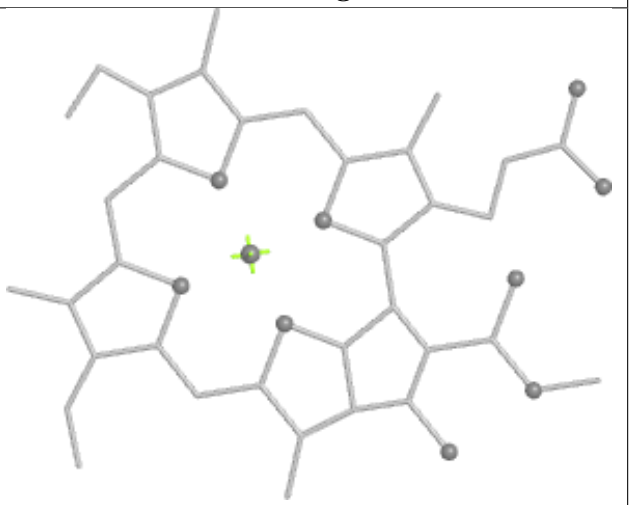
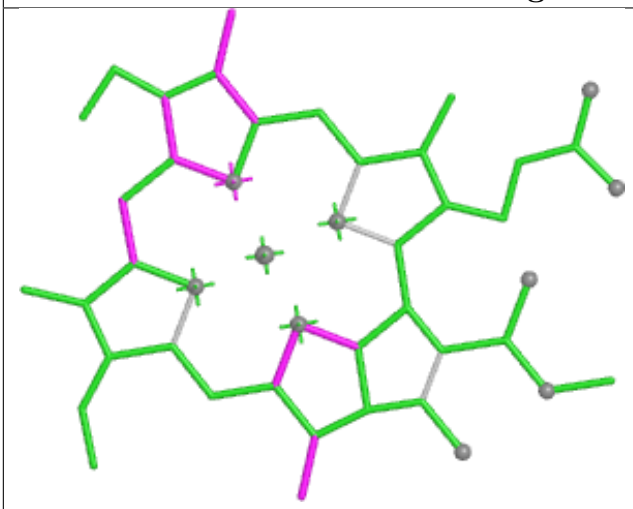


Rings

Ligand CLA d 512



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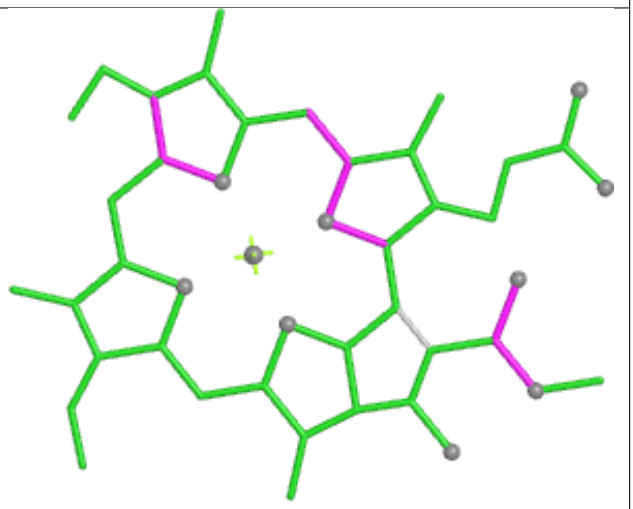
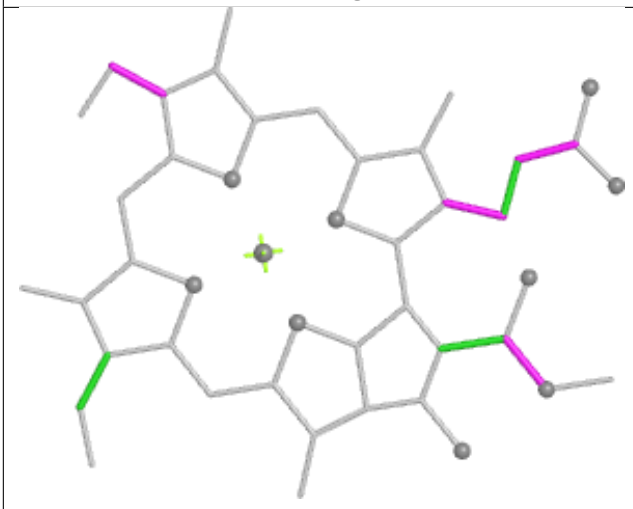


Bond angles



Torsions

Rings

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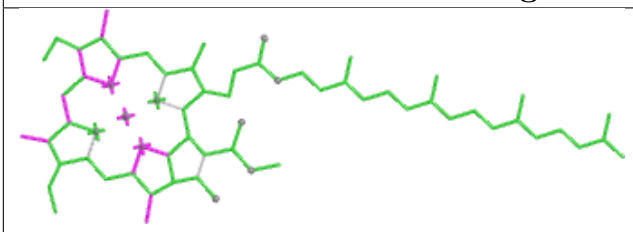

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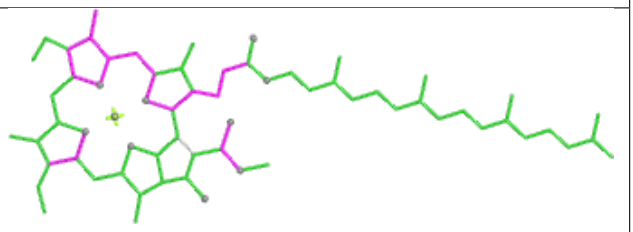

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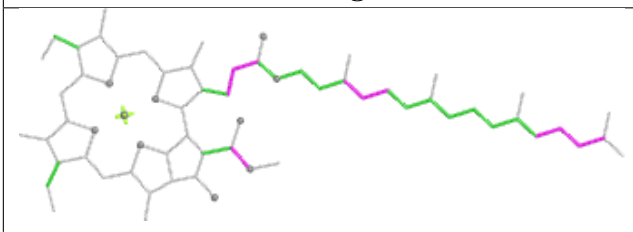

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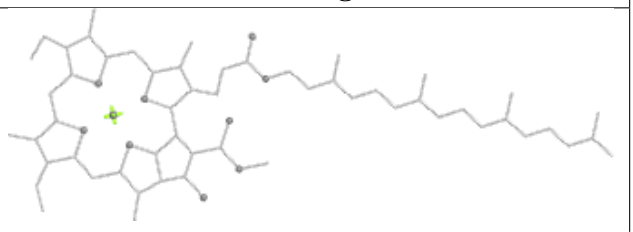
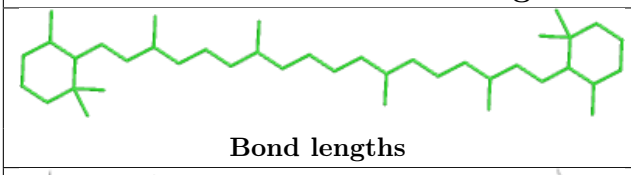


Rings

Ligand BCR V 4020



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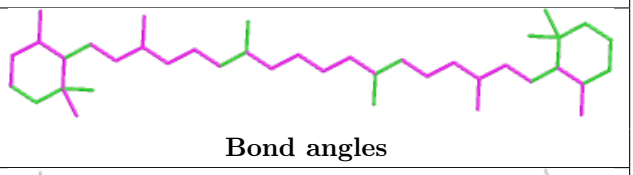

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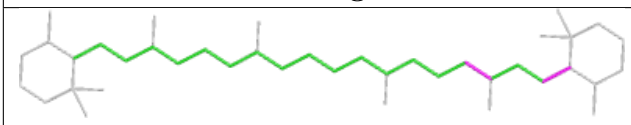

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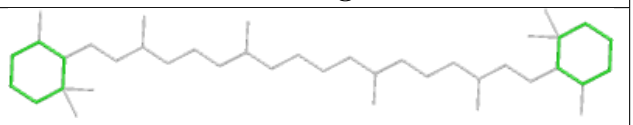
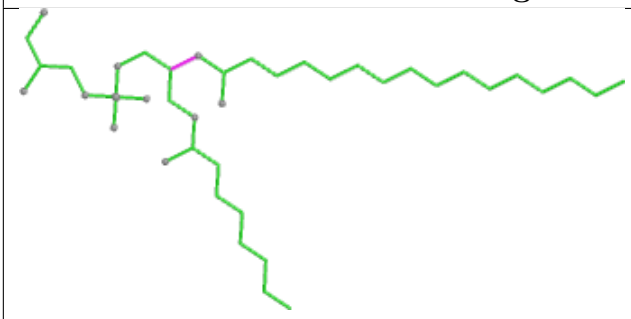


Rings

Ligand LHG A 5003



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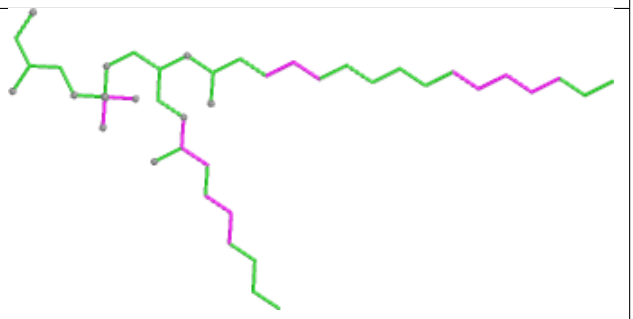

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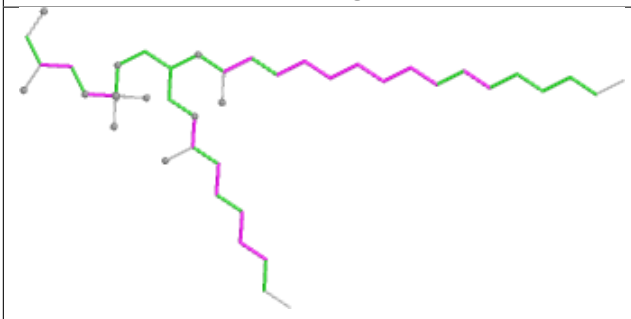

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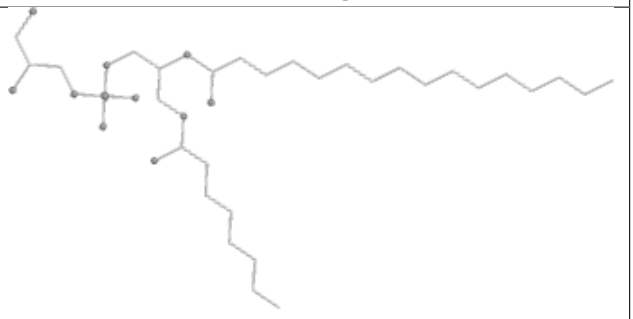

Rings

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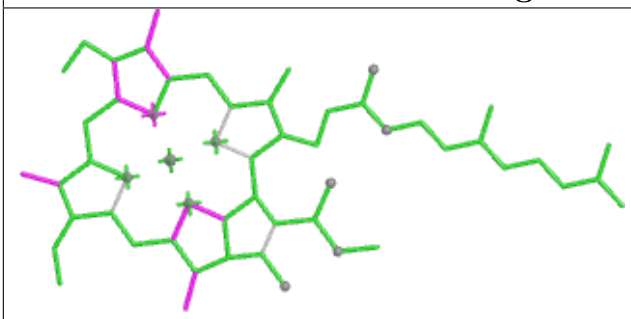
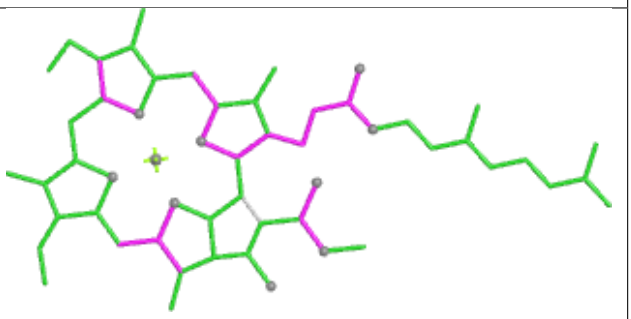
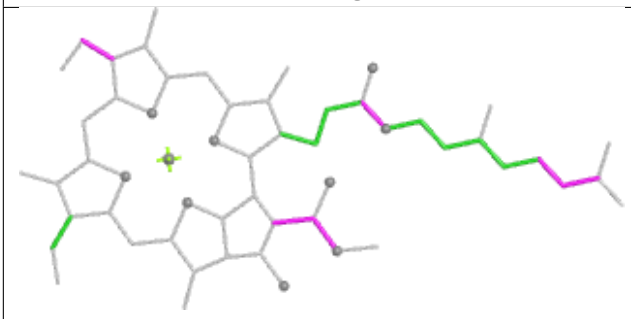
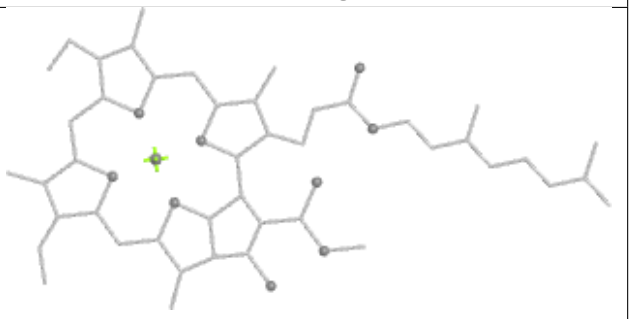
 Bond lengths	 Bond angles
 Torsions	 Rings

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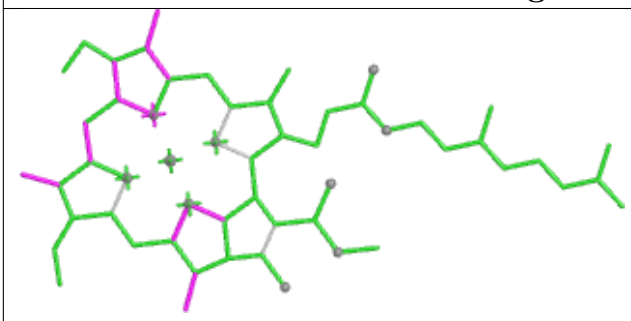
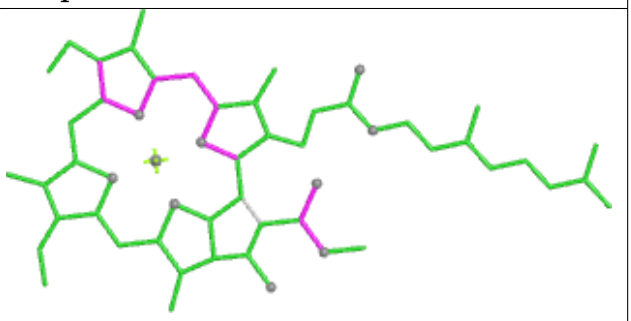
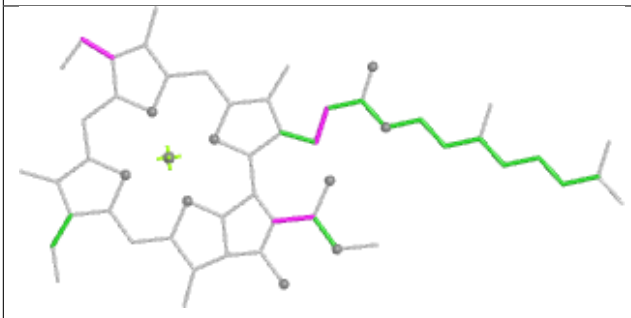
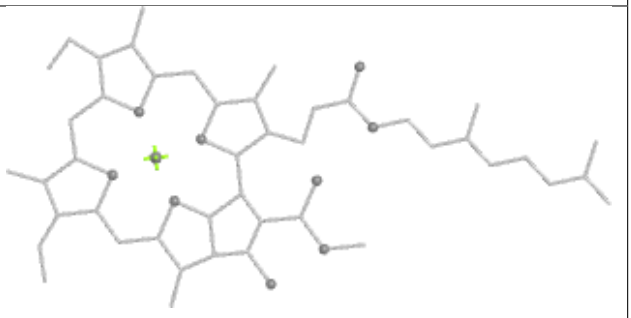
 Bond lengths	 Bond angles
 Torsions	 Rings

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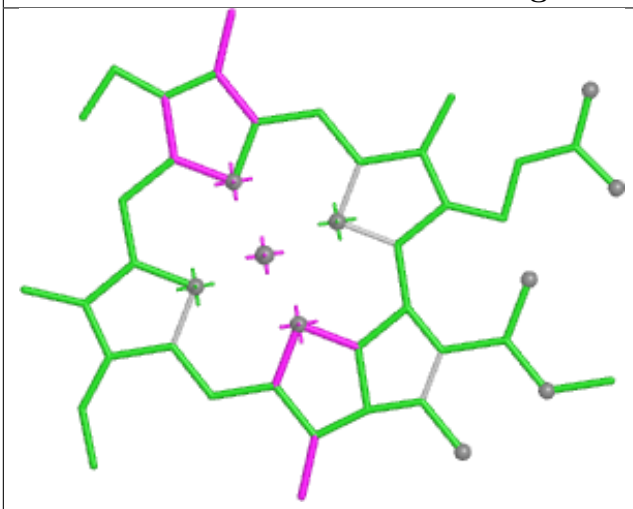

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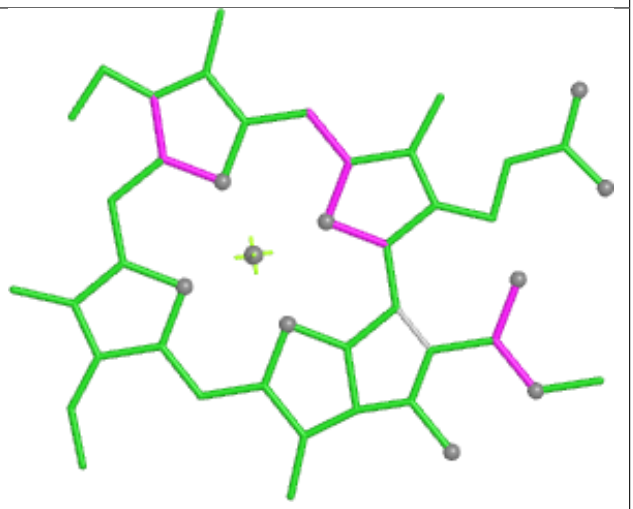
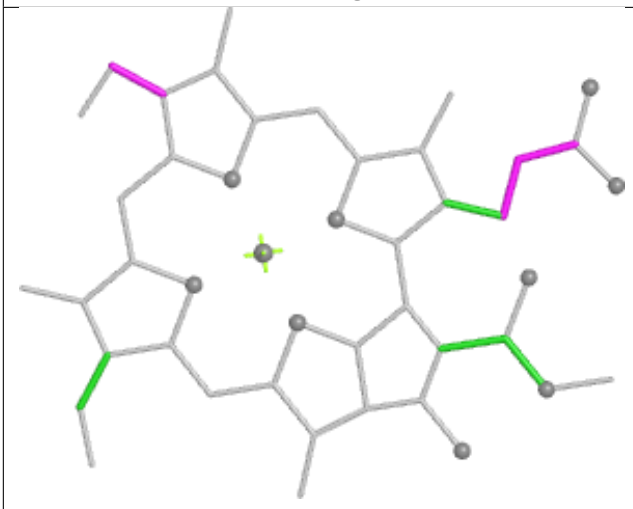
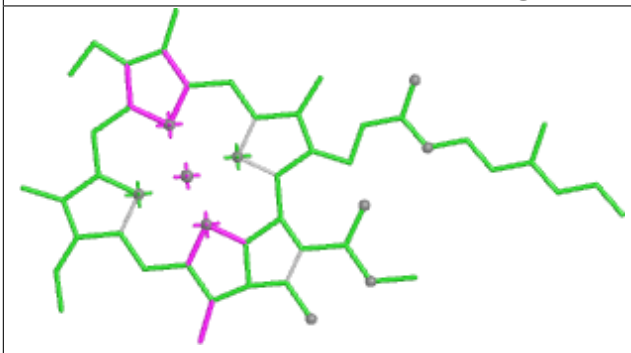
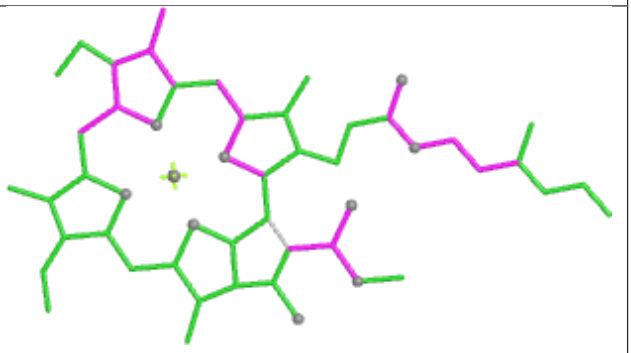
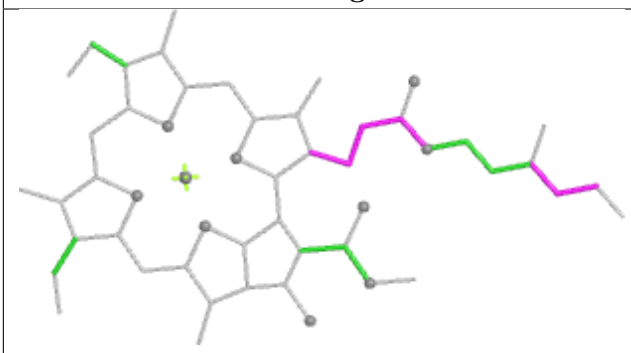
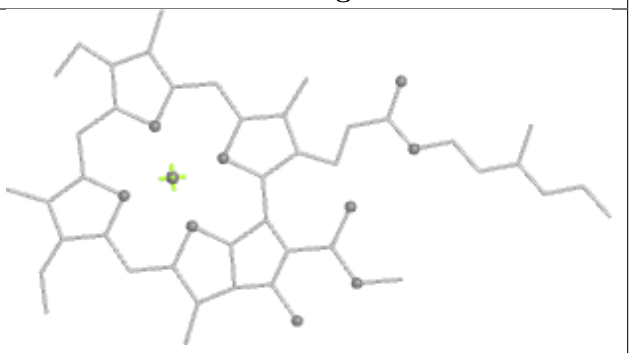


Bond angles



Torsions

Rings

Ligand CLA A 1135	
	
Bond lengths	Bond angles
	
Torsions	Rings

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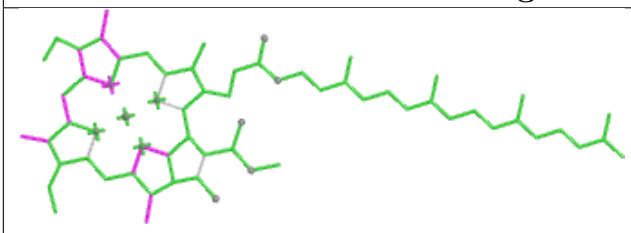	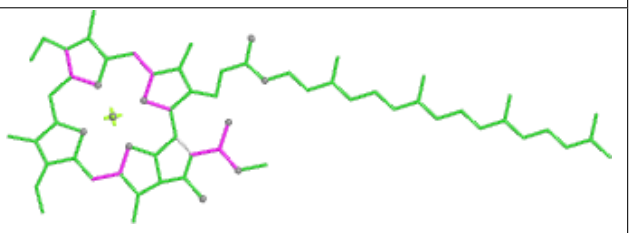
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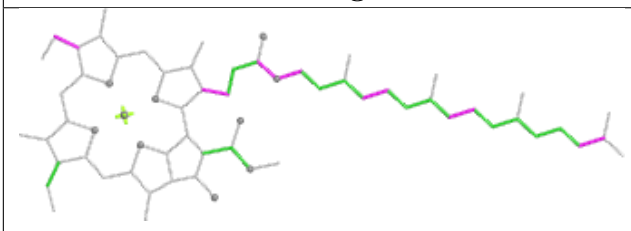
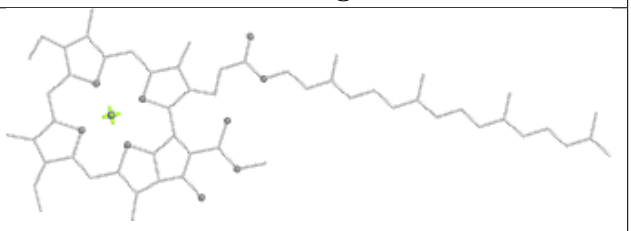
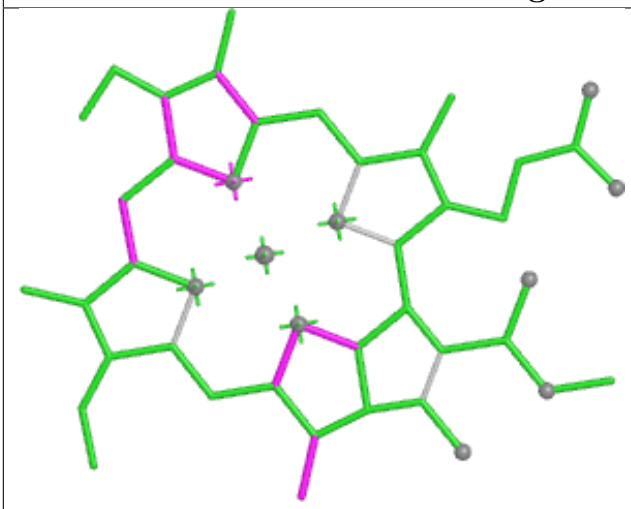
	
Torsions	Rings

Ligand CLA 6 509



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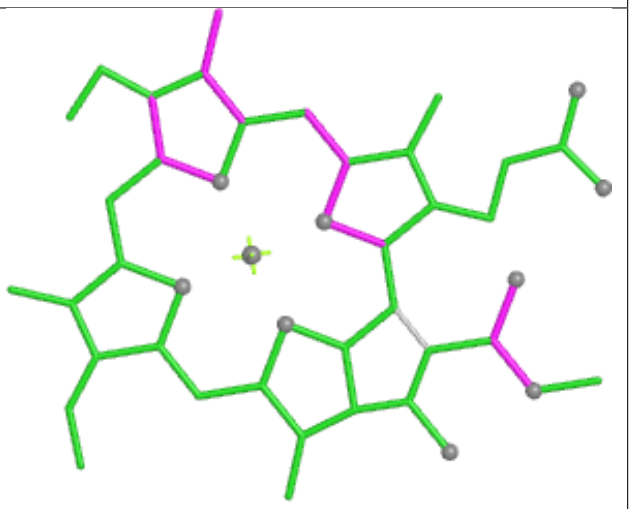

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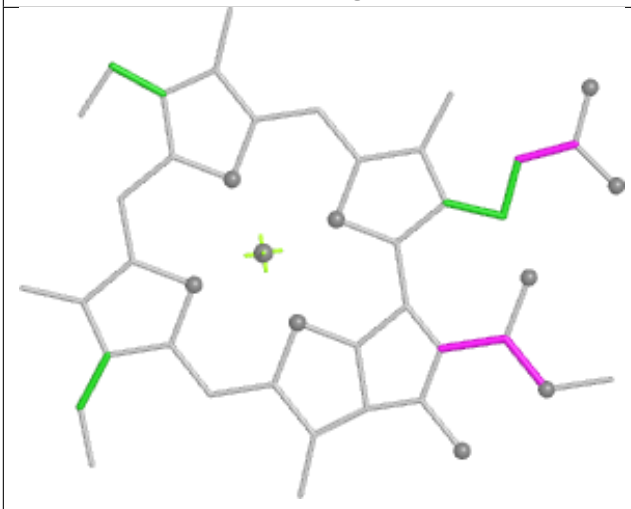
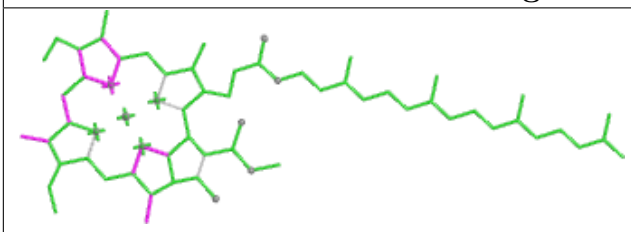


Torsions

Rings

Ligand CLA f 1213



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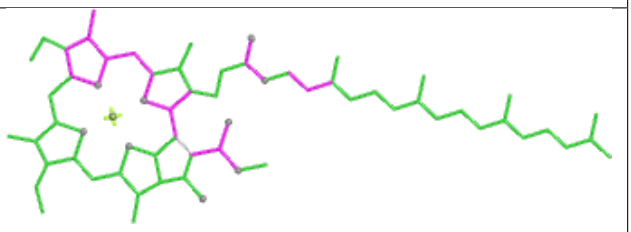
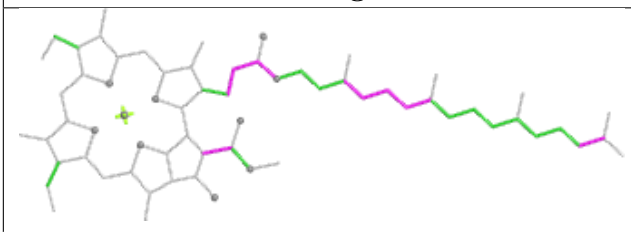
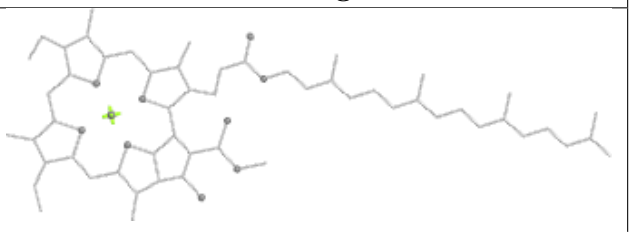


Bond angles

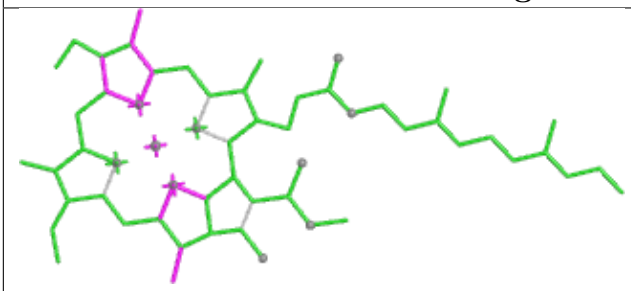


Torsions



Rings

Ligand CLA H 1217



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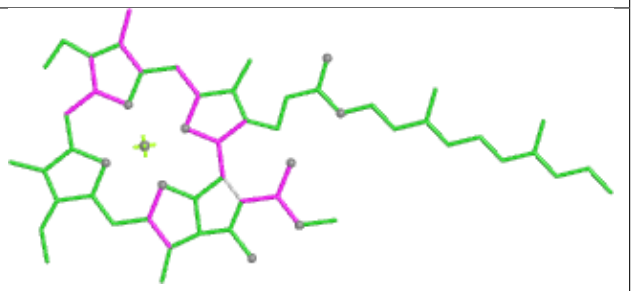
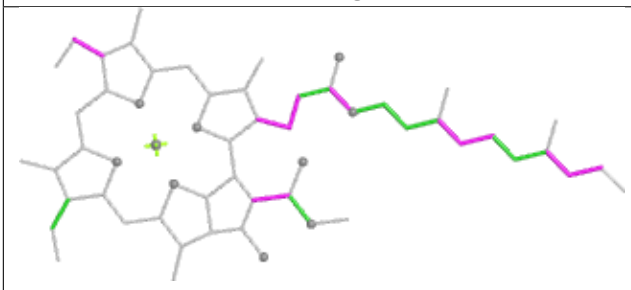
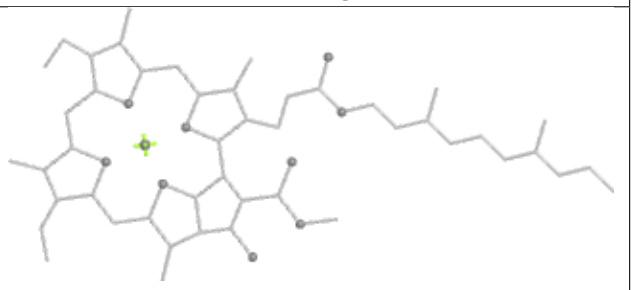


Bond angles

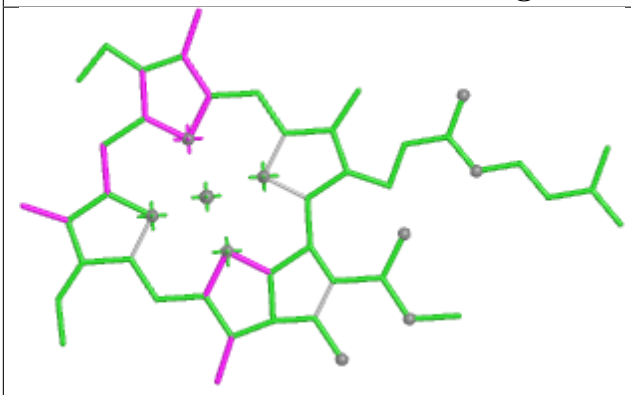


Torsions

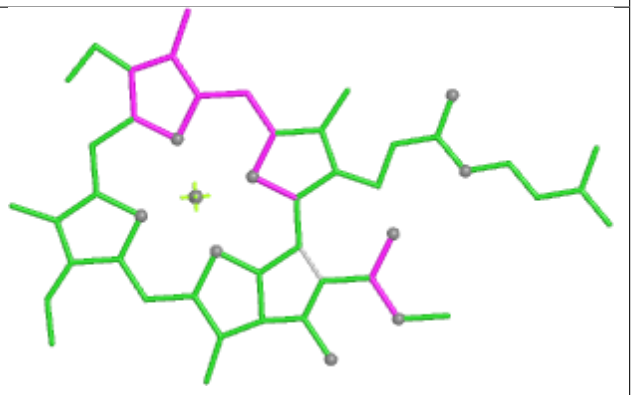


Rings

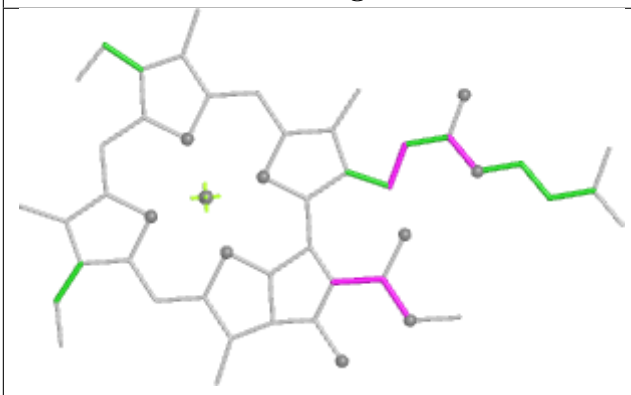
Ligand CLA B 1232



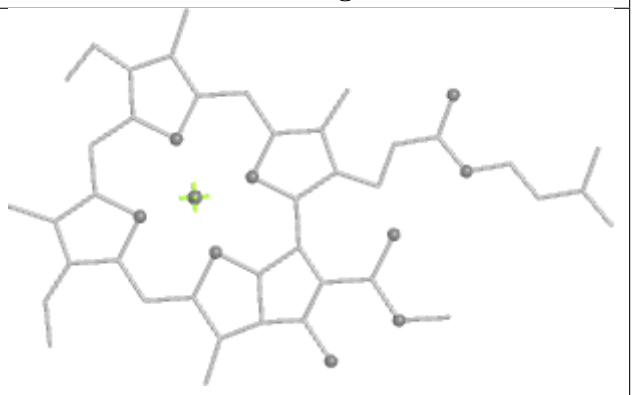
Bond lengths



Bond angles

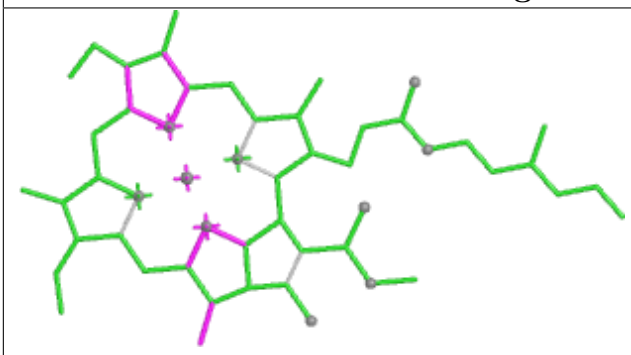


Torsions



Rings

Ligand CLA G 1135



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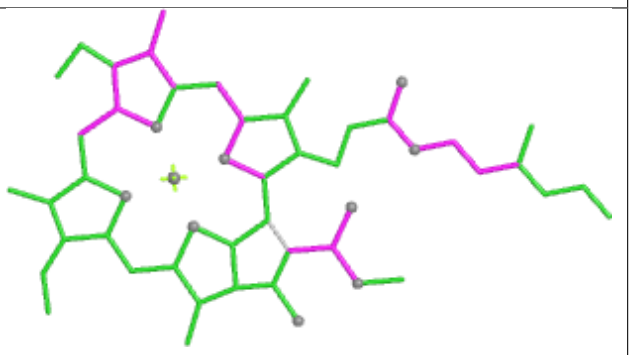

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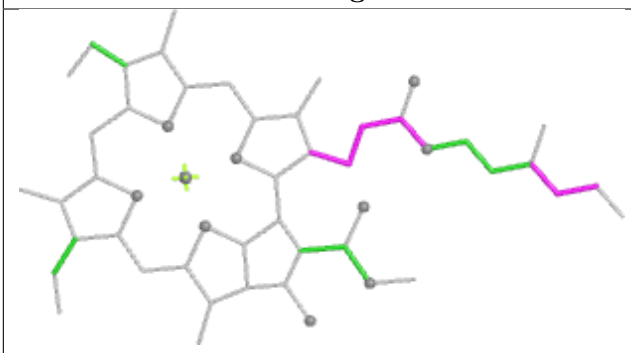

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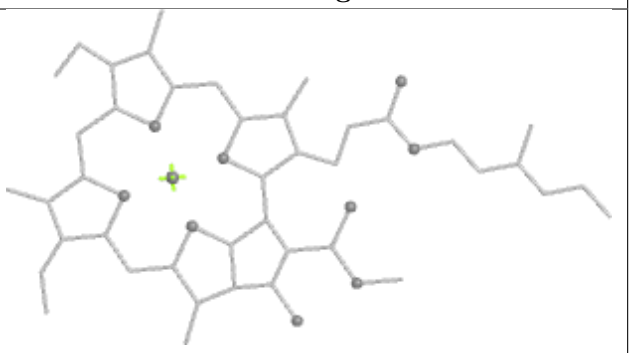
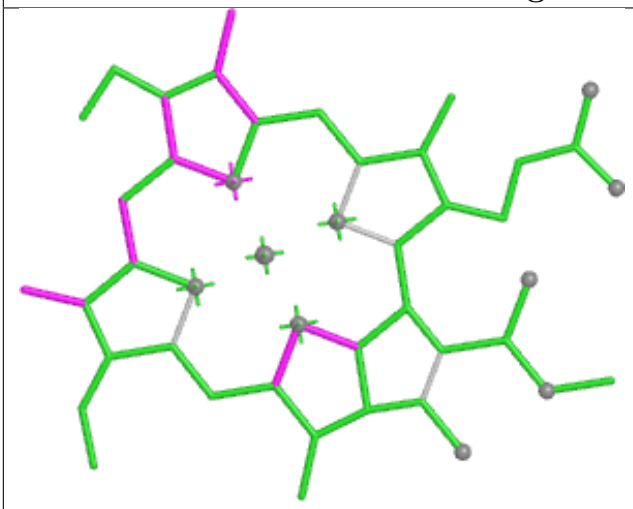


Rings

Ligand CLA u 506



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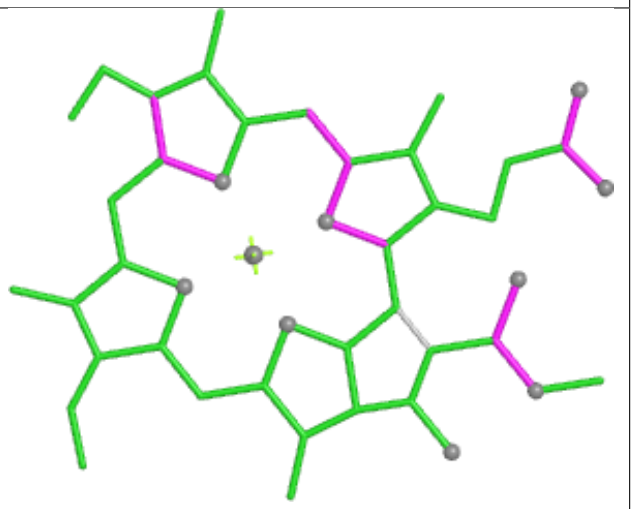

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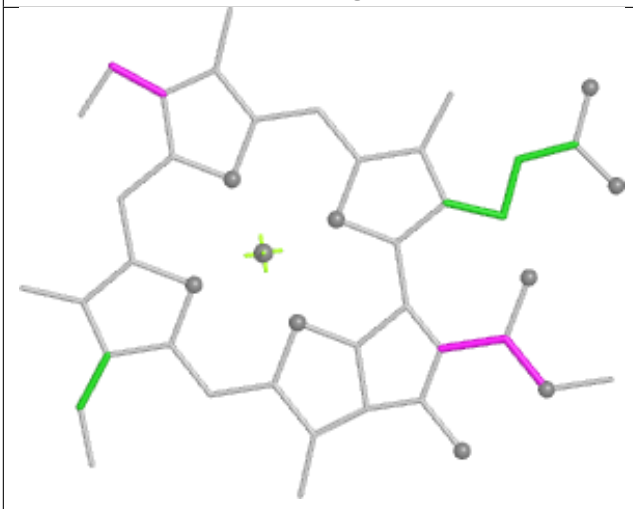
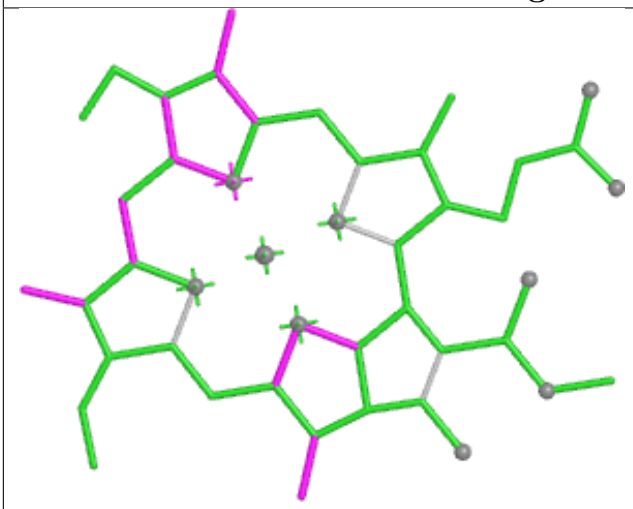


Torsions

Rings

Ligand CLA 2 517



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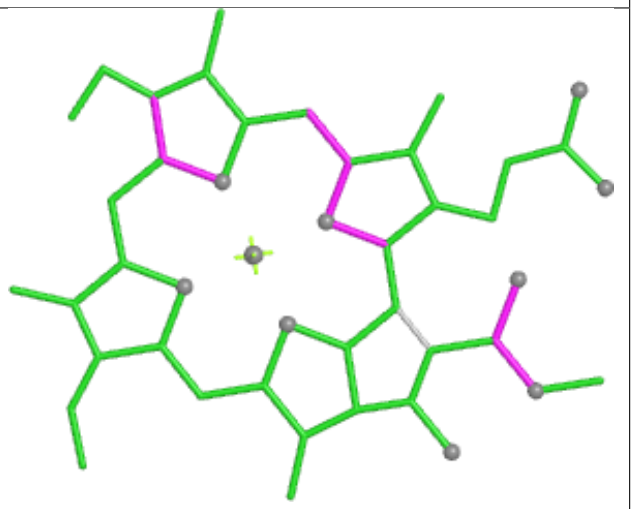

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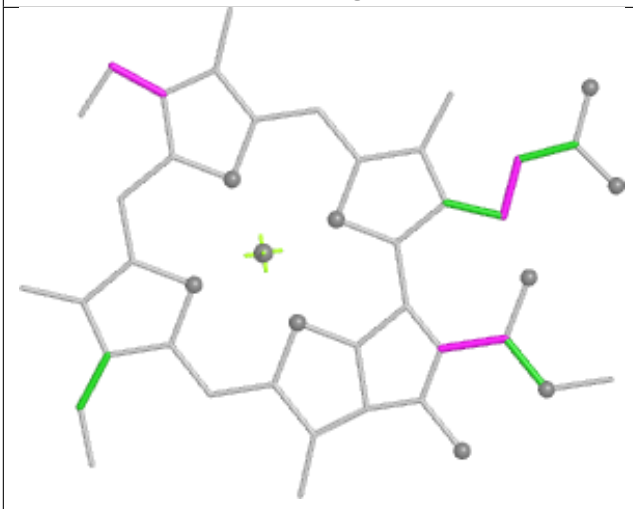
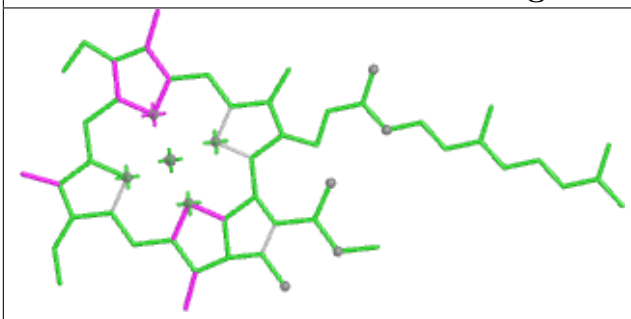


Torsions

Rings

Ligand CLA q 508



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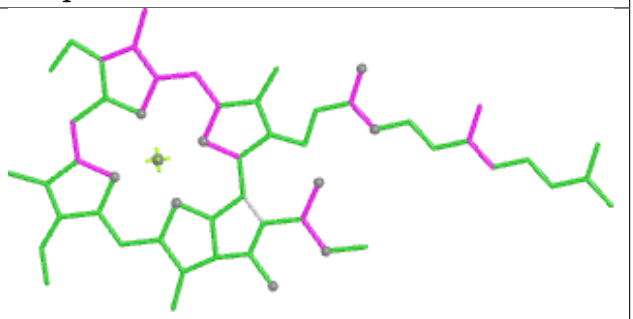
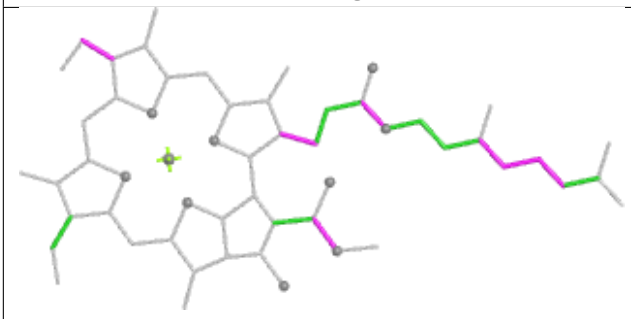


Bond angles



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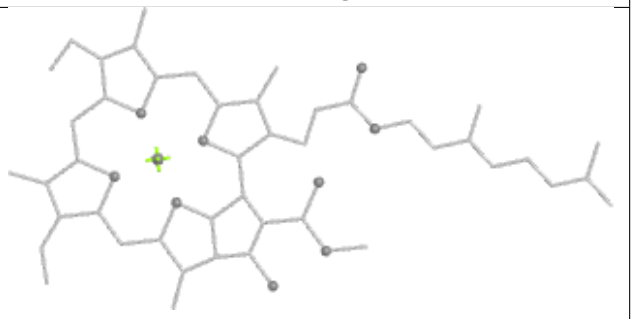
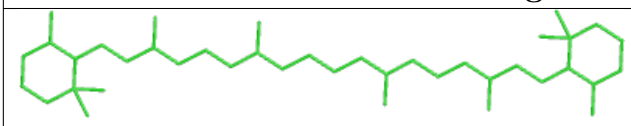


Rings

Ligand BCR u 521



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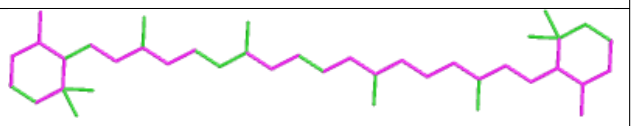

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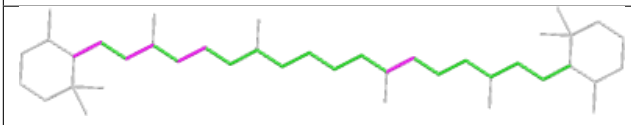

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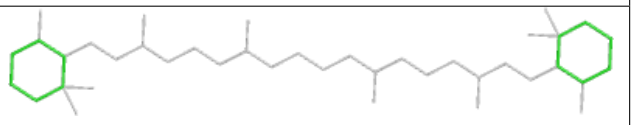
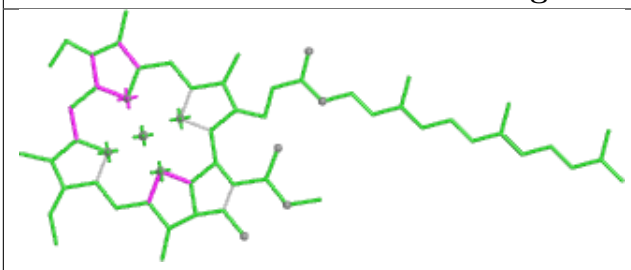


Rings

Ligand CLA t 501



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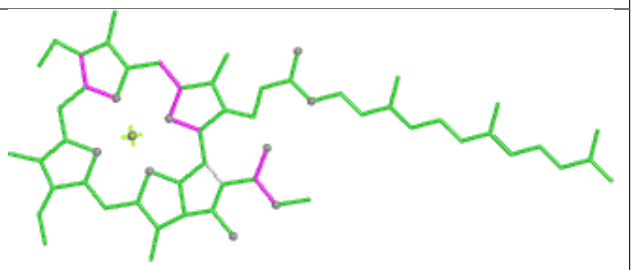

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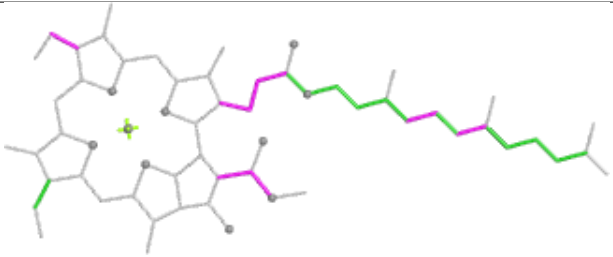

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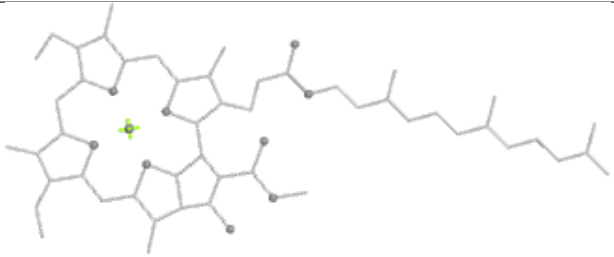
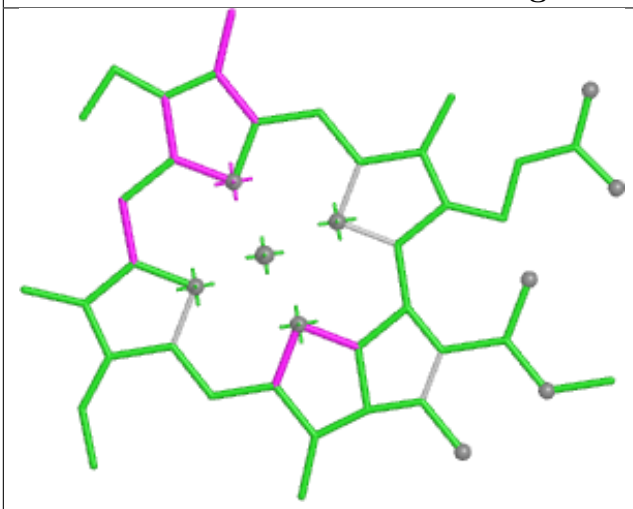


Rings

Ligand CLA c 504



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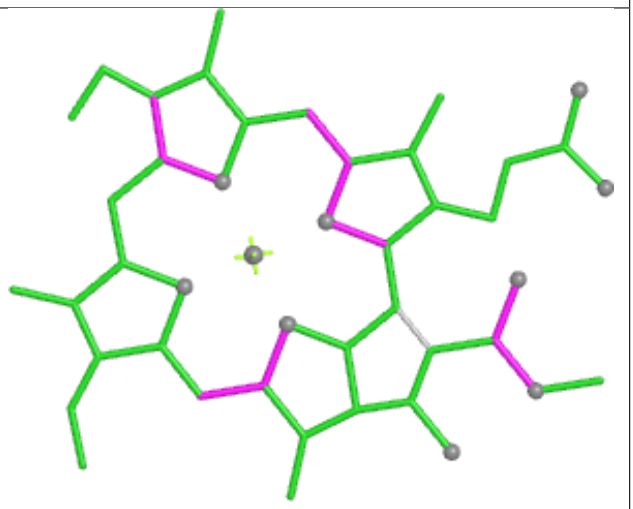

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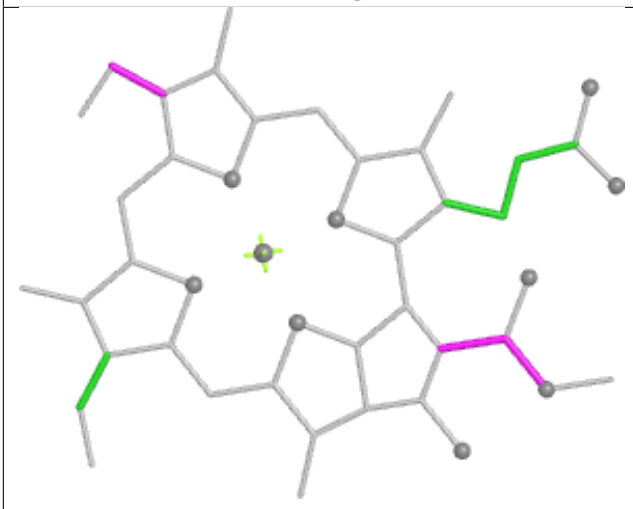

Torsions

Rings

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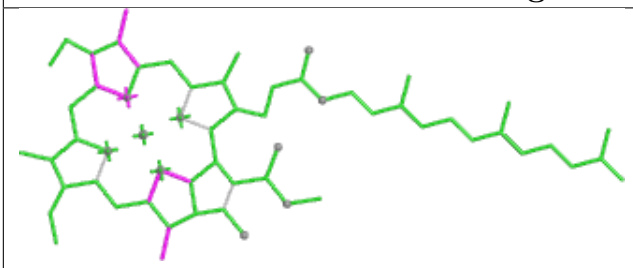

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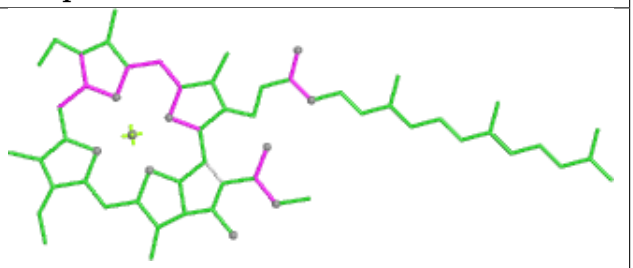

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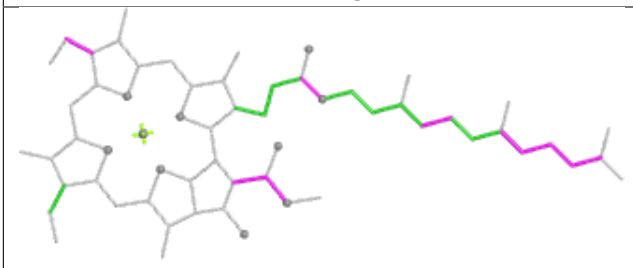

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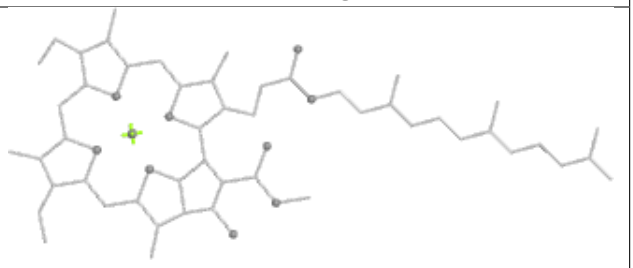
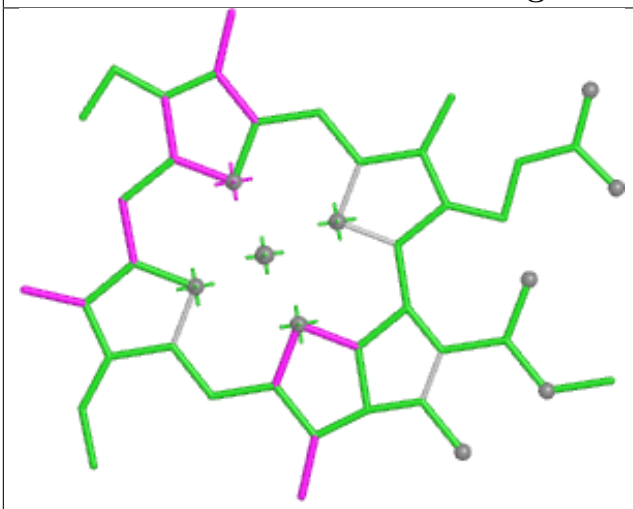


Rings

Ligand CLA u 517



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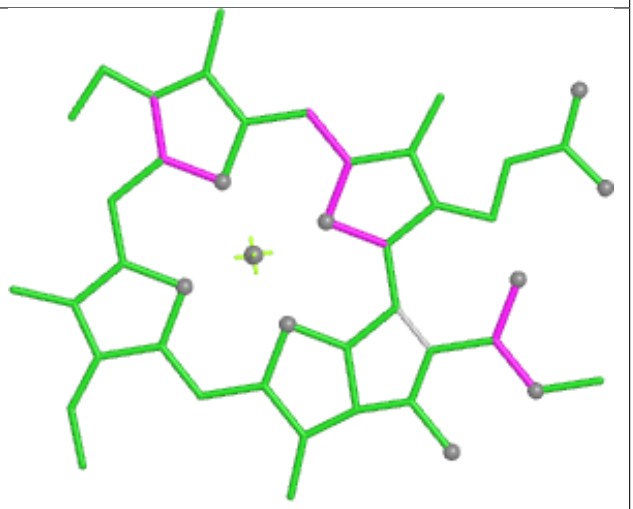

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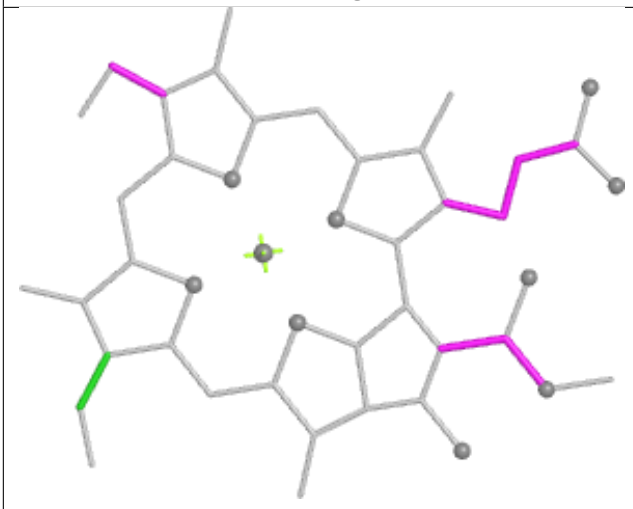
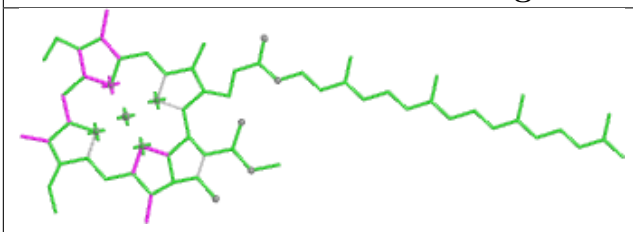


Torsions

Rings

Ligand CLA H 1227



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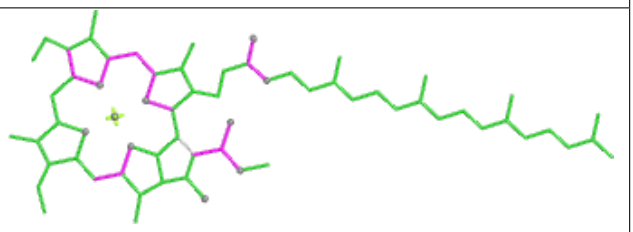

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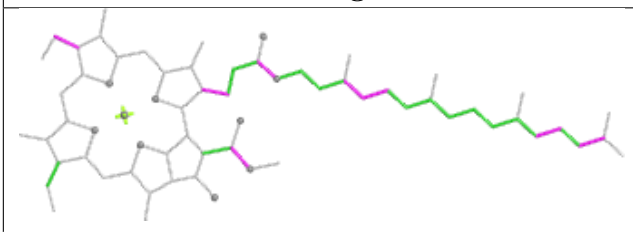

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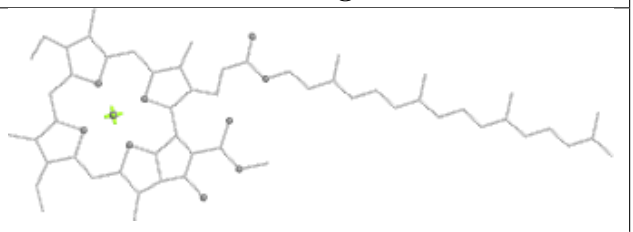
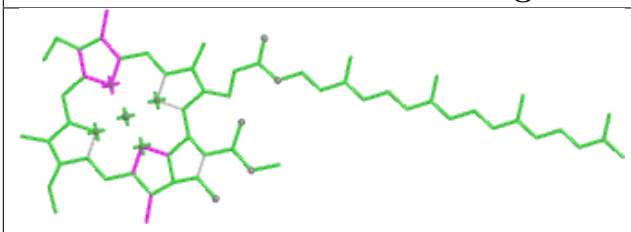


Rings

Ligand CLA H 1239



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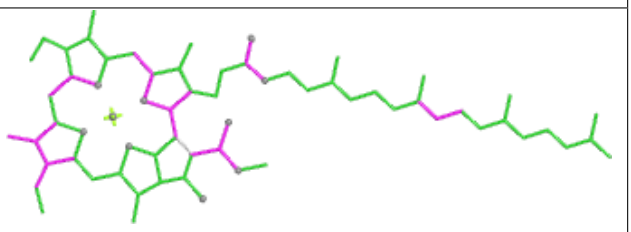
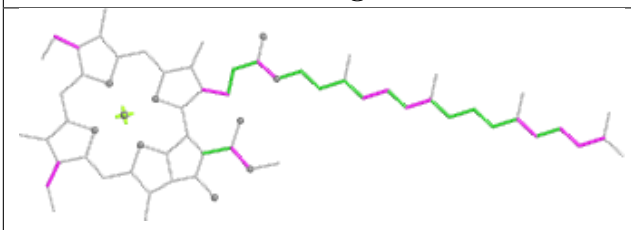


Bond angles



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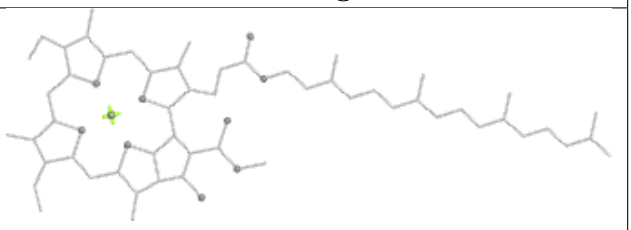
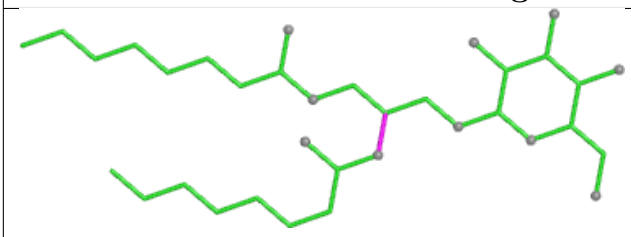


Rings

Ligand LMG T 5104



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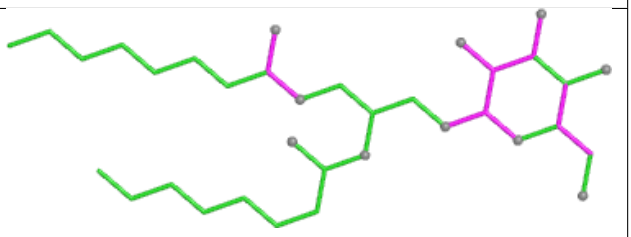
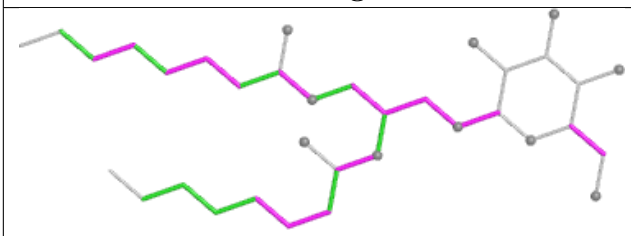


Bond angles



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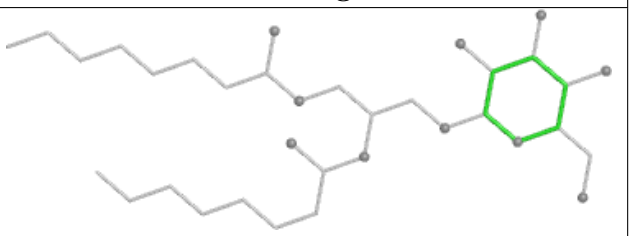
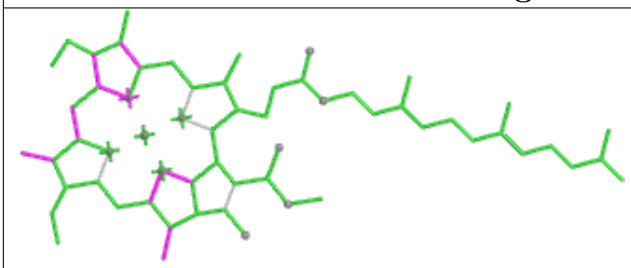
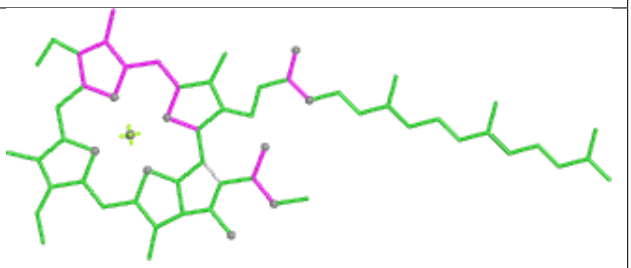
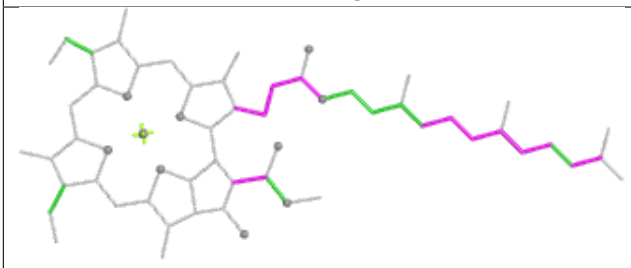
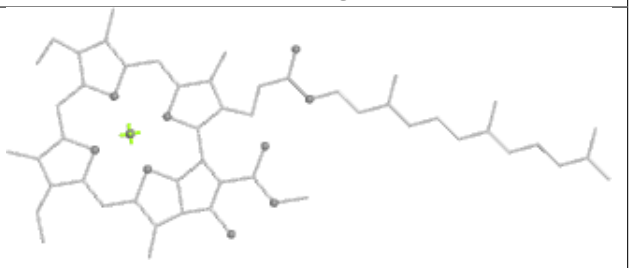


Rings

Ligand CLA A 1116	
	
Bond lengths	Bond angles
	
Torsions	Rings

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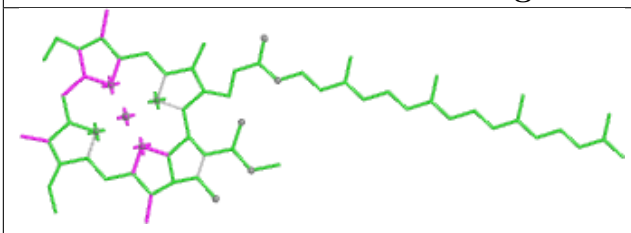
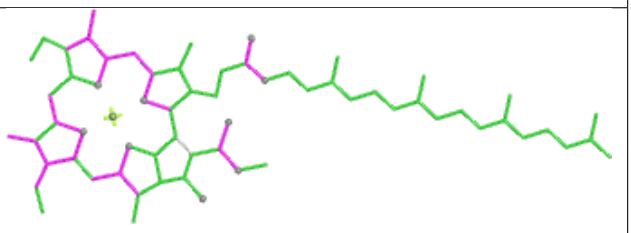
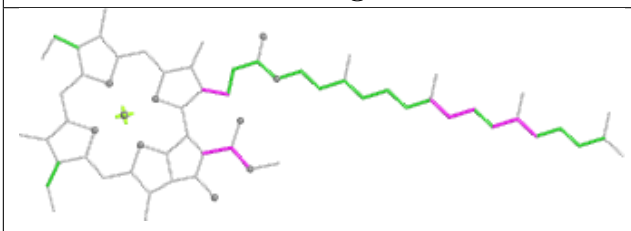
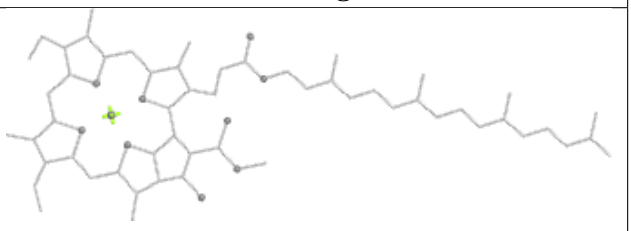
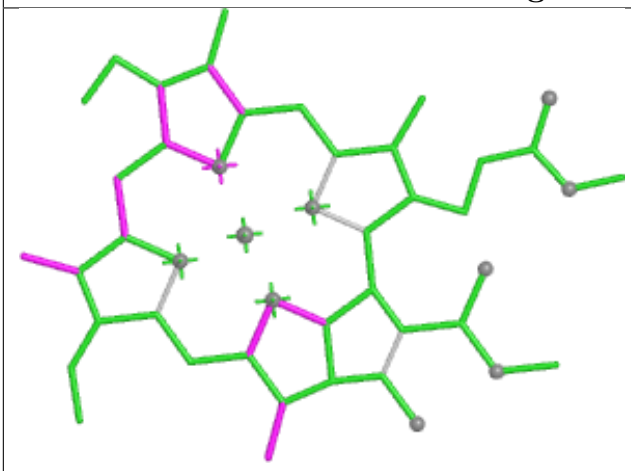
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 519



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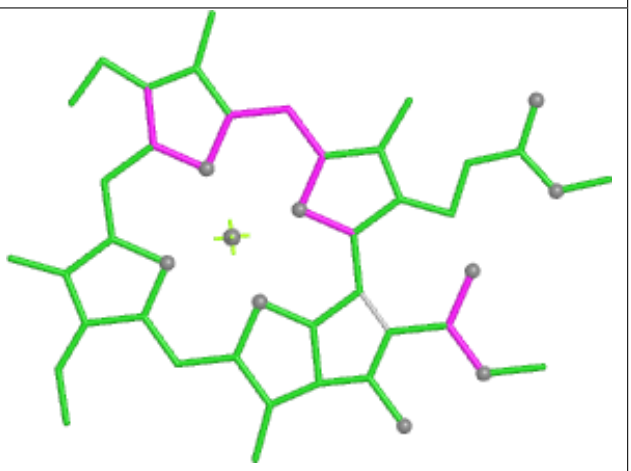

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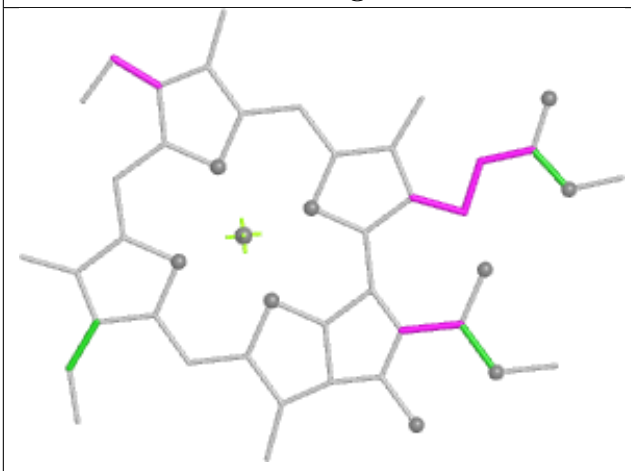

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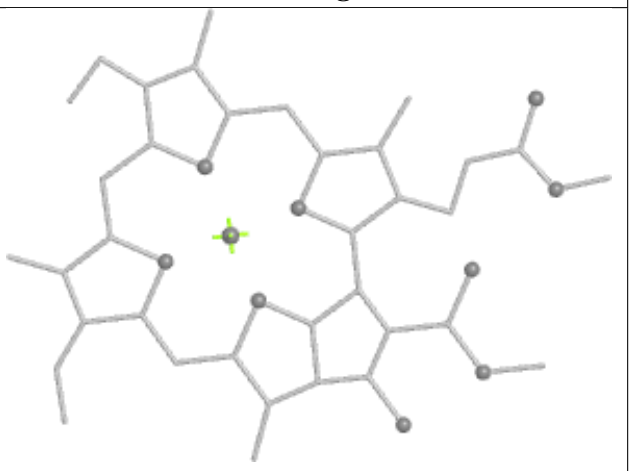
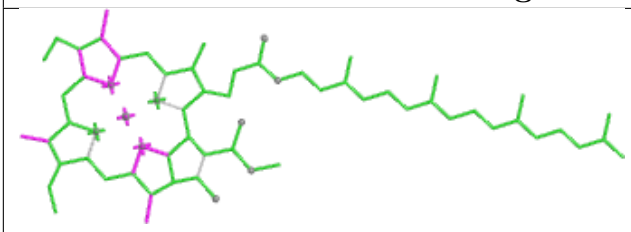


Rings

Ligand CLA A 1106



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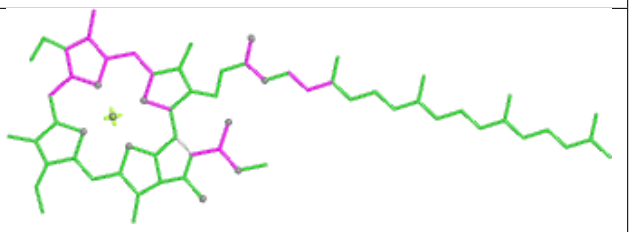

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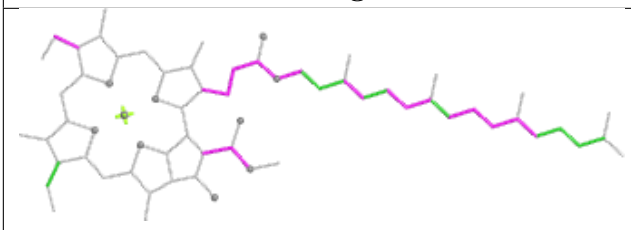

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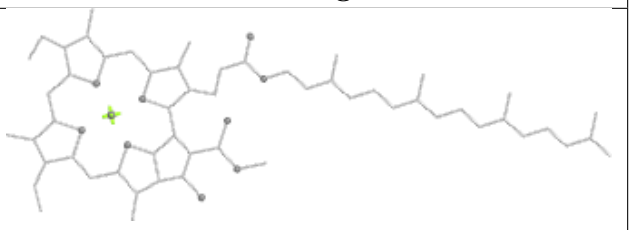
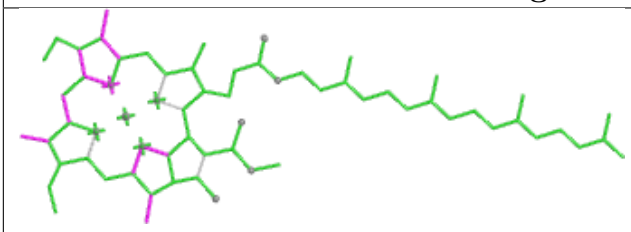
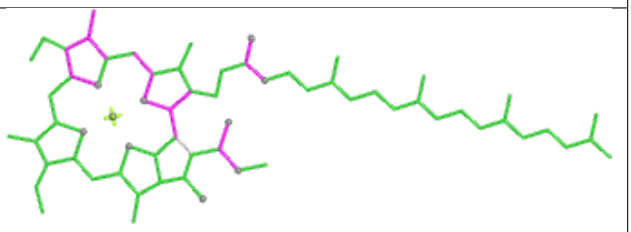
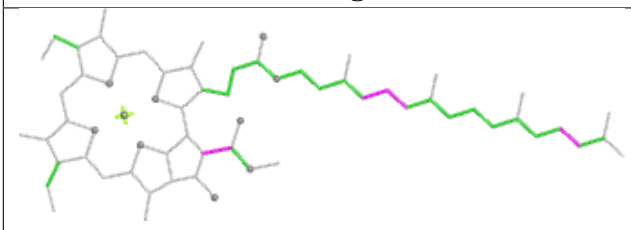
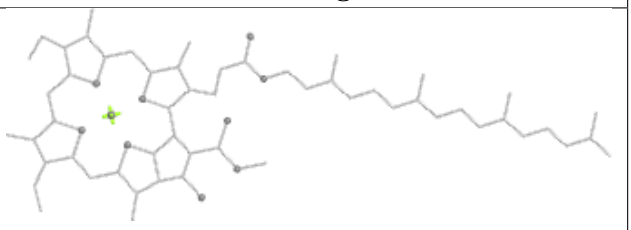


Rings

Ligand CLA s 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

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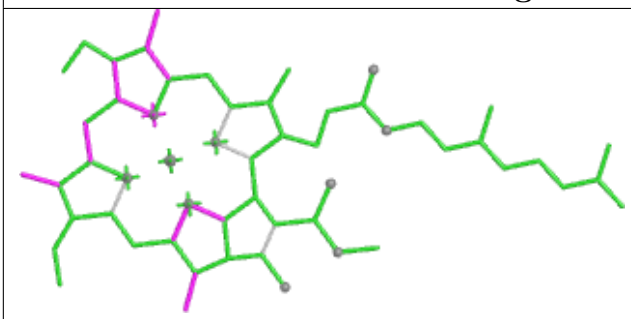
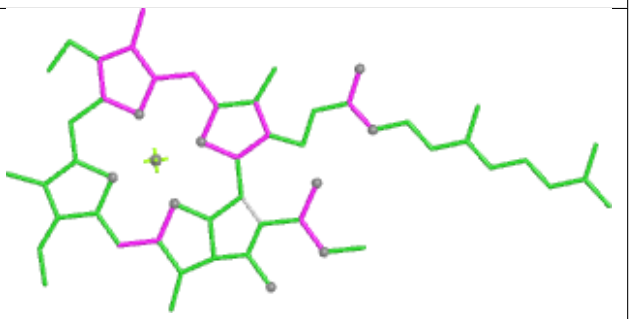
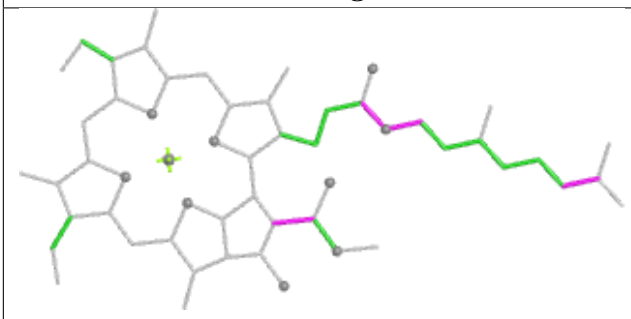
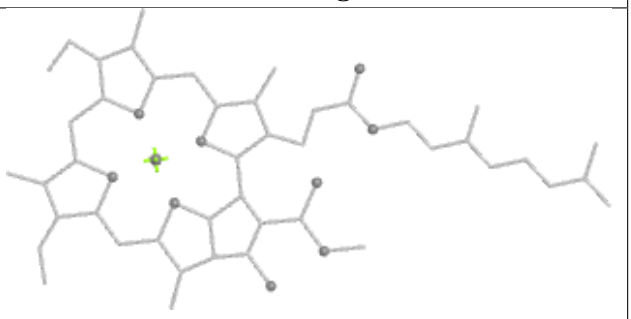
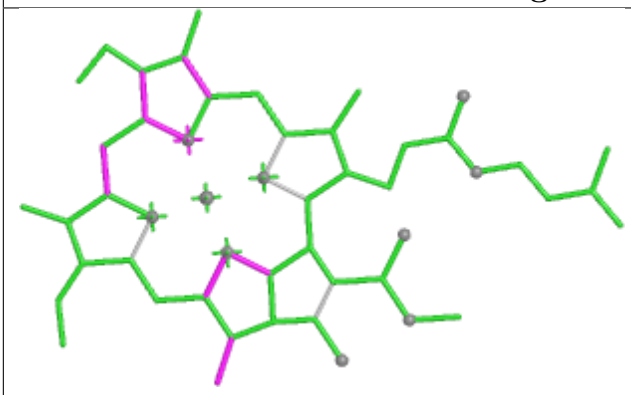
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA t 510



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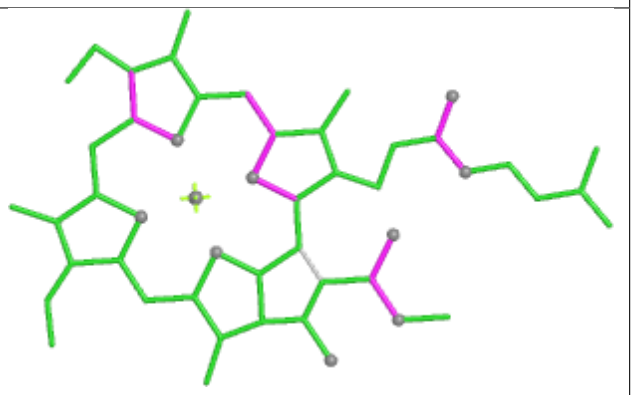

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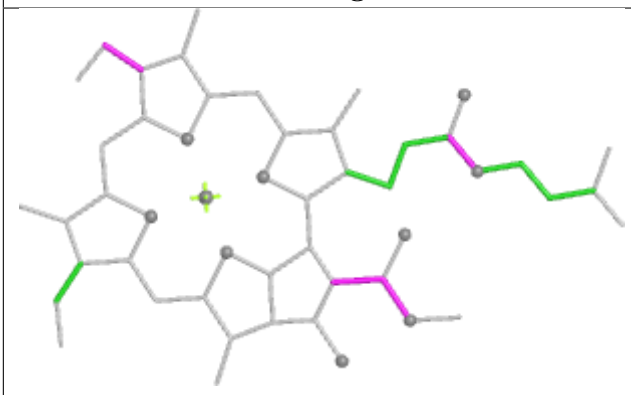

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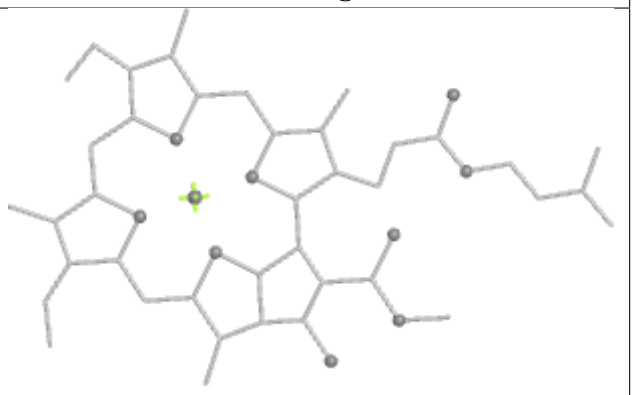
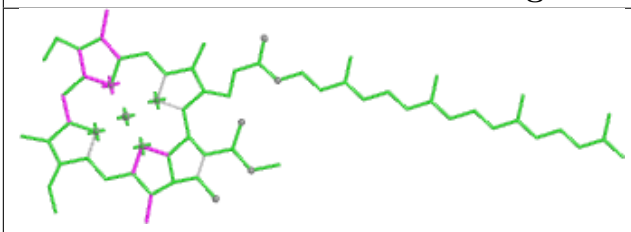


Rings

Ligand CLA Z 518



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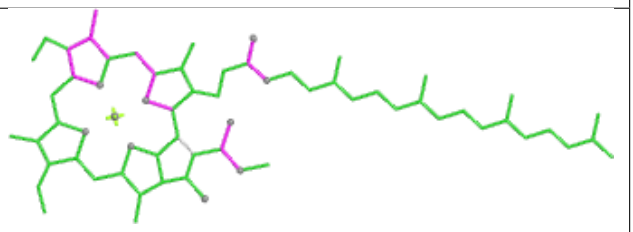

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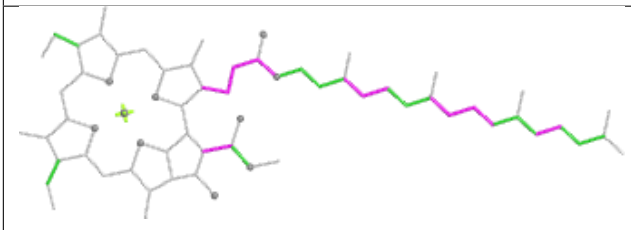

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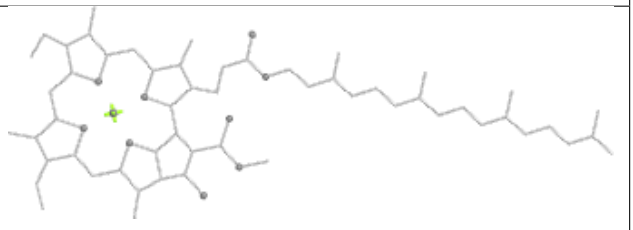

Rings

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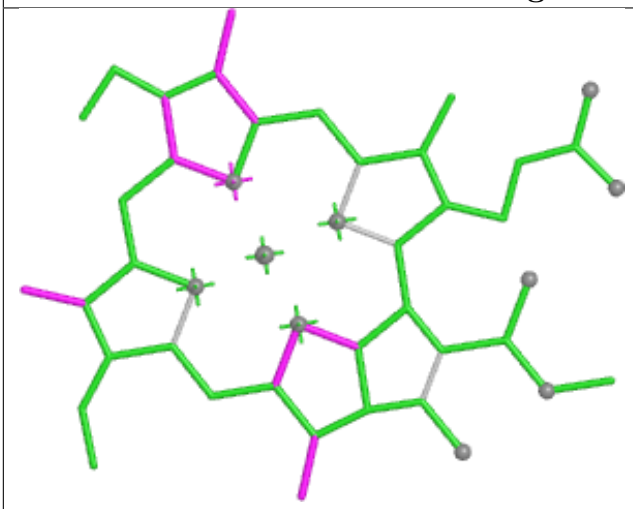

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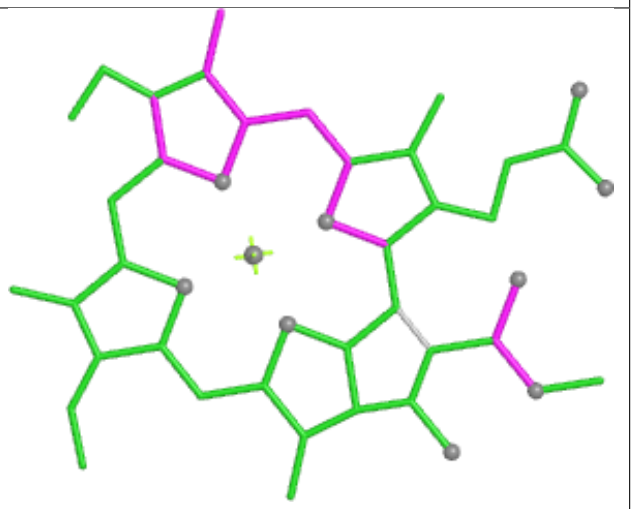

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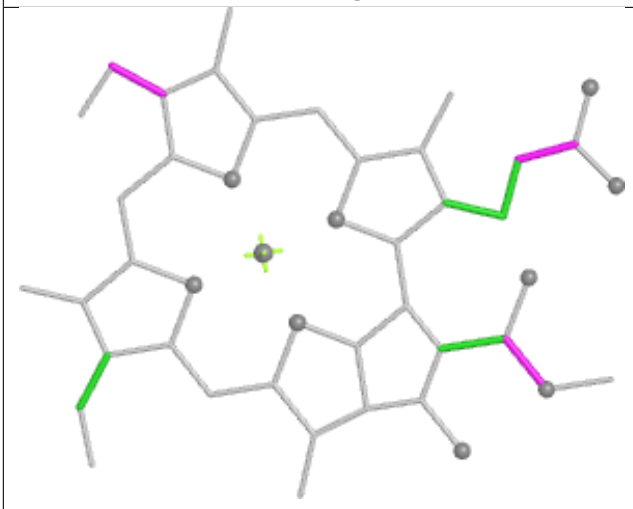
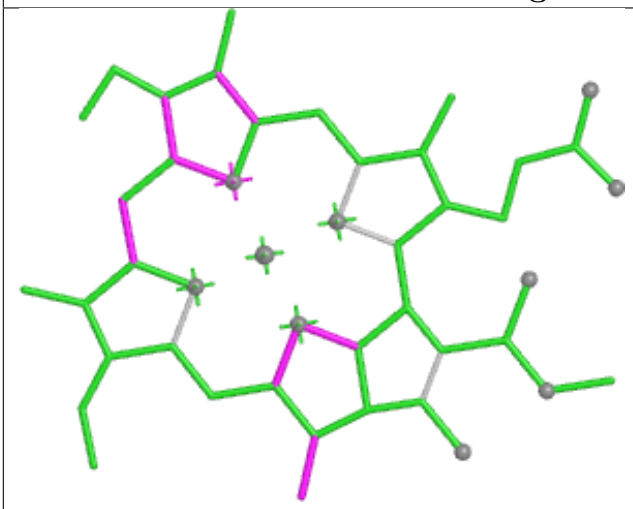


Torsions

Rings

Ligand CLA c 517



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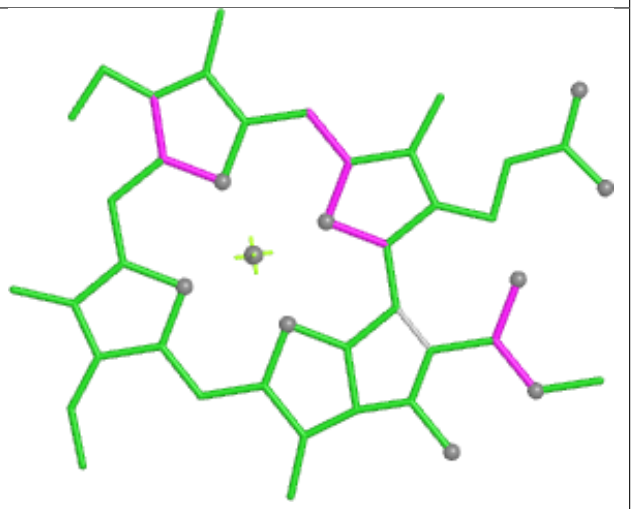

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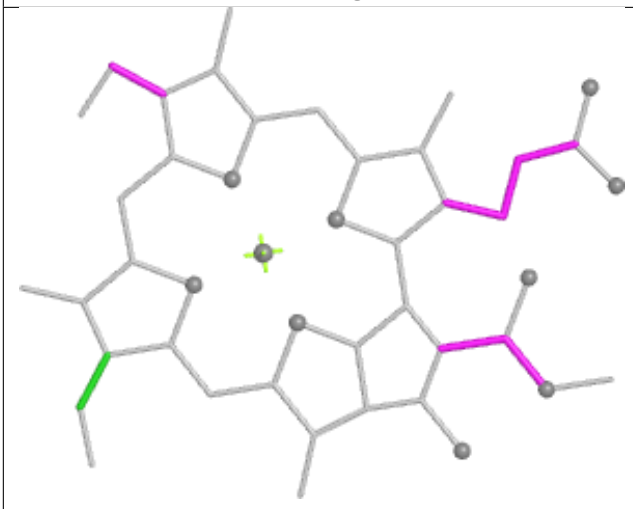
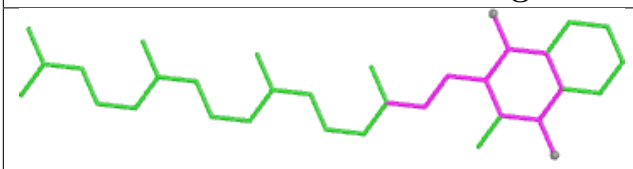


Torsions

Rings

Ligand PQN H 2002



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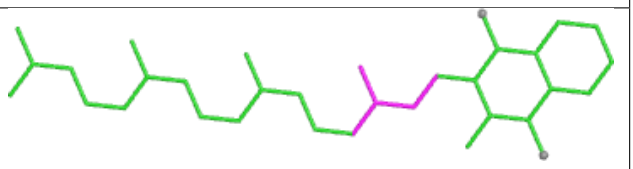

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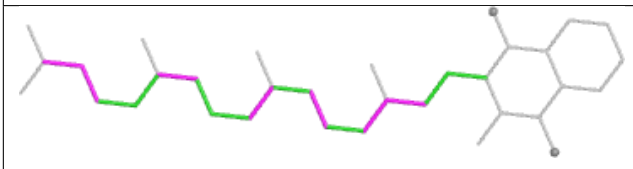

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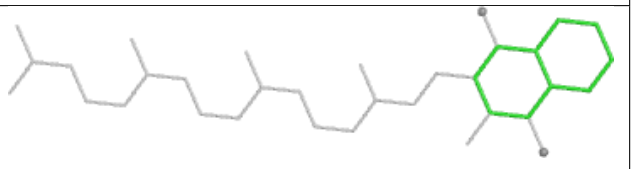
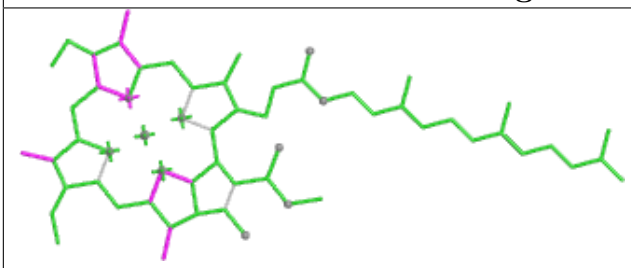
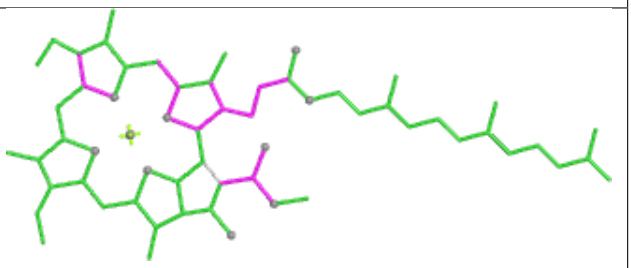
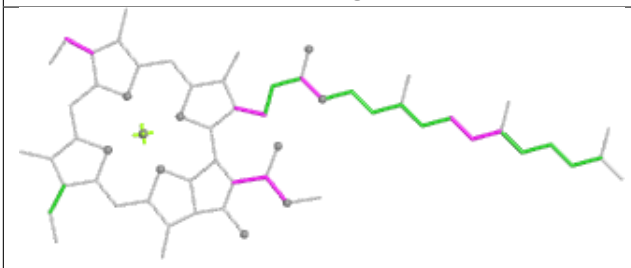
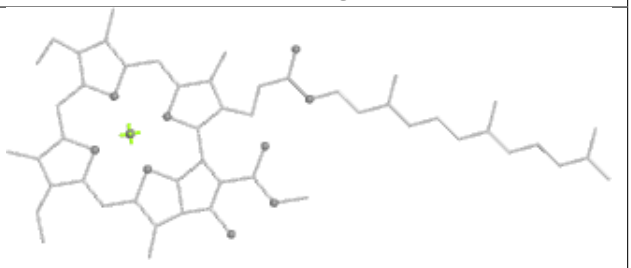
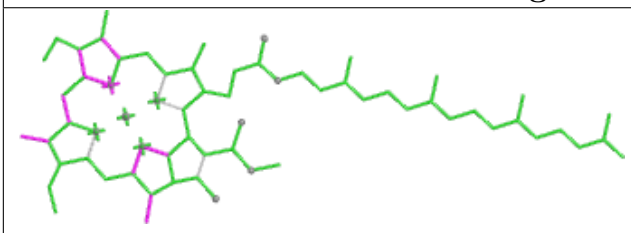
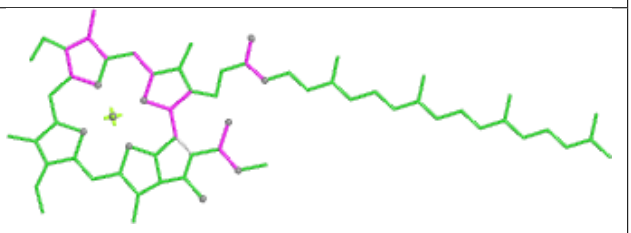


Rings

Ligand CLA B 1230	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 509	
	
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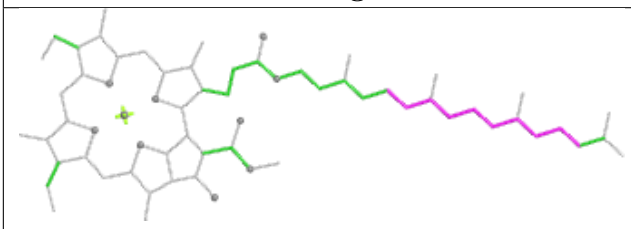
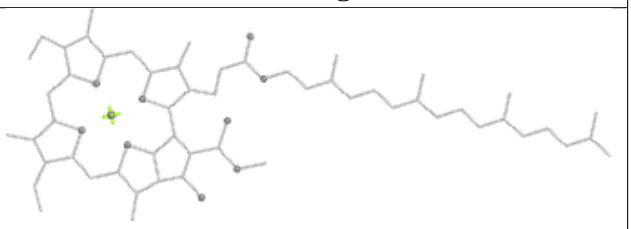
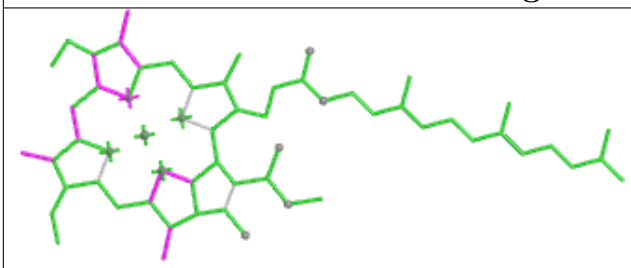
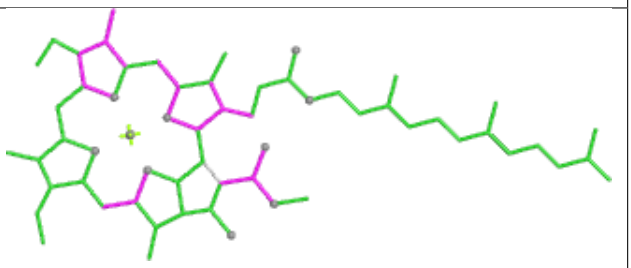
	
Torsions	Rings

Ligand CLA f 1222	
	
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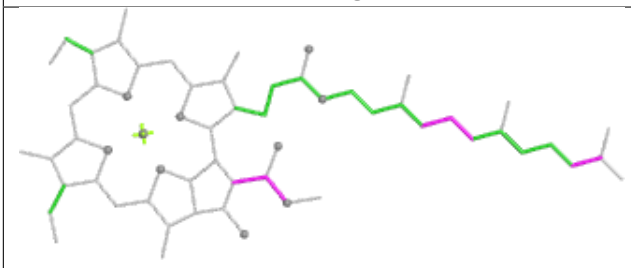	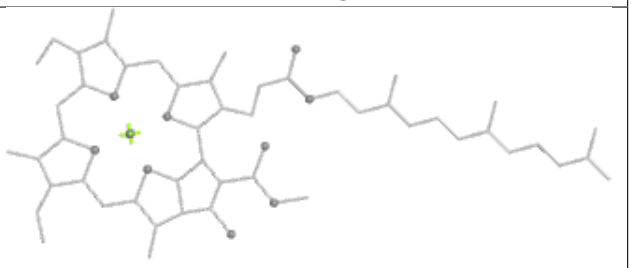
Torsions	Rings

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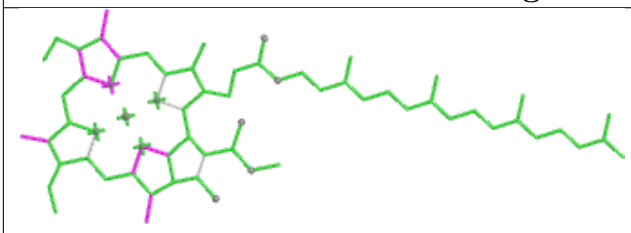
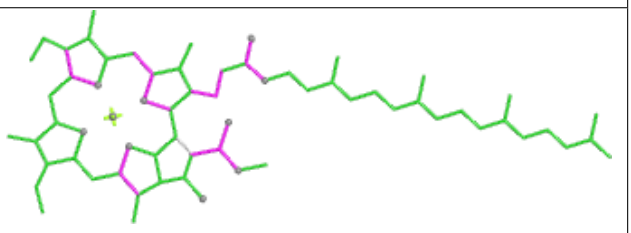
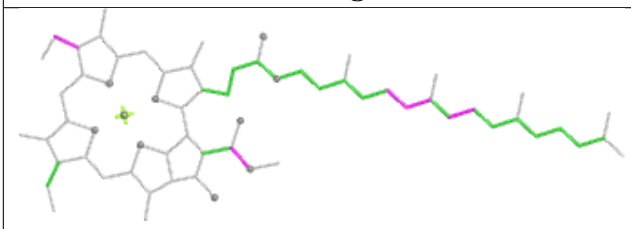
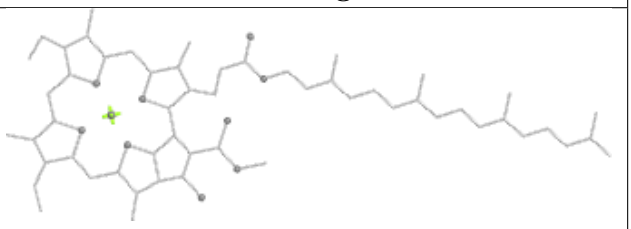
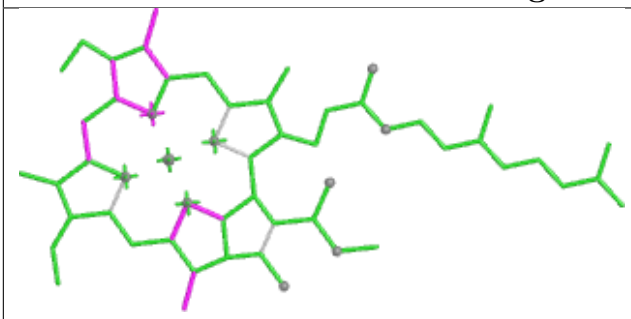
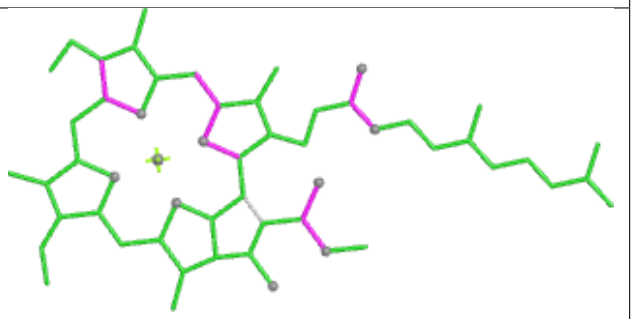
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 518



Bond lengths



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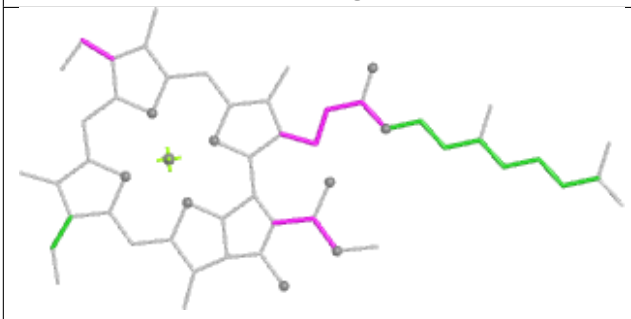
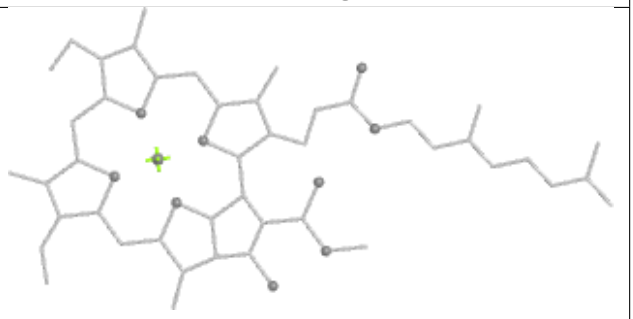
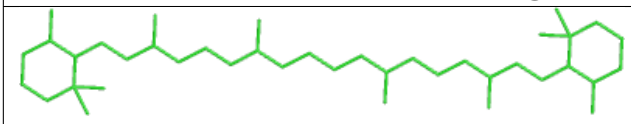


Torsions



Rings

Ligand BCR v 524



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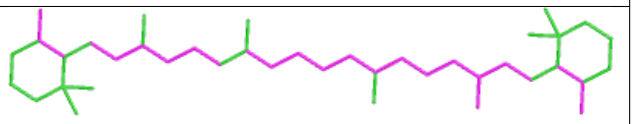

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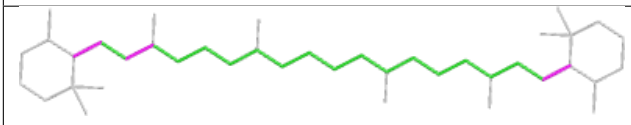

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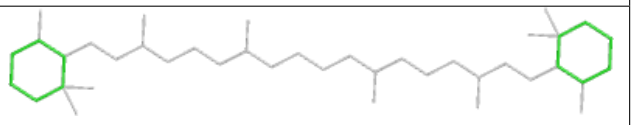
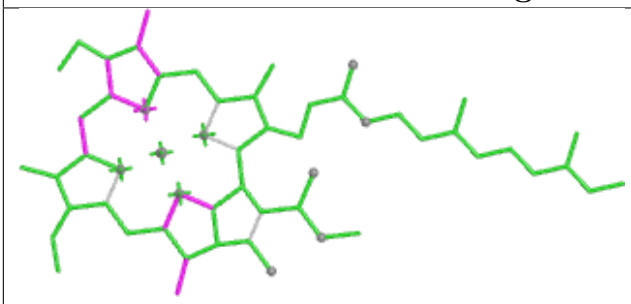


Rings

Ligand CLA A 1124



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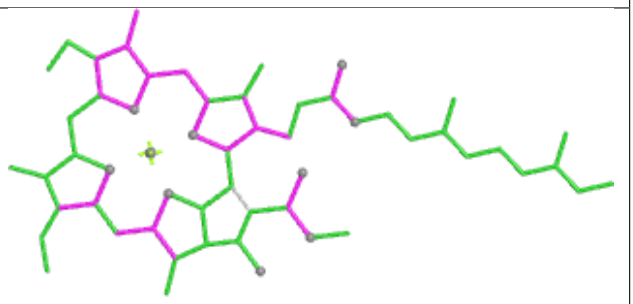

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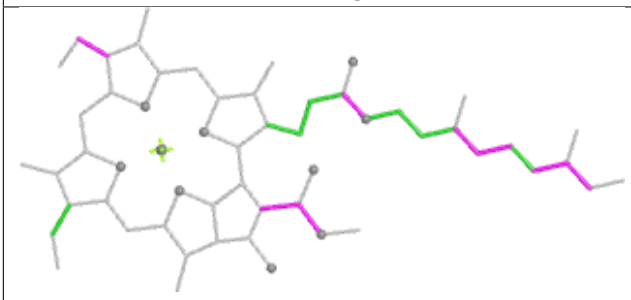

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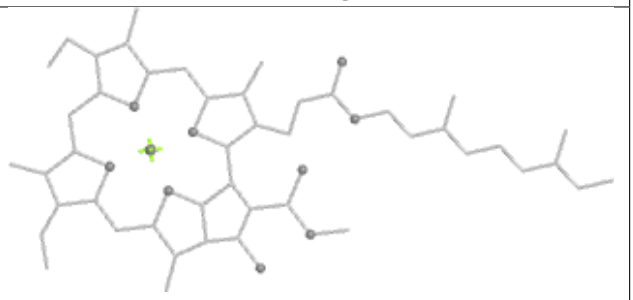
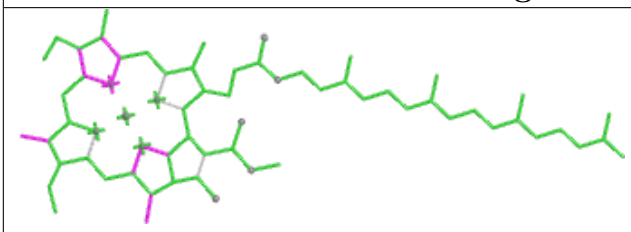


Rings

Ligand CLA H 1223



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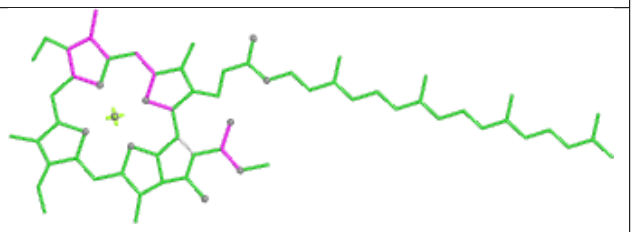
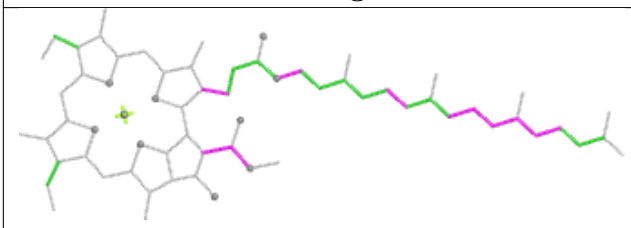


Bond angles



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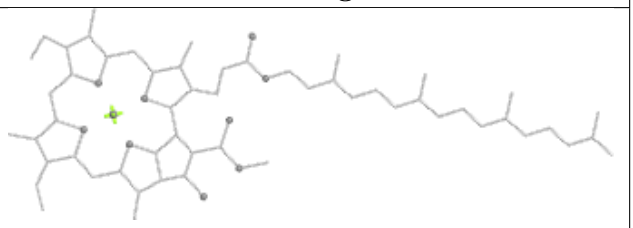
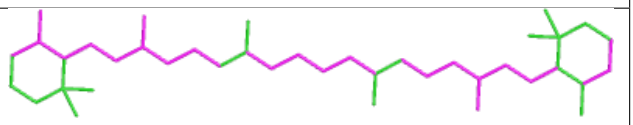


Rings

Ligand BCR 5 523

Bond lengths



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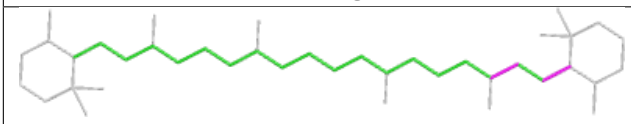

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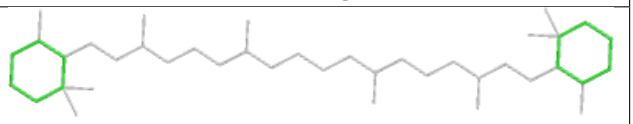
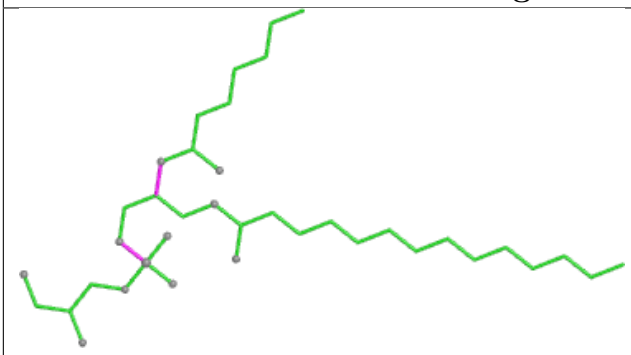


Rings

Ligand LHG V 5218



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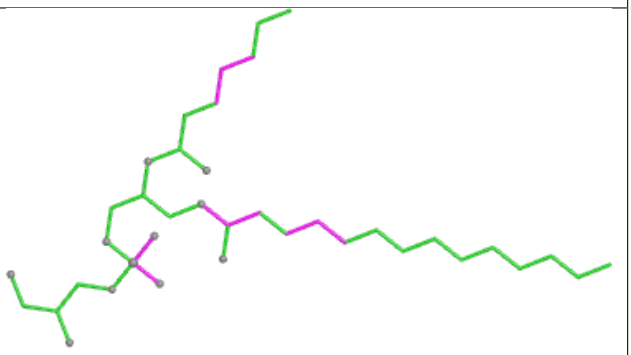

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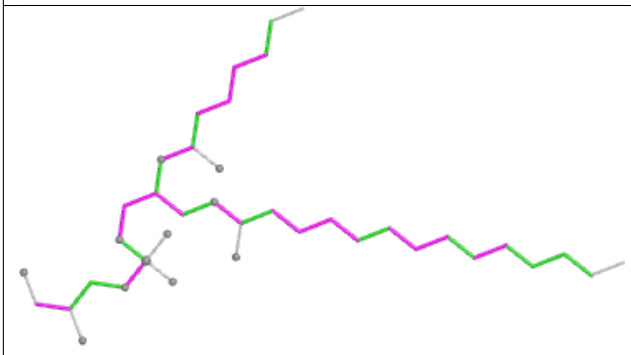

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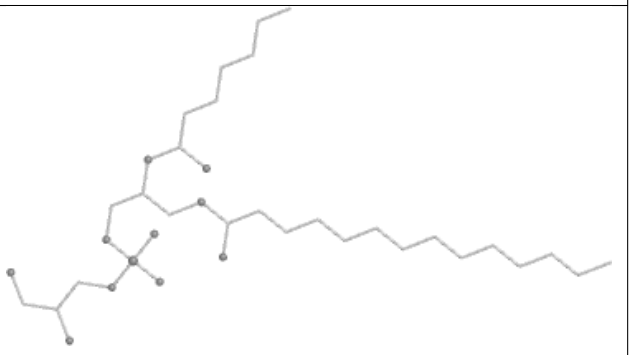
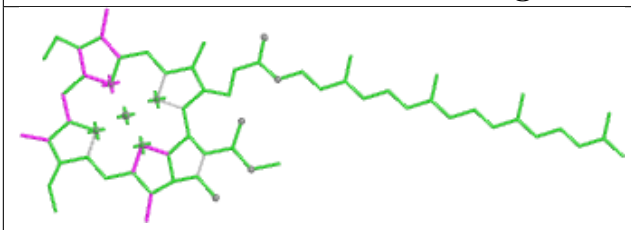


Rings

Ligand CLA G 1111



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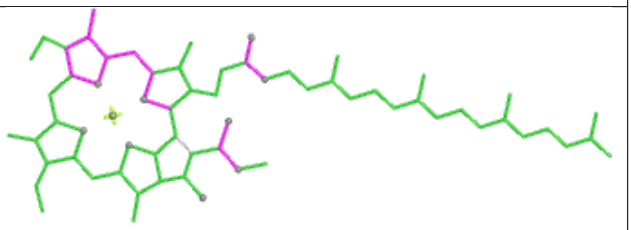

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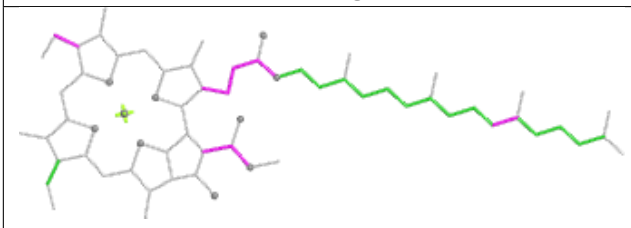

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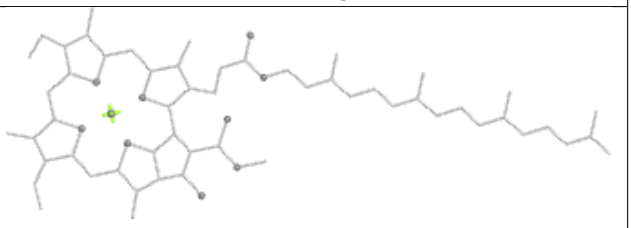
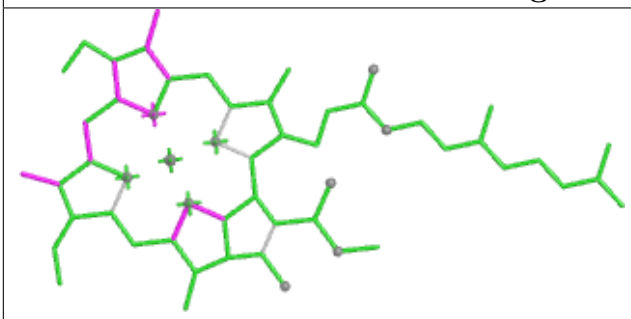
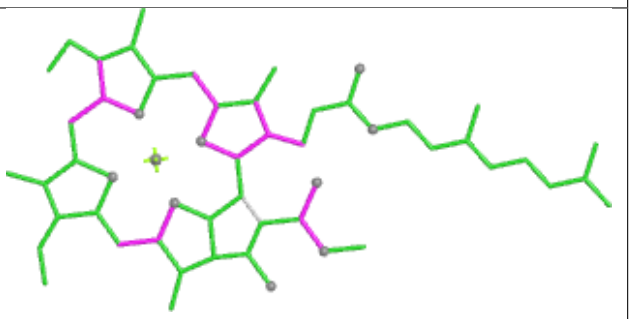
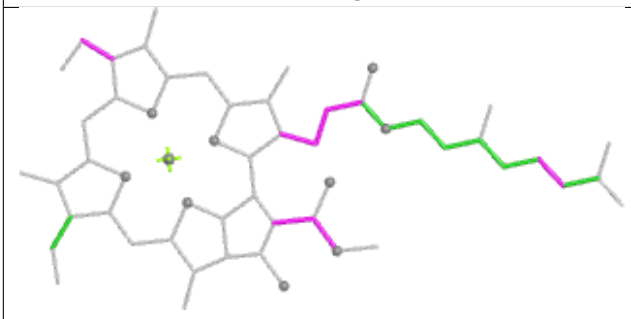
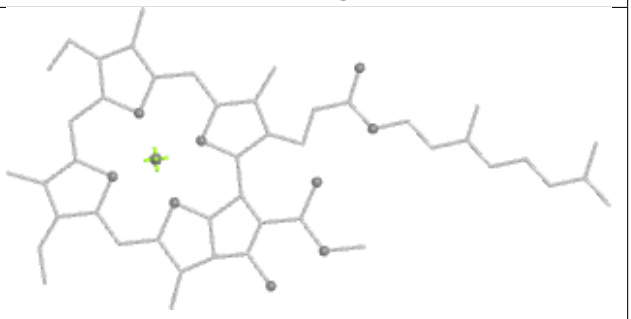
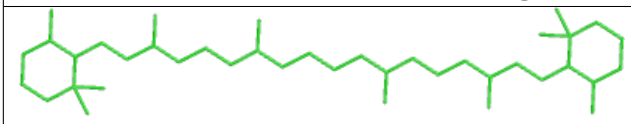
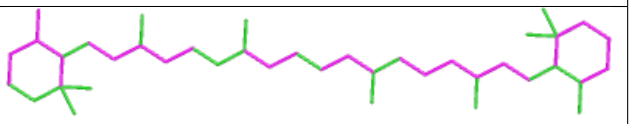
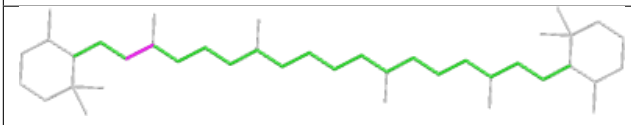
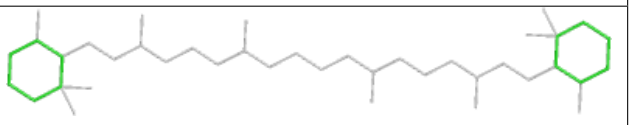
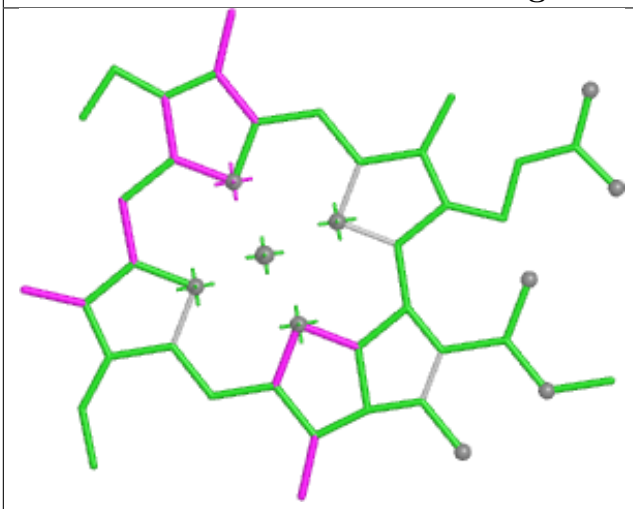


Rings

Ligand CLA r 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 4022	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 508



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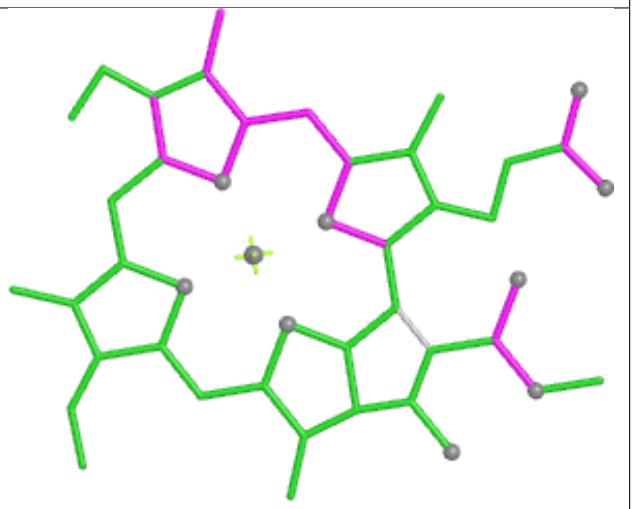

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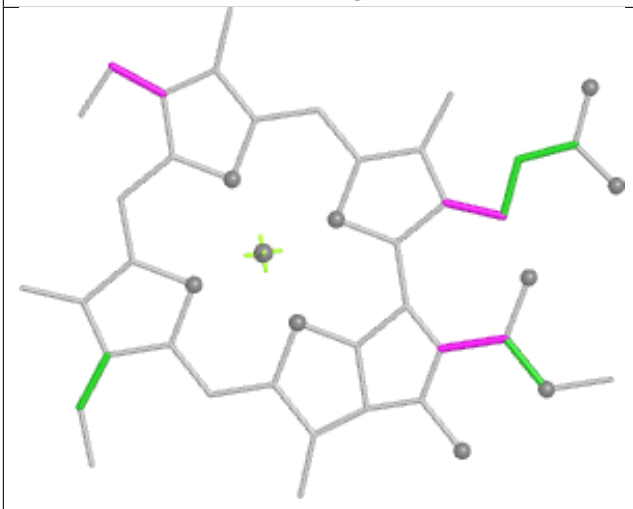
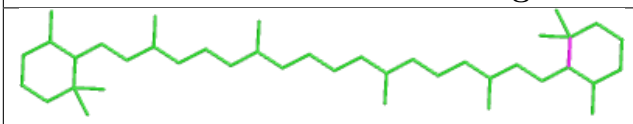


Torsions

Rings

Ligand BCR G 4002



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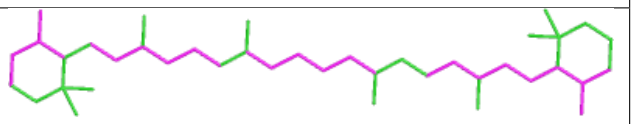
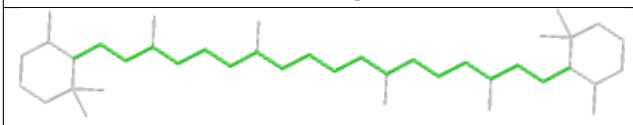


Bond angles



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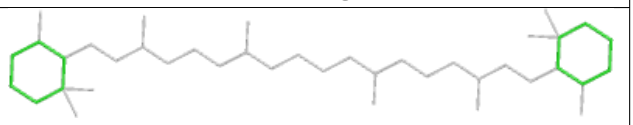
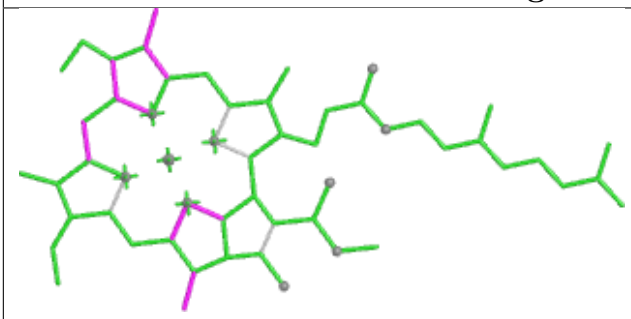


Rings

Ligand CLA u 503



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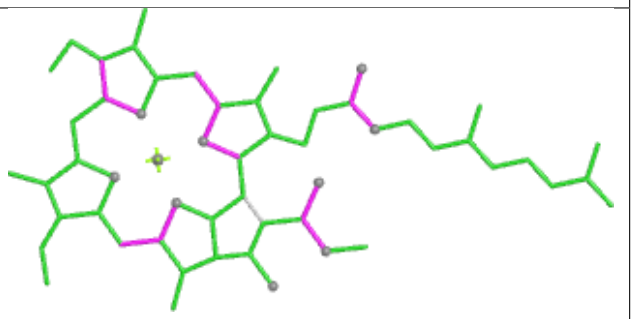
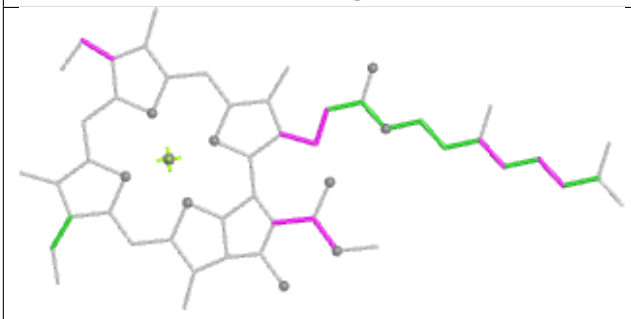


Bond angles



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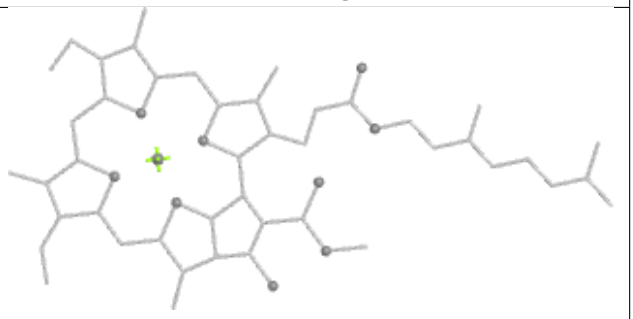
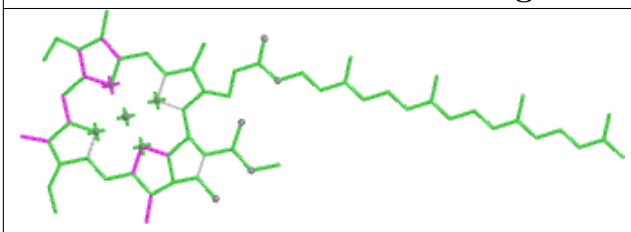


Rings

Ligand CLA B 1231



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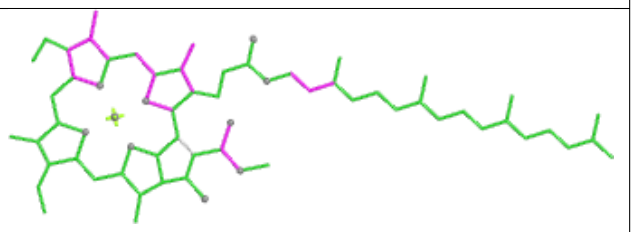
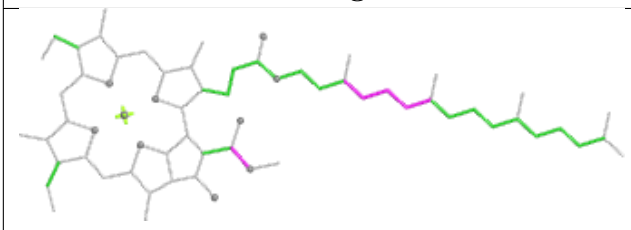


Bond angles



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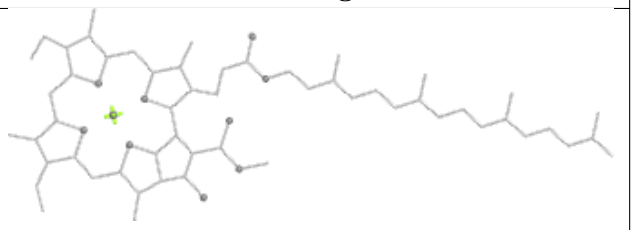
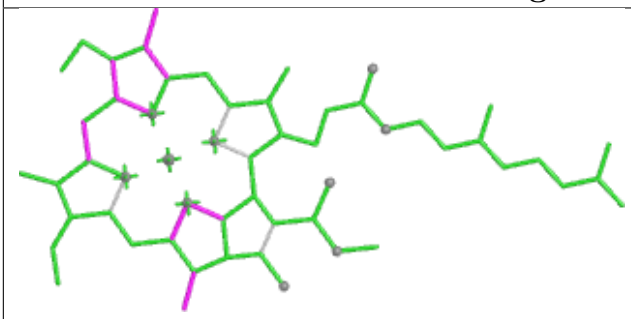


Rings

Ligand CLA c 503



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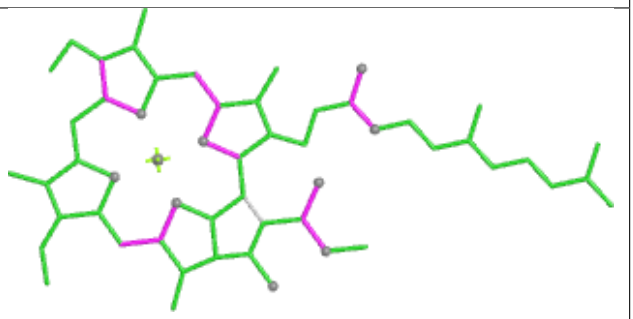
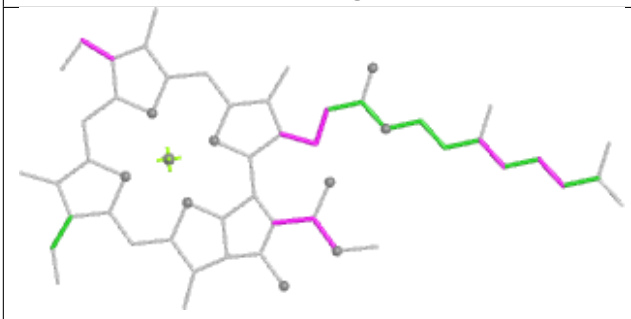
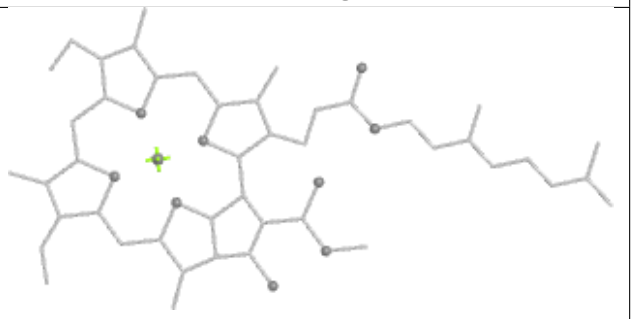


Bond angles

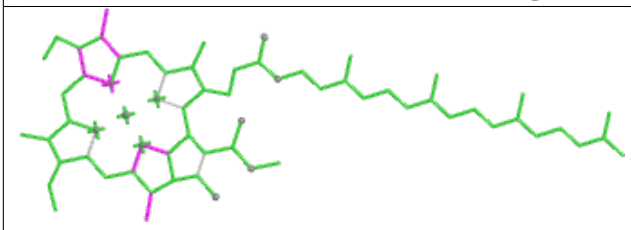


Torsions

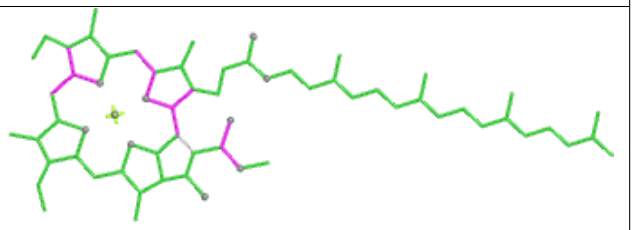


Rings

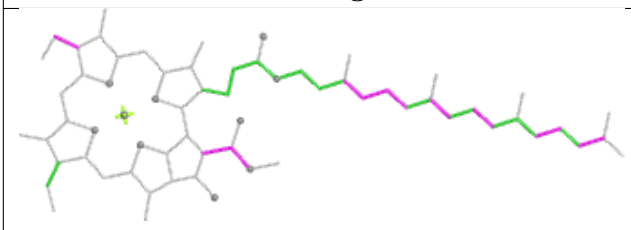
Ligand CLA Z 507



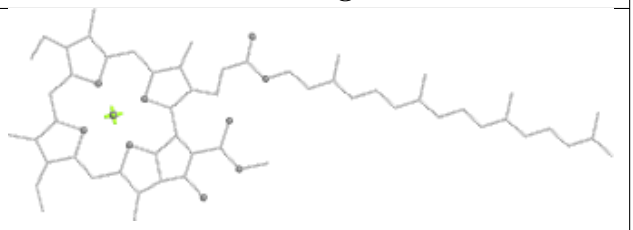
Bond lengths



Bond angles



Torsions



Rings

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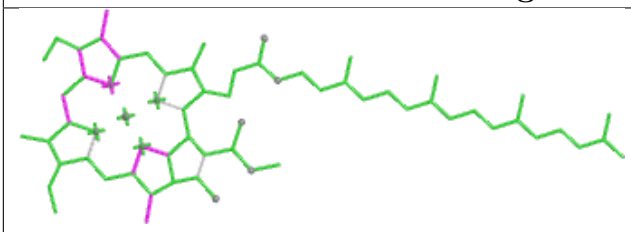
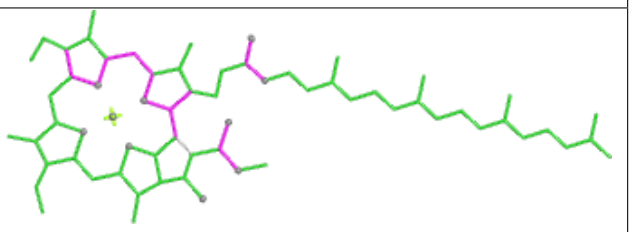
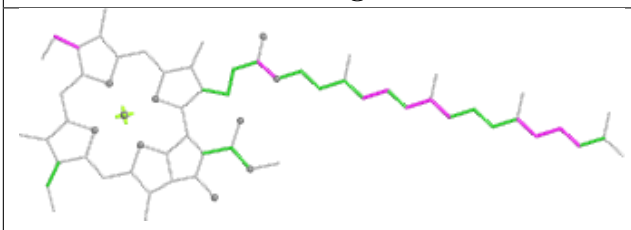
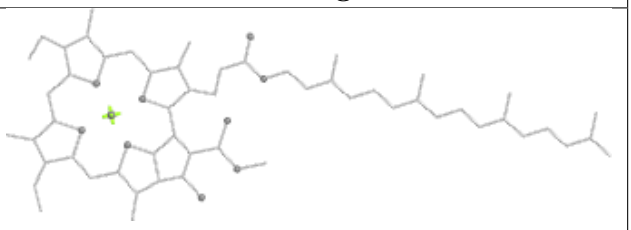
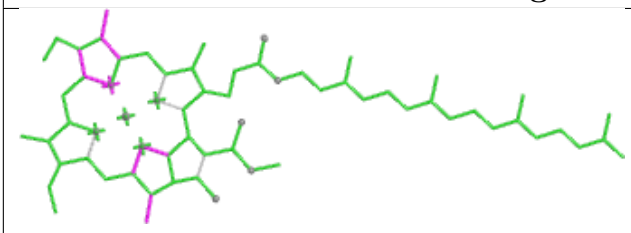
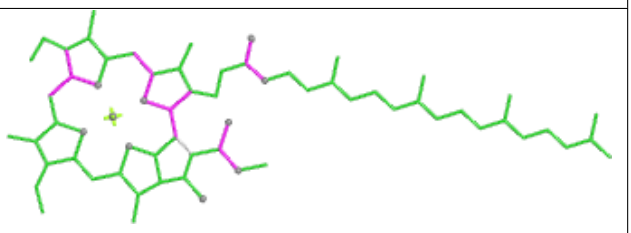
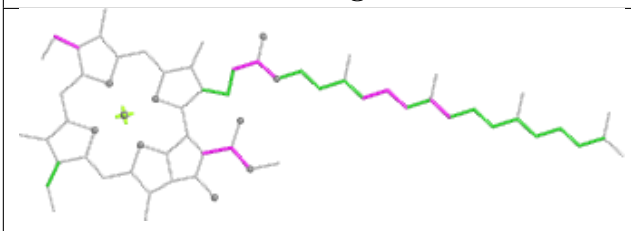
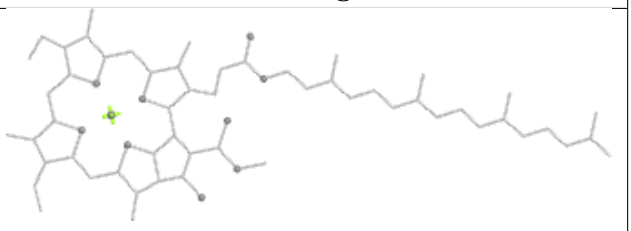
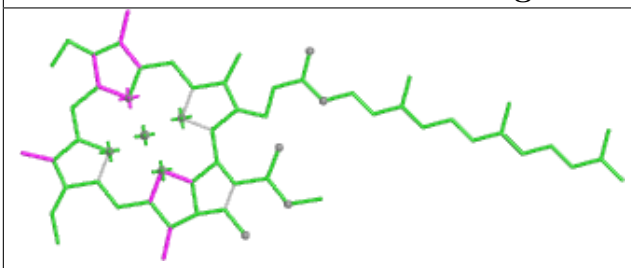
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1230



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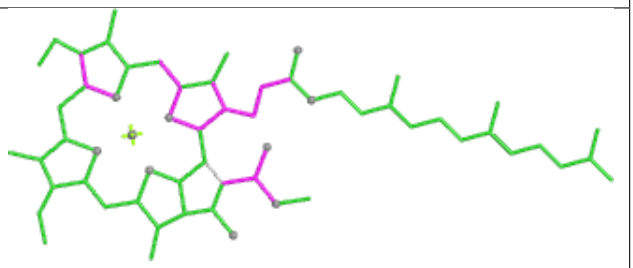
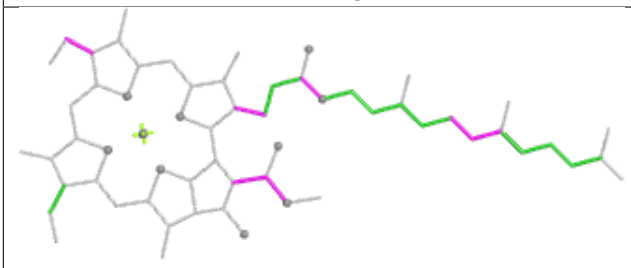


Bond angles



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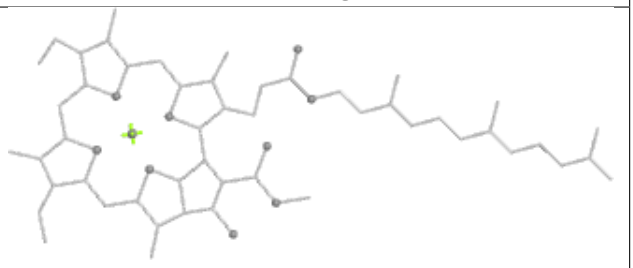
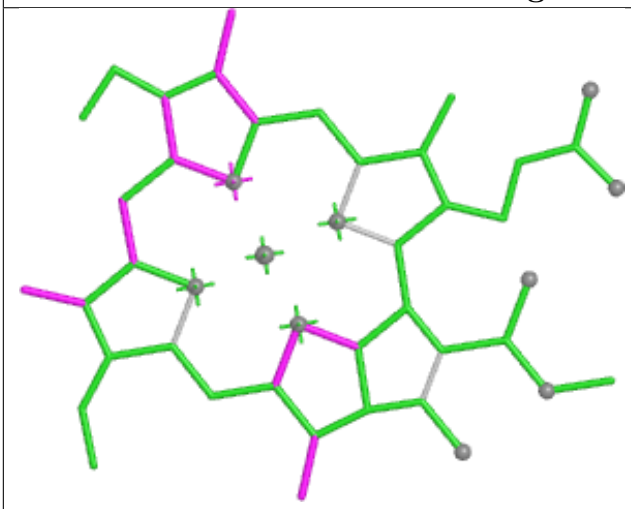


Rings

Ligand CLA u 513



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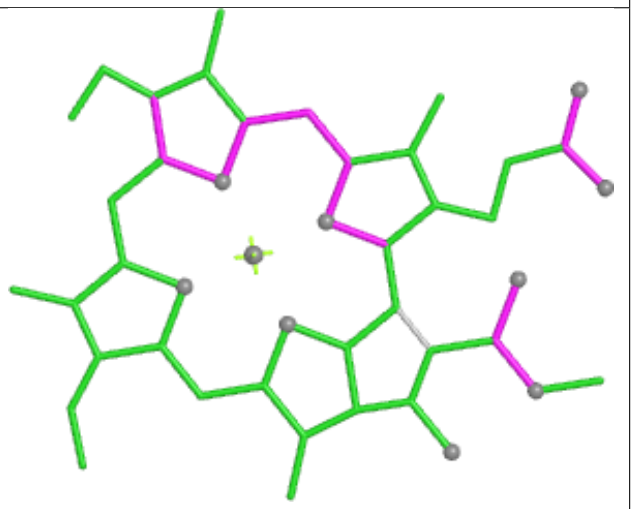
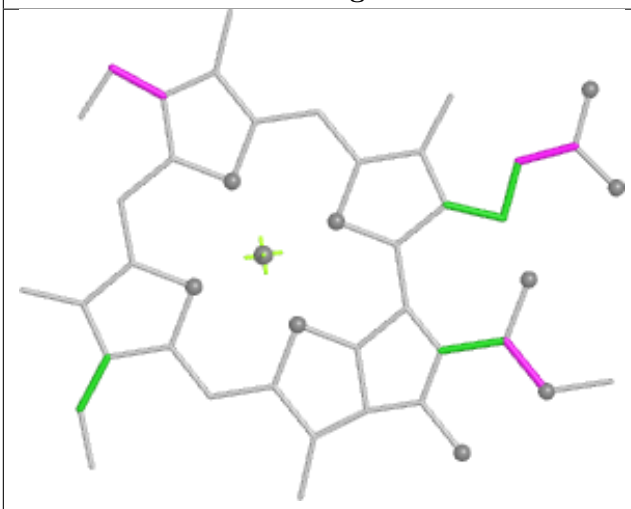


Bond angles



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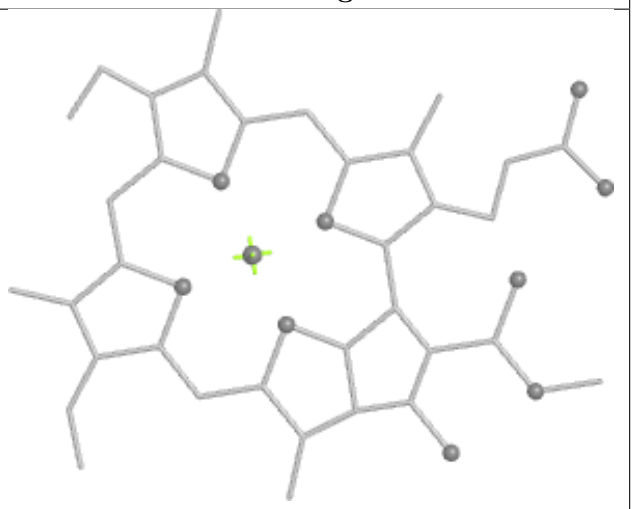
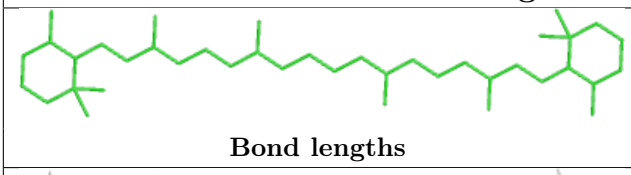


Rings

Ligand BCR e 4001



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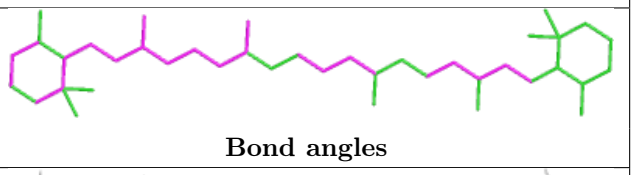

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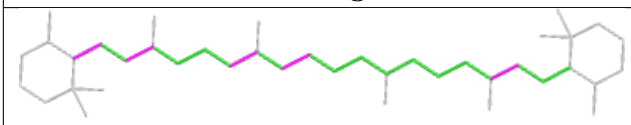

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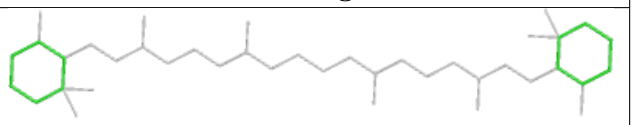
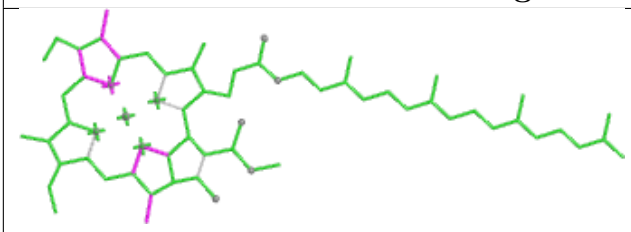


Rings

Ligand CLA G 1133



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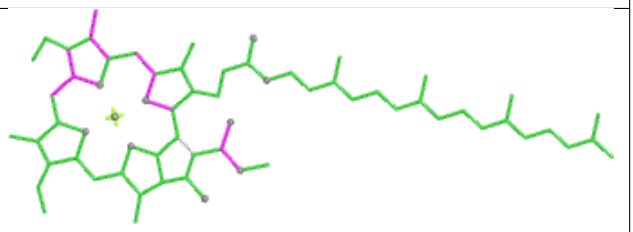
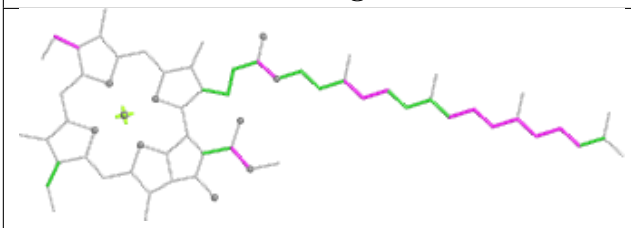


Bond angles



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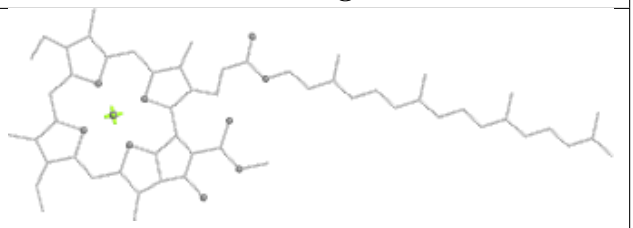
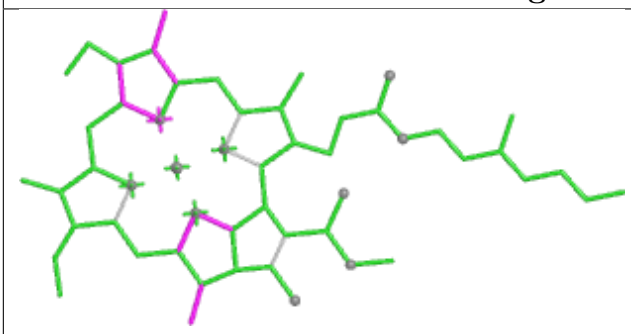


Rings

Ligand CLA 2 512



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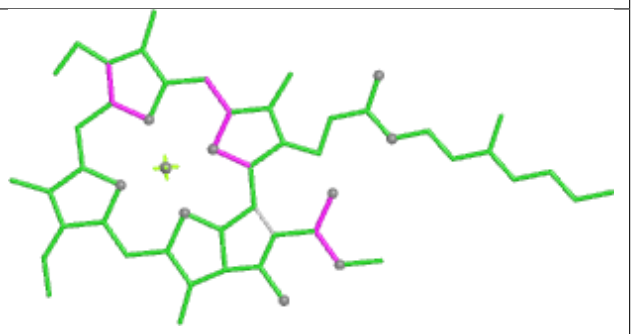
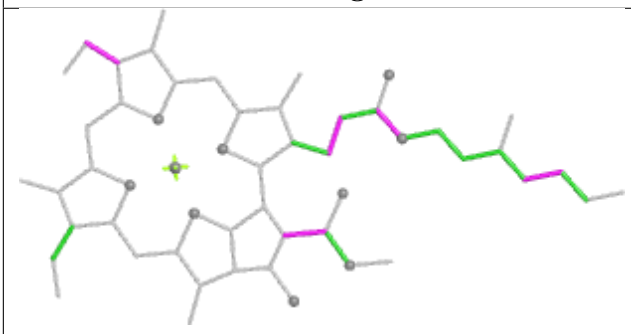


Bond angles



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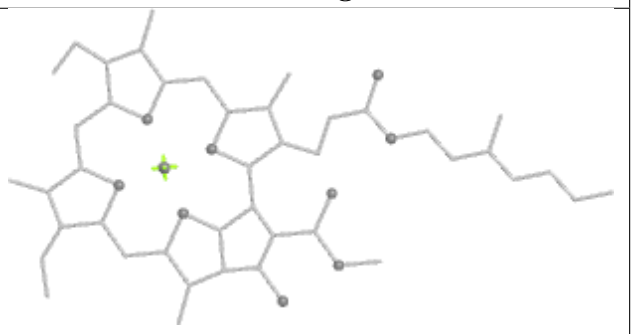
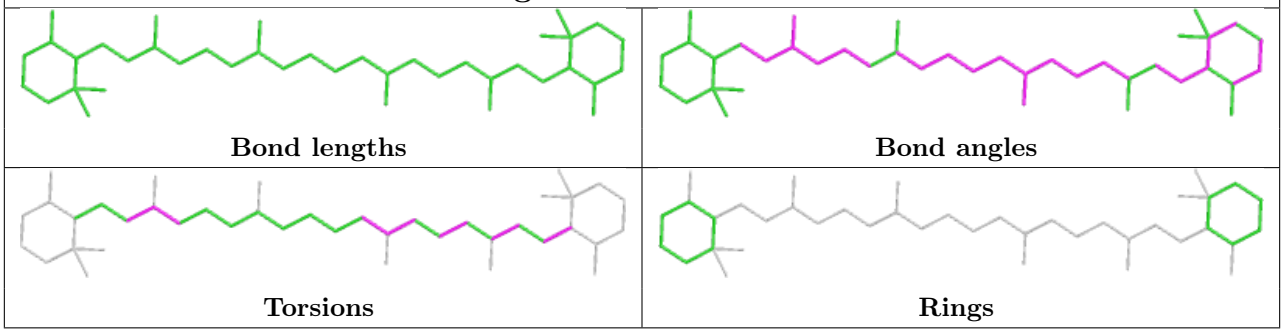


Rings

Ligand BCR A 4011



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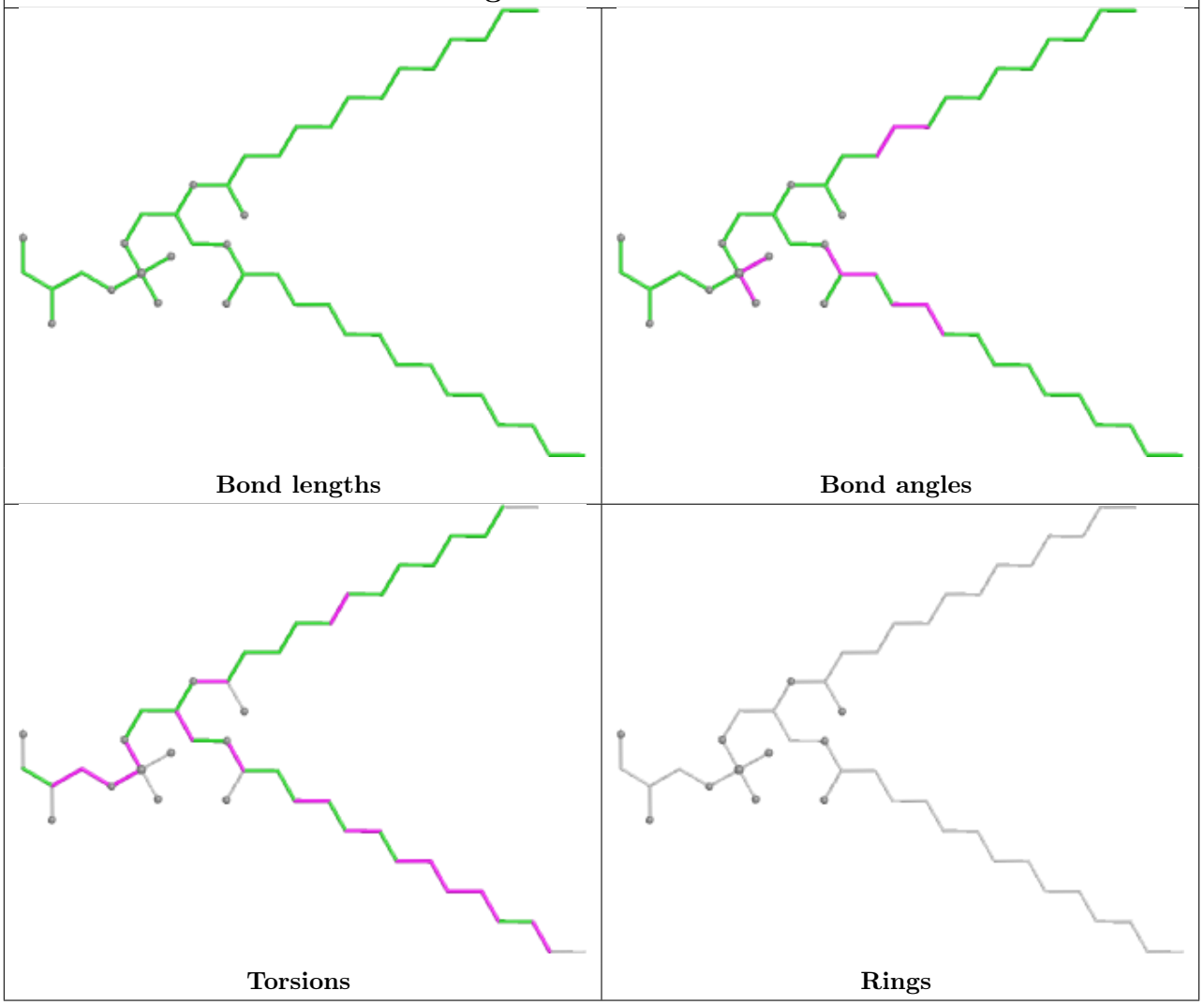

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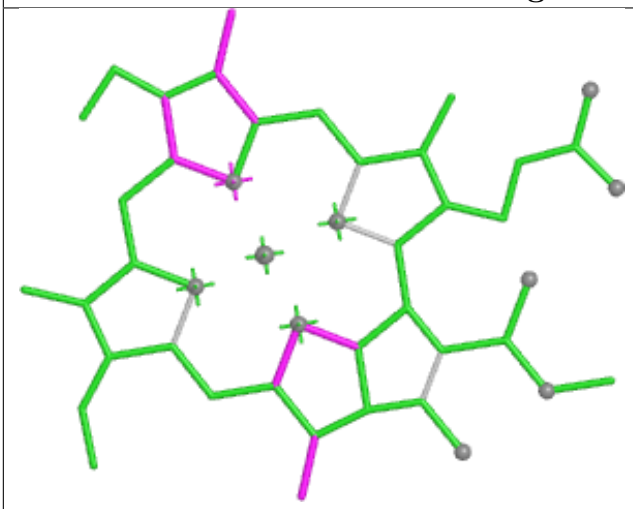
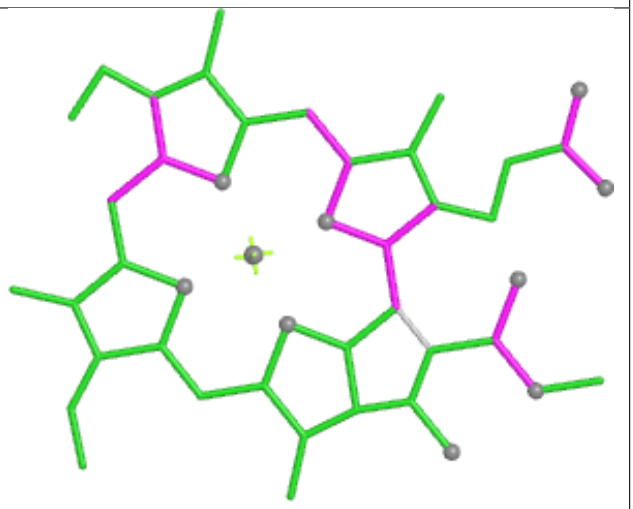
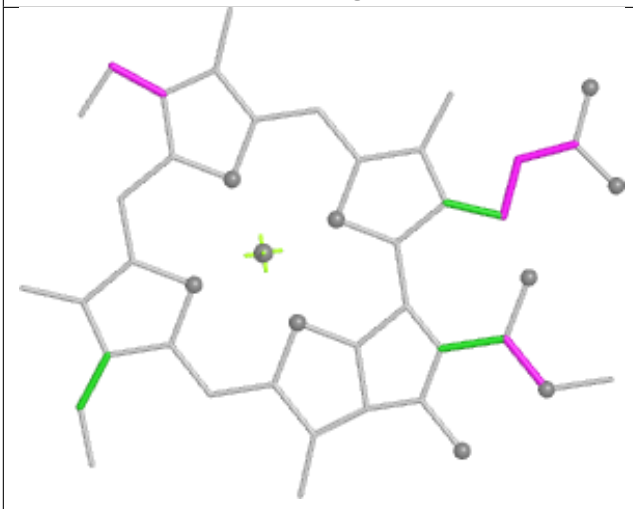


Bond lengths



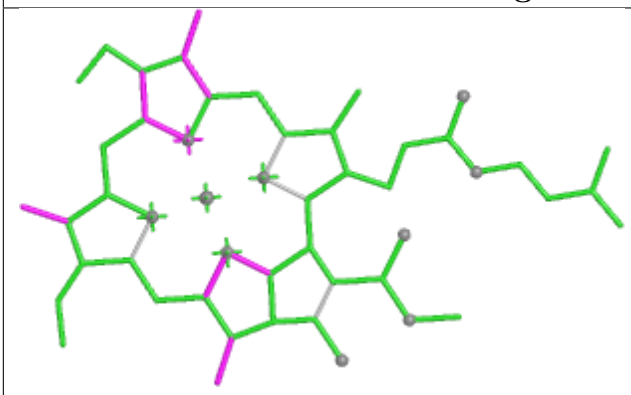
Bond angles



Torsions

Rings

Ligand CLA K 1103



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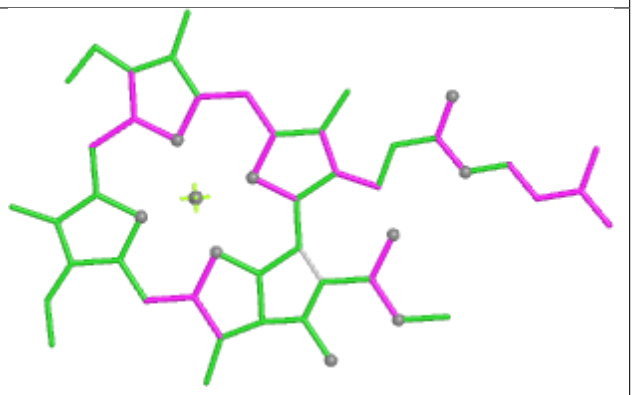

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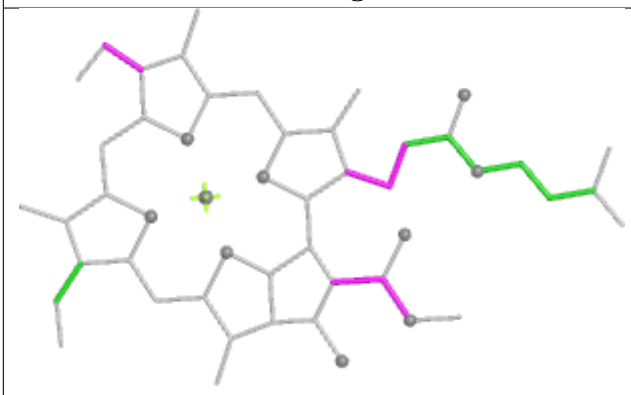
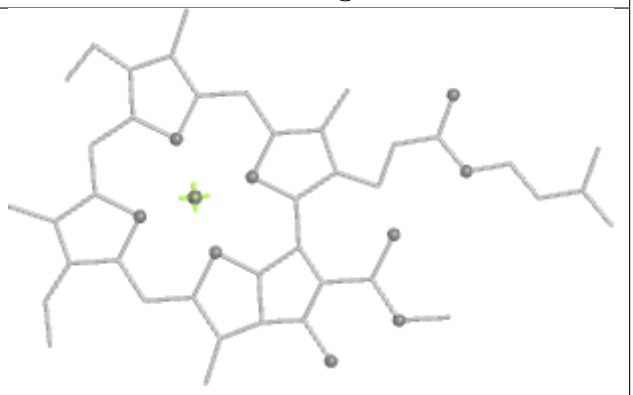
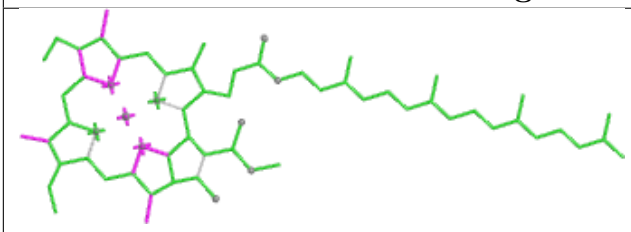


Torsions



Rings

Ligand CLA A 1128



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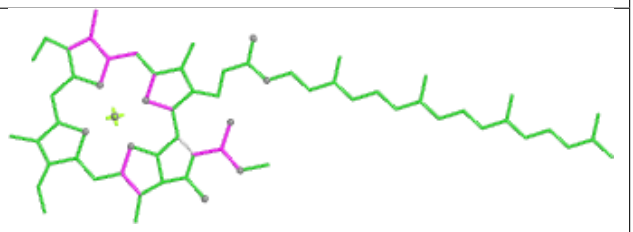
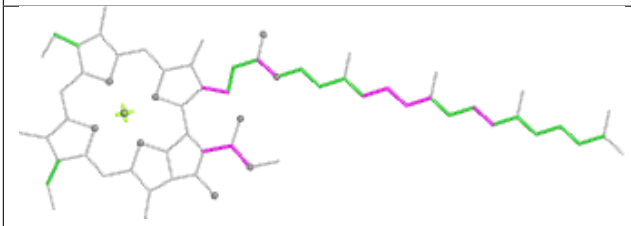


Bond angles



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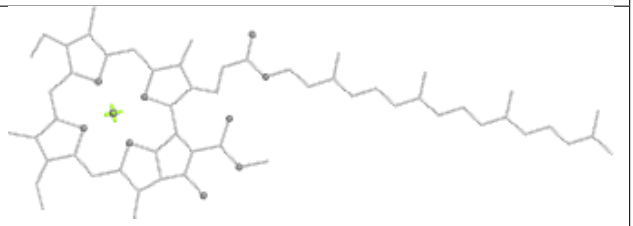
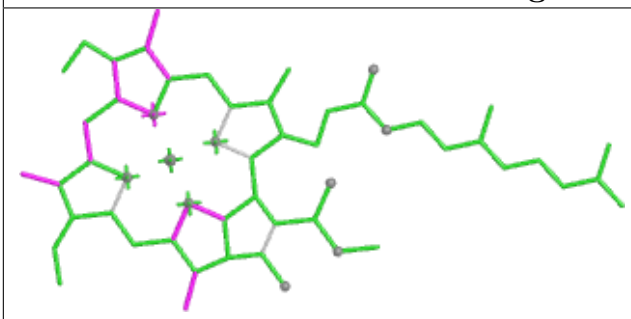


Rings

Ligand CLA a 518



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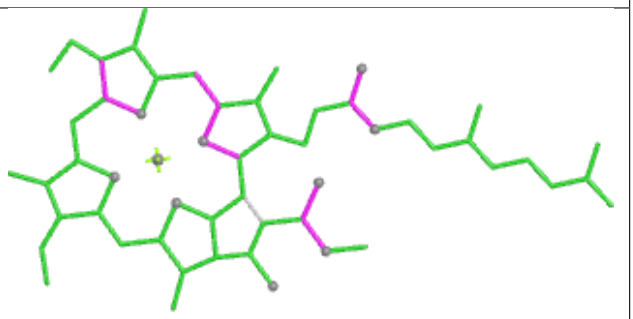
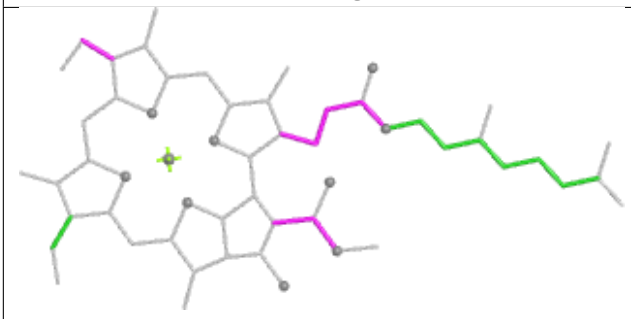


Bond angles



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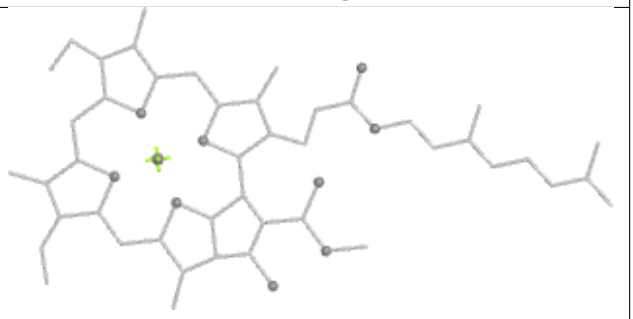
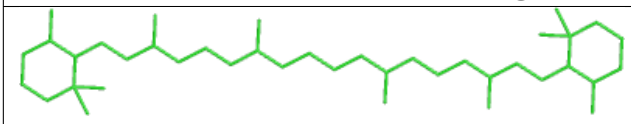


Rings

Ligand BCR H 4017



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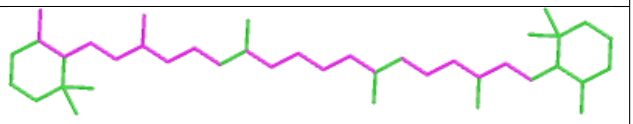
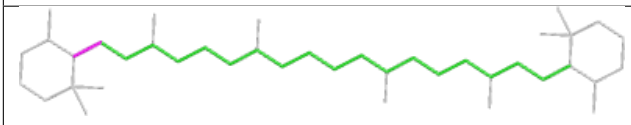
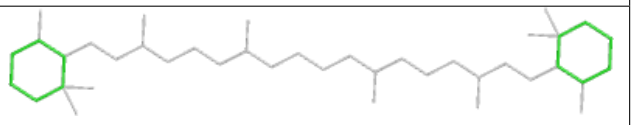


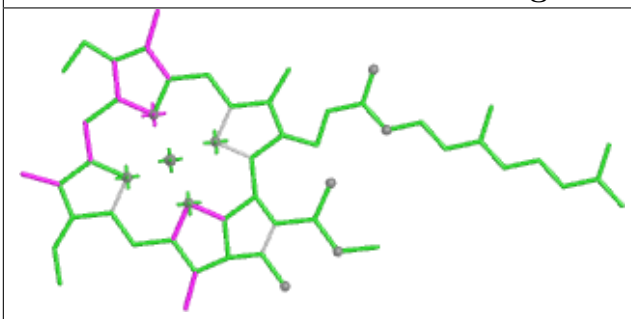
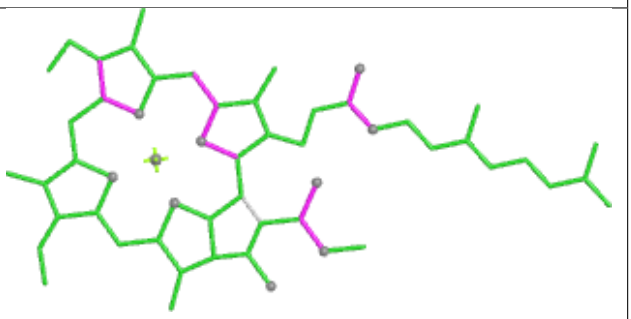
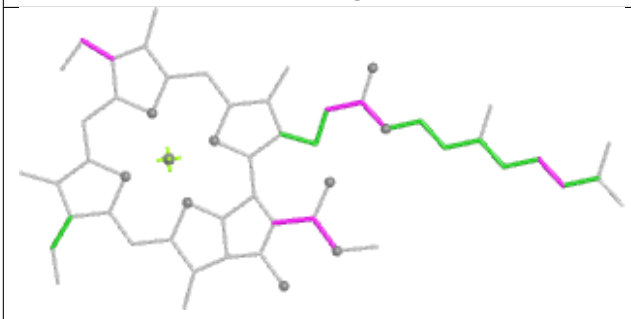
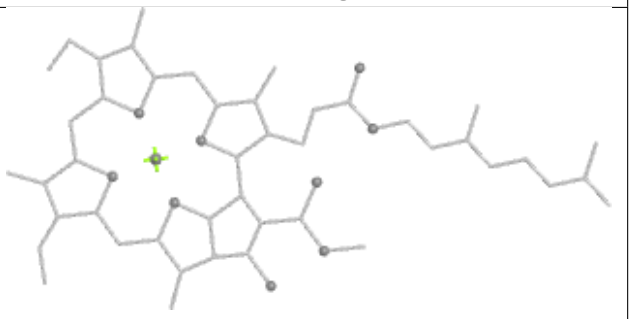
Bond angles



Torsions



Rings

Ligand CLA s 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

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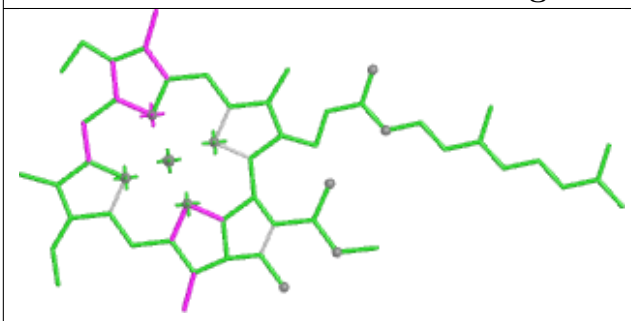
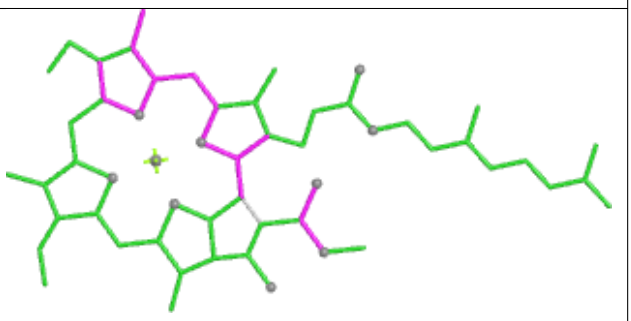
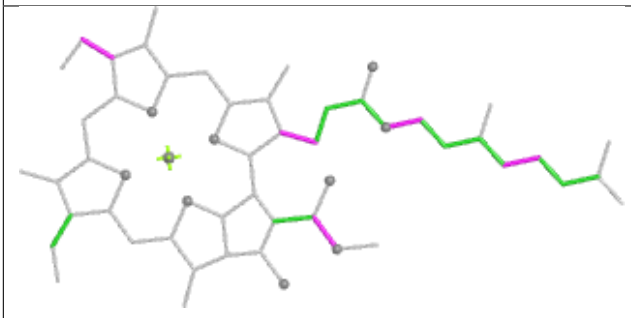
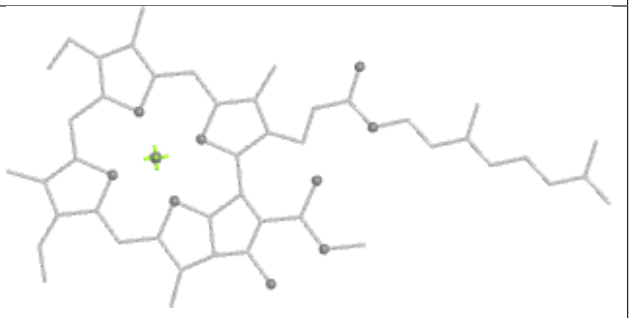
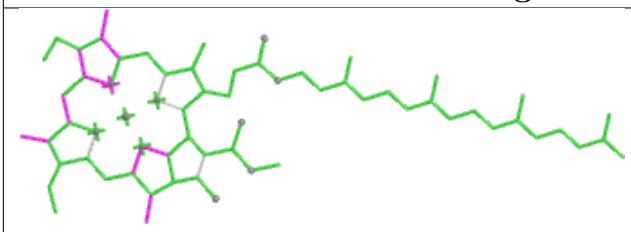
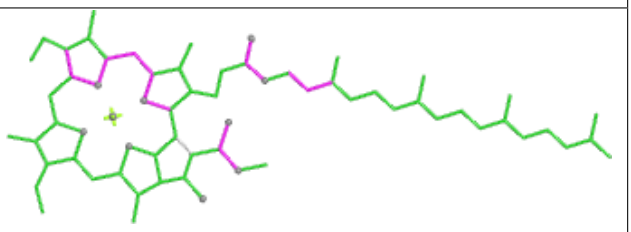
	
Bond lengths	Bond angles
	
Torsions	Rings

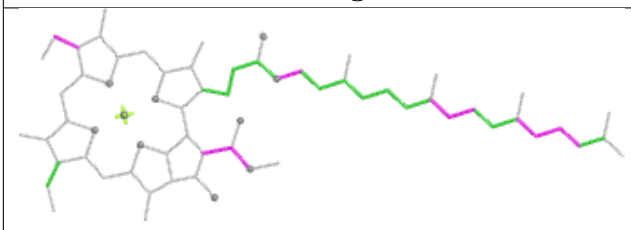
Ligand CLA G 1138



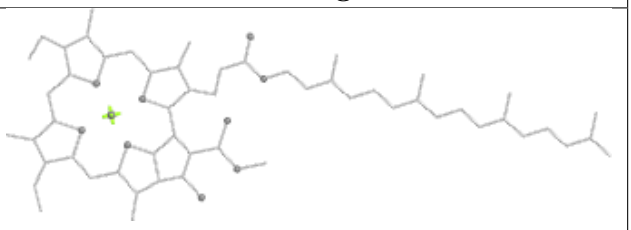
Bond lengths



Bond angles



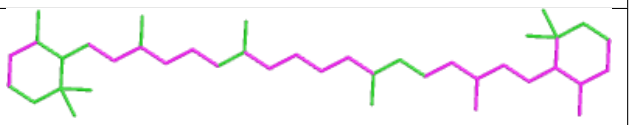
Torsions



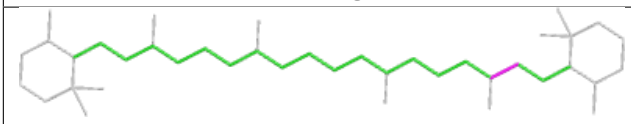
Rings

Ligand BCR K 4104

Bond lengths



Bond angles



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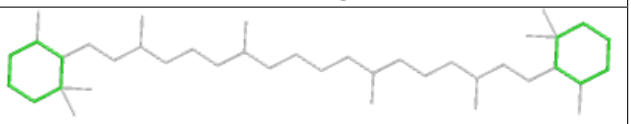
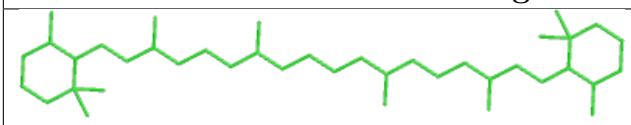
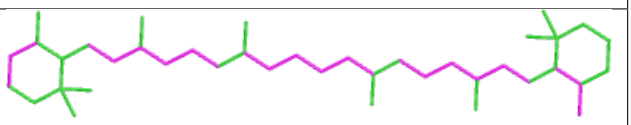


Rings

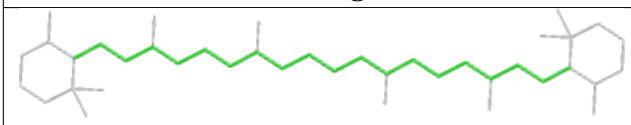
Ligand BCR G 4003



Bond lengths



Bond angles



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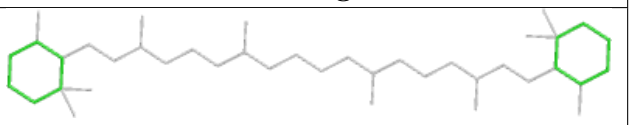
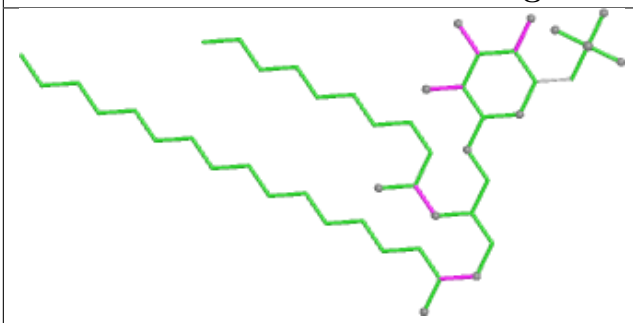


Rings

Ligand SQD Y 822



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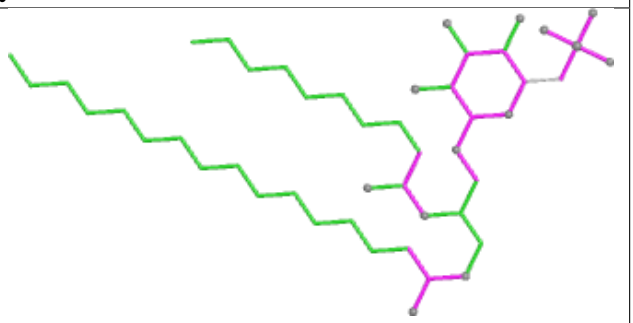
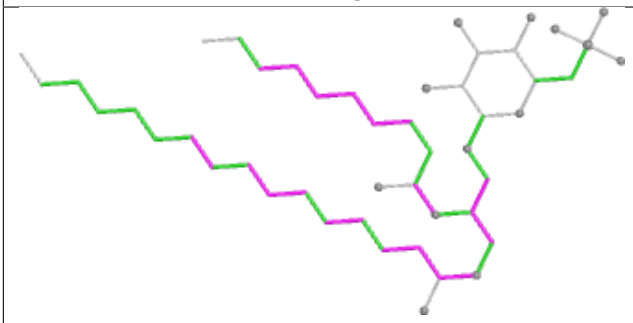


Bond angles



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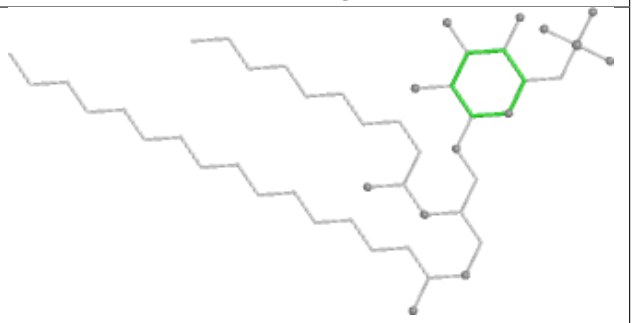
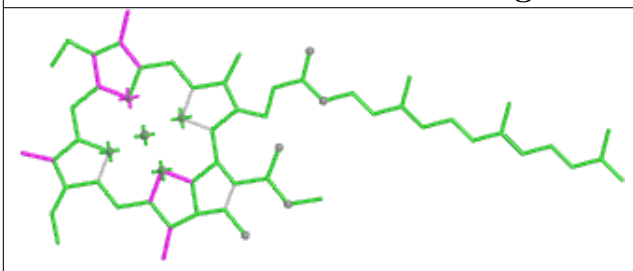


Rings

Ligand CLA A 1122



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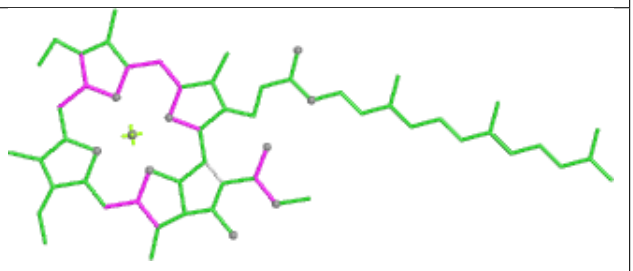
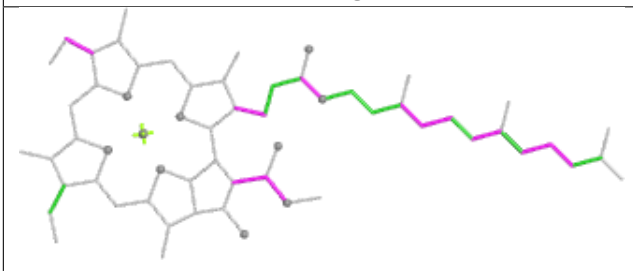


Bond angles



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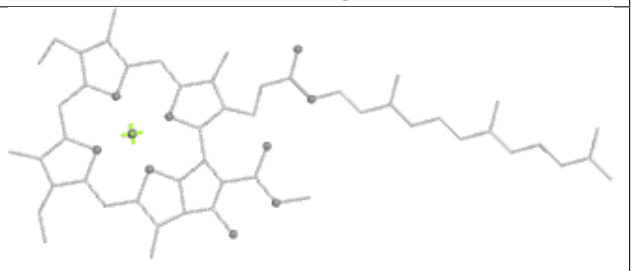
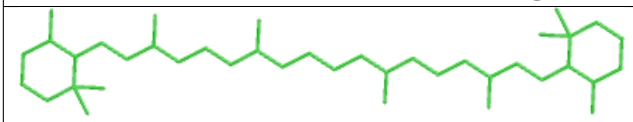
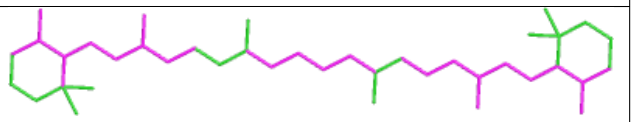


Rings

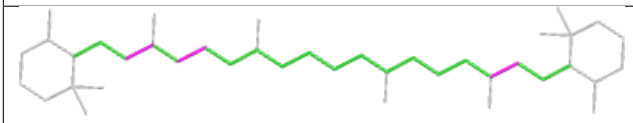
Ligand BCR s 524



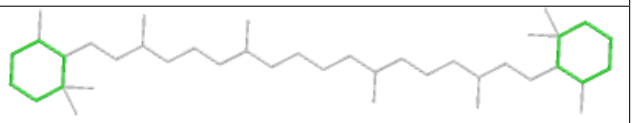
Bond lengths



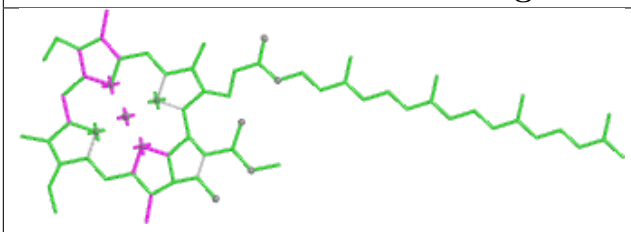
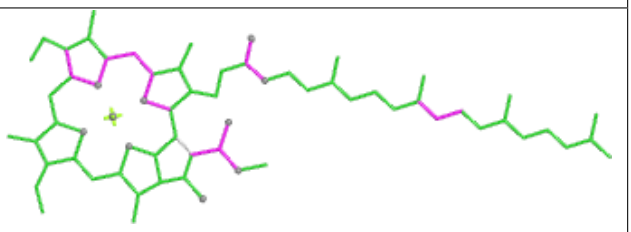
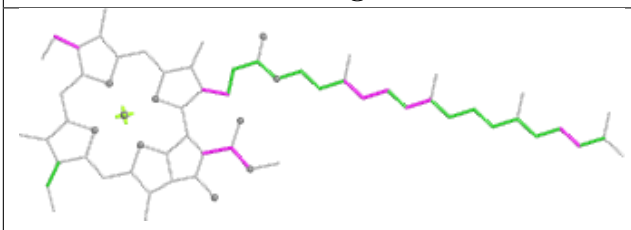
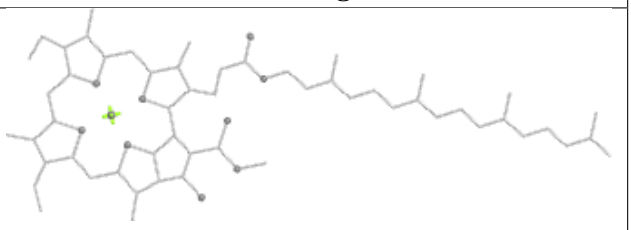
Bond angles

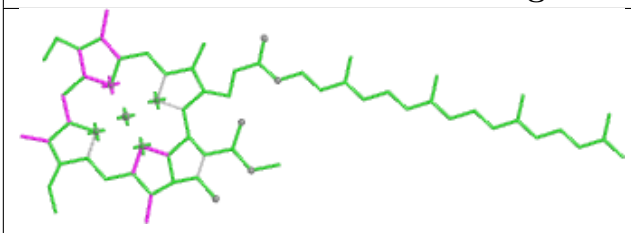
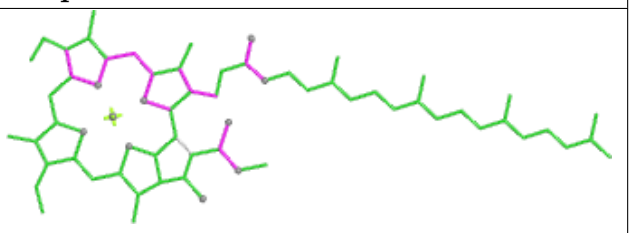
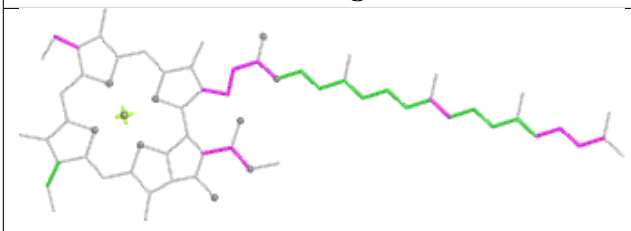
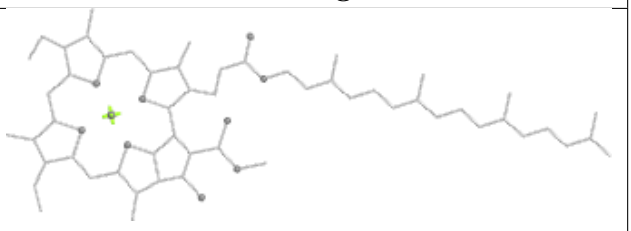


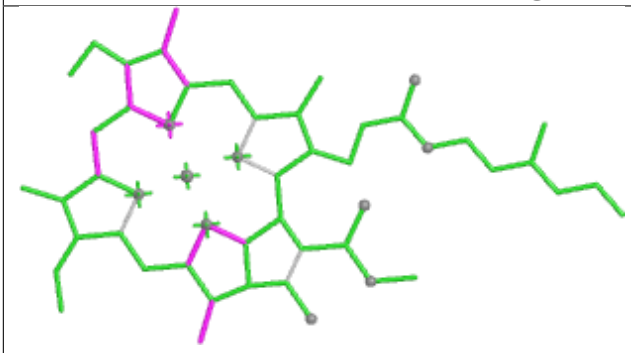
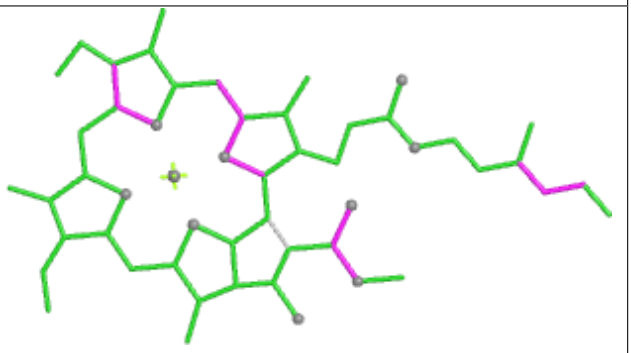
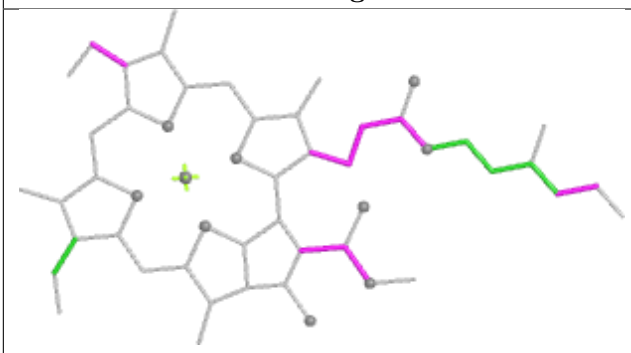
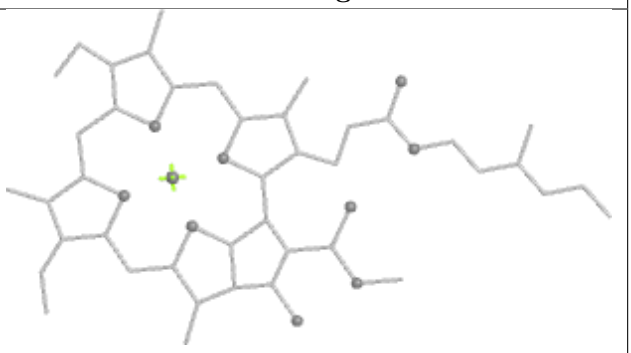
Torsions



Rings

Ligand CLA A 1139	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

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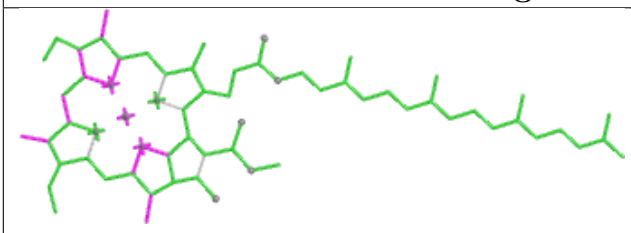
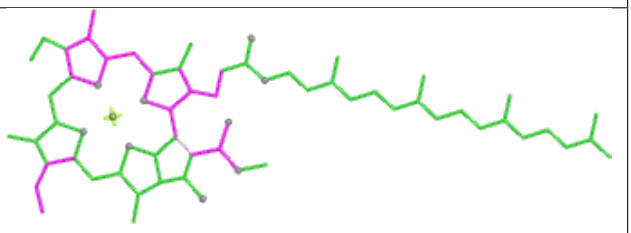
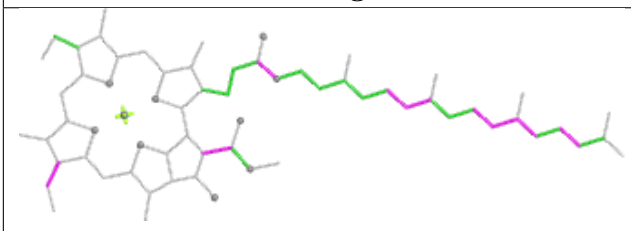
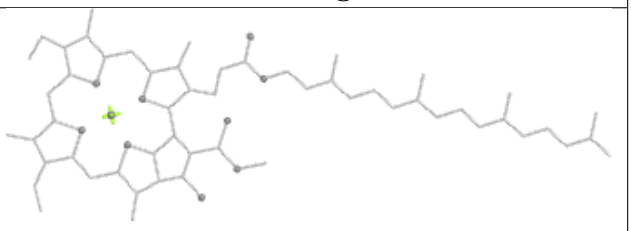
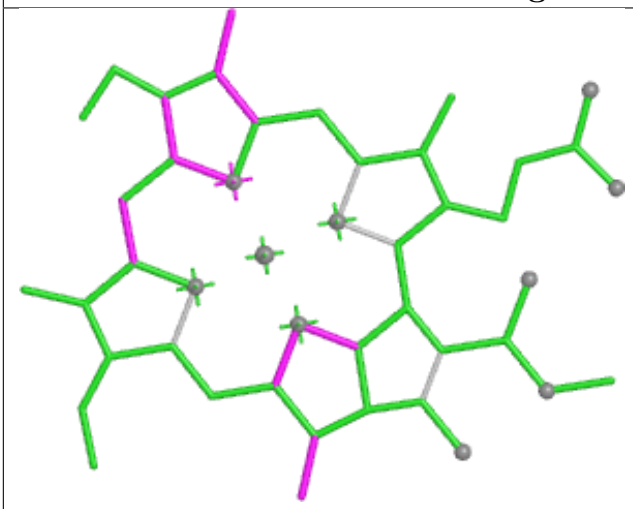
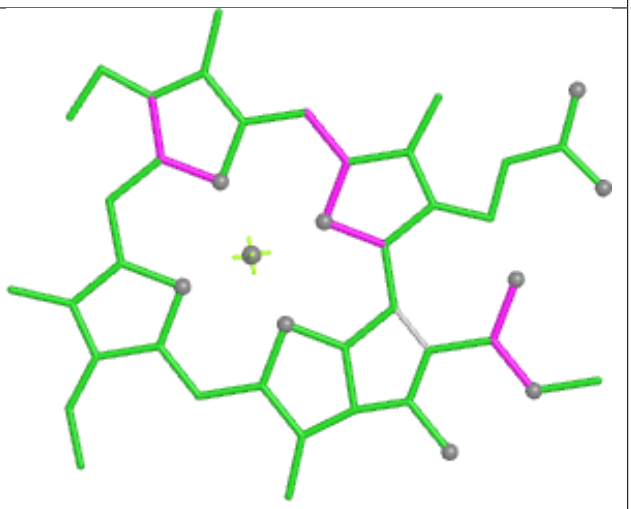
	
Bond lengths	Bond angles
	
Torsions	Rings

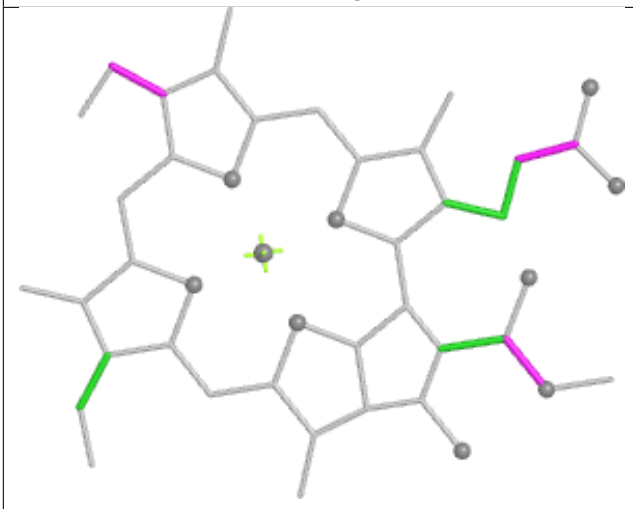
Ligand CLA 6 511



Bond lengths



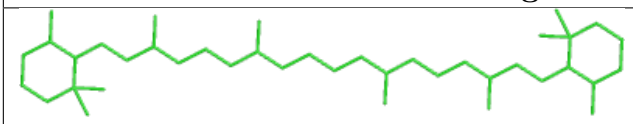
Bond angles



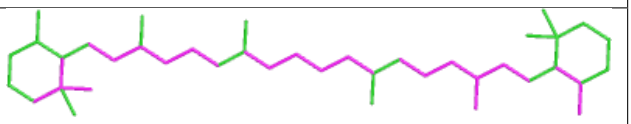
Torsions

Rings

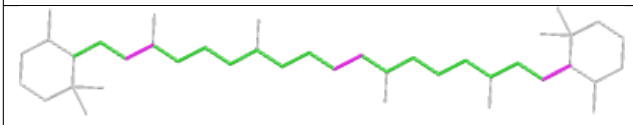
Ligand BCR l 4015



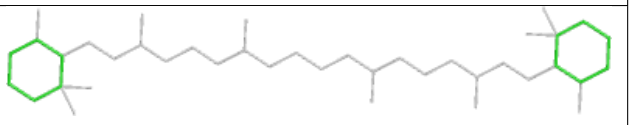
Bond lengths



Bond angles

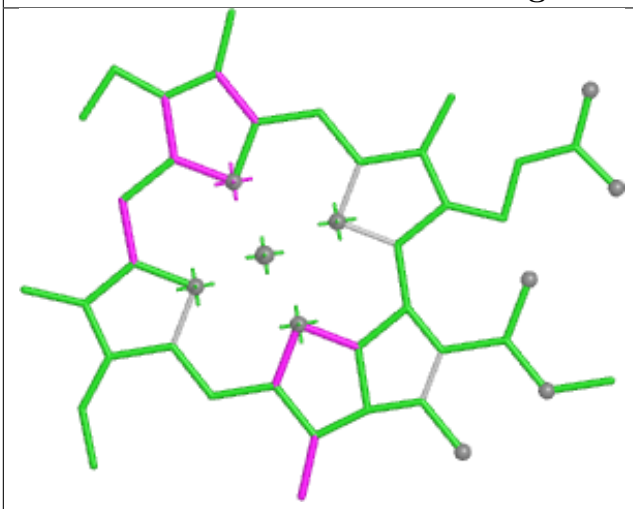


Torsions



Rings

Ligand CLA 2 516



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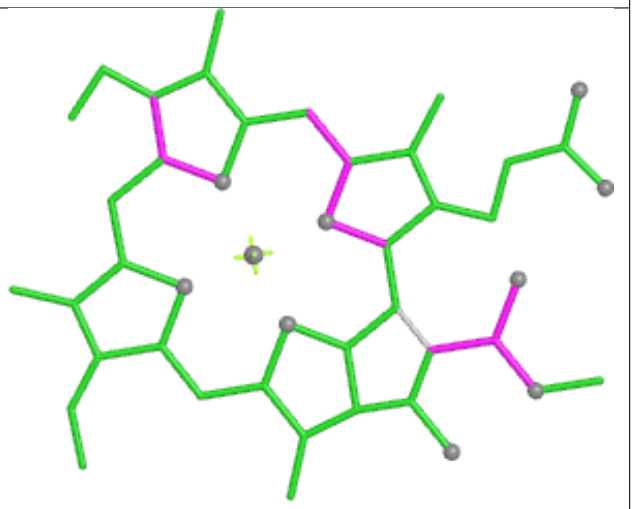

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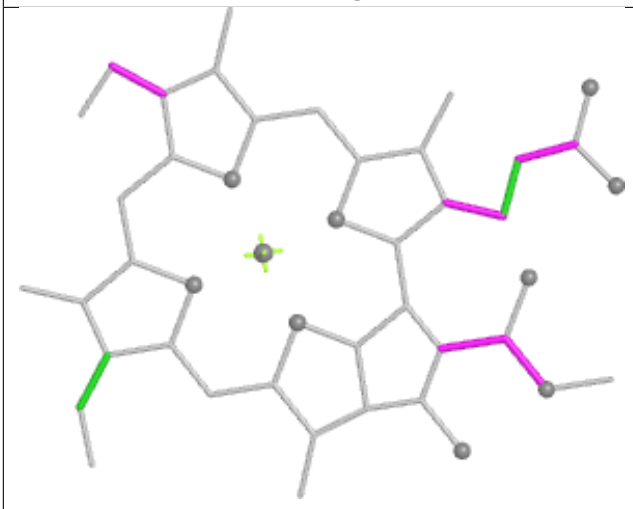
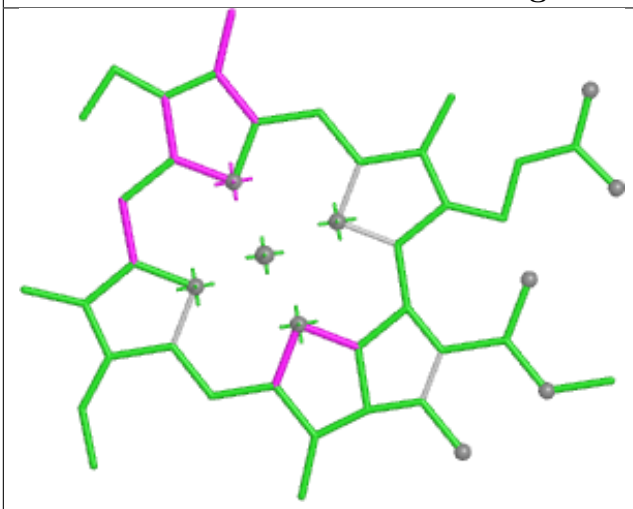


Torsions

Rings

Ligand CLA c 506



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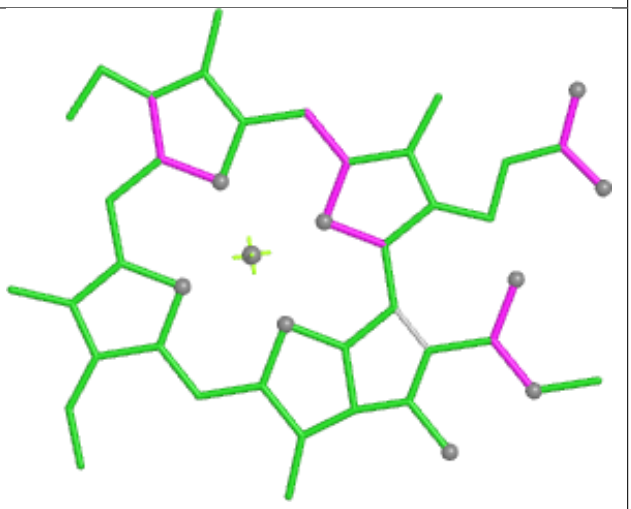
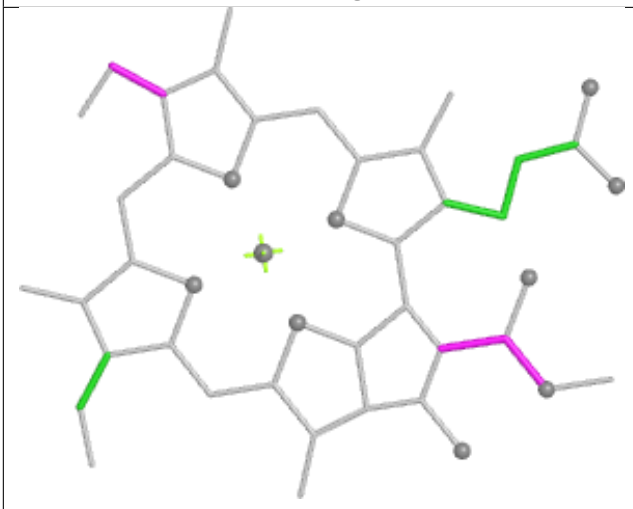


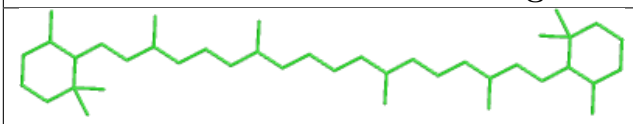
Bond angles



Torsions

Rings

Ligand BCR a 522



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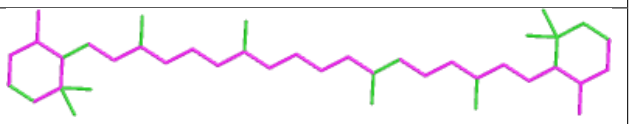

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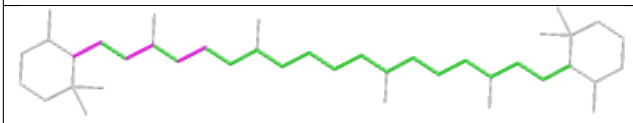
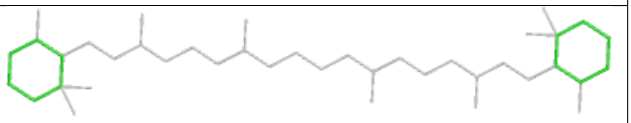
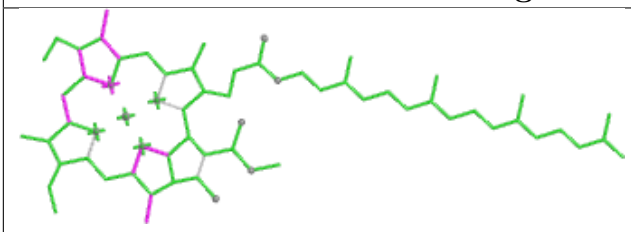


Torsions



Rings

Ligand CLA R 1301



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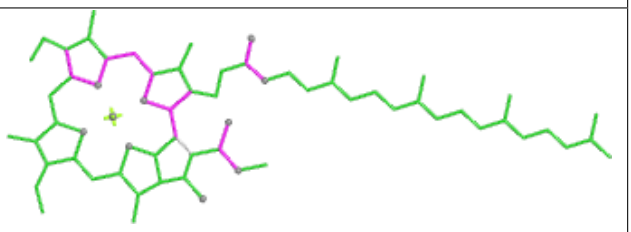
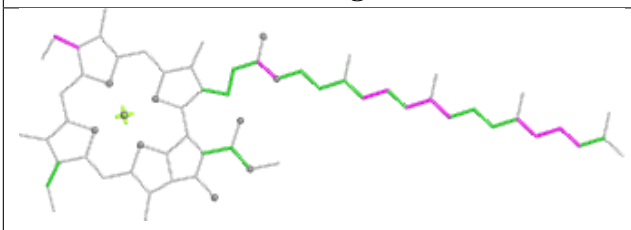


Bond angles



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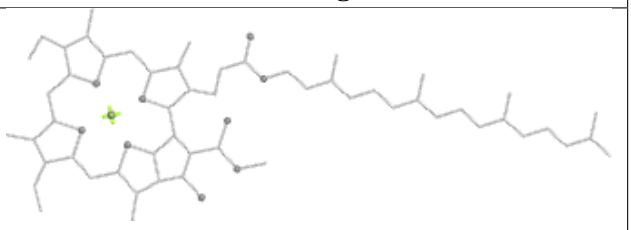
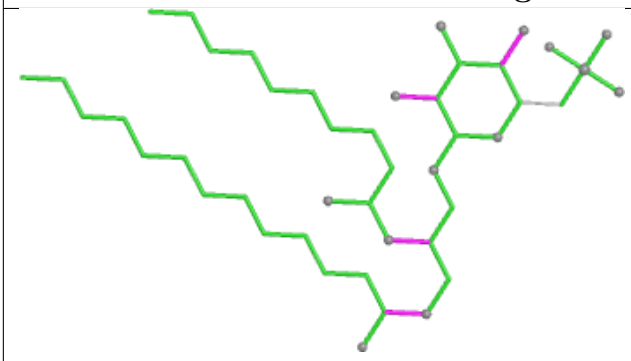


Rings

Ligand SQD H 1852



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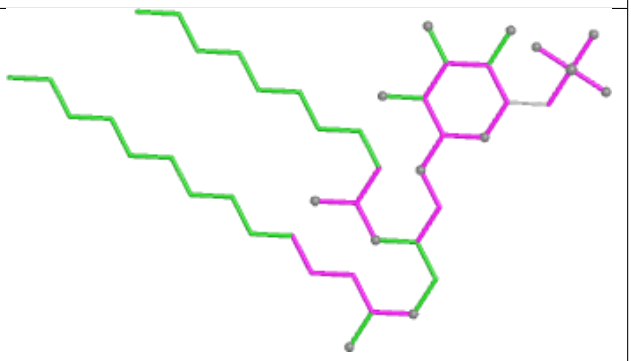

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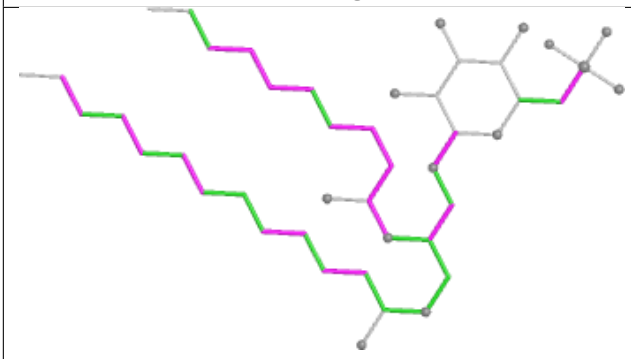

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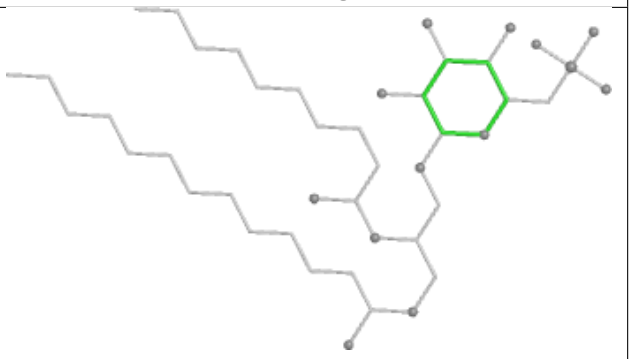
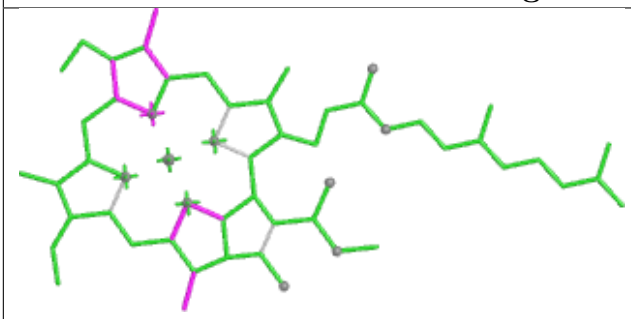


Rings

Ligand CLA f 1236



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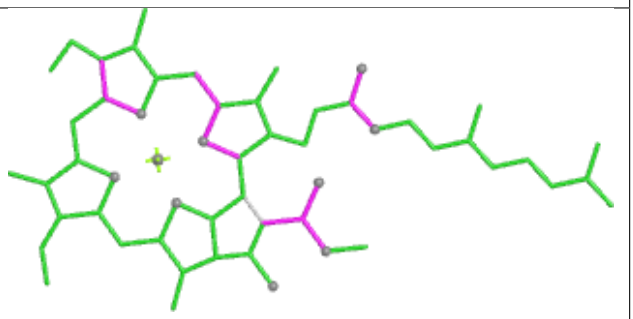

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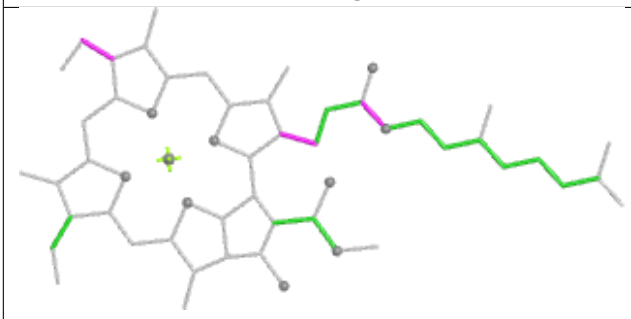

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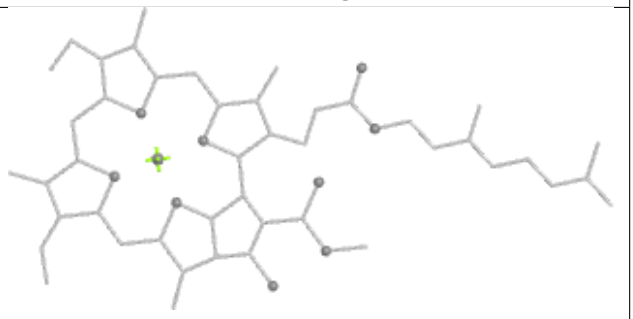
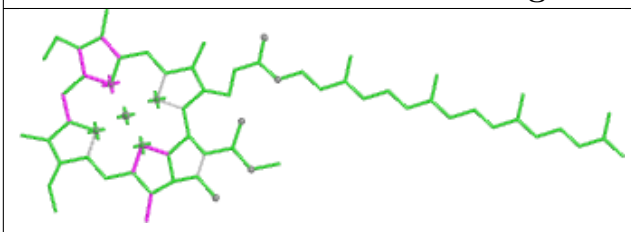


Rings

Ligand CLA 6 505



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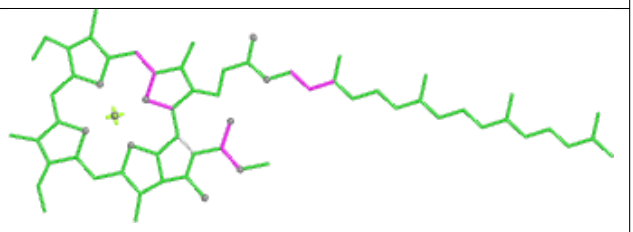

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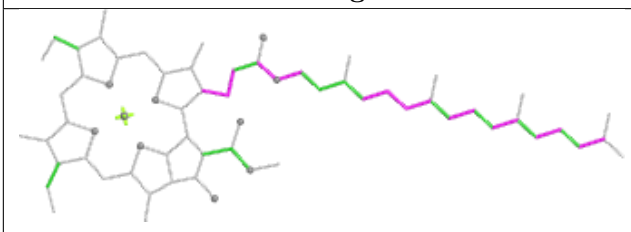

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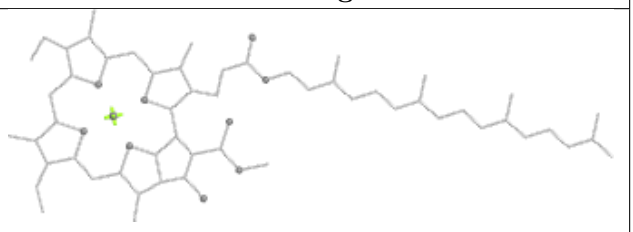
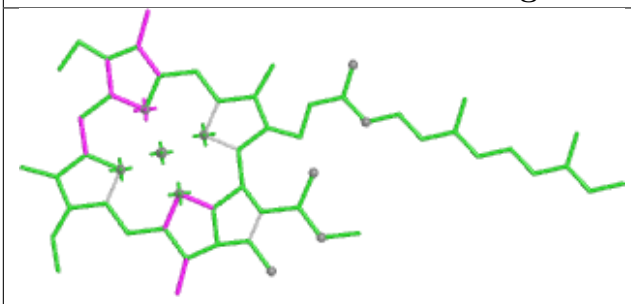
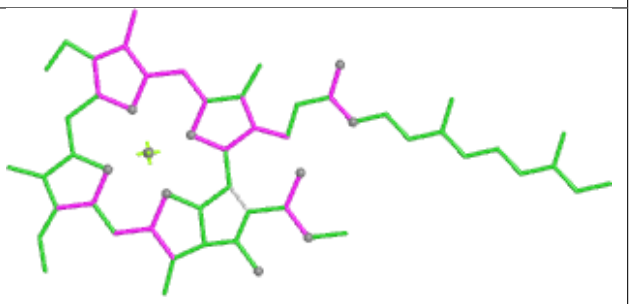
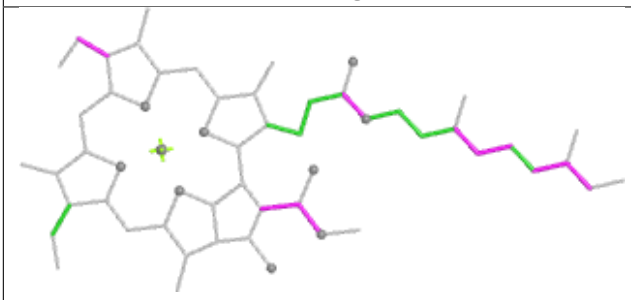
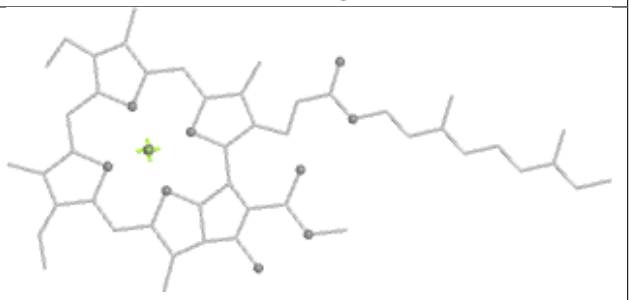


Rings

Ligand CLA e 1124	
	
Bond lengths	Bond angles
	
Torsions	Rings

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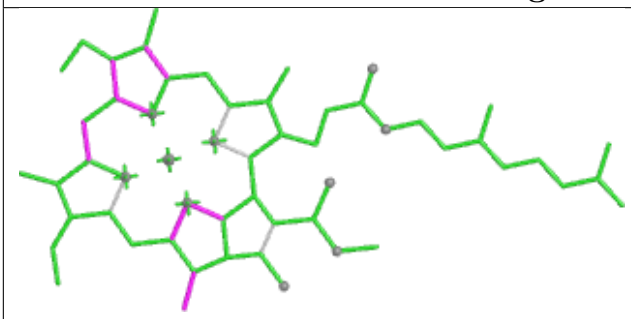
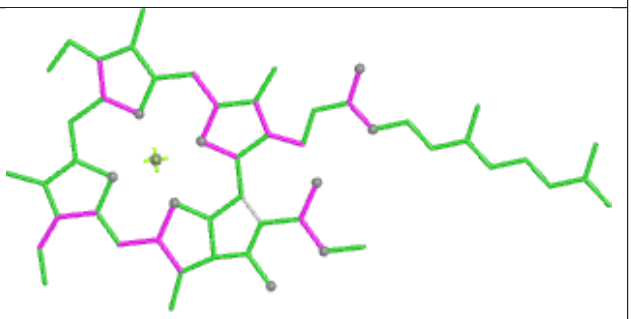
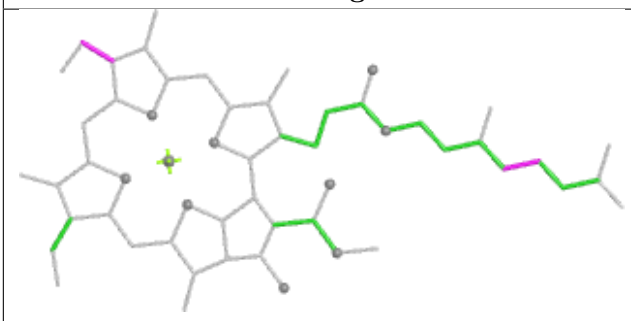
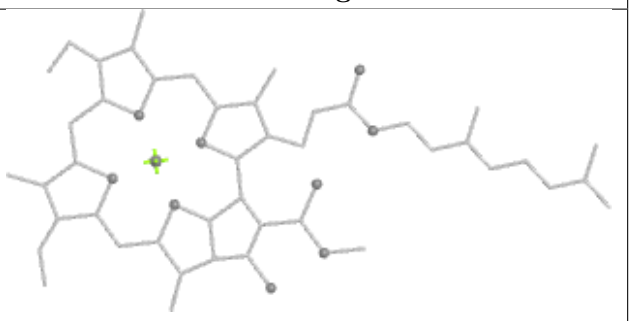
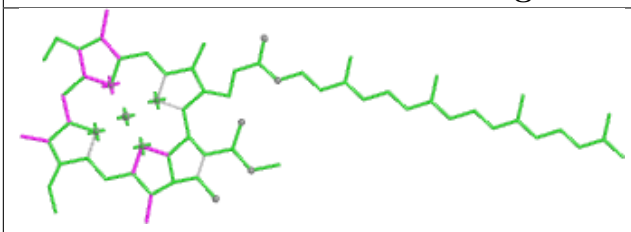
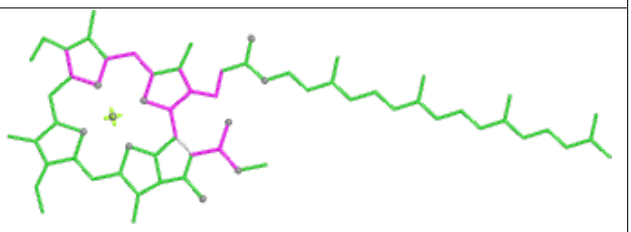
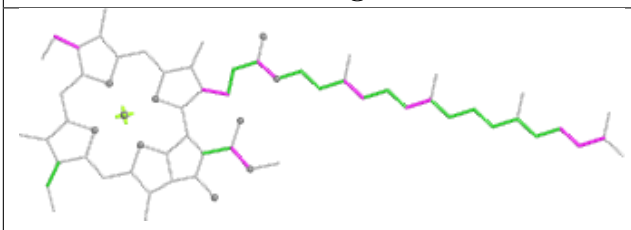
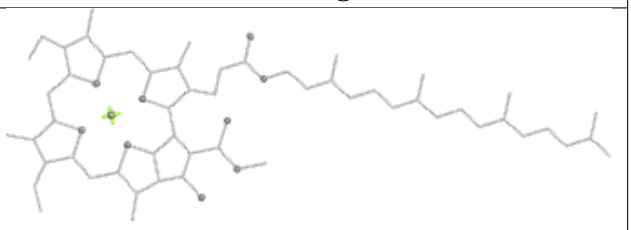
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1140	
 Bond lengths	 Bond angles
 Torsions	 Rings

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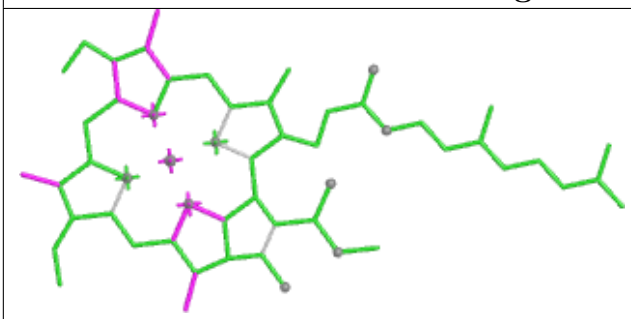
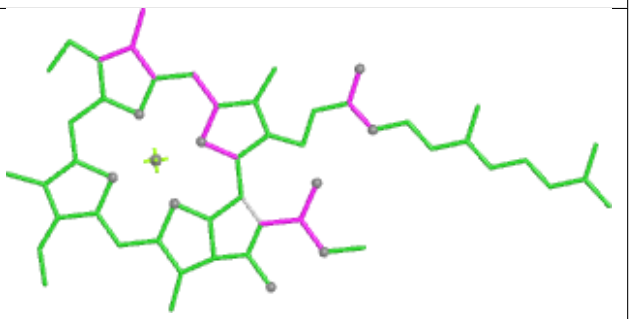
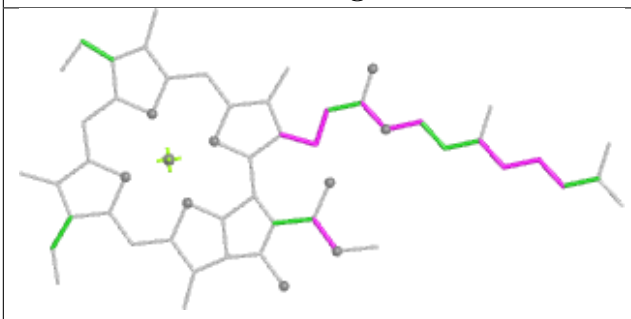
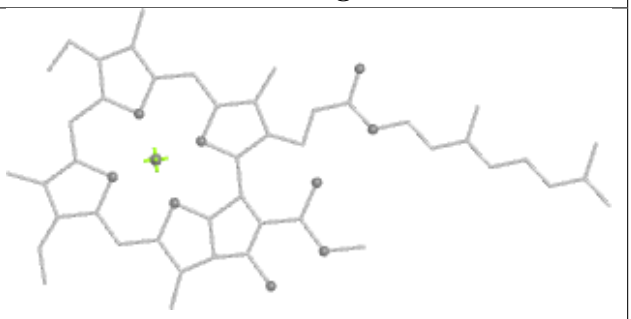
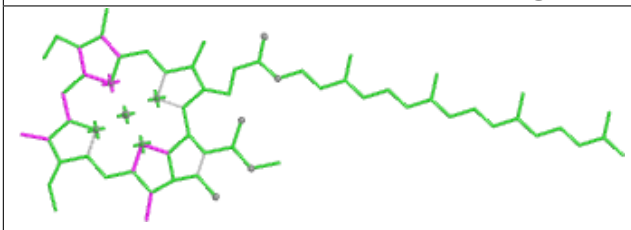
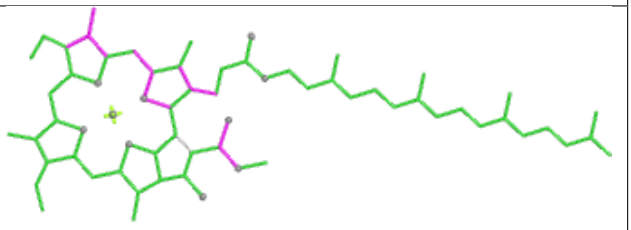
 Bond lengths	 Bond angles
 Torsions	 Rings

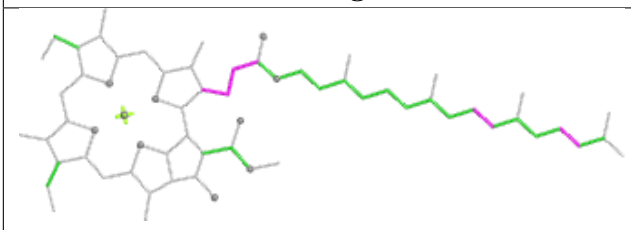
Ligand CLA s 501



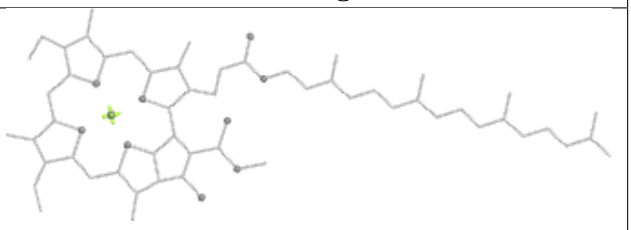
Bond lengths



Bond angles

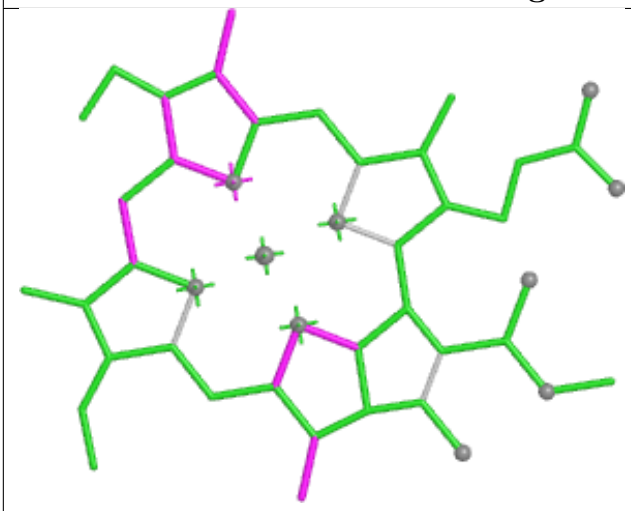


Torsions



Rings

Ligand CLA 5 516



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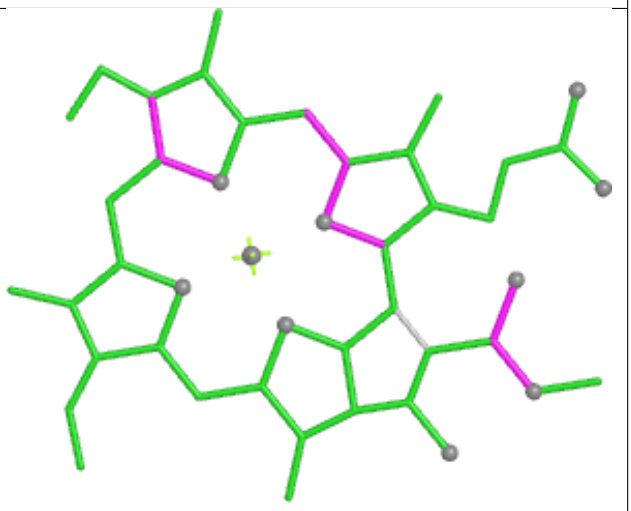
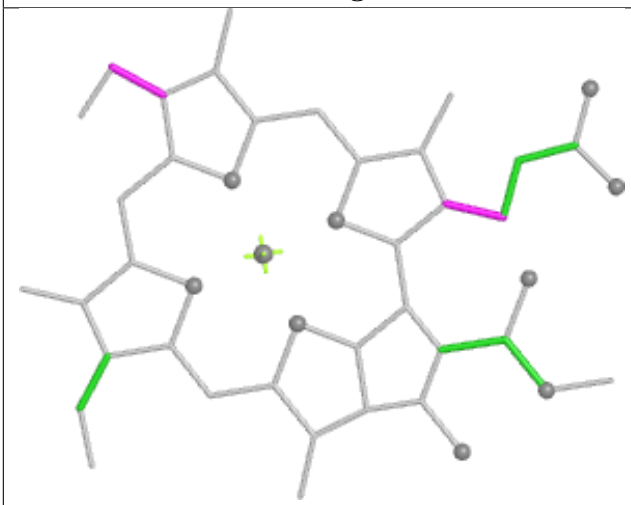
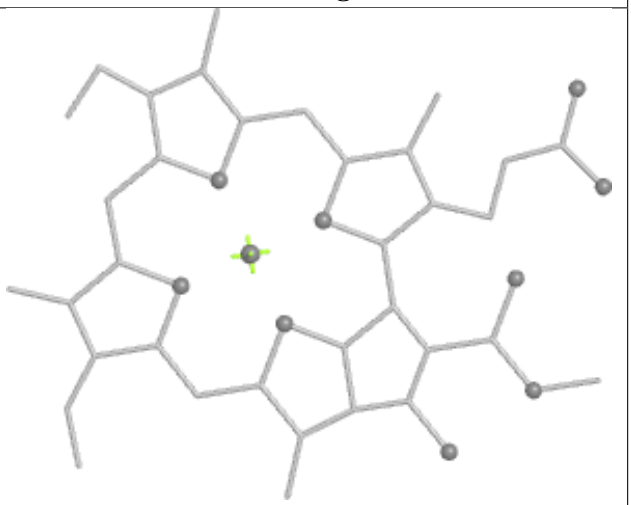


Bond angles

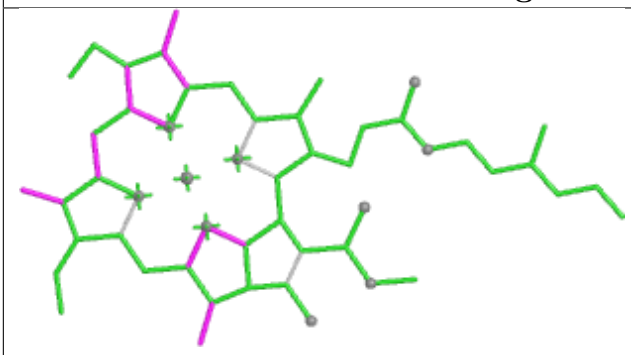


Torsions

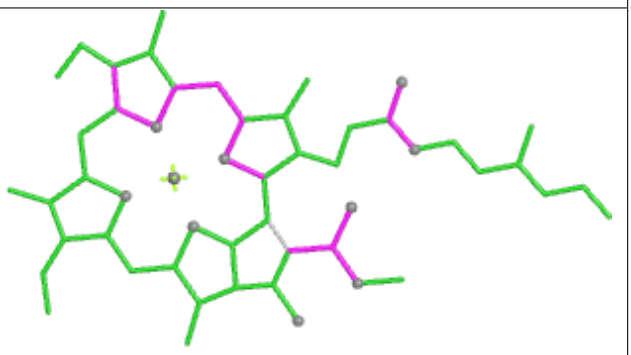


Rings

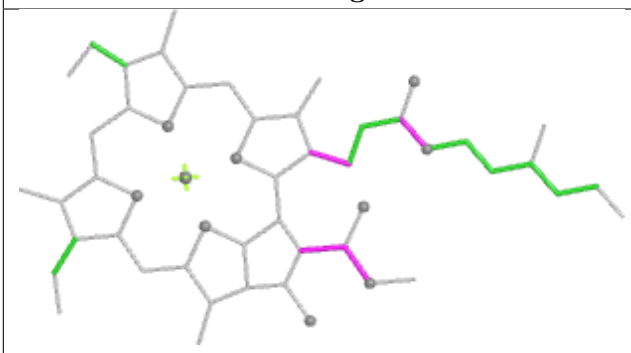
Ligand CLA B 1209



Bond lengths



Bond angles



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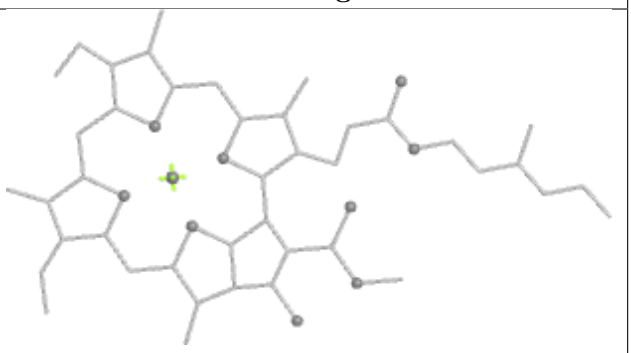
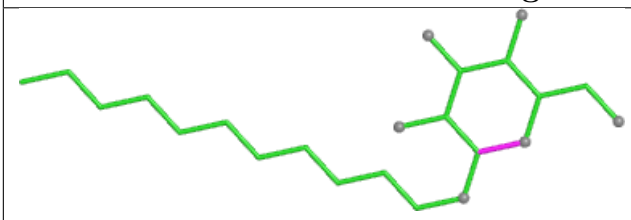


Rings

Ligand LMU Z 901



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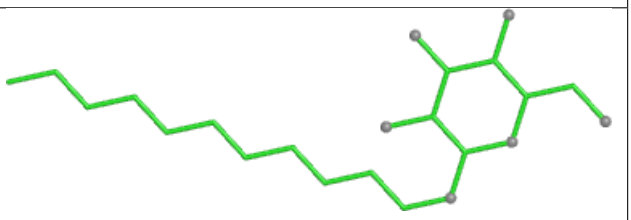
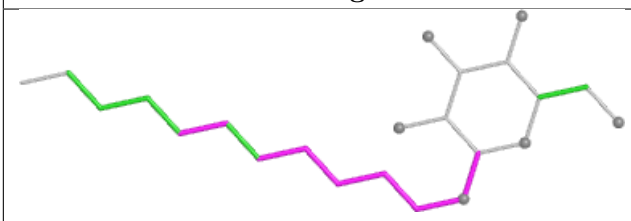


Bond angles



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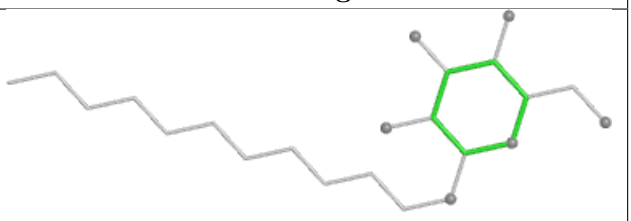
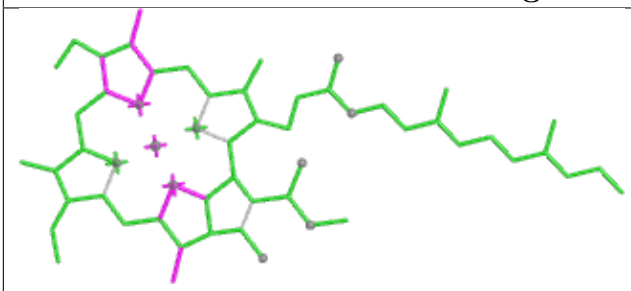


Rings

Ligand CLA f 1217



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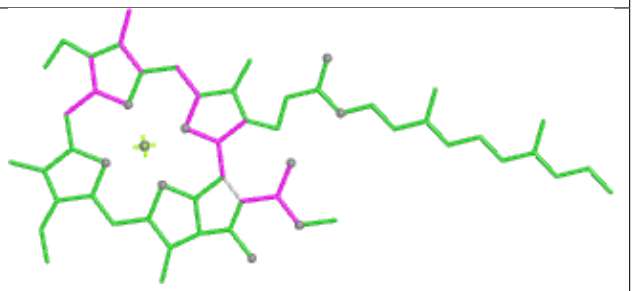
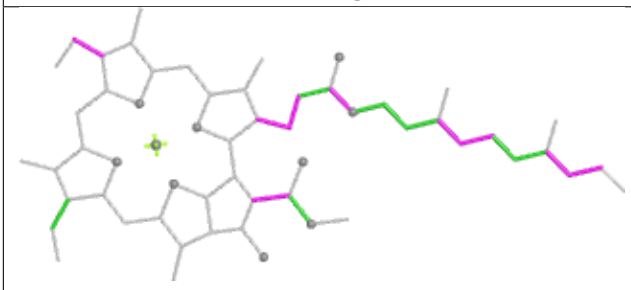


Bond angles



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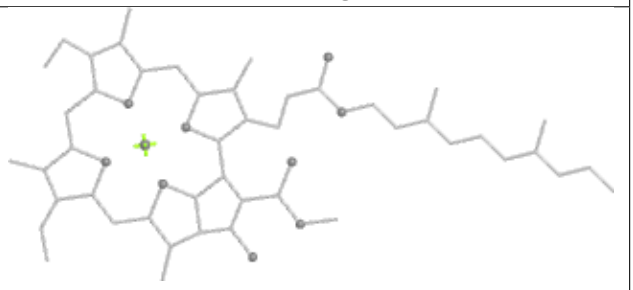
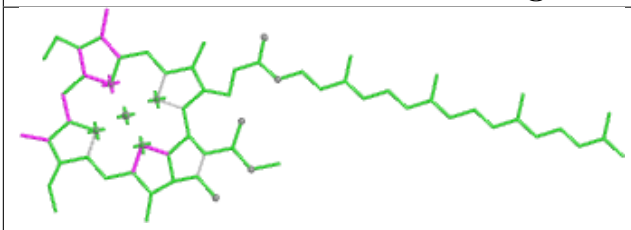


Rings

Ligand CLA u 501



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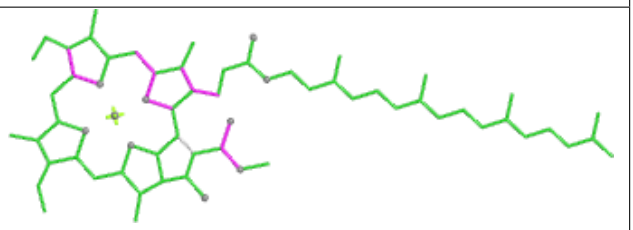
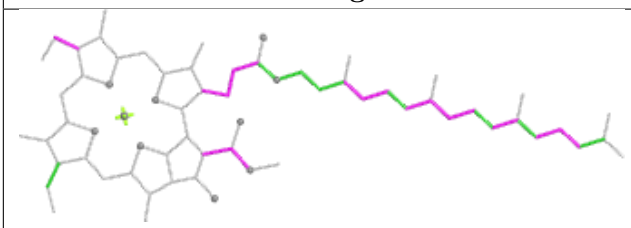


Bond angles



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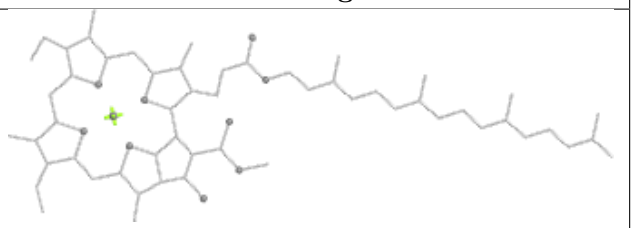
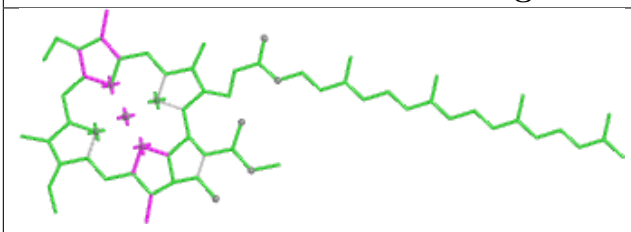


Rings

Ligand CLA A 1133



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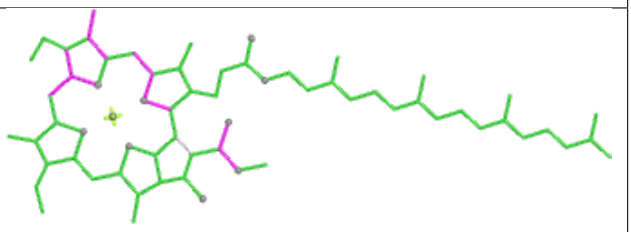

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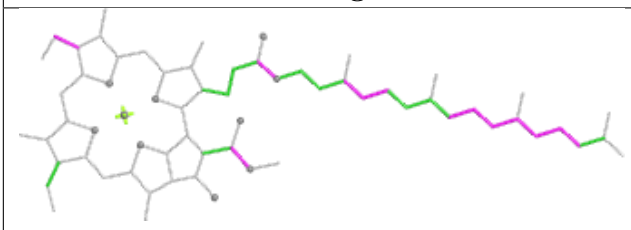

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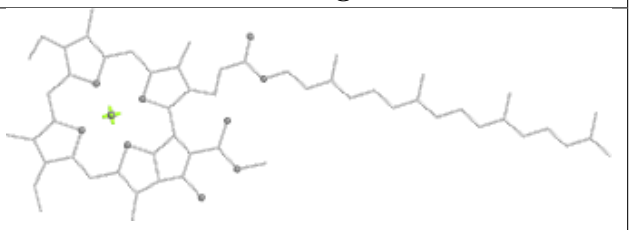
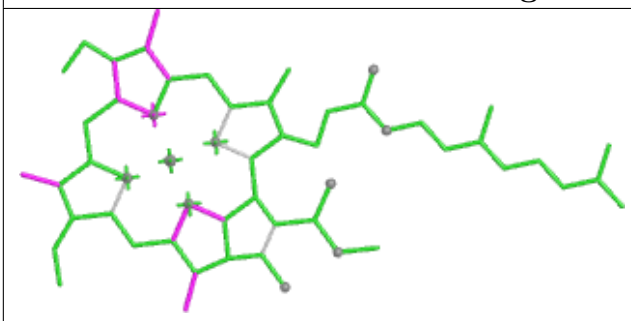


Rings

Ligand CLA e 1121



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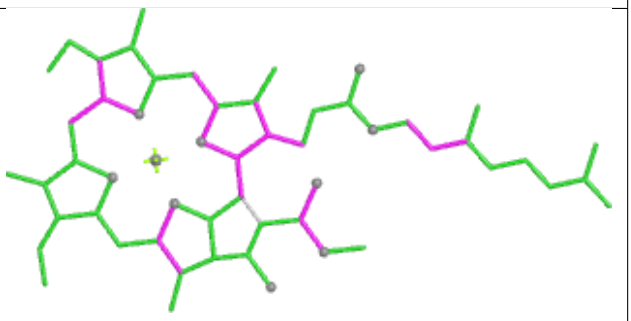

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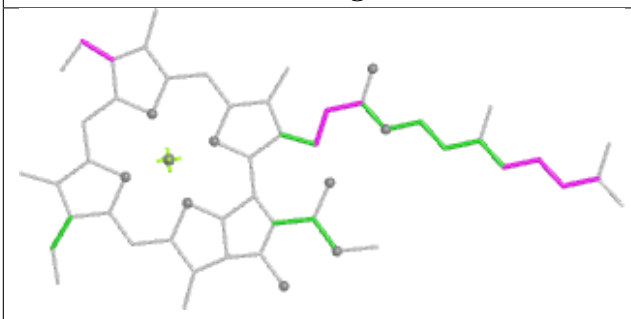

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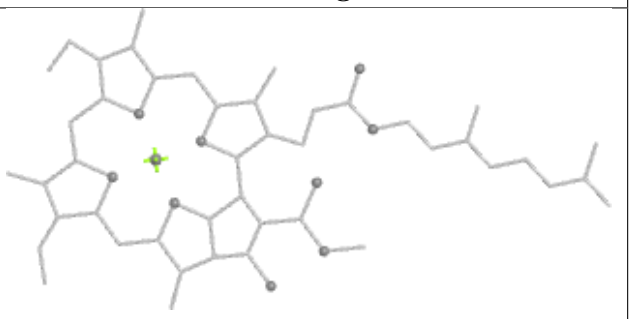
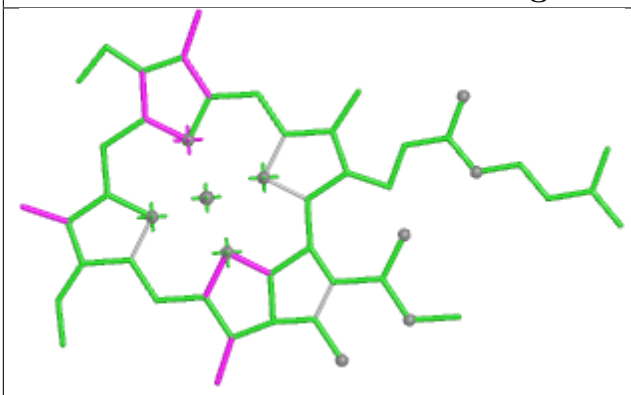


Rings

Ligand CLA s 506



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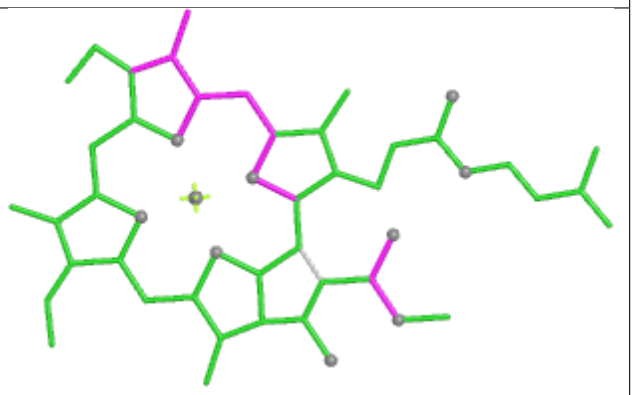
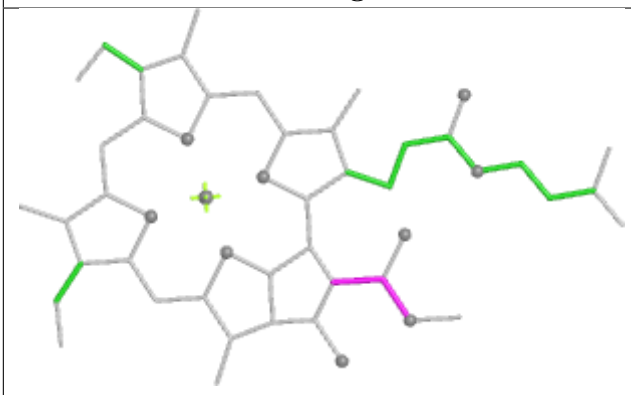


Bond angles



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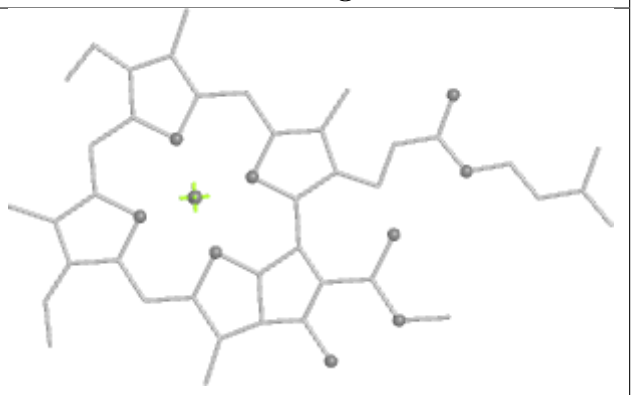
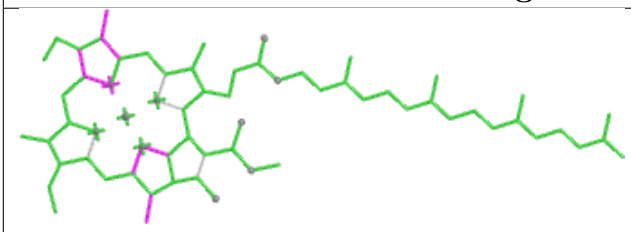


Rings

Ligand CLA B 1239



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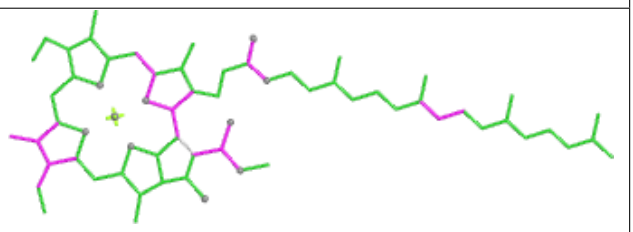
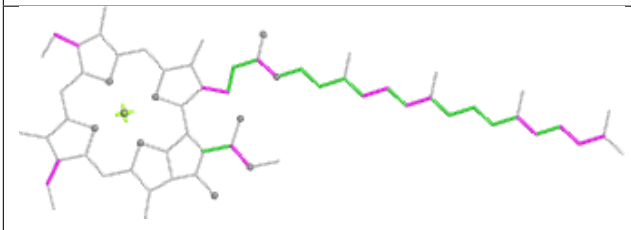


Bond angles



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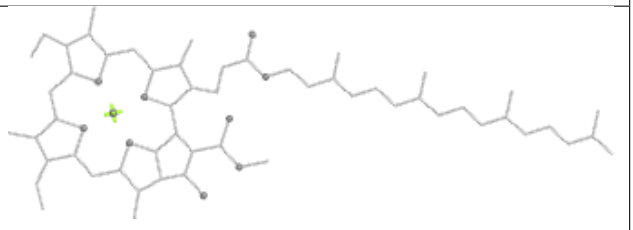
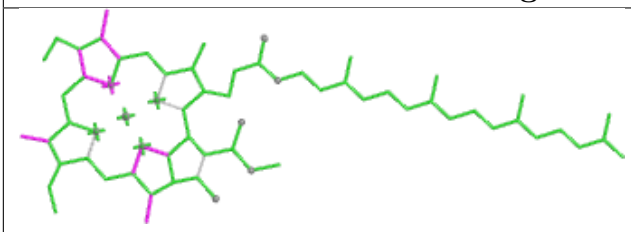


Rings

Ligand CLA e 1131



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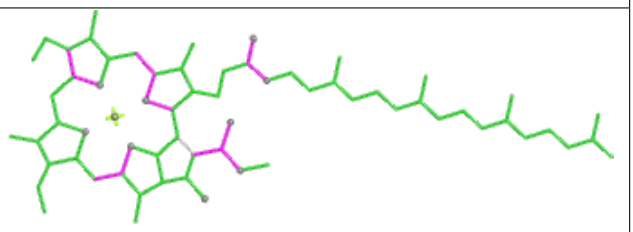
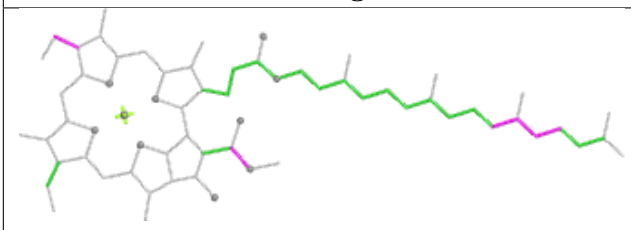


Bond angles



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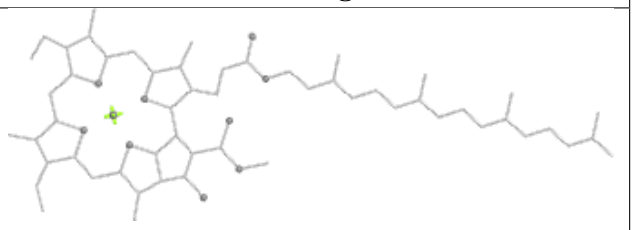
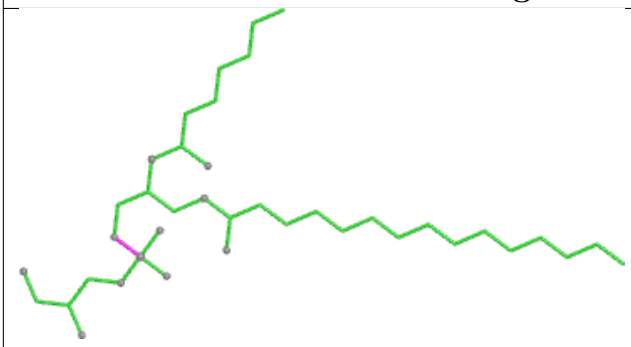


Rings

Ligand LHG A 5002



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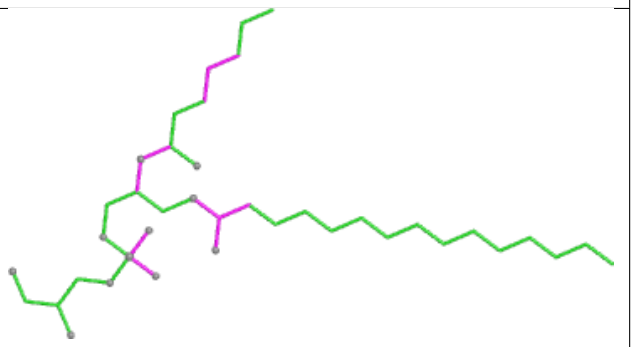
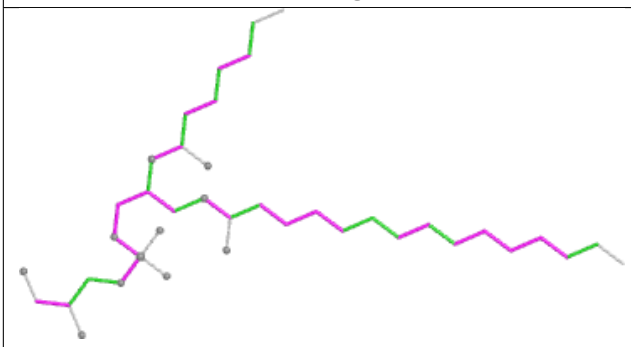


Bond angles



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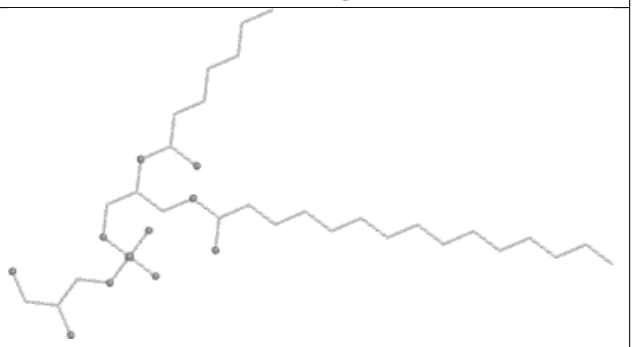
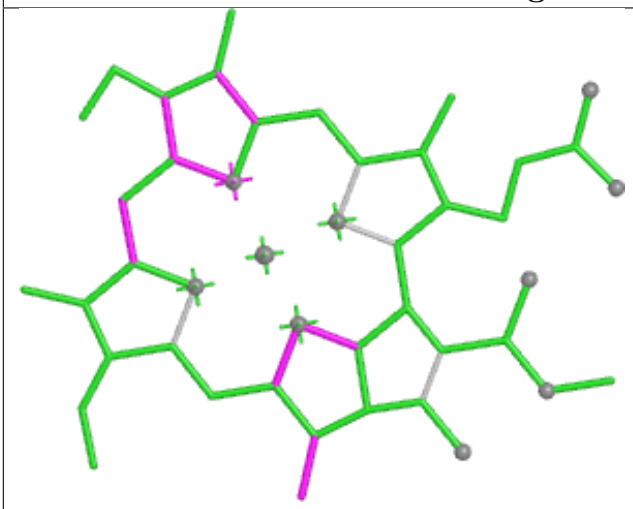


Rings

Ligand CLA q 516



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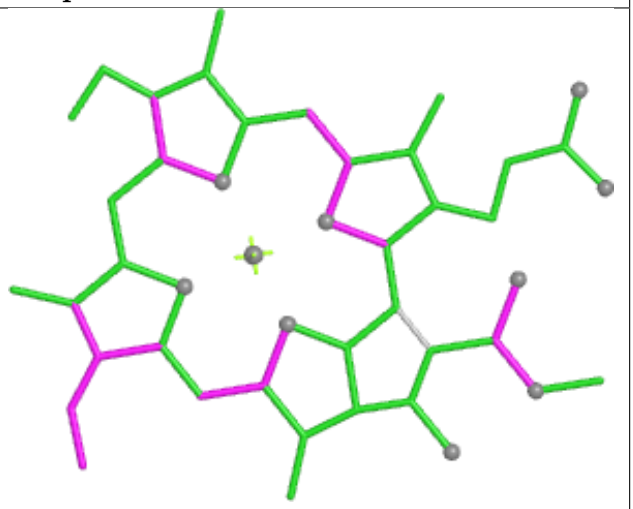
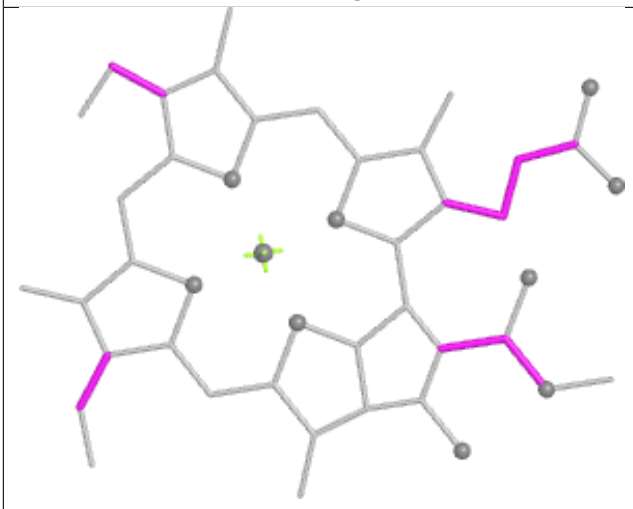


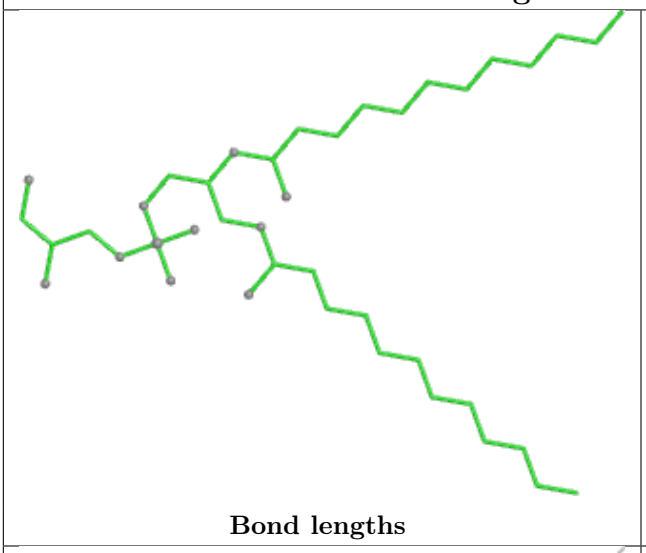
Bond angles



Torsions

Rings

Ligand LHG V 5220



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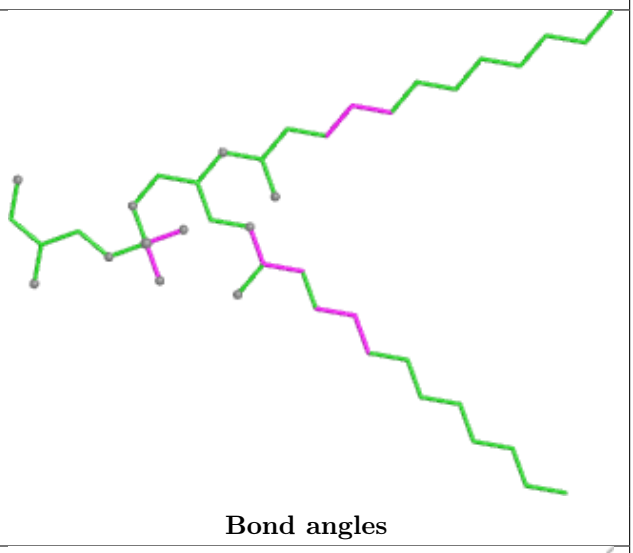
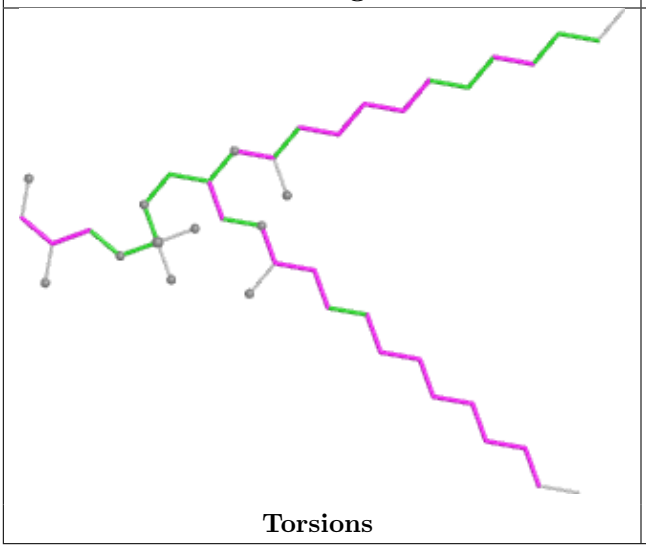
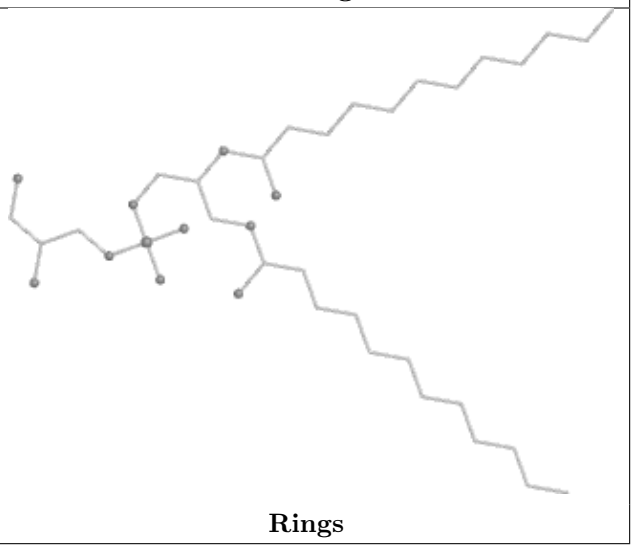


Bond angles

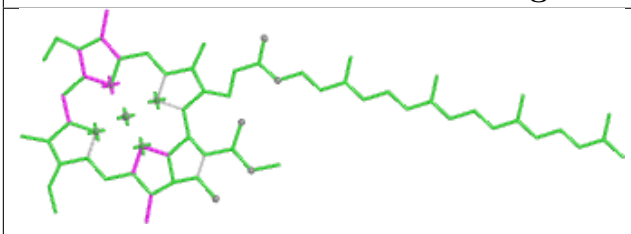


Torsions



Rings

Ligand CLA s 513



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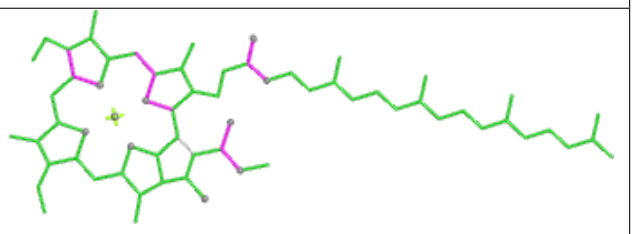
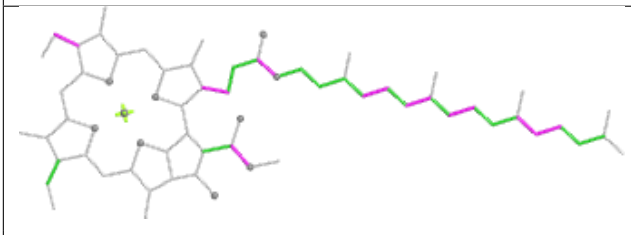


Bond angles



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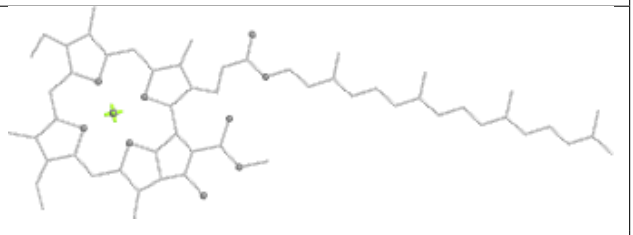
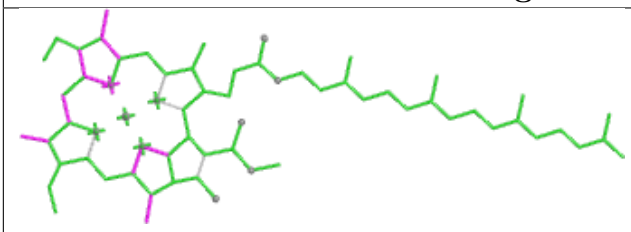
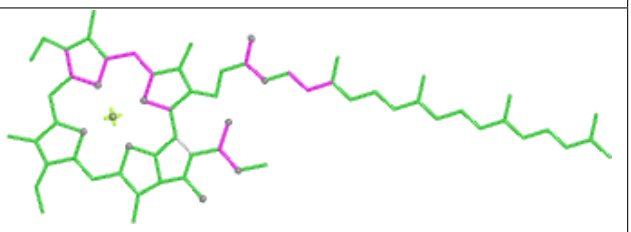


Rings

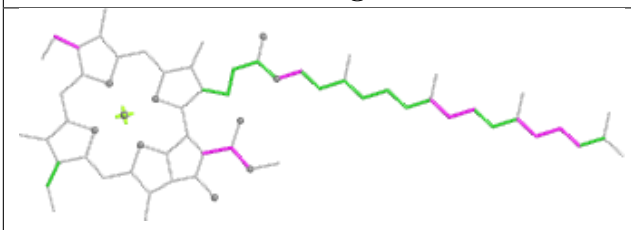
Ligand CLA A 1138



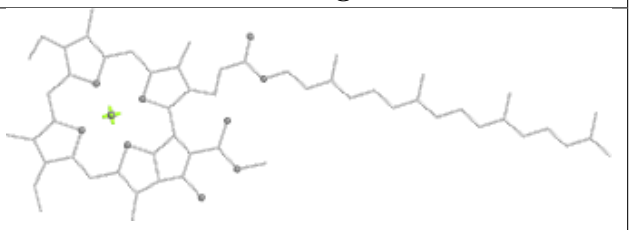
Bond lengths



Bond angles

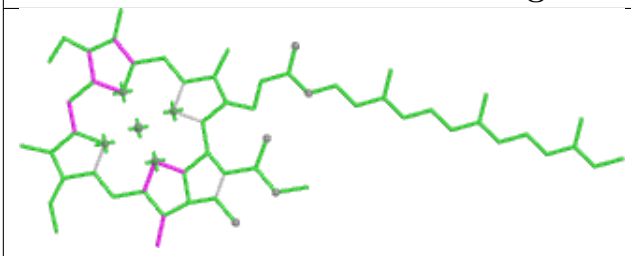


Torsions



Rings

Ligand CLA u 505



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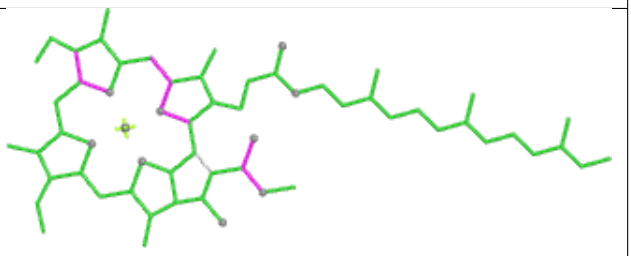
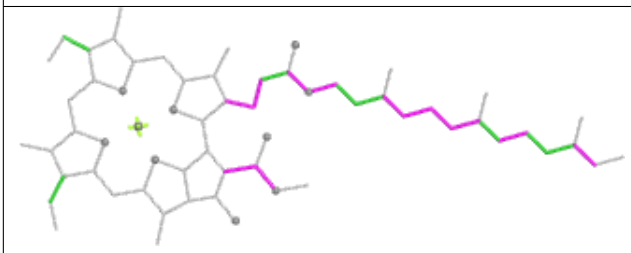


Bond angles



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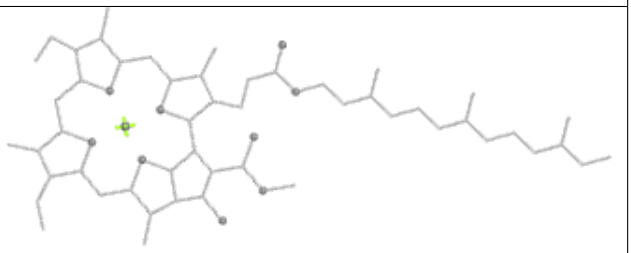
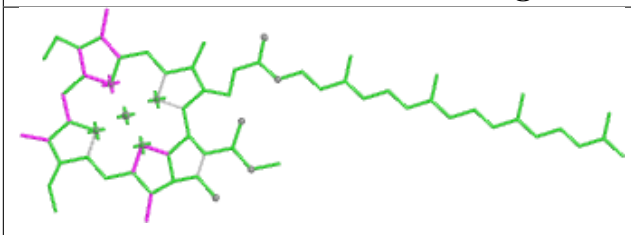


Rings

Ligand CLA H 1207



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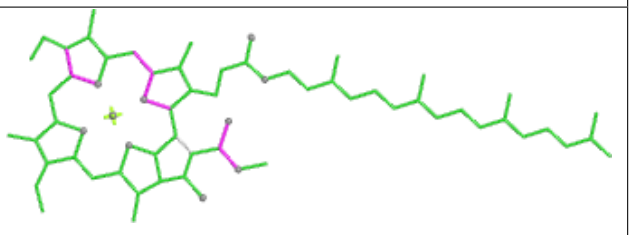

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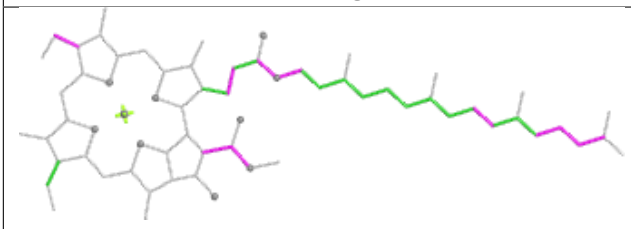

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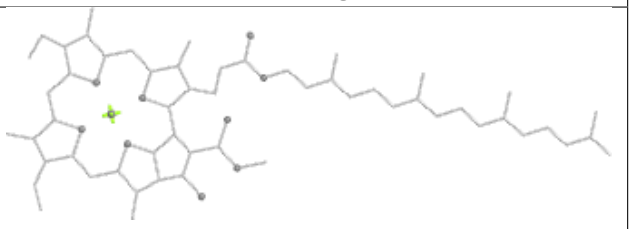
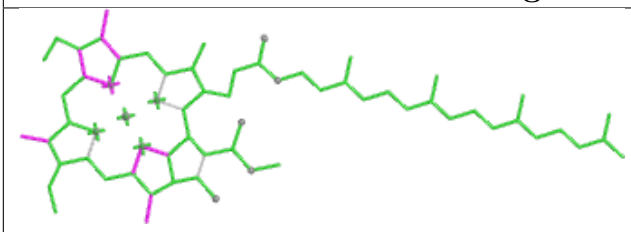


Rings

Ligand CLA l 1303



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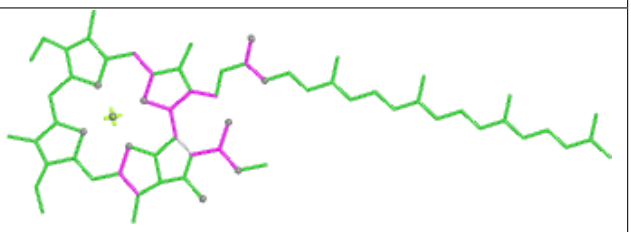
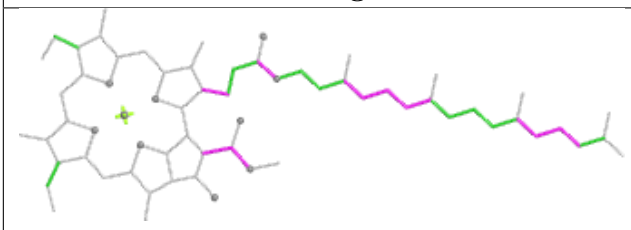


Bond angles



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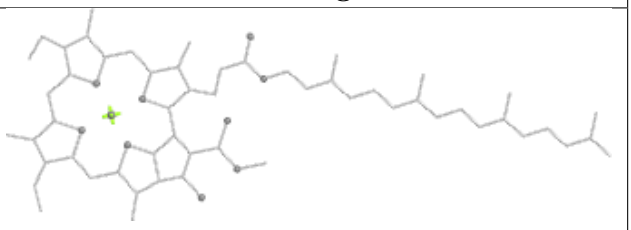
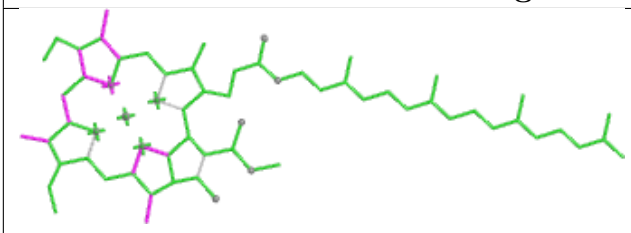


Rings

Ligand CLA A 1125



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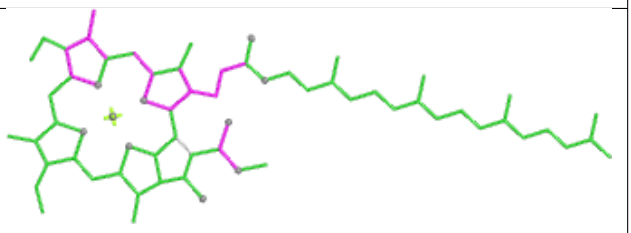

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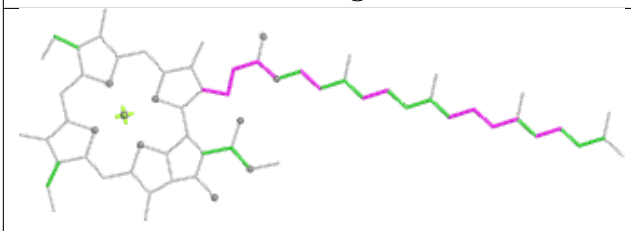

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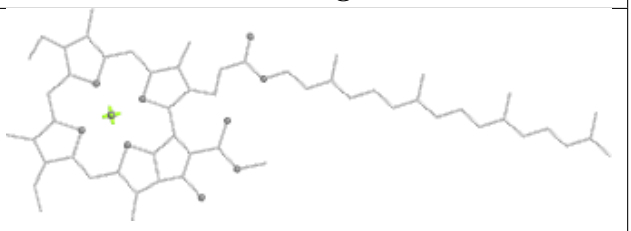
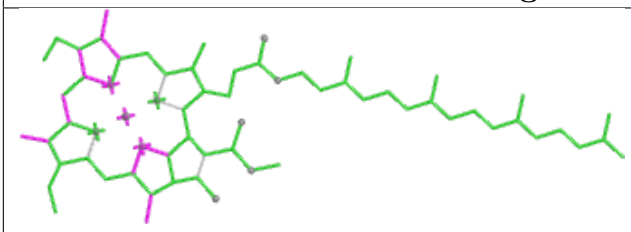


Rings

Ligand CLA e 1132



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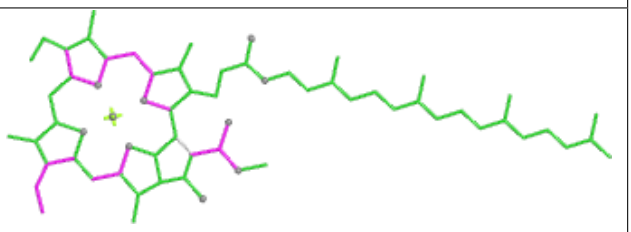
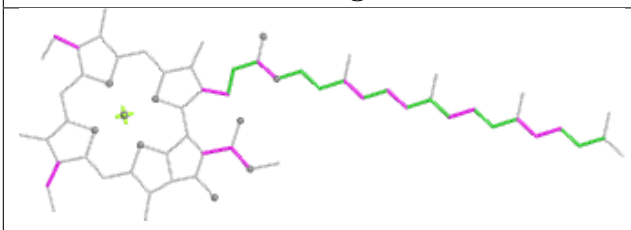


Bond angles



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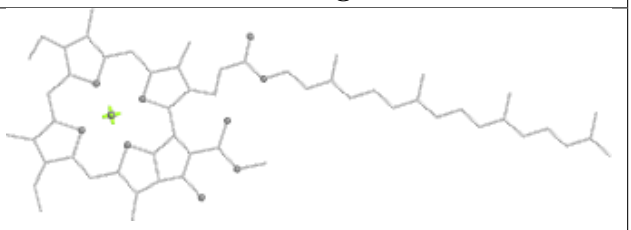
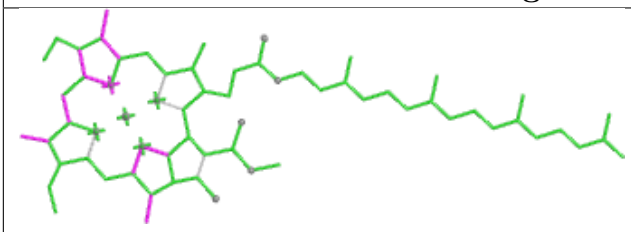
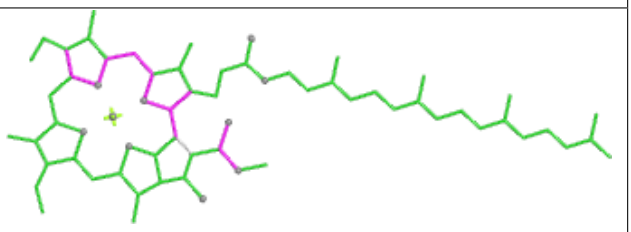
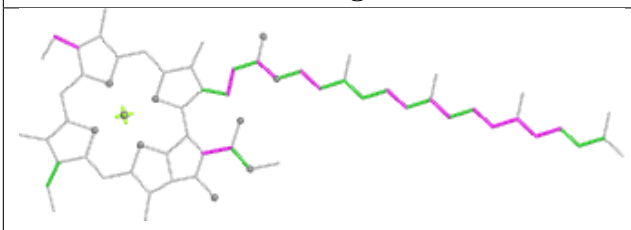
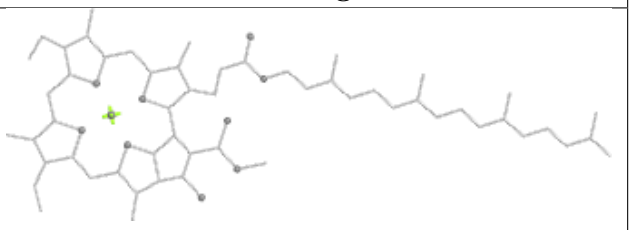


Rings

Ligand CLA f 1214	
	
Bond lengths	Bond angles
	
Torsions	Rings

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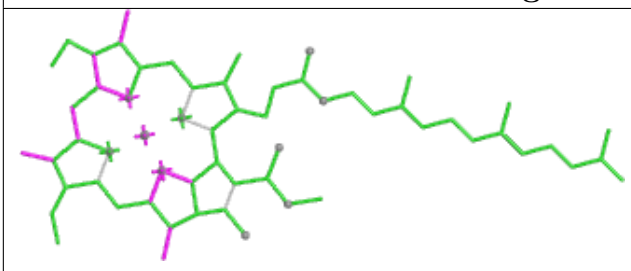
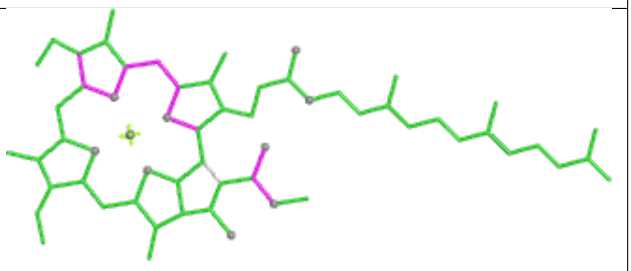
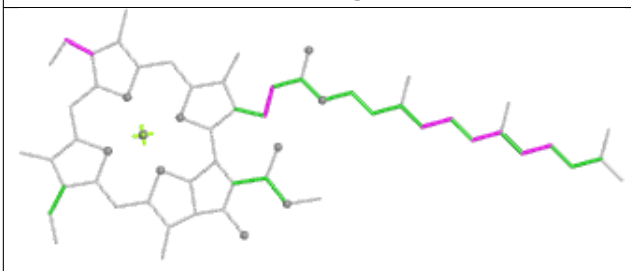
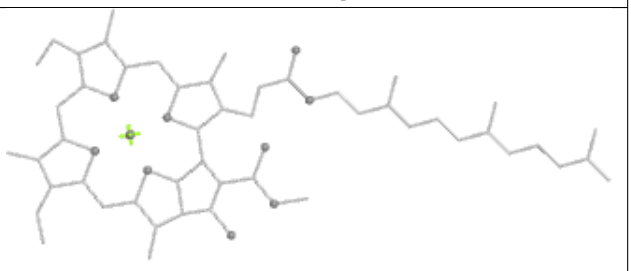
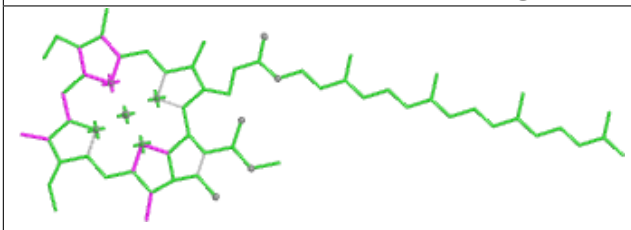
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1202



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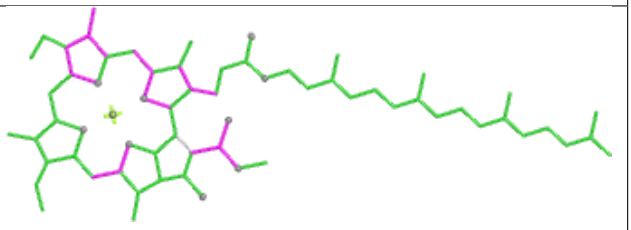
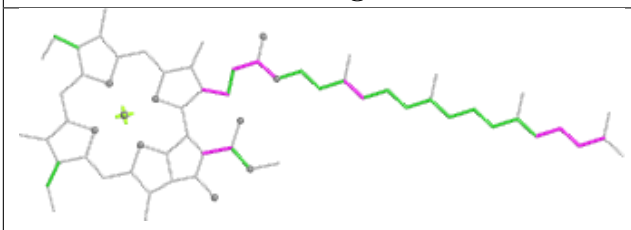


Bond angles



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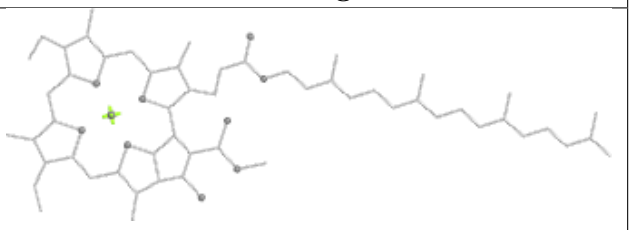
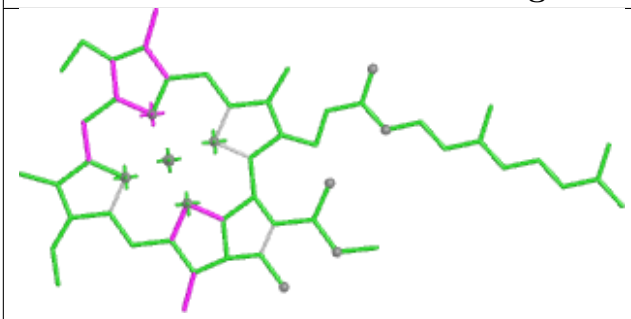


Rings

Ligand CLA 2 511



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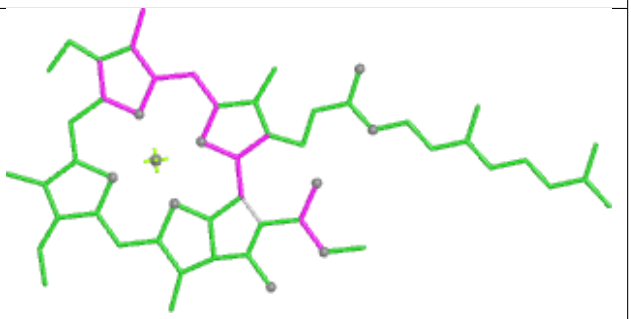
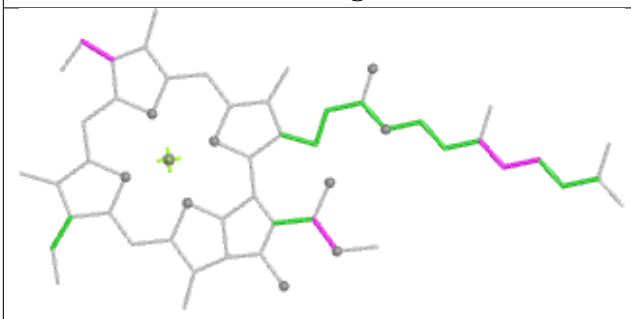


Bond angles



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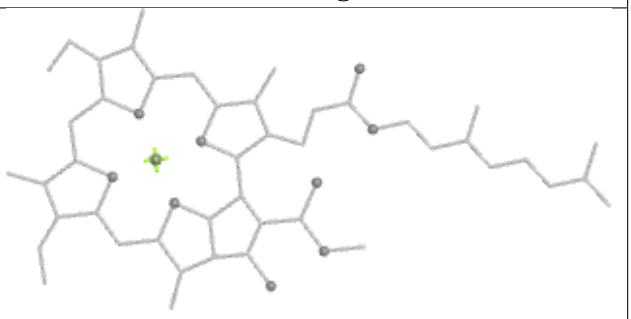
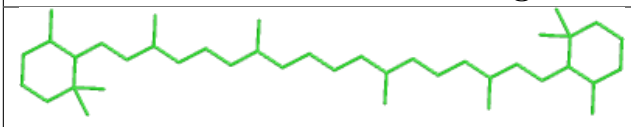


Rings

Ligand BCR V 4219



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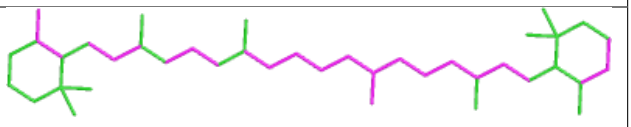
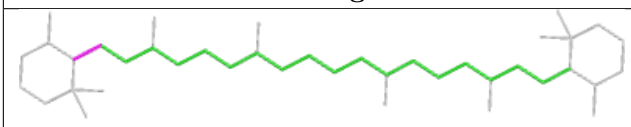
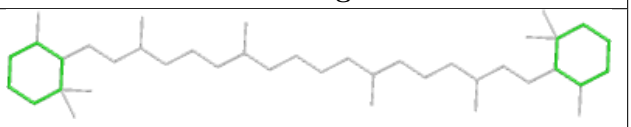


Bond angles

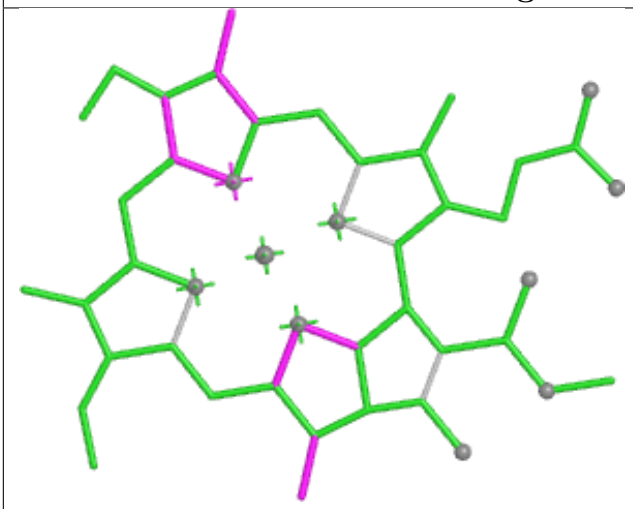


Torsions

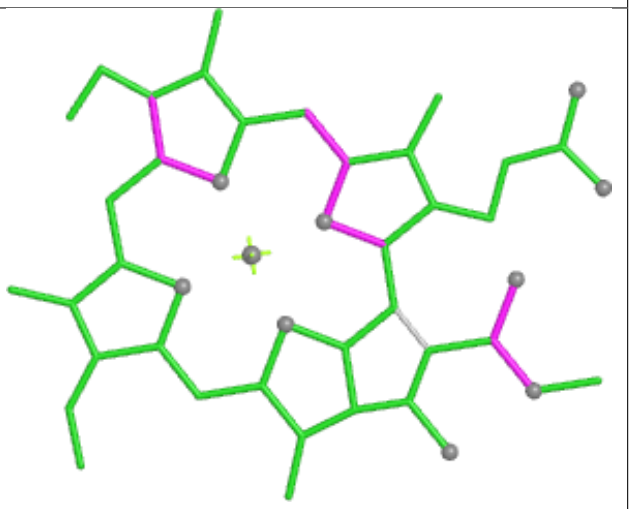


Rings

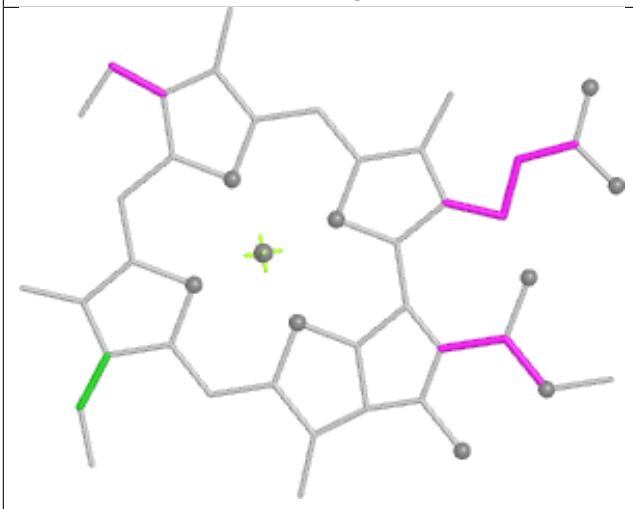
Ligand CLA F 1302



Bond lengths



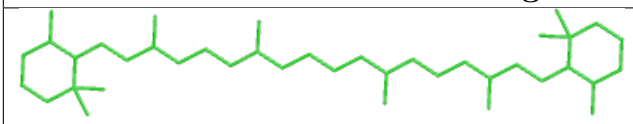
Bond angles



Torsions

Rings

Ligand BCR Y 522



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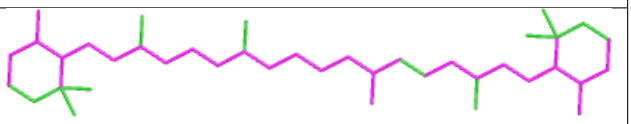
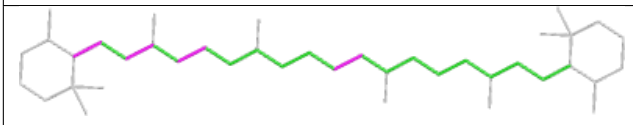
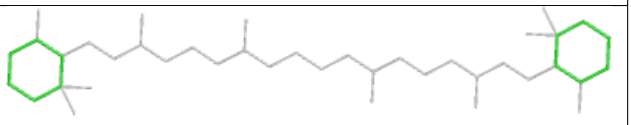


Bond angles

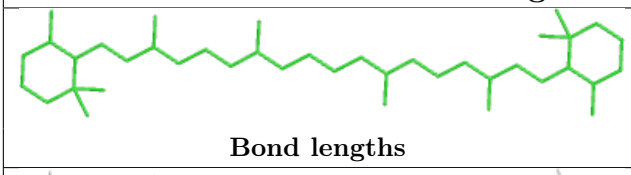


Torsions

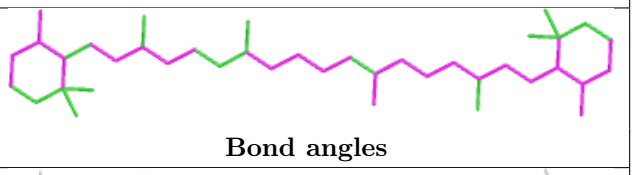


Rings

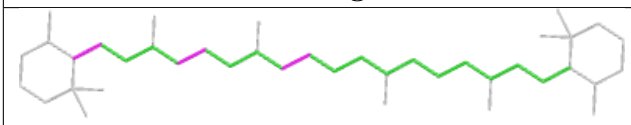
Ligand BCR t 522



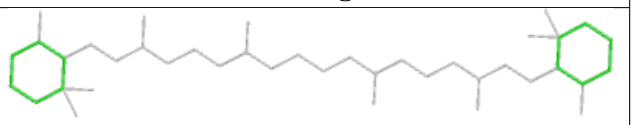
Bond lengths



Bond angles



Torsions



Rings

Ligand SQD Z 822

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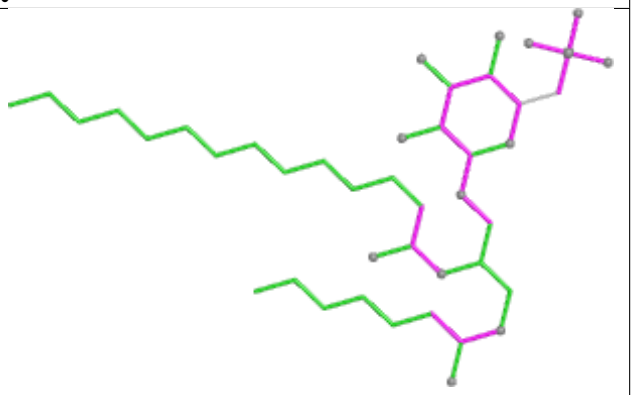

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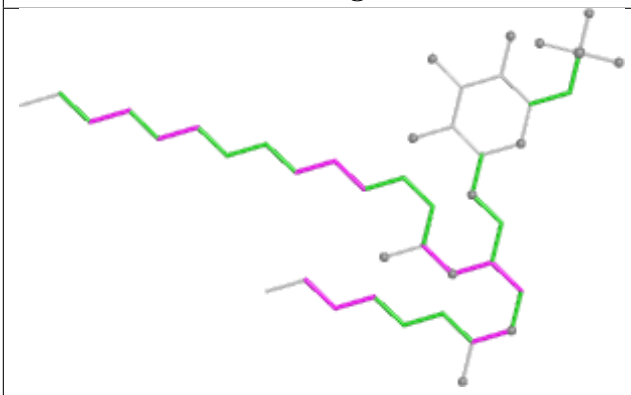

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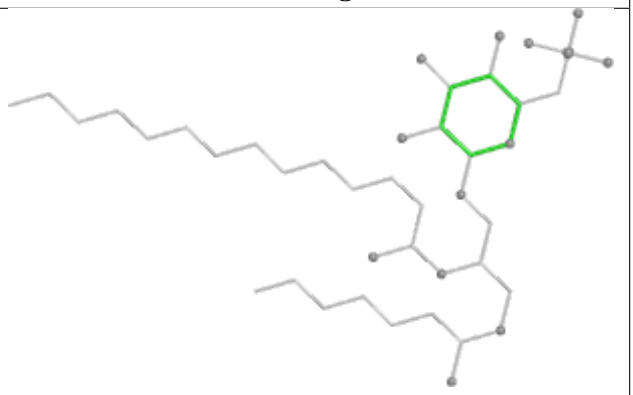
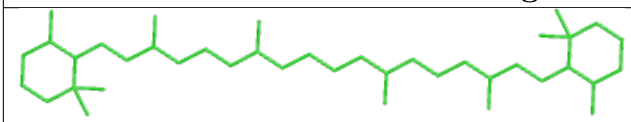


Rings

Ligand BCR f 4004



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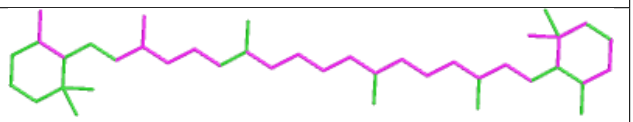
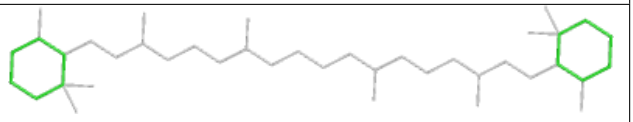


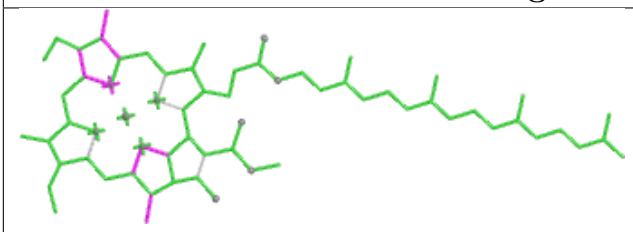
Bond angles

Torsions



Rings

Ligand CLA 2 507



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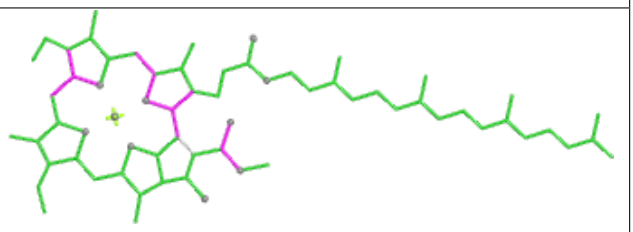

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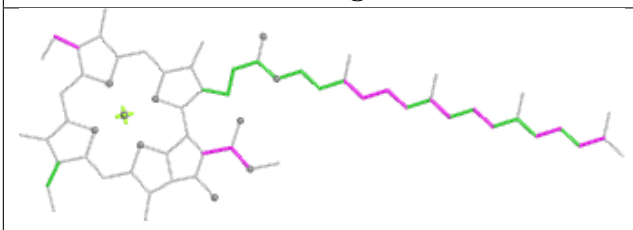

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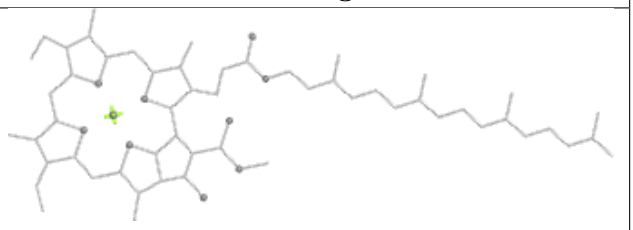
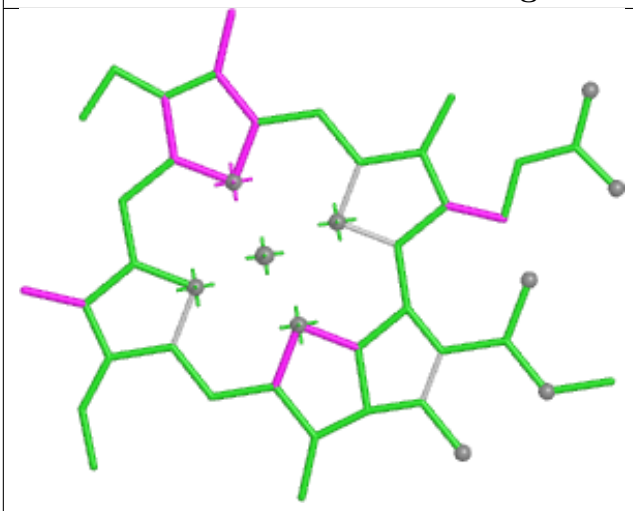


Rings

Ligand CLA e 1801



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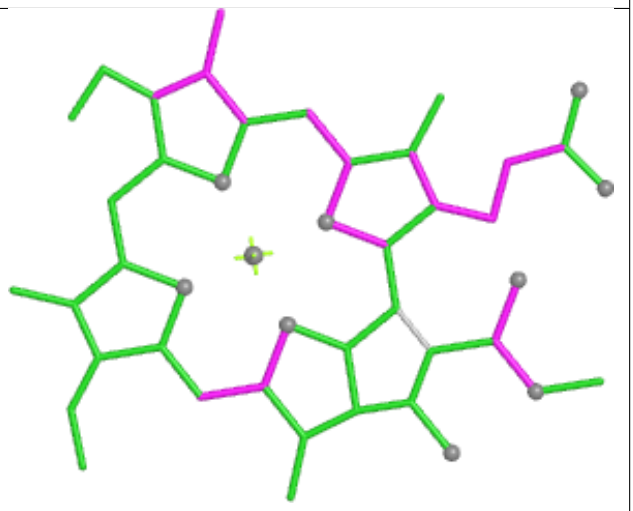

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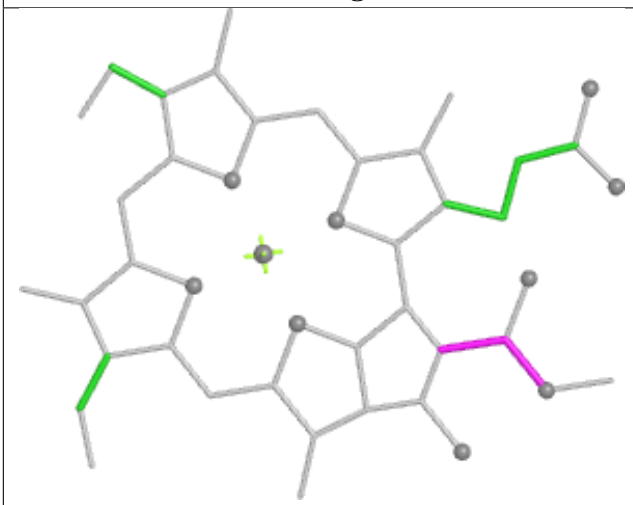

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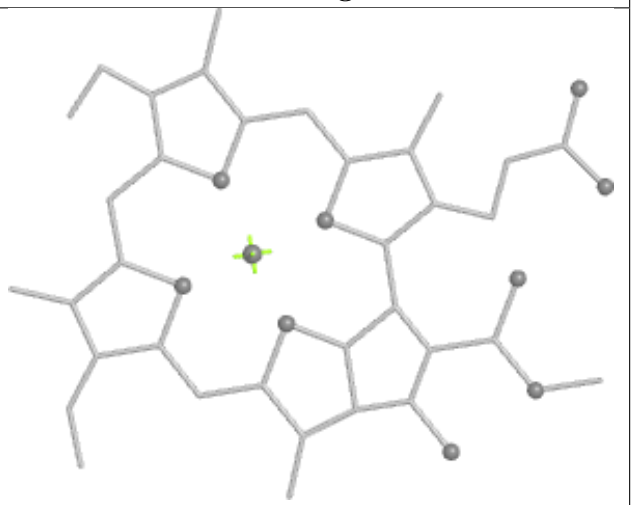
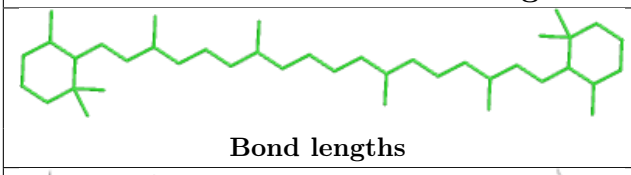


Rings

Ligand BCR l 4012



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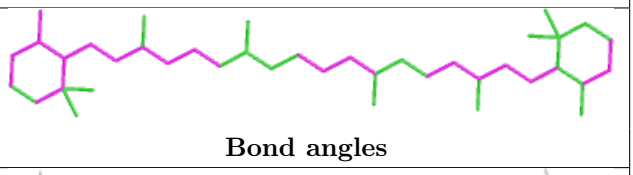

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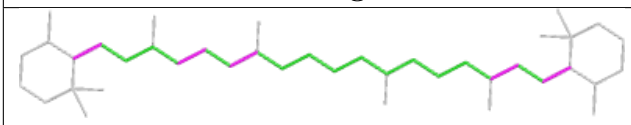

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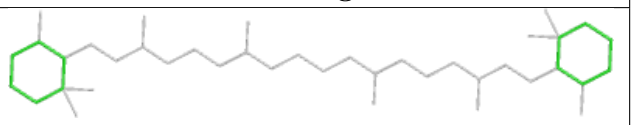

Rings

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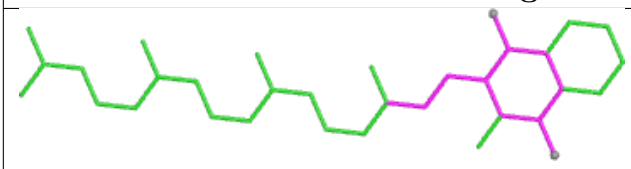

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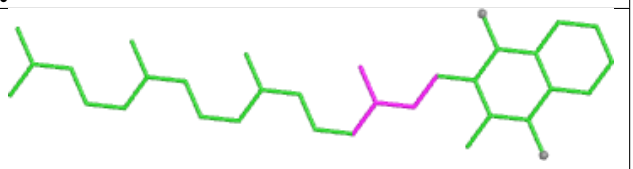

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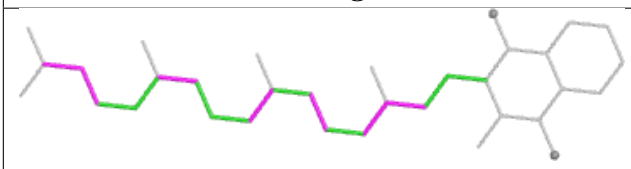

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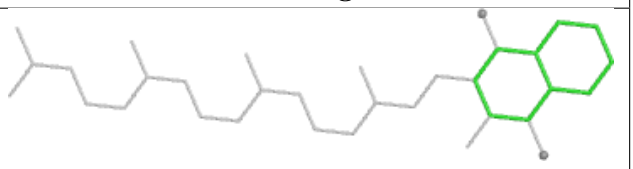
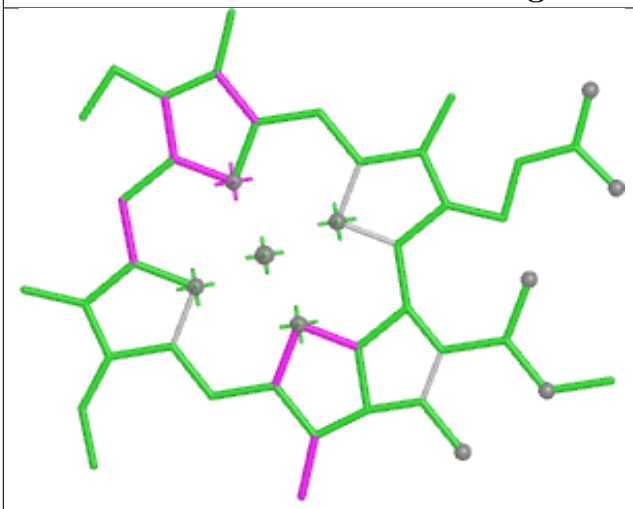


Rings

Ligand CLA u 516



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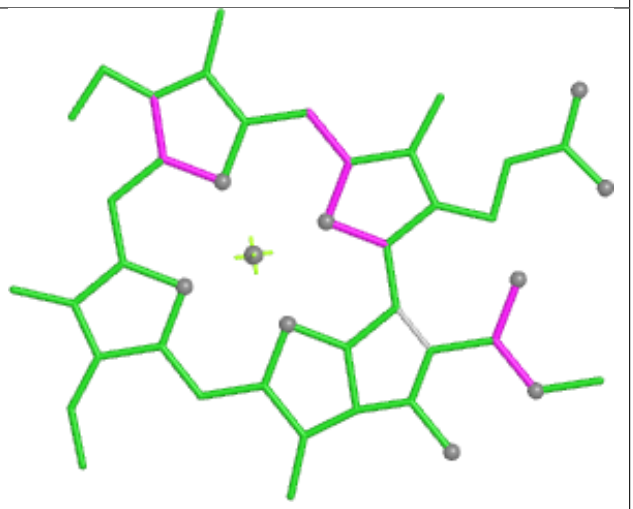

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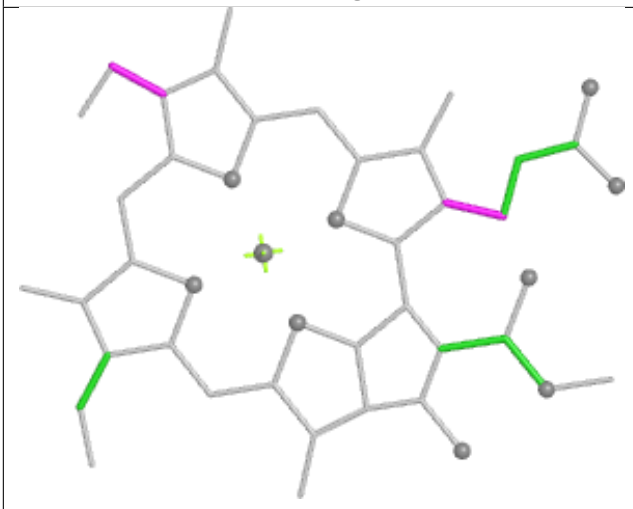
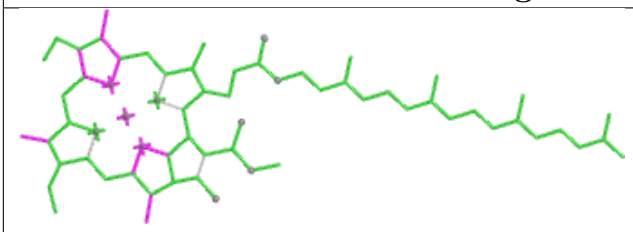


Torsions

Rings

Ligand CLA A 1107



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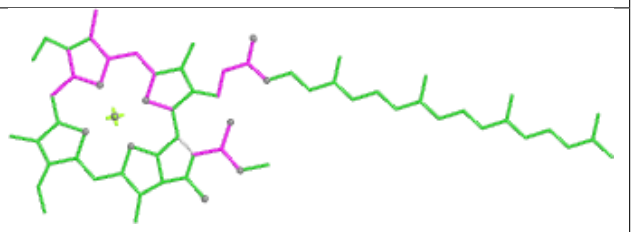

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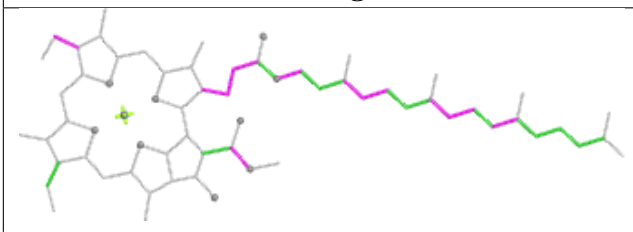

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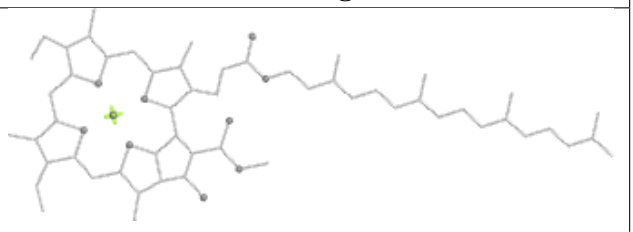

Rings

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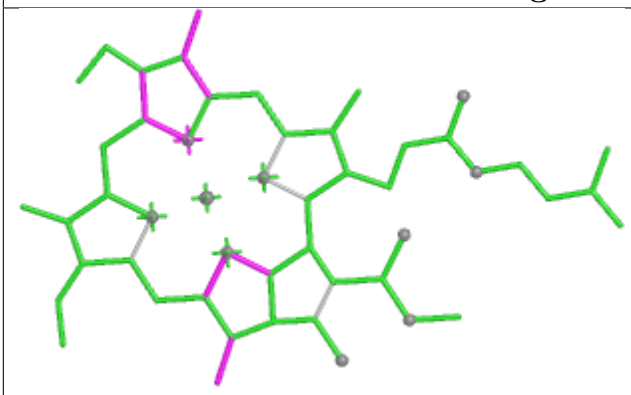

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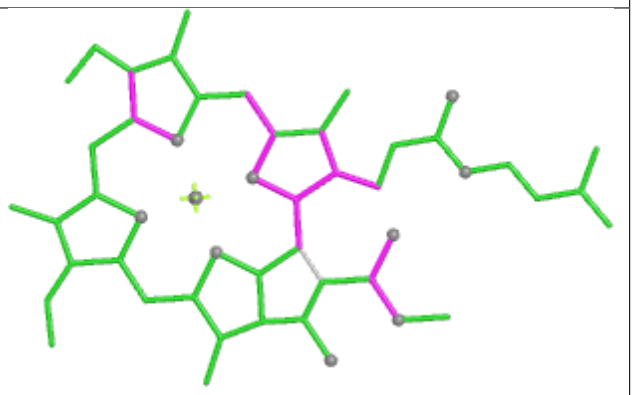

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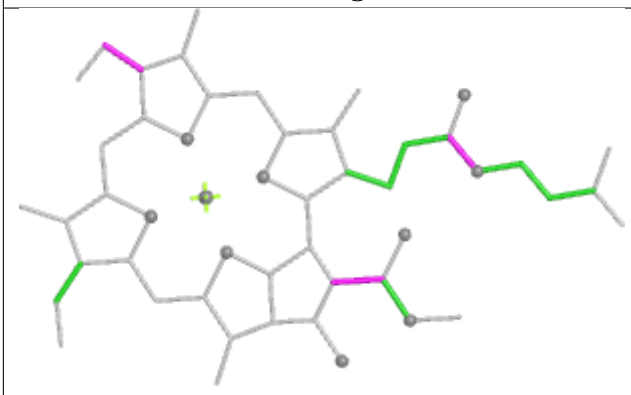

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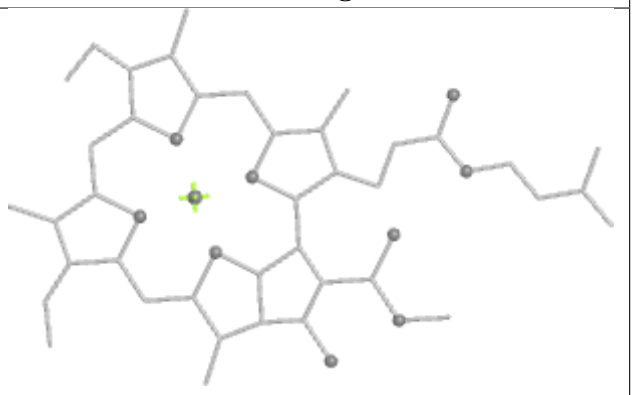

Rings

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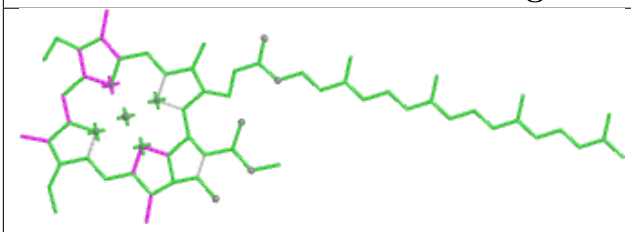

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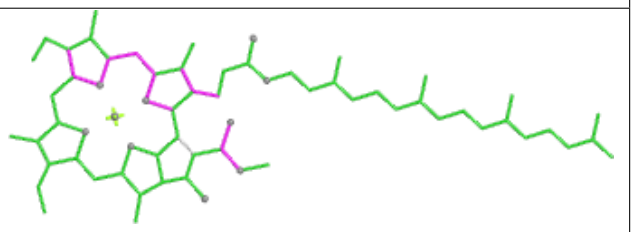

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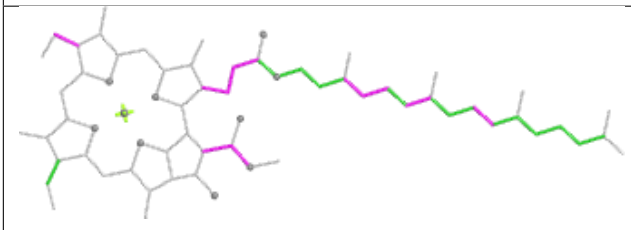

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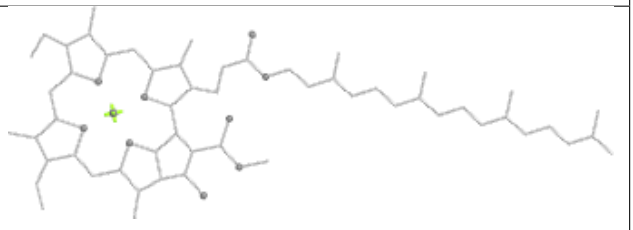

Rings

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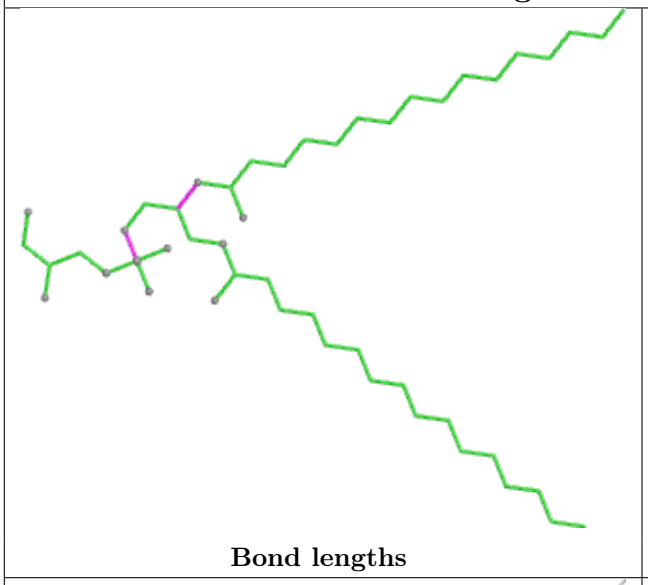

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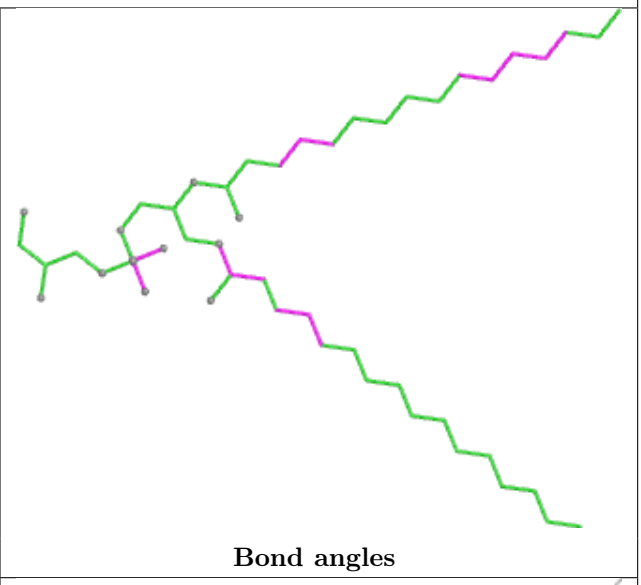
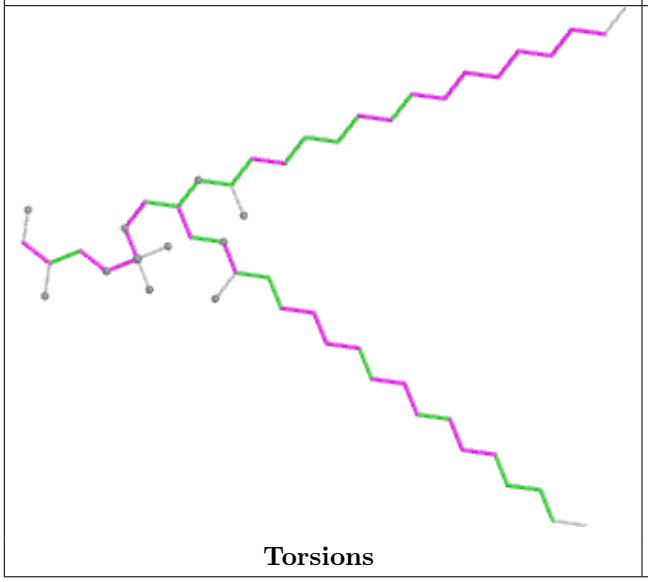


Bond angles



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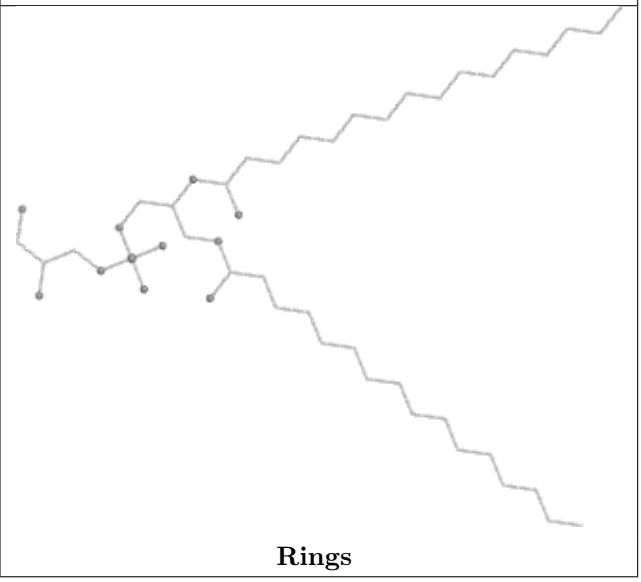

Rings

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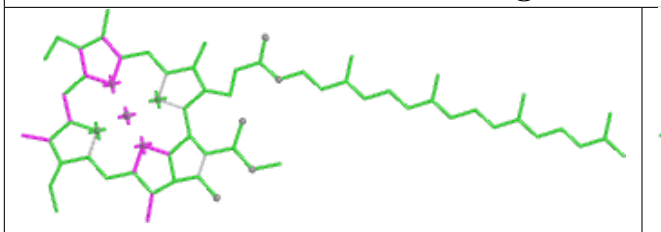

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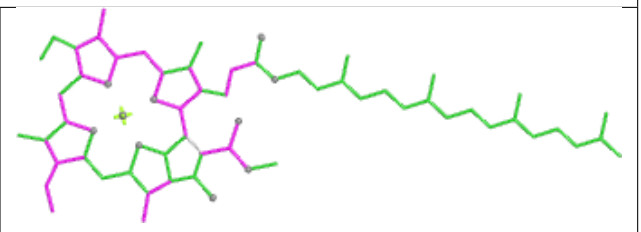
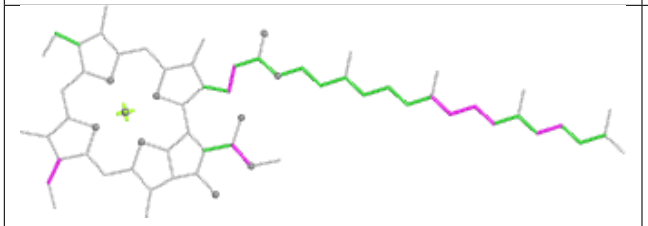


Bond angles



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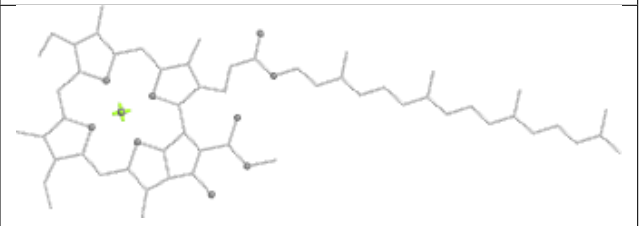
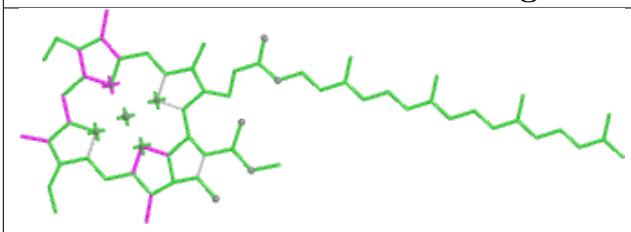


Rings

Ligand CLA e 1130



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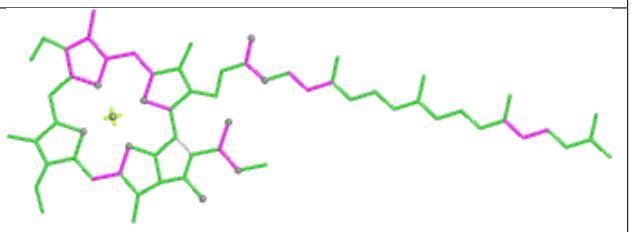
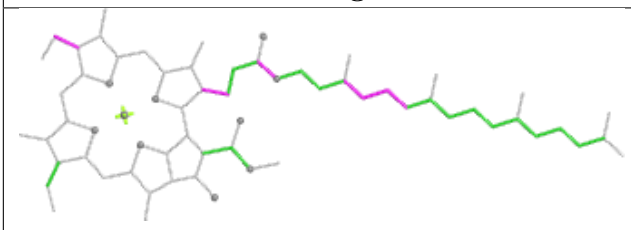


Bond angles



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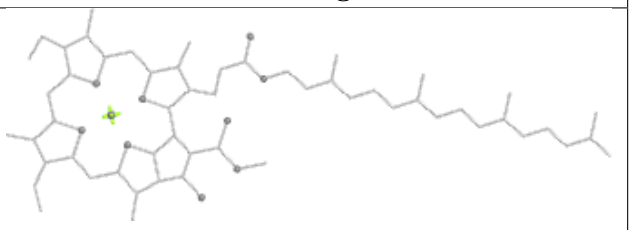

Rings

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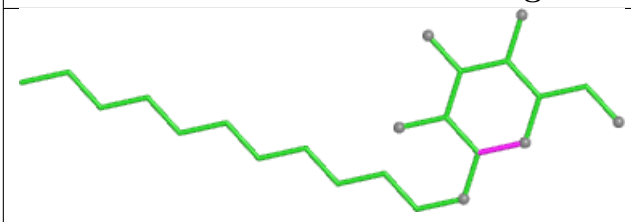
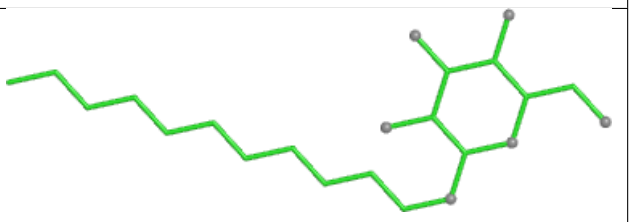
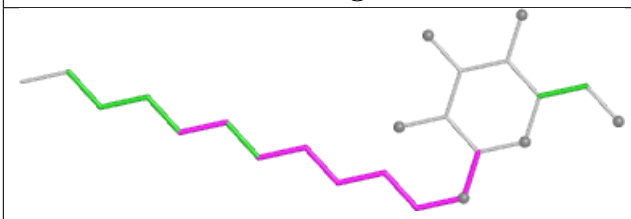


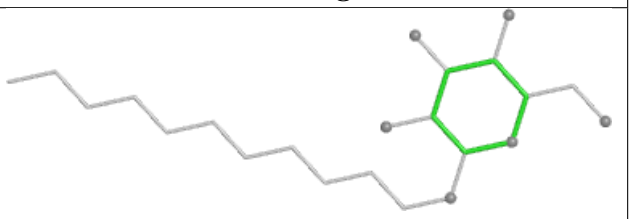
Bond lengths



Bond angles

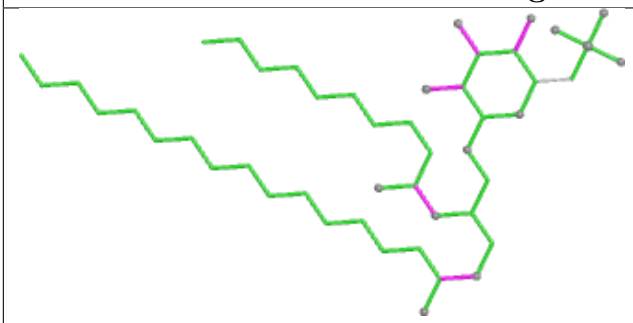


Torsions



Rings

Ligand SQD 1 822



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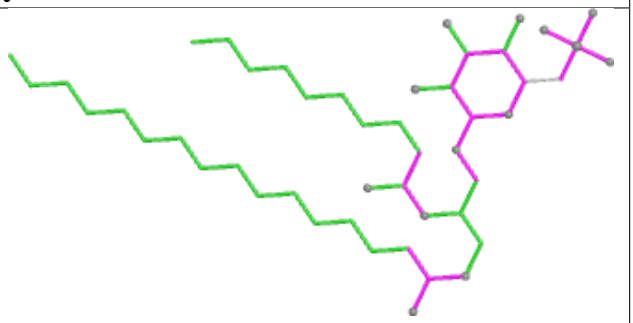

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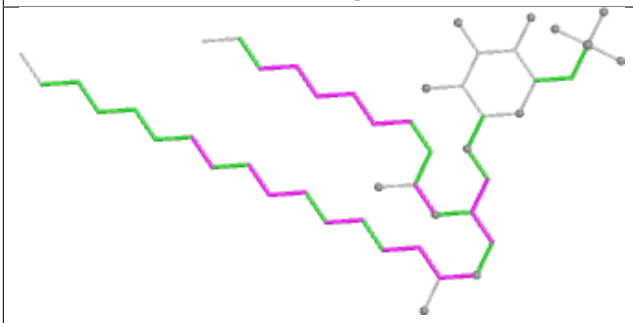

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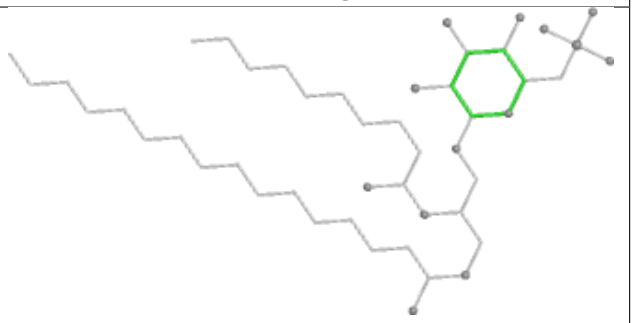
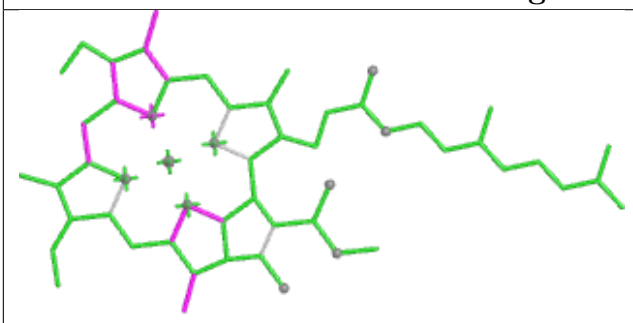


Rings

Ligand CLA 5 518



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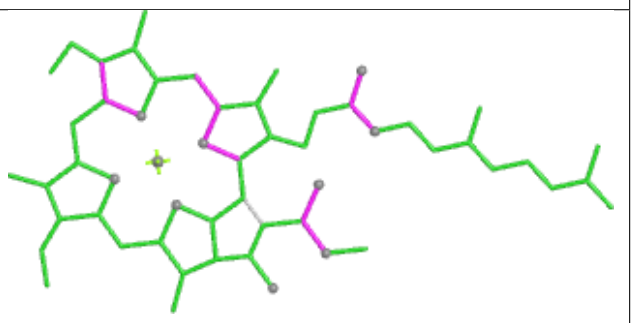
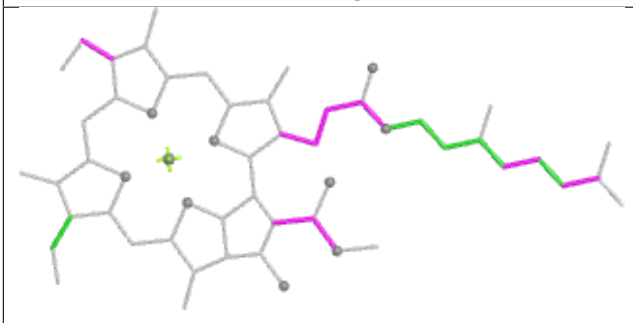


Bond angles



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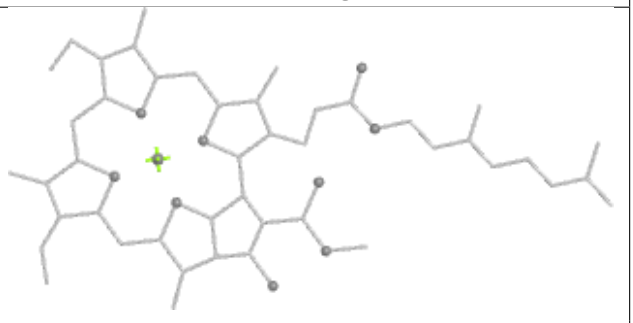
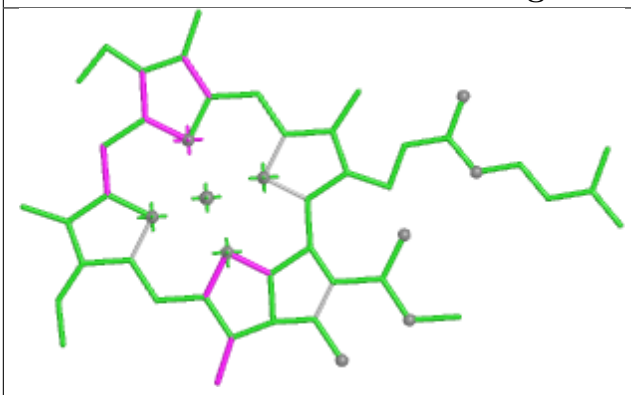


Rings

Ligand CLA b 510



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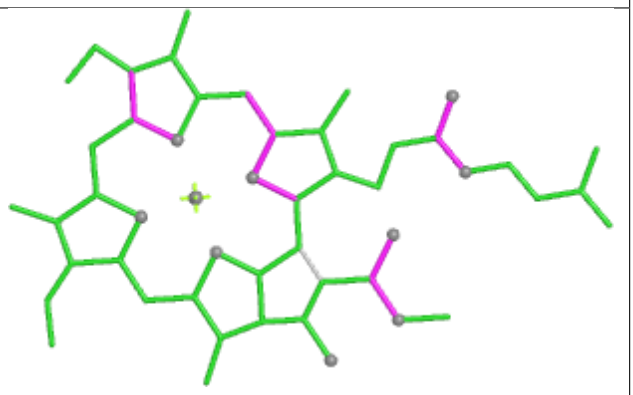

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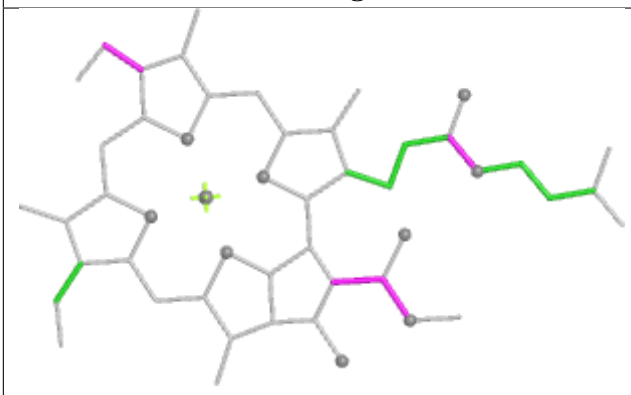

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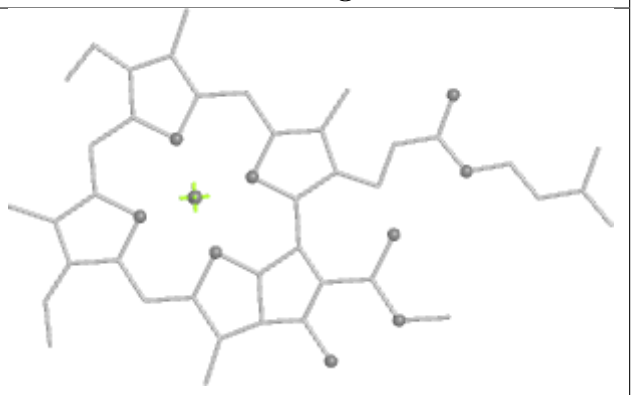
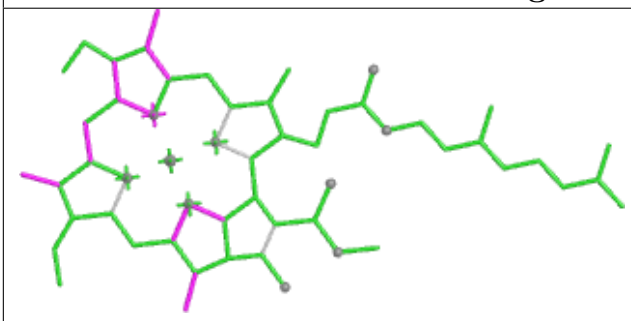


Rings

Ligand CLA 2 506



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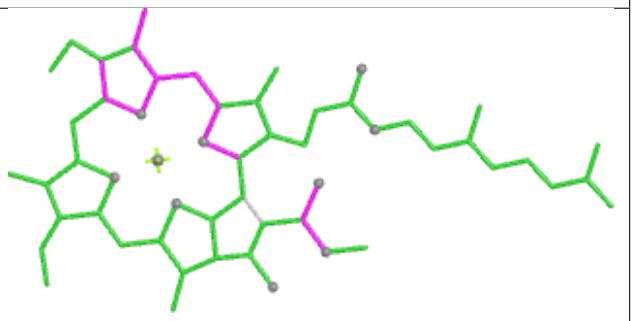

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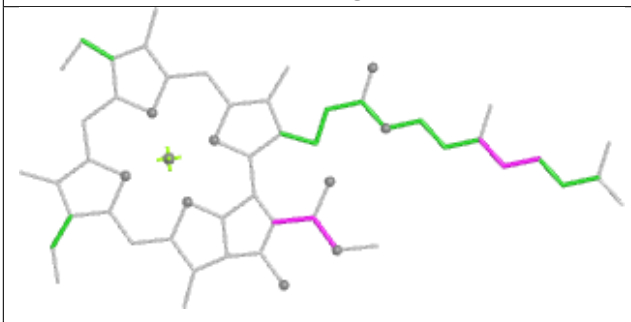

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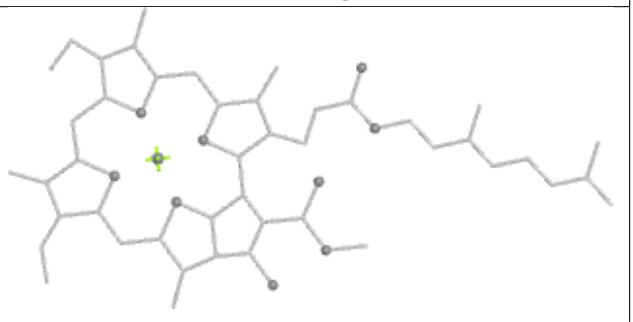

Rings

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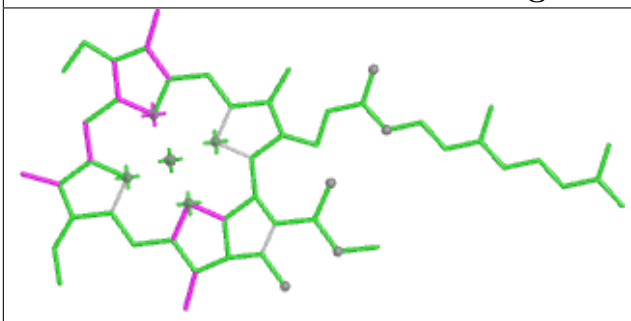

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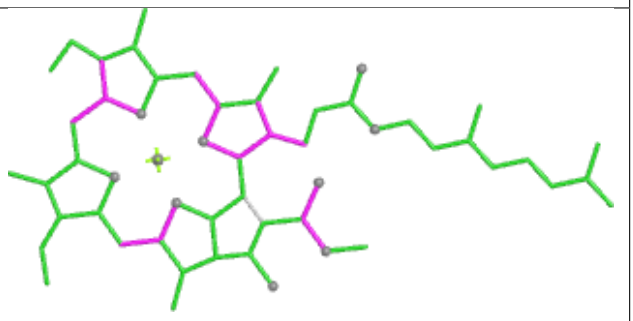

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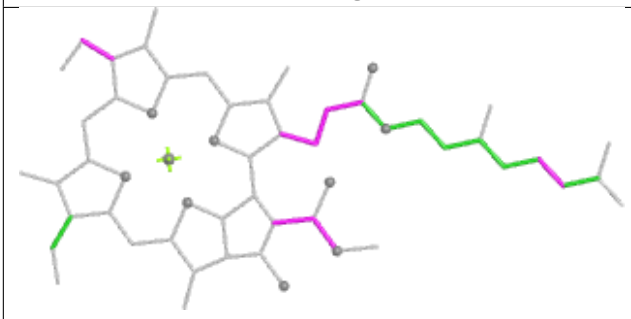

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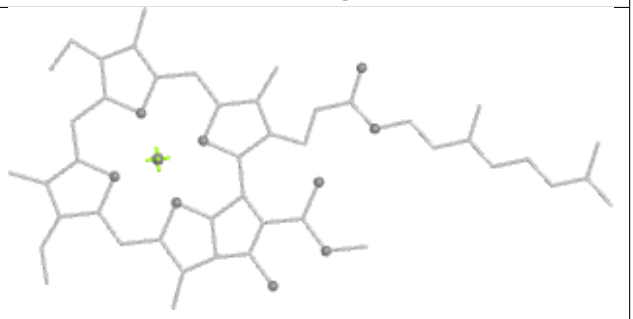
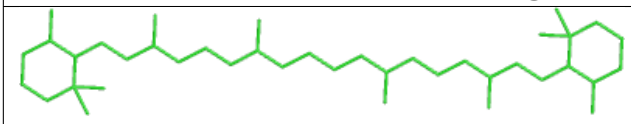


Rings

Ligand BCR u 522



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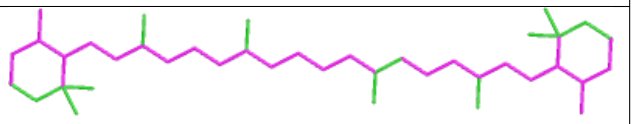
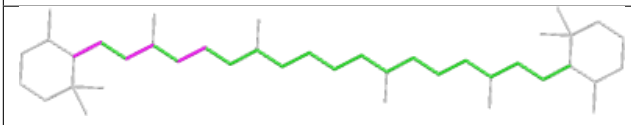


Bond angles



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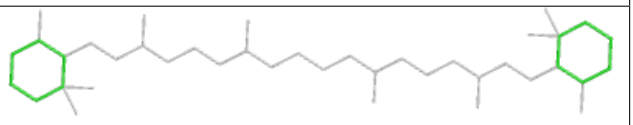
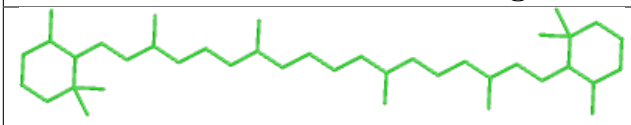


Rings

Ligand BCR M 4021



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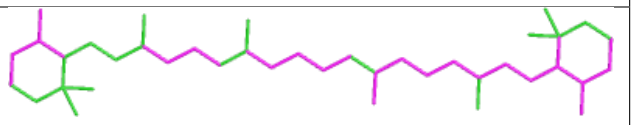

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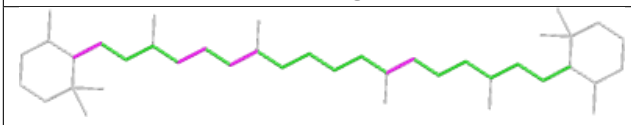

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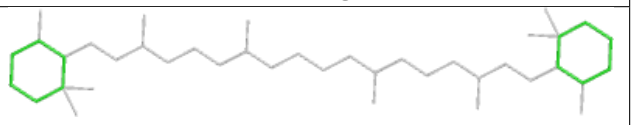
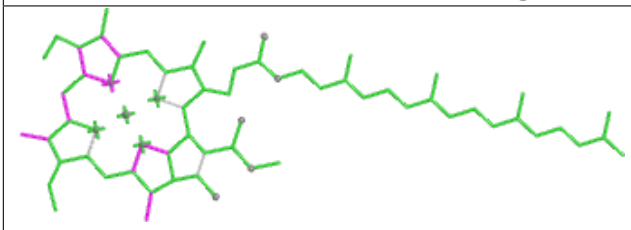


Rings

Ligand CLA H 1231



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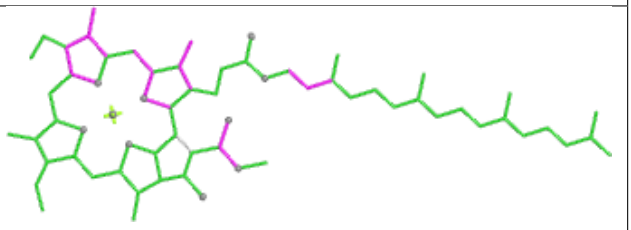
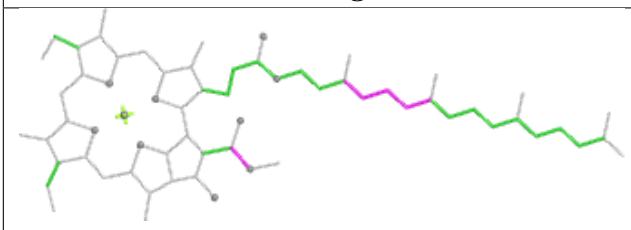


Bond angles



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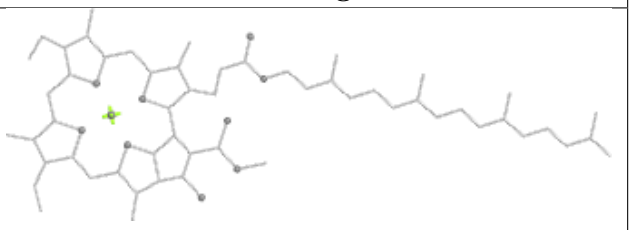
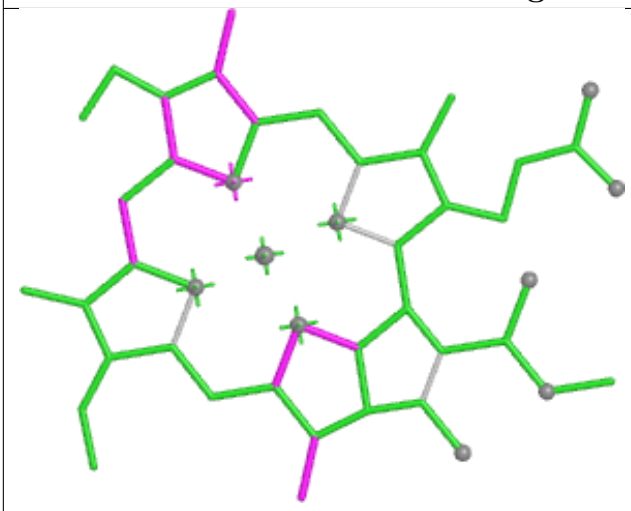


Rings

Ligand CLA b 506



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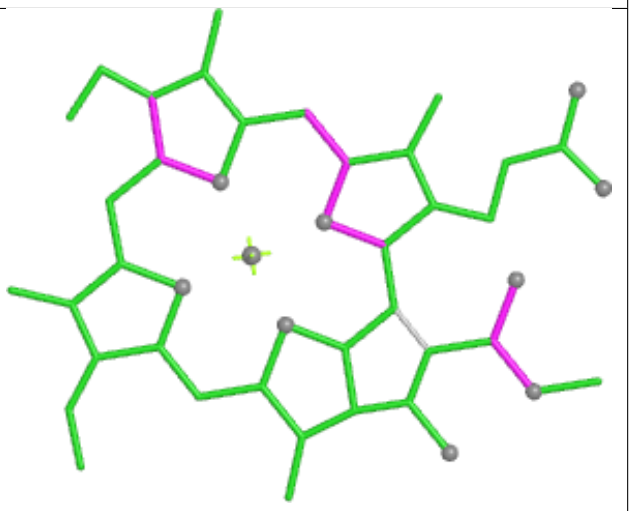

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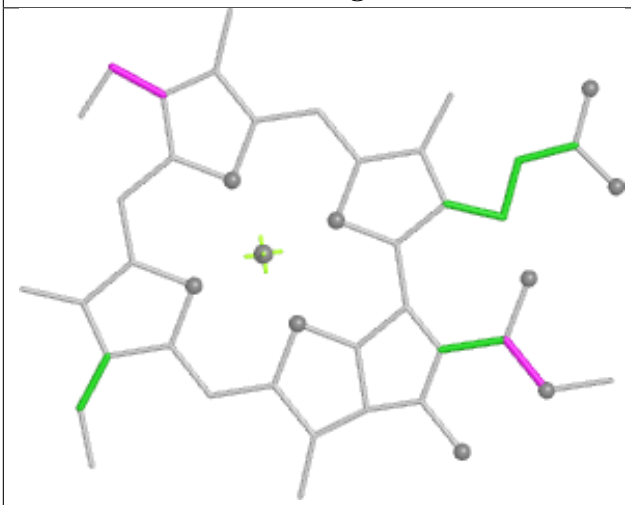

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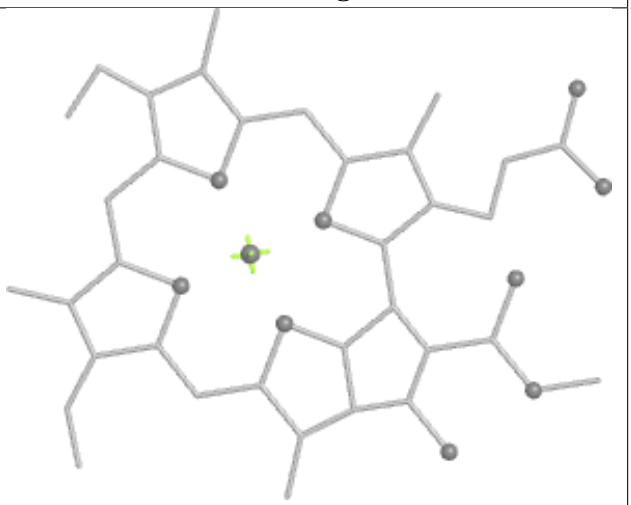
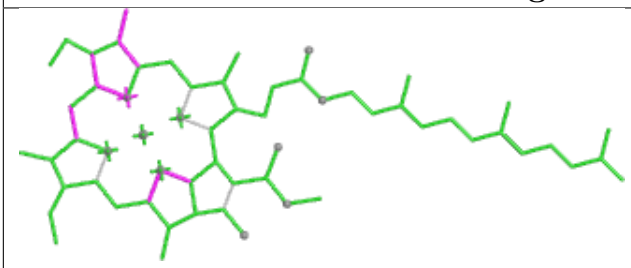


Rings

Ligand CLA 4 501



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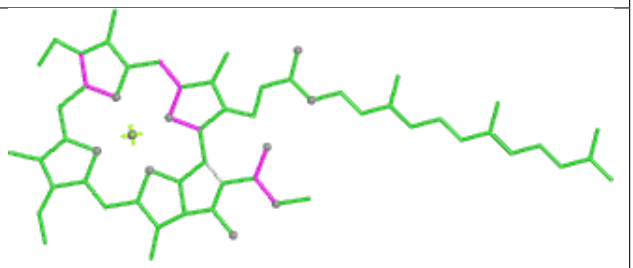
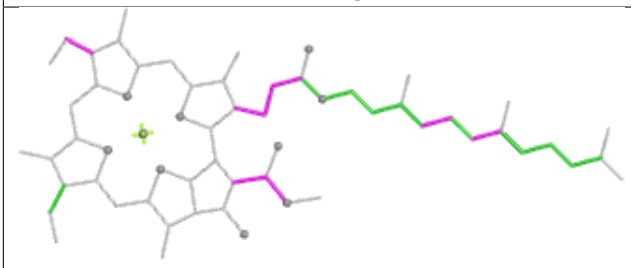


Bond angles



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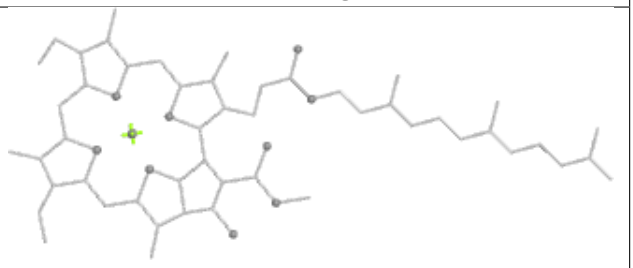
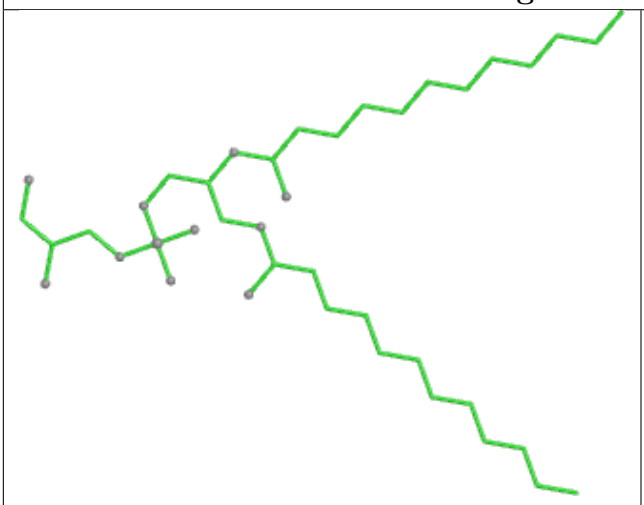


Rings

Ligand LHG n 5220



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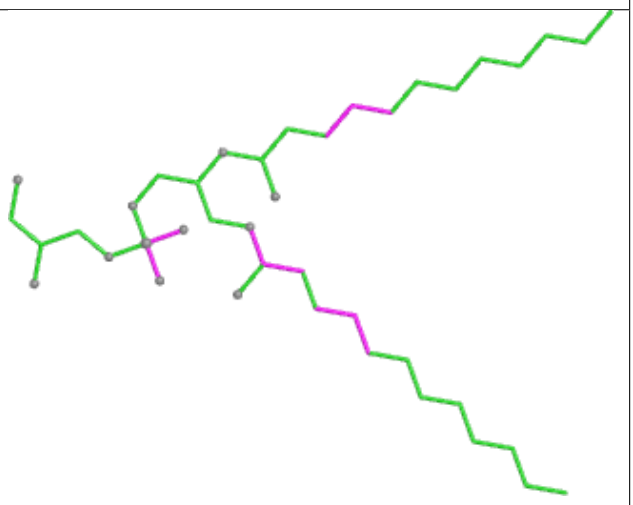
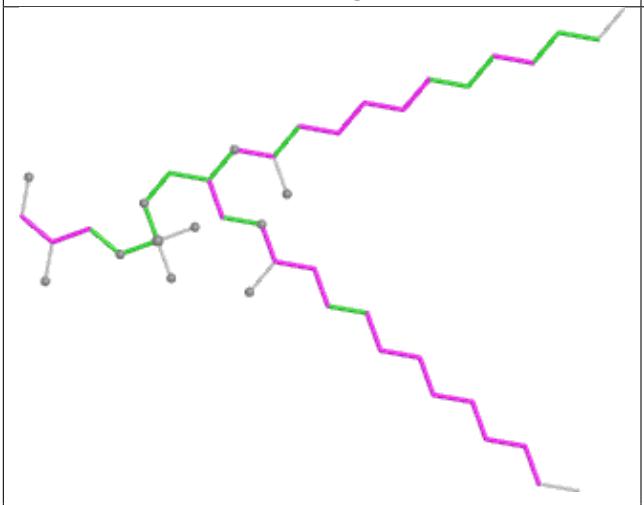


Bond angles



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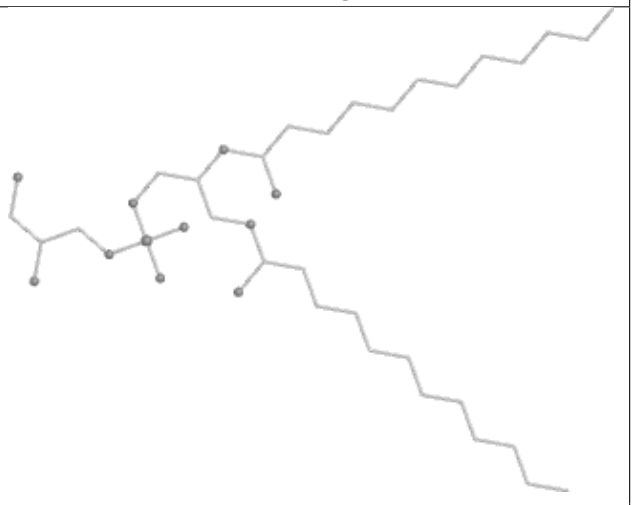
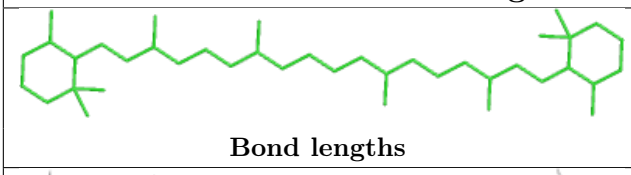


Rings

Ligand BCR W 4021



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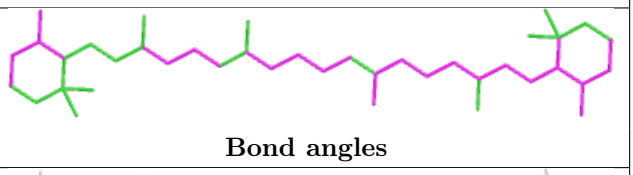
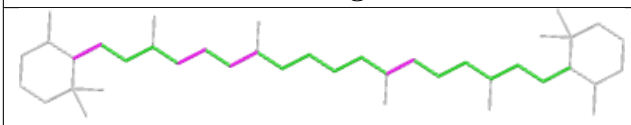


Bond angles



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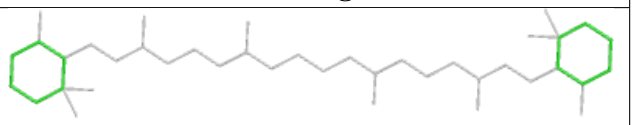
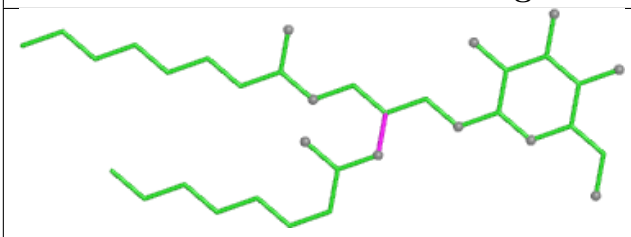
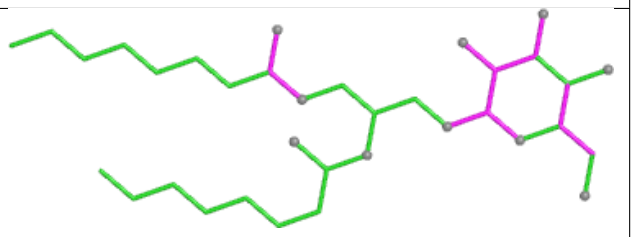


Rings

Ligand LMG J 5104



Bond lengths



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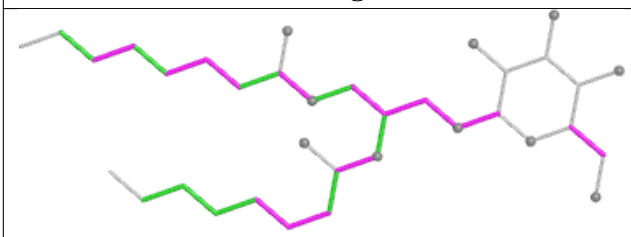
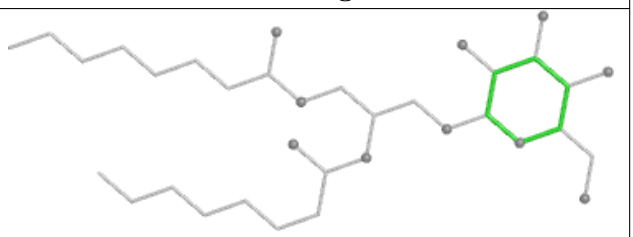
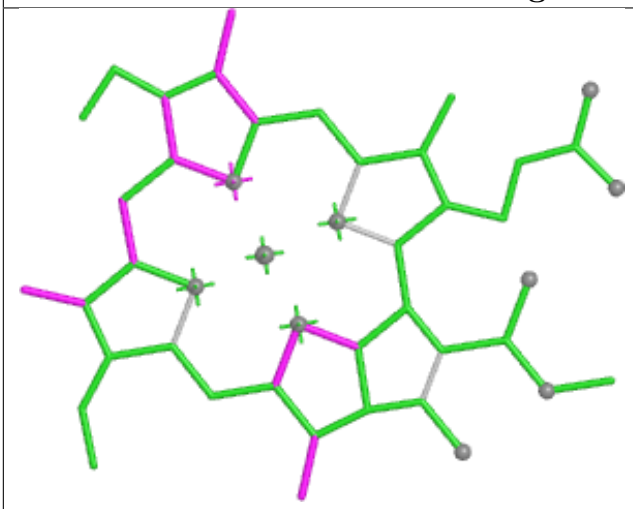


Torsions



Rings

Ligand CLA 1 517



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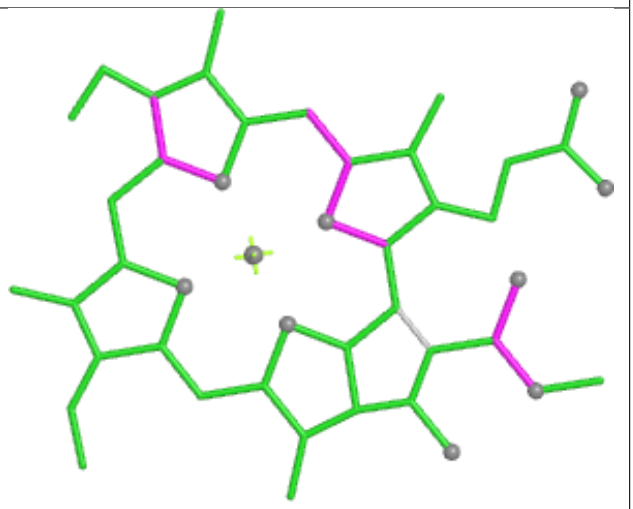

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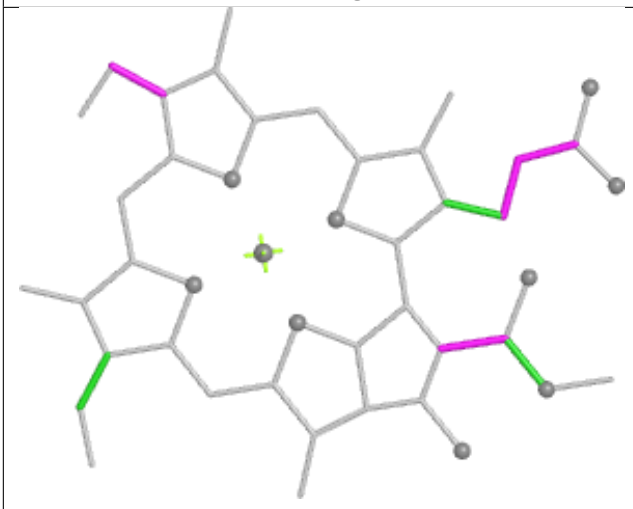
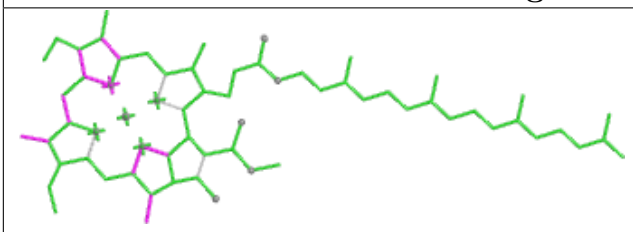


Torsions

Rings

Ligand CLA Z 510



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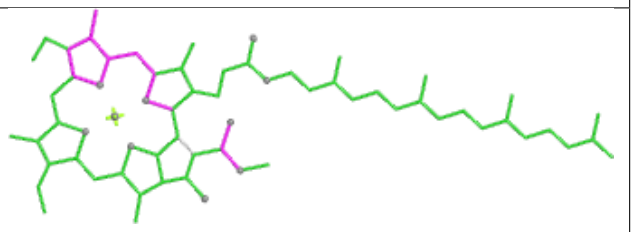

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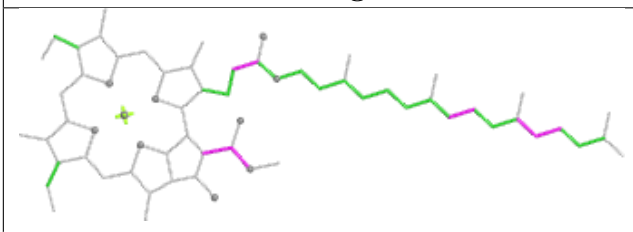

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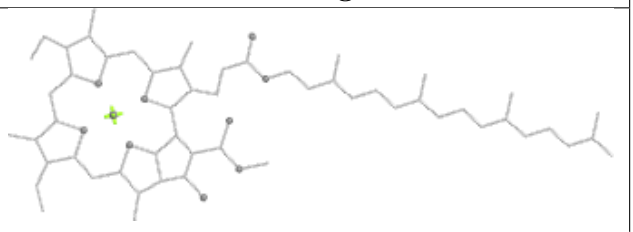
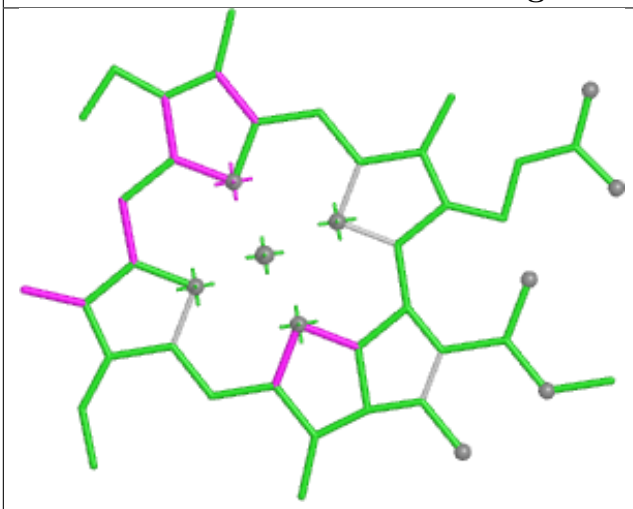


Rings

Ligand CLA b 517



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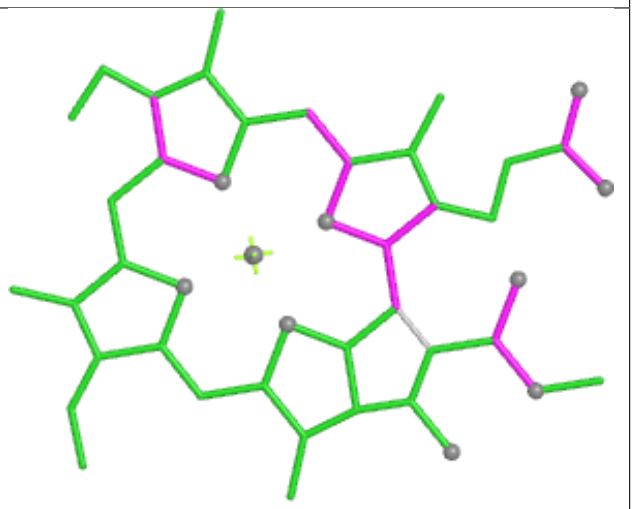

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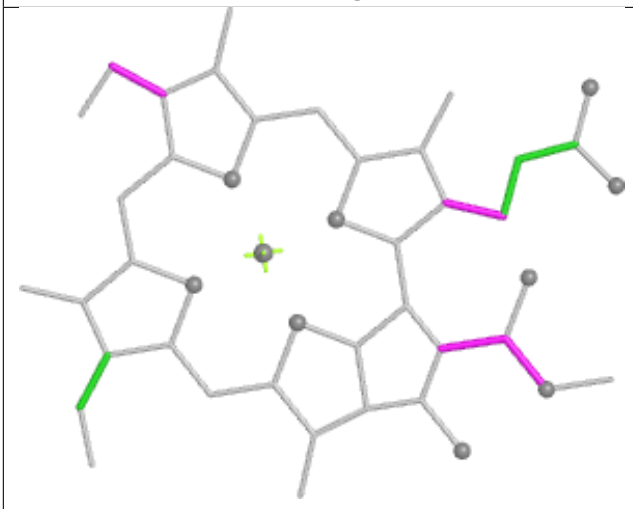
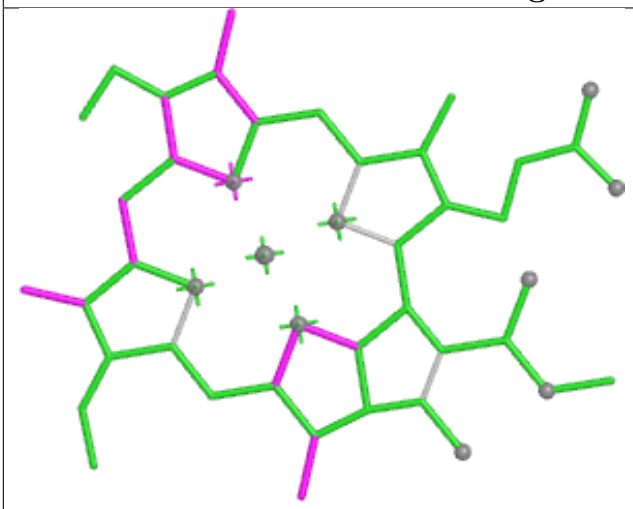


Torsions

Rings

Ligand CLA a 517



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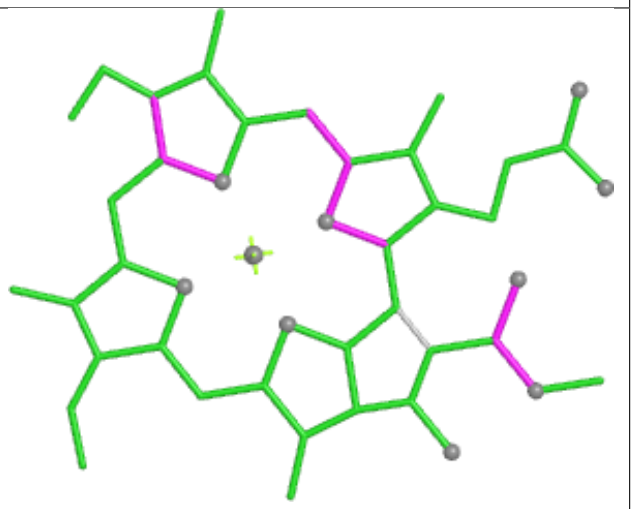
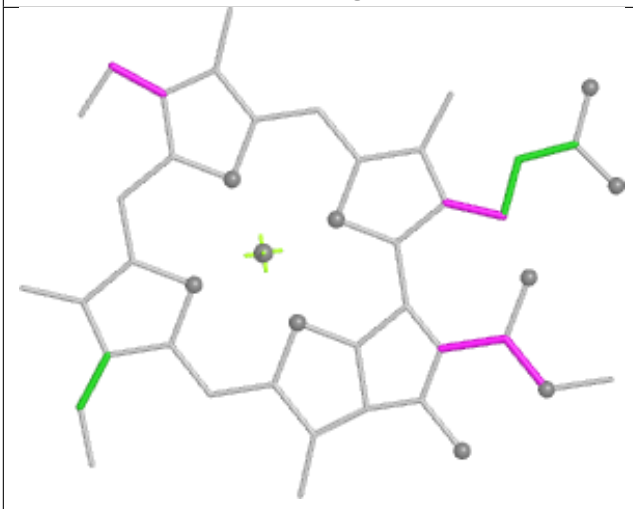


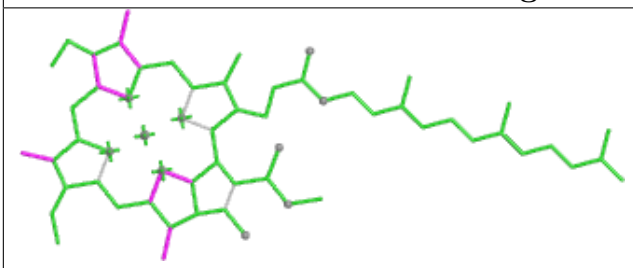
Bond angles



Torsions

Rings

Ligand CLA e 1136



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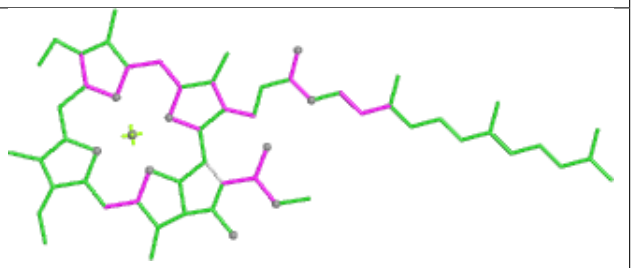
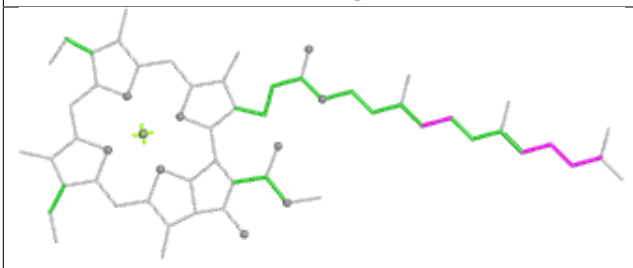


Bond angles



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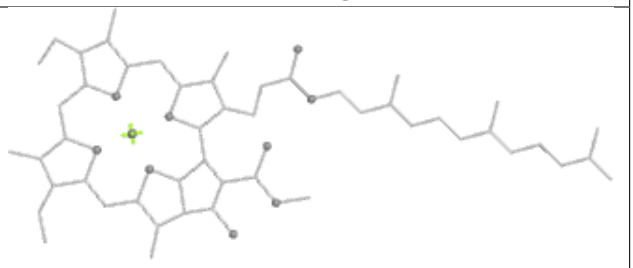
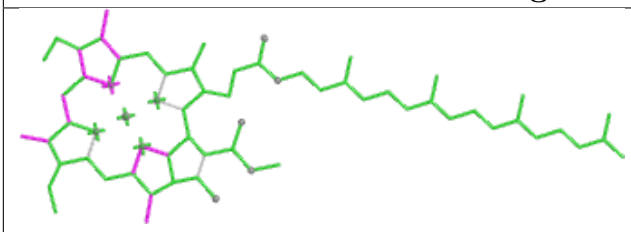


Rings

Ligand CLA r 518



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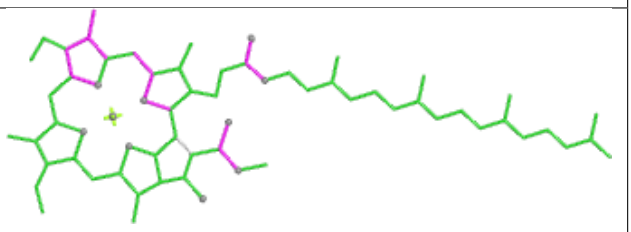
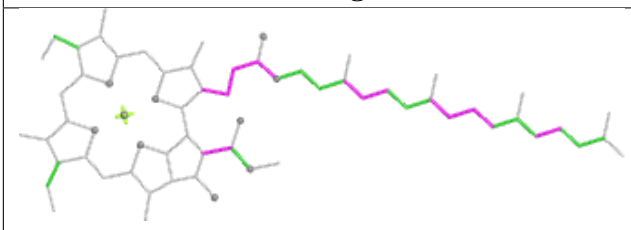


Bond angles



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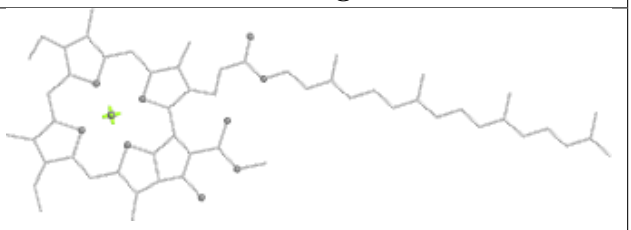
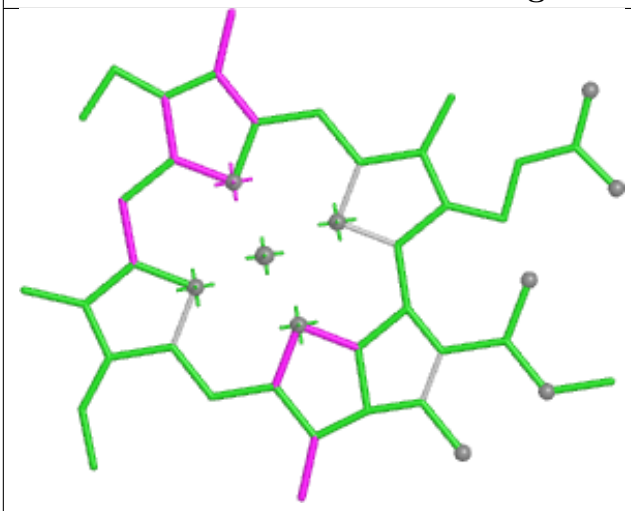


Rings

Ligand CLA v 511



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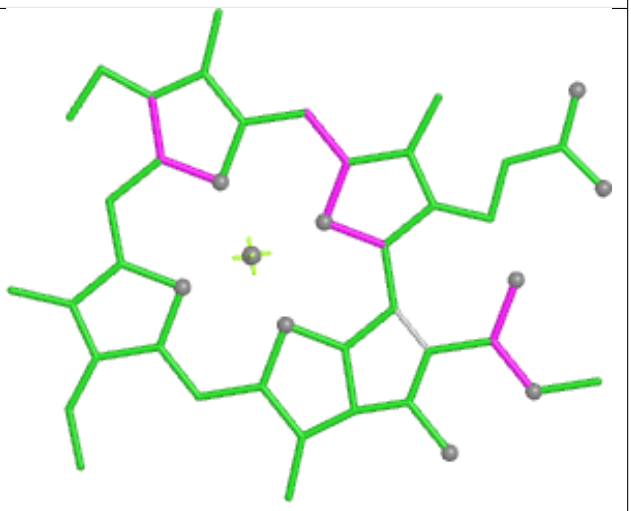

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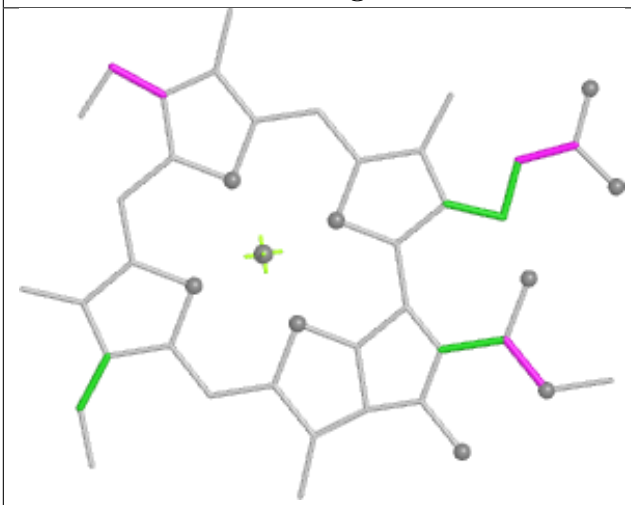

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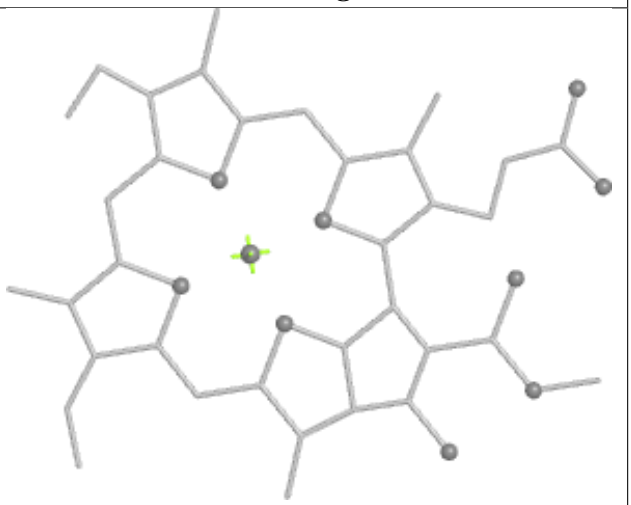
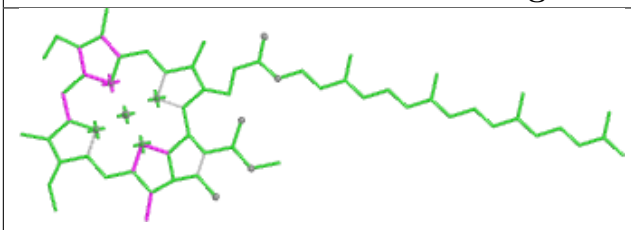


Rings

Ligand CLA a 505



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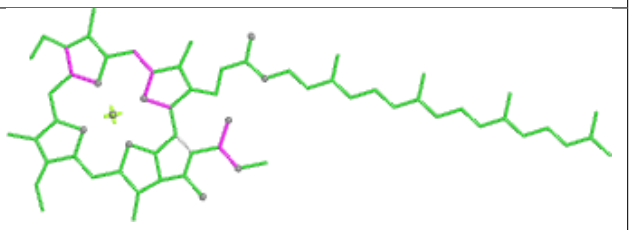
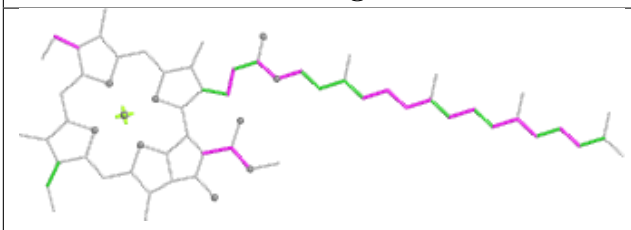


Bond angles



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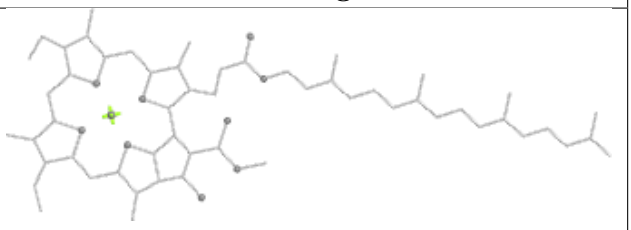
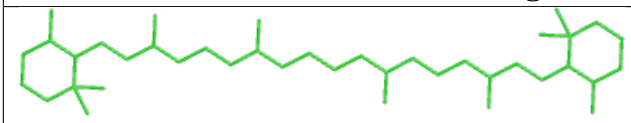


Rings

Ligand BCR Z 524



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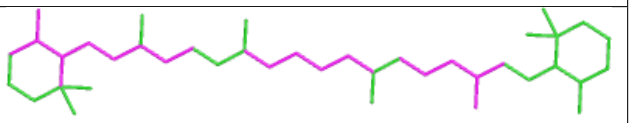
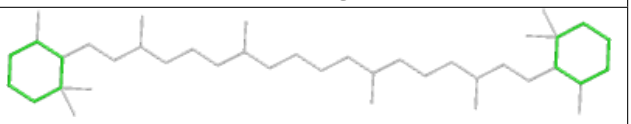


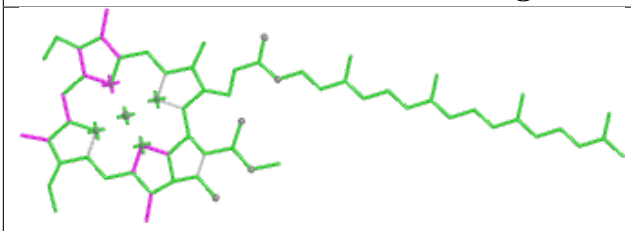
Bond angles

Torsions



Rings

Ligand CLA V 1502



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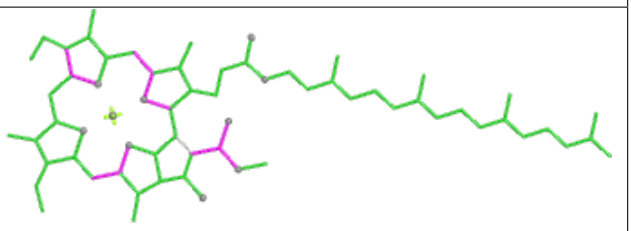
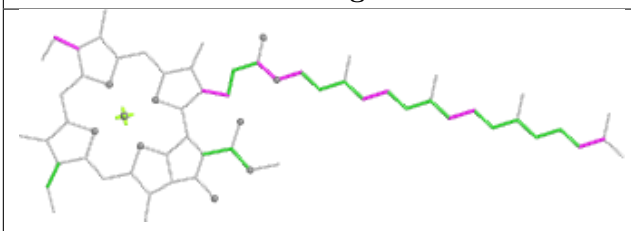


Bond angles



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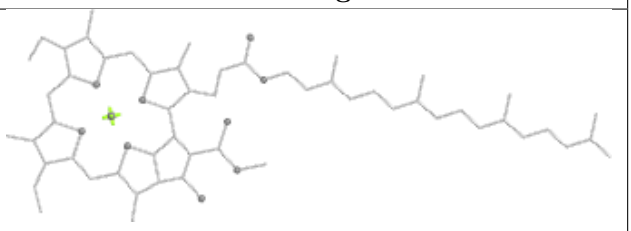
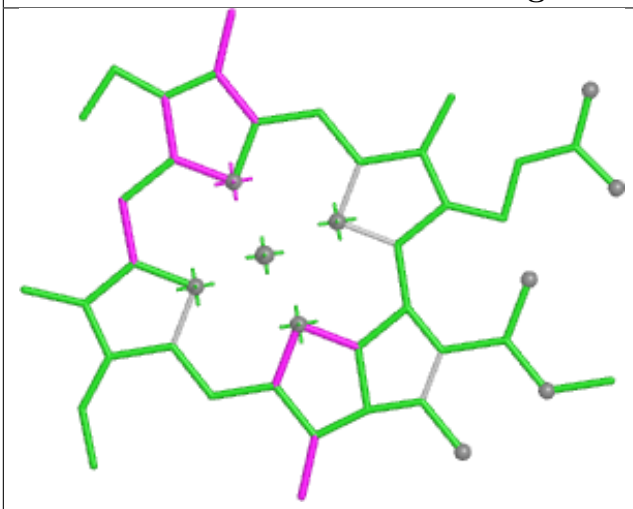


Rings

Ligand CLA v 507



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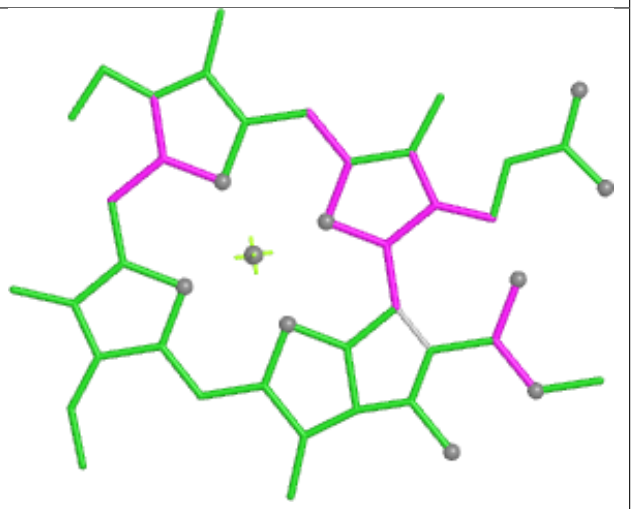
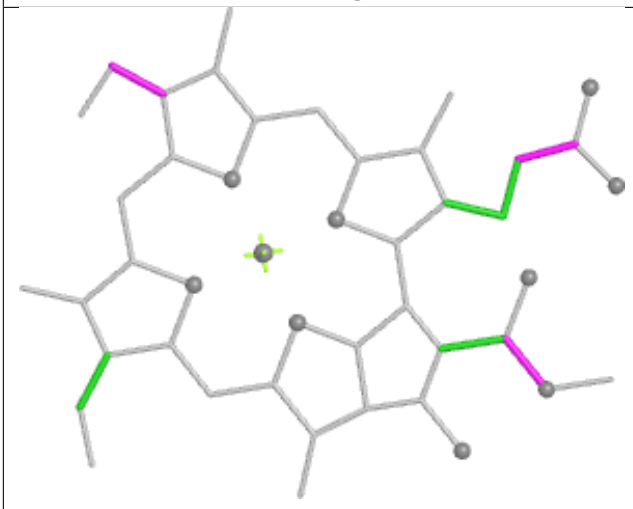


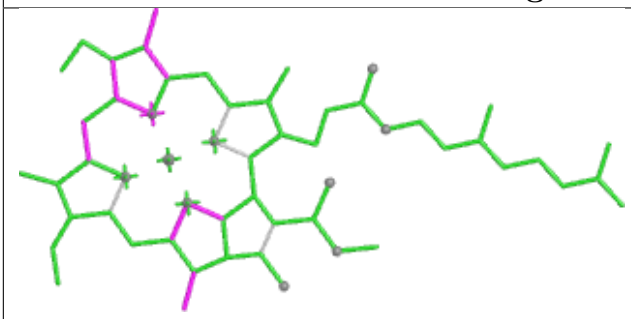
Bond angles



Torsions

Rings

Ligand CLA Z 511



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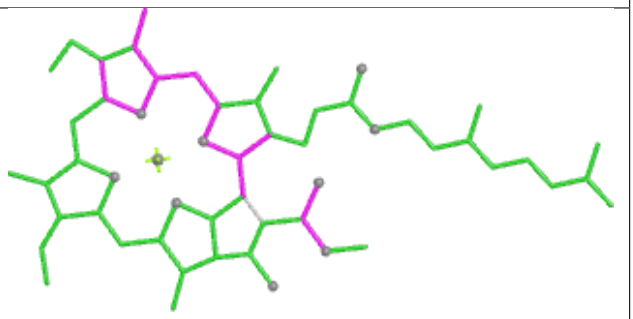
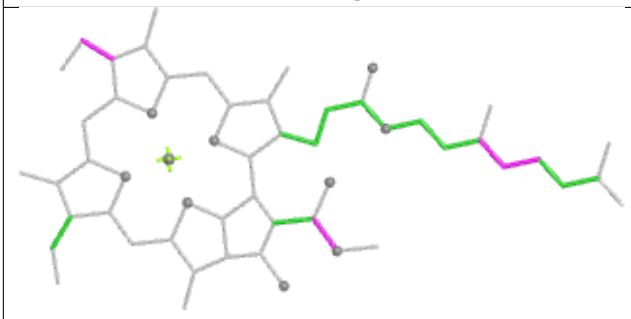


Bond angles



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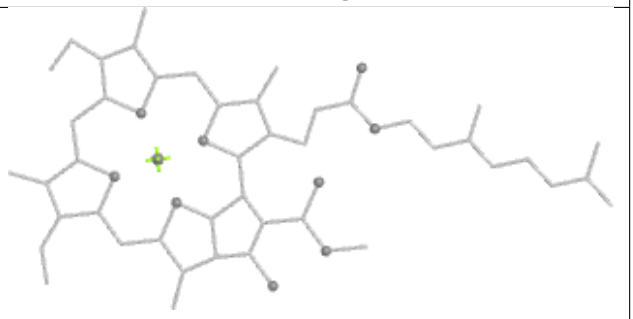
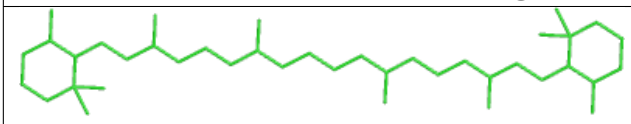


Rings

Ligand BCR H 4006



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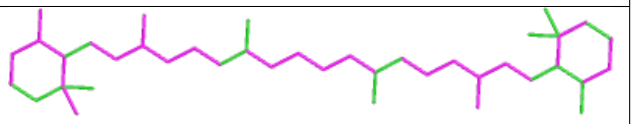
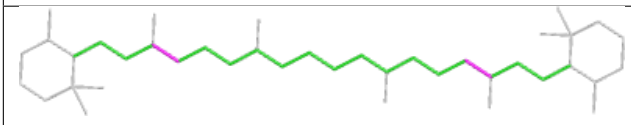


Bond angles



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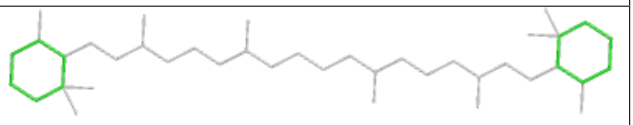
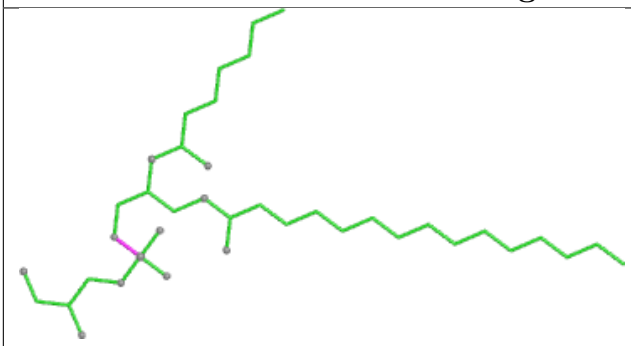
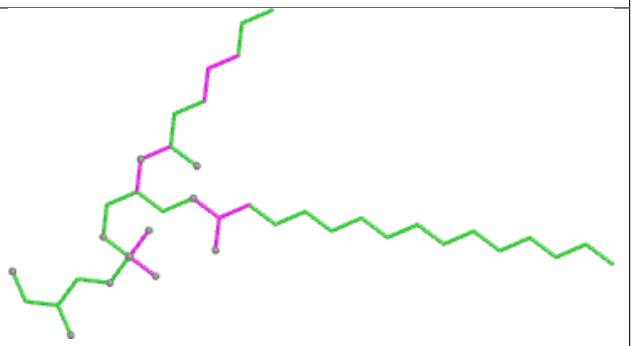


Rings

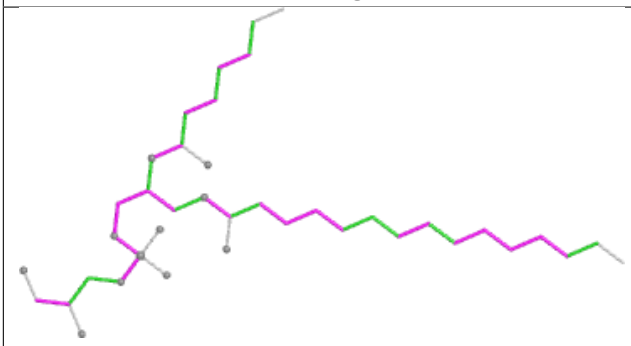
Ligand LHG e 5002



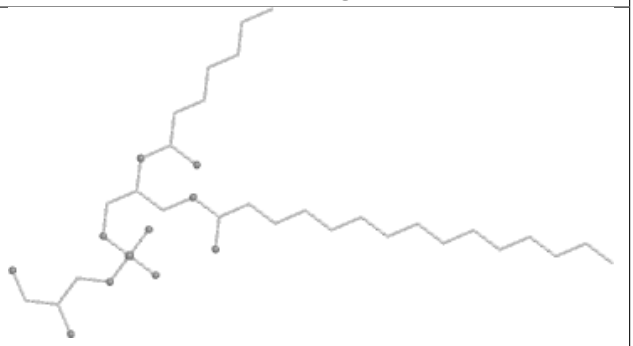
Bond lengths



Bond angles

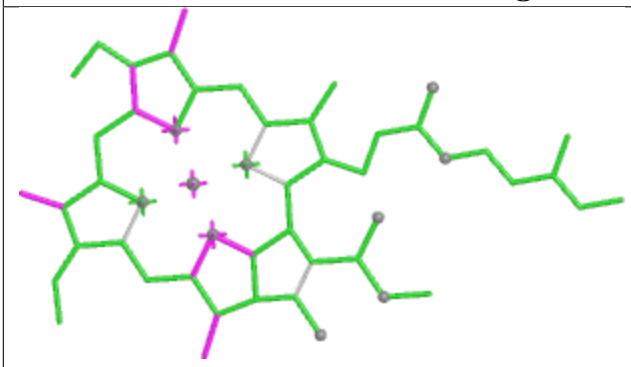


Torsions



Rings

Ligand CLA A 1129



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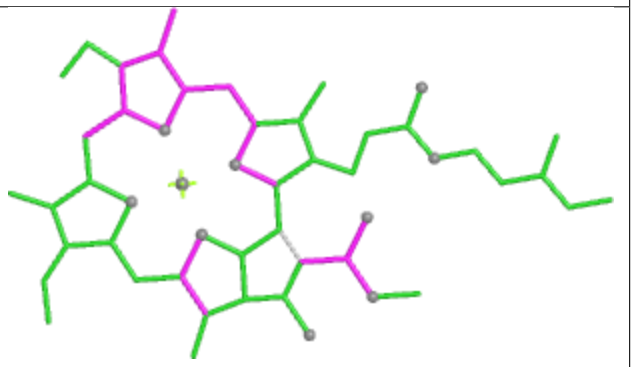

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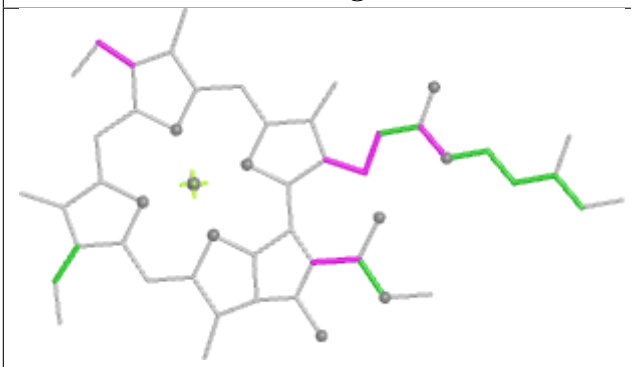

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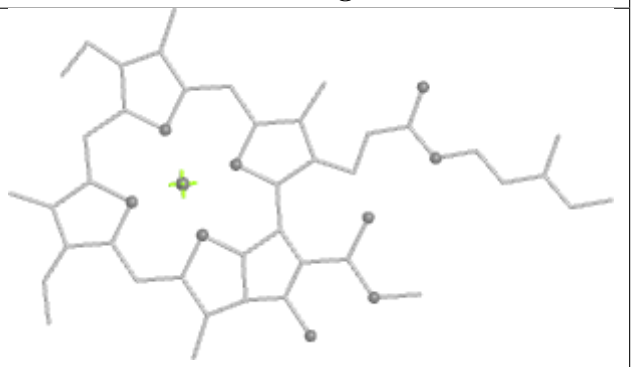
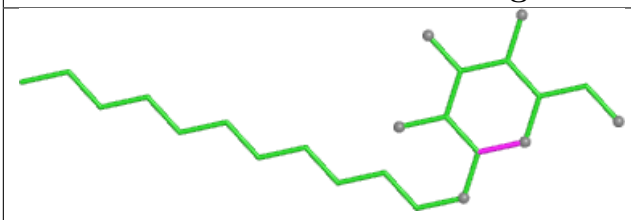


Rings

Ligand LMU G 1849



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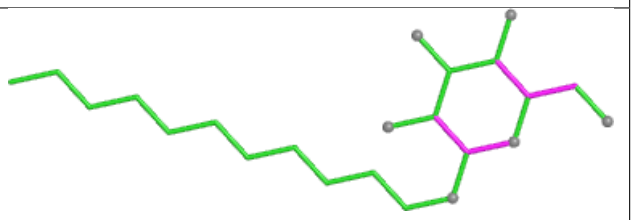

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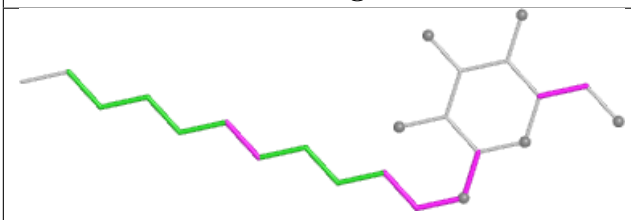

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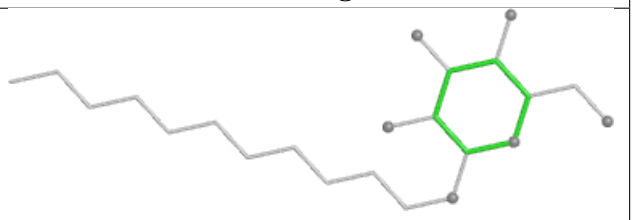
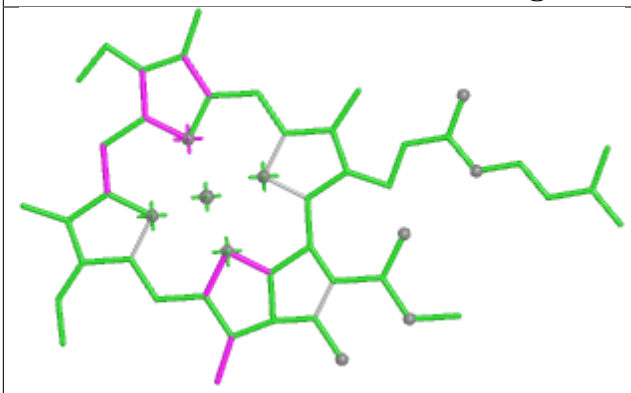


Rings

Ligand CLA 4 510



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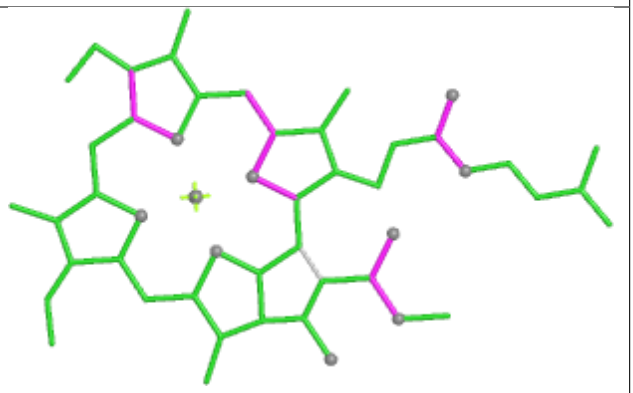

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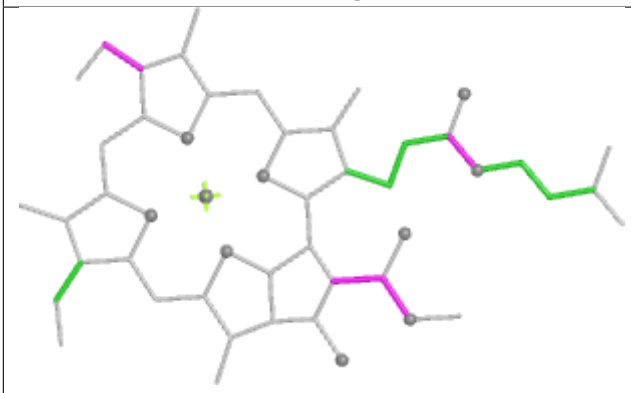

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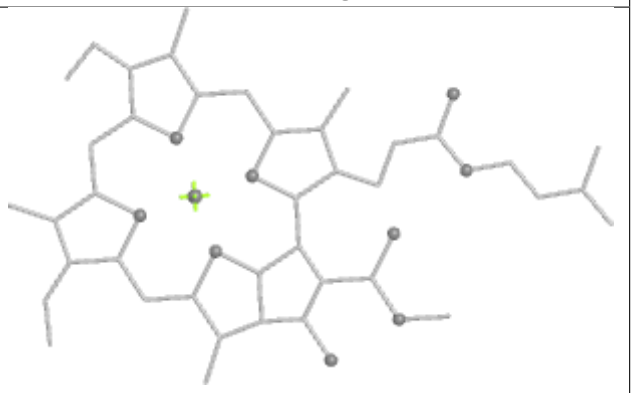
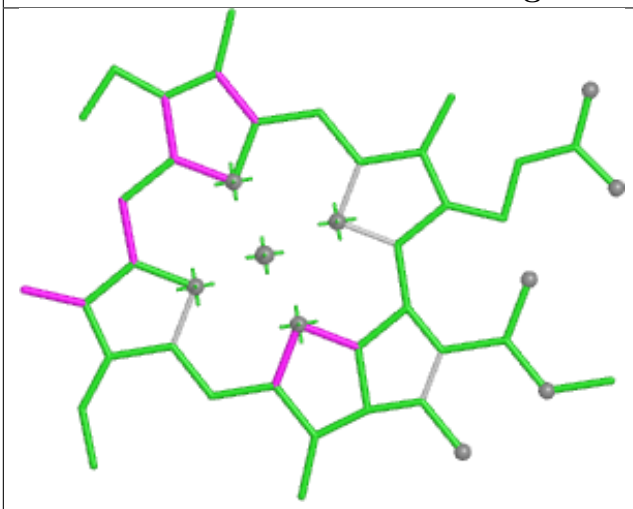


Rings

Ligand CLA Y 506



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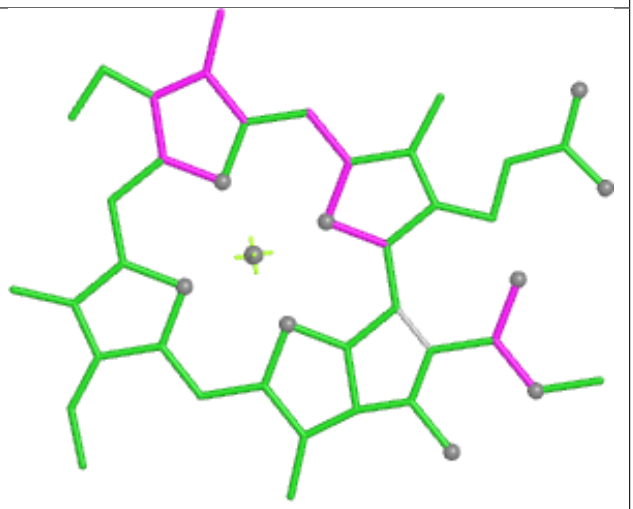

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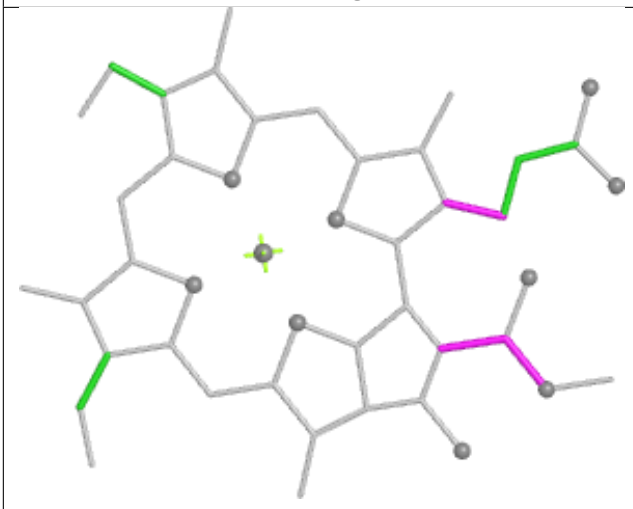
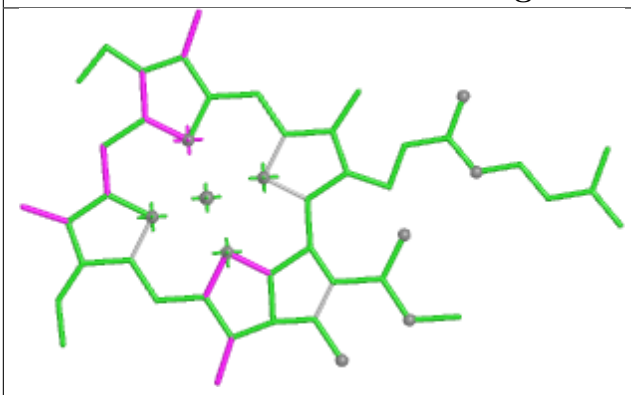


Torsions

Rings

Ligand CLA A 1112



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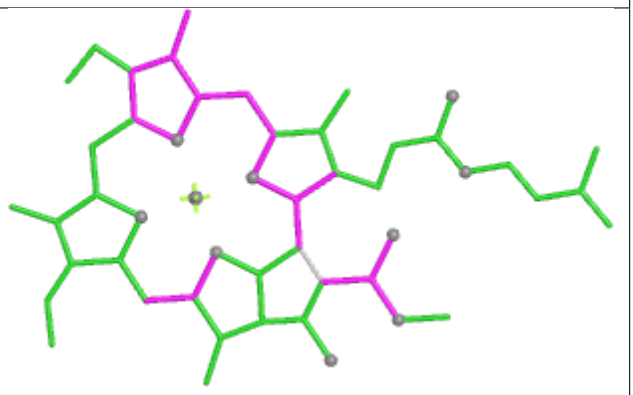

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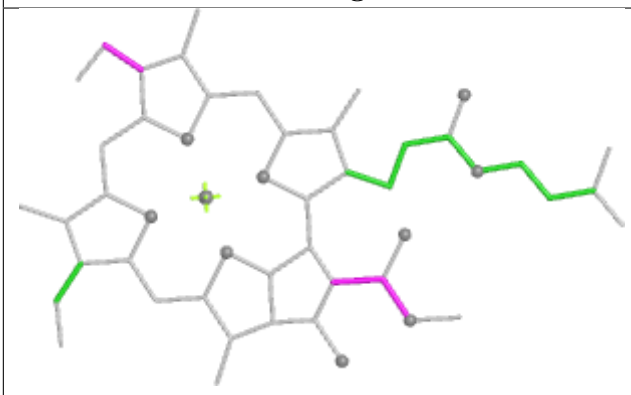

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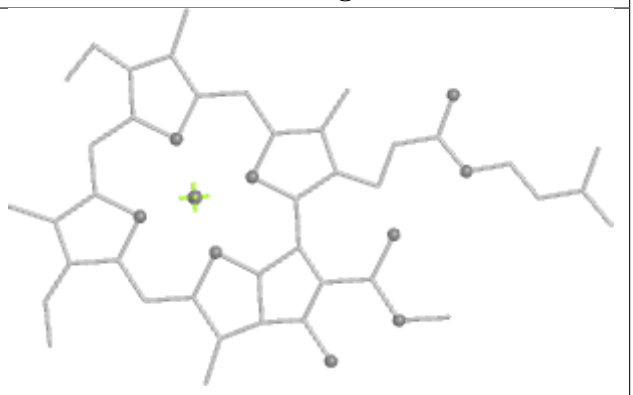
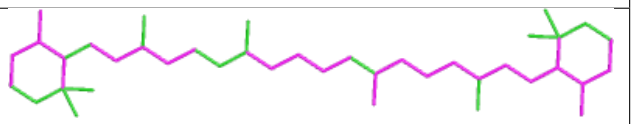


Rings

Ligand BCR b 522

Bond lengths



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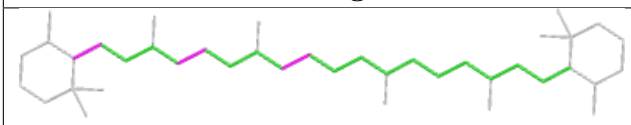

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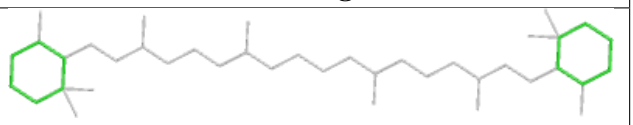
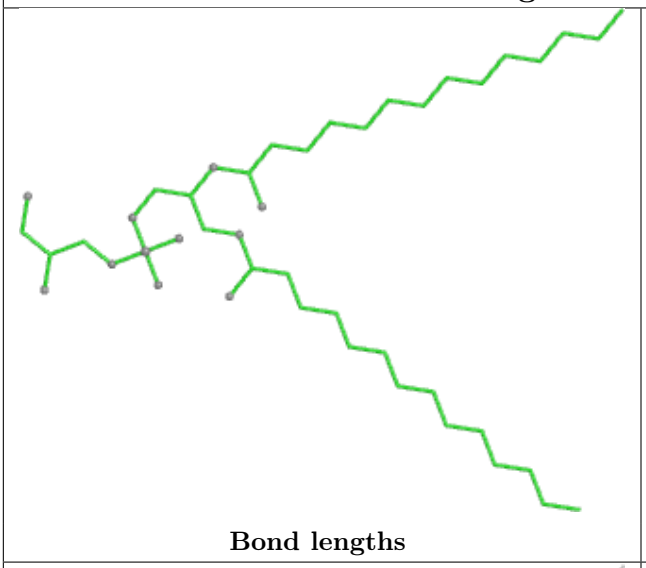


Rings

Ligand LHG e 5006



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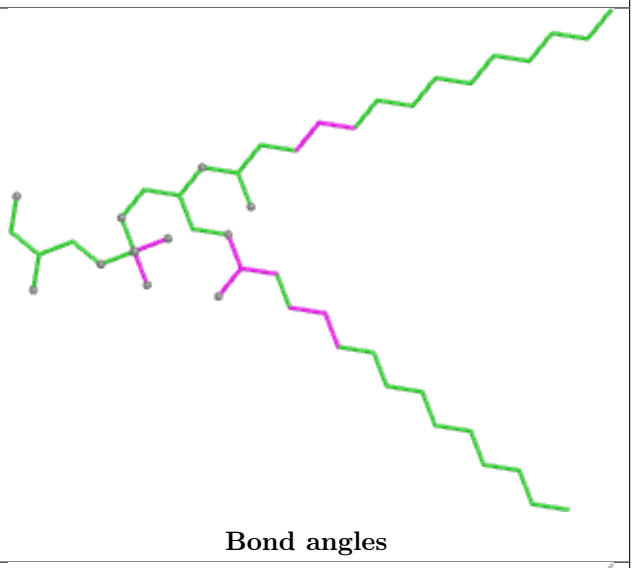

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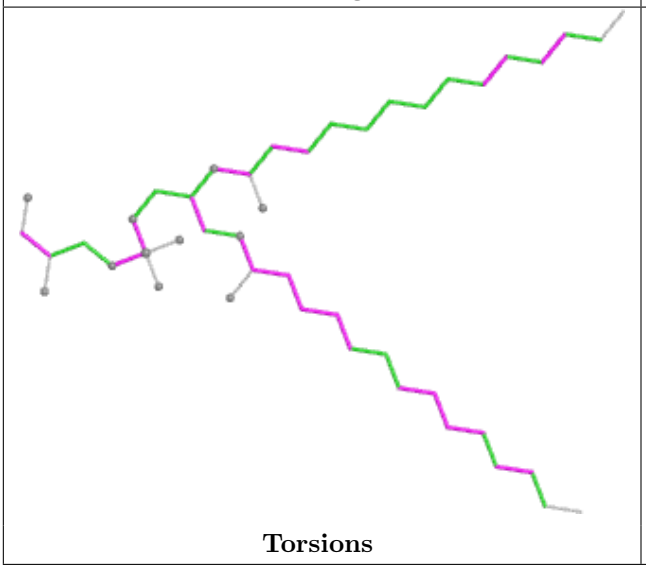

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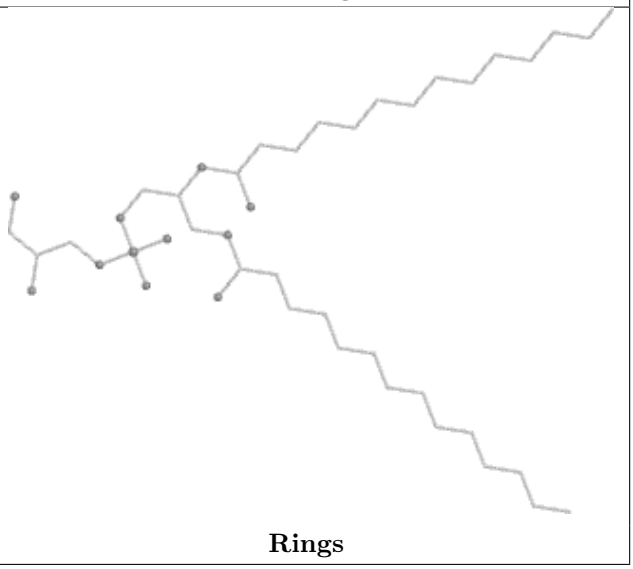
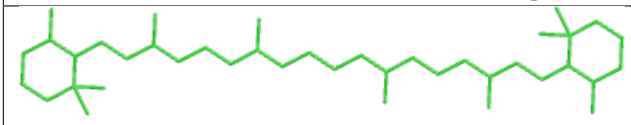


Rings

Ligand BCR b 521



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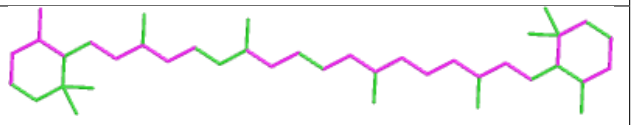
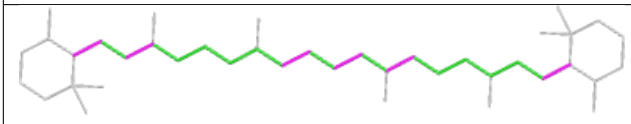


Bond angles



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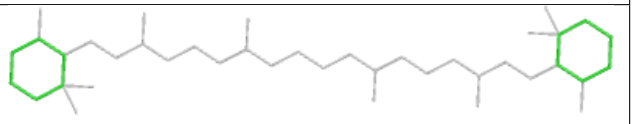
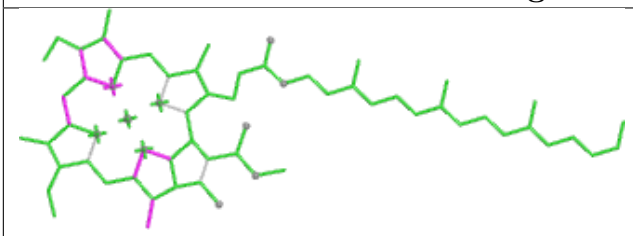


Rings

Ligand CLA q 503



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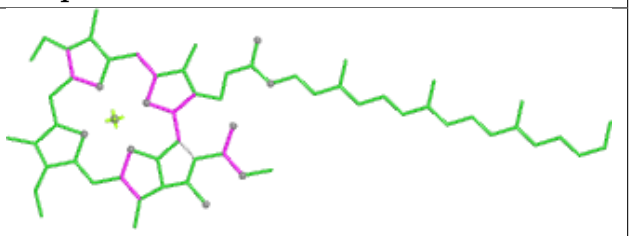

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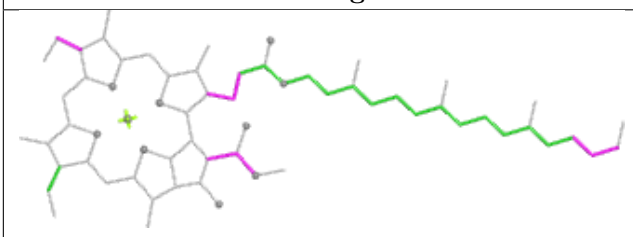

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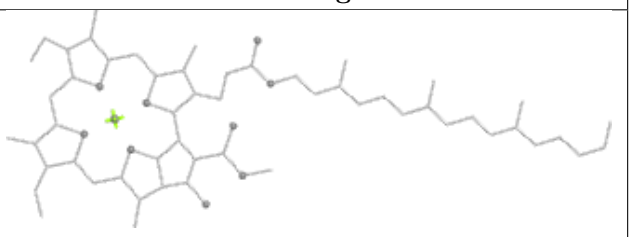
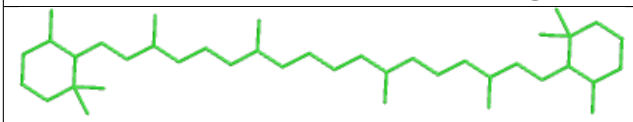


Rings

Ligand BCR 1 524



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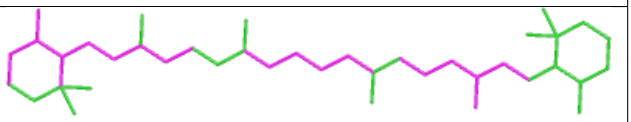

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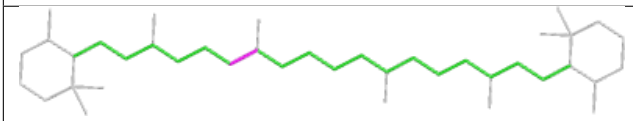

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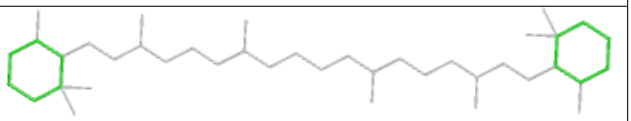
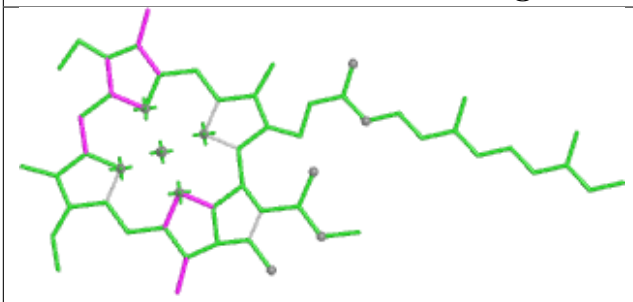


Rings

Ligand CLA G 1134



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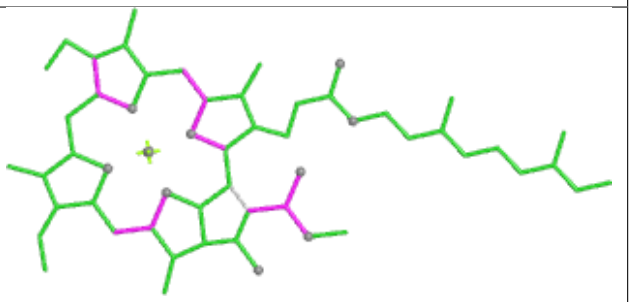

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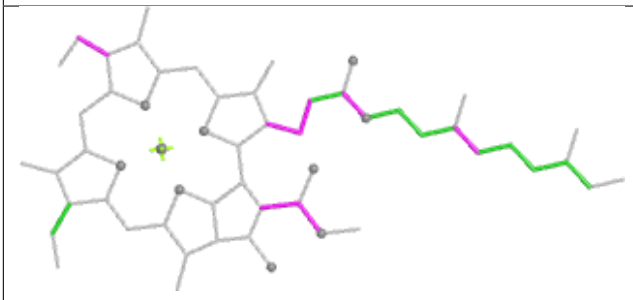

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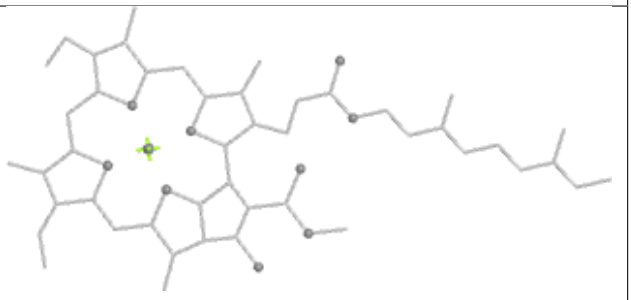
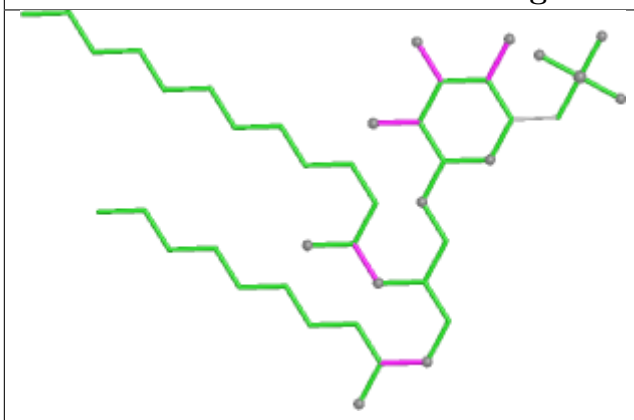


Rings

Ligand SQD a 822



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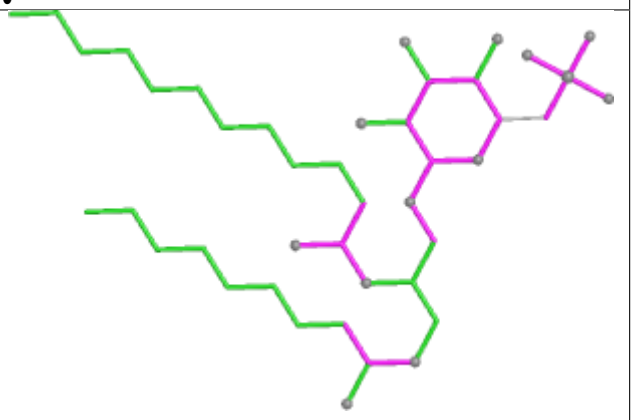
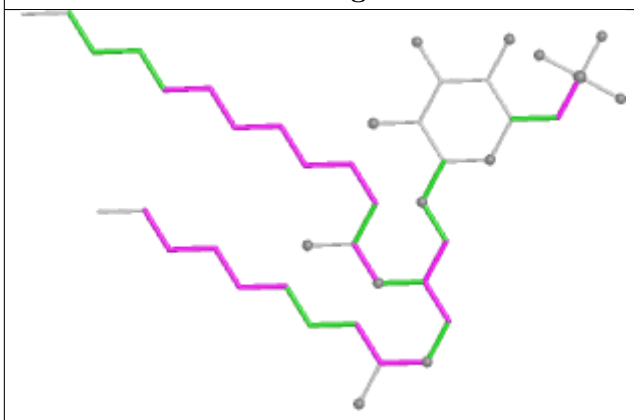


Bond angles



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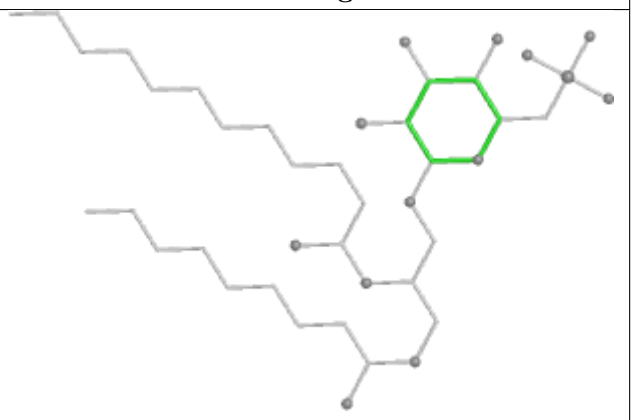
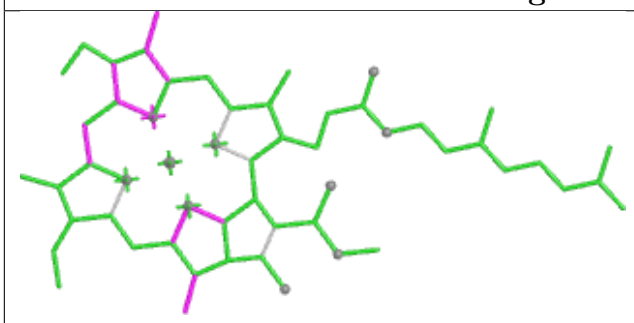


Rings

Ligand CLA u 511



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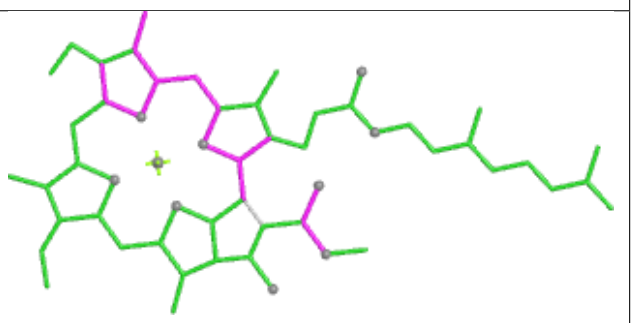
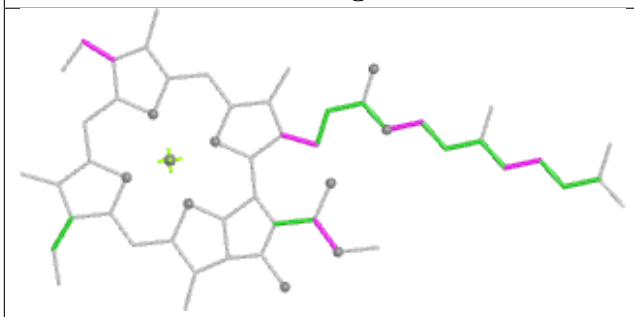


Bond angles



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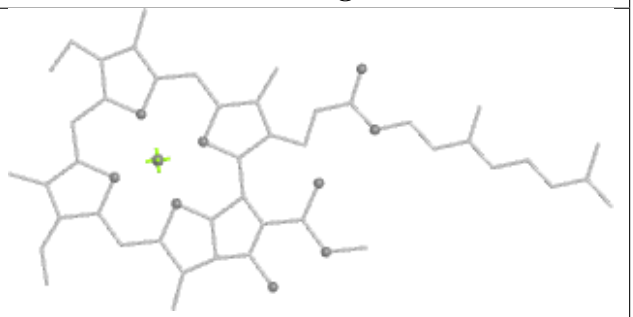
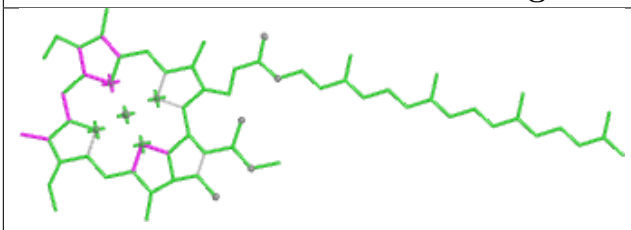


Rings

Ligand CLA 5 501



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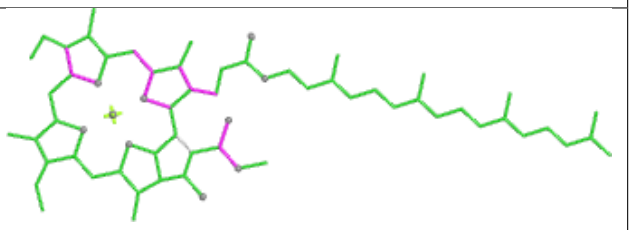

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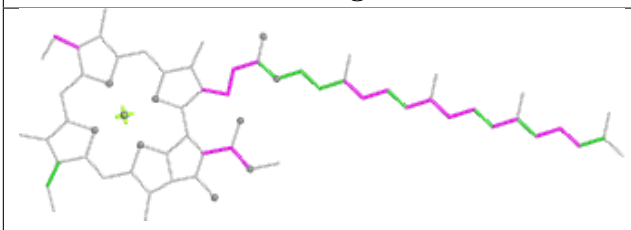
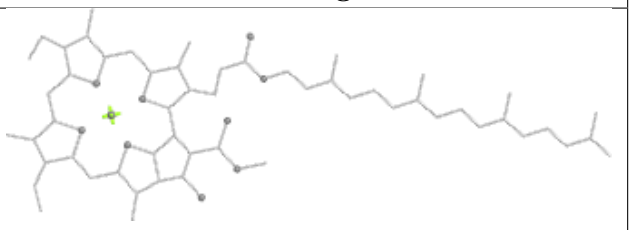


Torsions



Rings

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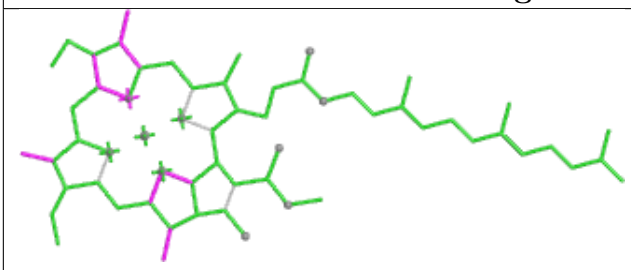

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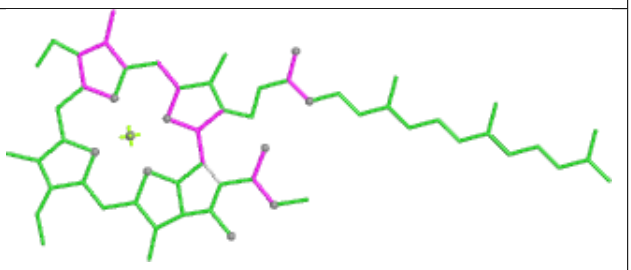

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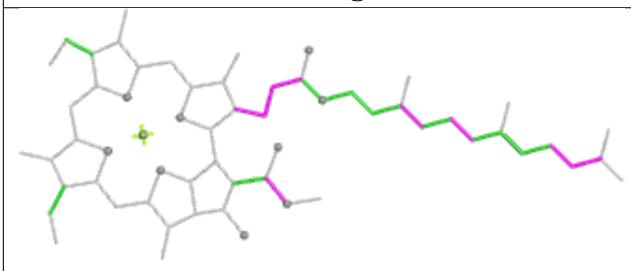

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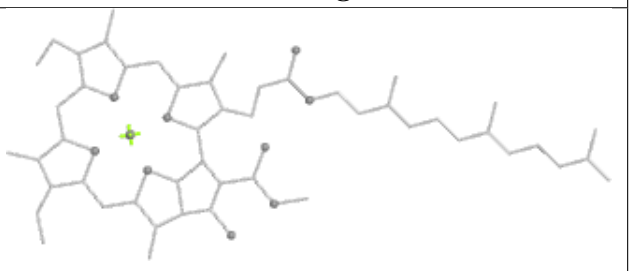

Rings

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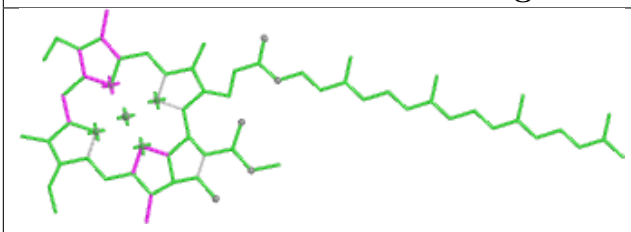

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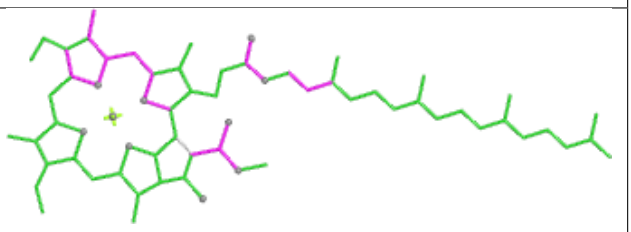

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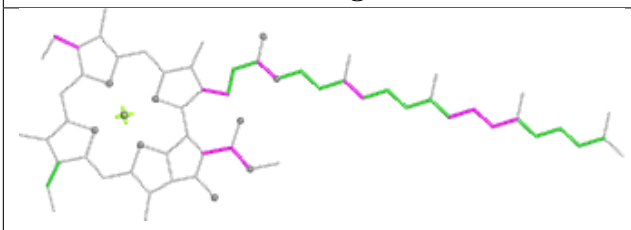

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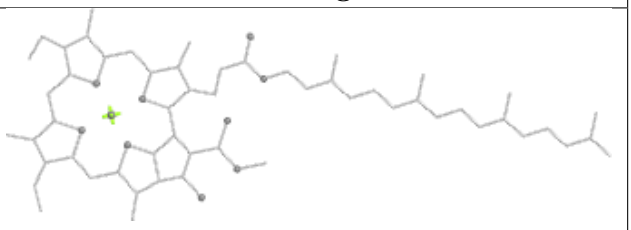

Rings

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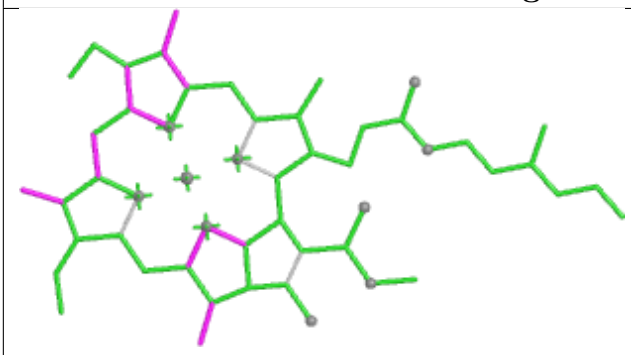

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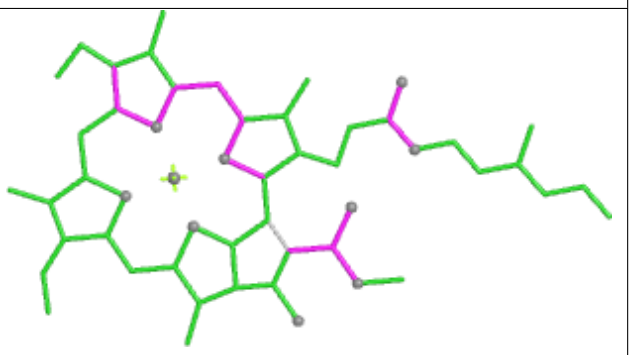

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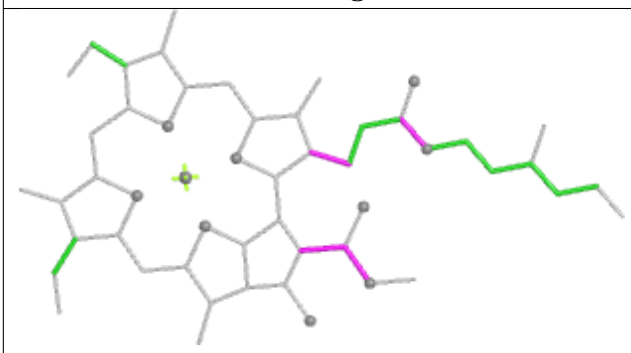

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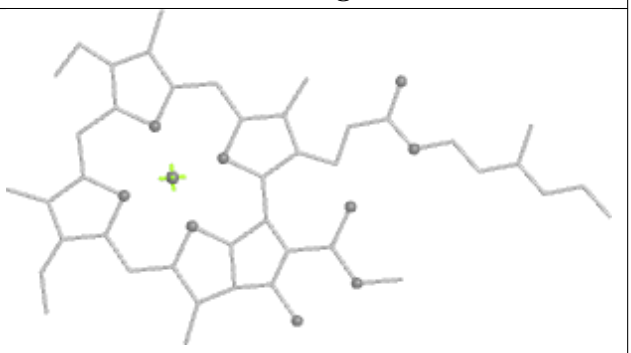
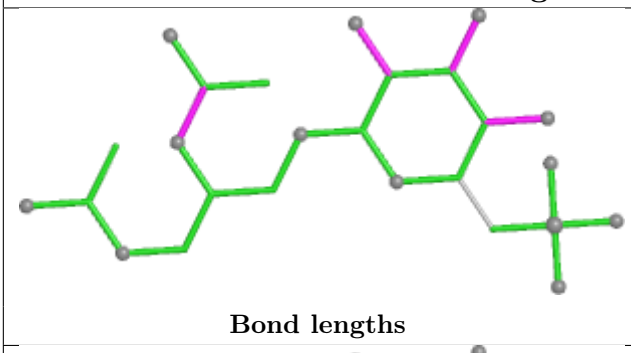


Rings

Ligand SQD t 822



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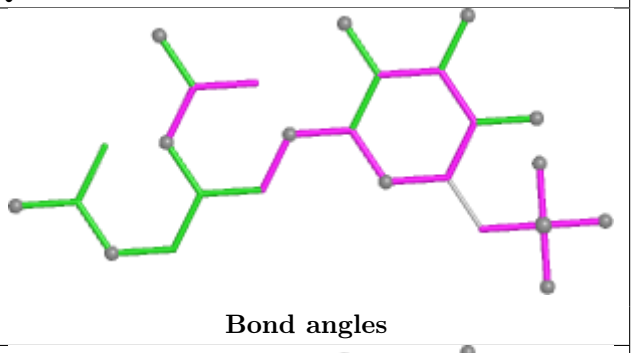

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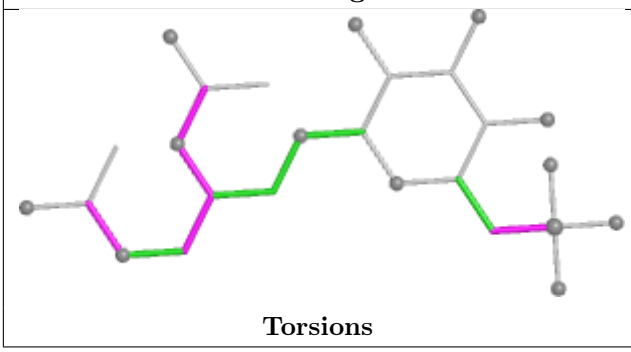

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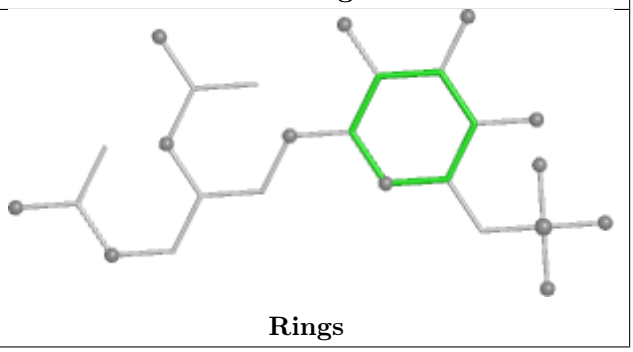
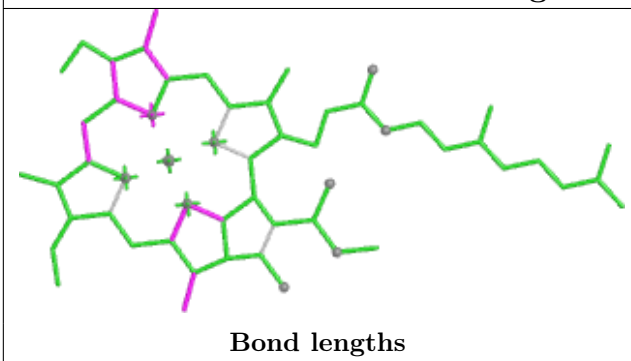


Rings

Ligand CLA c 518



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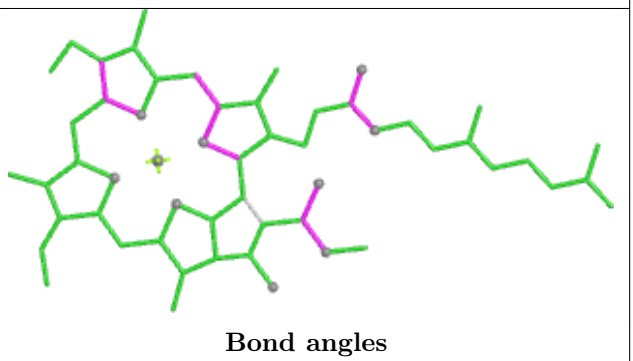

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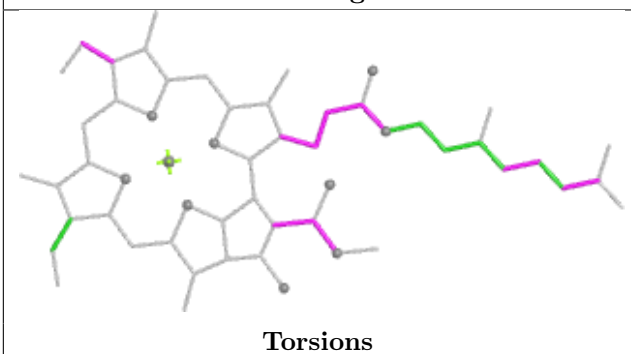

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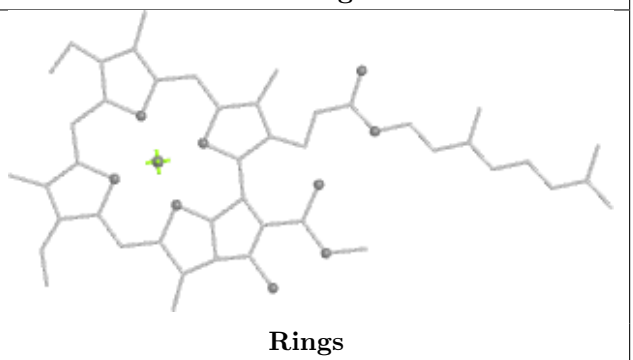
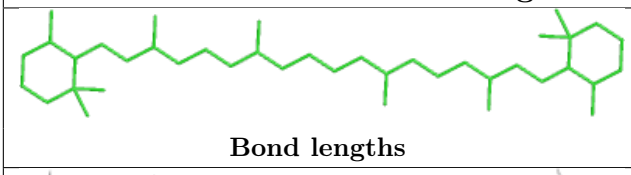


Rings

Ligand BCR S 4018



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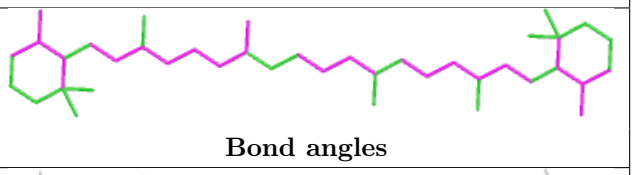

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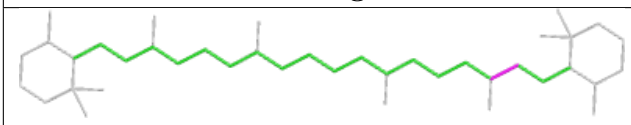

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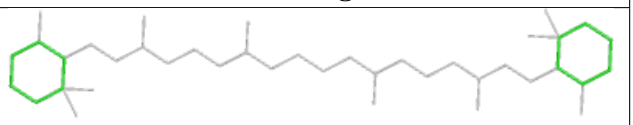
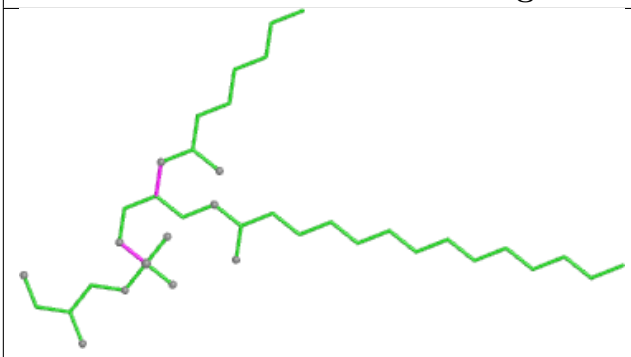


Rings

Ligand LHG n 5218



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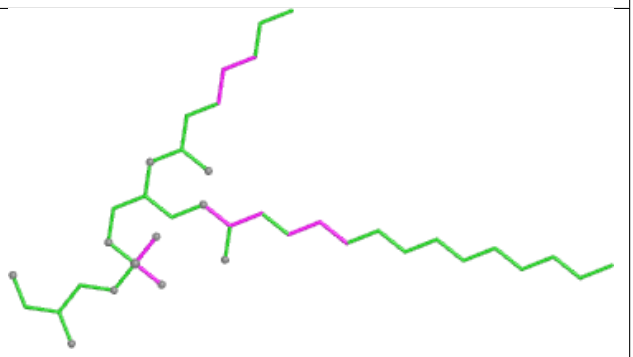

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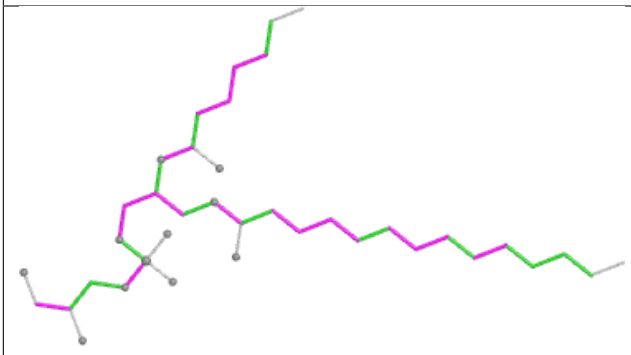

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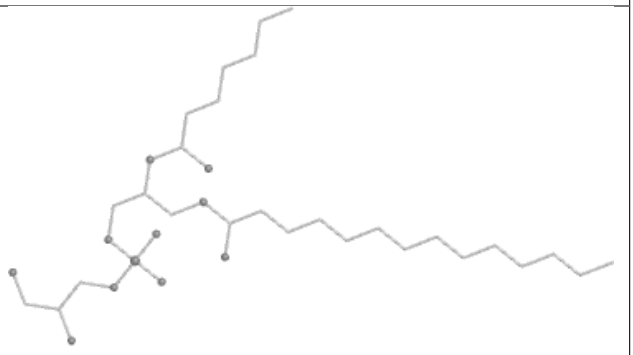
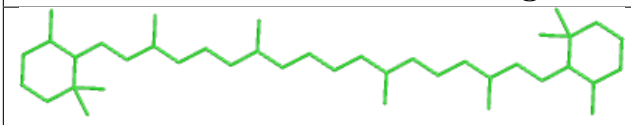


Rings

Ligand BCR f 4009



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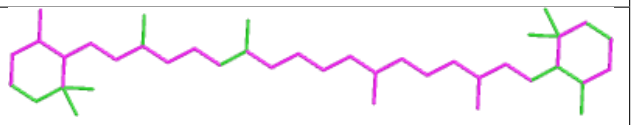

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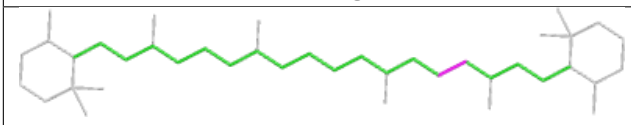

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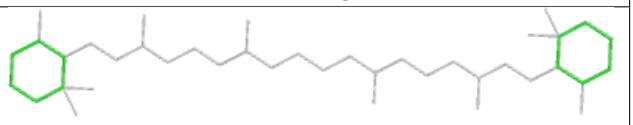
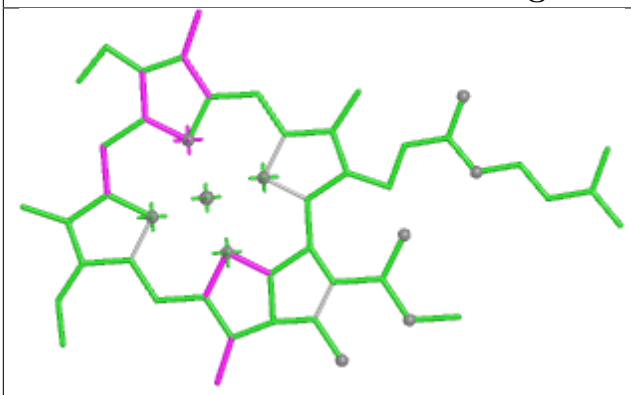


Rings

Ligand CLA 3 511



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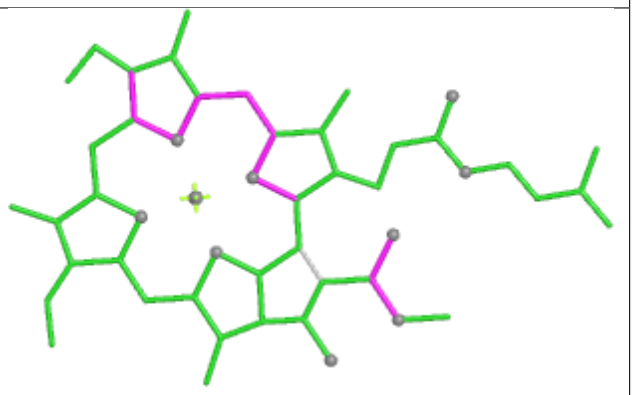

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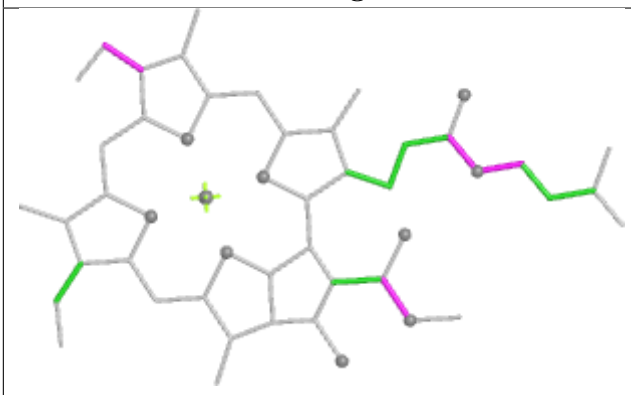

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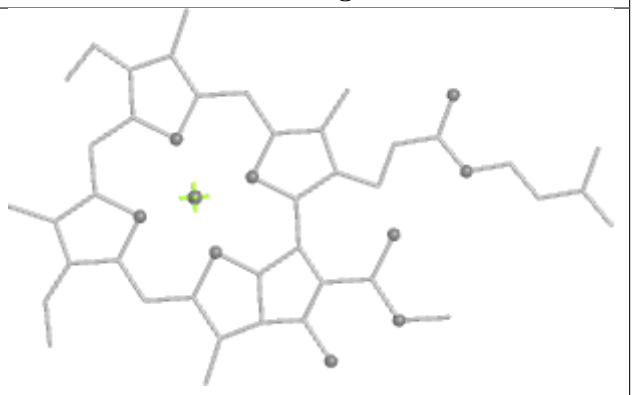
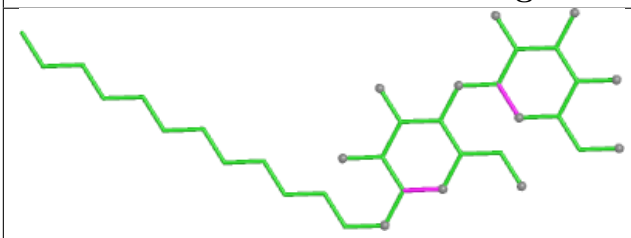


Rings

Ligand LMU e 1848



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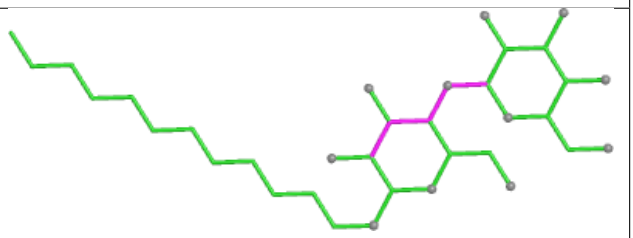
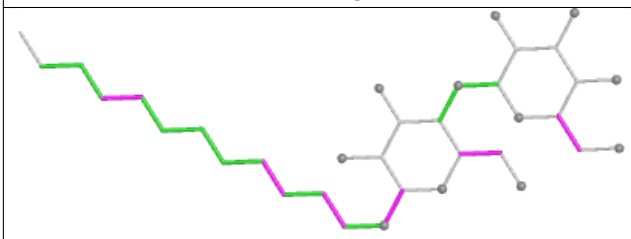


Bond angles



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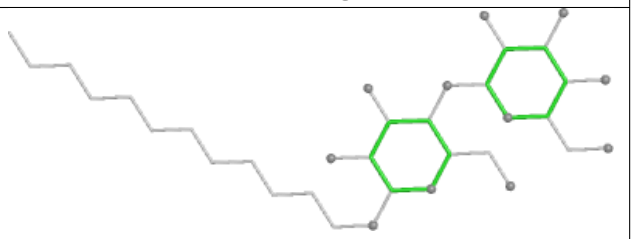
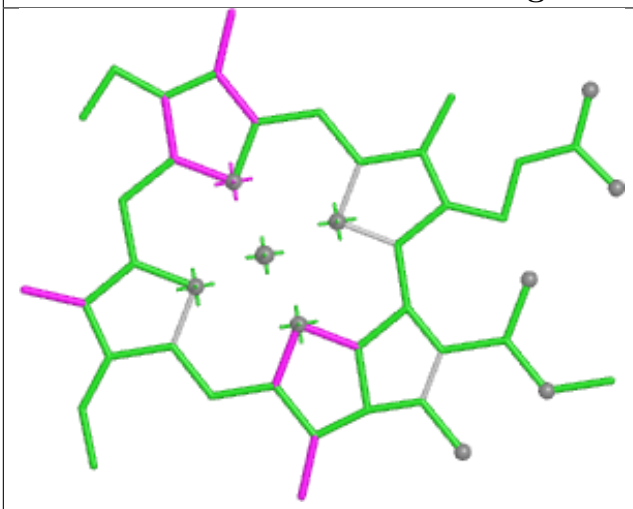


Rings

Ligand CLA b 508



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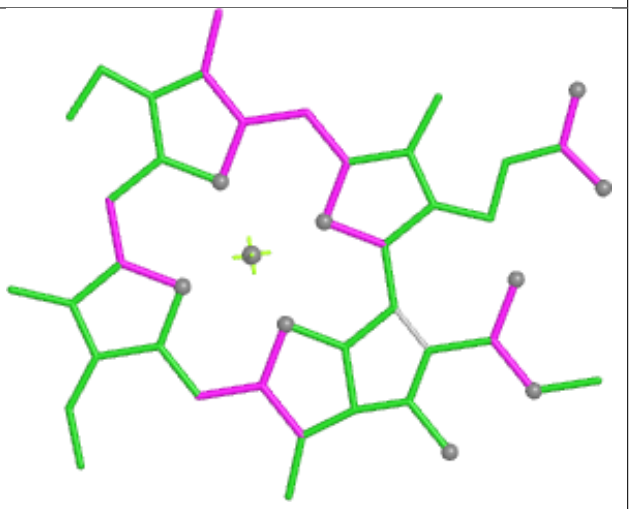
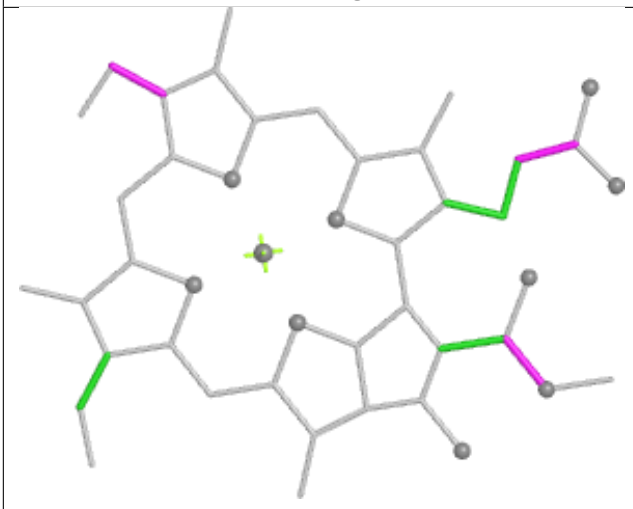


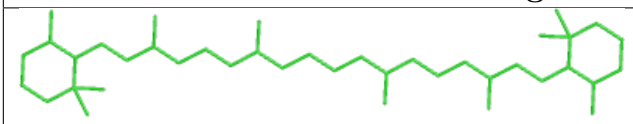
Bond angles



Torsions

Rings

Ligand BCR 4 523



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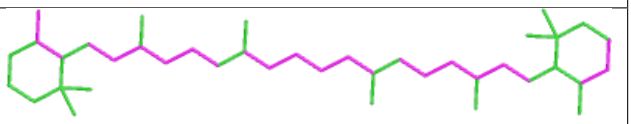
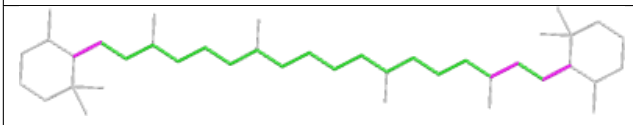


Bond angles



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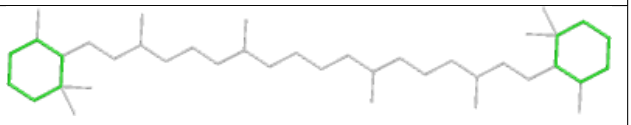
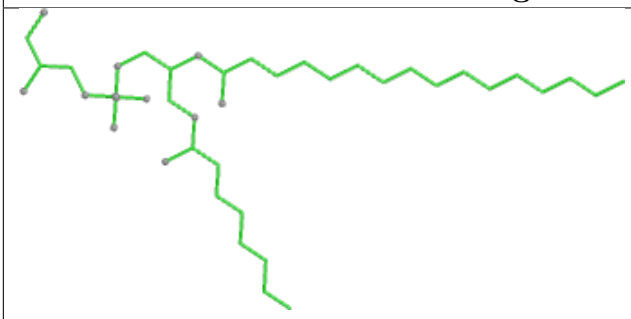


Rings

Ligand LHG G 5003



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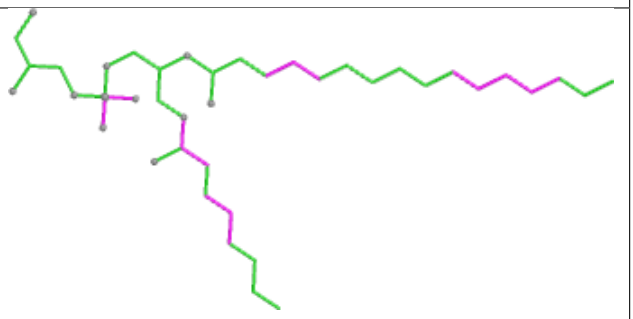
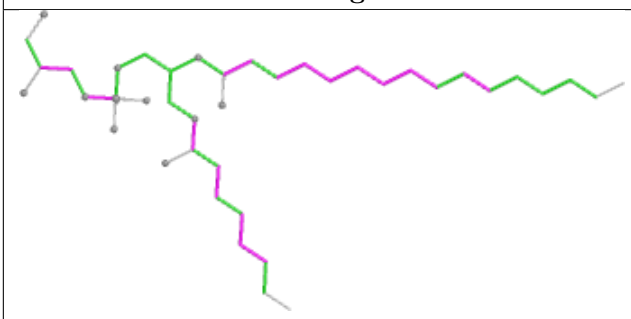
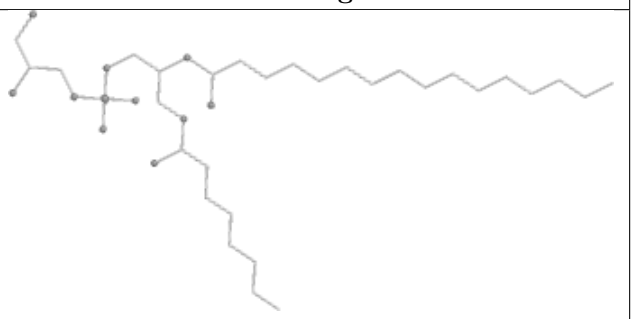


Bond angles

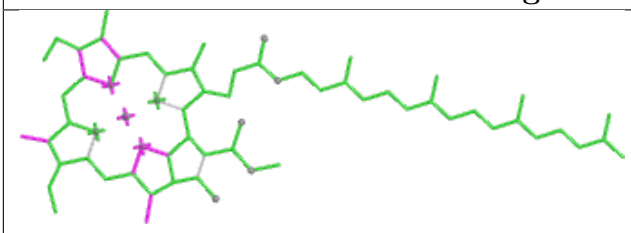


Torsions

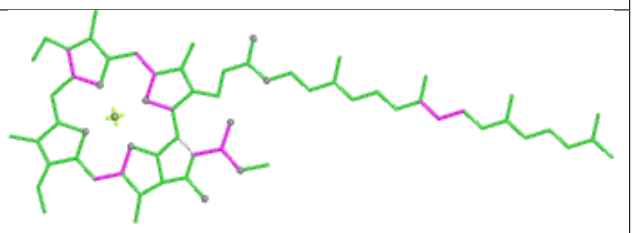


Rings

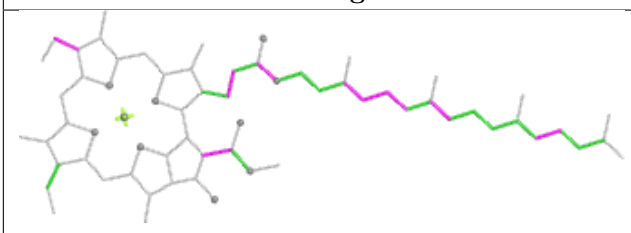
Ligand CLA f 1204



Bond lengths



Bond angles



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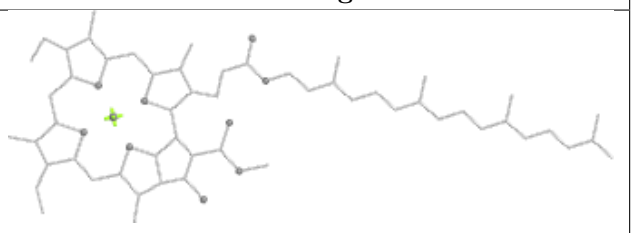
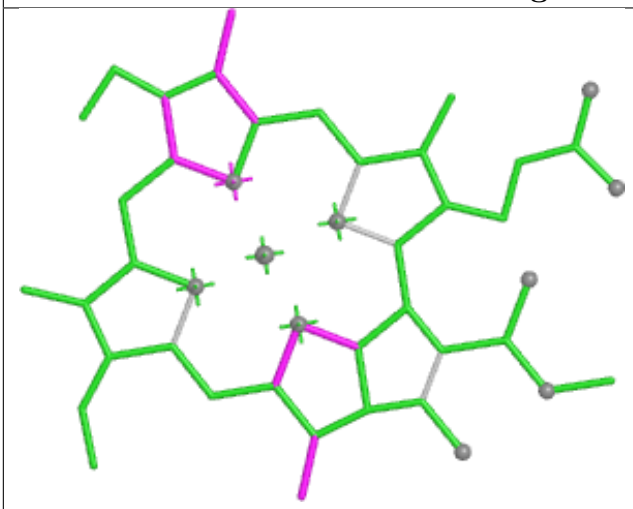


Rings

Ligand CLA t 512



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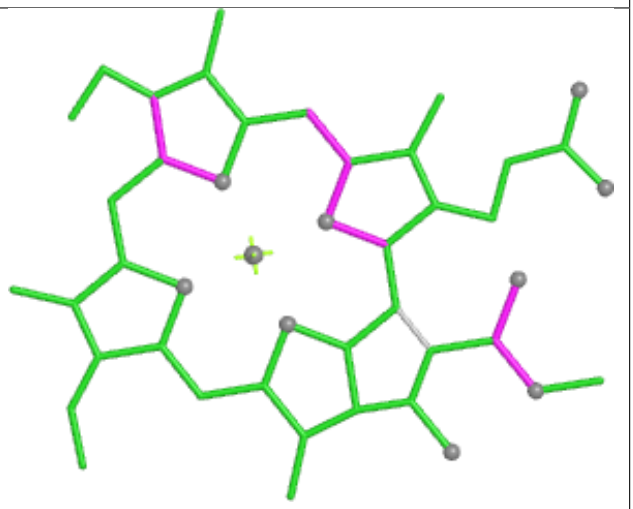
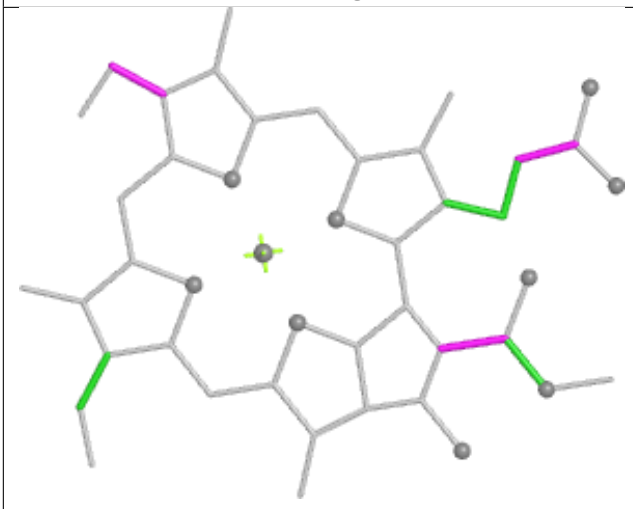


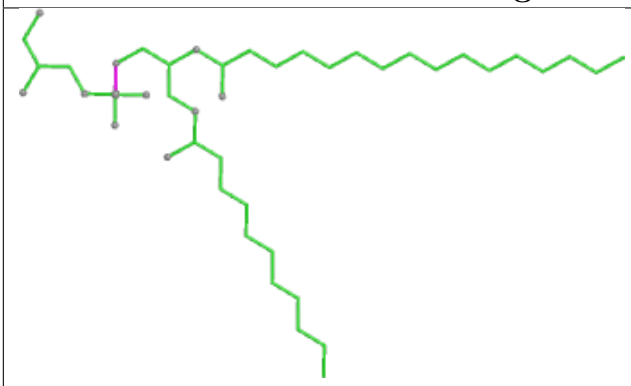
Bond angles



Torsions

Rings

Ligand LHG B 1855



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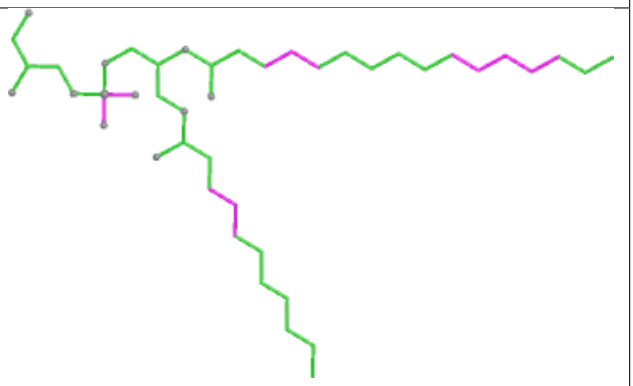

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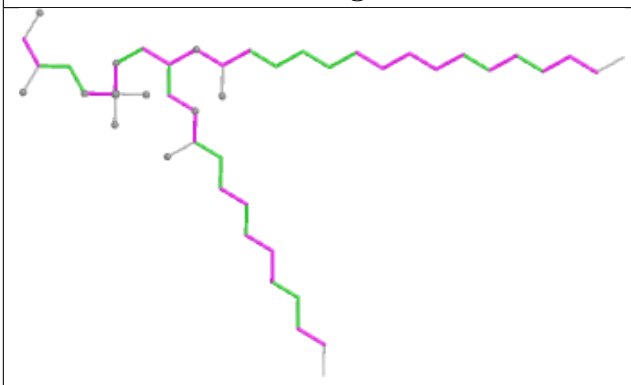

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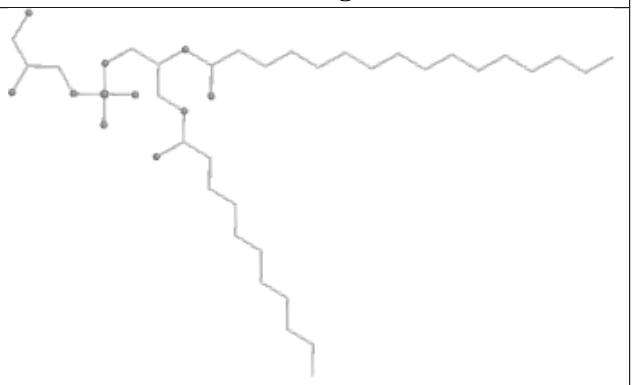
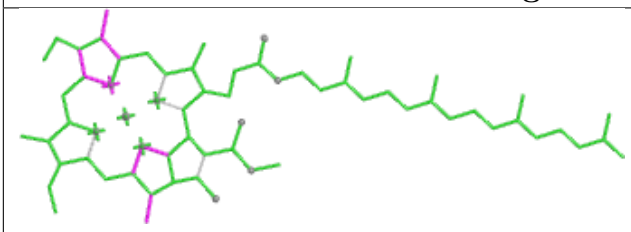


Rings

Ligand CLA f 1208



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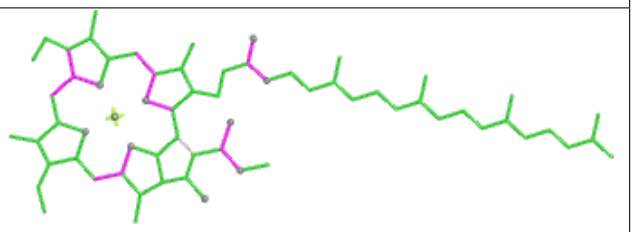
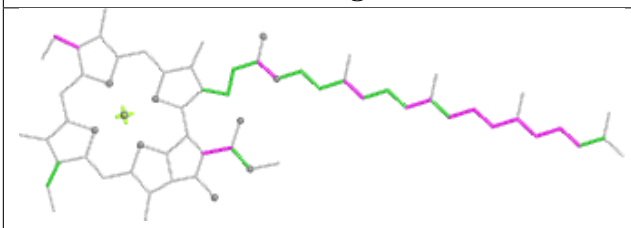


Bond angles



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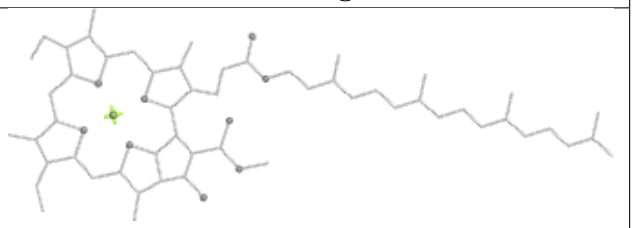
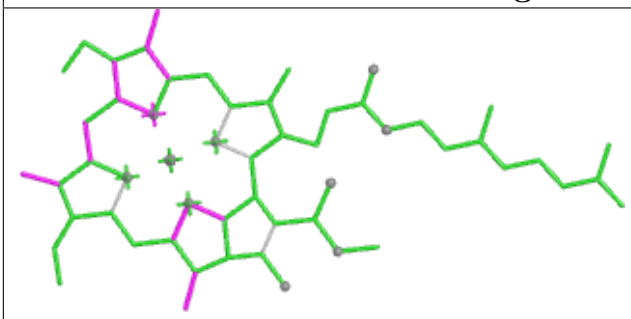
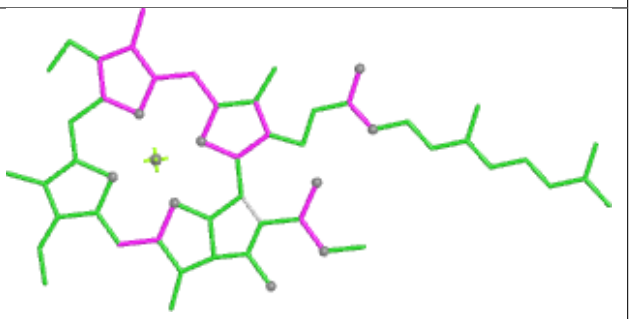
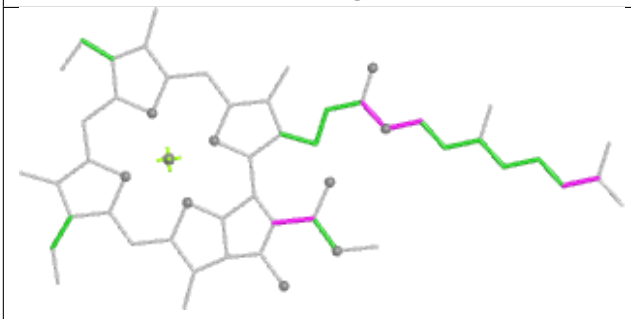
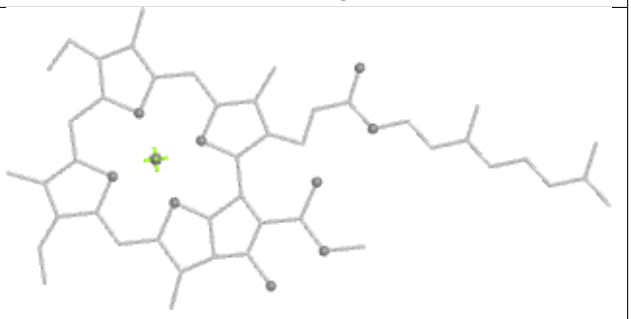


Rings

Ligand CLA G 1105	
 Bond lengths	 Bond angles
 Torsions	 Rings

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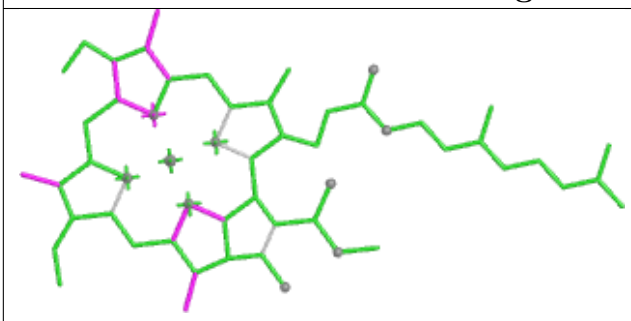
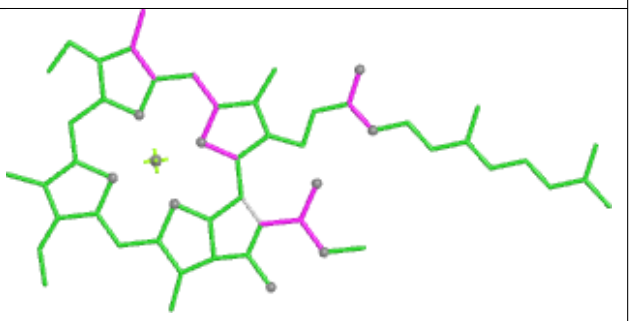
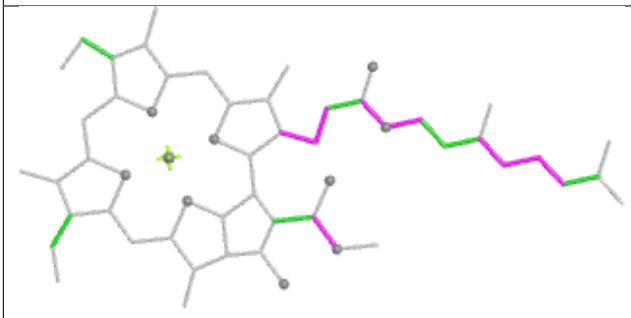
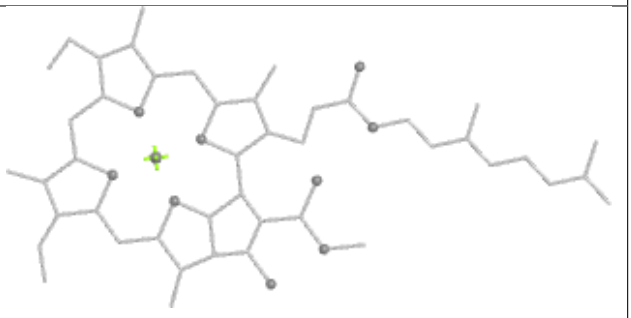
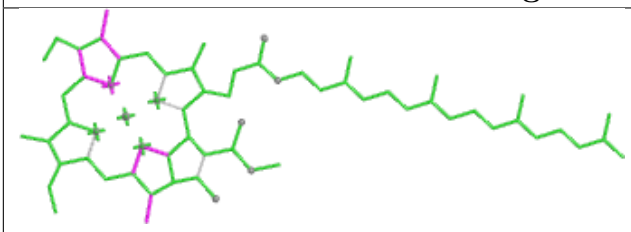
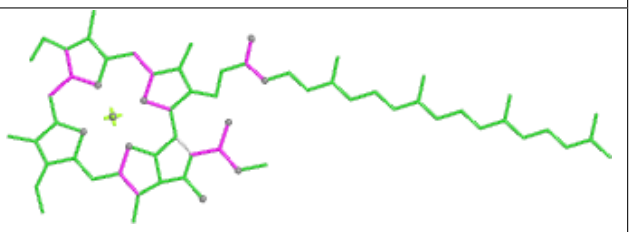
 Bond lengths	 Bond angles
 Torsions	 Rings

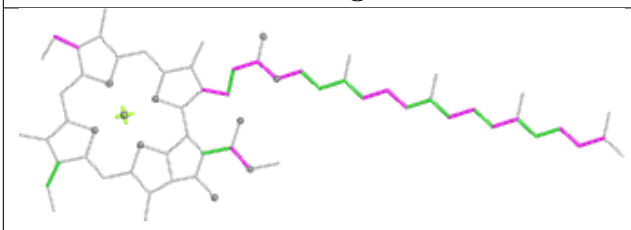
Ligand CLA f 1219



Bond lengths



Bond angles



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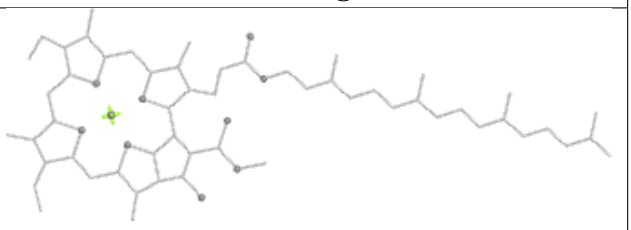
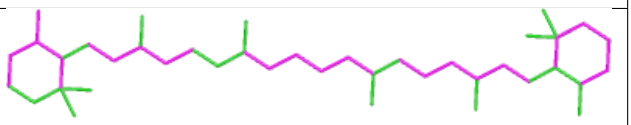


Rings

Ligand BCR n 4022

Bond lengths



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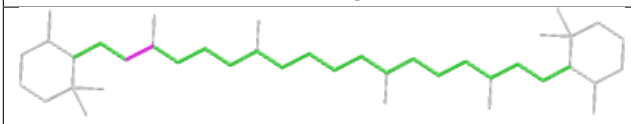

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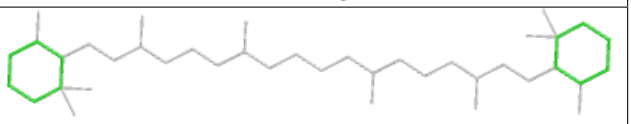
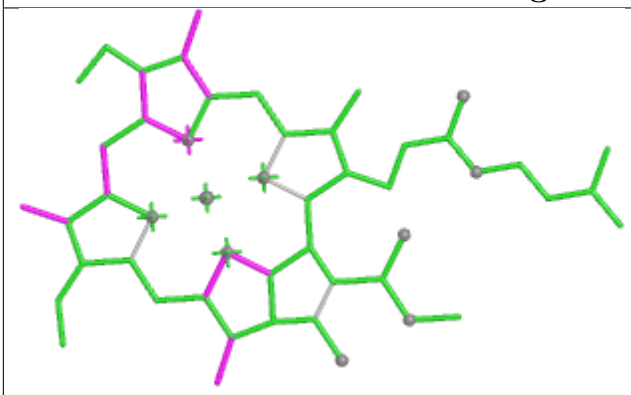


Rings

Ligand CLA r 504



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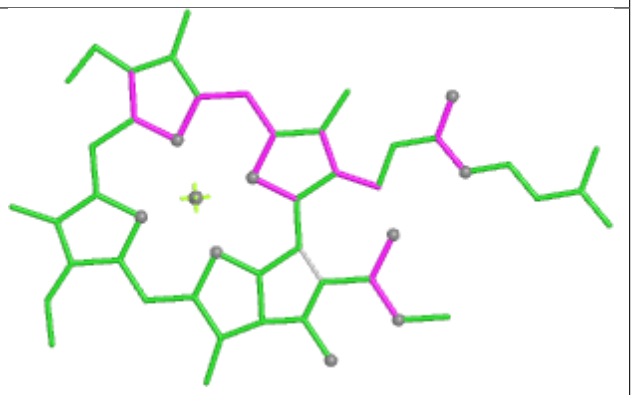
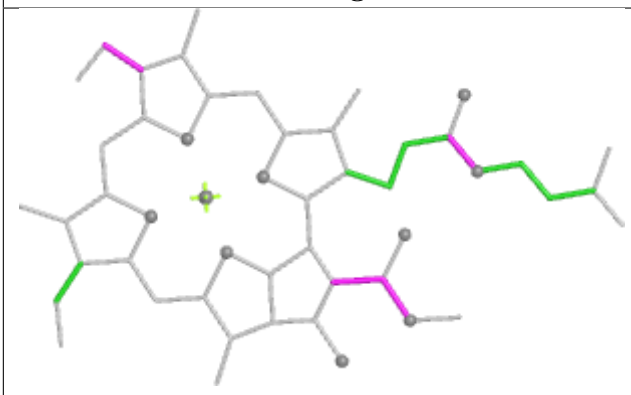


Bond angles



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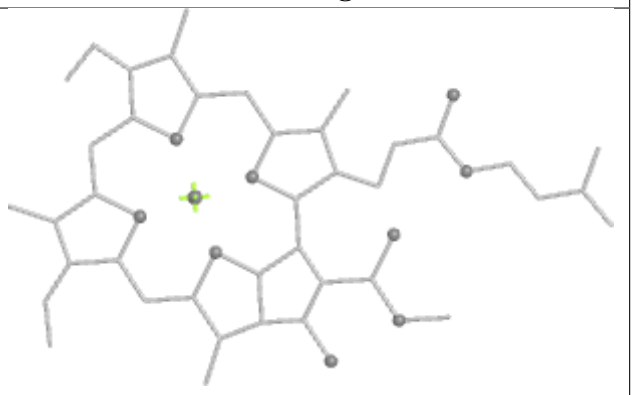
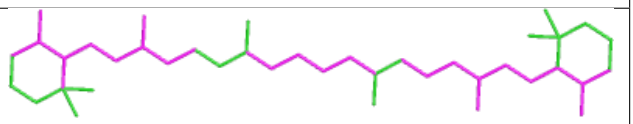


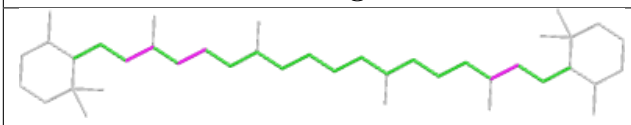
Rings

Ligand BCR a 524

Bond lengths



Bond angles



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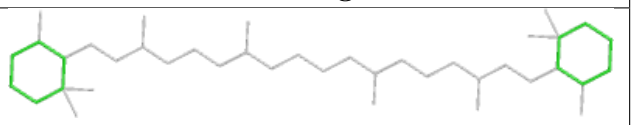
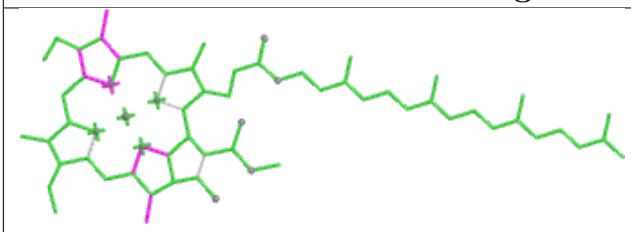


Rings

Ligand CLA G 1011



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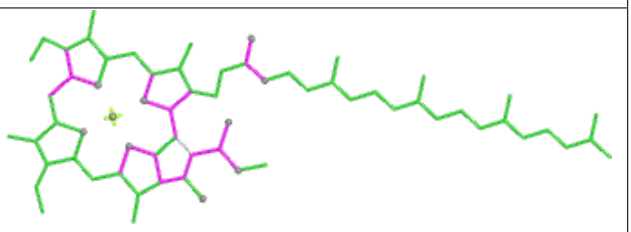
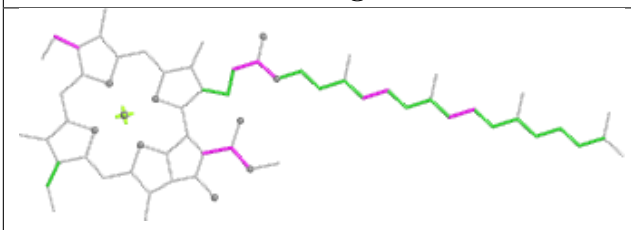
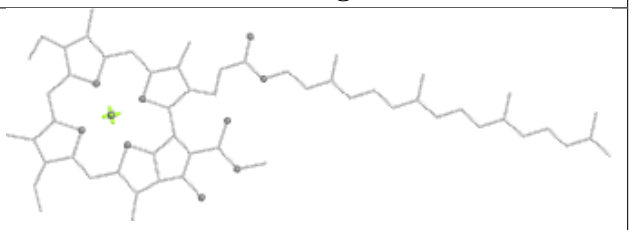


Bond angles

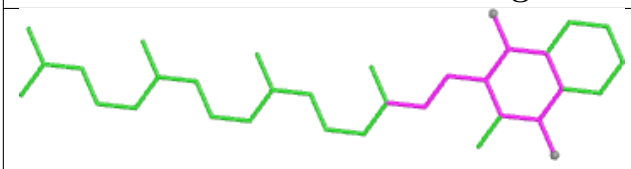


Torsions



Rings

Ligand PQN G 2001



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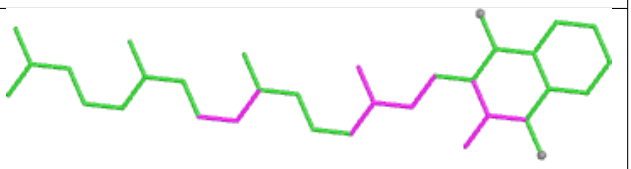
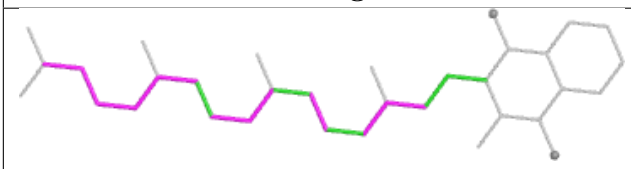
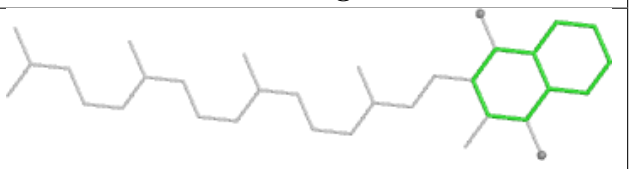


Bond angles

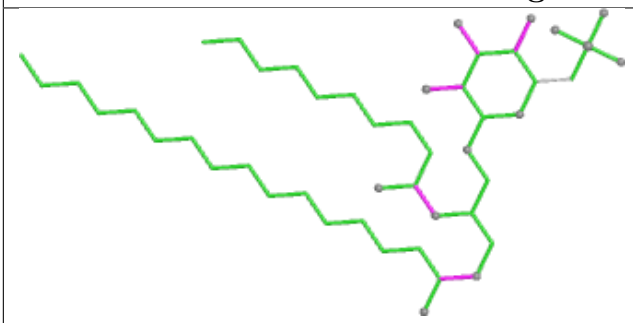


Torsions



Rings

Ligand SQD q 822



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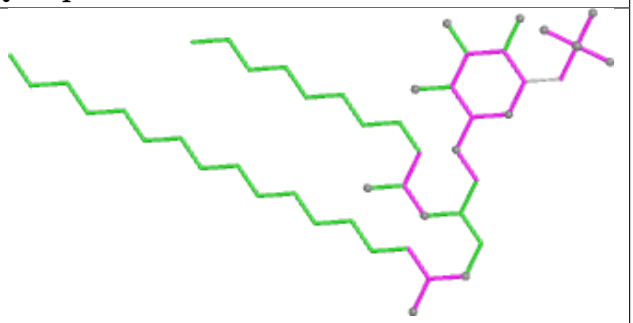
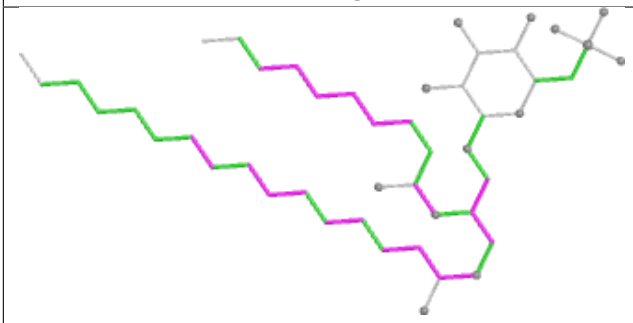


Bond angles



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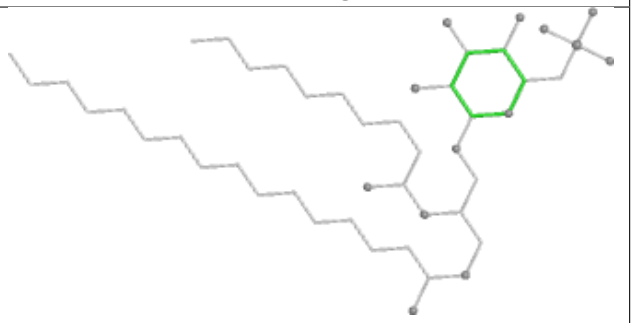
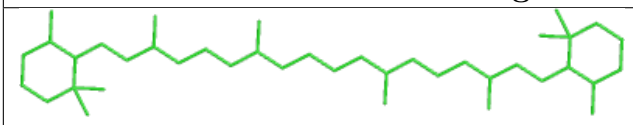
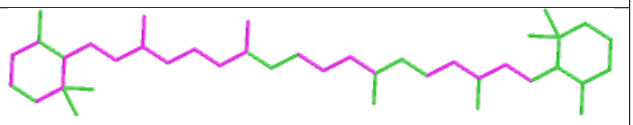


Rings

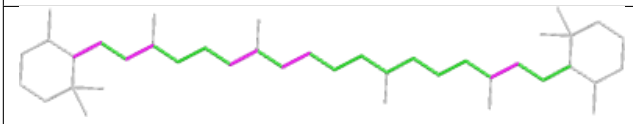
Ligand BCR G 4001



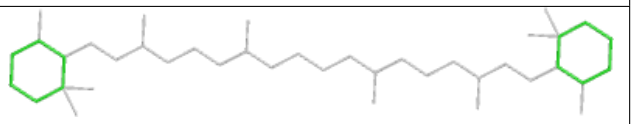
Bond lengths



Bond angles

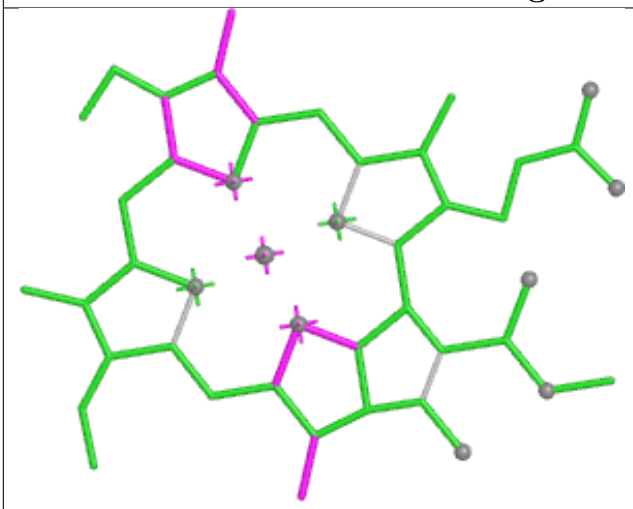


Torsions



Rings

Ligand CLA a 512



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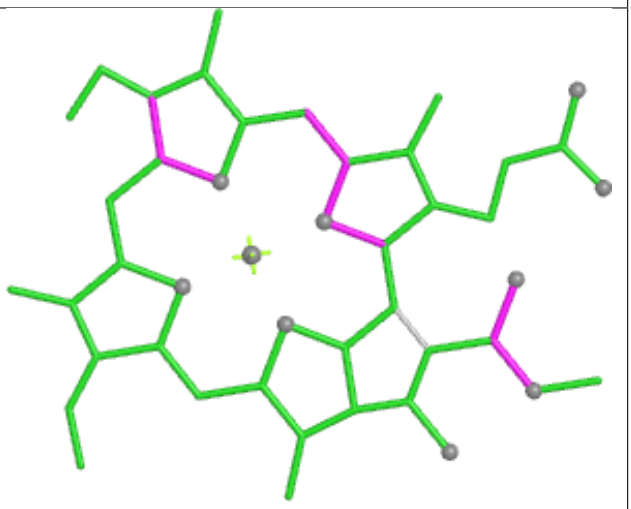
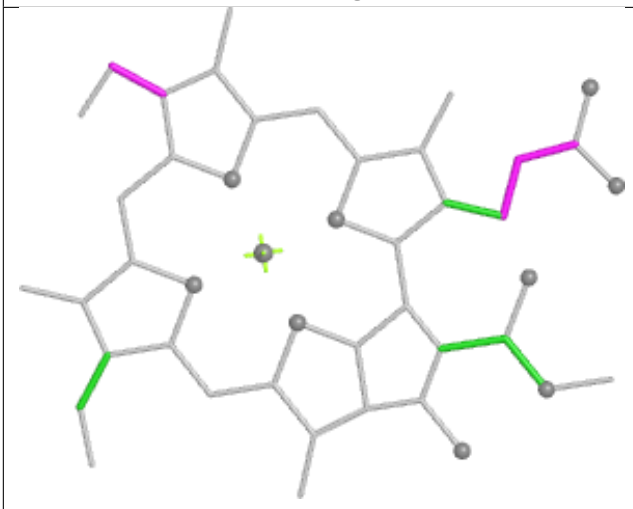


Bond angles



Torsions

Rings

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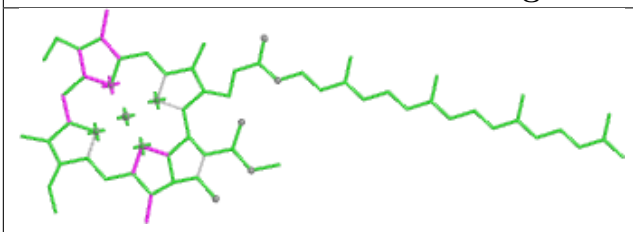

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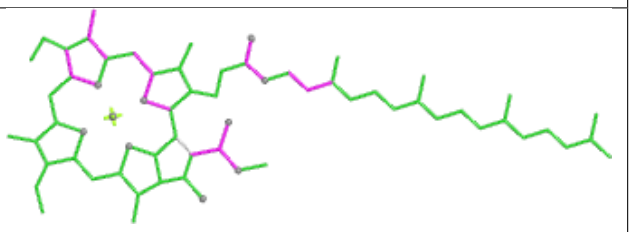
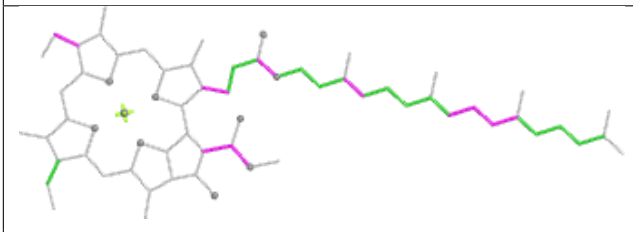


Bond angles



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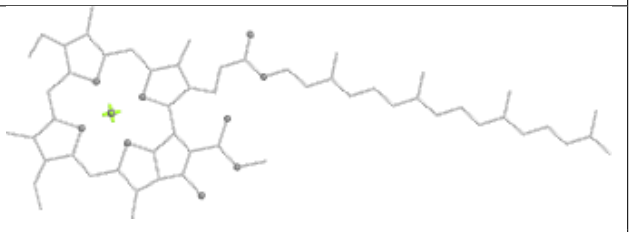
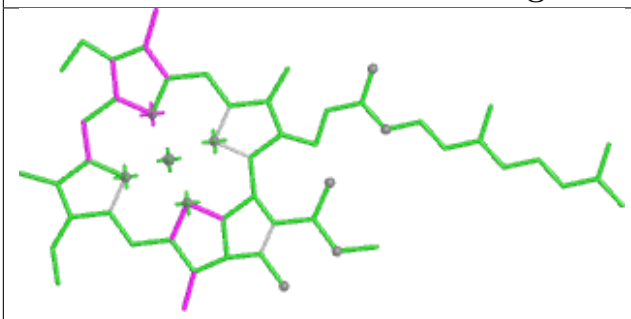


Rings

Ligand CLA b 518



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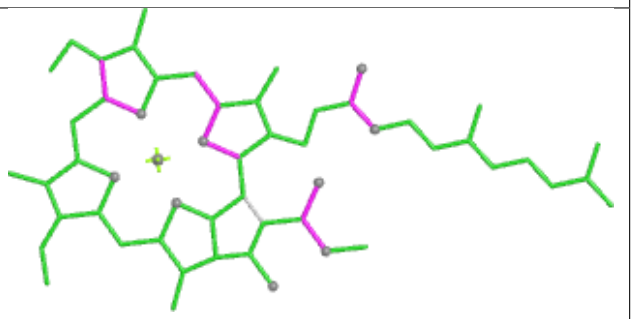
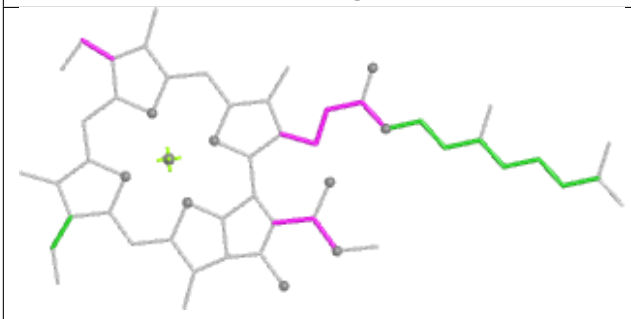


Bond angles



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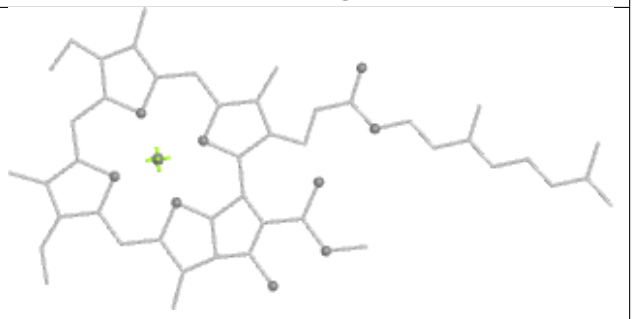
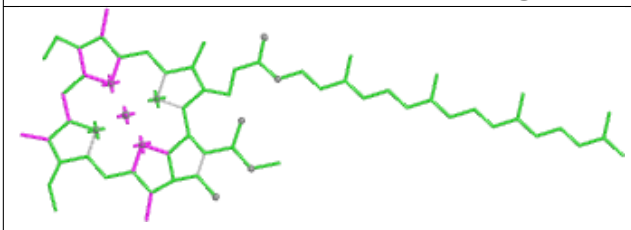


Rings

Ligand CLA B 1012



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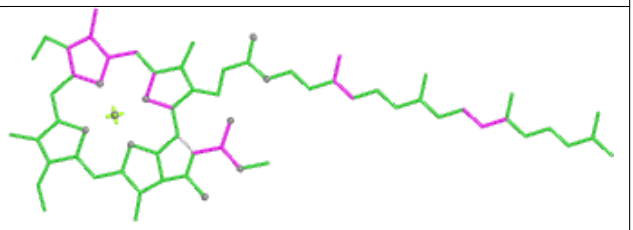
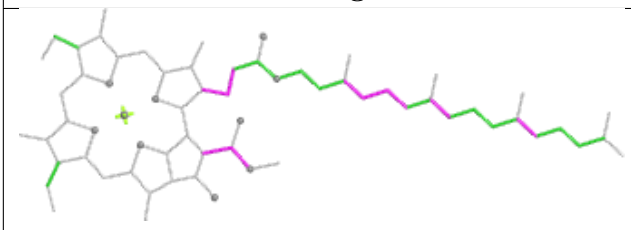


Bond angles



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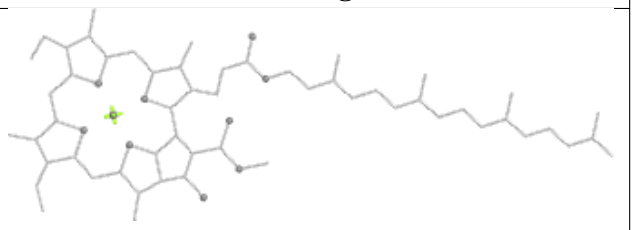
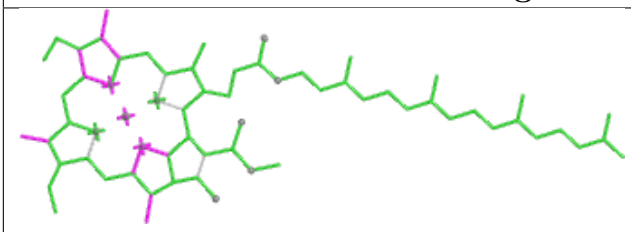


Rings

Ligand CLA H 1205



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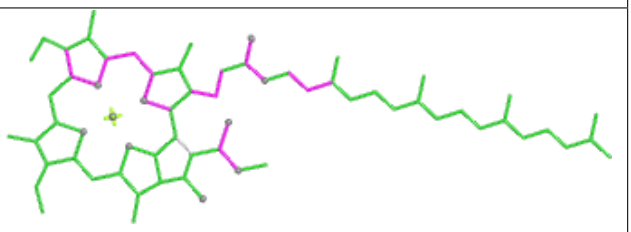
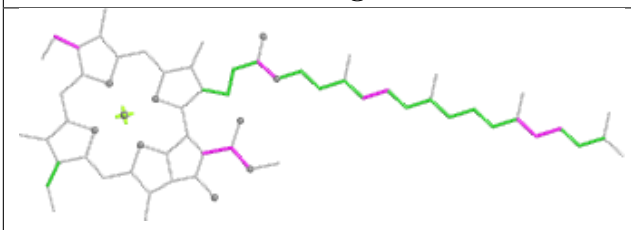


Bond angles



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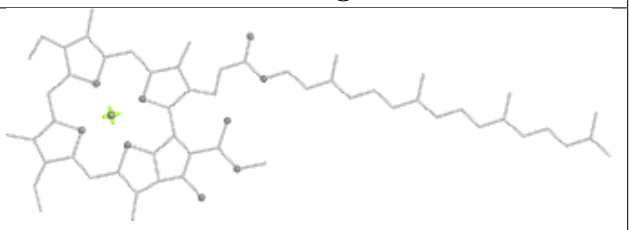
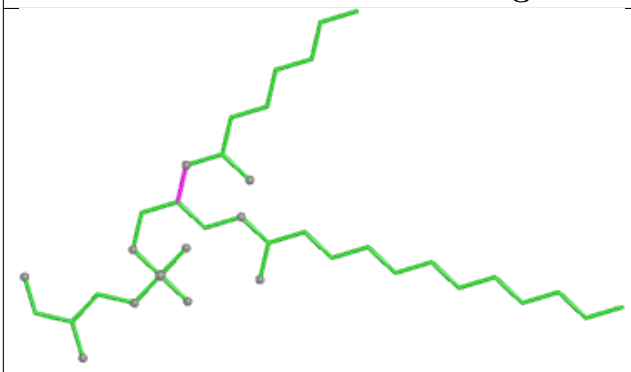


Rings

Ligand LHG G 5004



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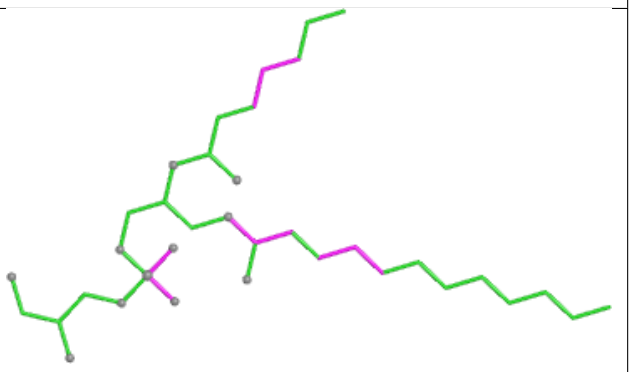
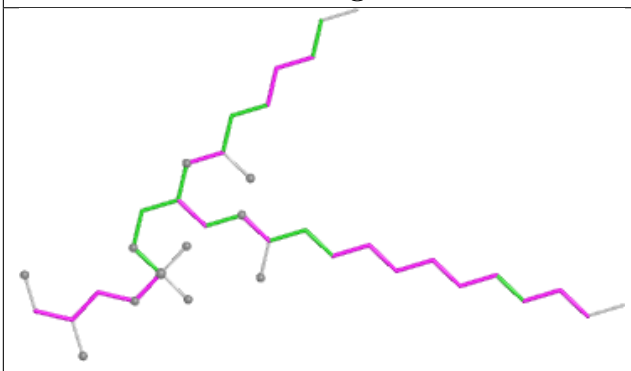


Bond angles



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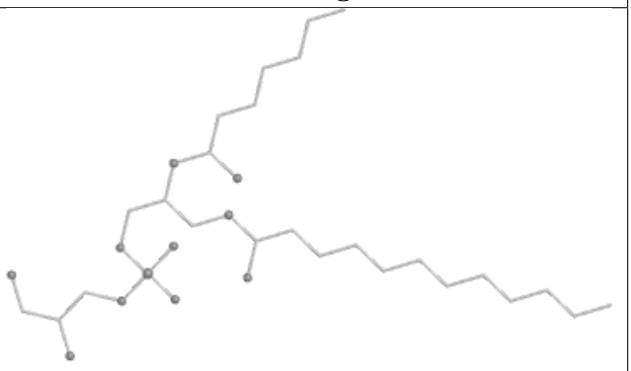
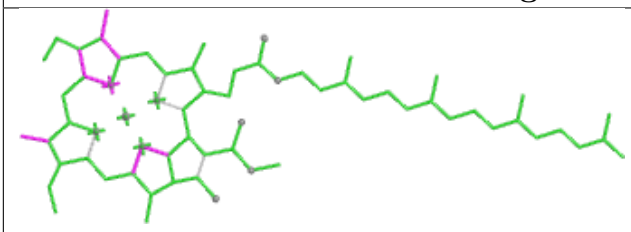


Rings

Ligand CLA e 1137



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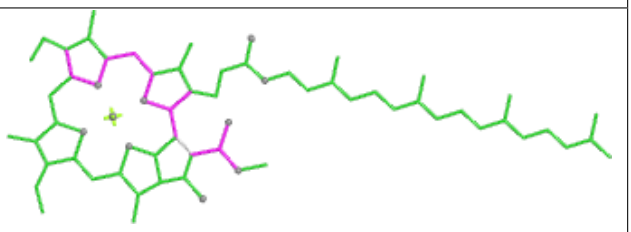
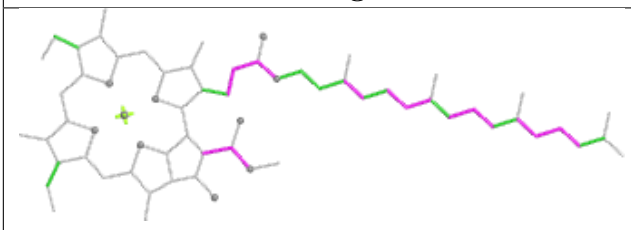


Bond angles



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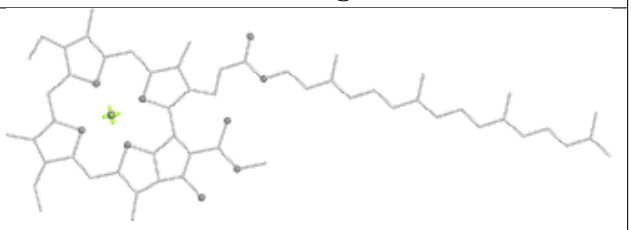
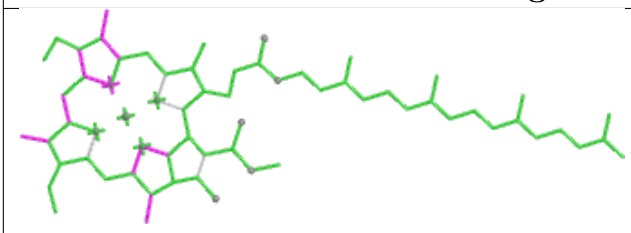


Rings

Ligand CLA 2 509



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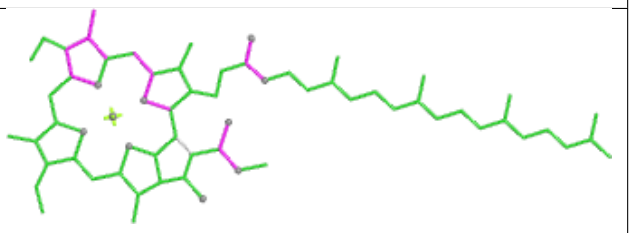
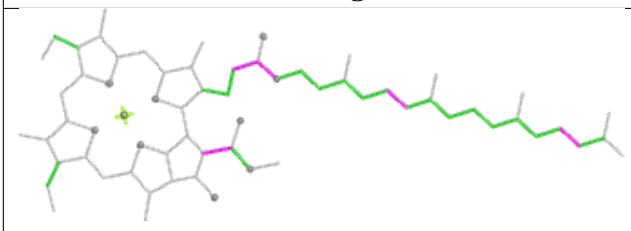


Bond angles



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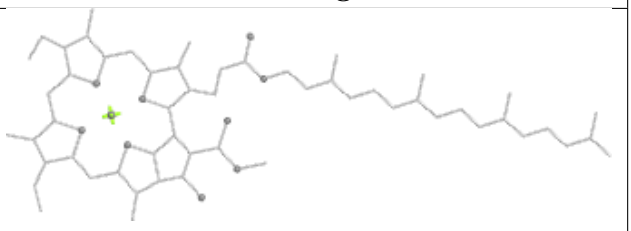
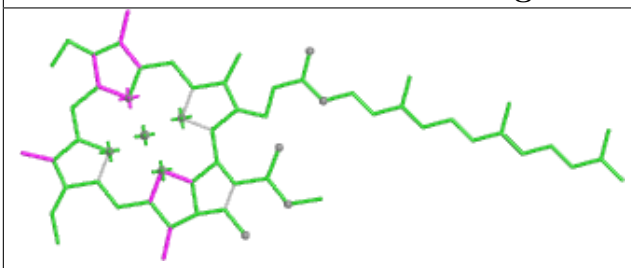


Rings

Ligand CLA A 1118



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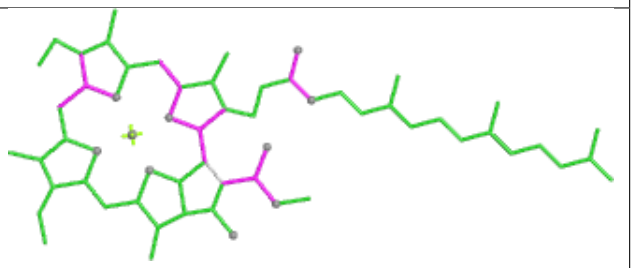

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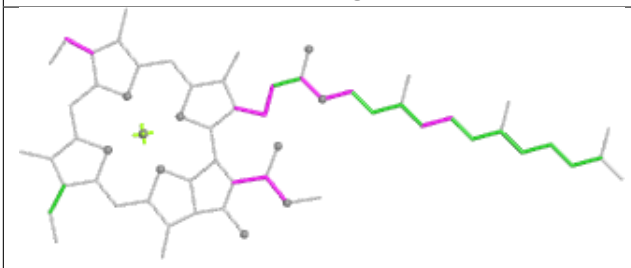

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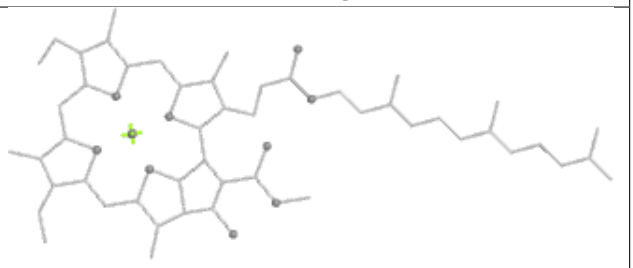
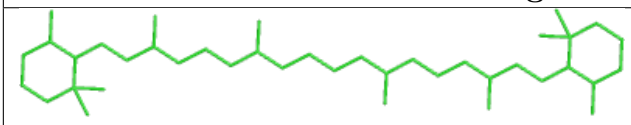


Rings

Ligand BCR 4 524



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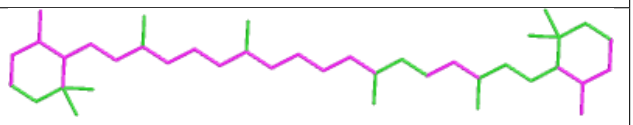
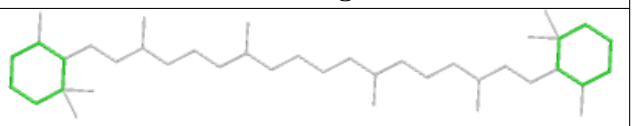


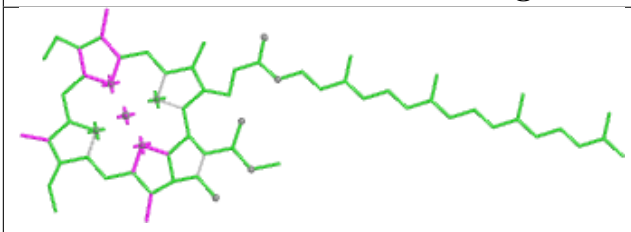
Bond angles

Torsions



Rings

Ligand CLA A 1117



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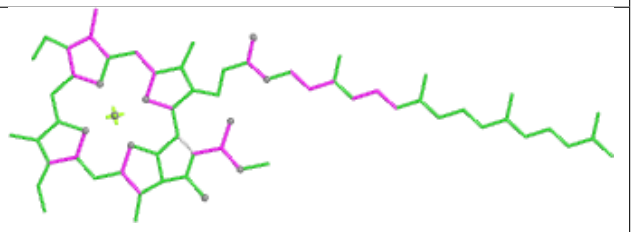
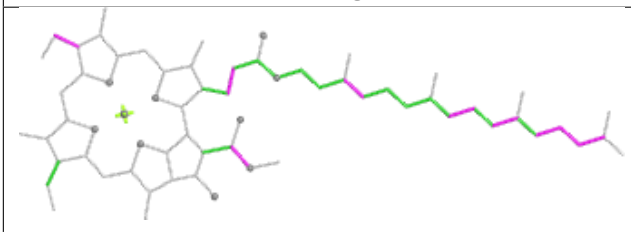


Bond angles



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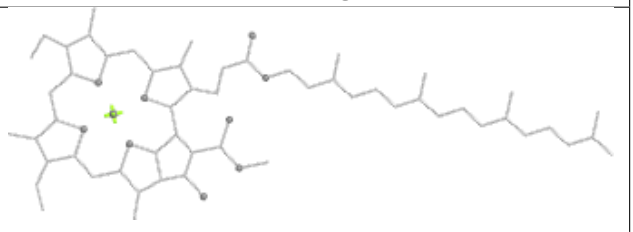
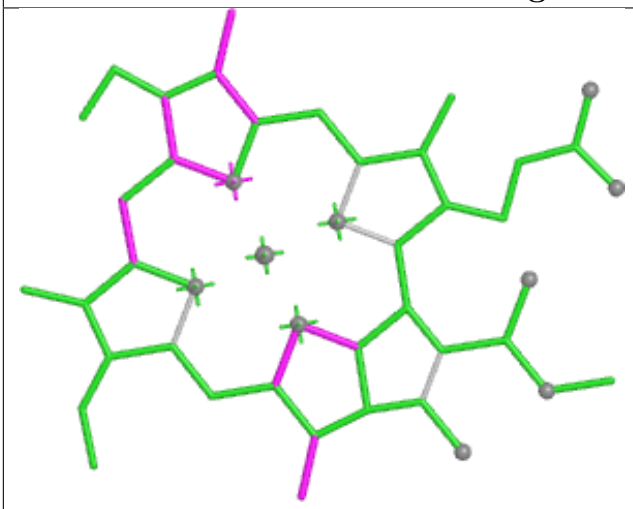


Rings

Ligand CLA 4 506



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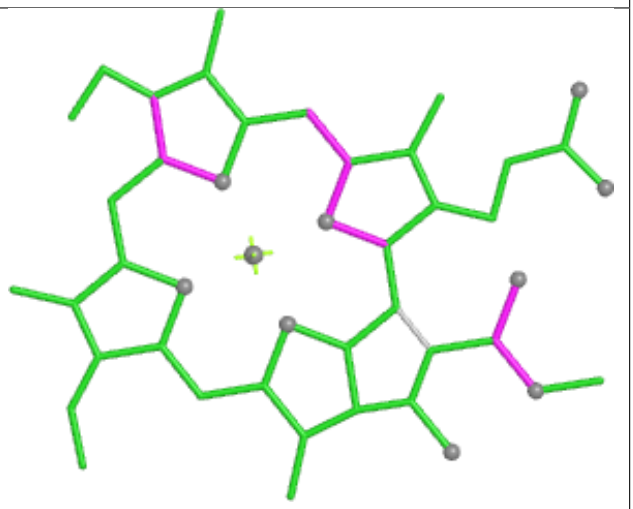
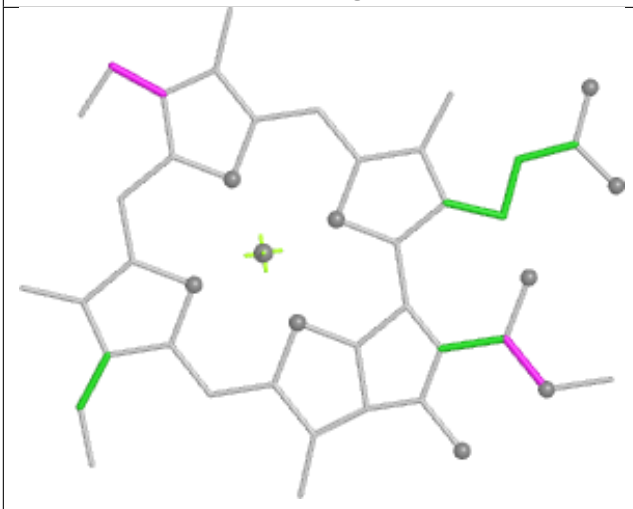


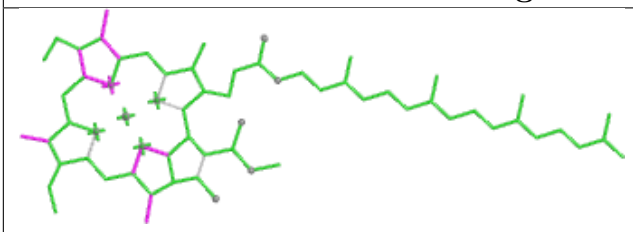
Bond angles



Torsions

Rings

Ligand CLA T 1303



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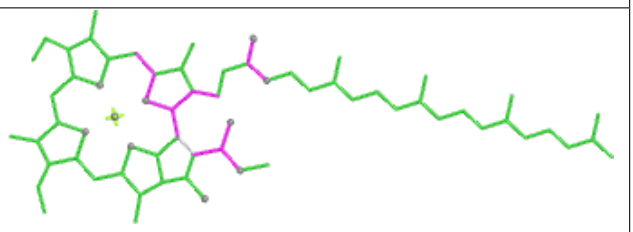
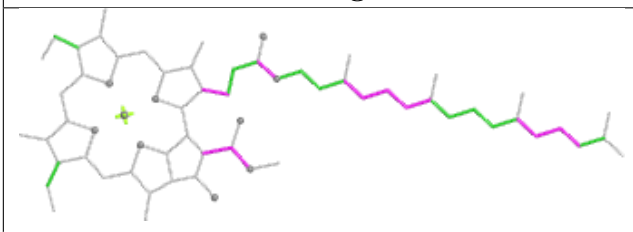
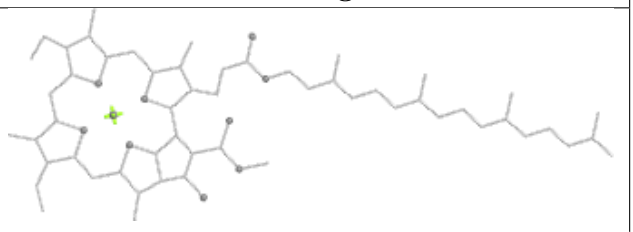


Bond angles

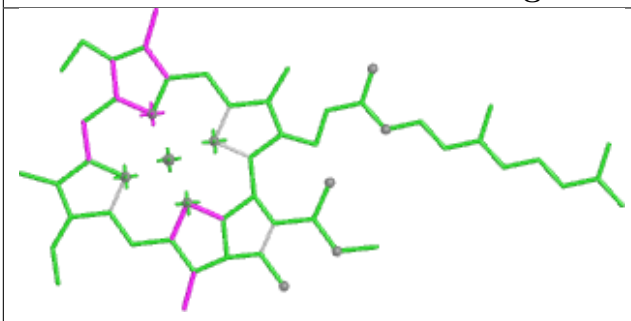


Torsions

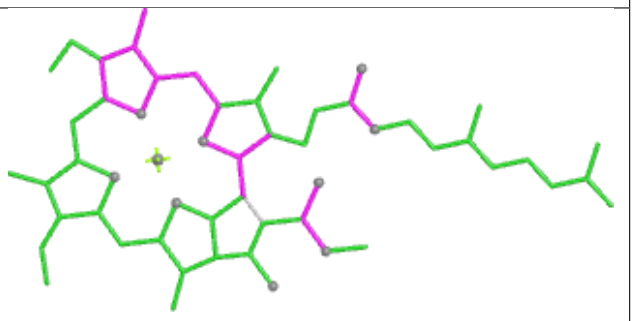


Rings

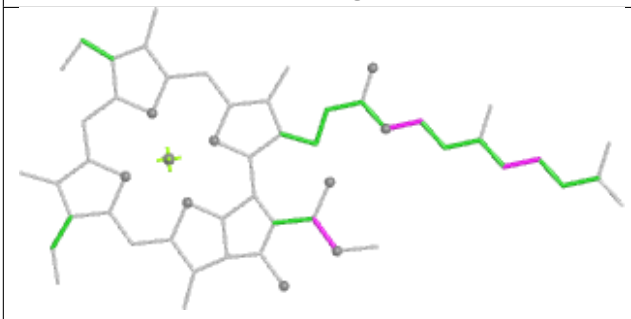
Ligand CLA Y 511



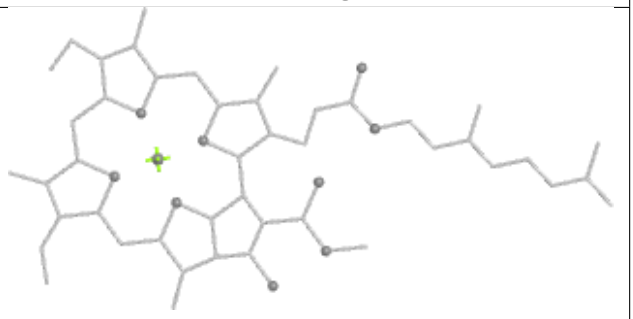
Bond lengths



Bond angles

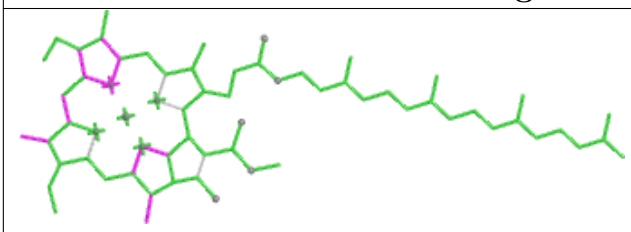


Torsions



Rings

Ligand CLA B 1202



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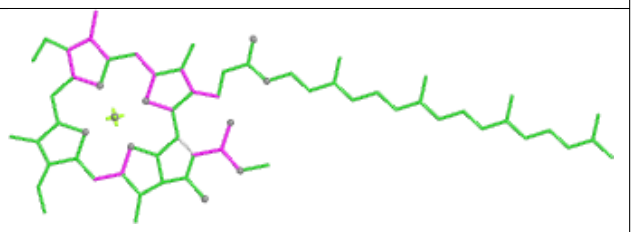
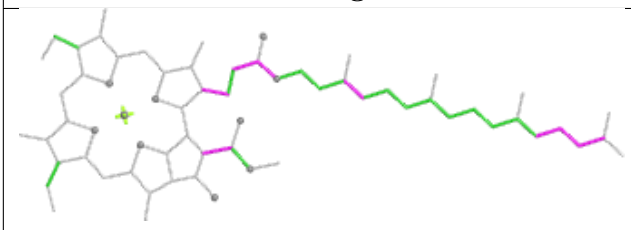
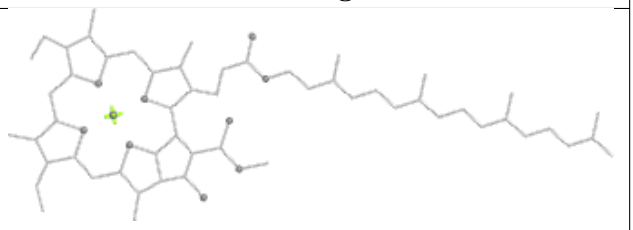


Bond angles

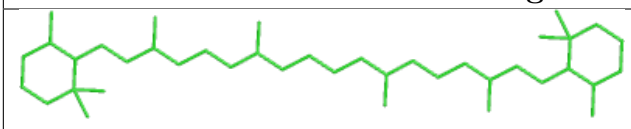


Torsions



Rings

Ligand BCR 6 521



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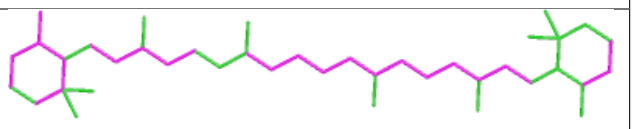
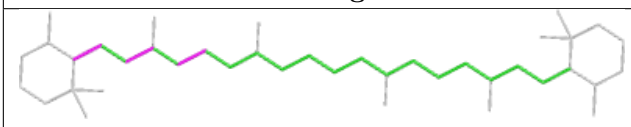
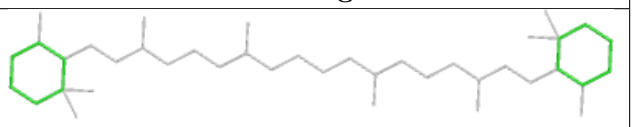


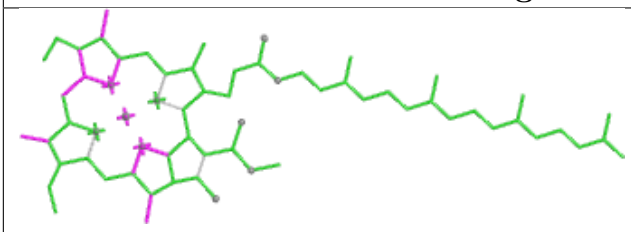
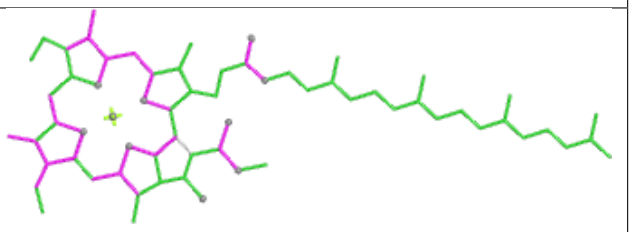
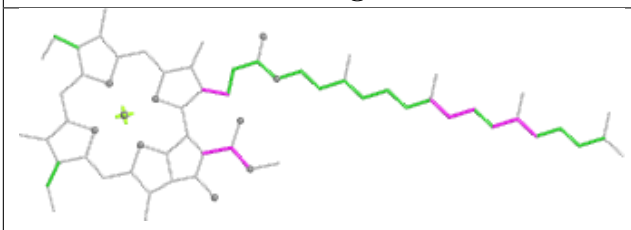
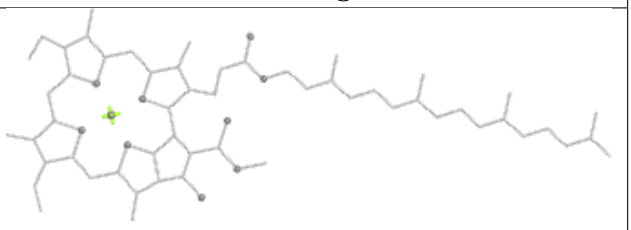
Bond angles

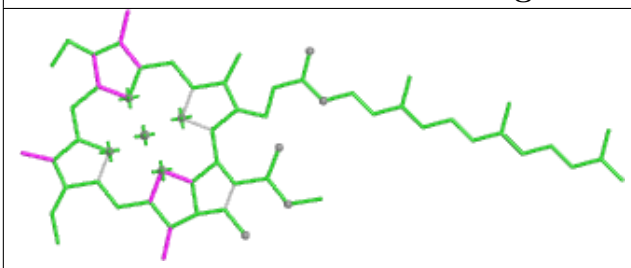
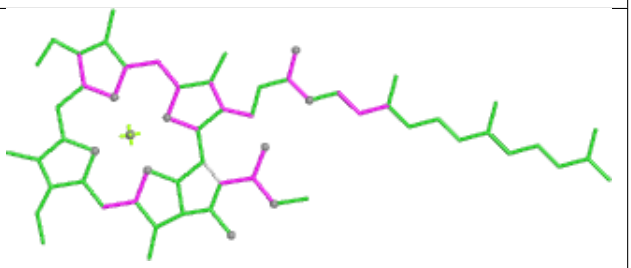
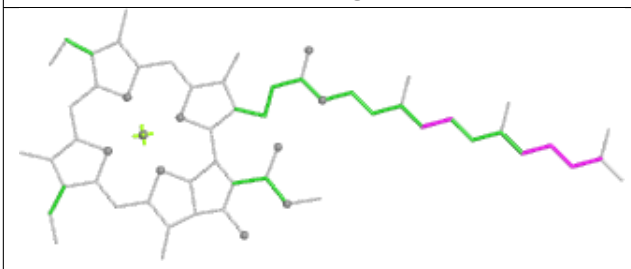
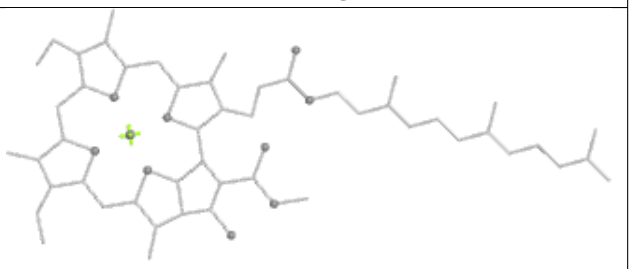


Torsions

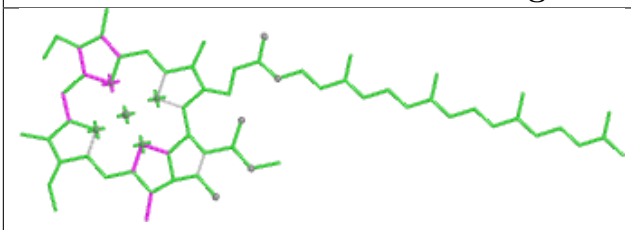


Rings

Ligand CLA B 1226	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 513



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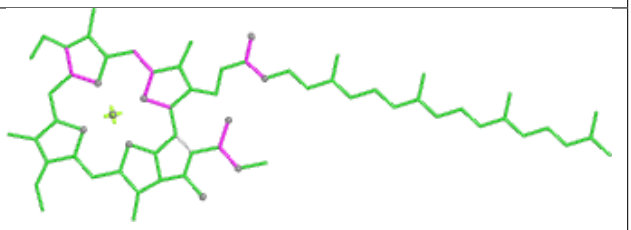
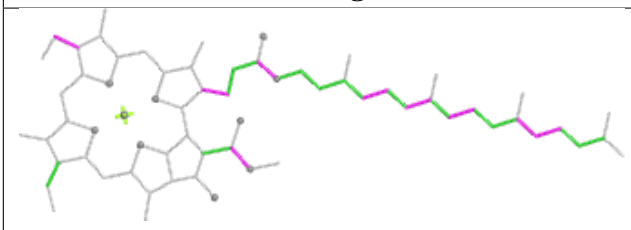
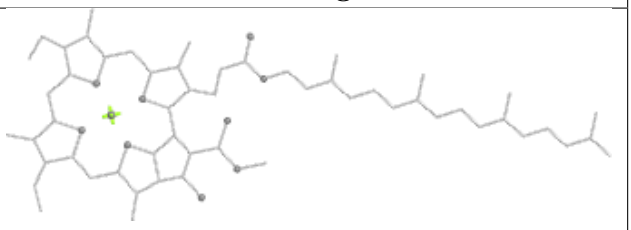


Bond angles

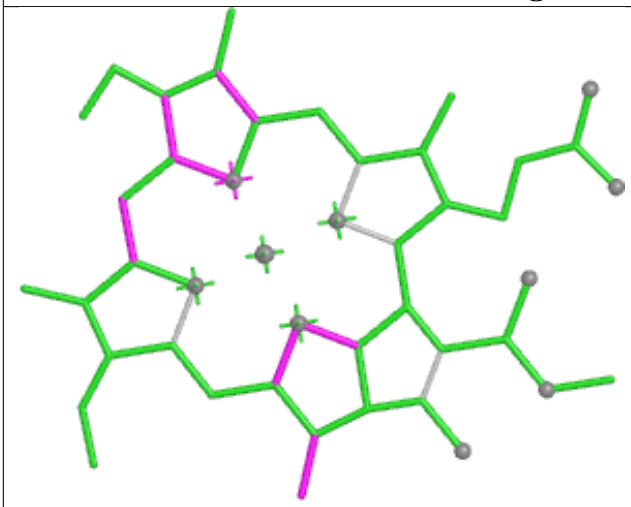


Torsions



Rings

Ligand CLA v 509



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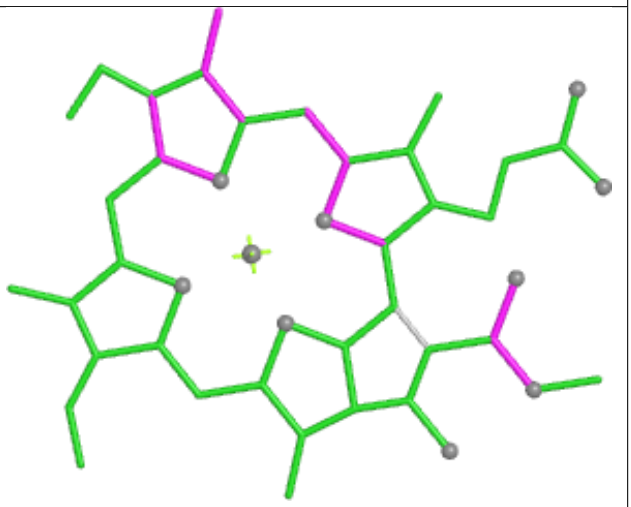

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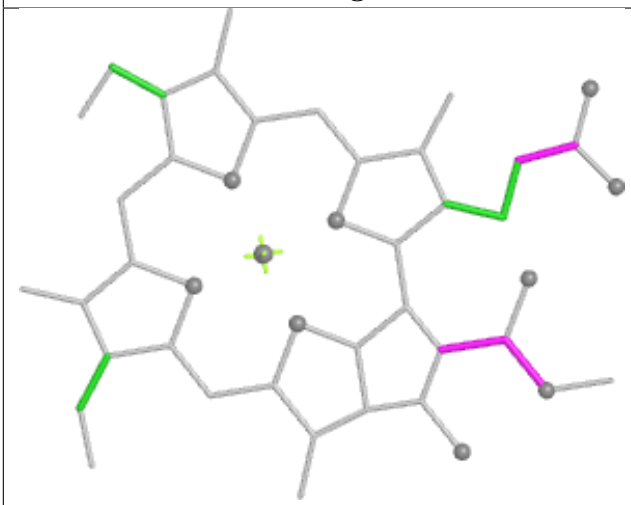

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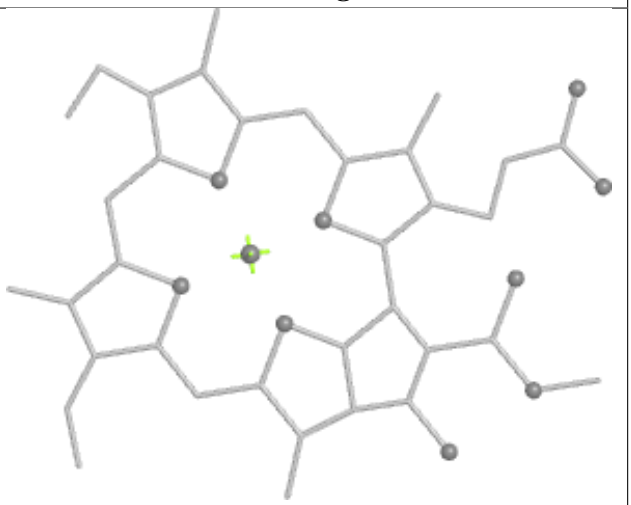
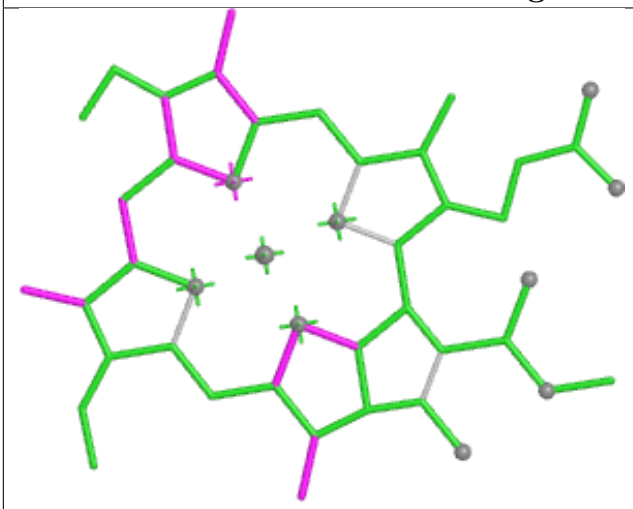


Rings

Ligand CLA q 504



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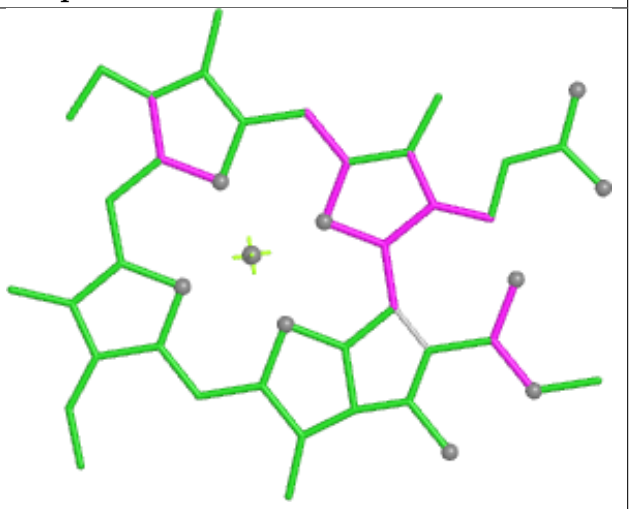
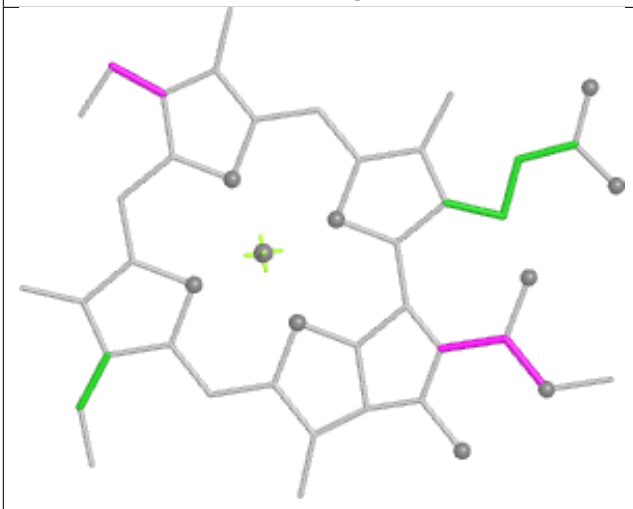


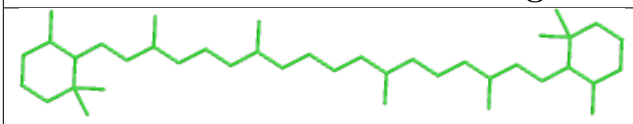
Bond angles



Torsions

Rings

Ligand BCR 1 521



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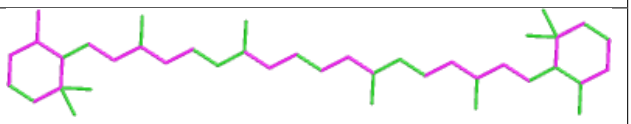
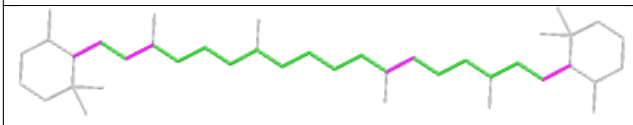
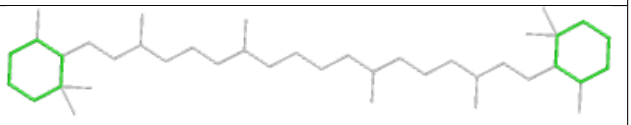


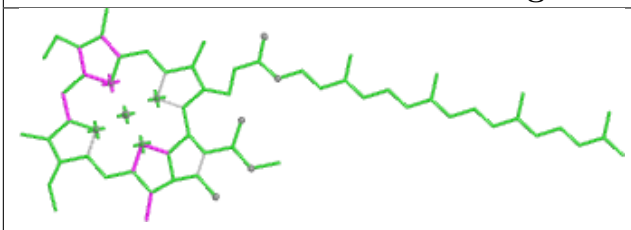
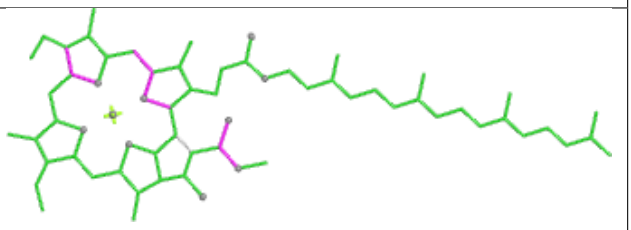
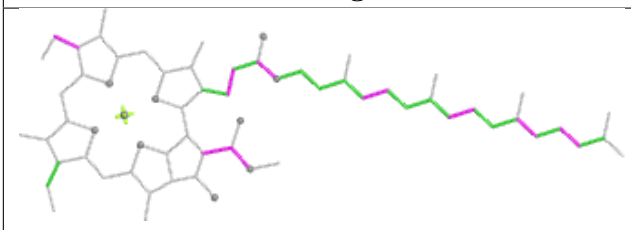
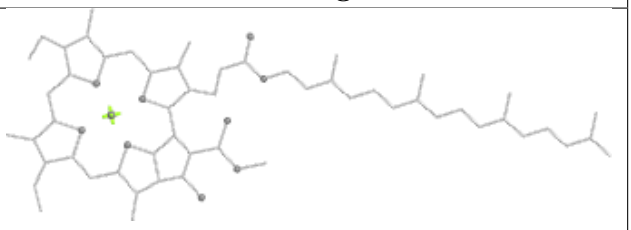
Bond angles

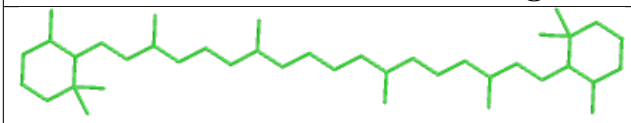
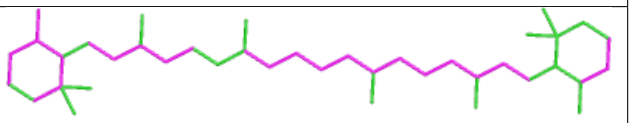
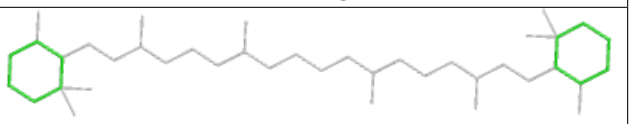


Torsions

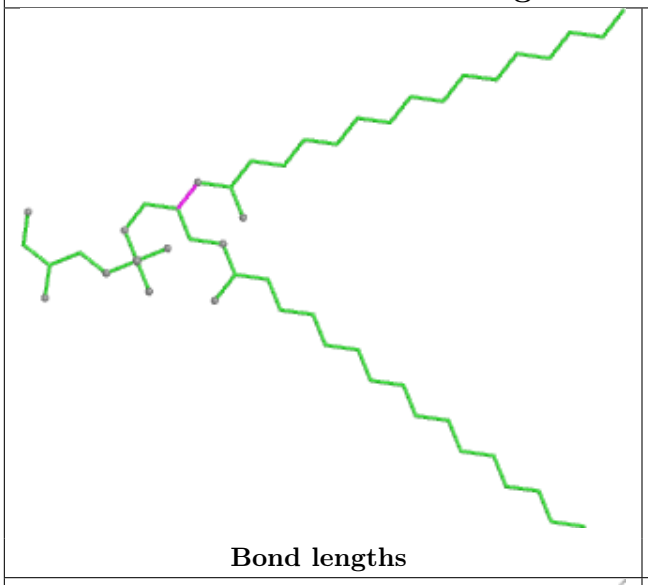


Rings

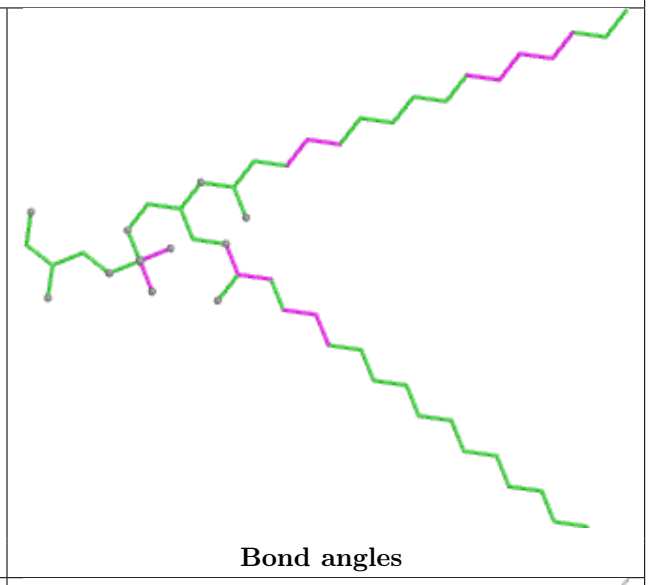
Ligand CLA b 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR d 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

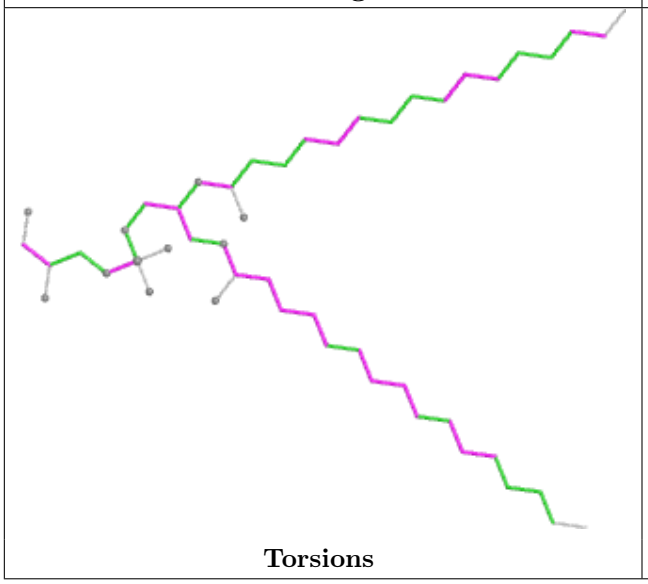
Ligand LHG A 5001



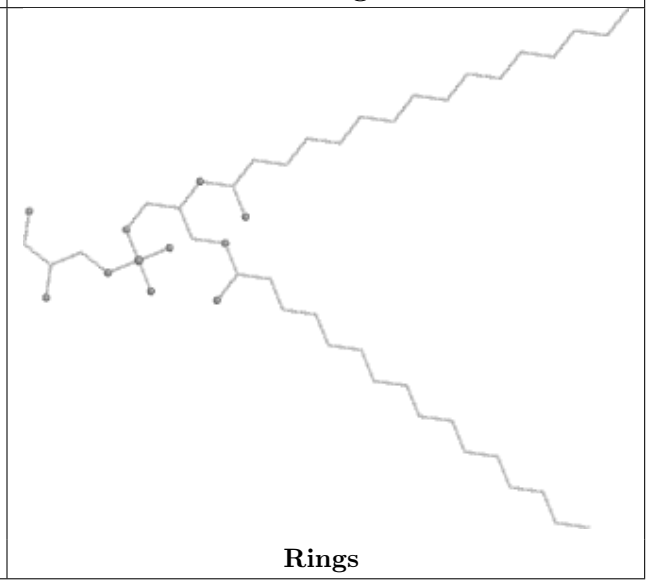
Bond lengths



Bond angles

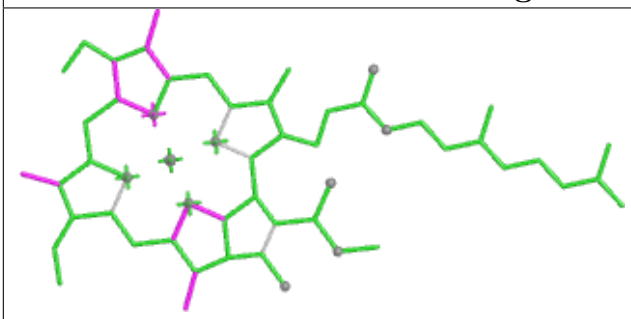


Torsions

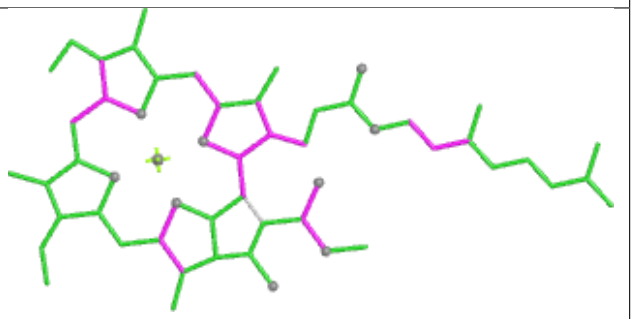


Rings

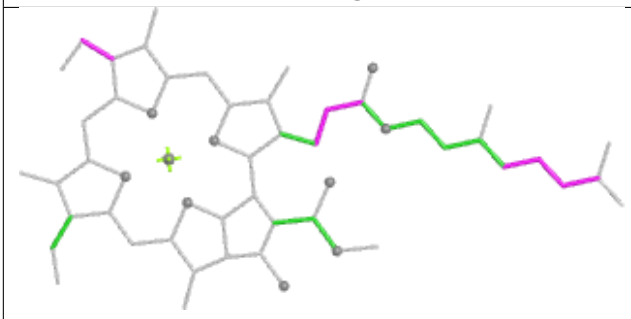
Ligand CLA A 1121



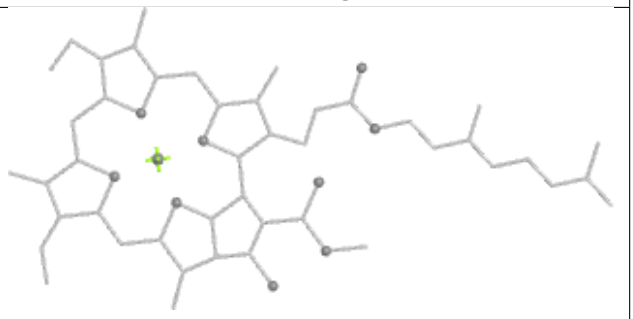
Bond lengths



Bond angles

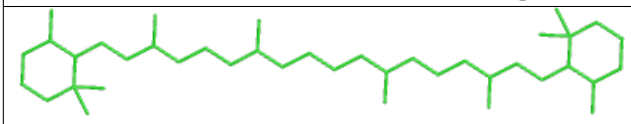


Torsions

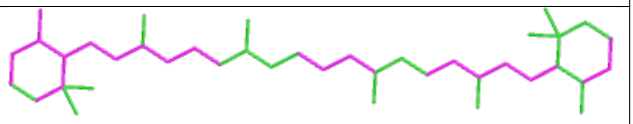


Rings

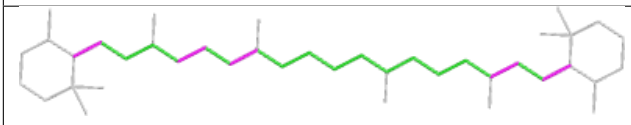
Ligand BCR T 4012



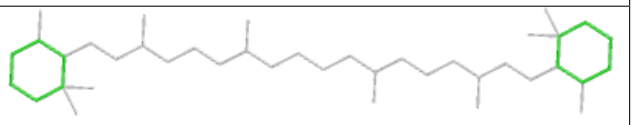
Bond lengths



Bond angles

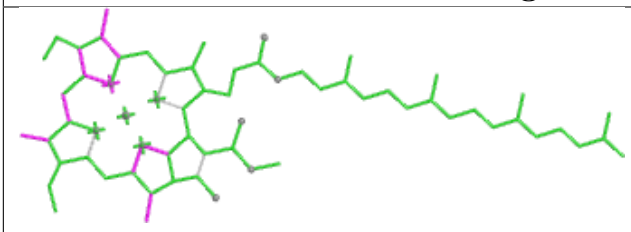


Torsions



Rings

Ligand CLA e 1125



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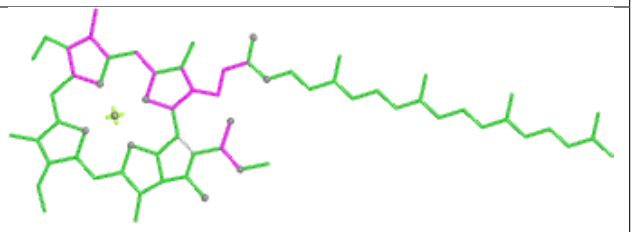
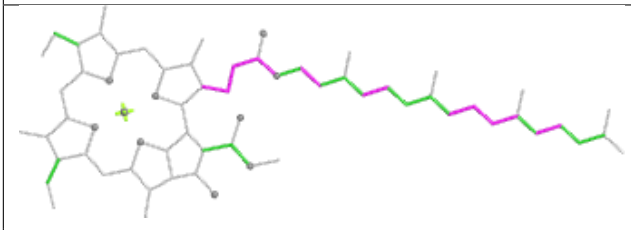


Bond angles



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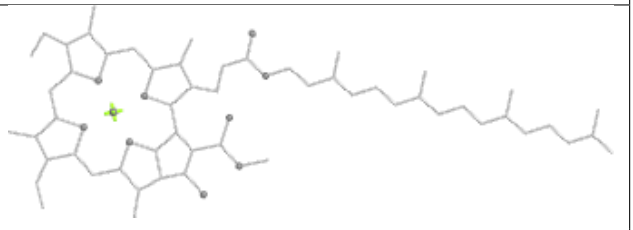
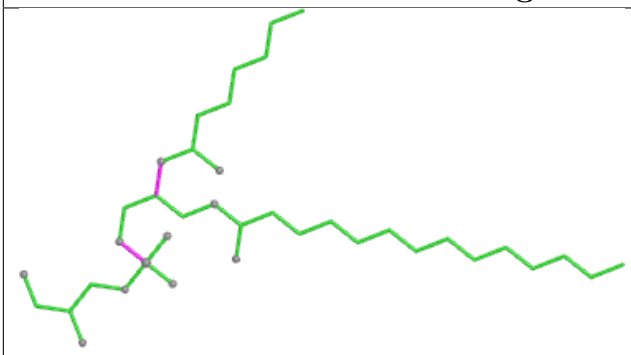


Rings

Ligand LHG L 5218



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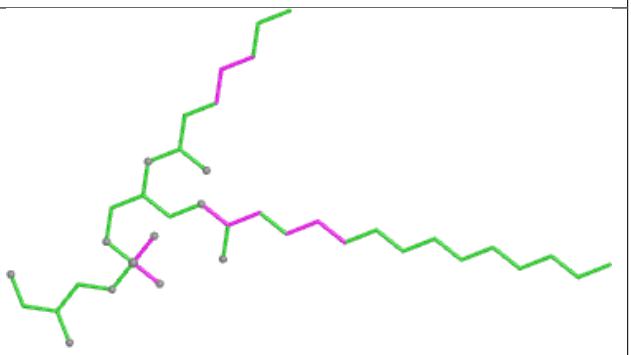

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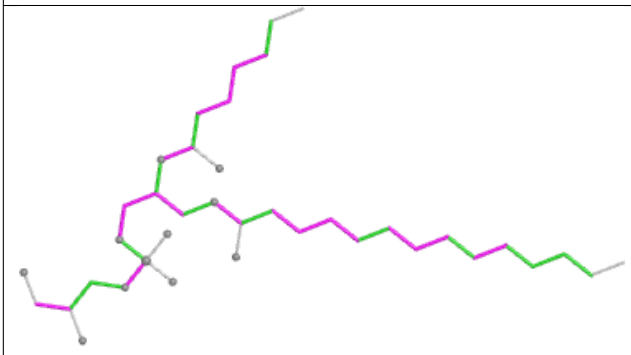

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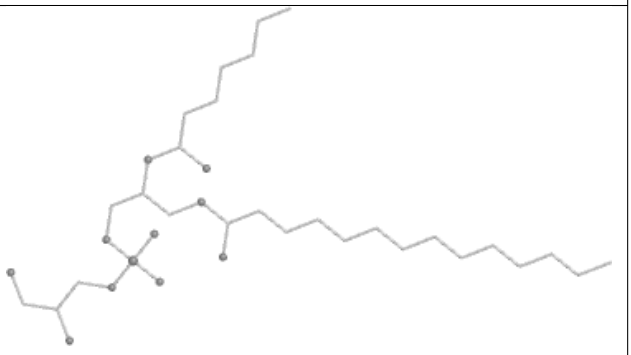

Rings

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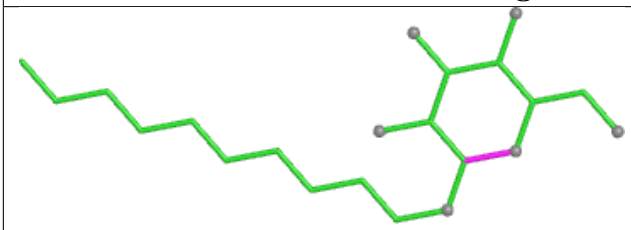

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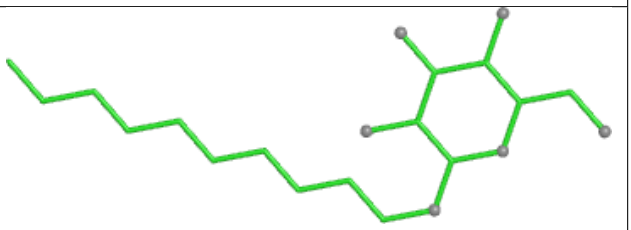

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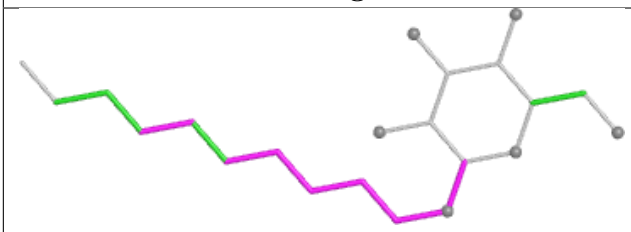

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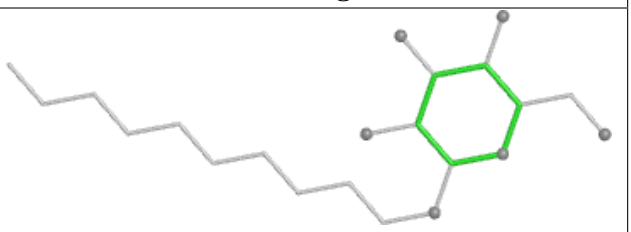
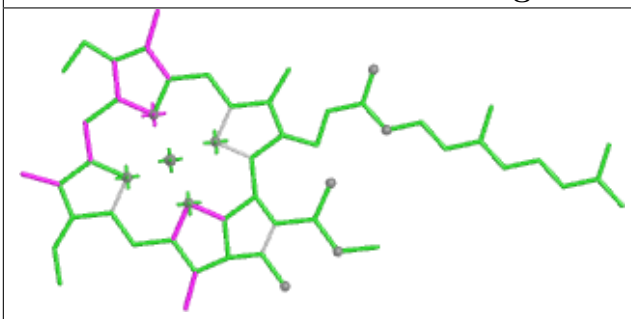


Rings

Ligand CLA m 1401



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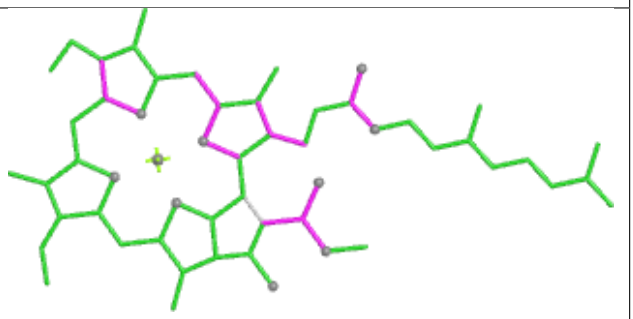

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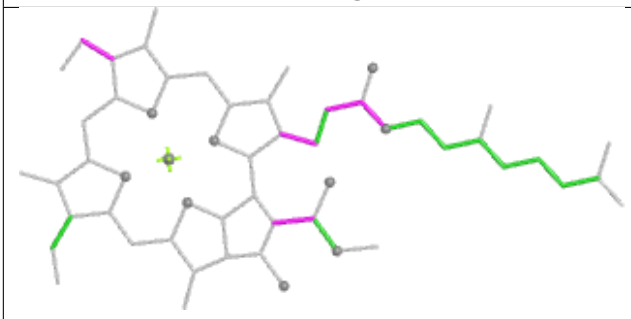

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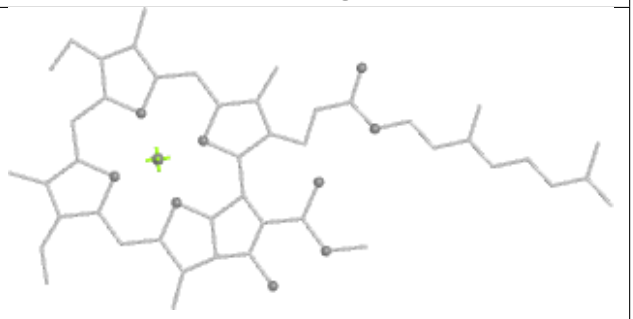
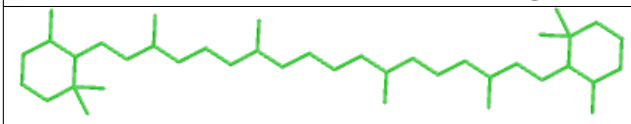


Rings

Ligand BCR q 524



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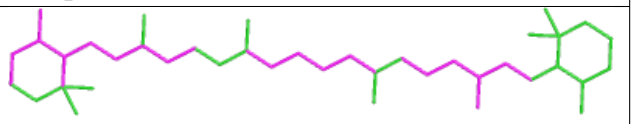

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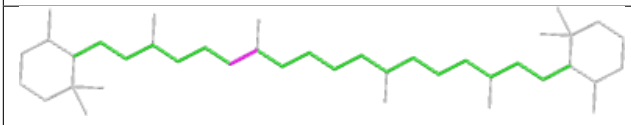

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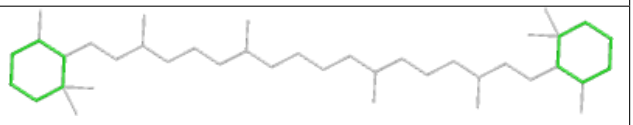

Rings

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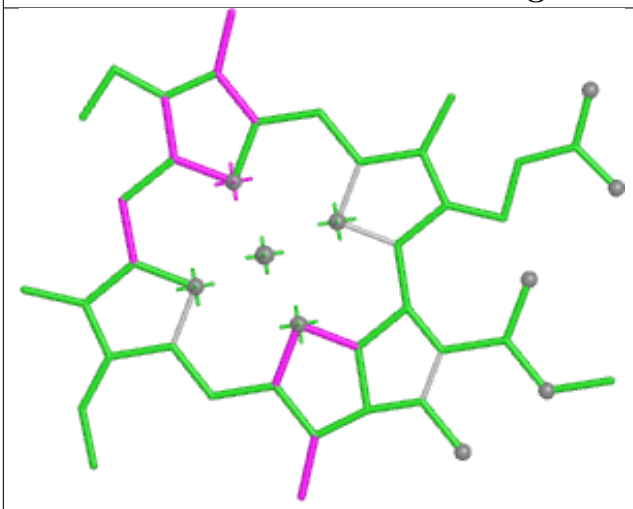

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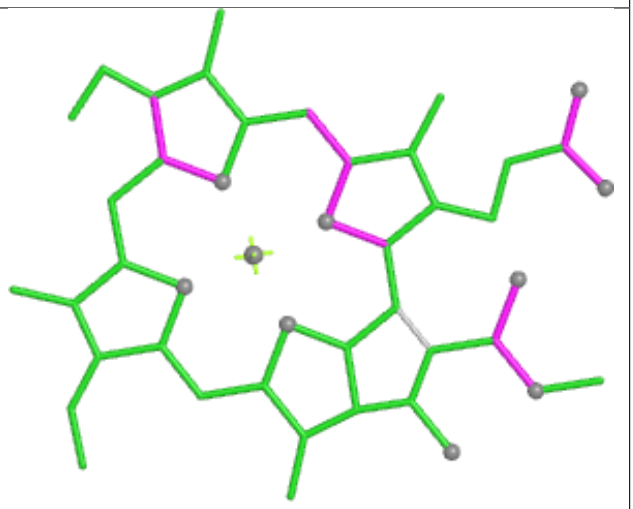

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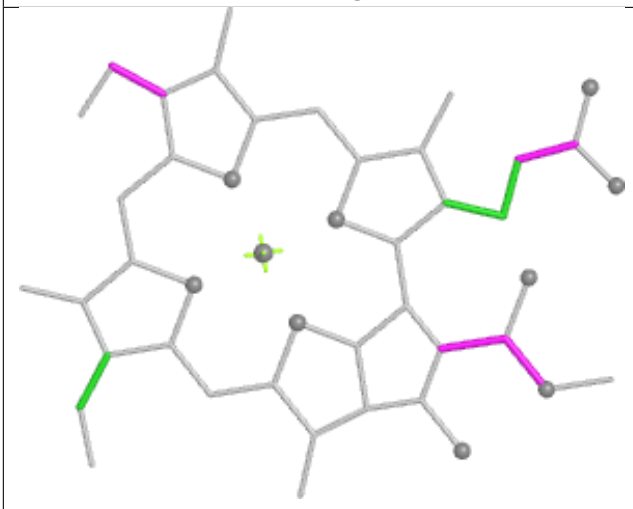

Torsions

Rings

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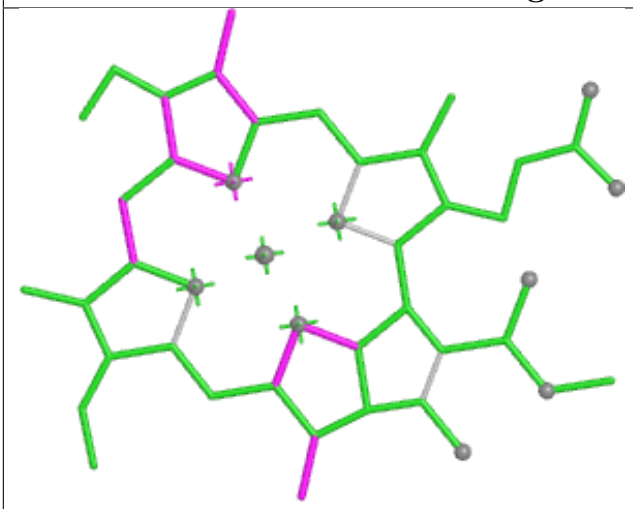

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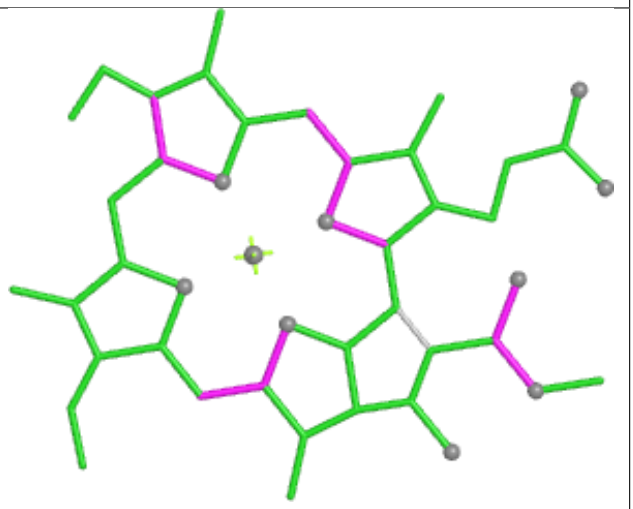

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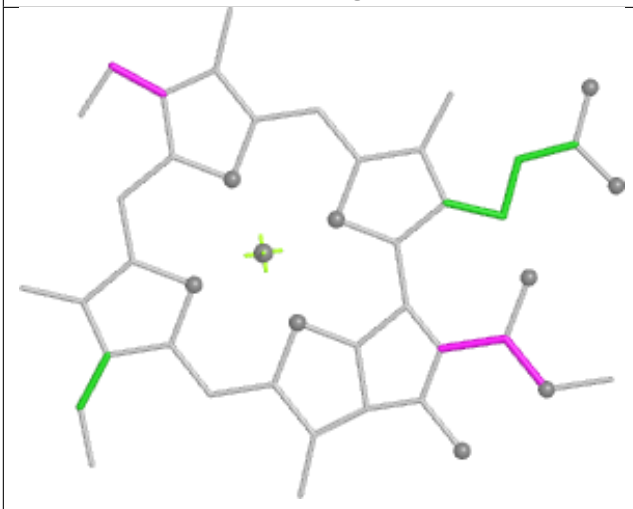

Torsions

Rings

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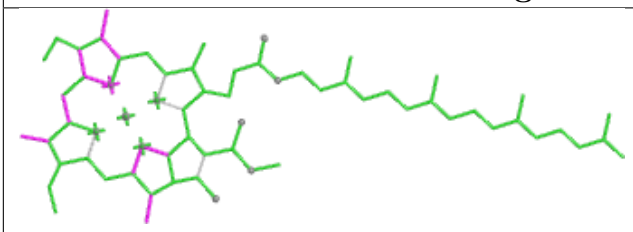

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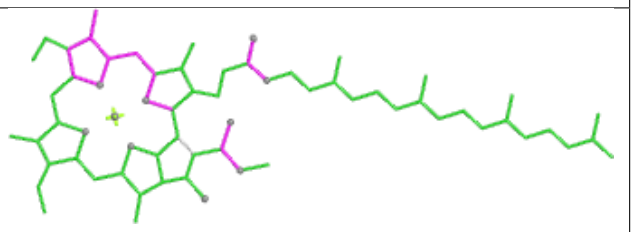

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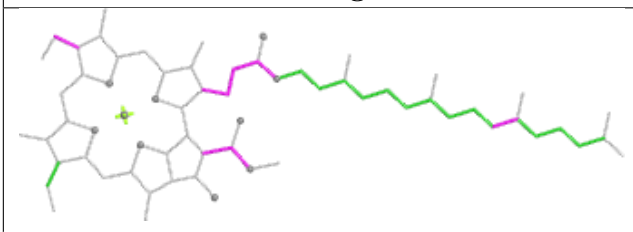

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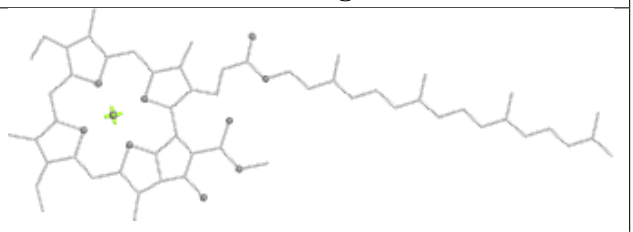

Rings

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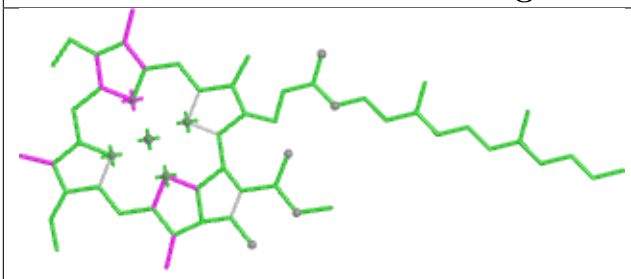

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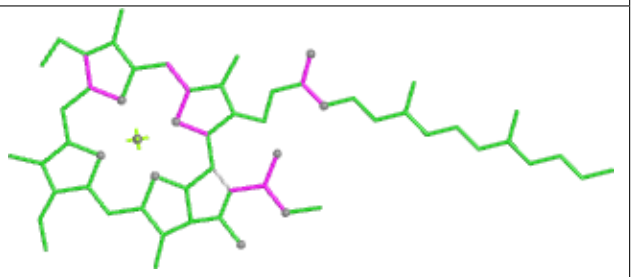

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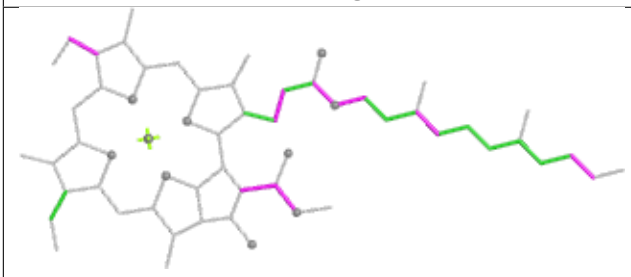

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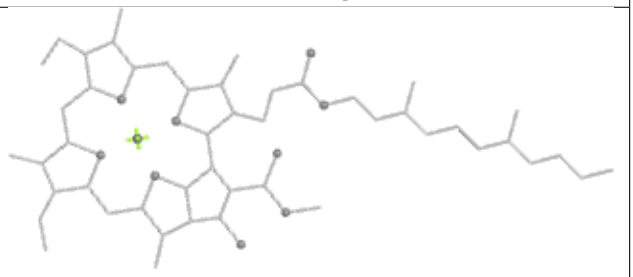

Rings

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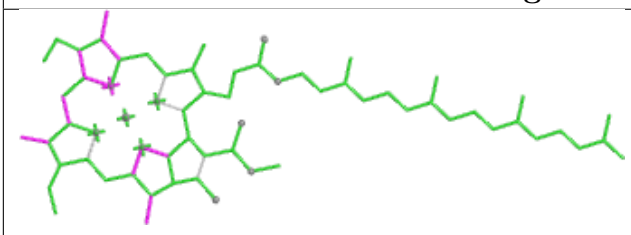

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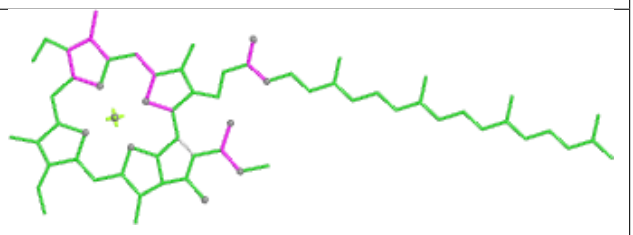

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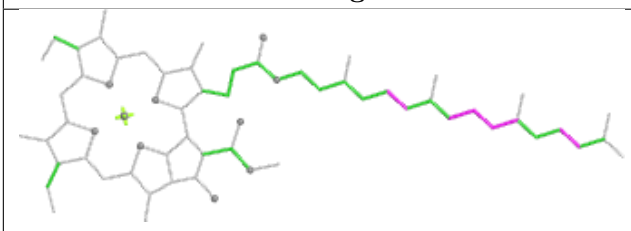

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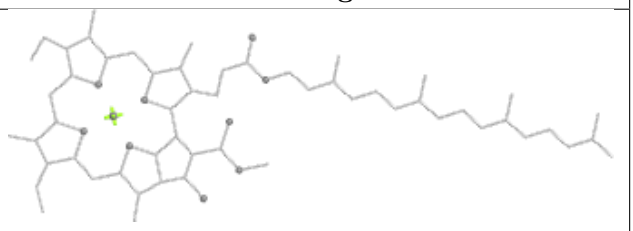

Rings

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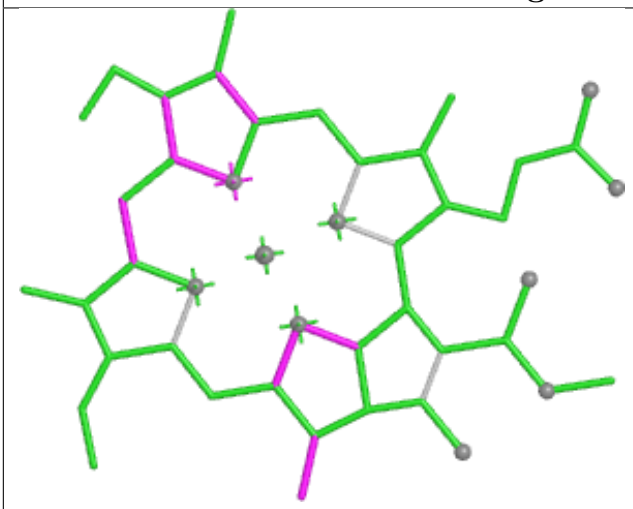

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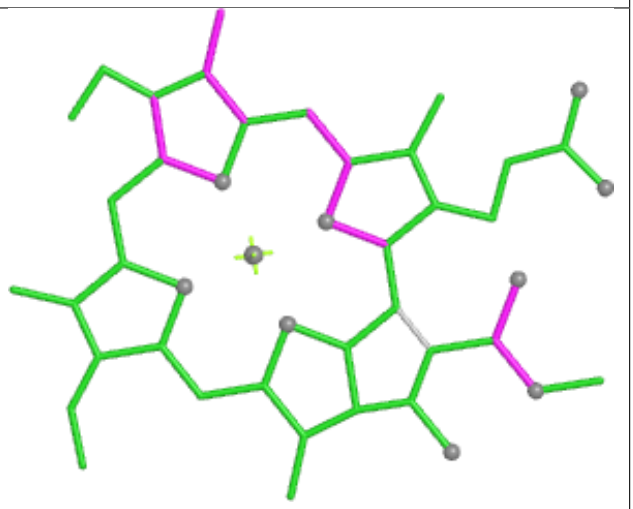

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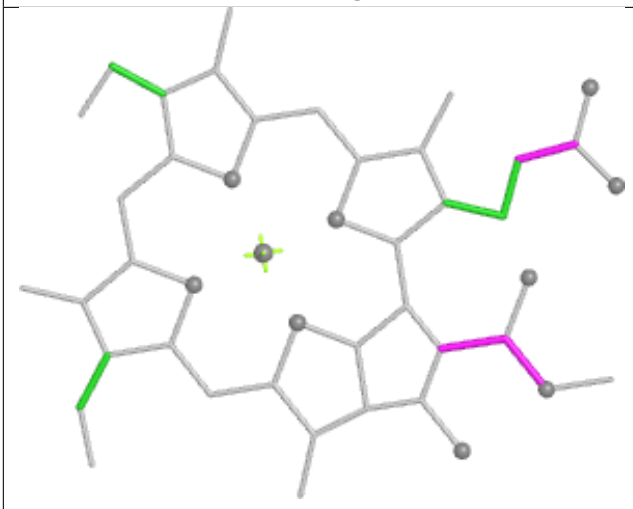

Torsions

Rings

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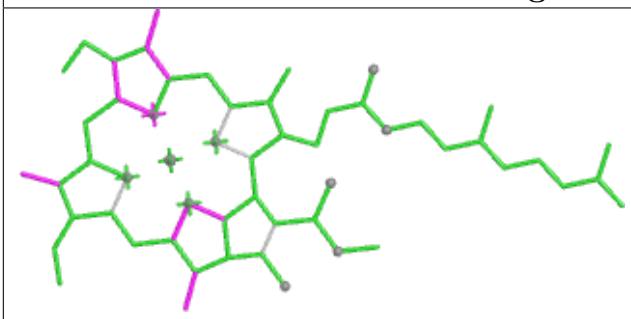

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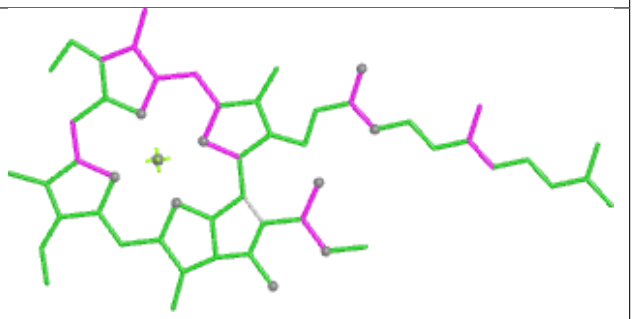

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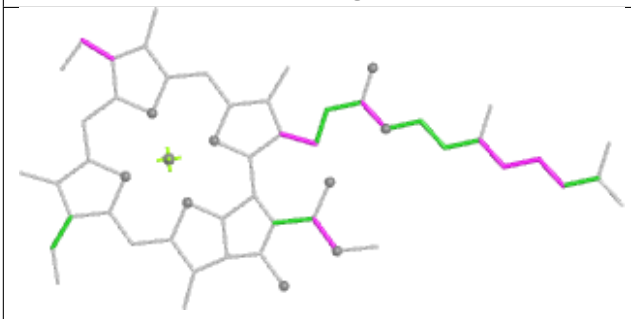

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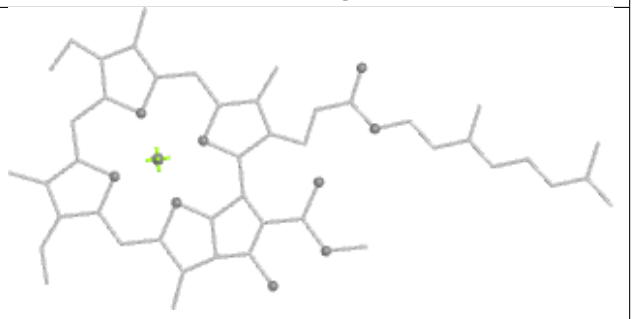

Rings

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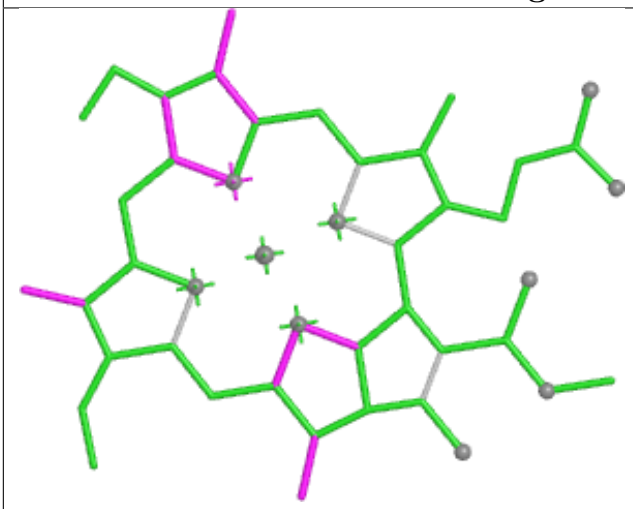

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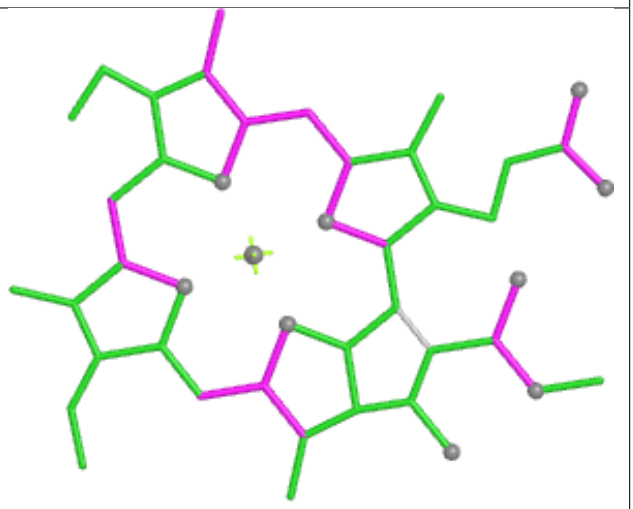

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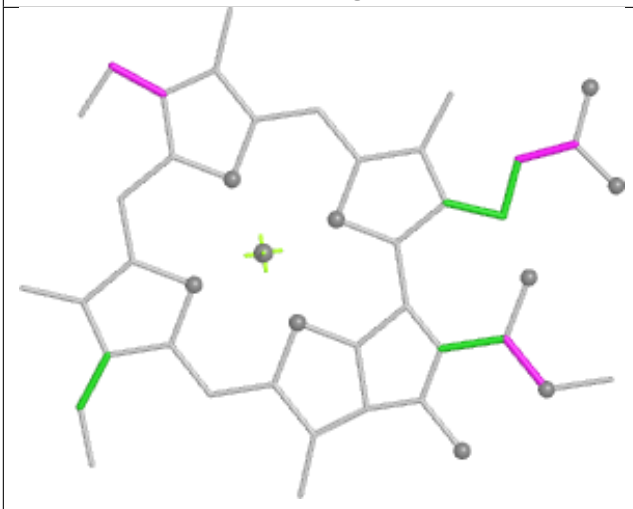
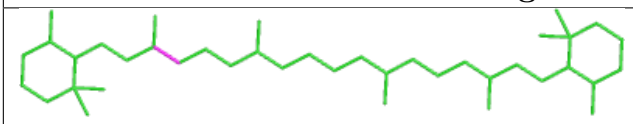


Torsions

Rings

Ligand BCR e 4008



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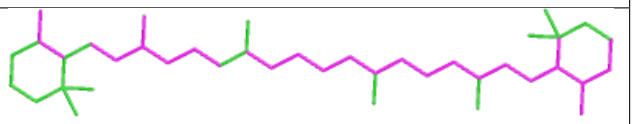

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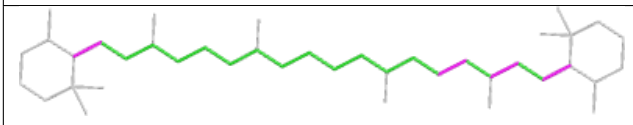
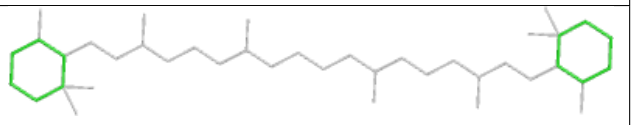
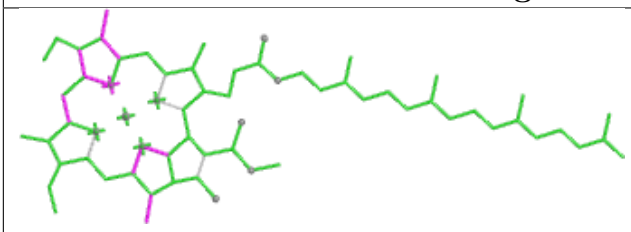


Torsions

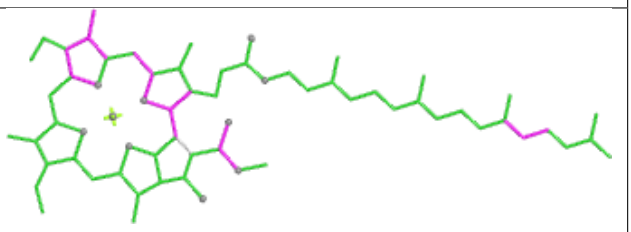


Rings

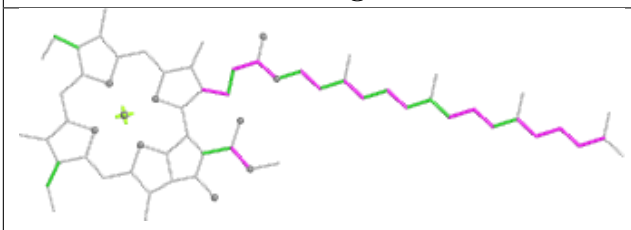
Ligand CLA G 1126



Bond lengths



Bond angles



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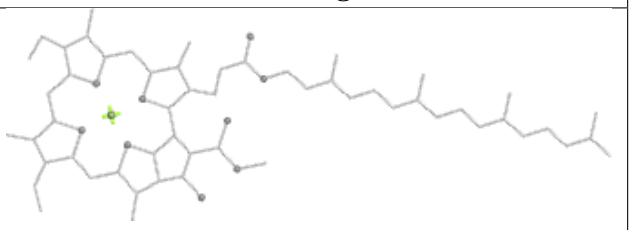
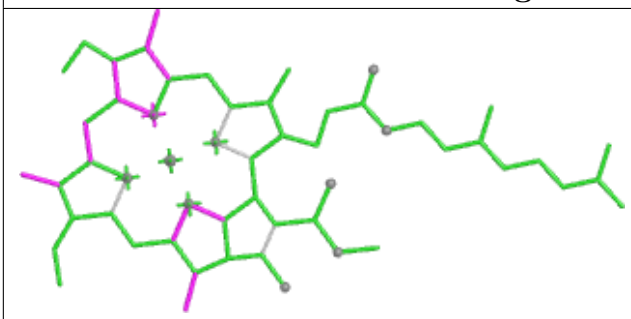


Rings

Ligand CLA U 1401



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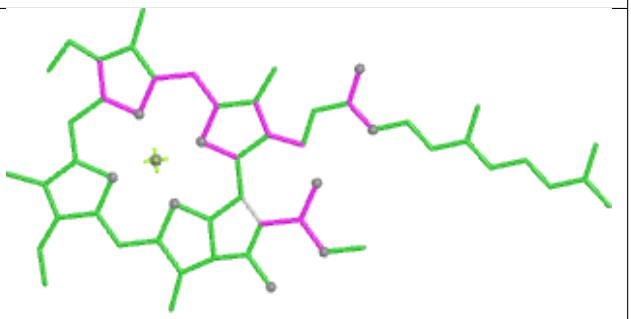

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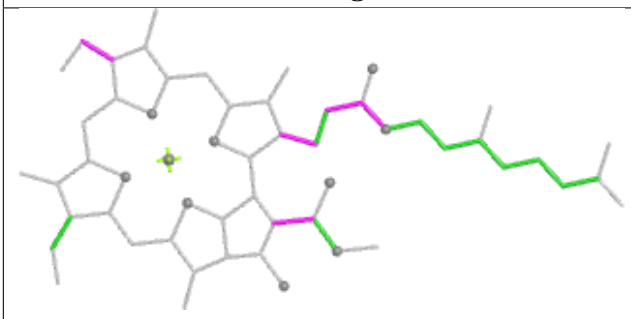

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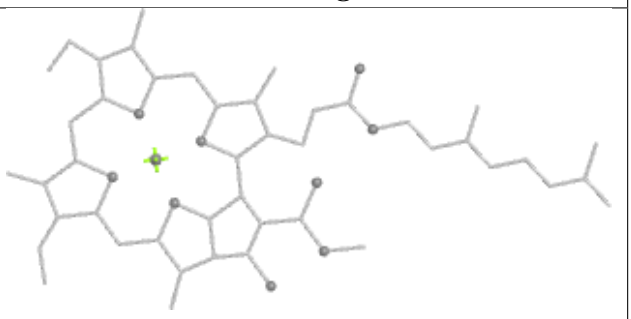
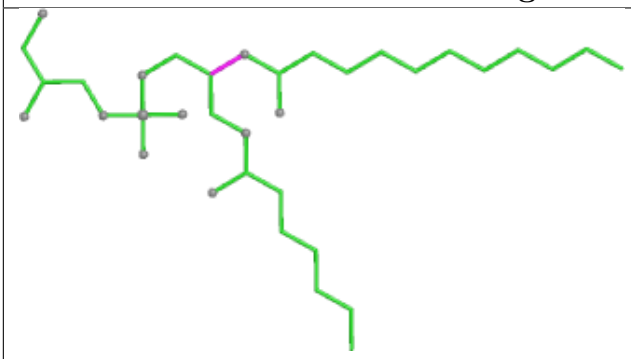


Rings

Ligand LHG e 5008



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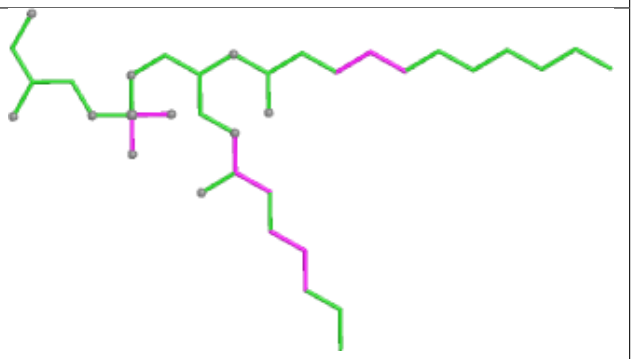
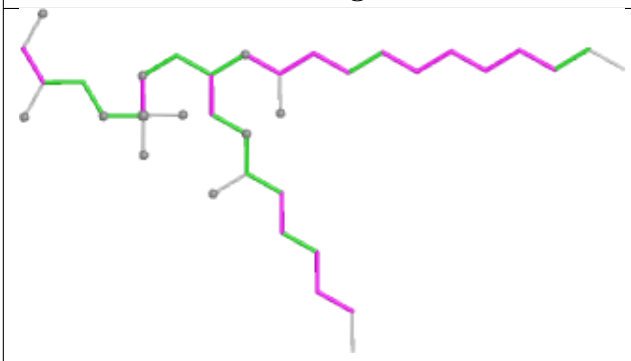


Bond angles



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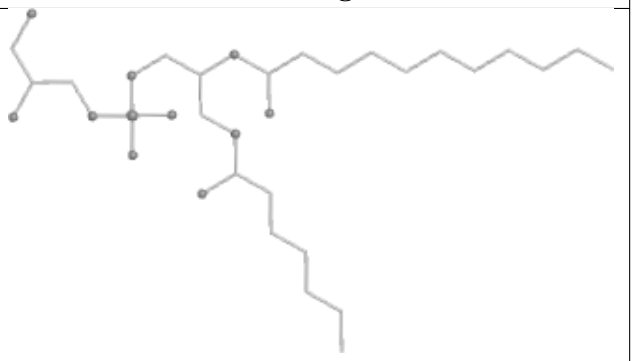
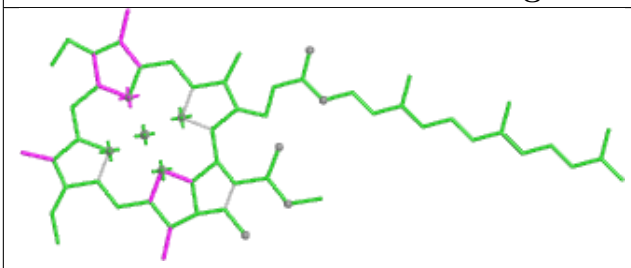


Rings

Ligand CLA Y 518



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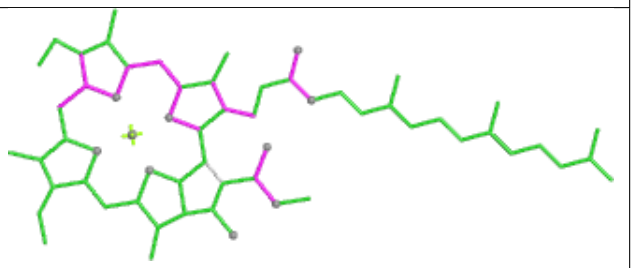

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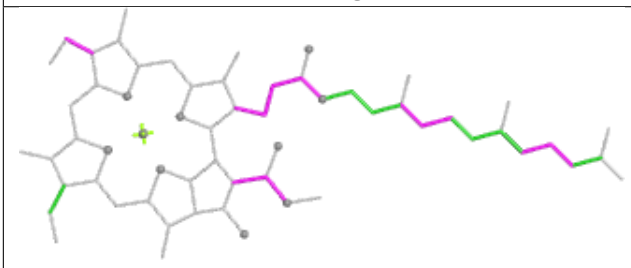

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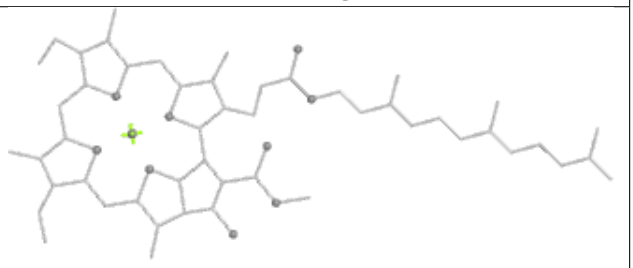
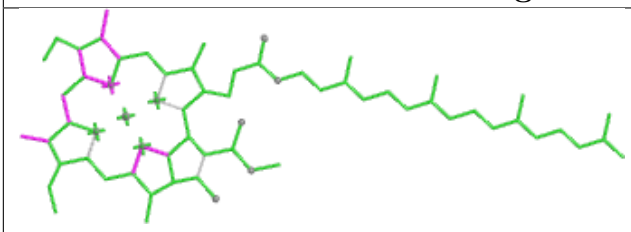


Rings

Ligand CLA A 1102



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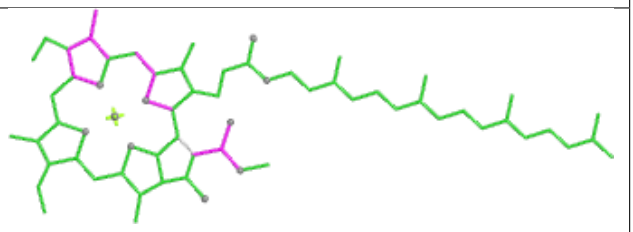
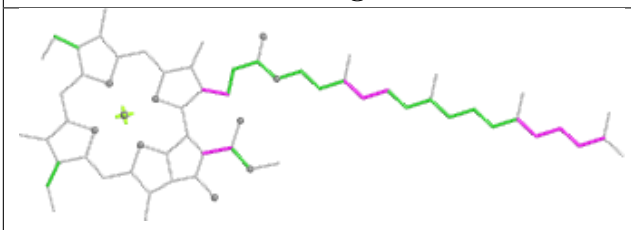


Bond angles



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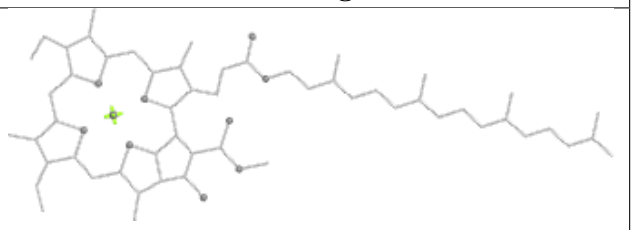
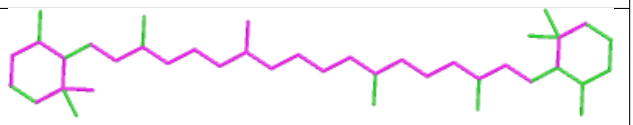


Rings

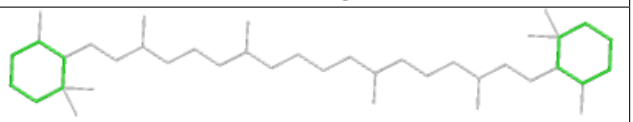
Ligand BCR T 4013

Bond lengths



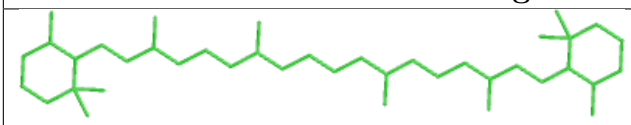
Bond angles

Torsions



Rings

Ligand BCR U 4104



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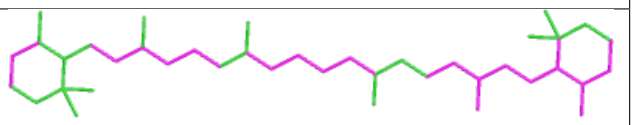
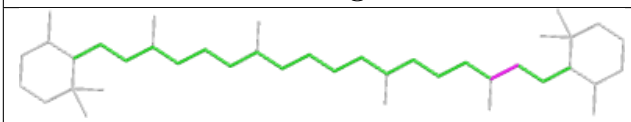


Bond angles



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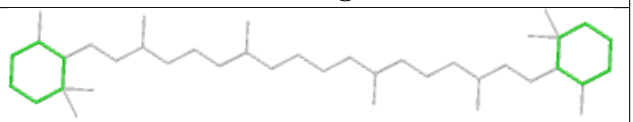
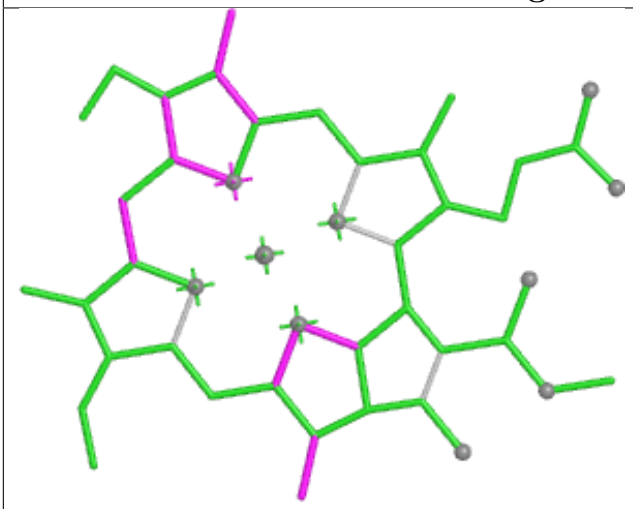


Rings

Ligand CLA 6 512



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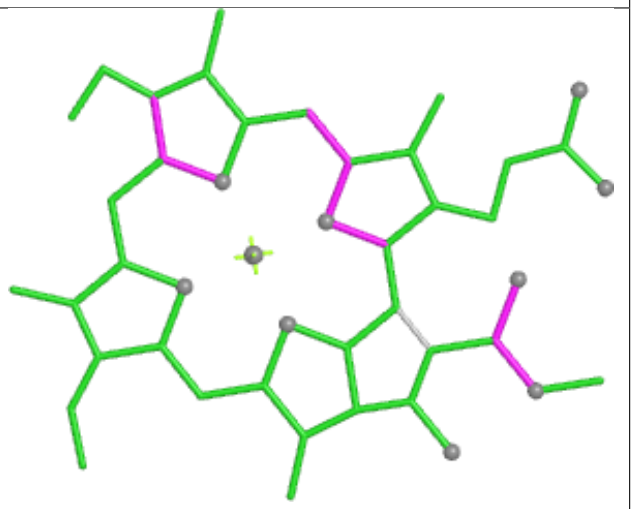

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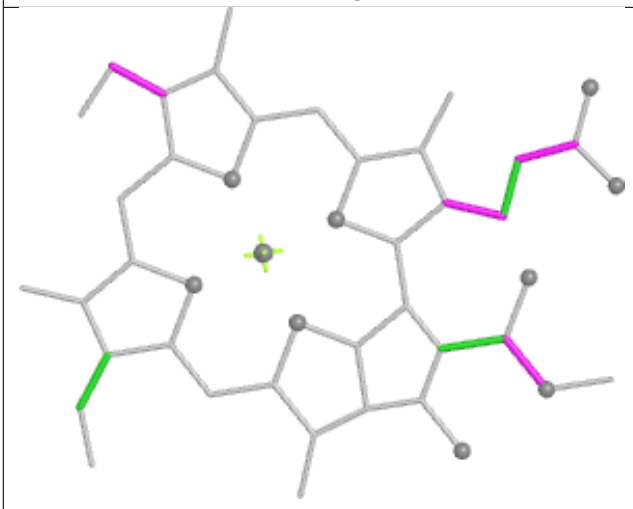
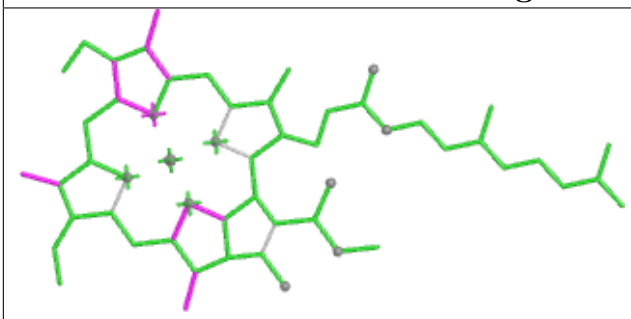


Torsions

Rings

Ligand CLA B 1228



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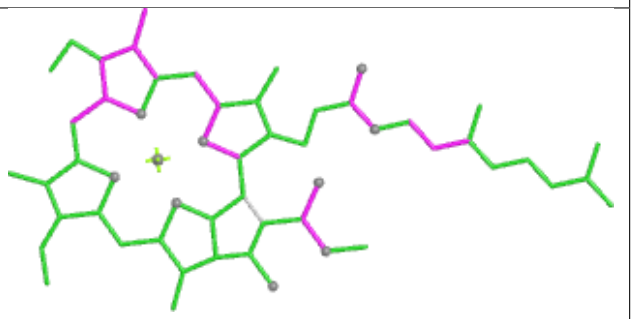
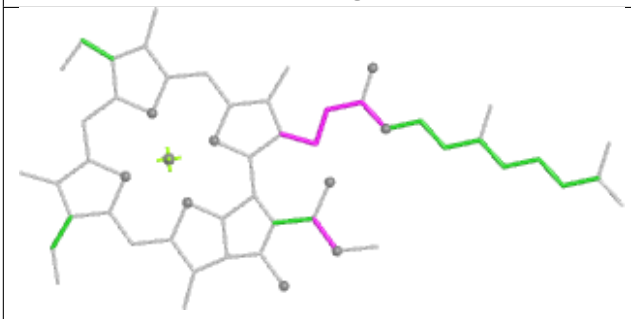


Bond angles



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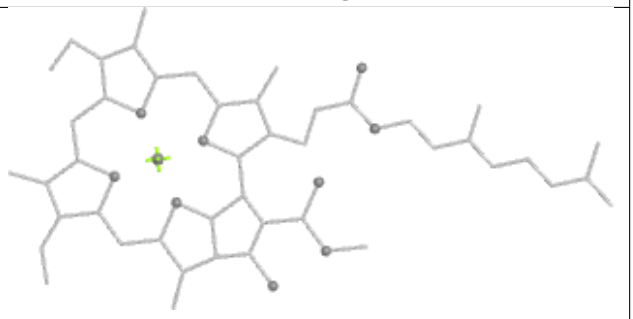
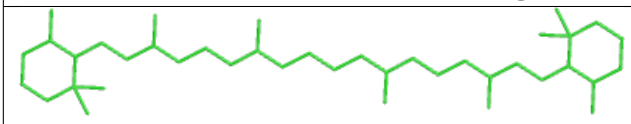


Rings

Ligand BCR G 4007



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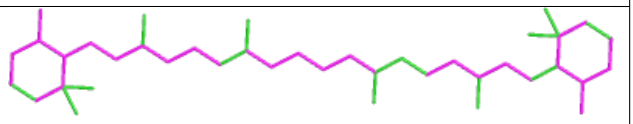

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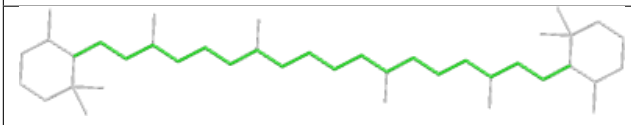

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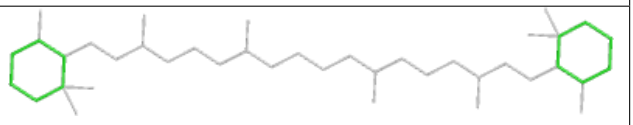
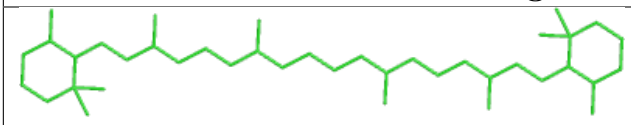


Rings

Ligand BCR a 521



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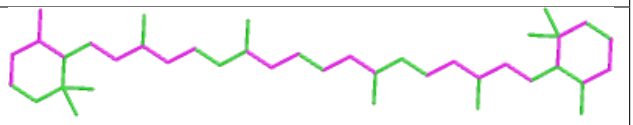
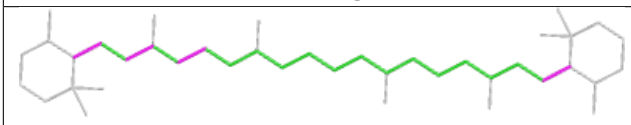


Bond angles



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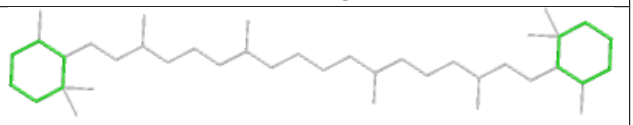
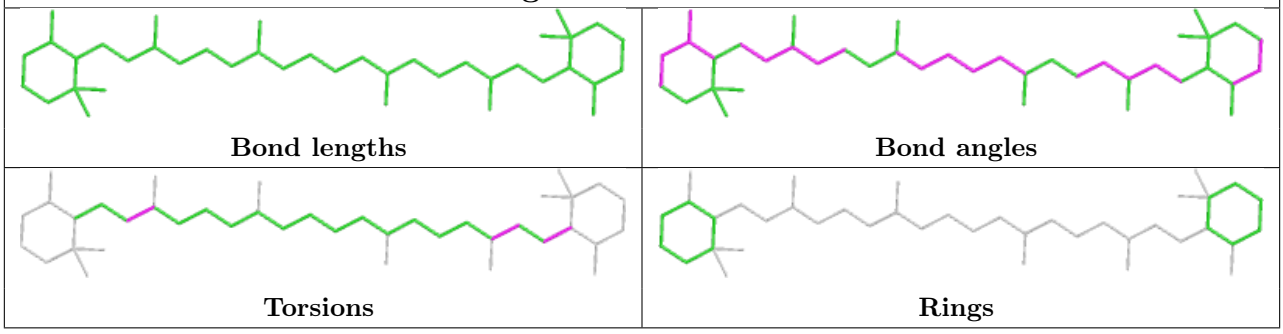
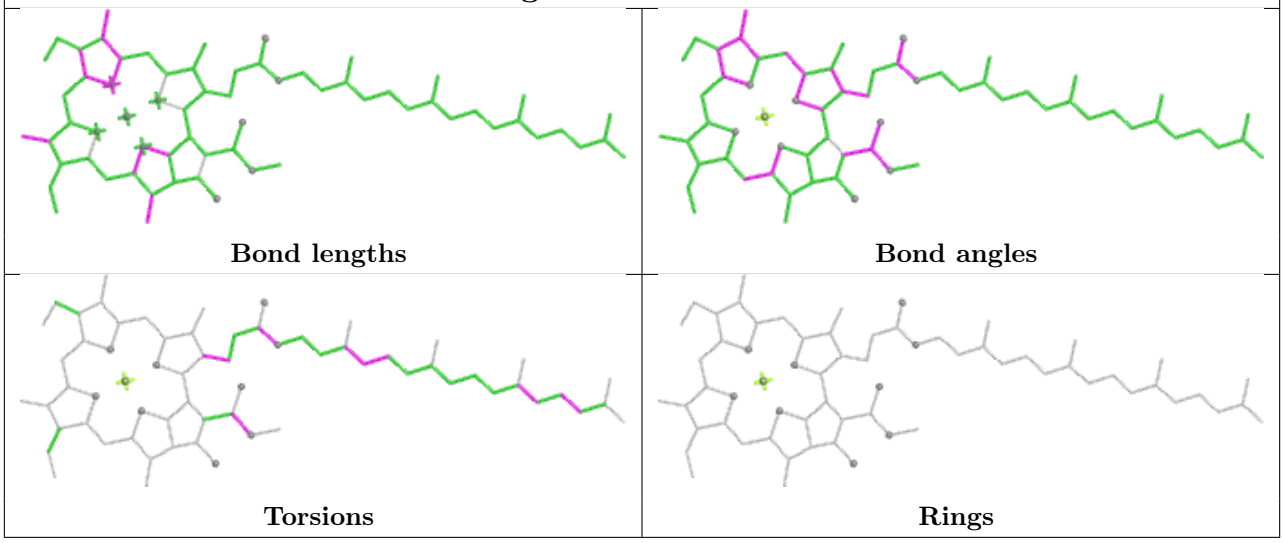


Rings

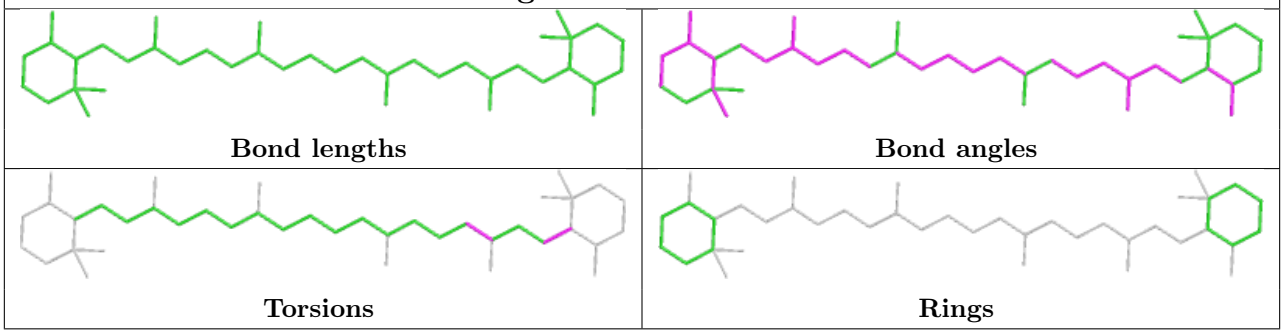
Ligand BCR f 4005



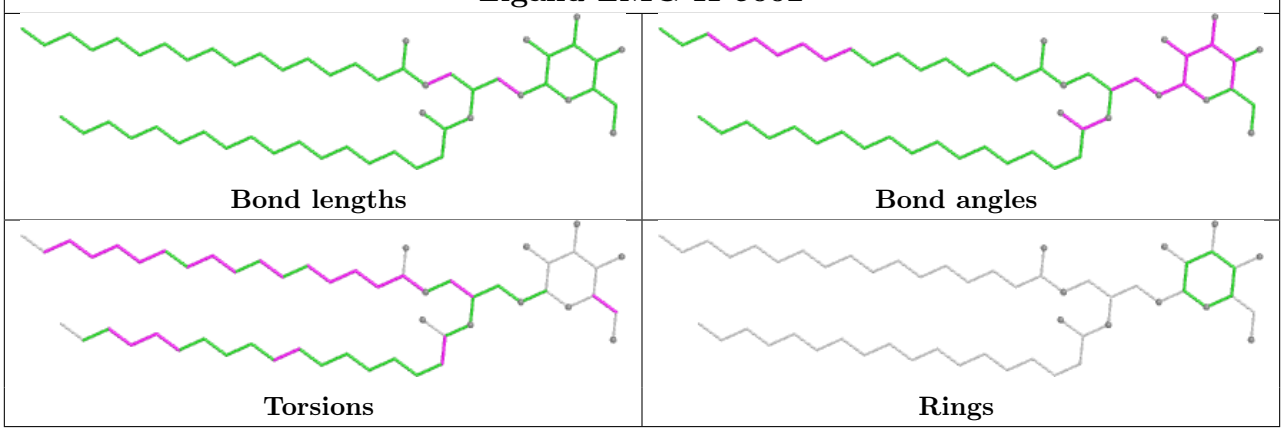
Ligand CLA e 1104



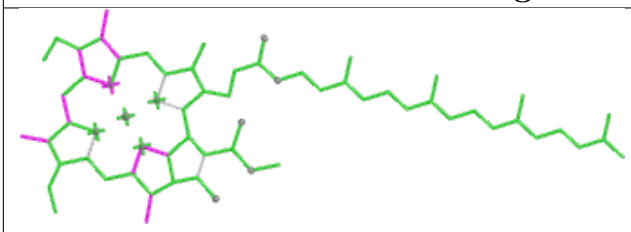
Ligand BCR n 4020



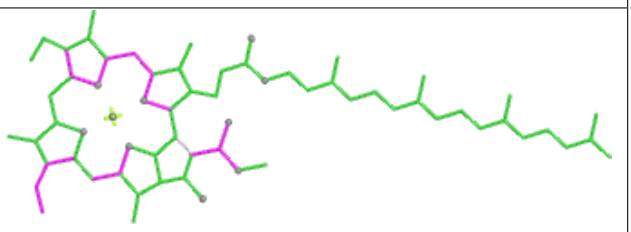
Ligand LMG H 5002



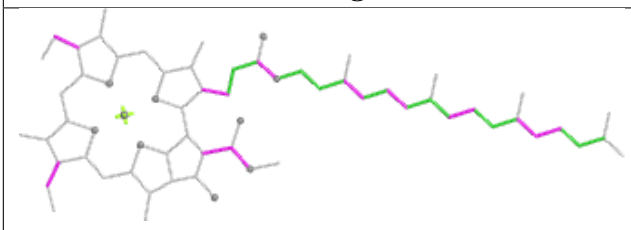
Ligand CLA G 1132



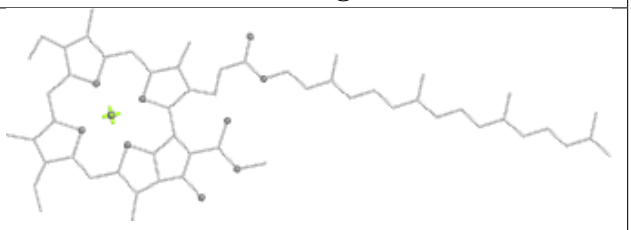
Bond lengths



Bond angles

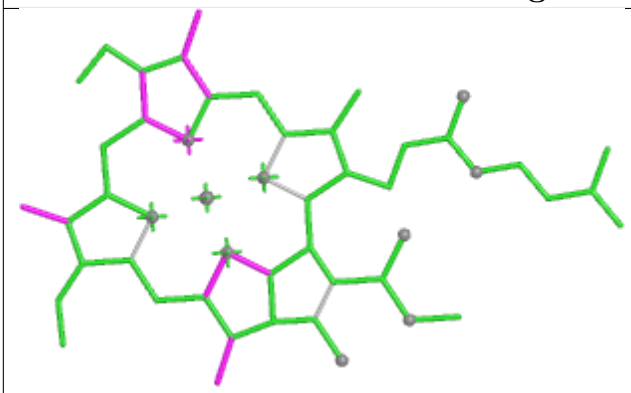


Torsions



Rings

Ligand CLA 3 506



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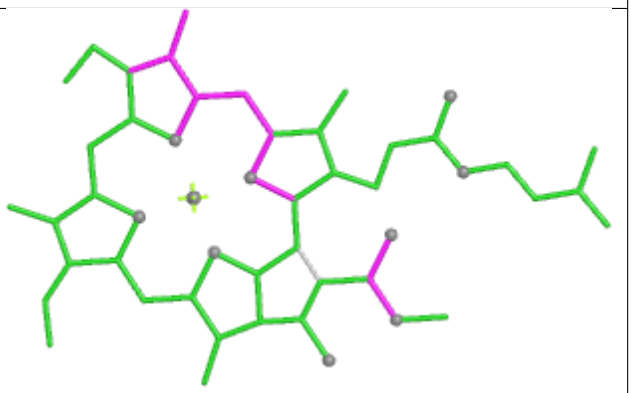
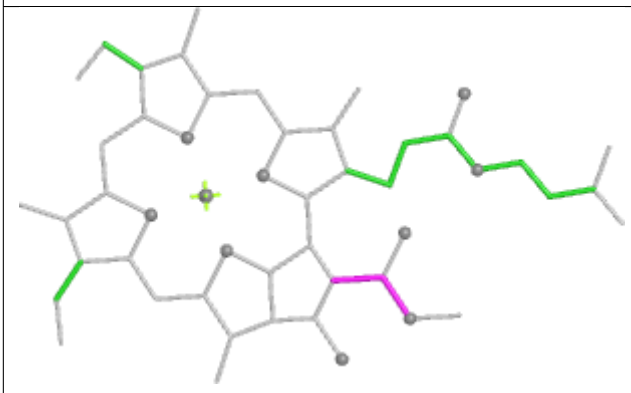
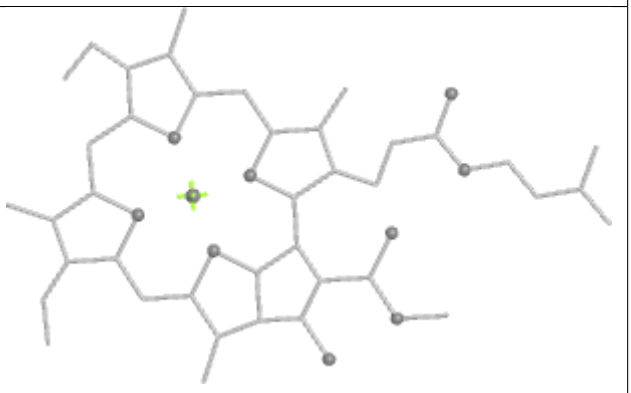


Bond angles

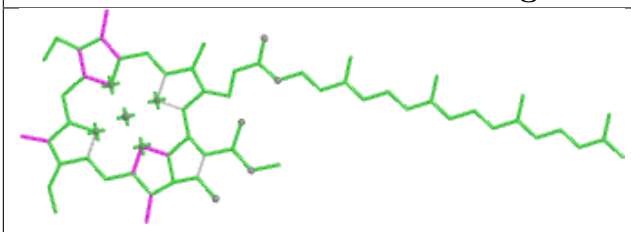


Torsions

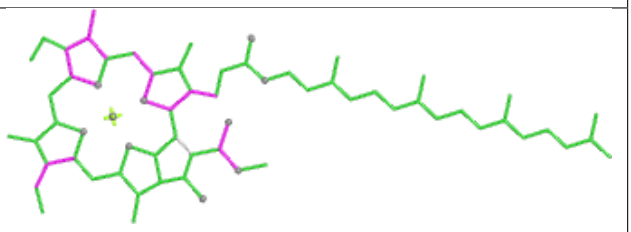


Rings

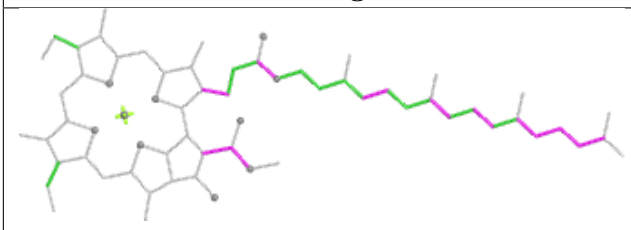
Ligand CLA e 1103



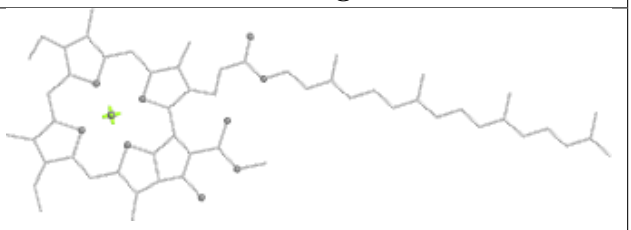
Bond lengths



Bond angles

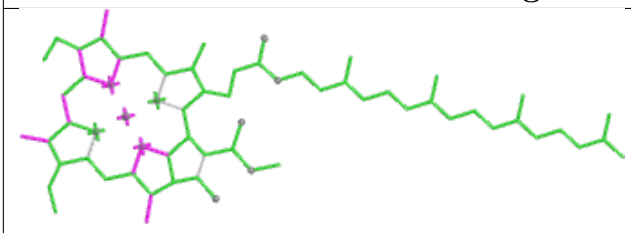


Torsions



Rings

Ligand CLA f 1221



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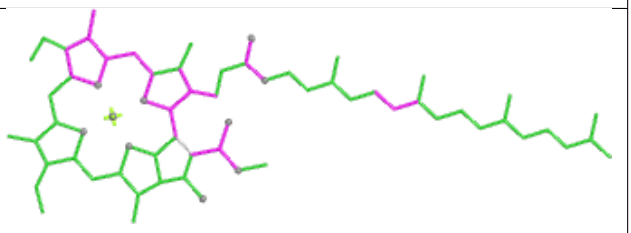
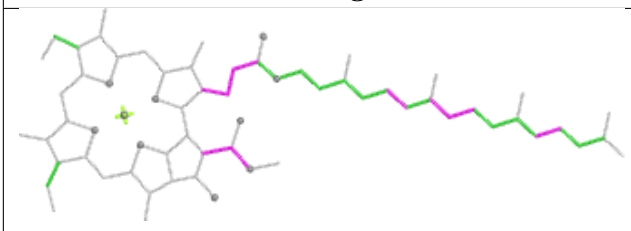


Bond angles



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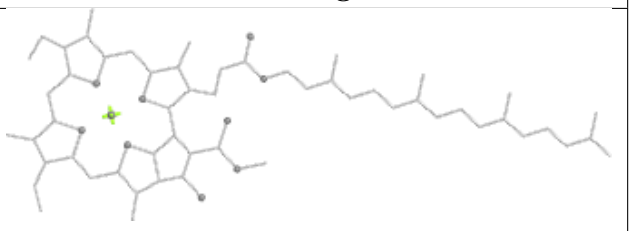
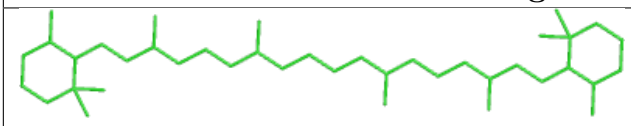


Rings

Ligand BCR t 521



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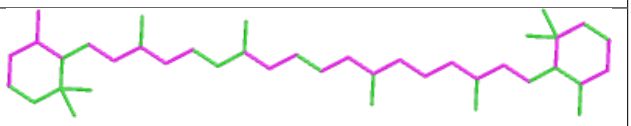
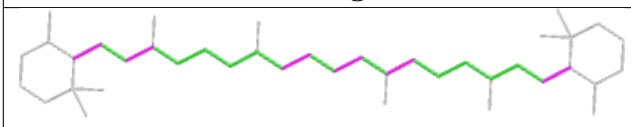


Bond angles



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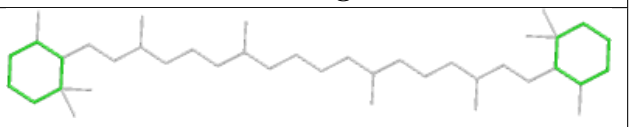
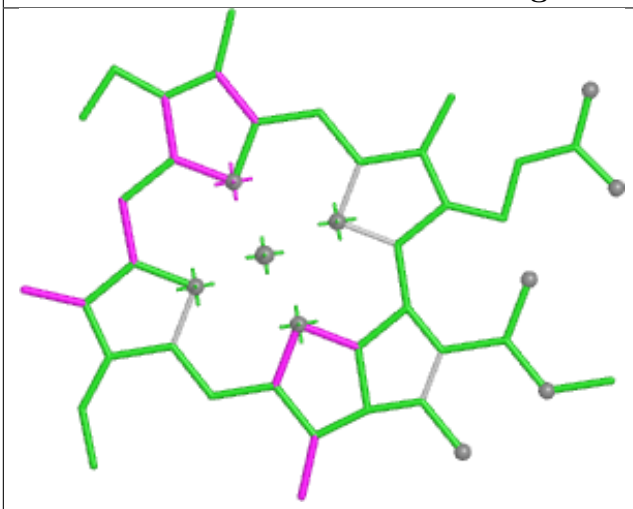


Rings

Ligand CLA t 517



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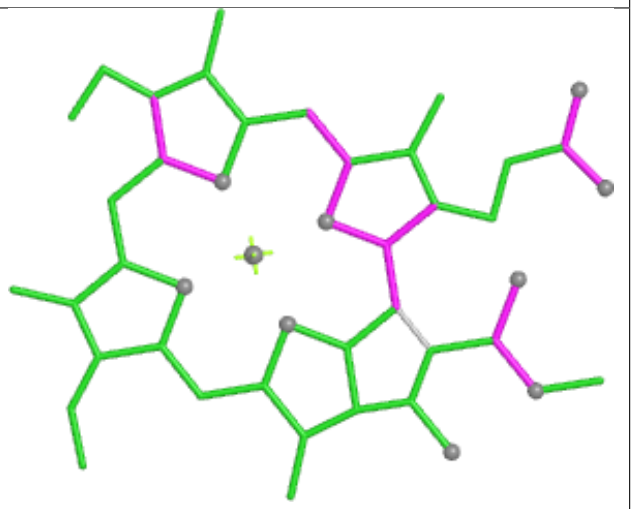
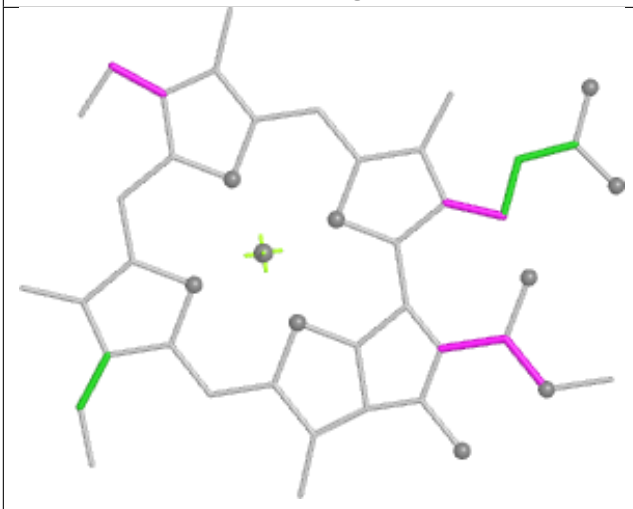


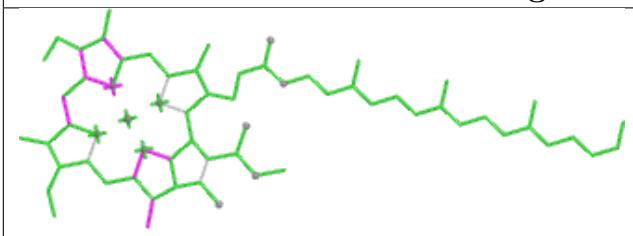
Bond angles



Torsions

Rings

Ligand CLA 1 503



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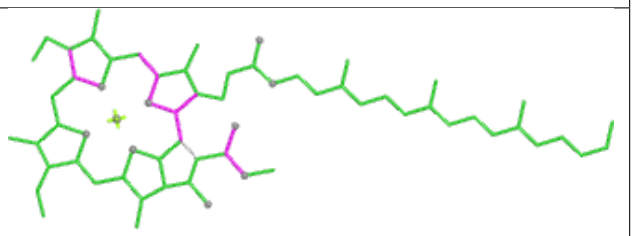
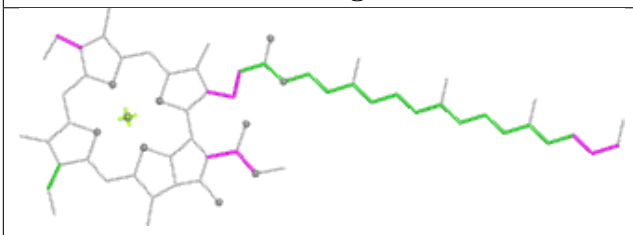
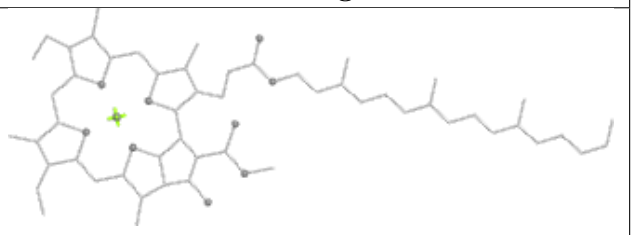


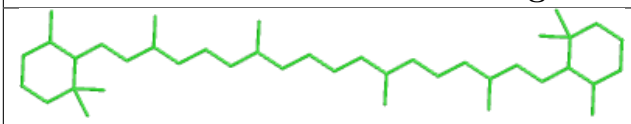
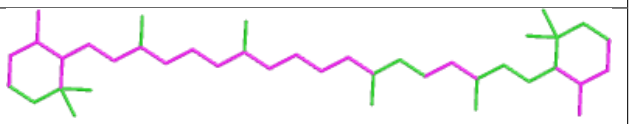
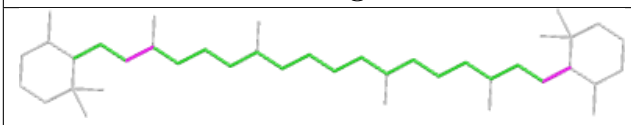
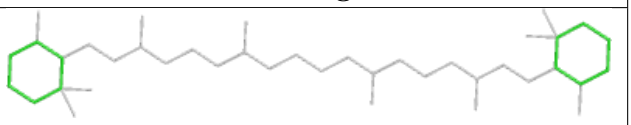
Bond angles

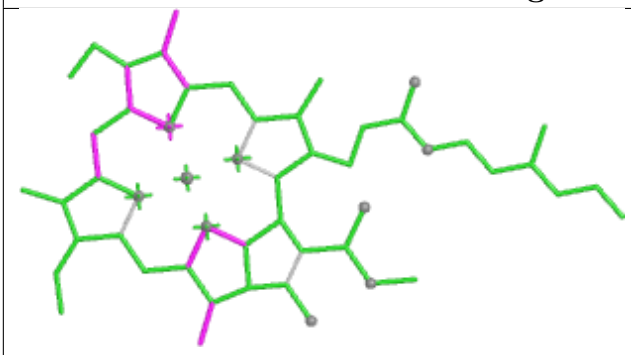
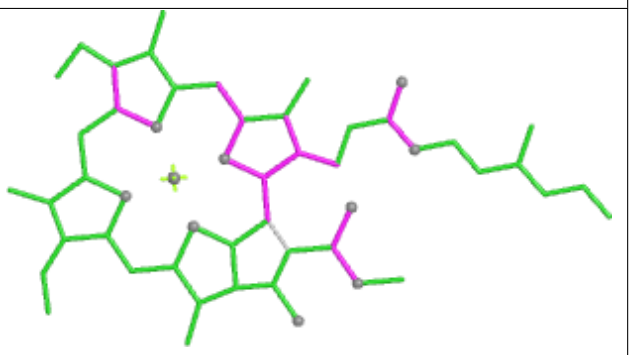
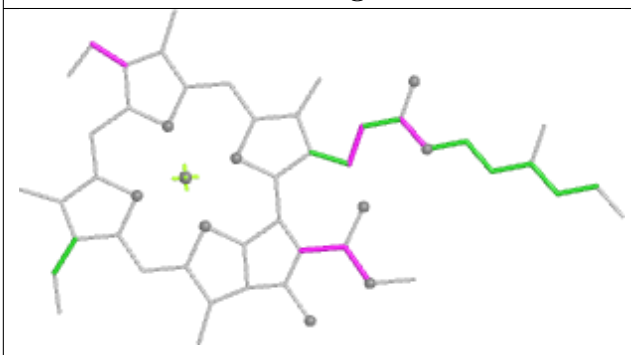
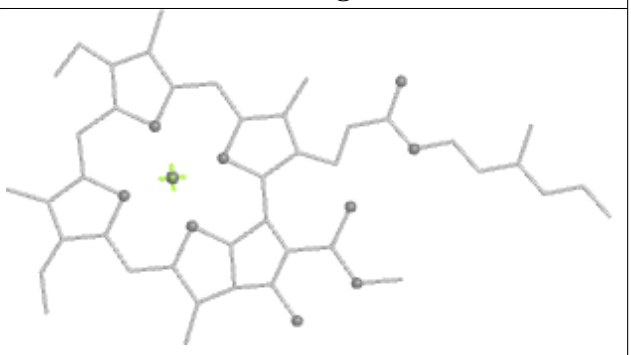


Torsions

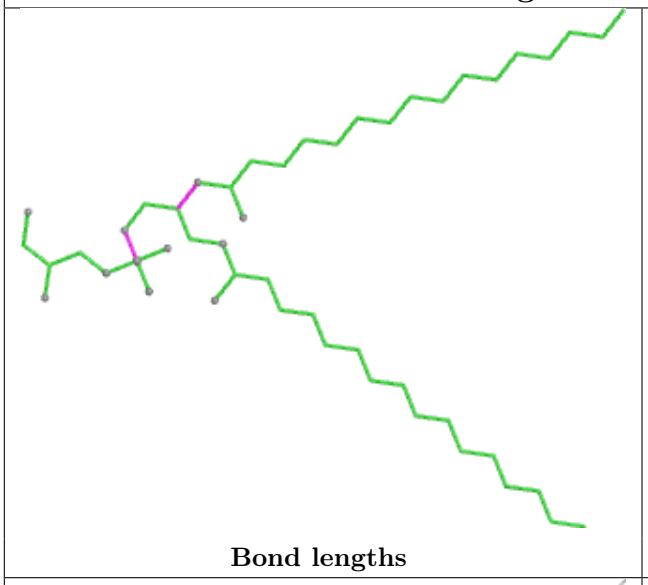


Rings

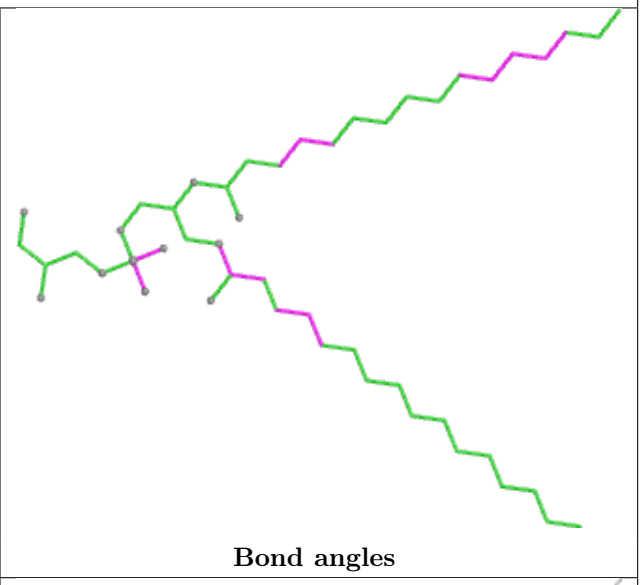
Ligand BCR t 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

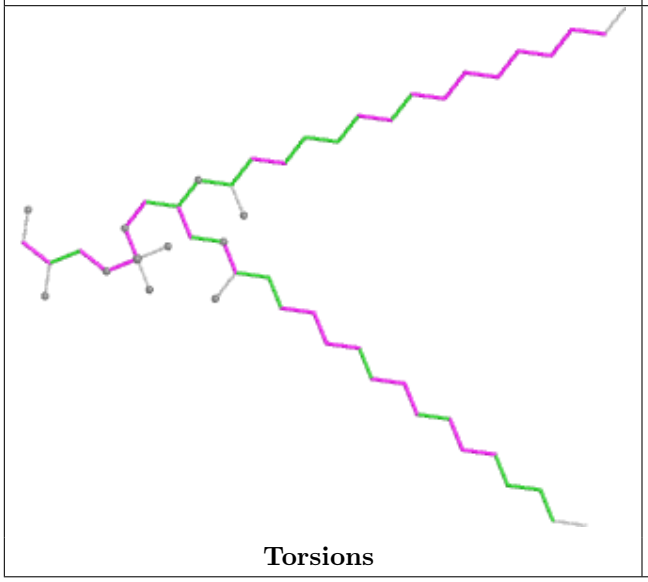
Ligand LHG L 5221



Bond lengths



Bond angles



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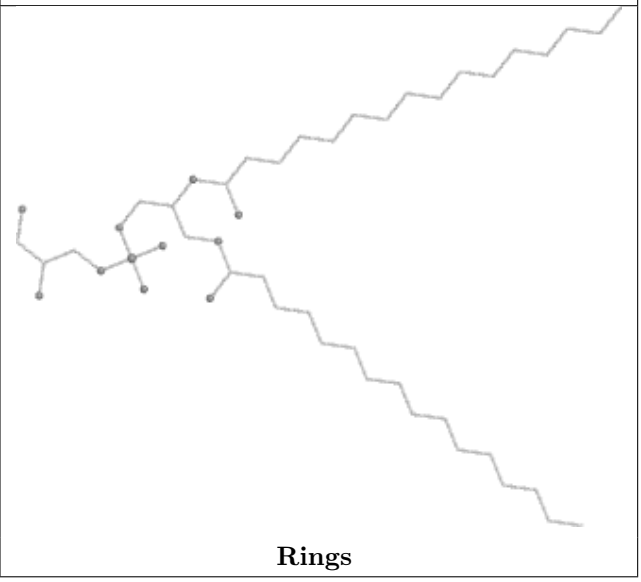
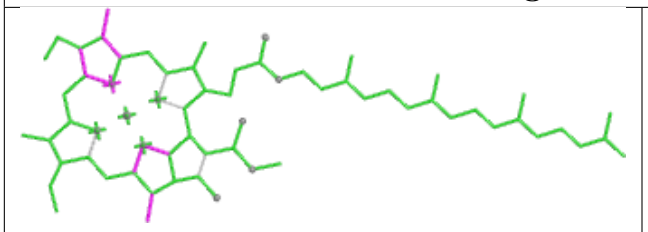


Rings

Ligand CLA f 1239



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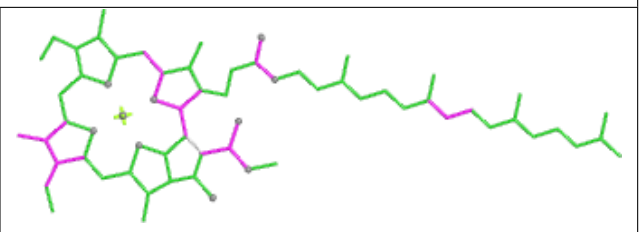

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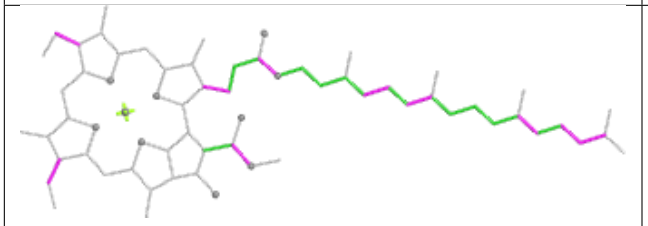

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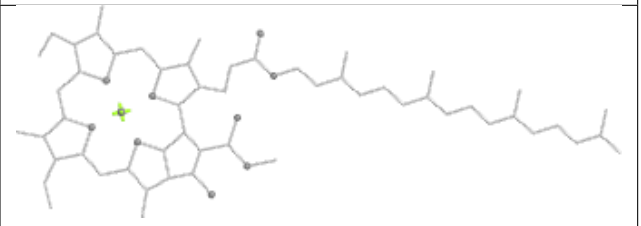
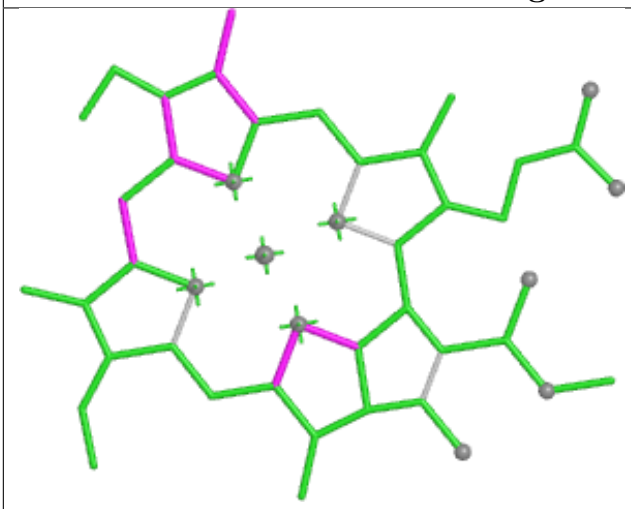


Rings

Ligand CLA 6 513



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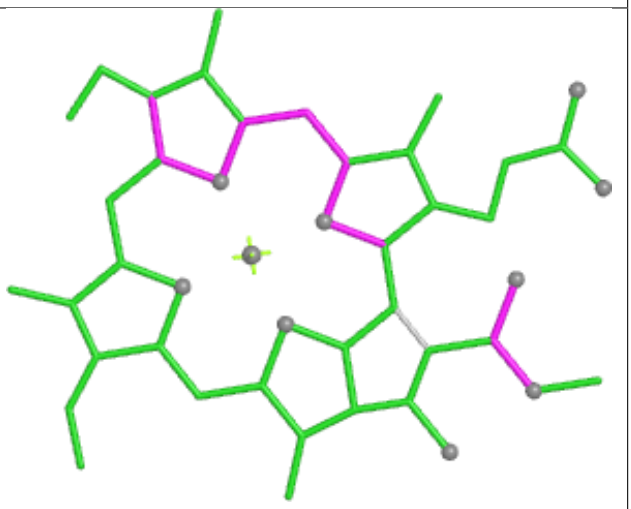
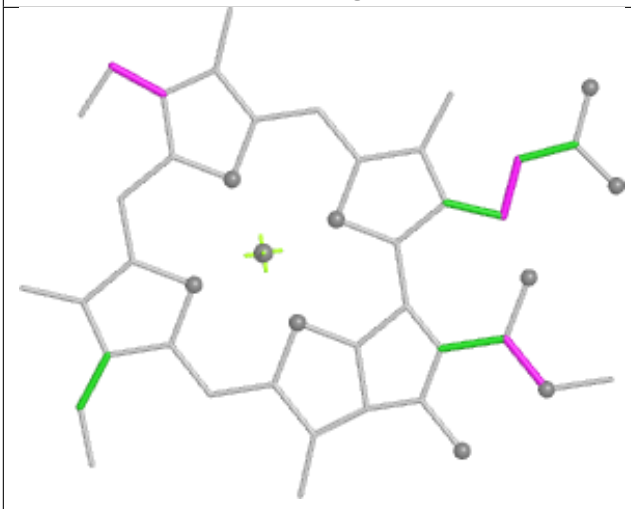


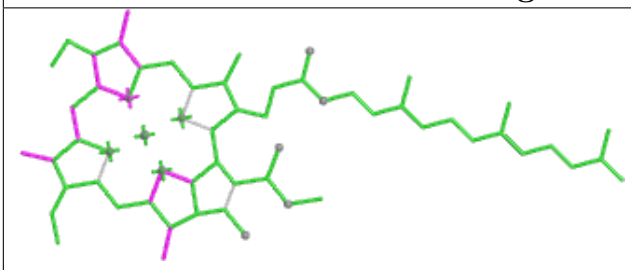
Bond angles



Torsions

Rings

Ligand CLA L 1503



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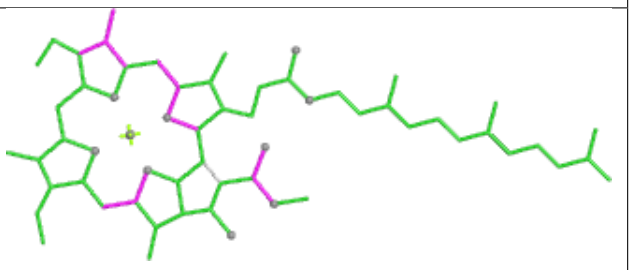
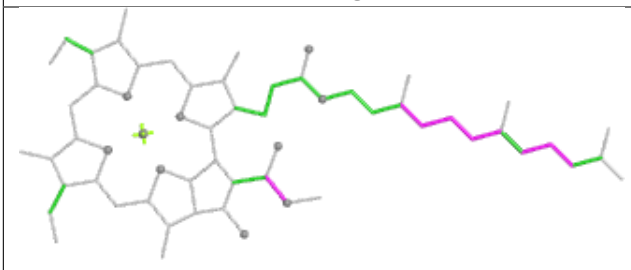


Bond angles



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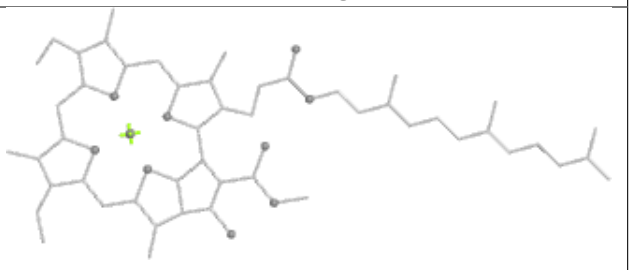
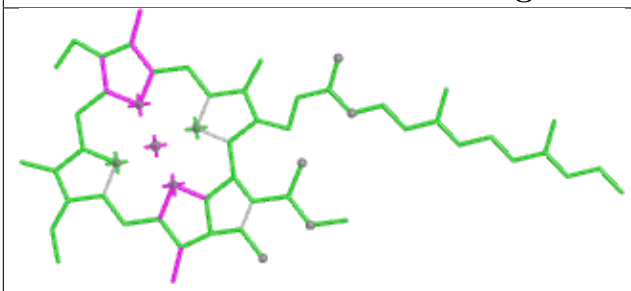


Rings

Ligand CLA B 1217



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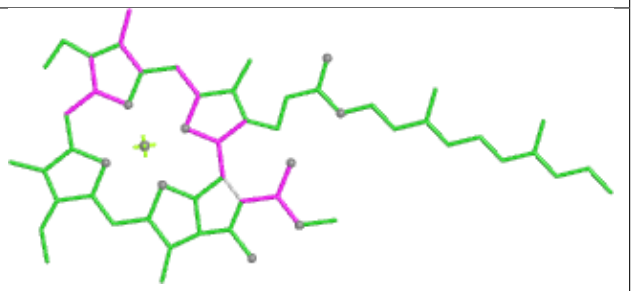
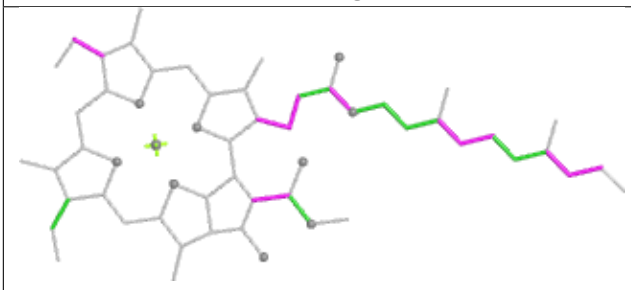


Bond angles



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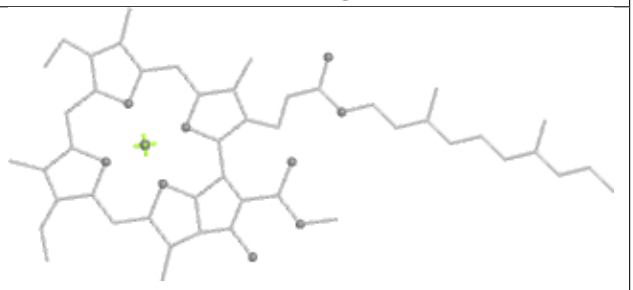
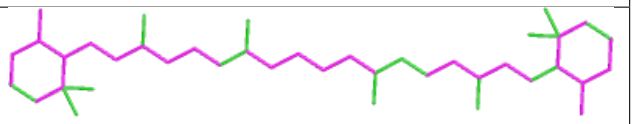


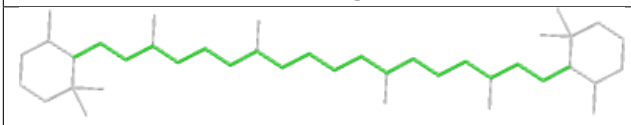
Rings

Ligand BCR e 4007

Bond lengths



Bond angles



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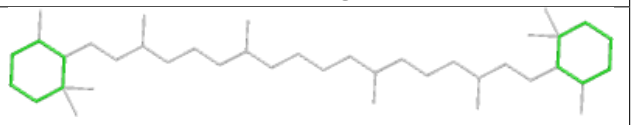
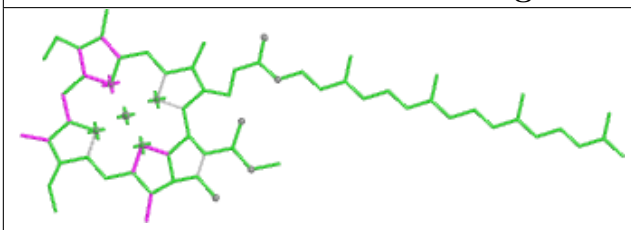
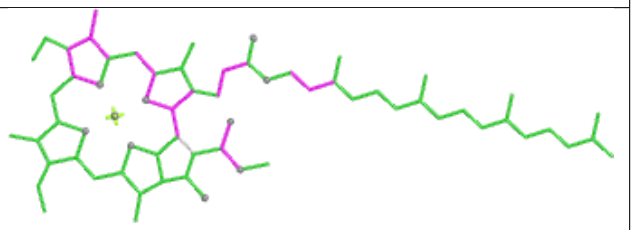


Rings

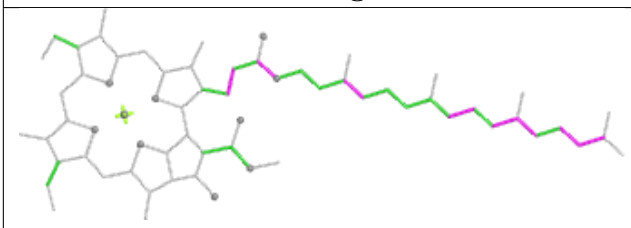
Ligand CLA A 1127



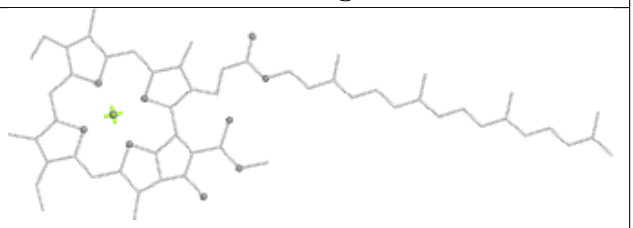
Bond lengths



Bond angles

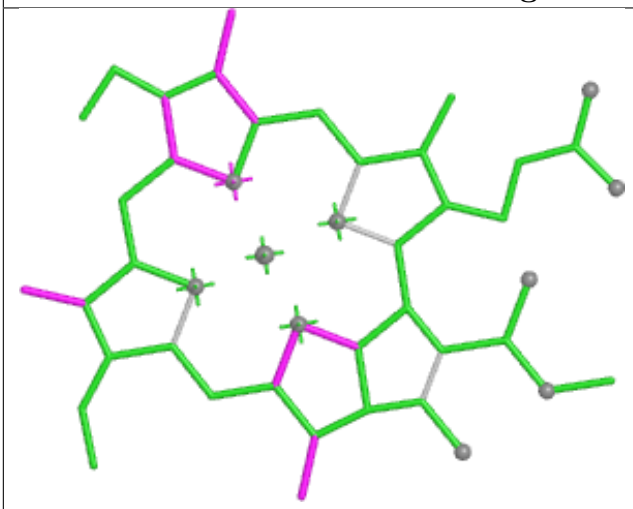


Torsions



Rings

Ligand CLA e 1113



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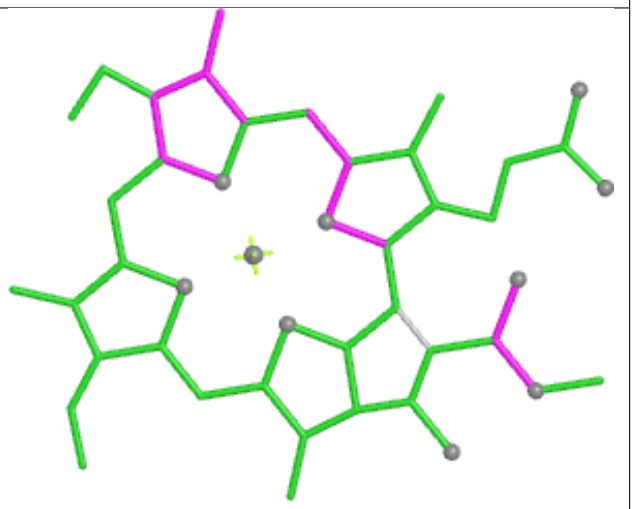

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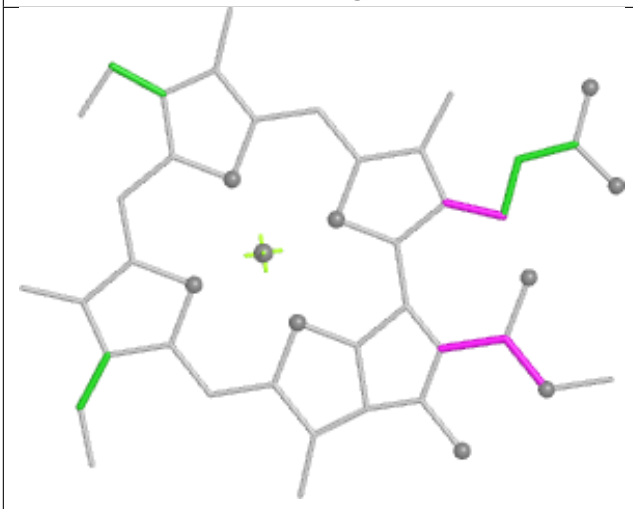
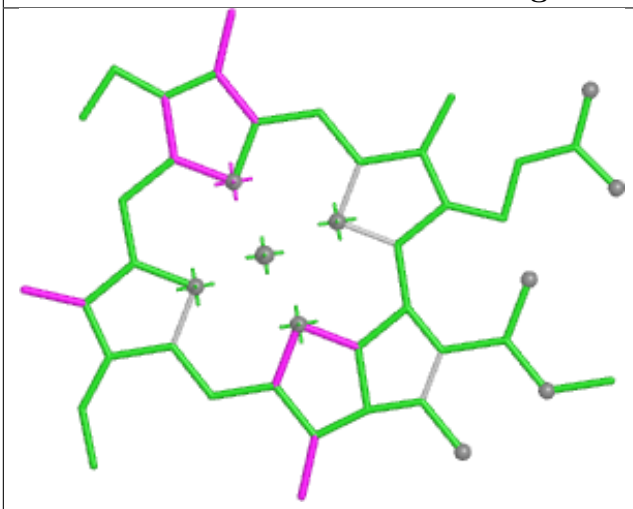


Torsions

Rings

Ligand CLA t 508



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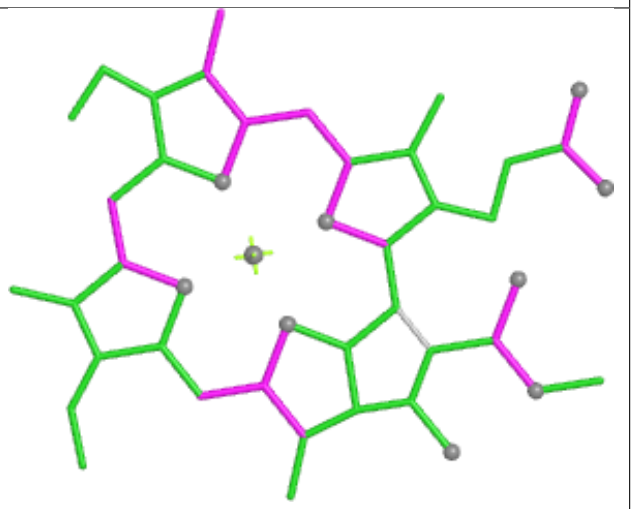

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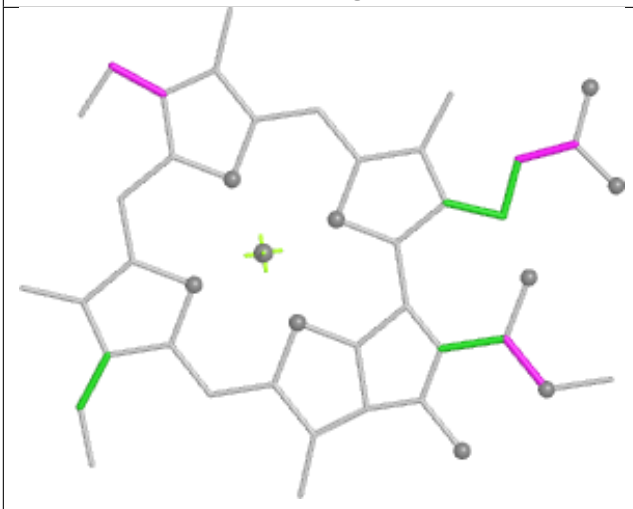
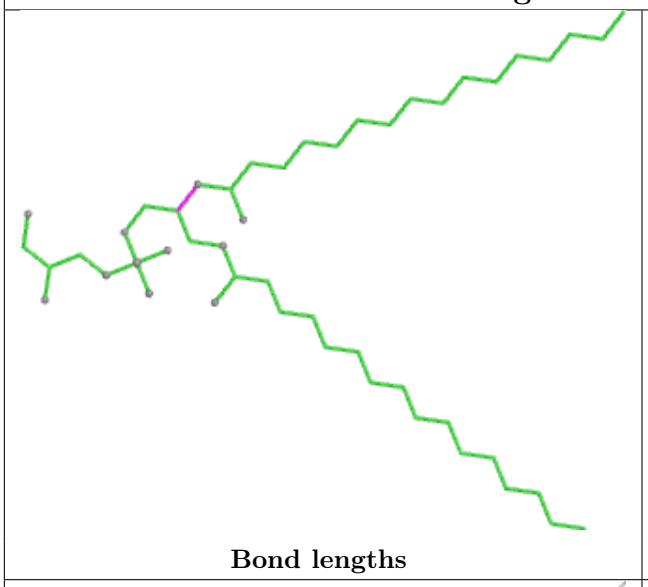


Torsions

Rings

Ligand LHG G 5001



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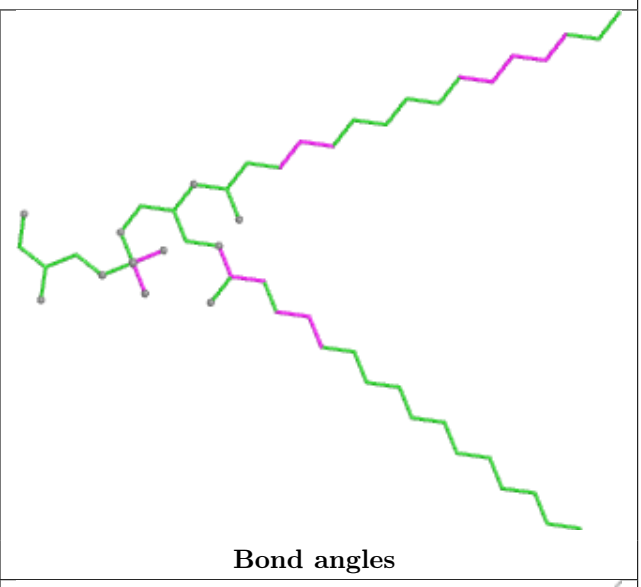
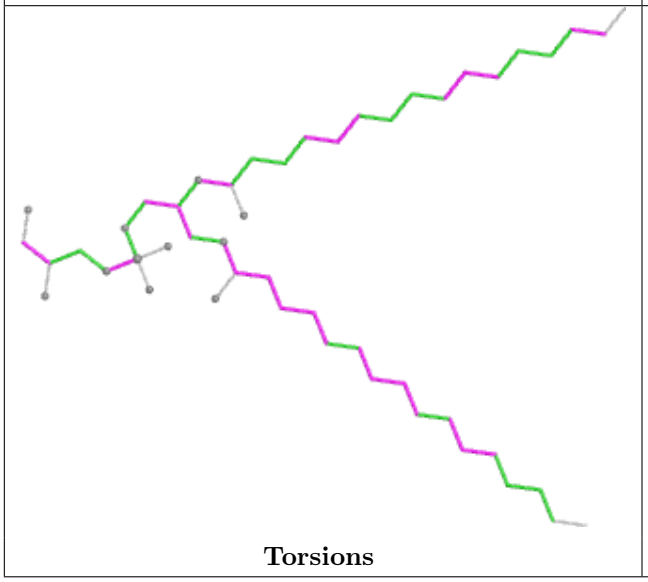


Bond angles



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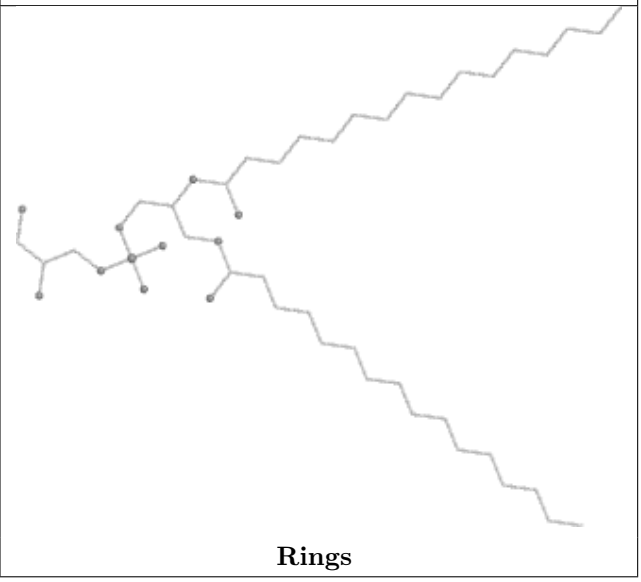
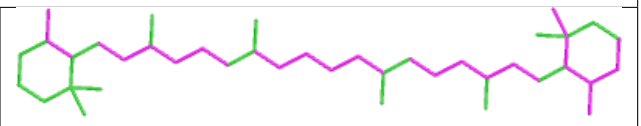


Rings

Ligand BCR V 4019

Bond lengths



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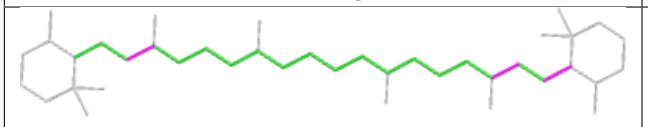

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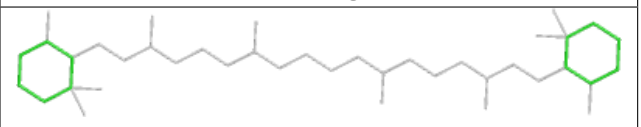
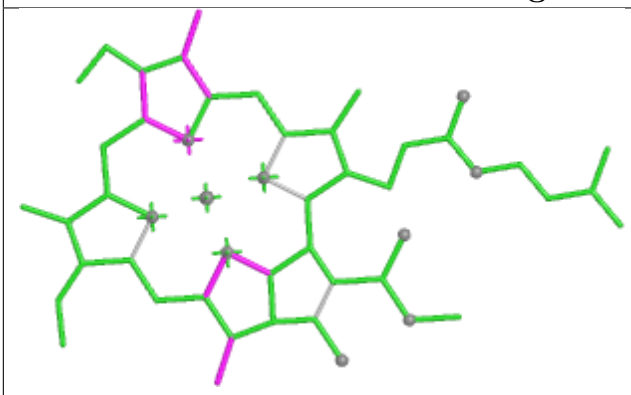


Rings

Ligand CLA 3 502



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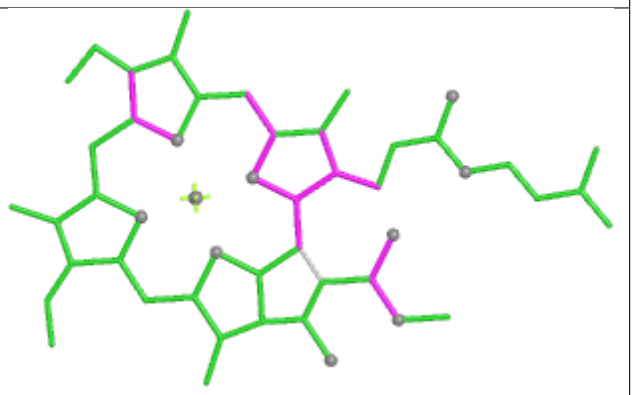

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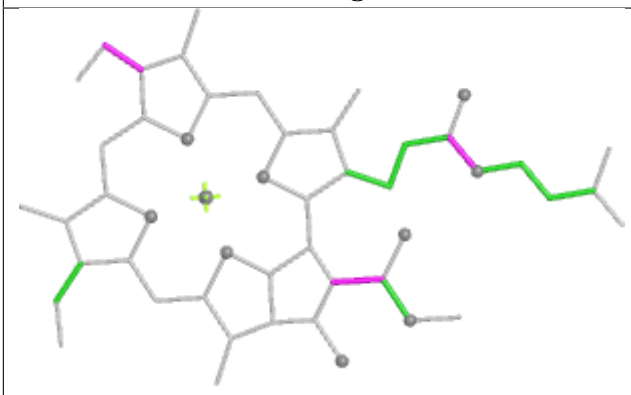

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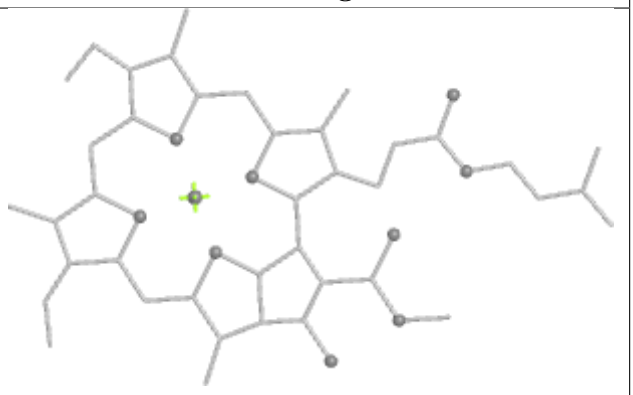
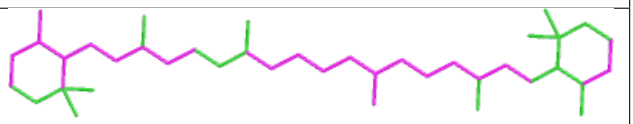


Rings

Ligand BCR a 523

Bond lengths



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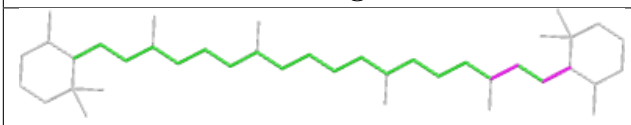

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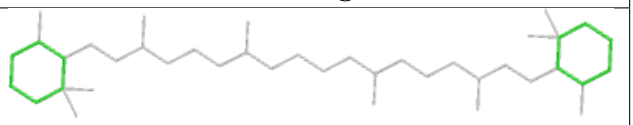
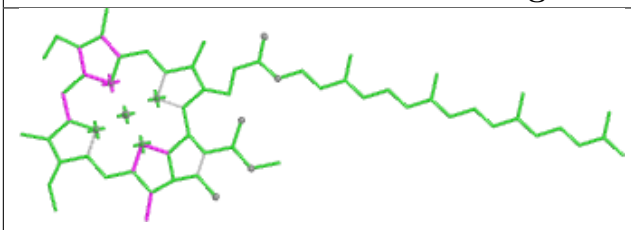
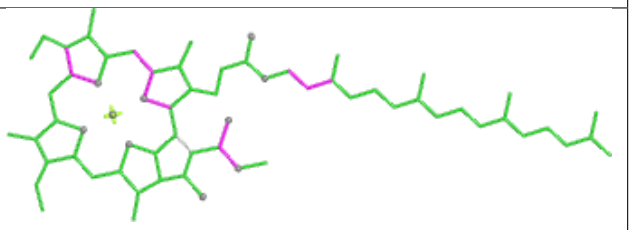
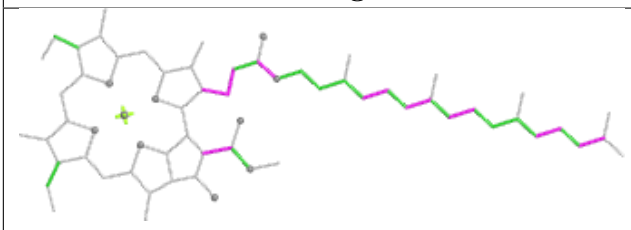
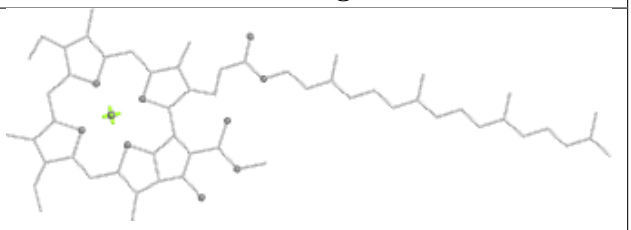
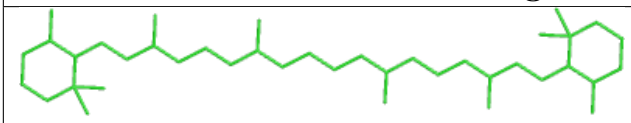
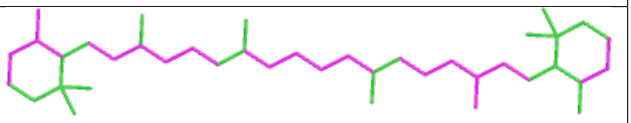


Rings

Ligand CLA 1 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Z 523	
	
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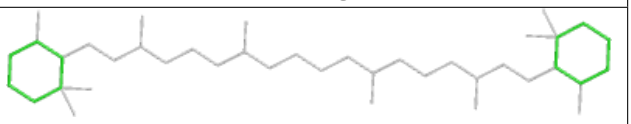
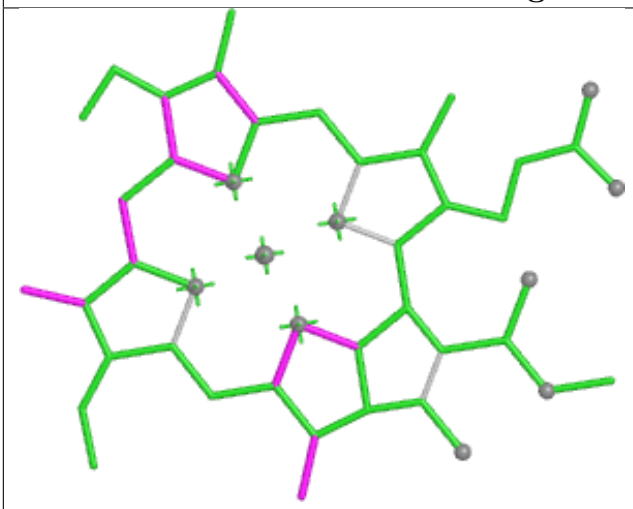
	
Torsions	Rings

Ligand CLA q 506



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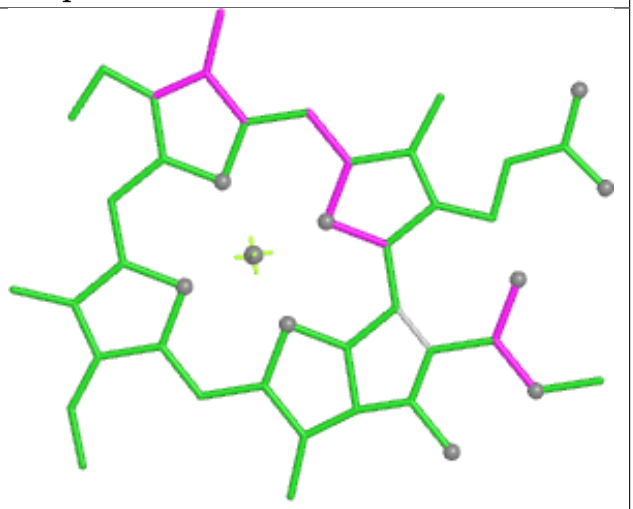
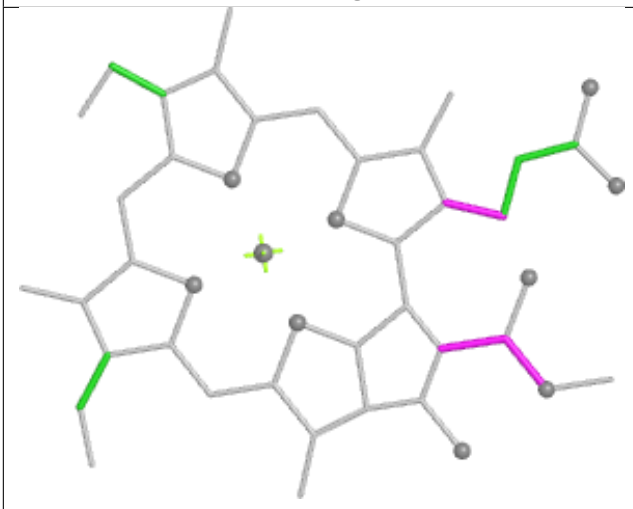


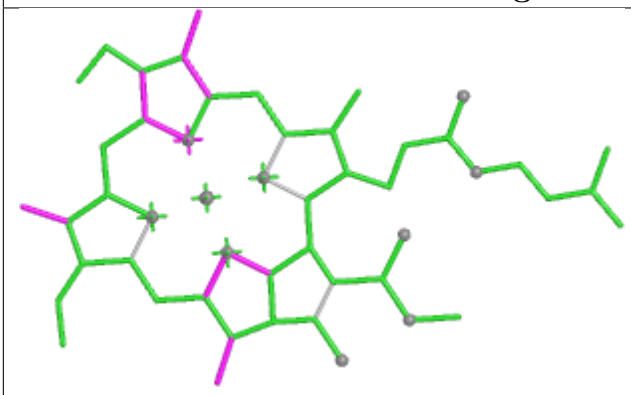
Bond angles



Torsions

Rings

Ligand CLA m 1103



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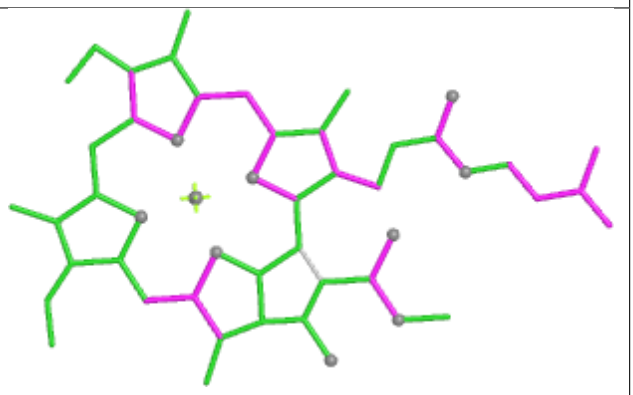

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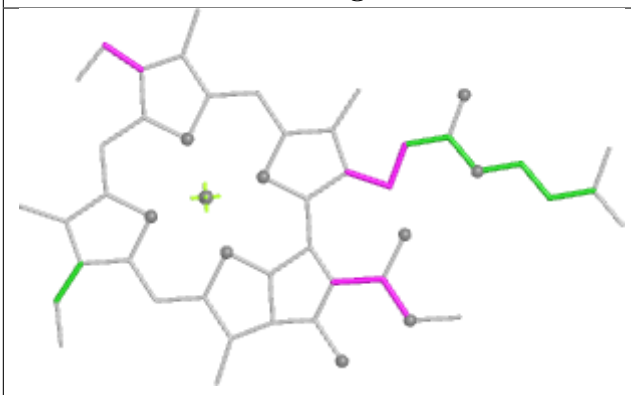
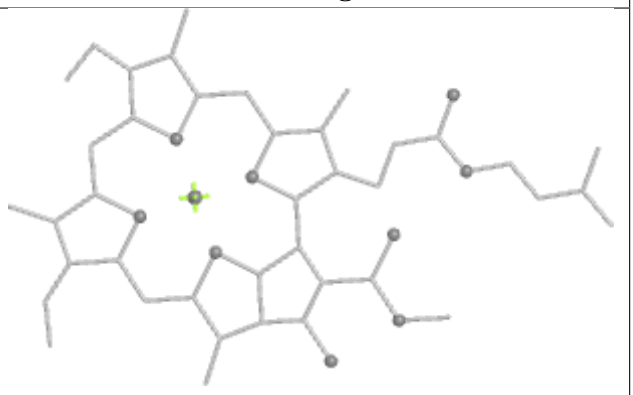
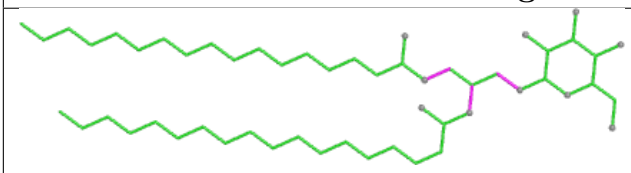


Torsions



Rings

Ligand LMG f 5002



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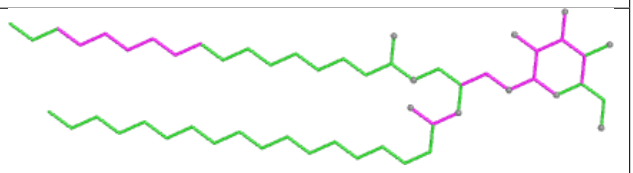
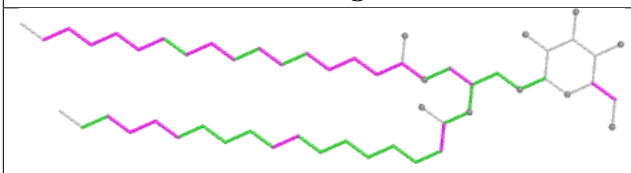


Bond angles



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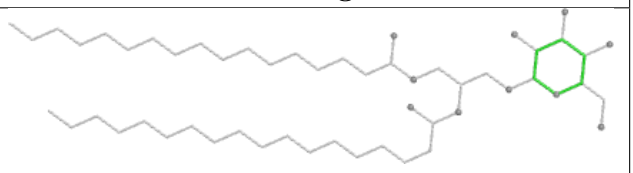
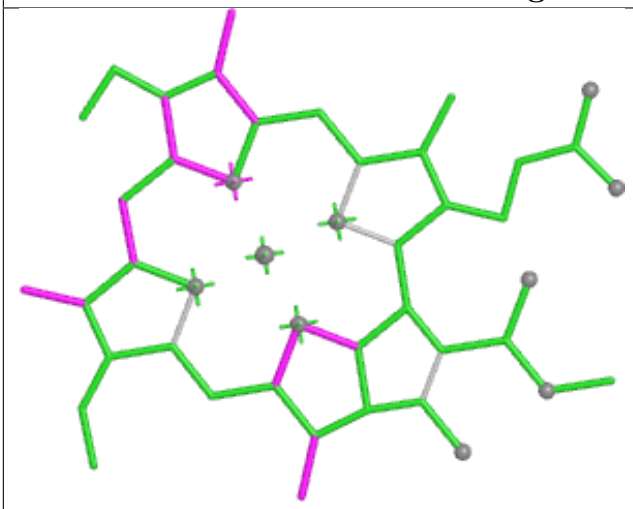


Rings

Ligand CLA q 517



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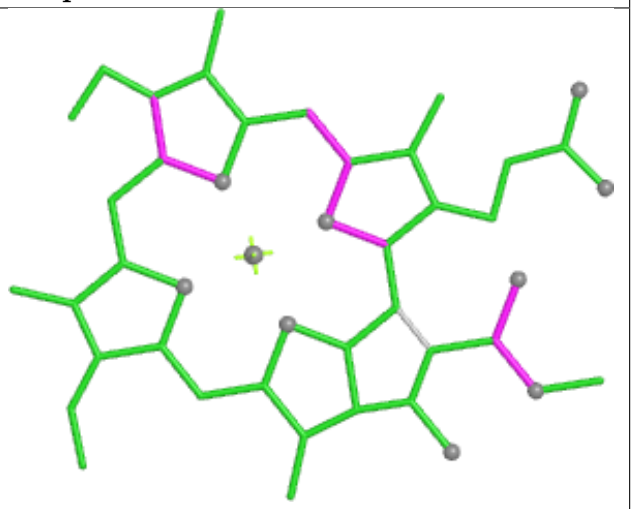
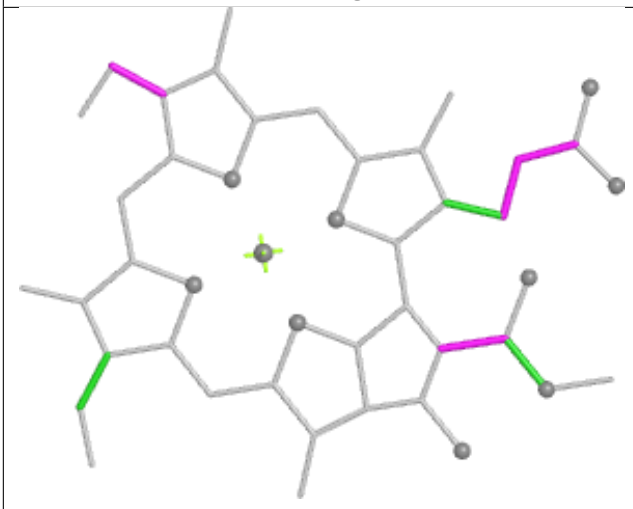


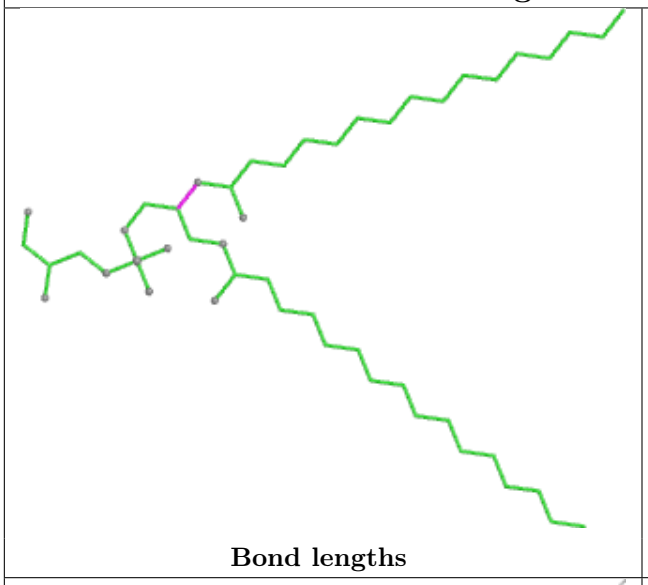
Bond angles



Torsions

Rings

Ligand LHG A 5009



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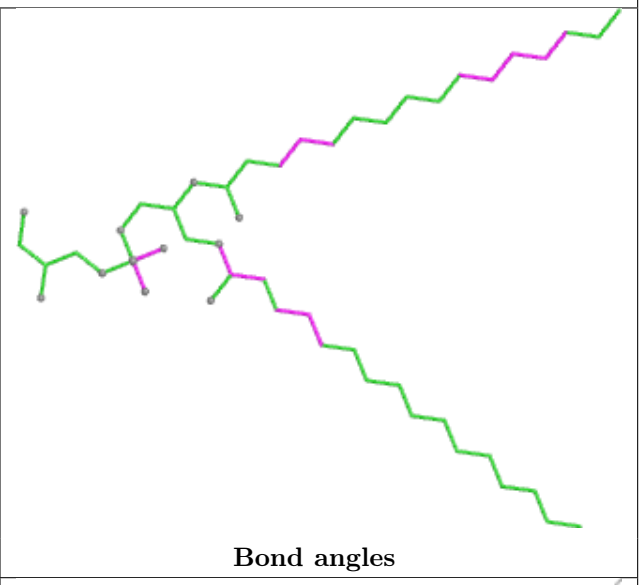
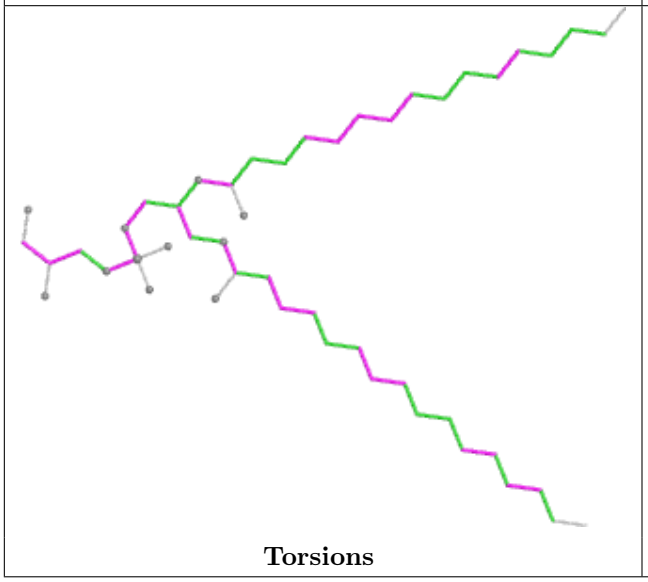


Bond angles



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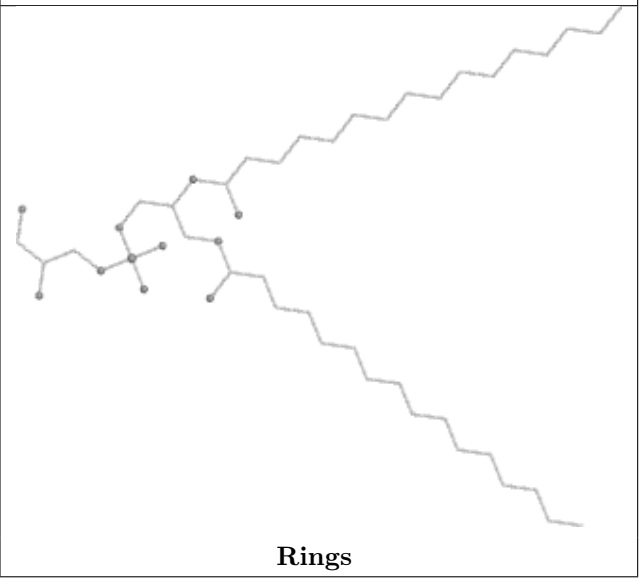
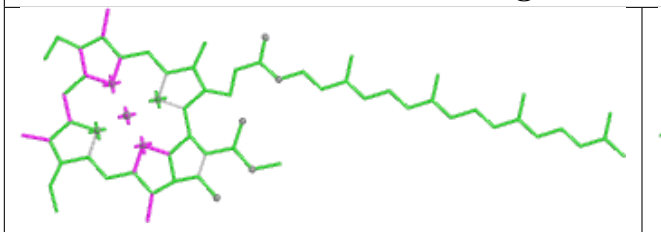
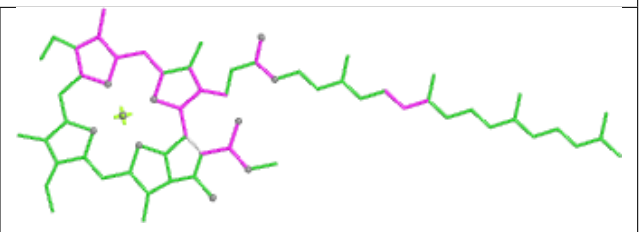


Rings

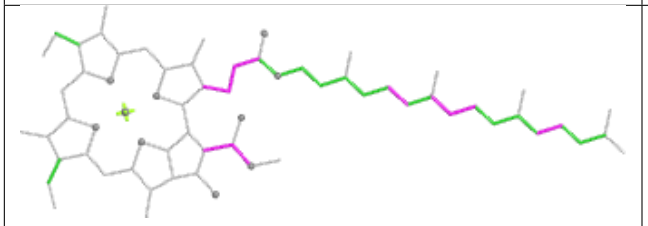
Ligand CLA H 1221



Bond lengths



Bond angles



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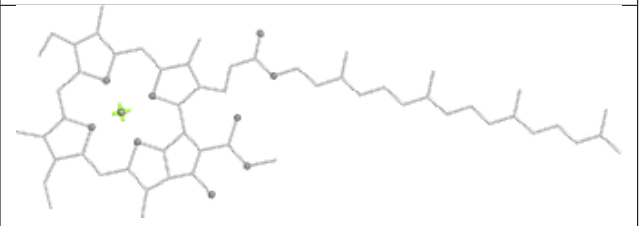
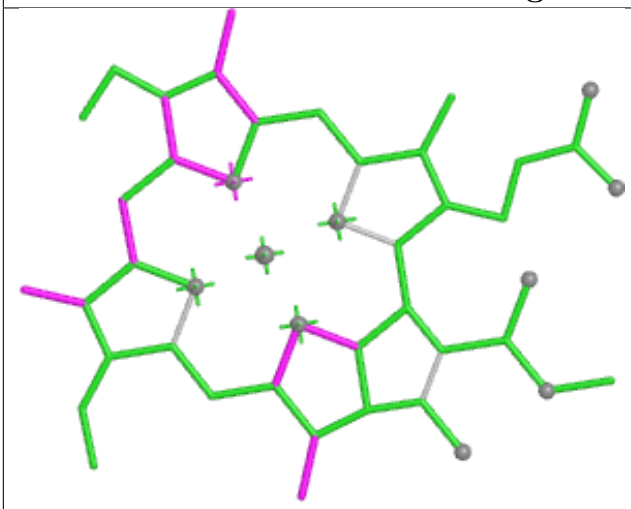
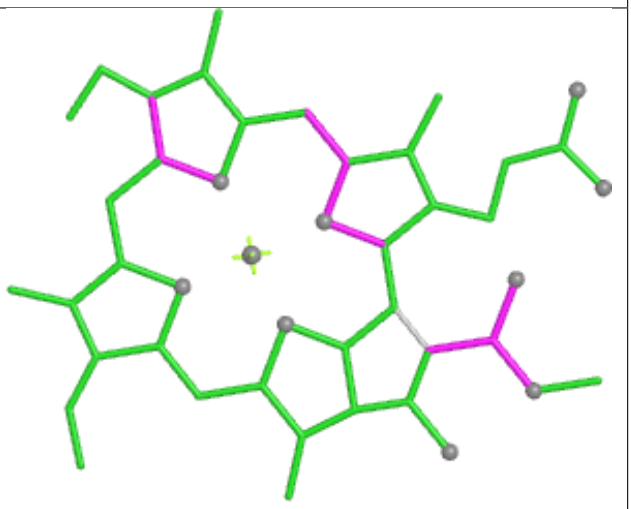


Rings

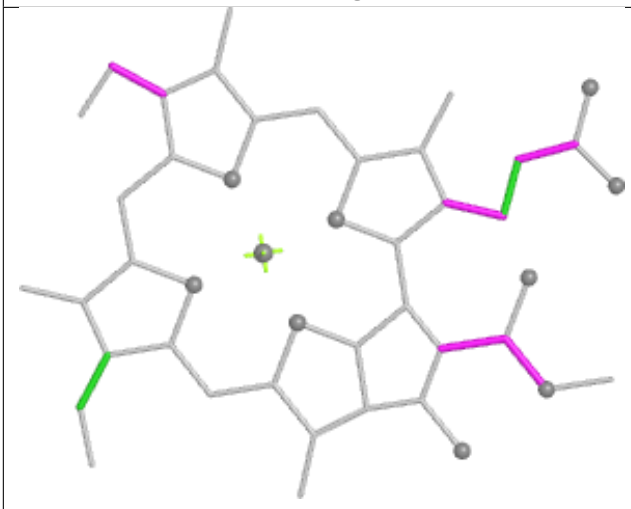
Ligand CLA Z 516



Bond lengths



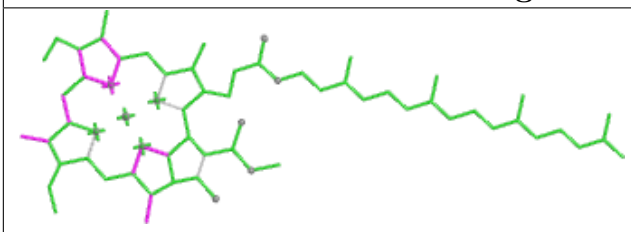
Bond angles



Torsions

Rings

Ligand CLA B 1229



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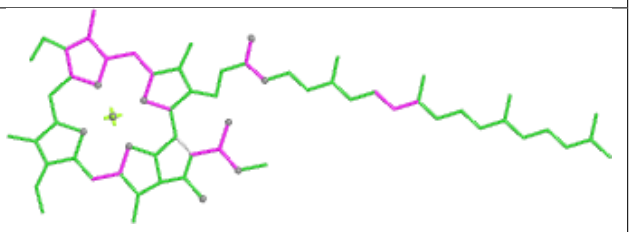
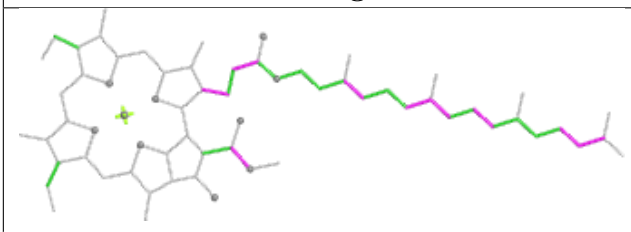
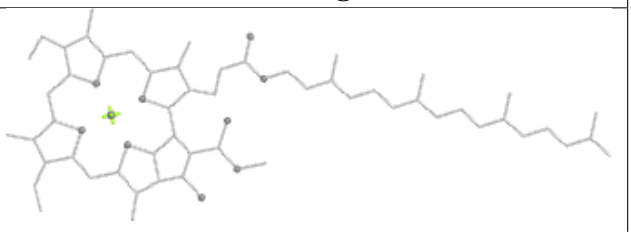


Bond angles

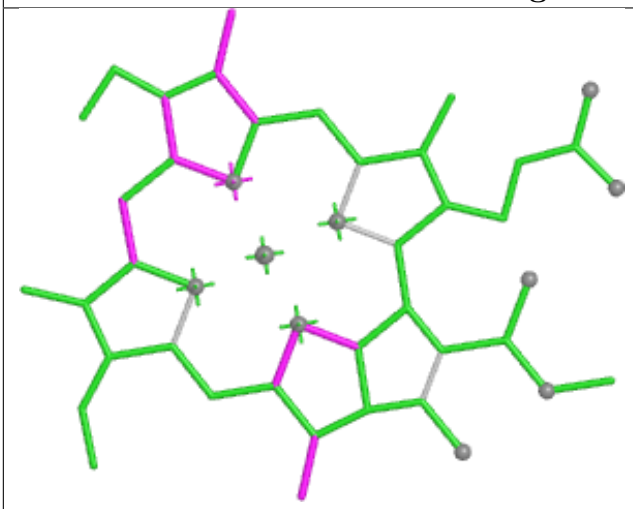


Torsions



Rings

Ligand CLA c 510



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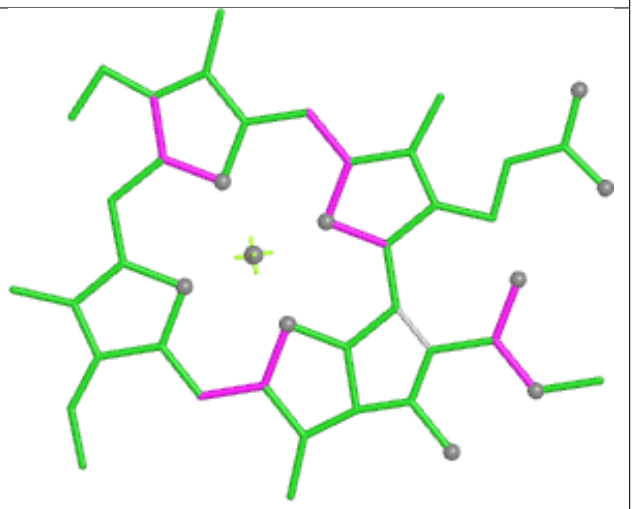
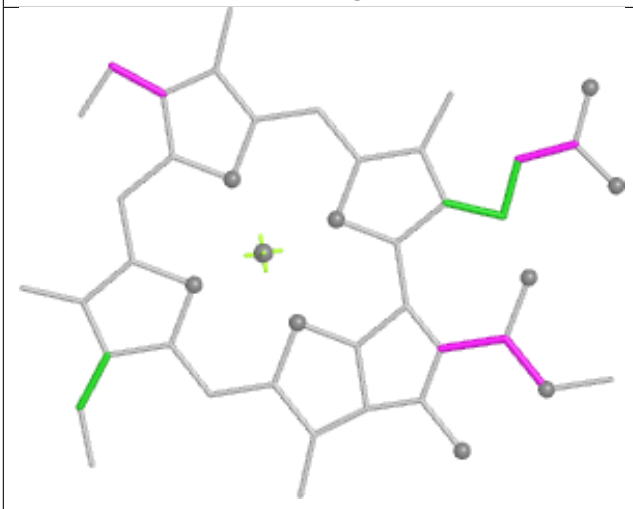


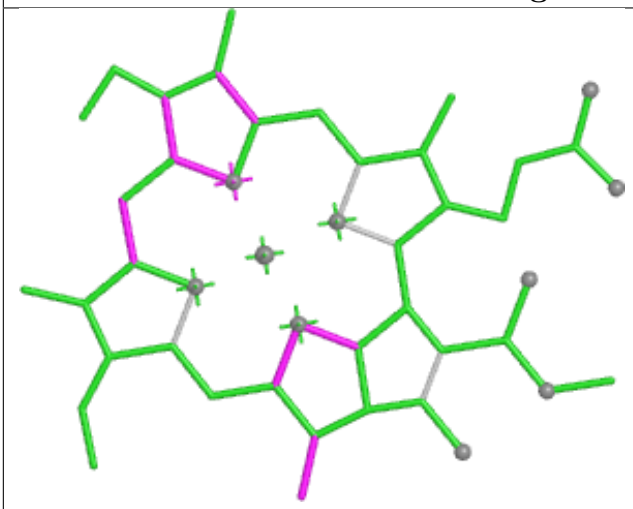
Bond angles



Torsions

Rings

Ligand CLA s 516



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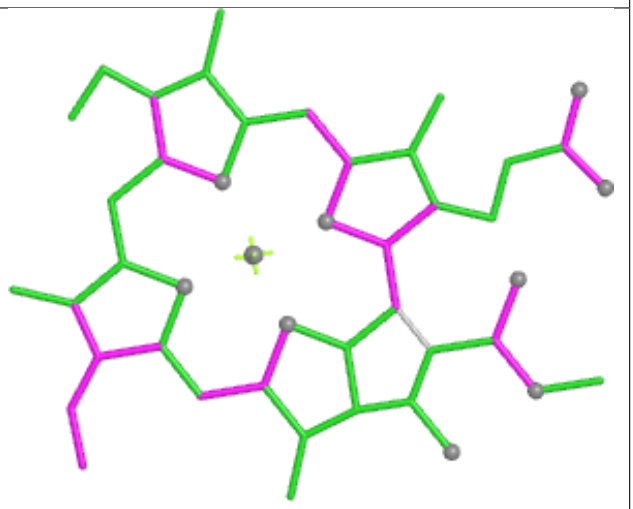
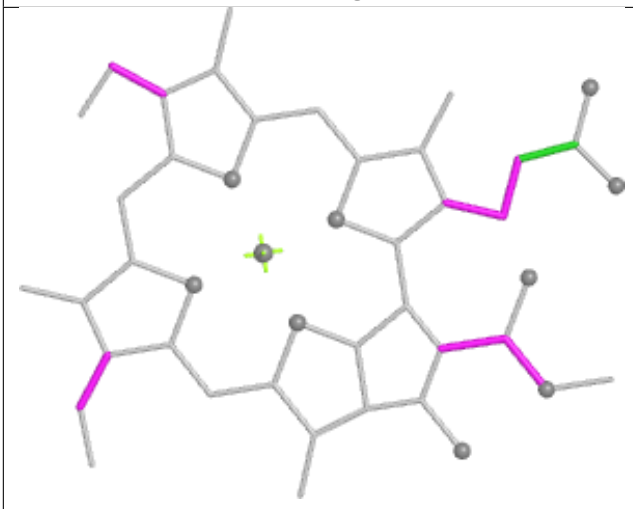


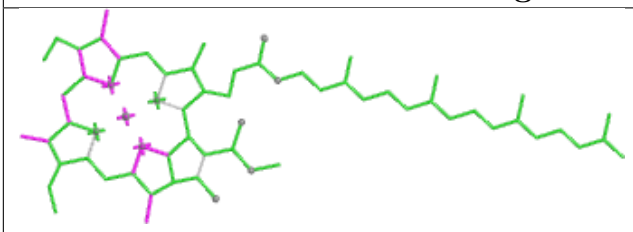
Bond angles



Torsions

Rings

Ligand CLA H 1225



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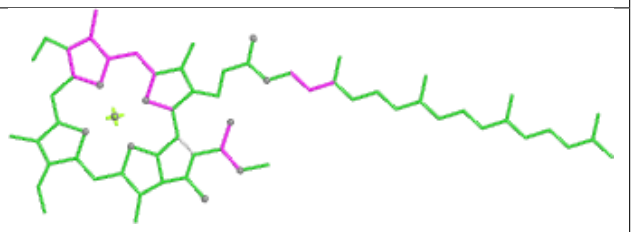

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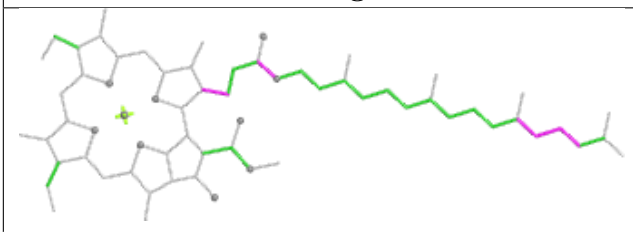

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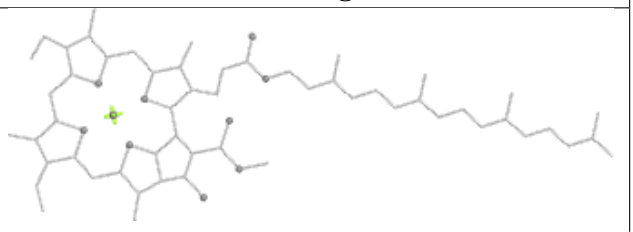
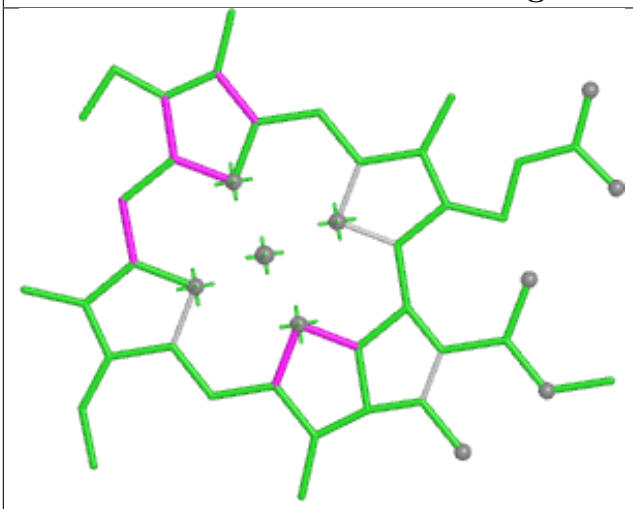


Rings

Ligand CLA d 513



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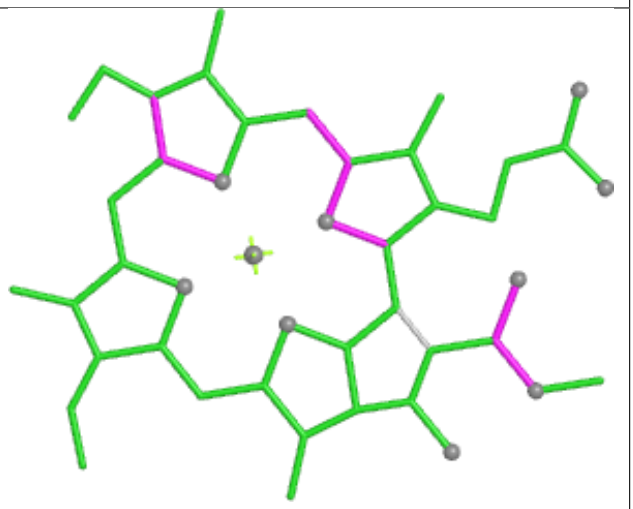
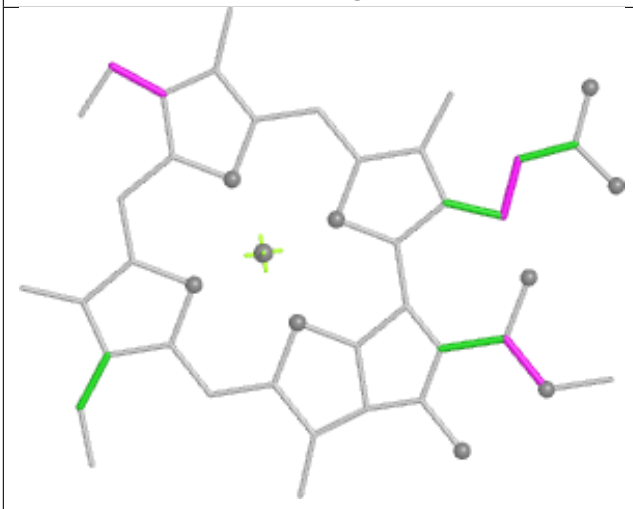


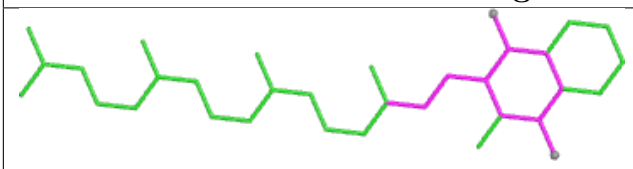
Bond angles



Torsions

Rings

Ligand PQN B 2002



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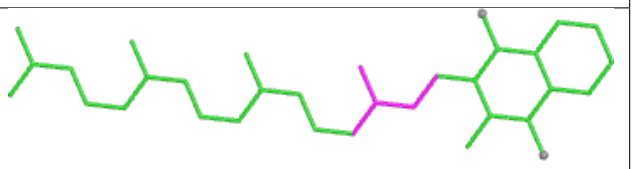
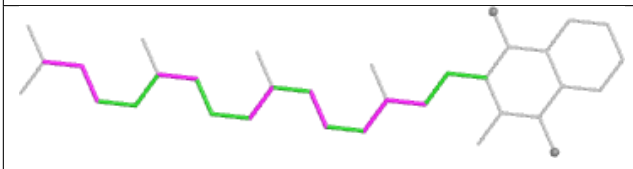


Bond angles



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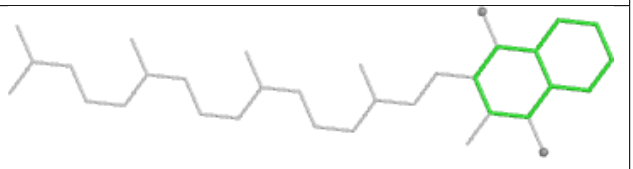
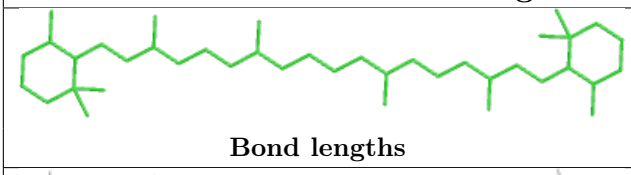


Rings

Ligand BCR L 4219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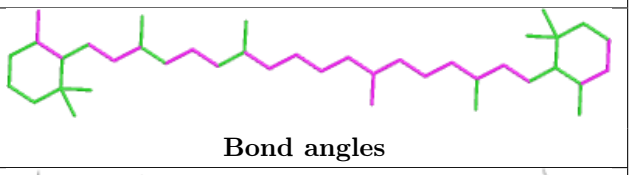
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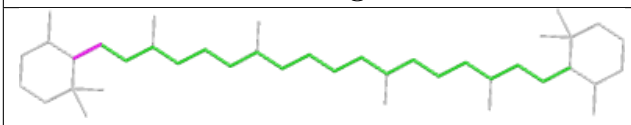
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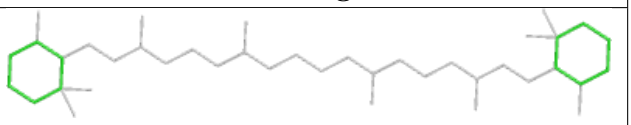
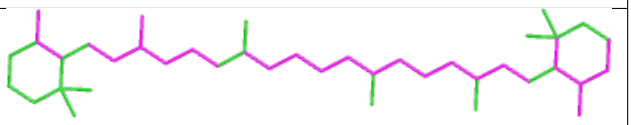
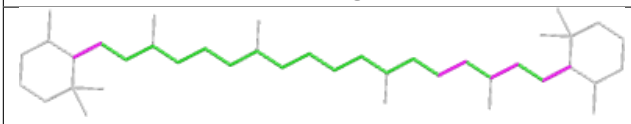

Rings

Ligand BCR G 4008

Bond lengths


Bond angles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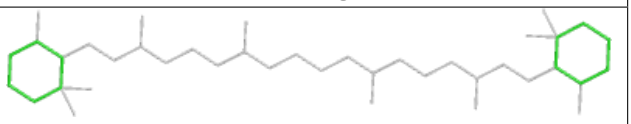
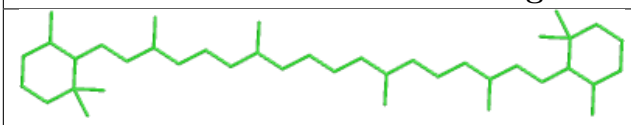

Rings

Ligand BCR q 522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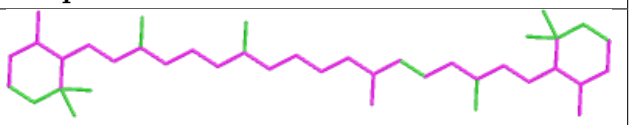
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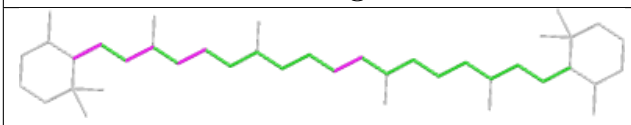
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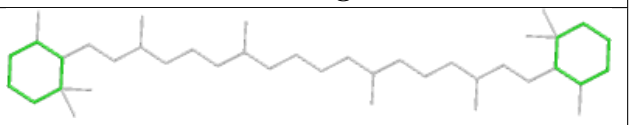
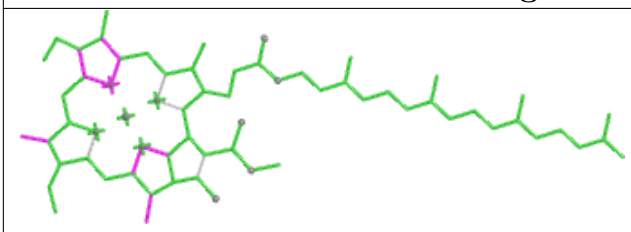

Rings

Ligand CLA e 1123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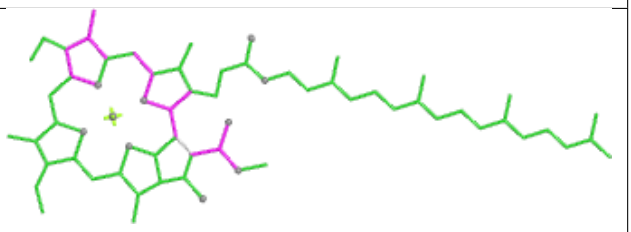
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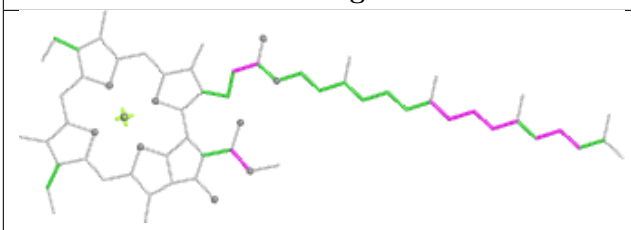
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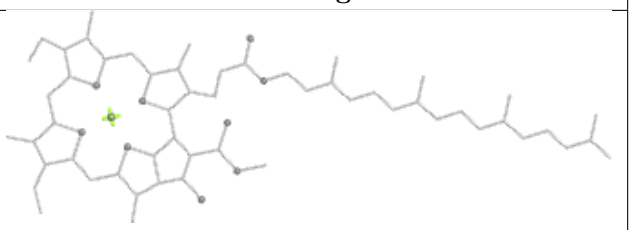
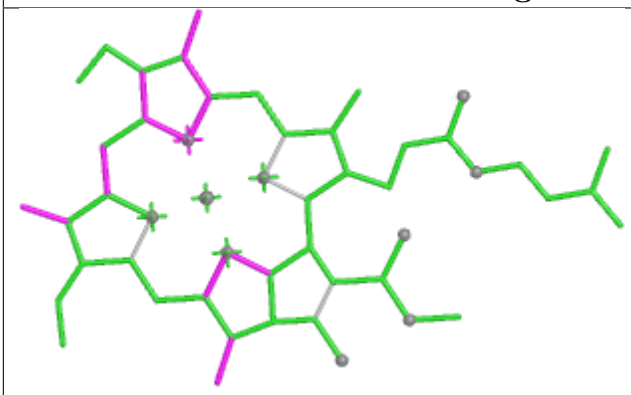

Rings

Ligand CLA H 1232



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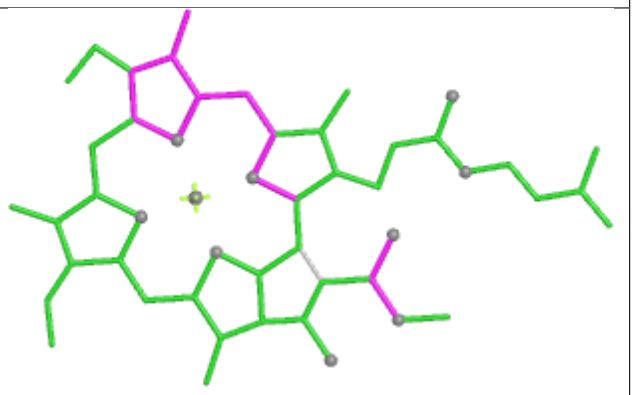
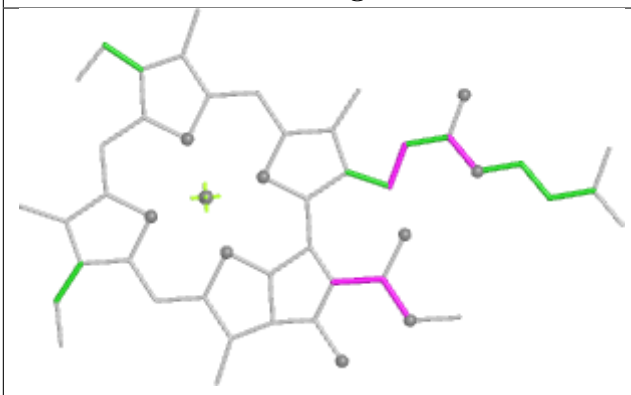


Bond angles



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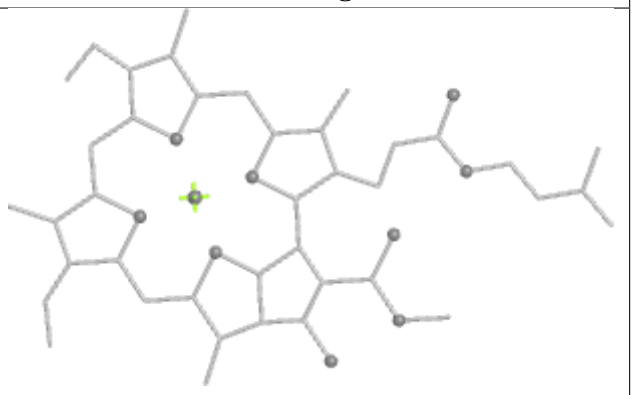
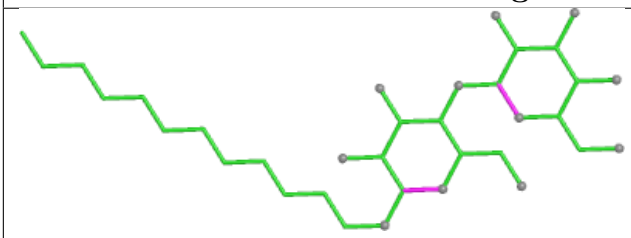


Rings

Ligand LMU B 1843



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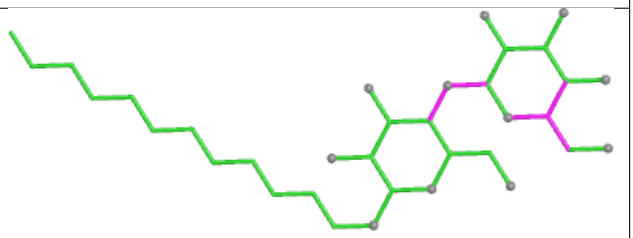
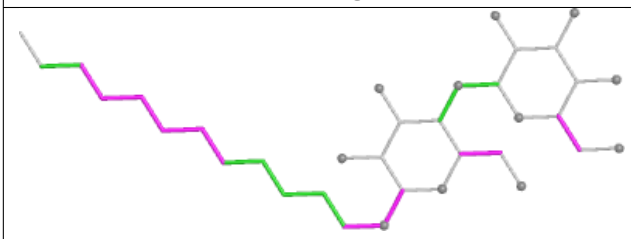
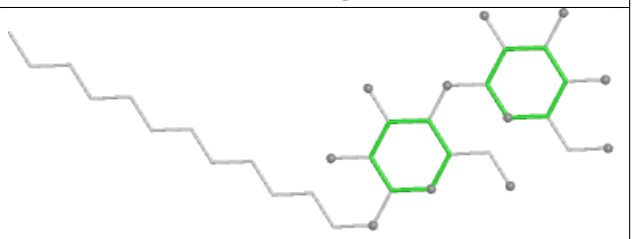


Bond angles

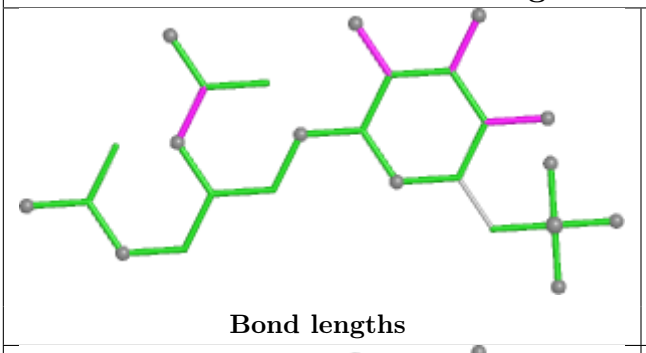


Torsions



Rings

Ligand SQD 4 822



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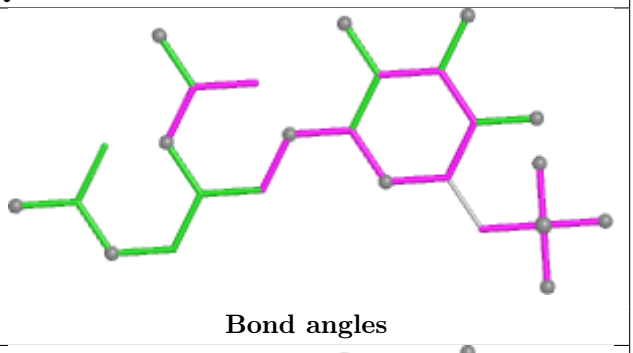
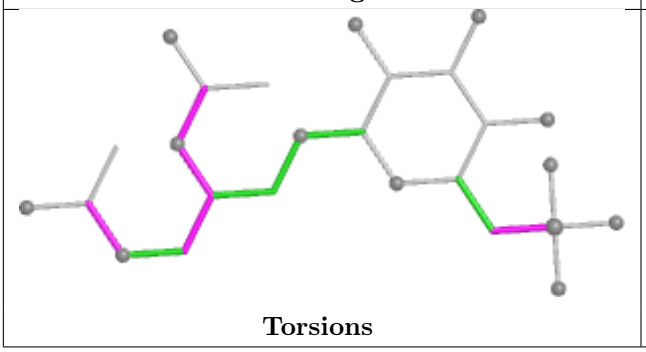
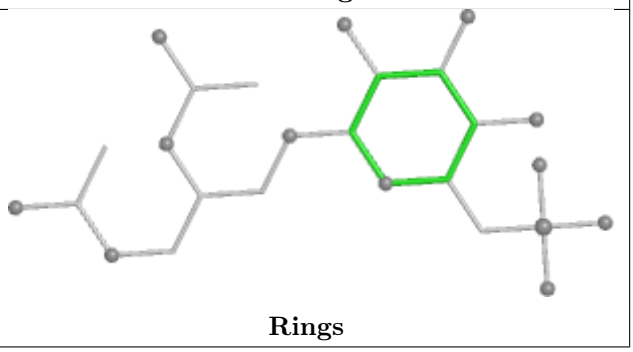


Bond angles

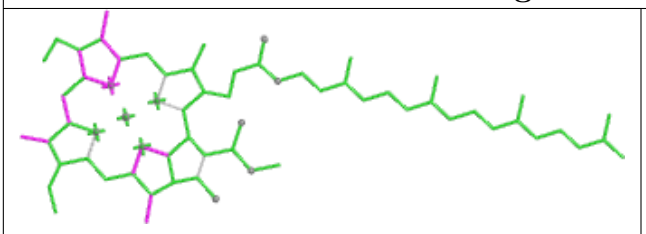


Torsions



Rings

Ligand CLA H 1213



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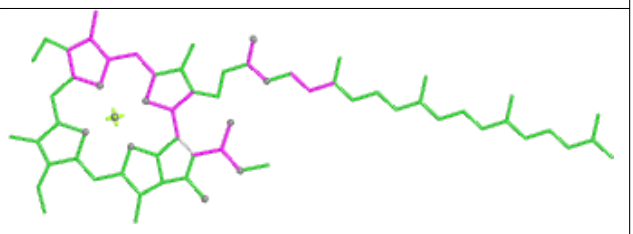
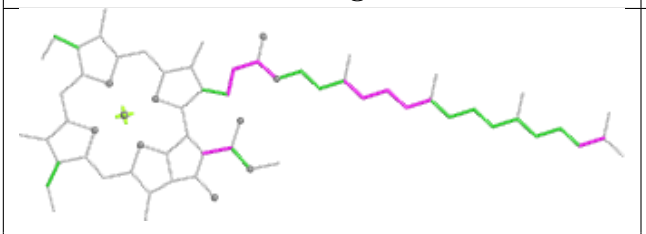
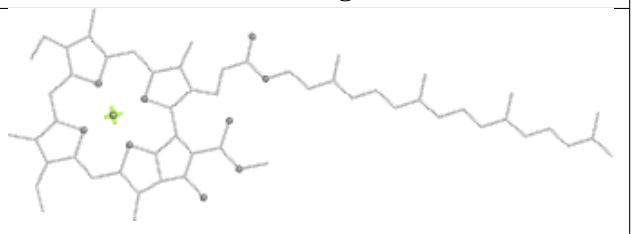


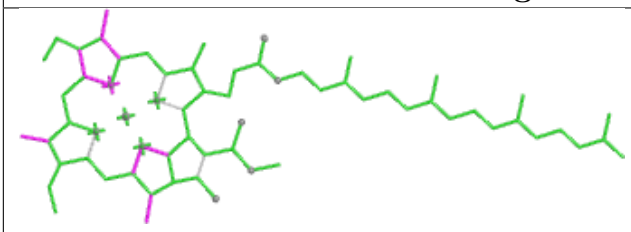
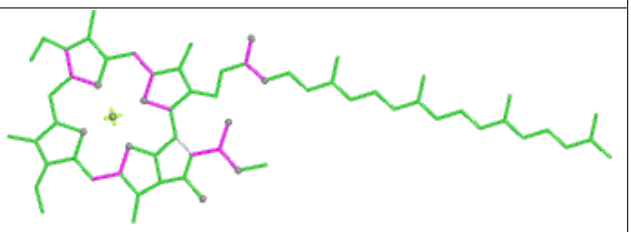
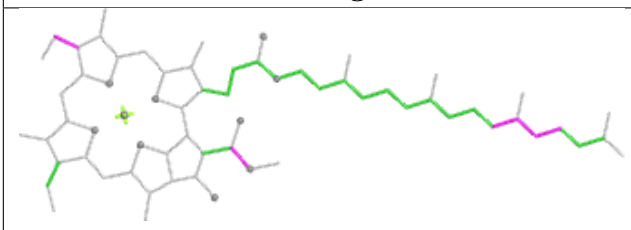
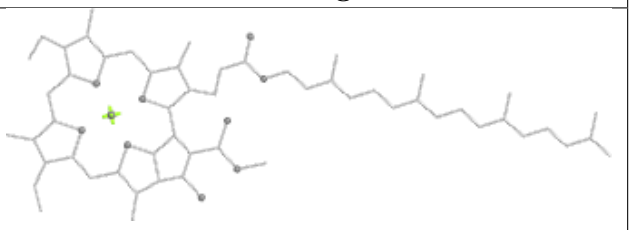
Bond angles

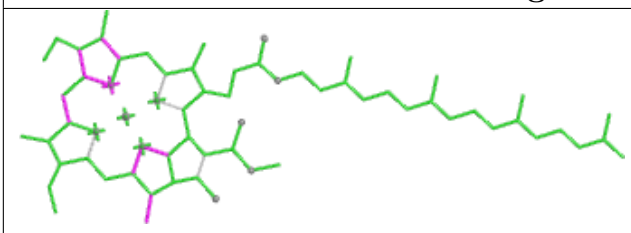
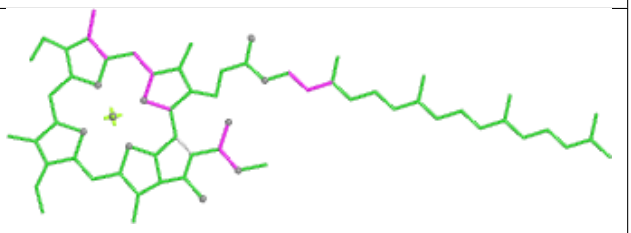
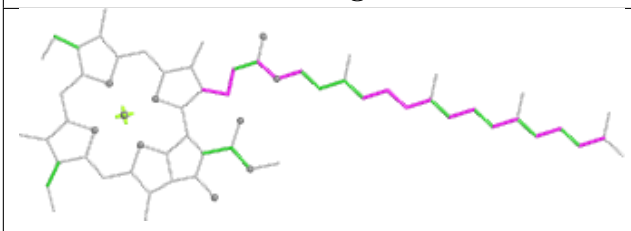
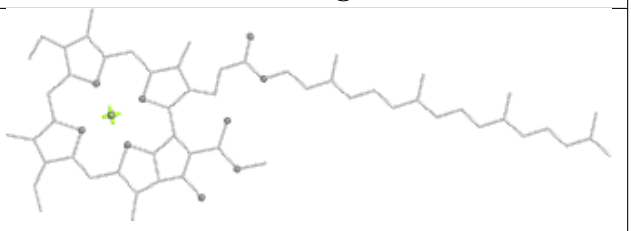


Torsions



Rings

Ligand CLA G 1131	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA v 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

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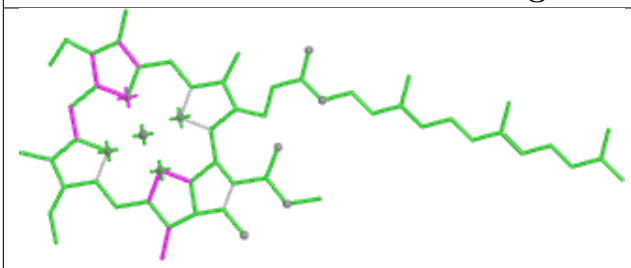	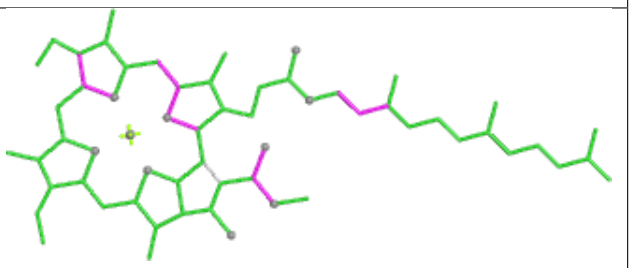
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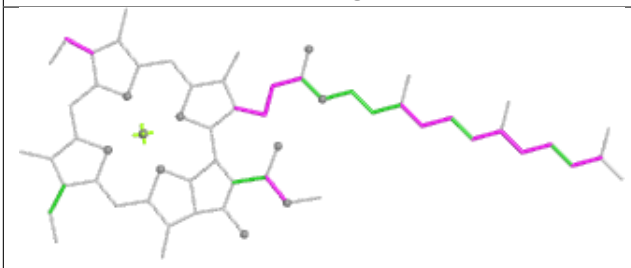	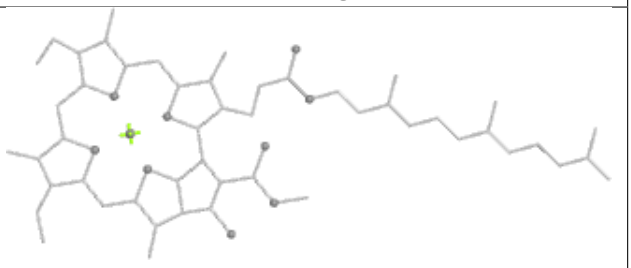
Torsions	**Rings**

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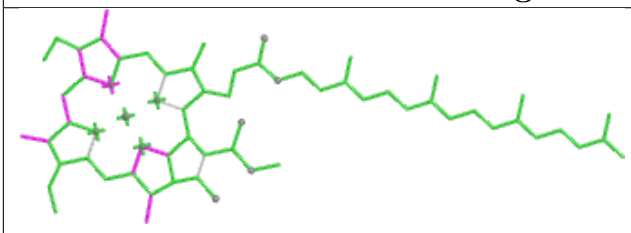
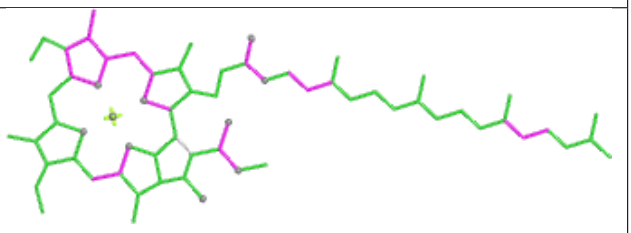
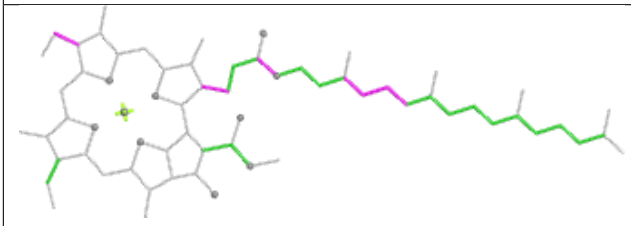
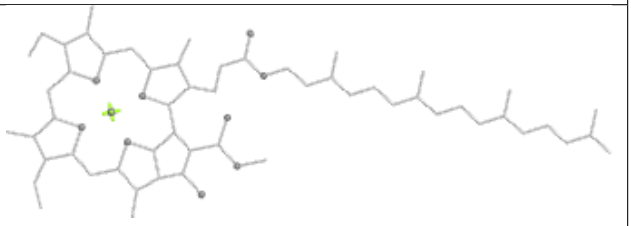
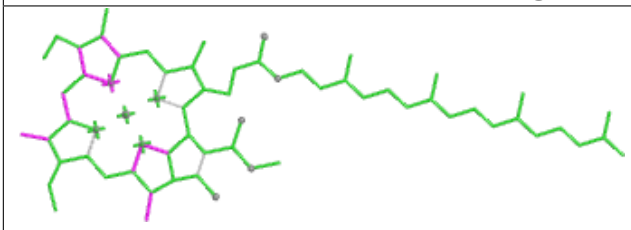
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA r 510



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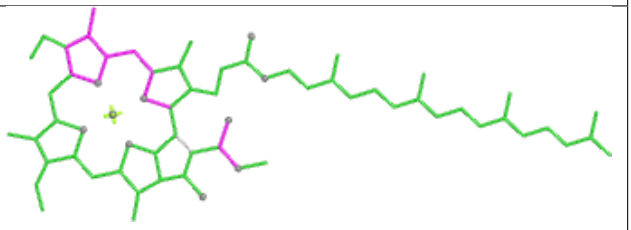
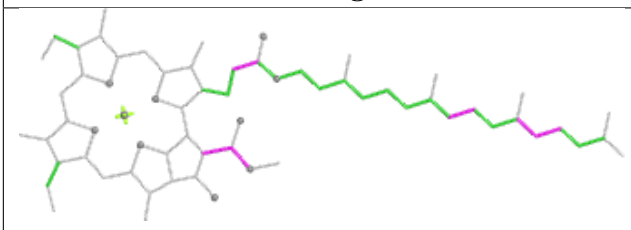


Bond angles



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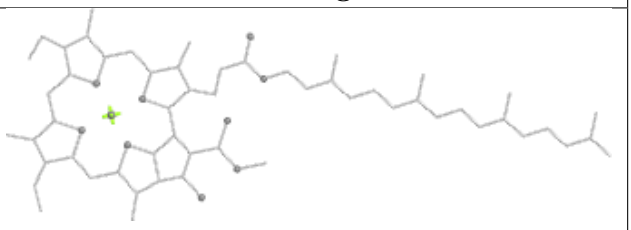
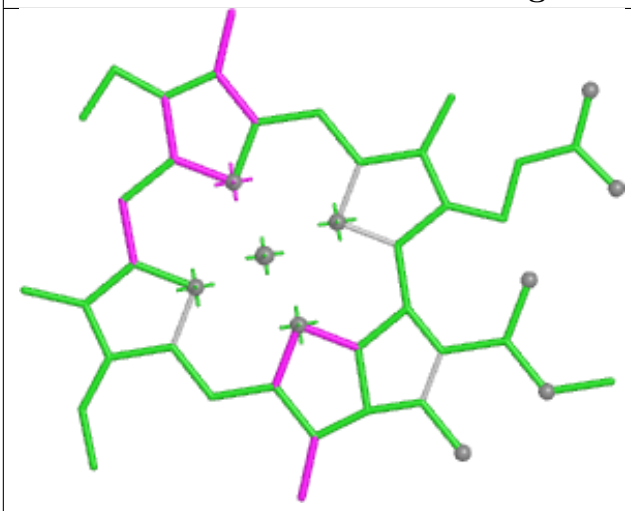


Rings

Ligand CLA 5 512



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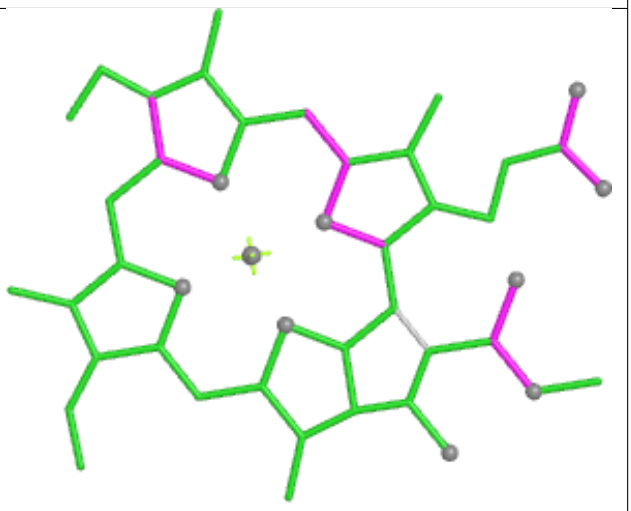
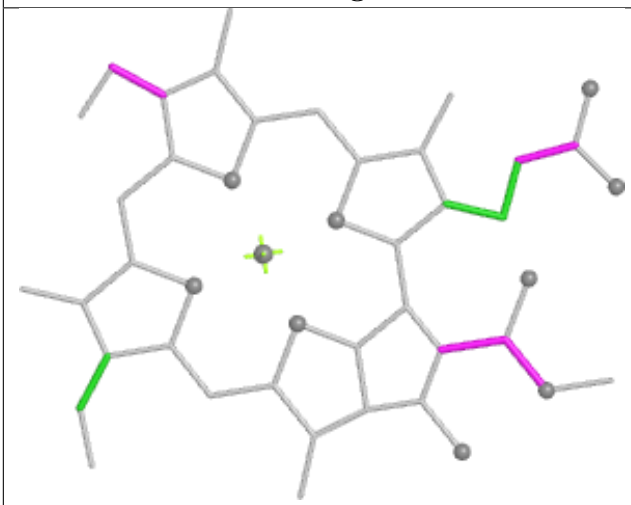


Bond angles



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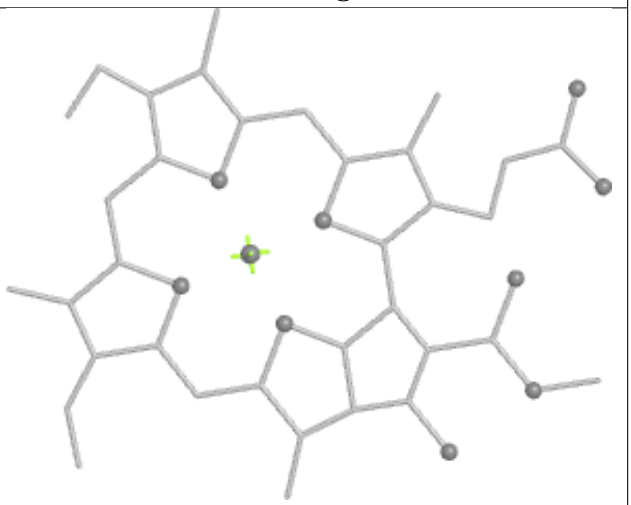
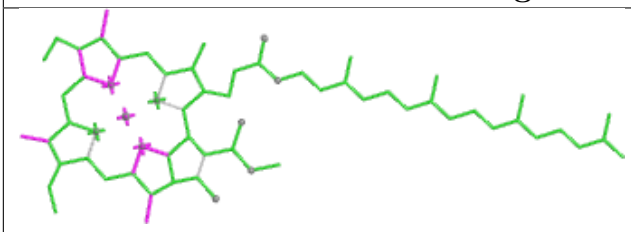


Rings

Ligand CLA G 1119



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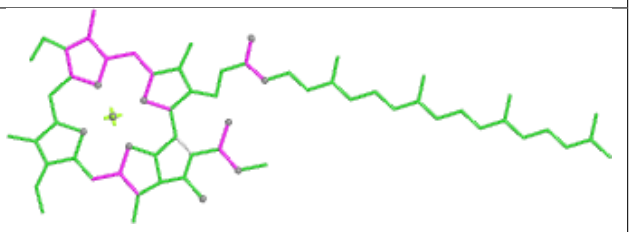
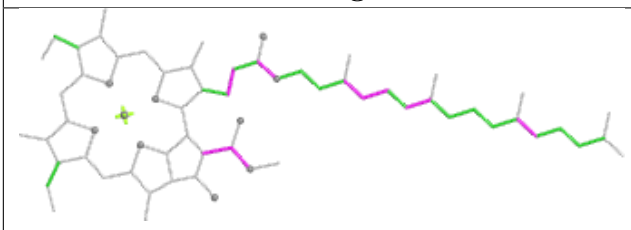


Bond angles



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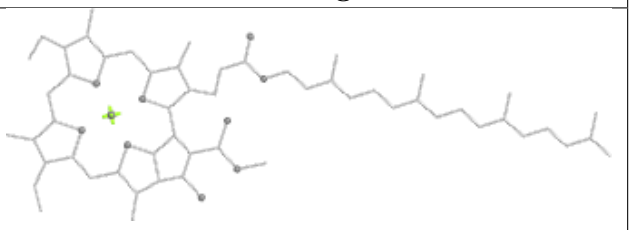
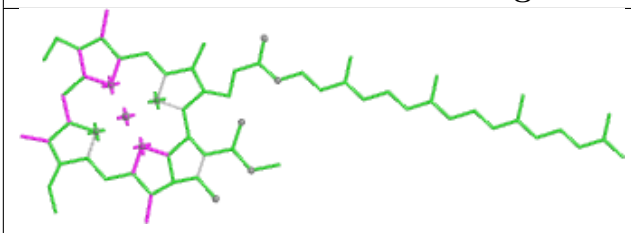


Rings

Ligand CLA G 1013



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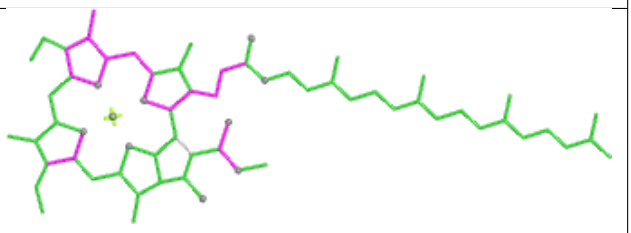
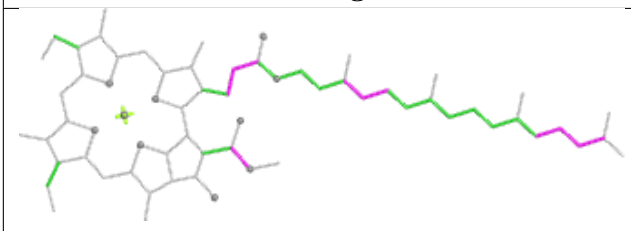


Bond angles



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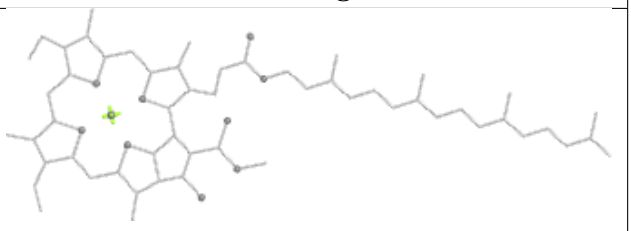

Rings

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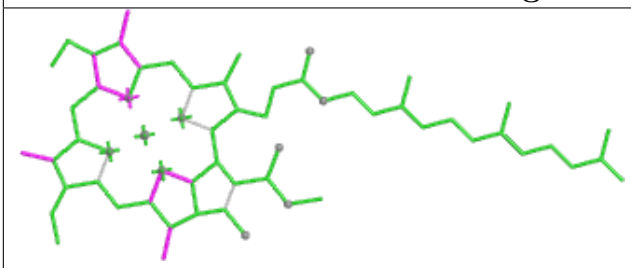

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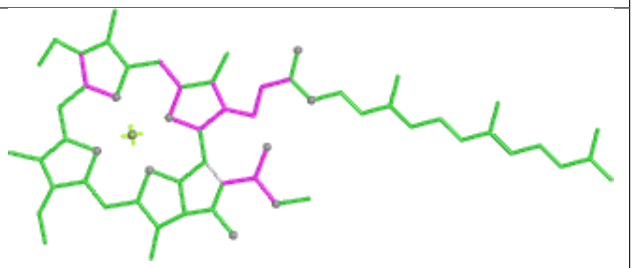
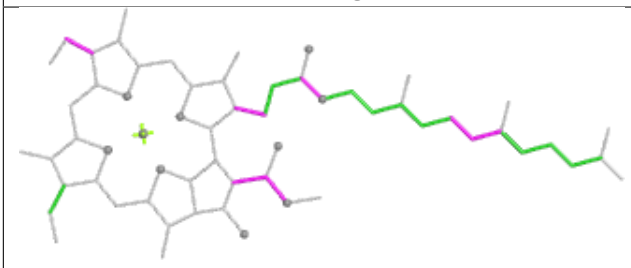


Bond angles



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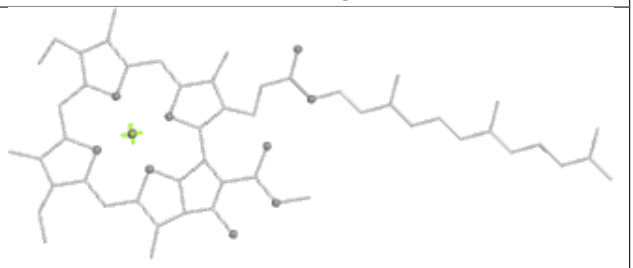
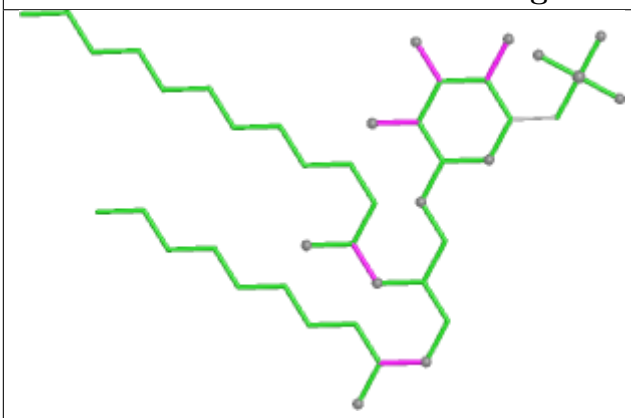


Rings

Ligand SQD s 822



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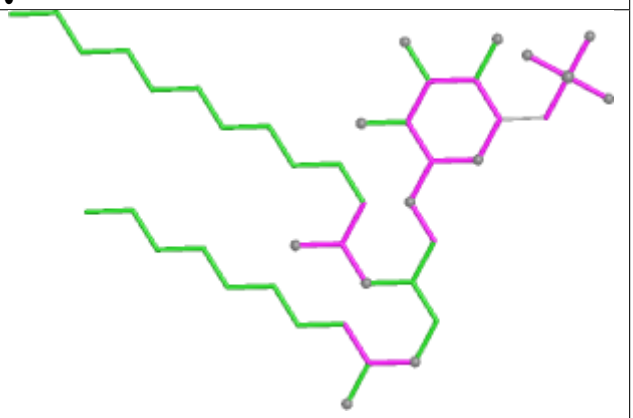
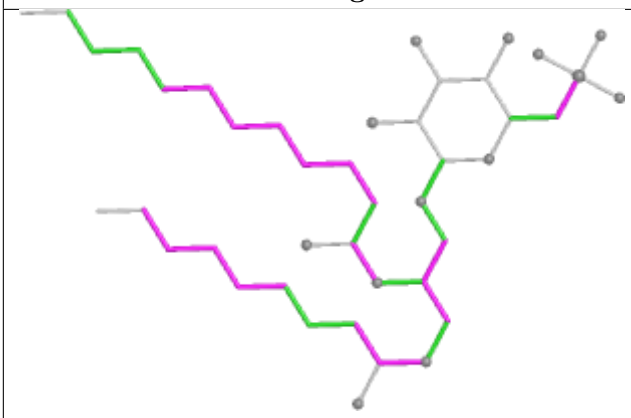


Bond angles



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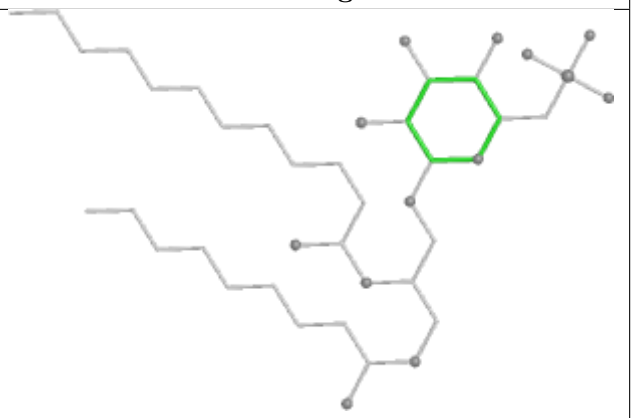

Rings

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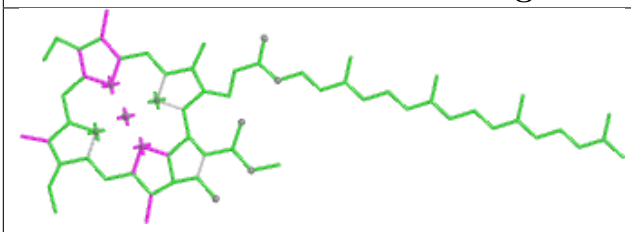

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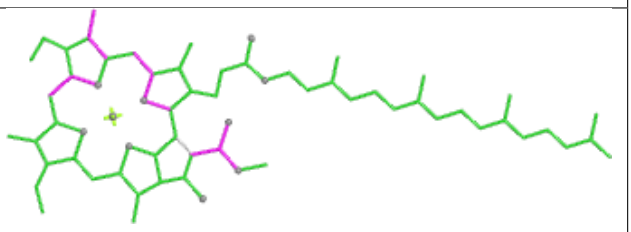
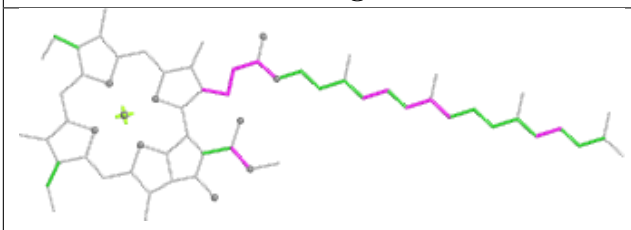


Bond angles



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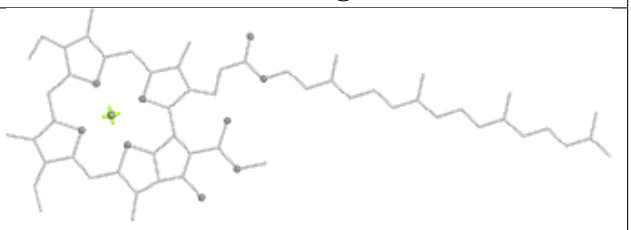
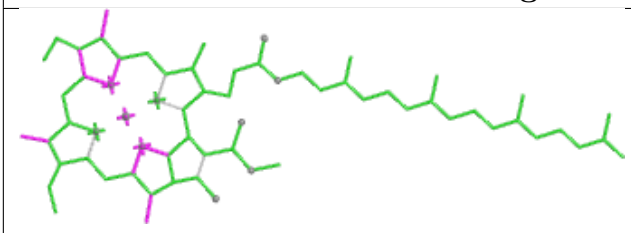


Rings

Ligand CLA e 1119



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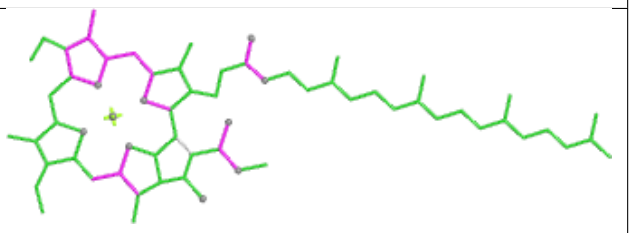
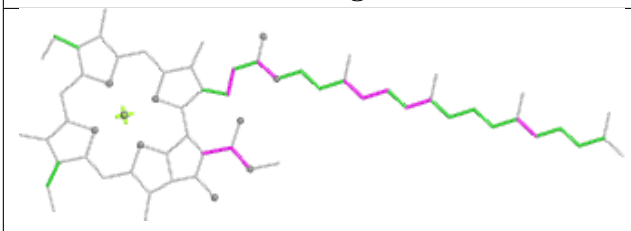


Bond angles



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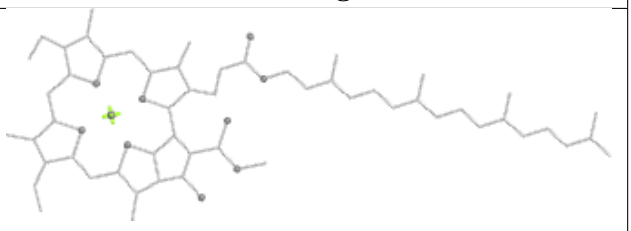
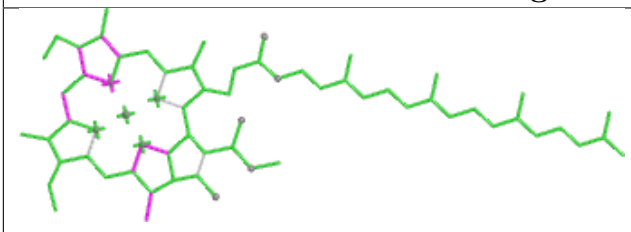


Rings

Ligand CLA t 505



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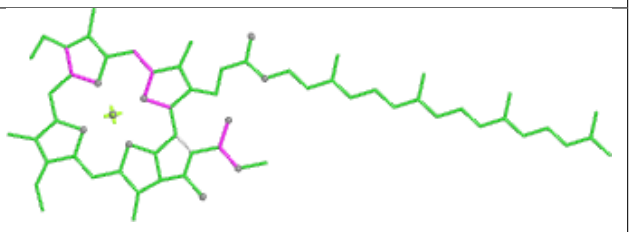
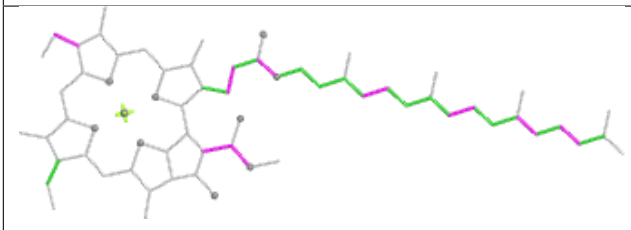
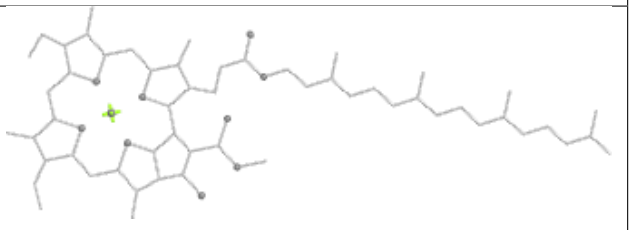


Bond angles

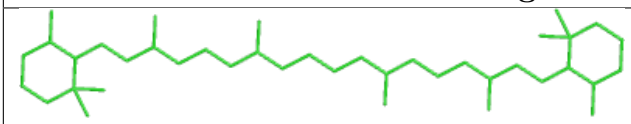


Torsions



Rings

Ligand BCR e 4011



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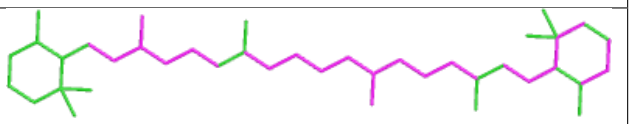

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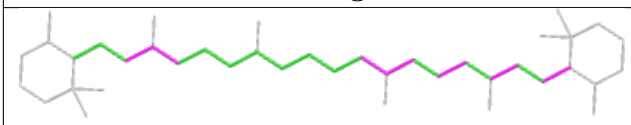

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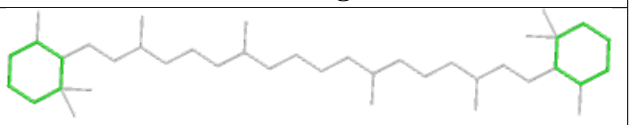
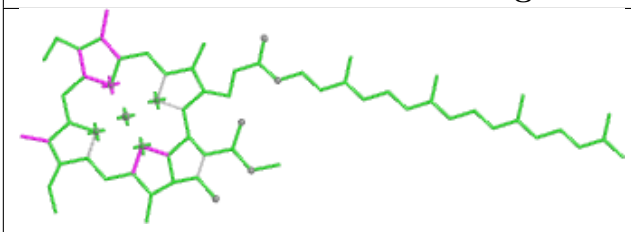


Rings

Ligand CLA A 1137



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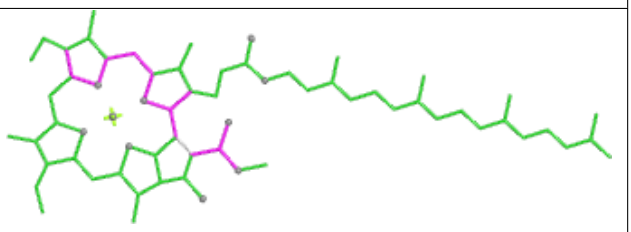

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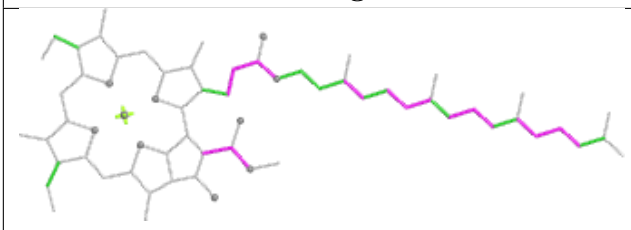

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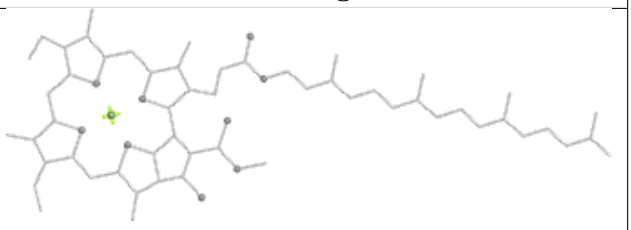
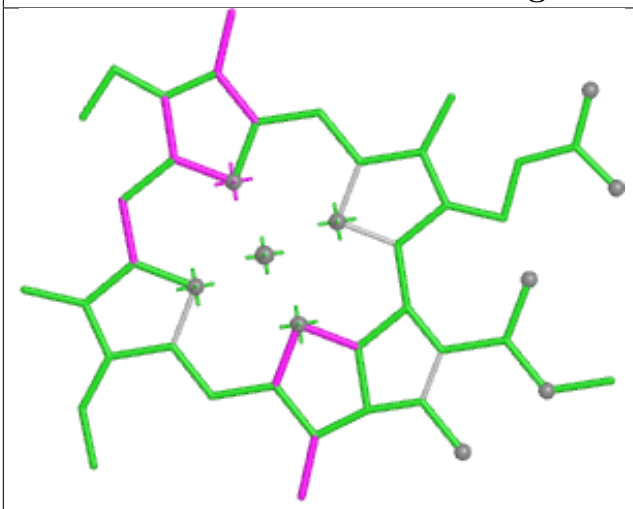


Rings

Ligand CLA 6 510



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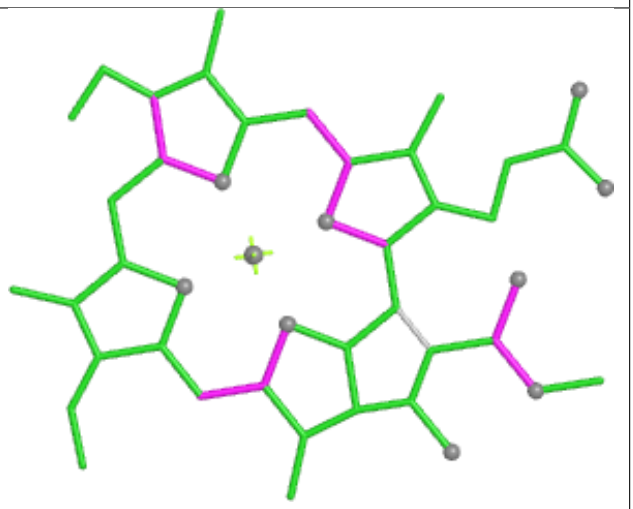

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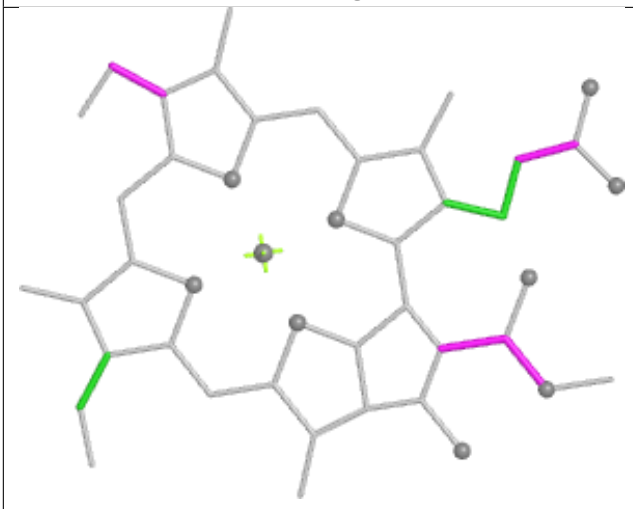
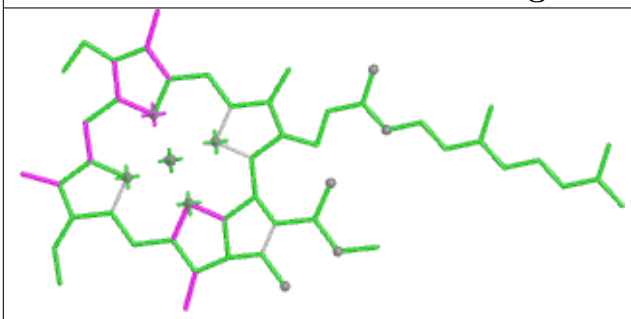


Torsions

Rings

Ligand CLA a 519



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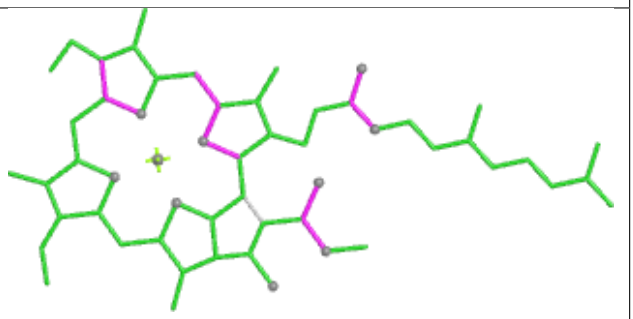

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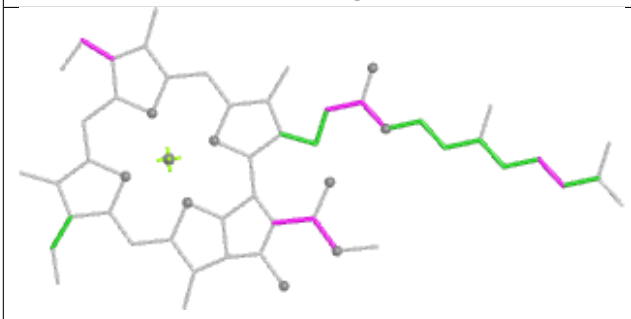

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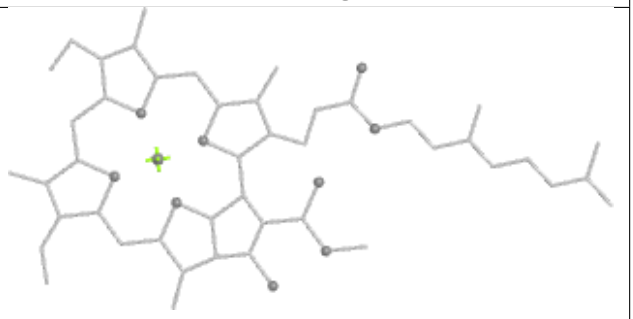
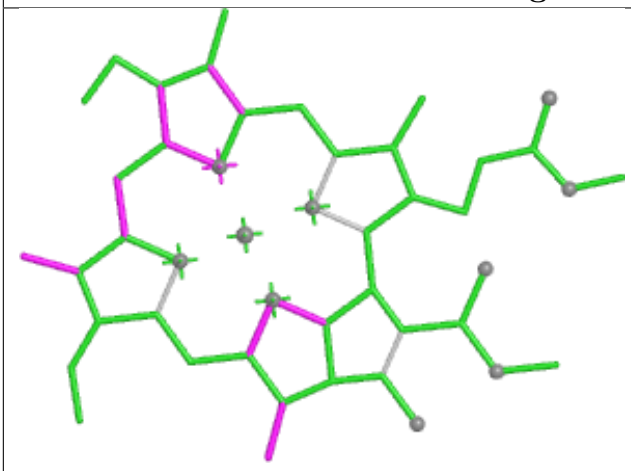


Rings

Ligand CLA c 519



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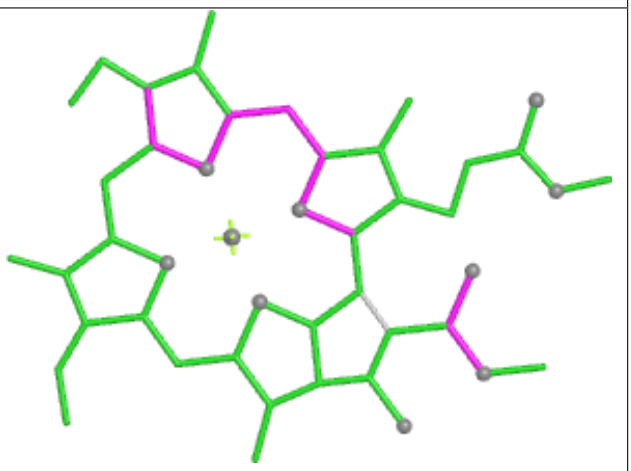

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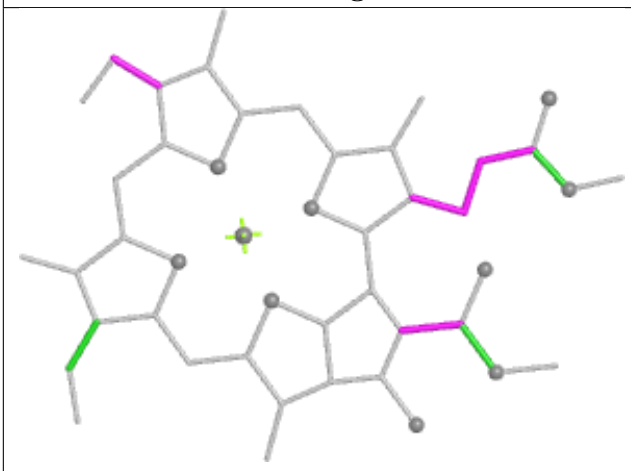

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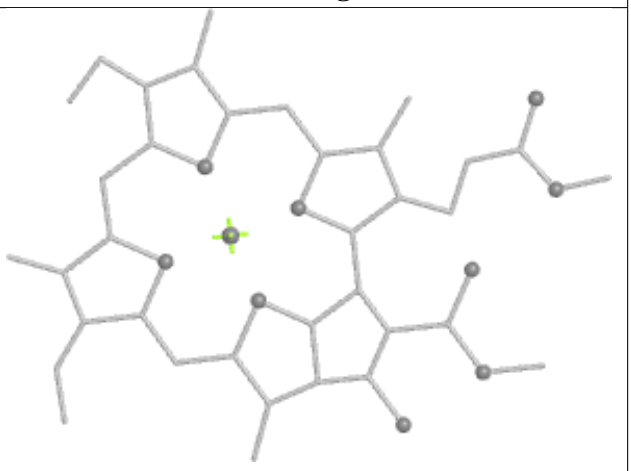
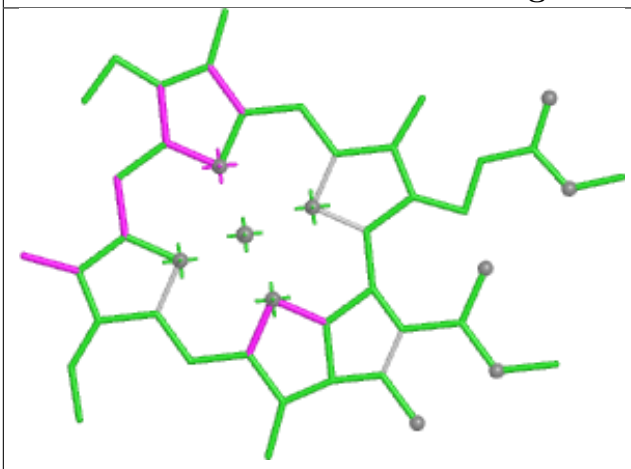


Rings

Ligand CLA 6 519



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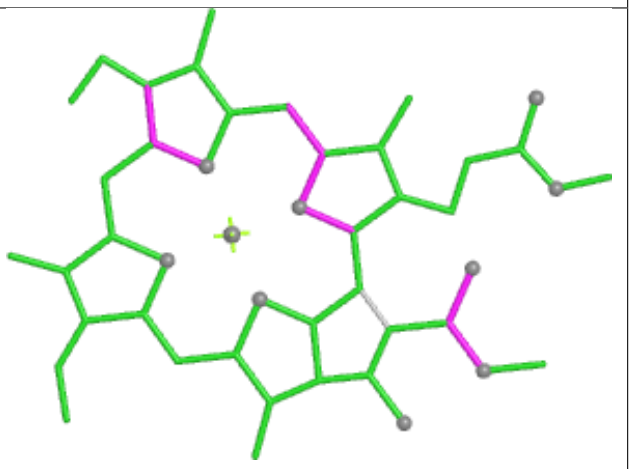

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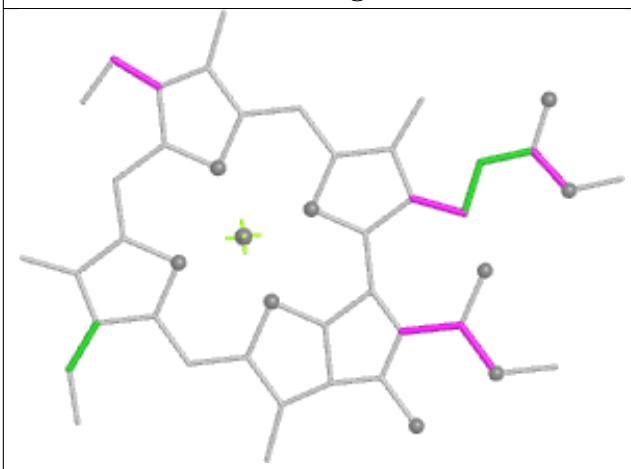

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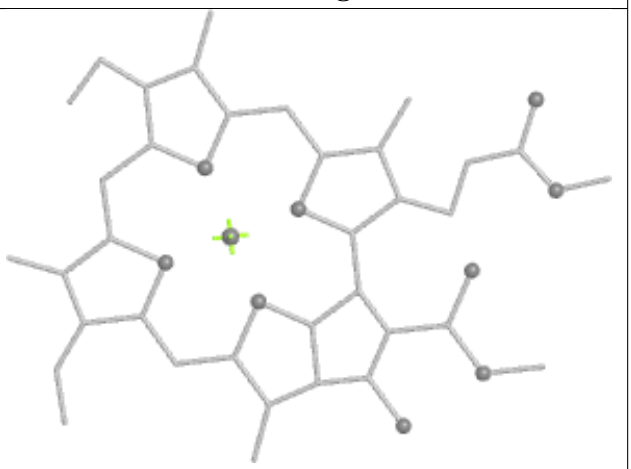
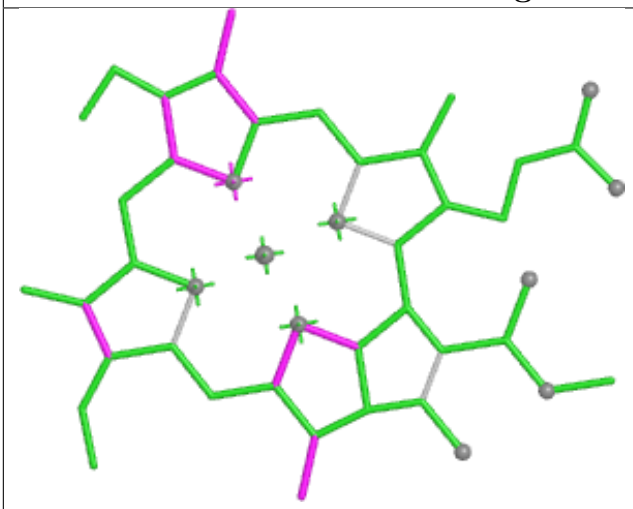


Rings

Ligand CLA U 1105



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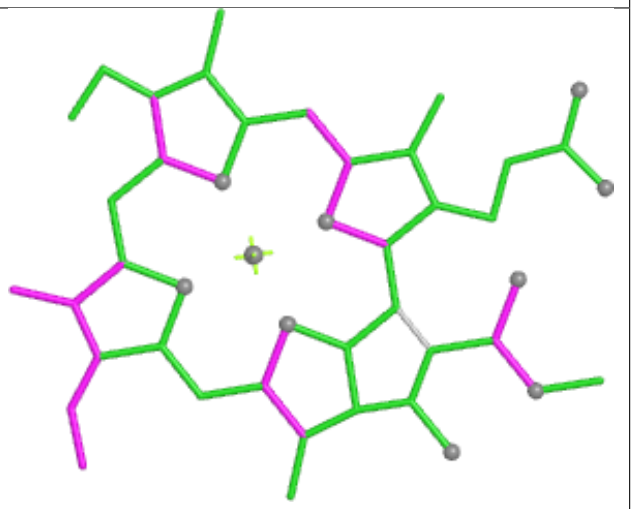

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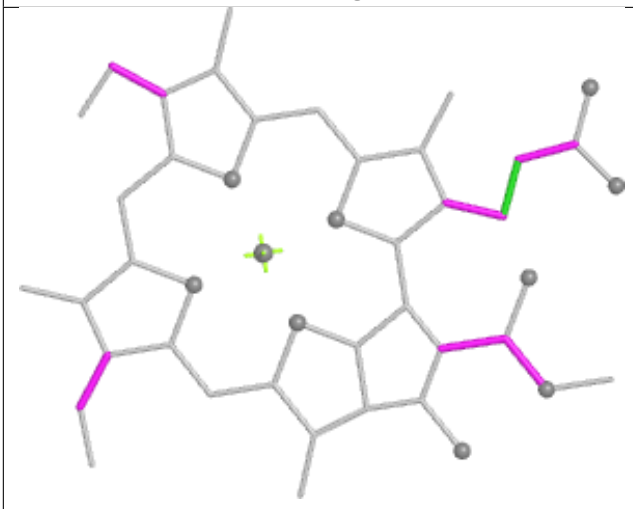
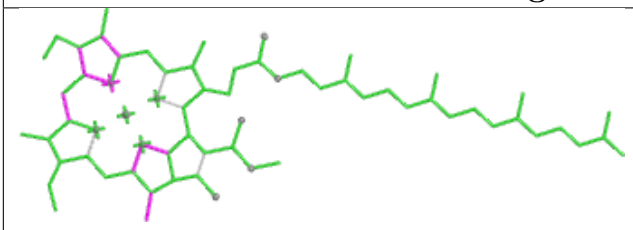


Torsions

Rings

Ligand CLA 4 505



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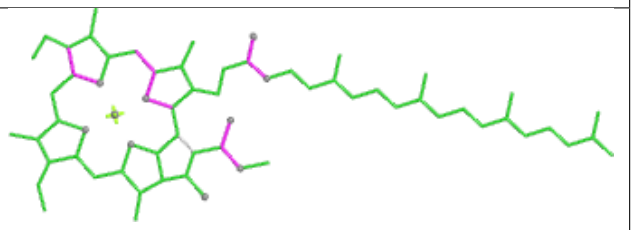

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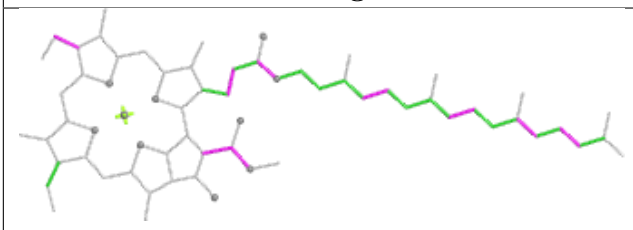

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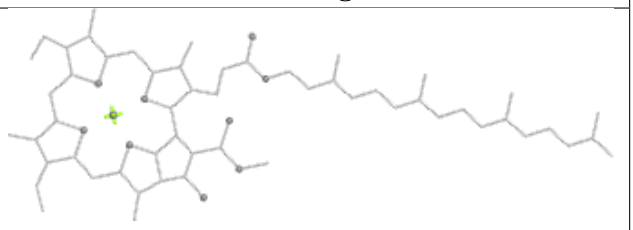
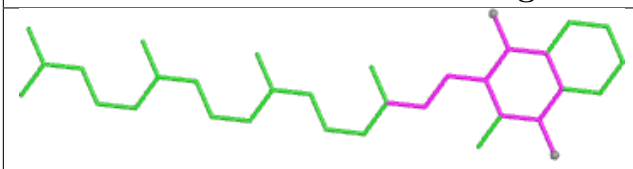


Rings

Ligand PQN e 2001



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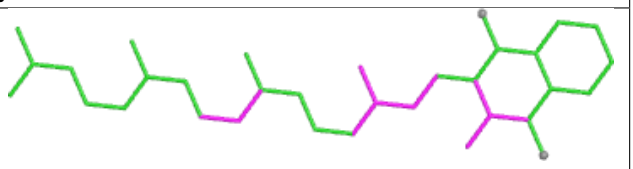

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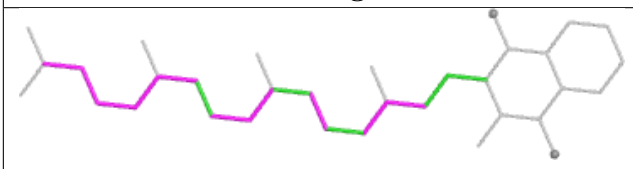

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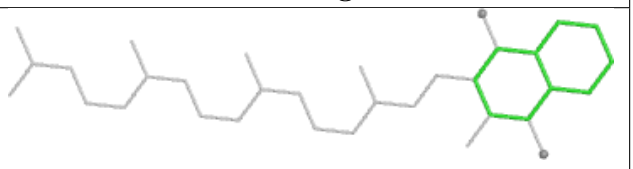
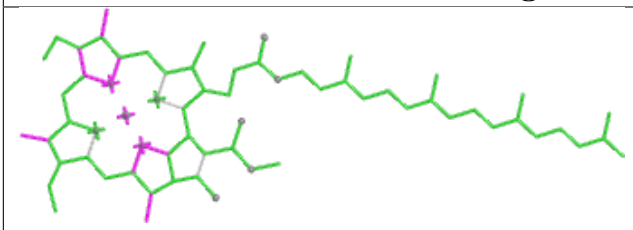


Rings

Ligand CLA e 1128



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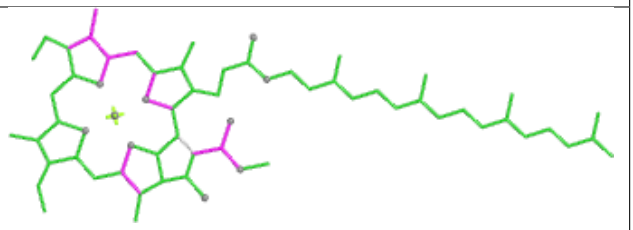

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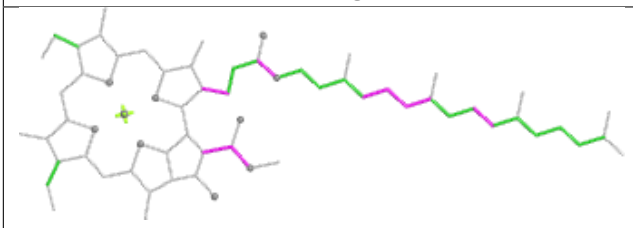

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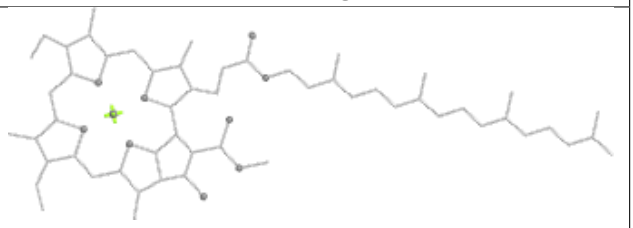
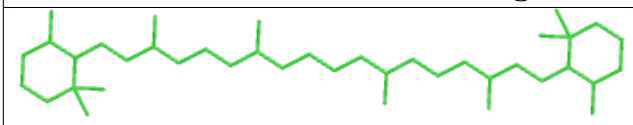


Rings

Ligand BCR H 4005



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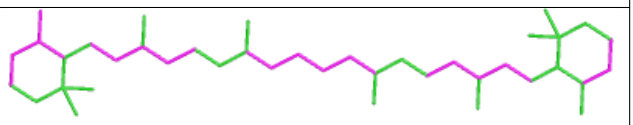
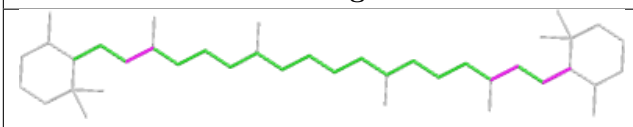


Bond angles



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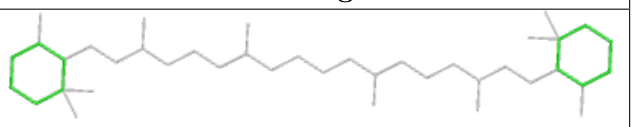
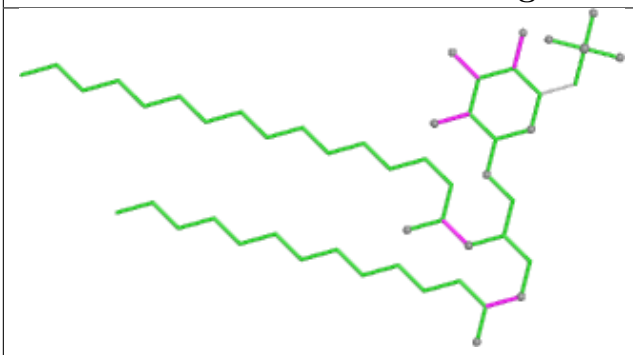


Rings

Ligand SQD n 5216



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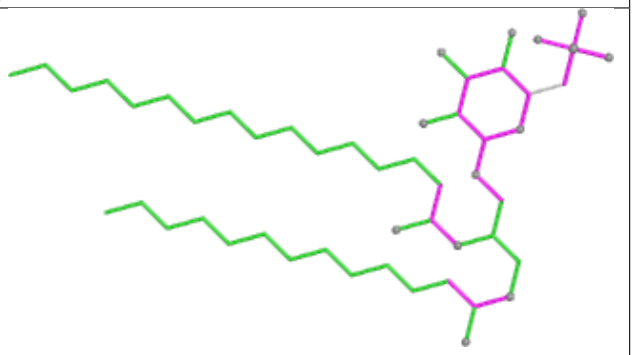
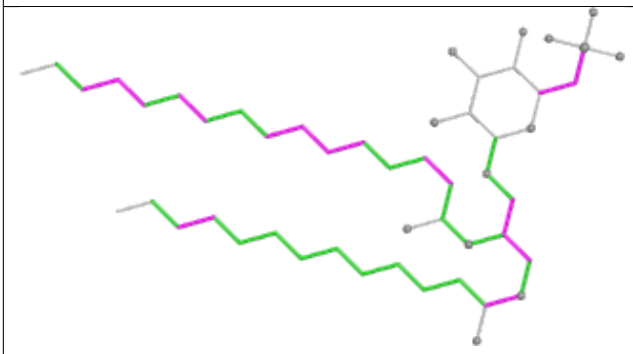


Bond angles



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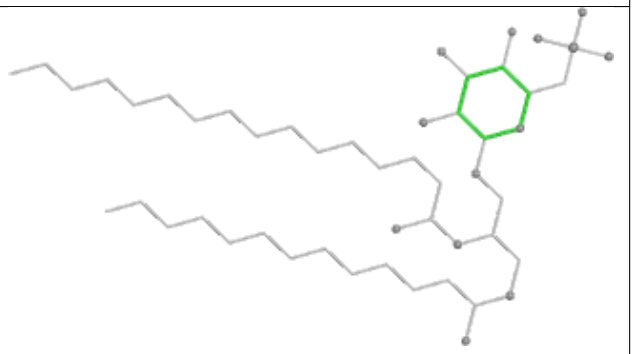
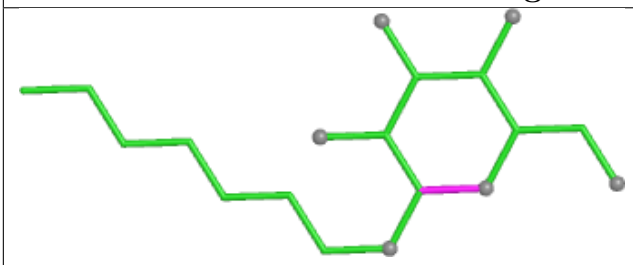


Rings

Ligand LMU 1 902



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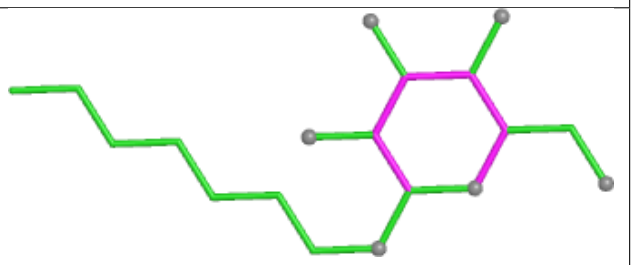
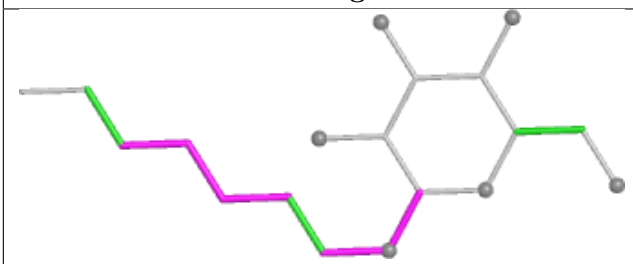


Bond angles



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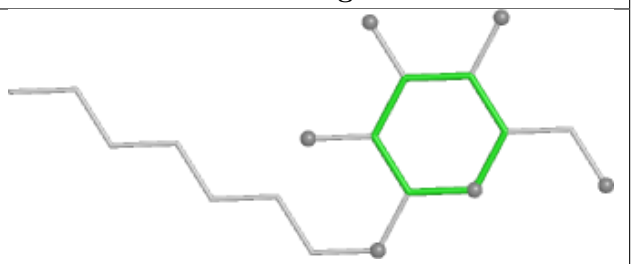
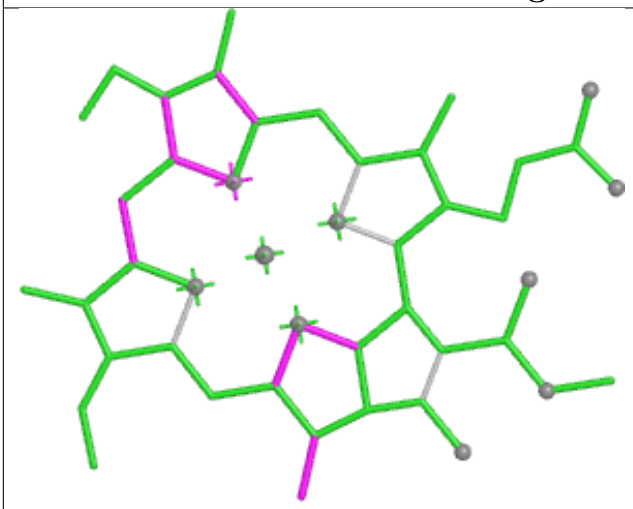
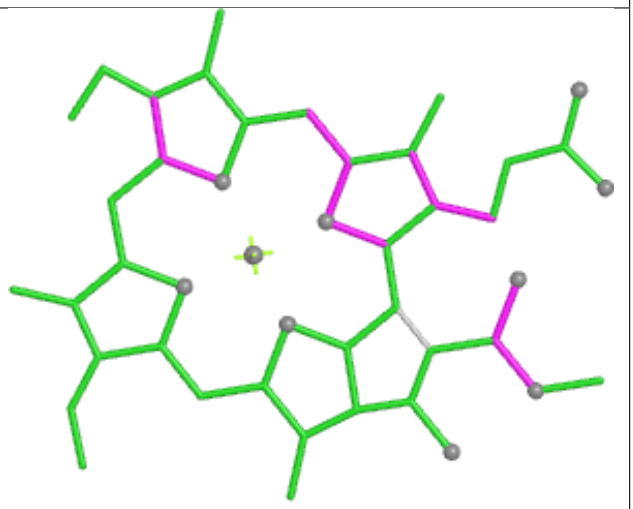


Rings

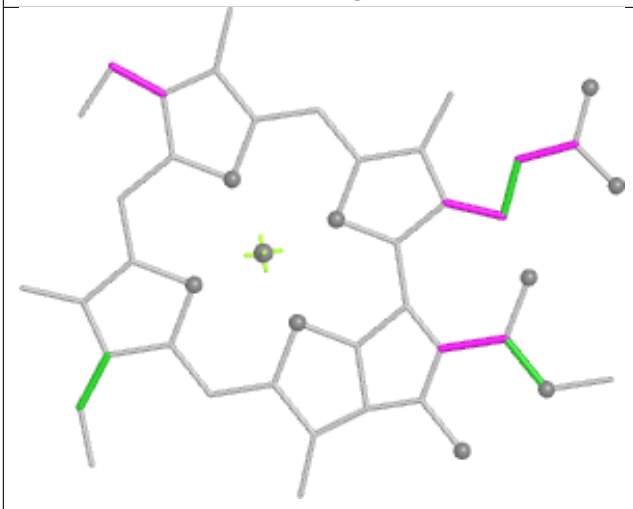
Ligand CLA 4 516



Bond lengths



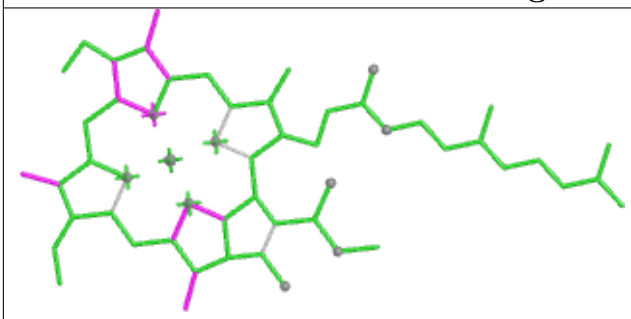
Bond angles



Torsions

Rings

Ligand CLA a 508



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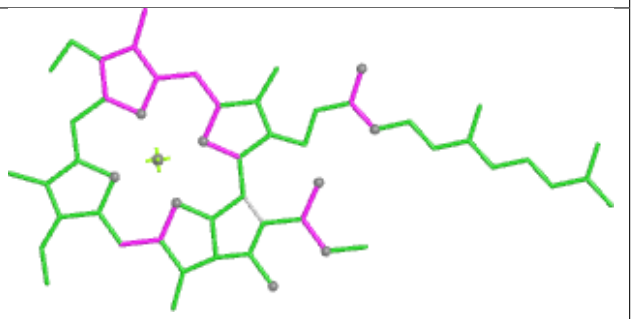

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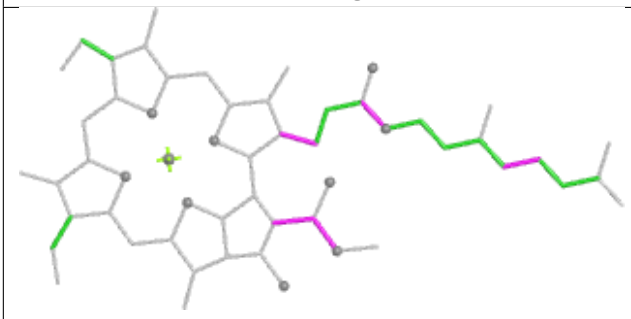
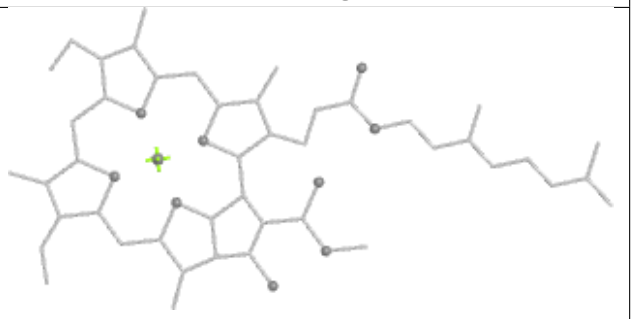
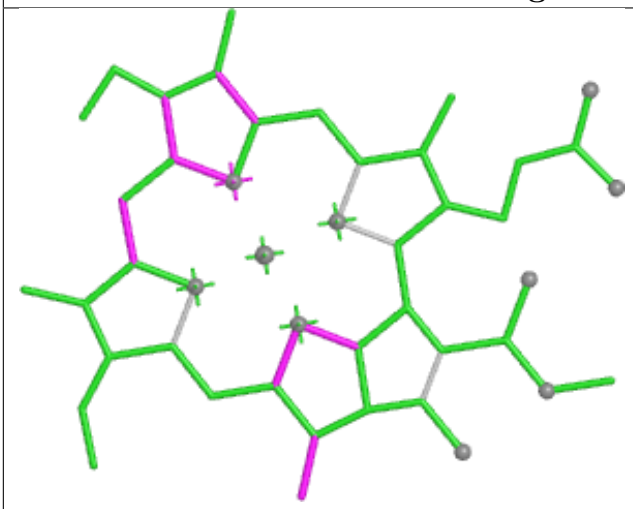


Torsions



Rings

Ligand CLA a 516



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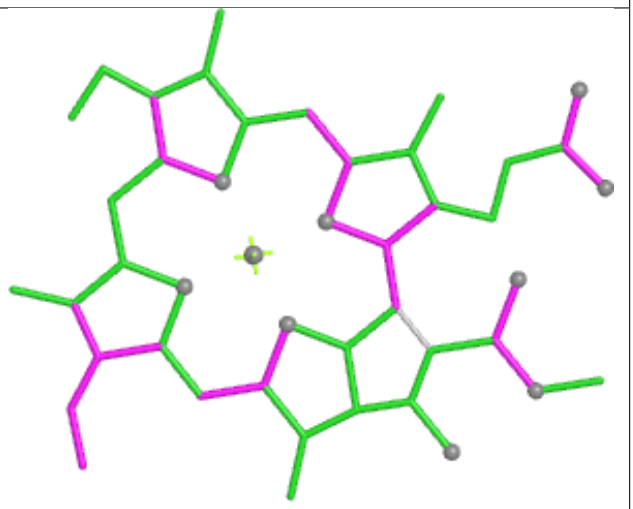
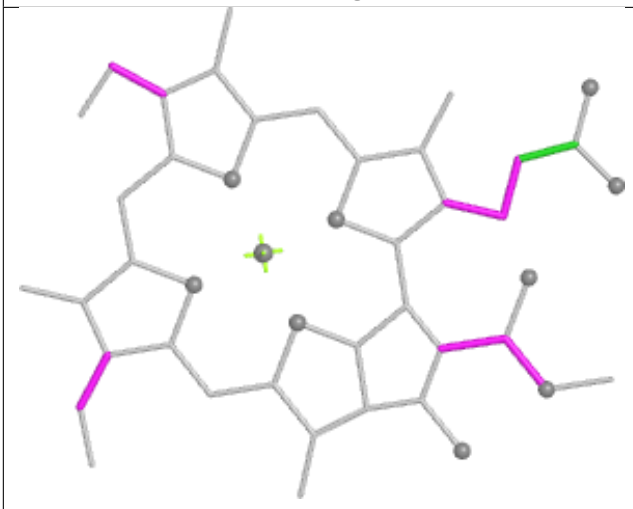


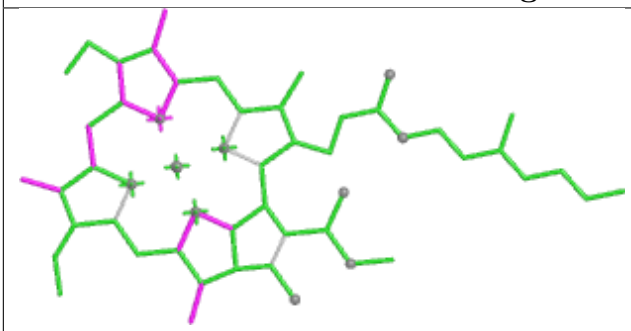
Bond angles



Torsions

Rings

Ligand CLA e 1120



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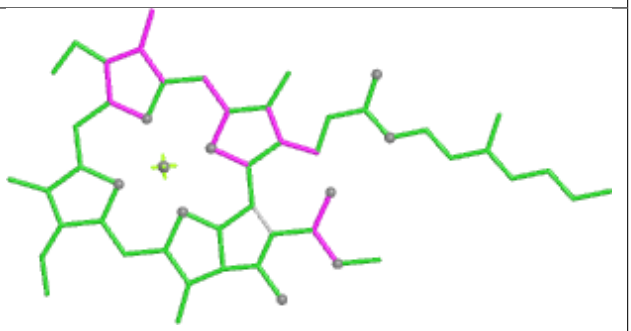
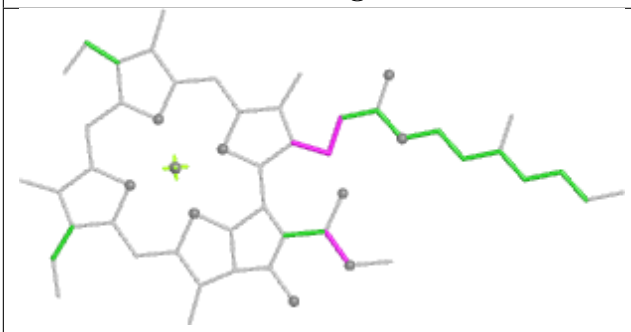
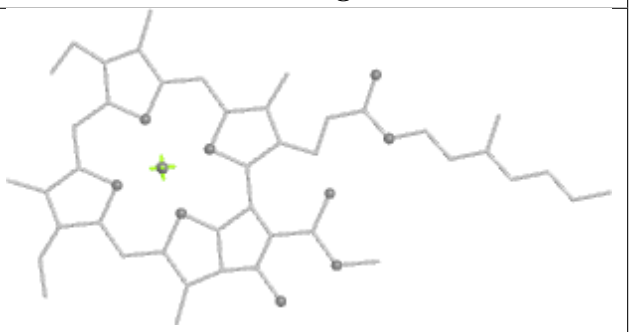


Bond angles



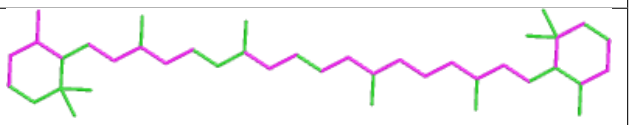
Torsions



Rings

Ligand BCR Z 521

Bond lengths



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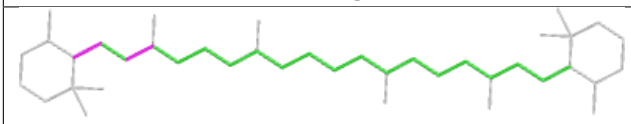

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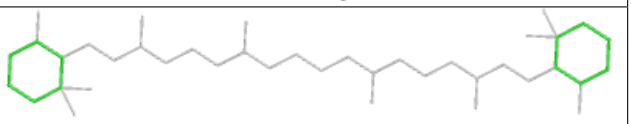
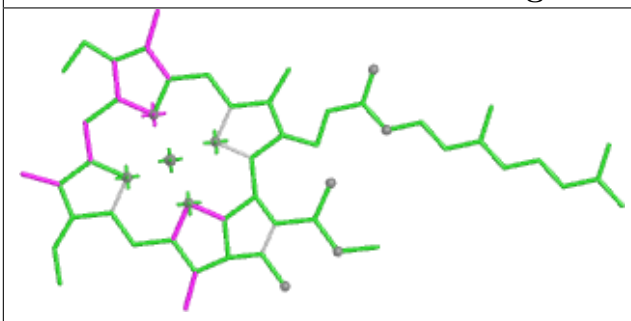


Rings

Ligand CLA Z 508



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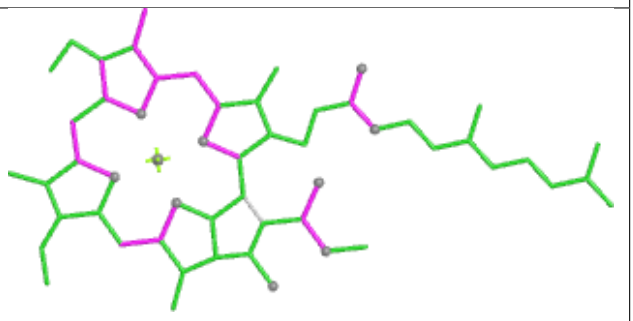

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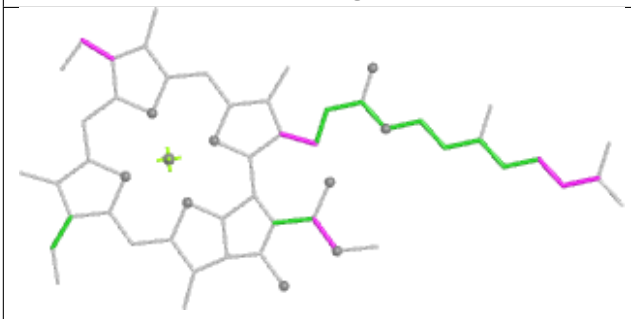

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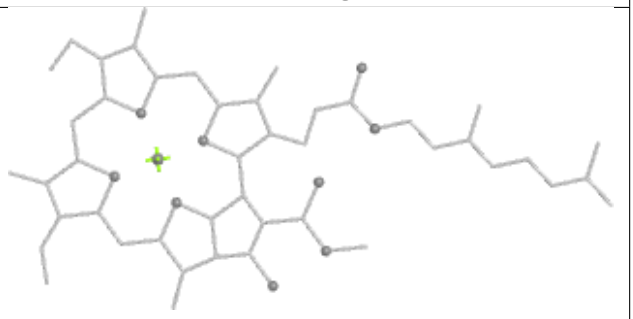
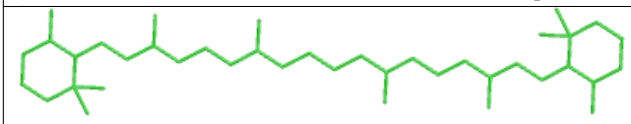


Rings

Ligand BCR t 523



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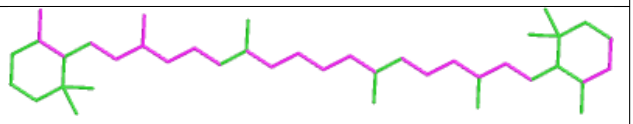
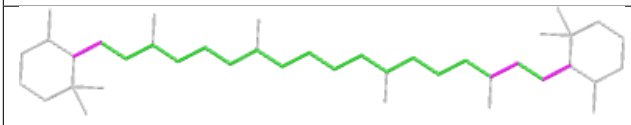


Bond angles



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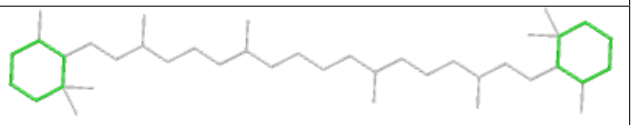
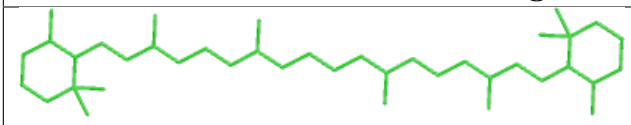


Rings

Ligand BCR r 522



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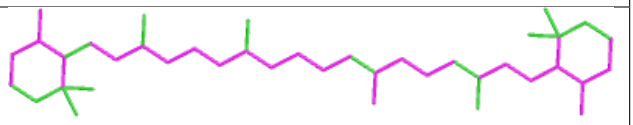

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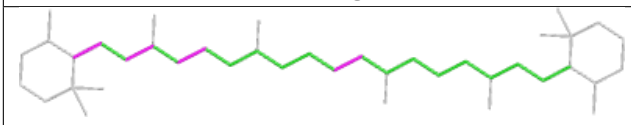

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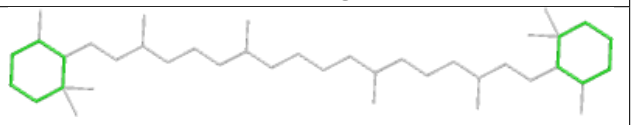
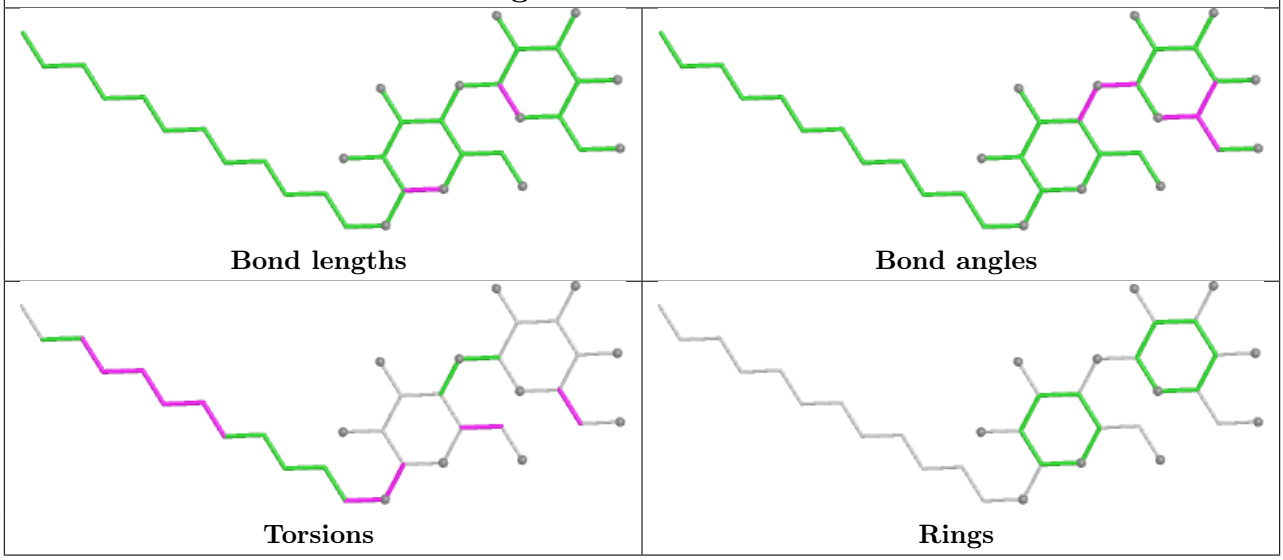
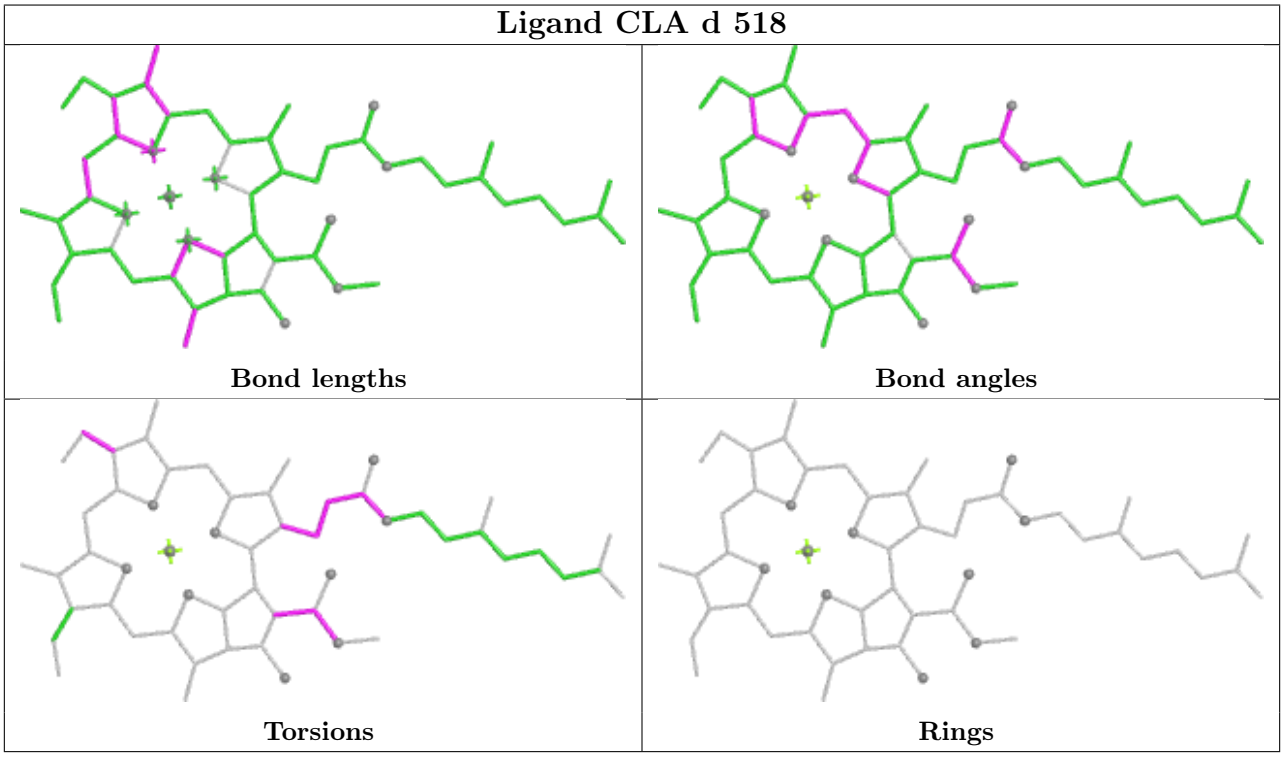


Rings

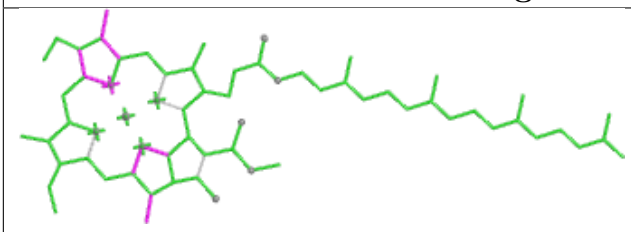
Ligand LMU H 1843



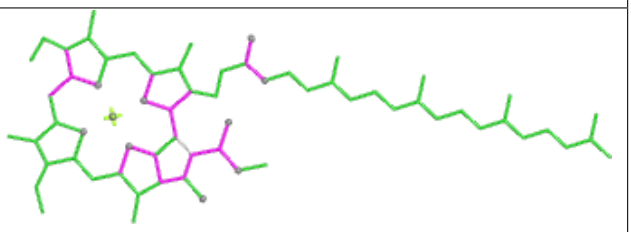
Ligand CLA d 518



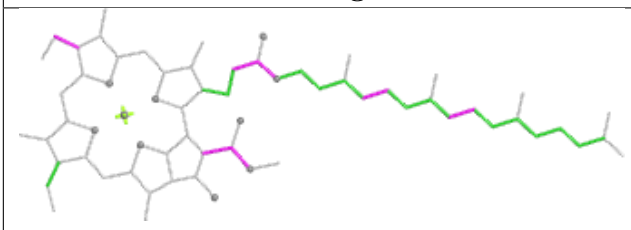
Ligand CLA A 1011



Bond lengths



Bond angles



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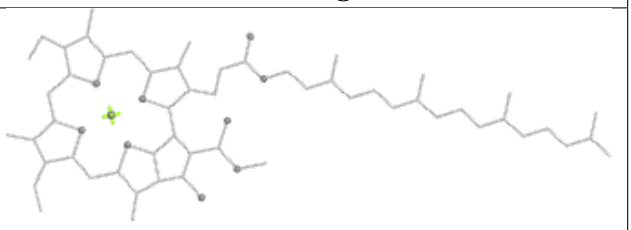
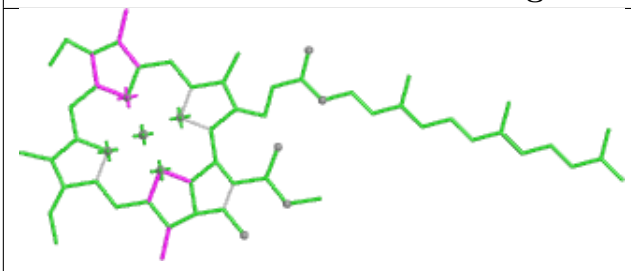


Rings

Ligand CLA Z 502



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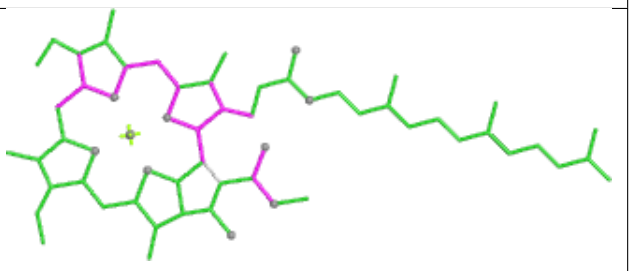

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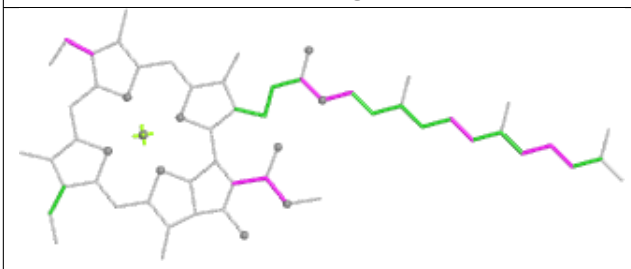

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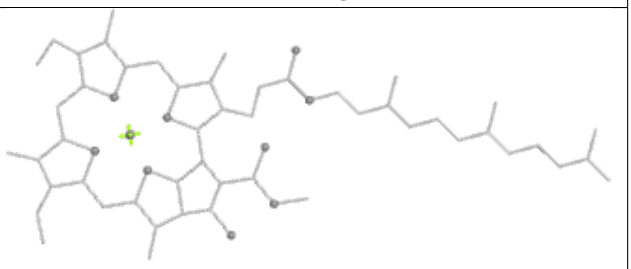
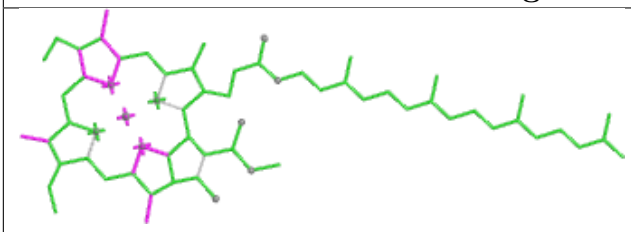


Rings

Ligand CLA f 1215



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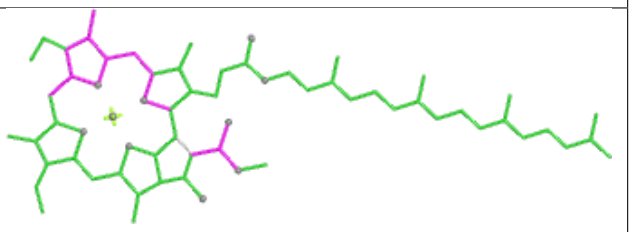
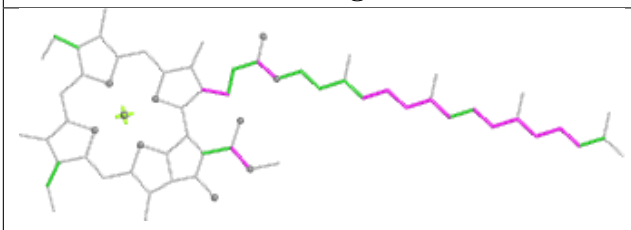


Bond angles



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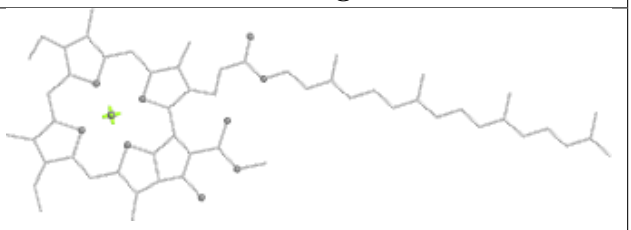
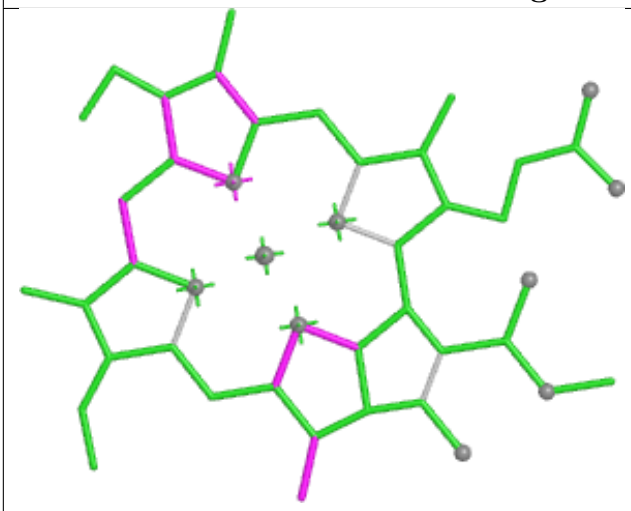


Rings

Ligand CLA t 516



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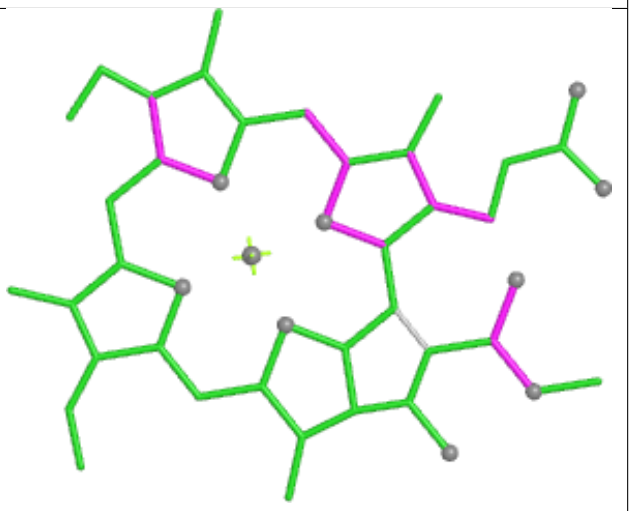
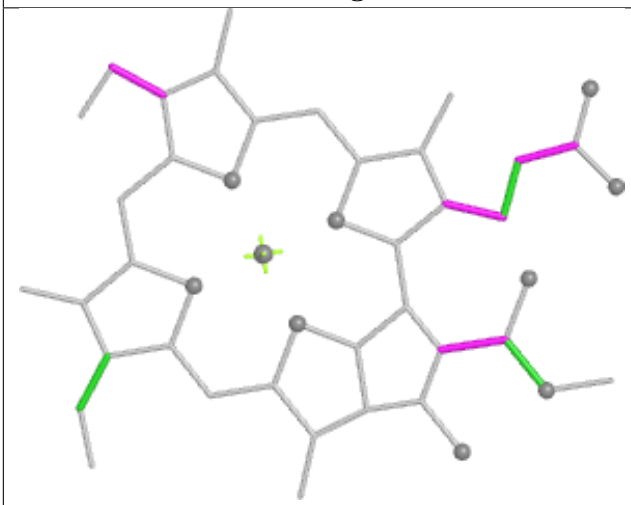
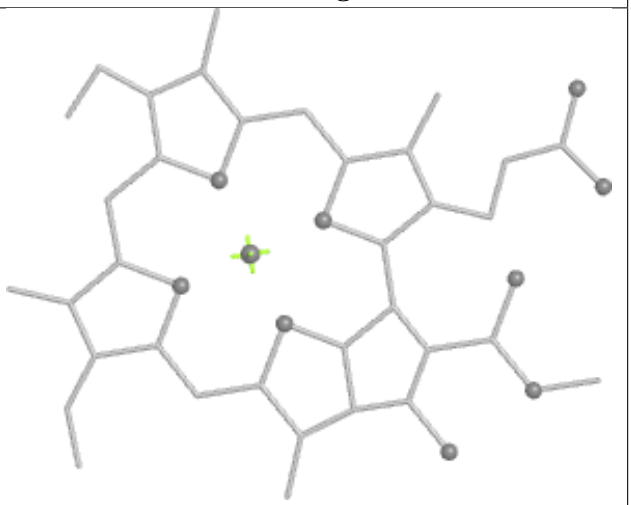


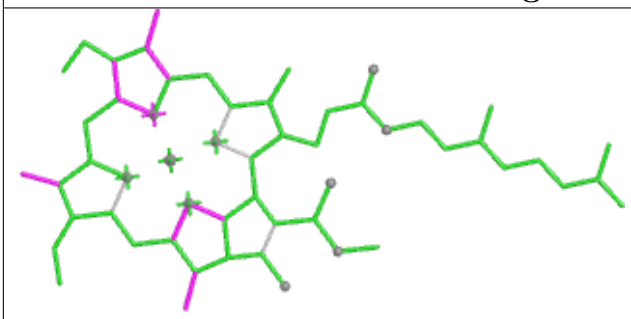
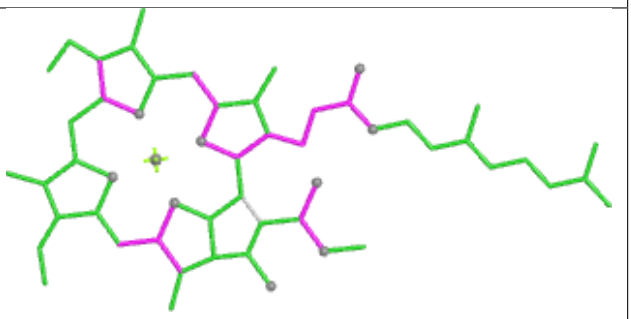
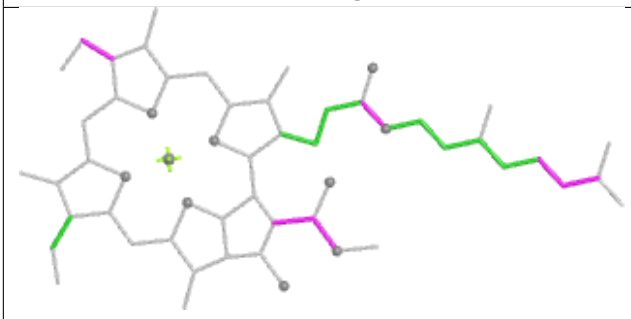
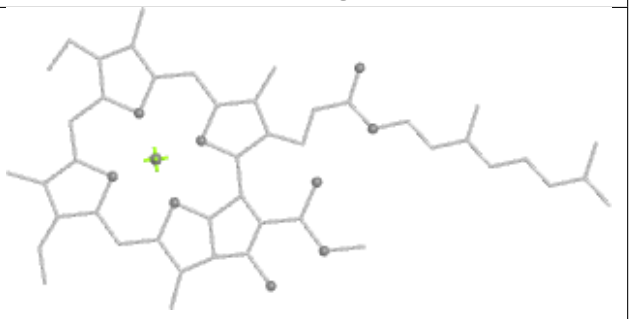
Bond angles

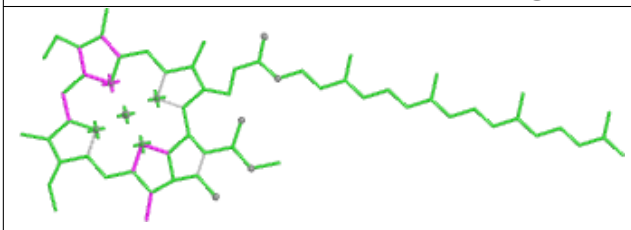
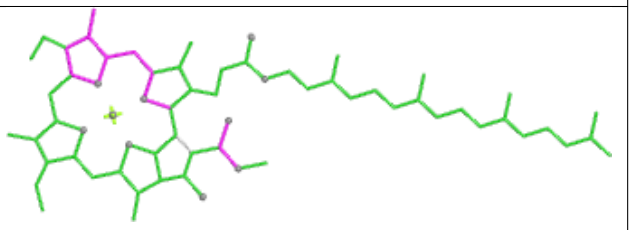
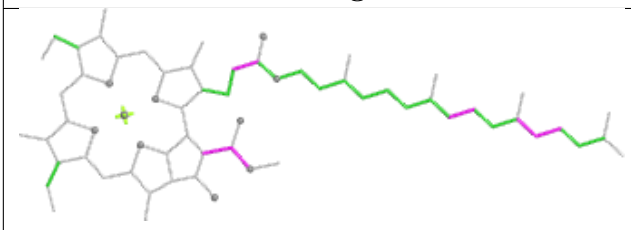
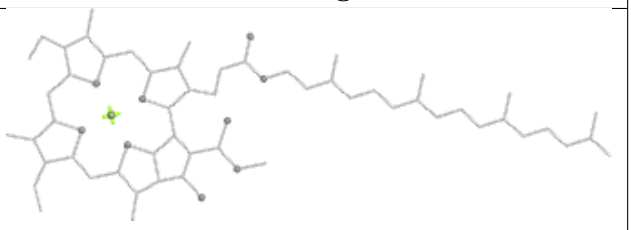


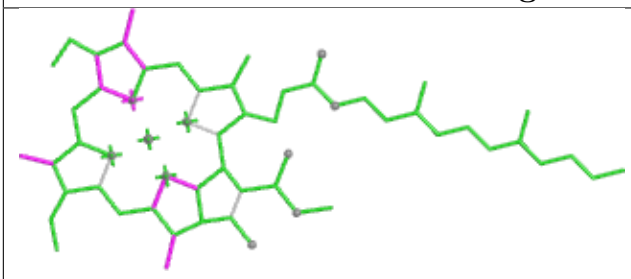
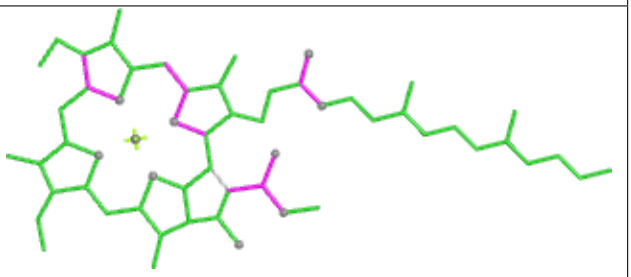
Torsions



Rings

Ligand CLA f 1220	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA J 1302	
	
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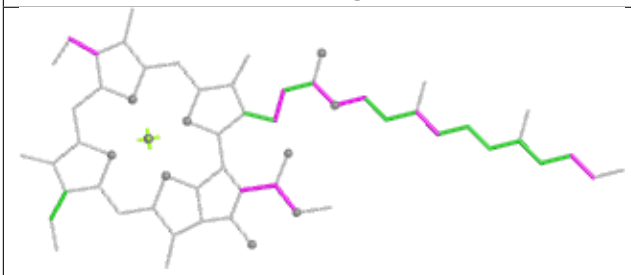	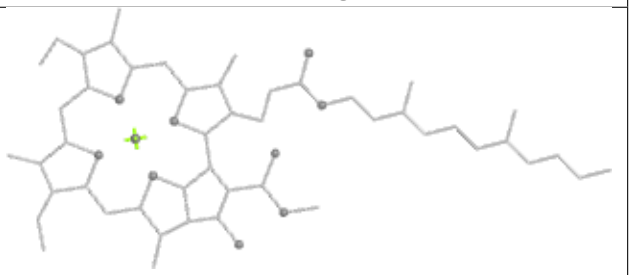
Torsions	Rings

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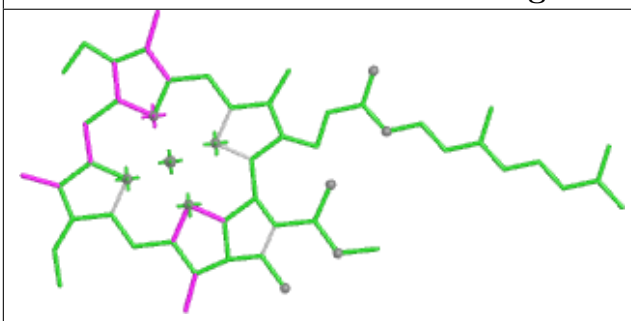
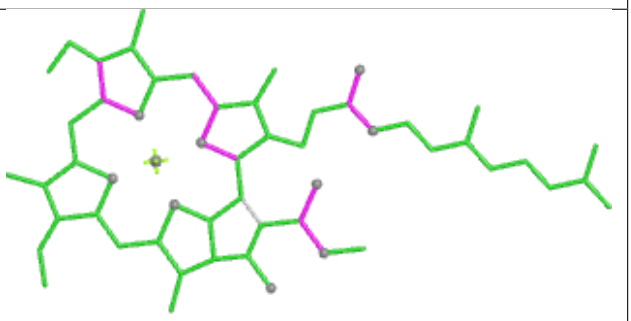
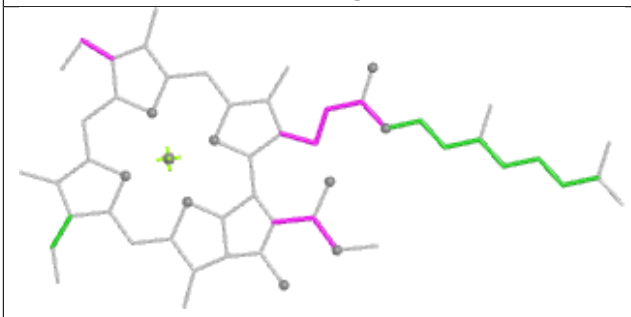
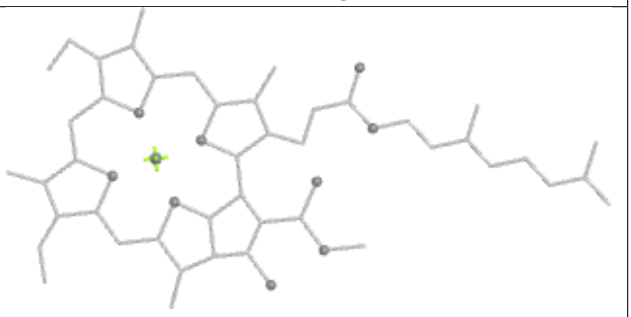
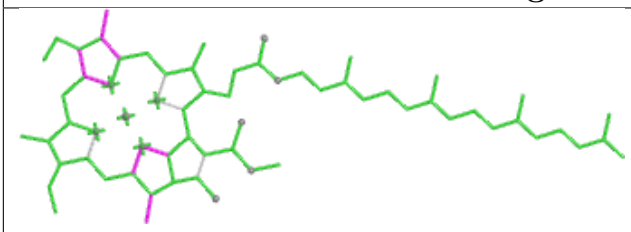
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 509



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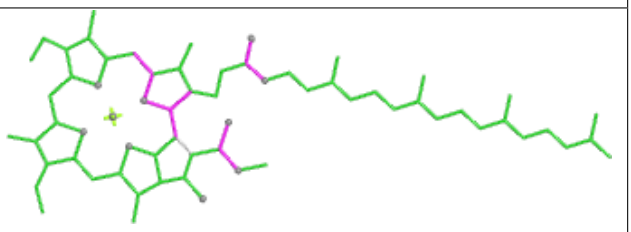

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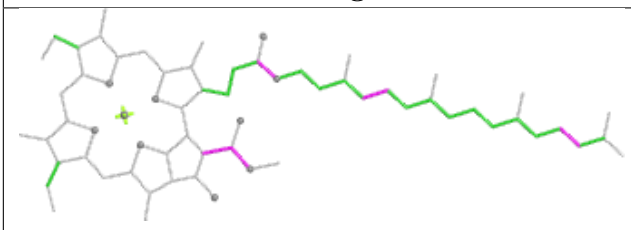
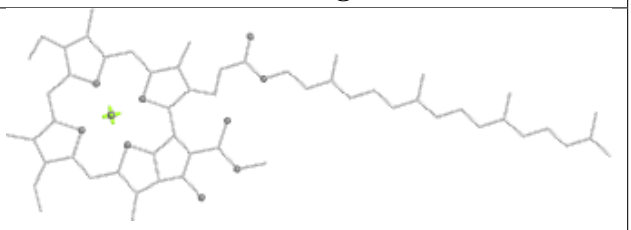
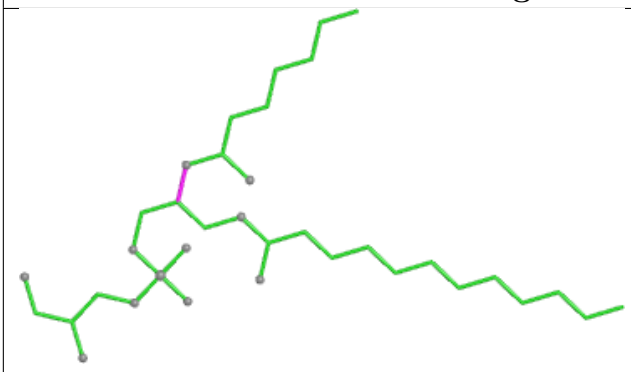


Torsions



Rings

Ligand LHG A 5004



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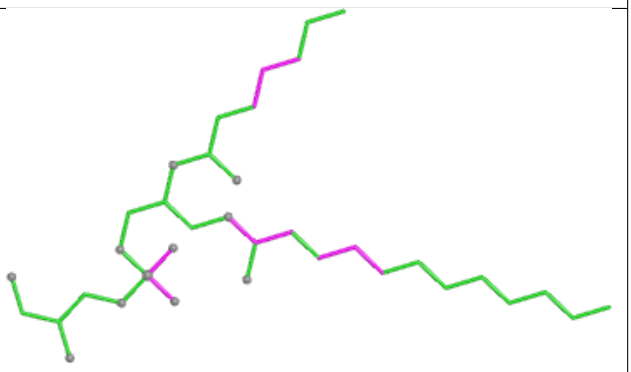
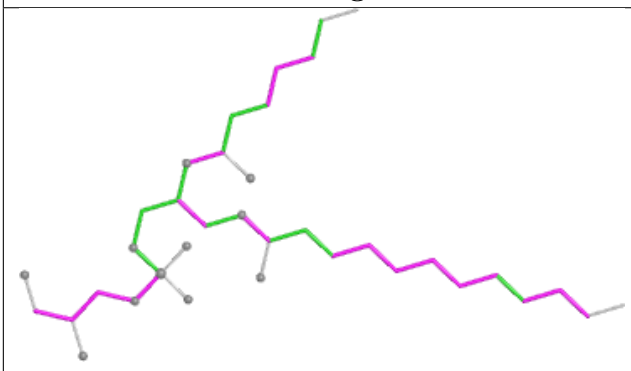


Bond angles



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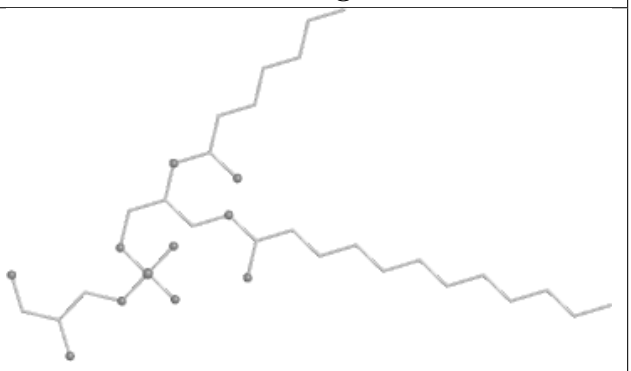
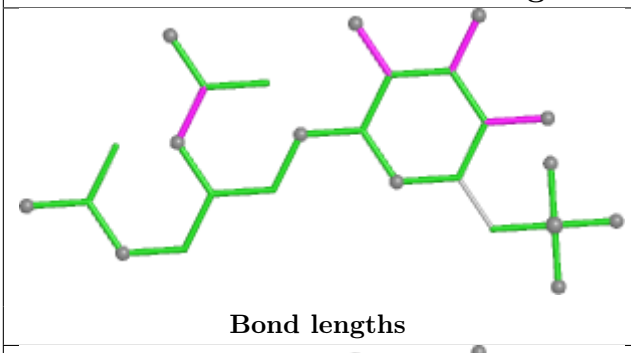


Rings

Ligand SQD b 822



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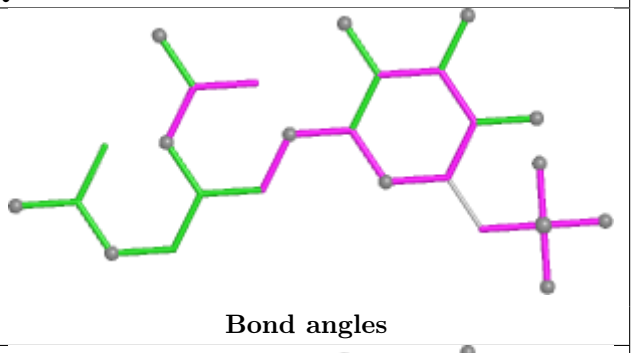

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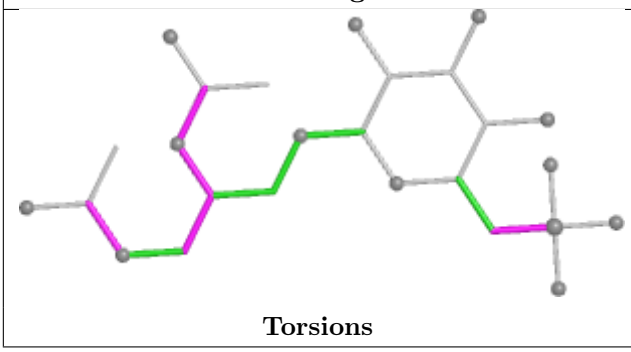

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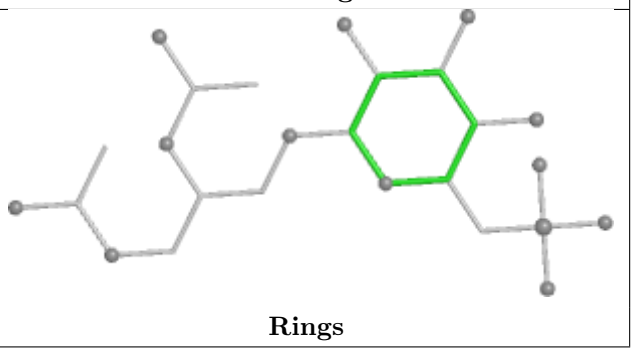
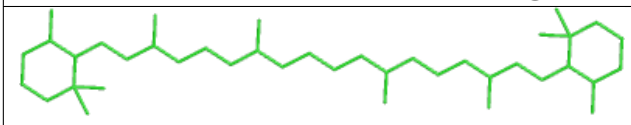


Rings

Ligand BCR 6 522



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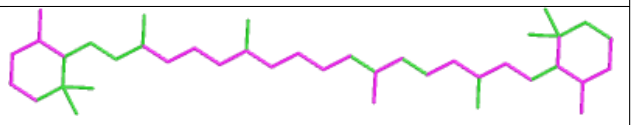
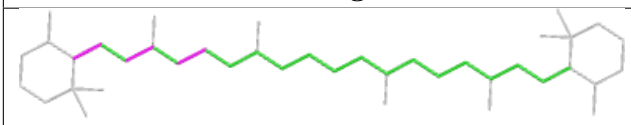


Bond angles



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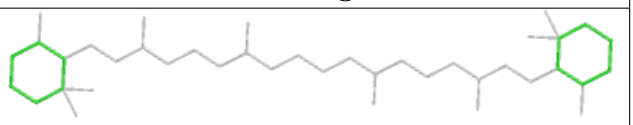
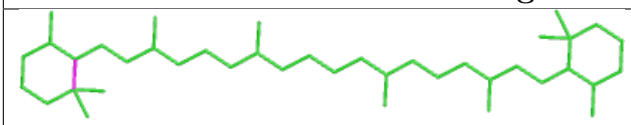


Rings

Ligand BCR k 4018



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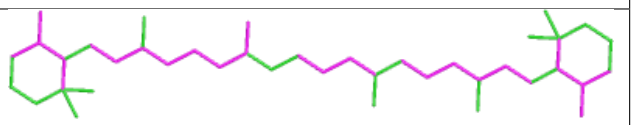

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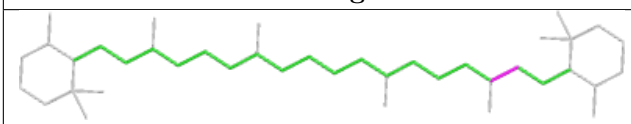

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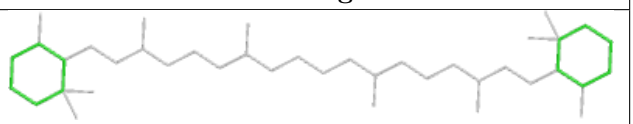
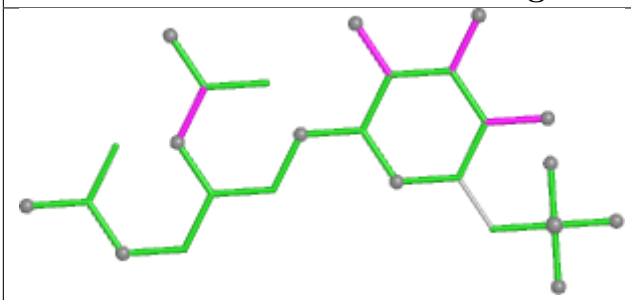


Rings

Ligand SQD v 822



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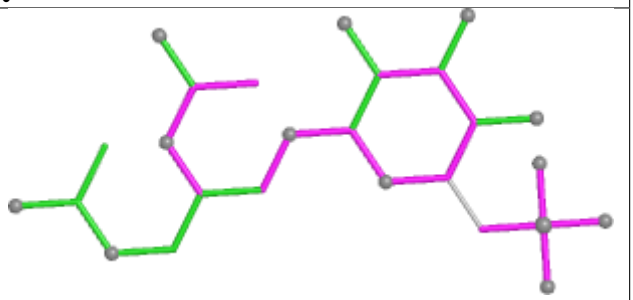

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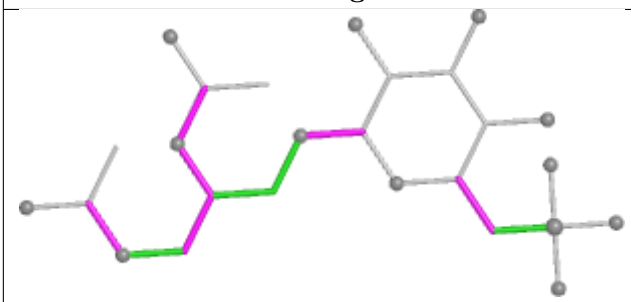

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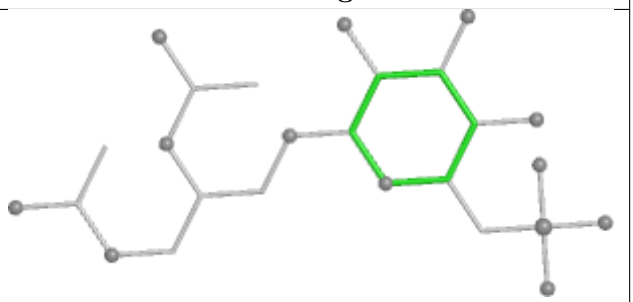
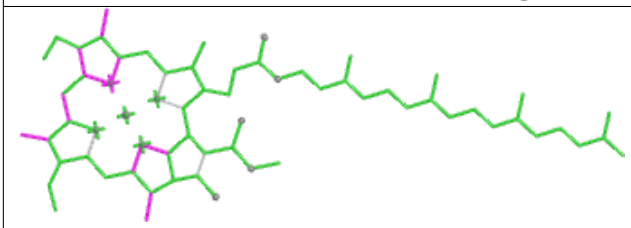


Rings

Ligand CLA B 1238



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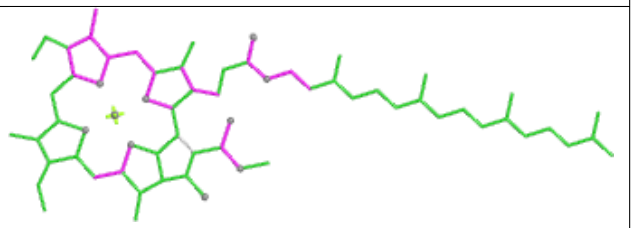

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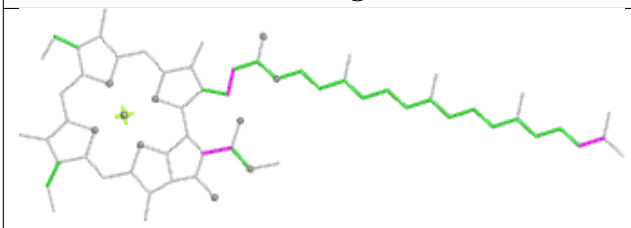

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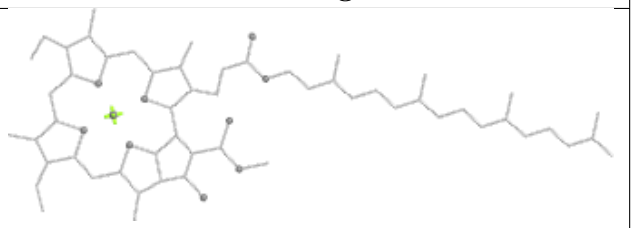
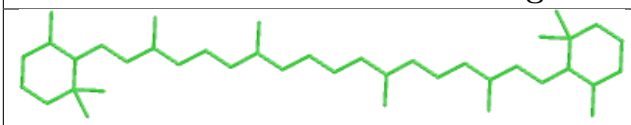


Rings

Ligand BCR 1 522



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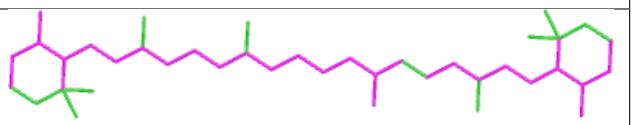
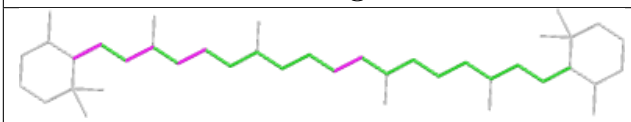


Bond angles



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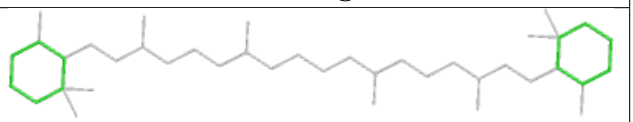
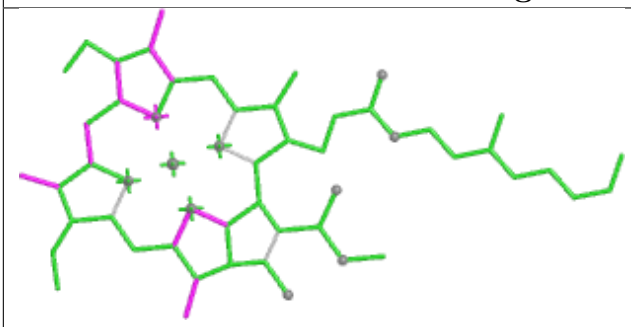


Rings

Ligand CLA A 1108



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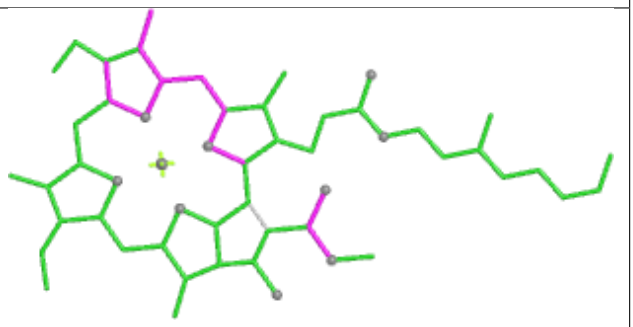
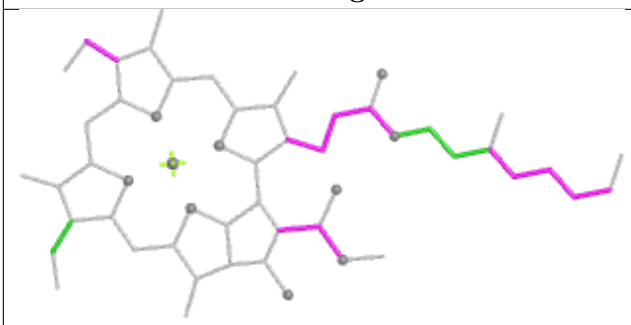


Bond angles



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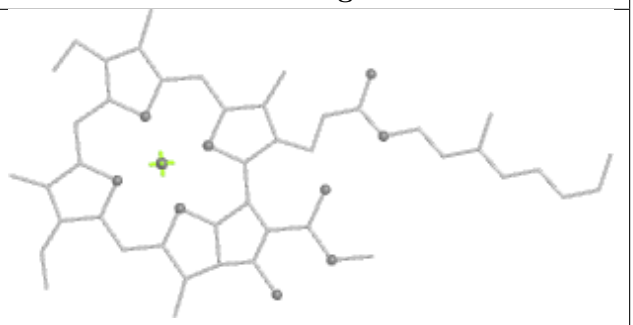
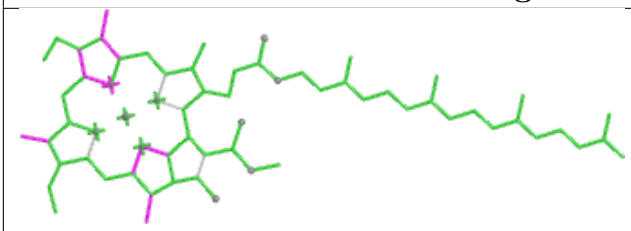


Rings

Ligand CLA H 1210



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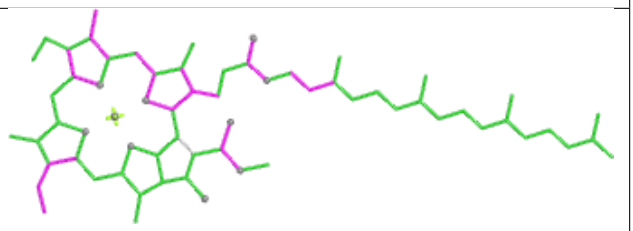
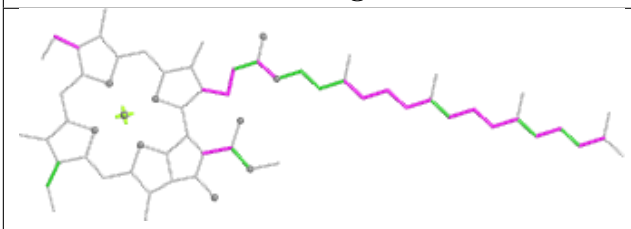
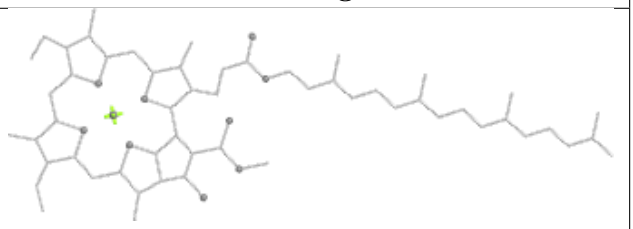


Bond angles

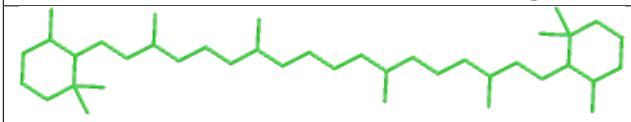


Torsions

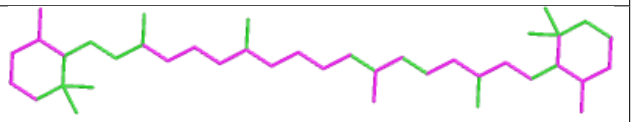


Rings

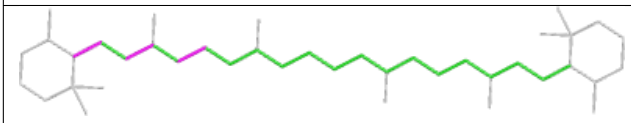
Ligand BCR d 522



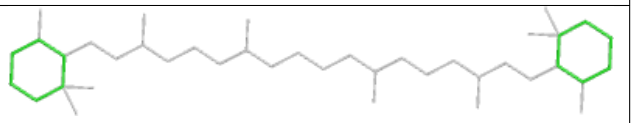
Bond lengths



Bond angles

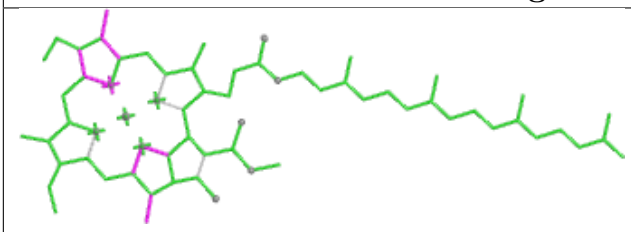


Torsions



Rings

Ligand CLA 3 507



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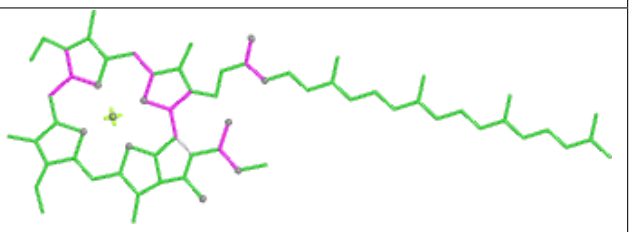

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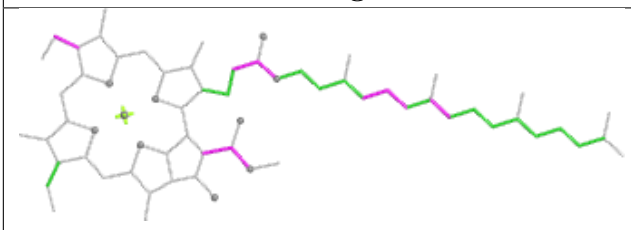

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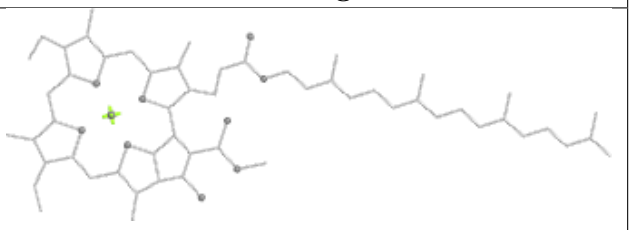
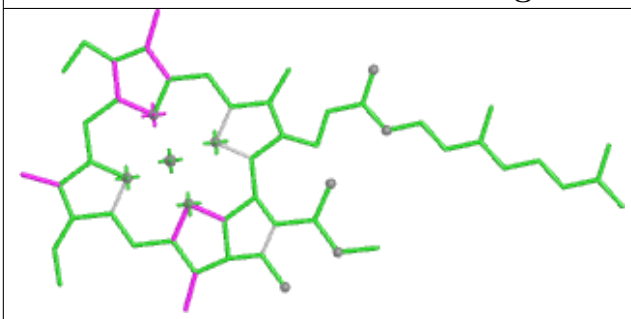


Rings

Ligand CLA H 1220



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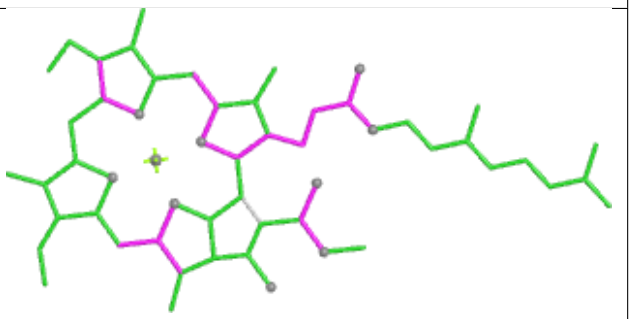

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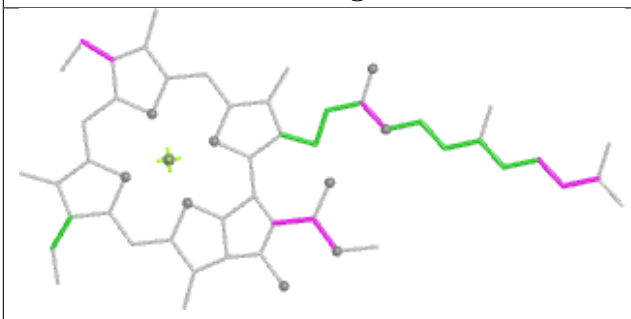

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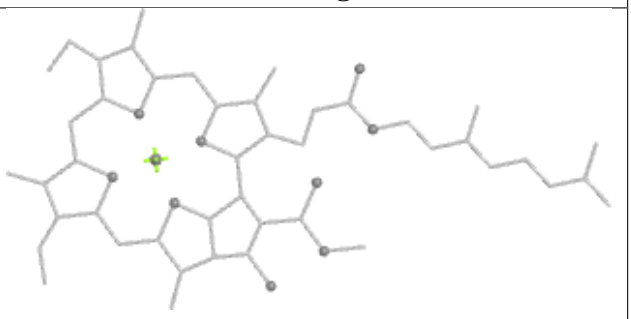
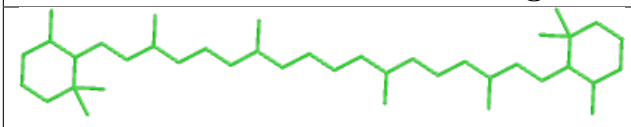


Rings

Ligand BCR u 524



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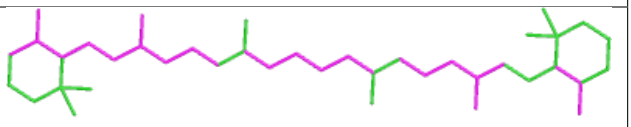

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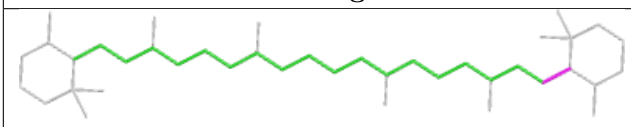

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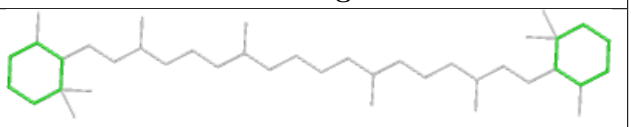
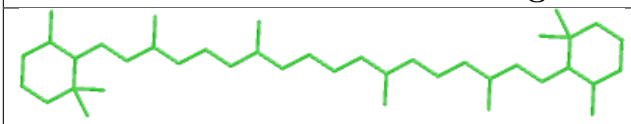
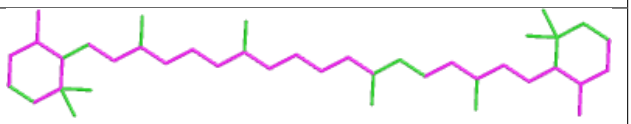
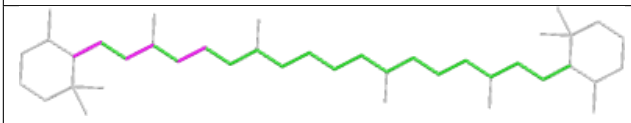
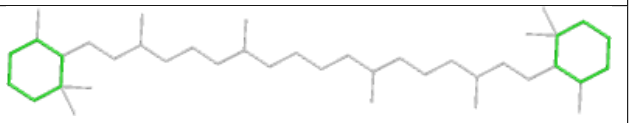


Rings

Ligand BCR s 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

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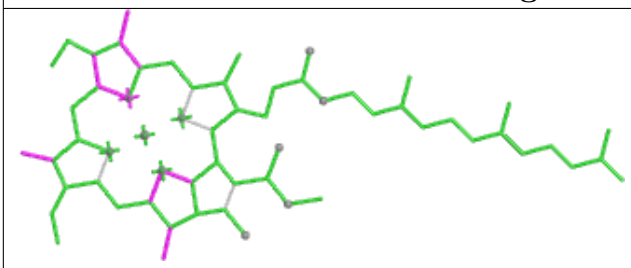
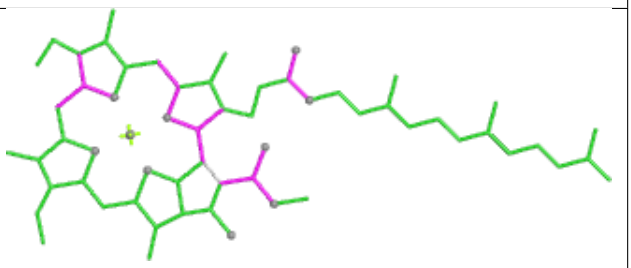
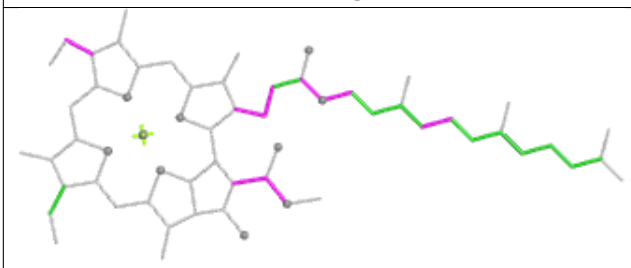
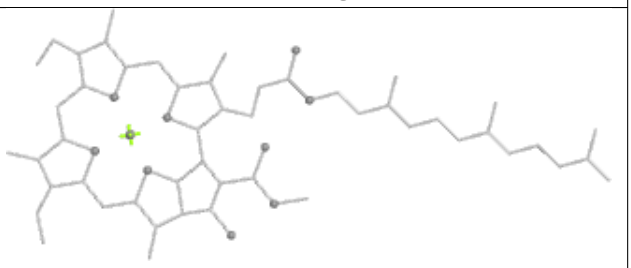
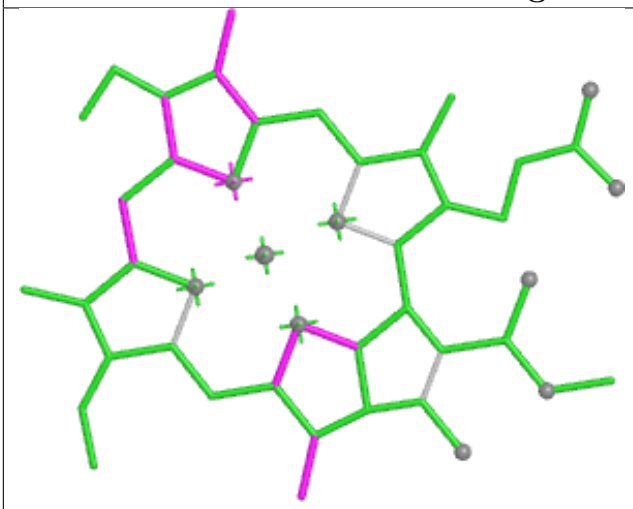
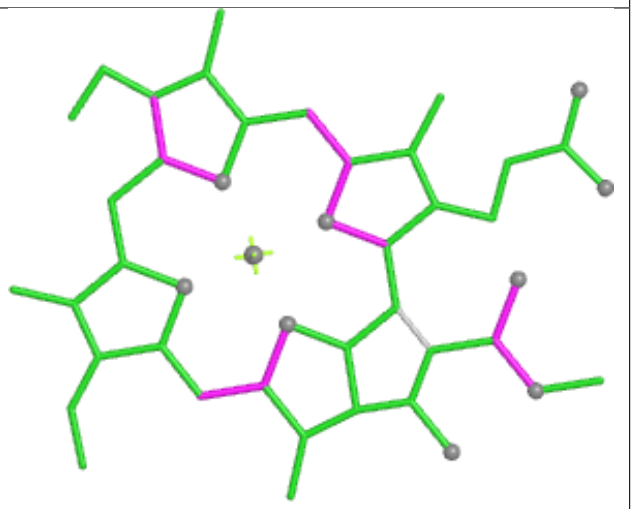
 Bond lengths	 Bond angles
 Torsions	 Rings

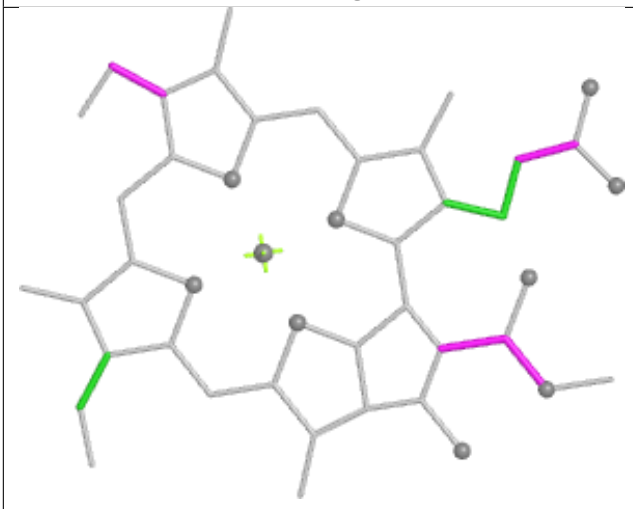
Ligand CLA 5 510



Bond lengths



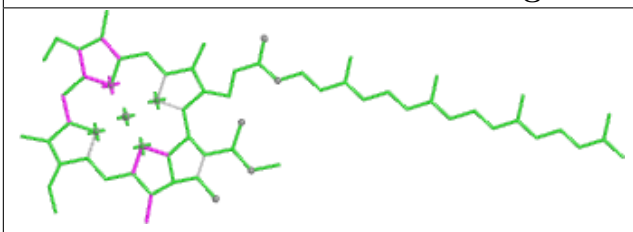
Bond angles



Torsions

Rings

Ligand CLA Y 510



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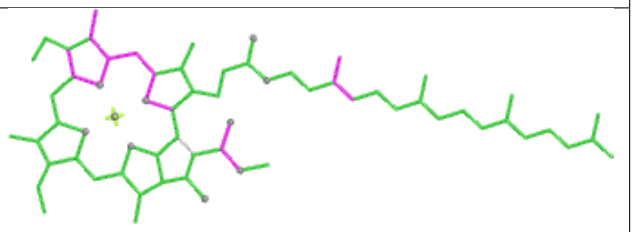

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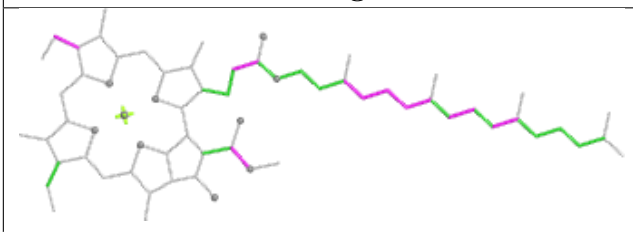

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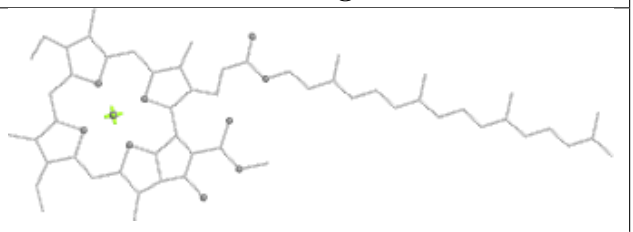
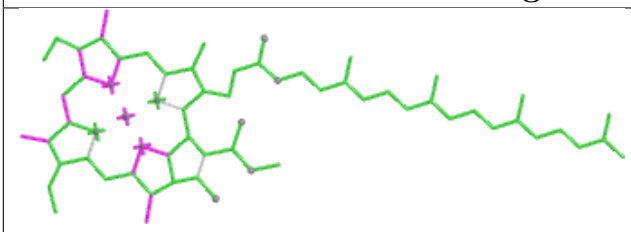


Rings

Ligand CLA f 1012



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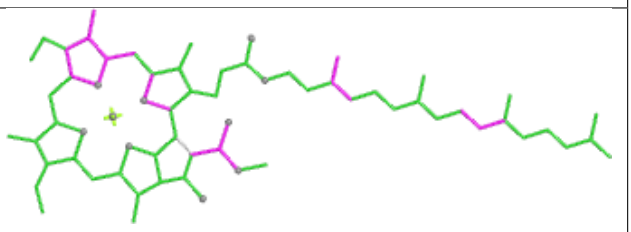
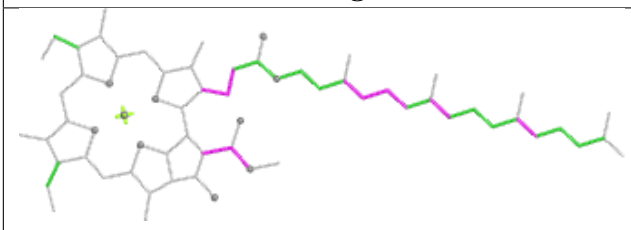


Bond angles



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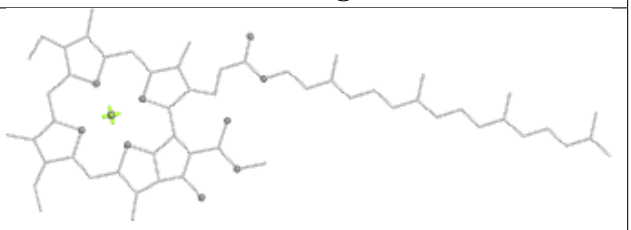
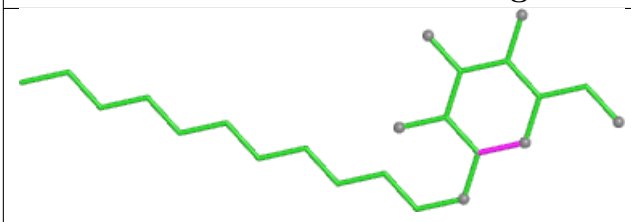


Rings

Ligand LMU A 1849



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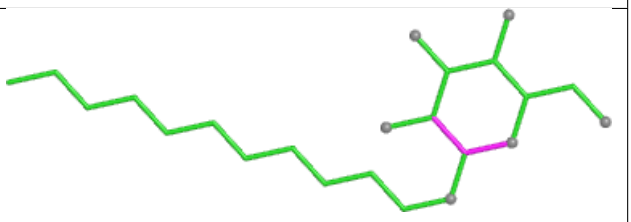

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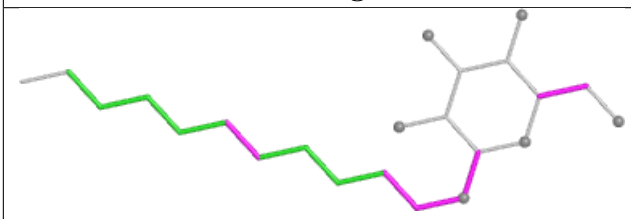

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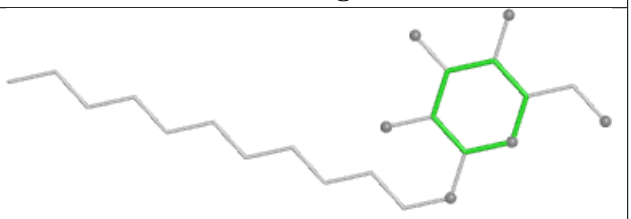

Rings

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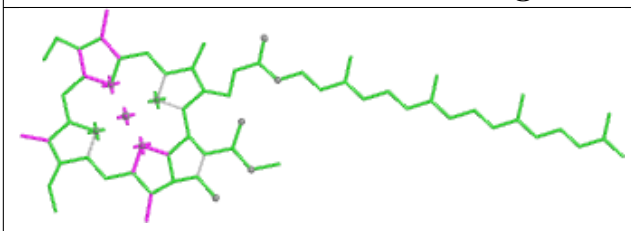

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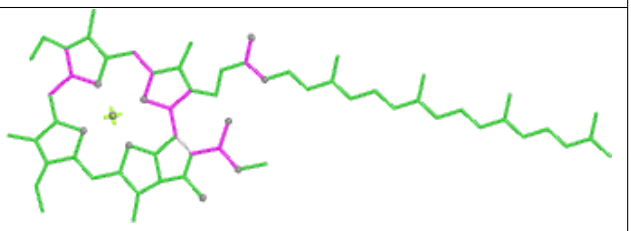

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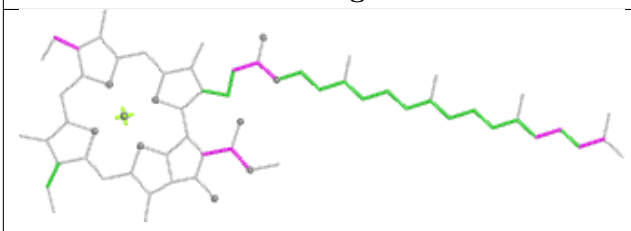

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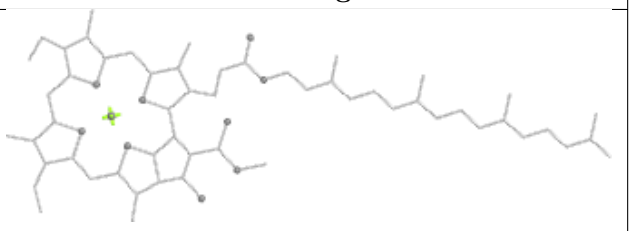
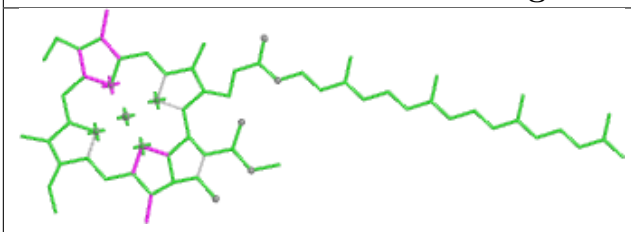


Rings

Ligand CLA a 507



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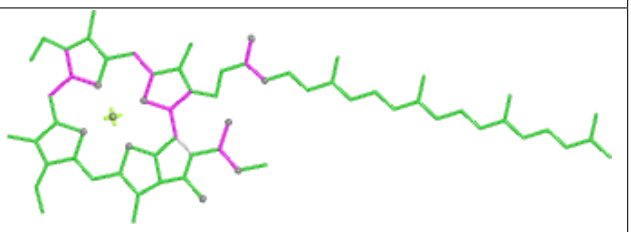

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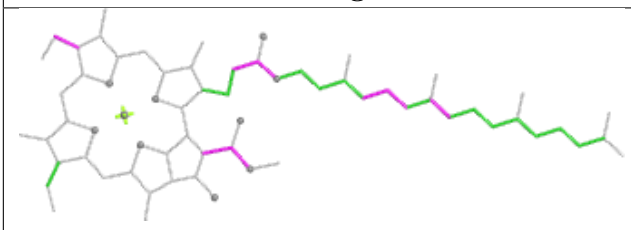

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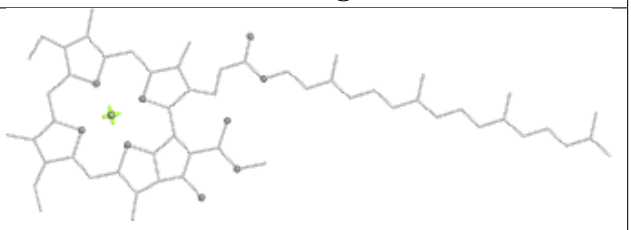

Rings

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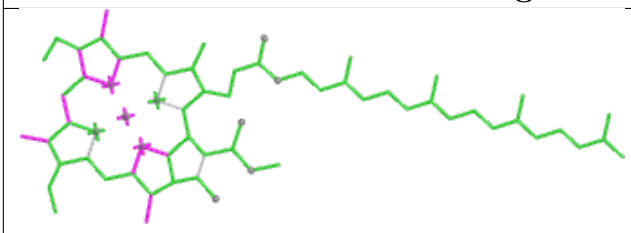

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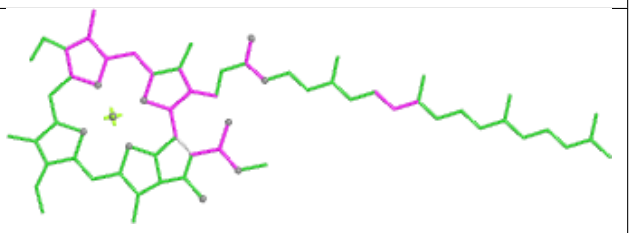
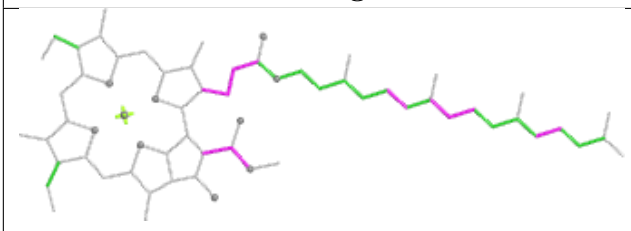


Bond angles



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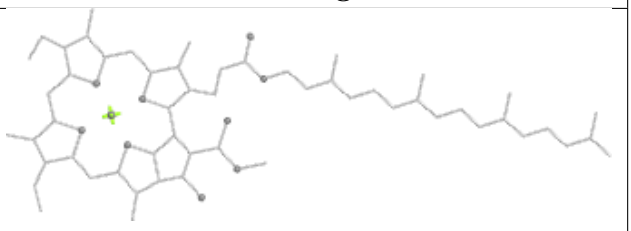

Rings

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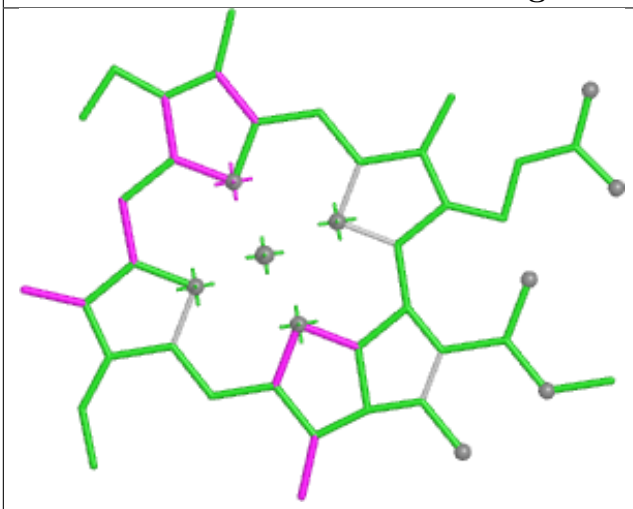

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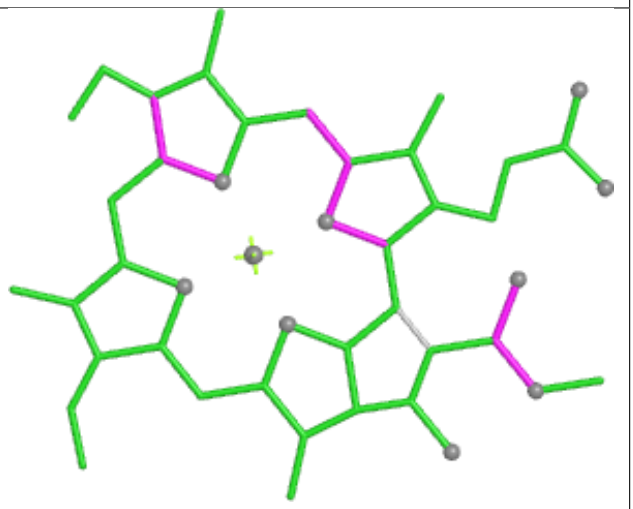
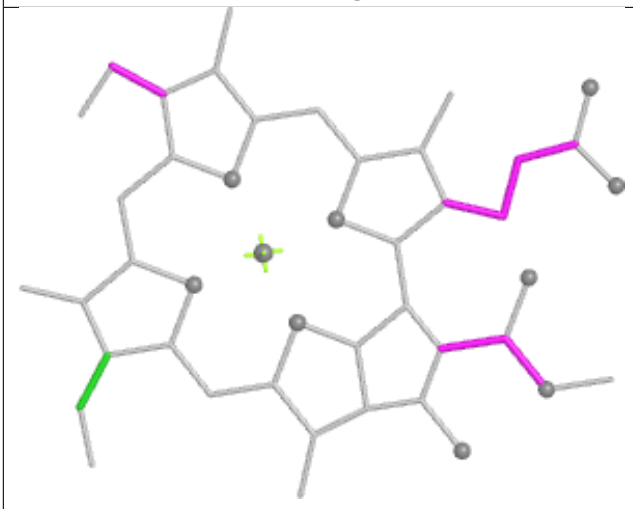


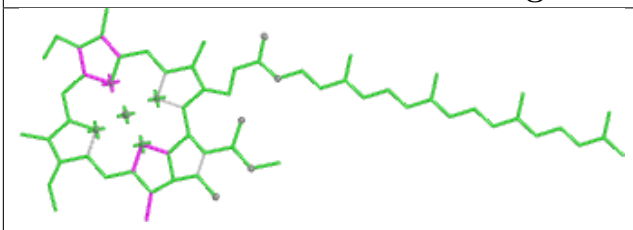
Bond angles



Torsions

Rings

Ligand CLA Z 505



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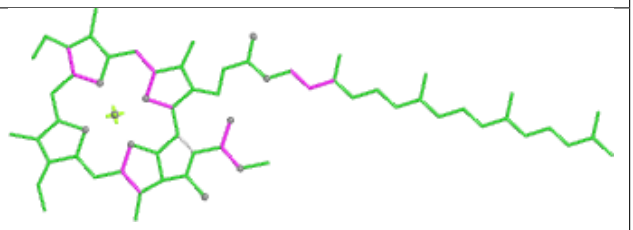

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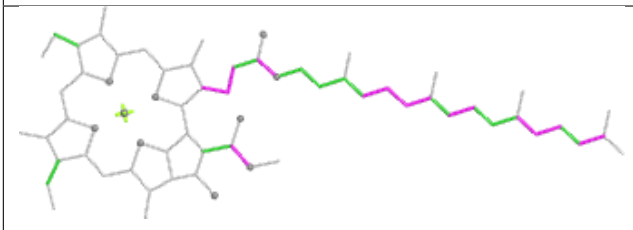

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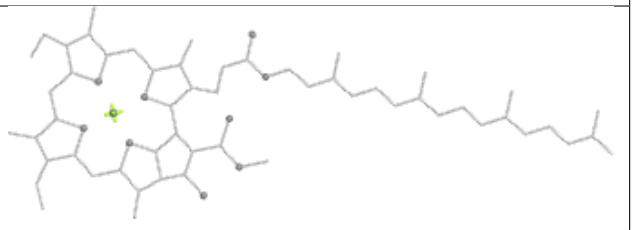
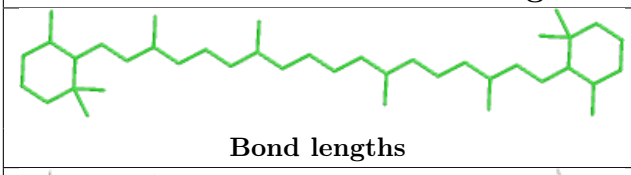


Rings

Ligand BCR 6 524



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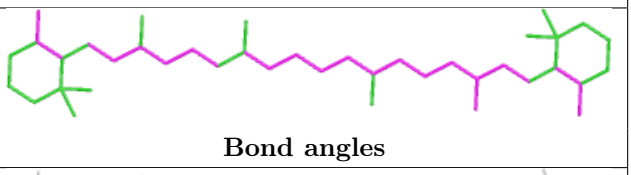

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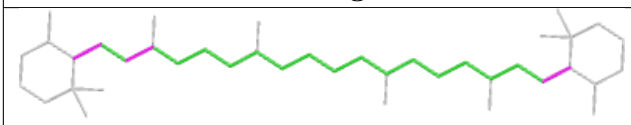

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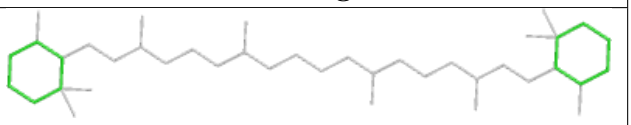
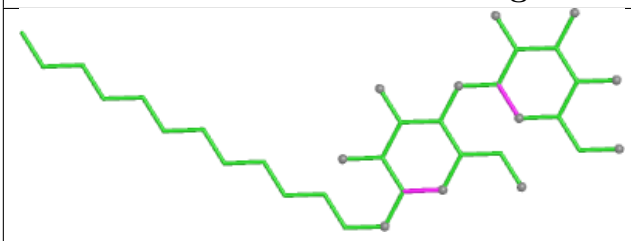


Rings

Ligand LMU G 1848



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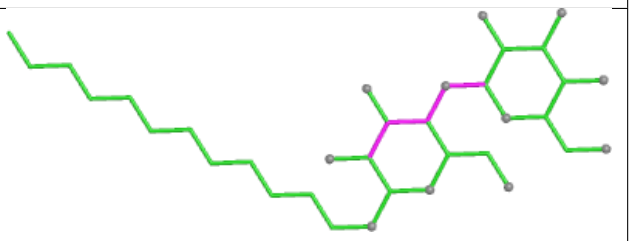

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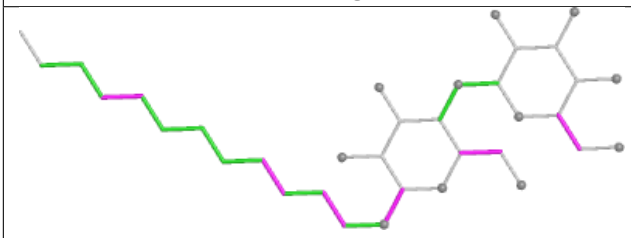

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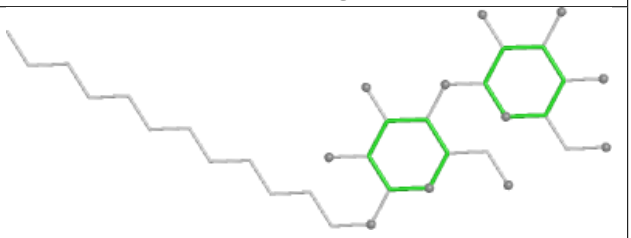
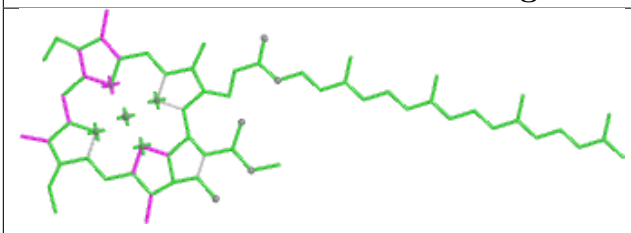


Rings

Ligand CLA e 1102



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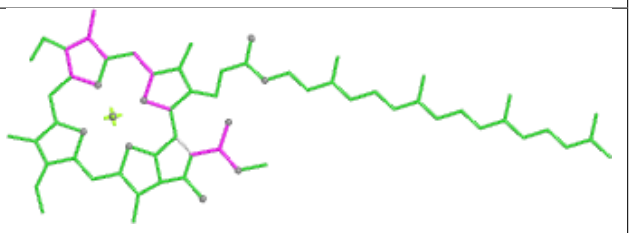

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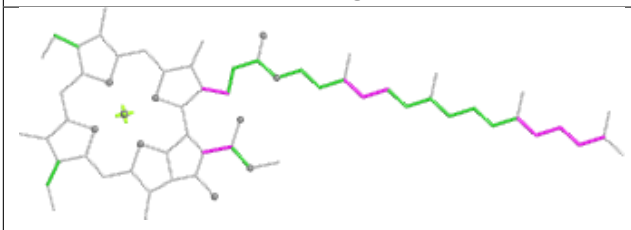

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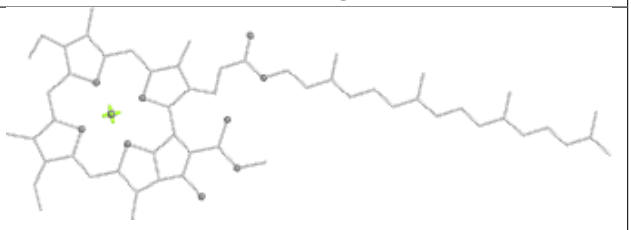
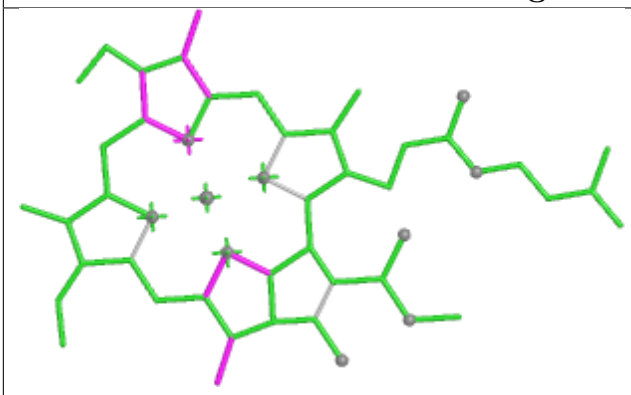


Rings

Ligand CLA a 502



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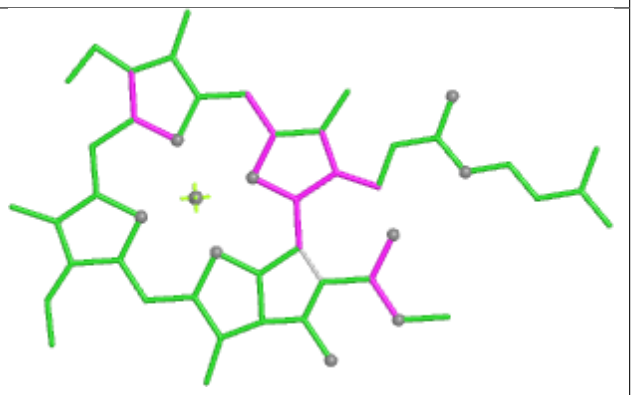

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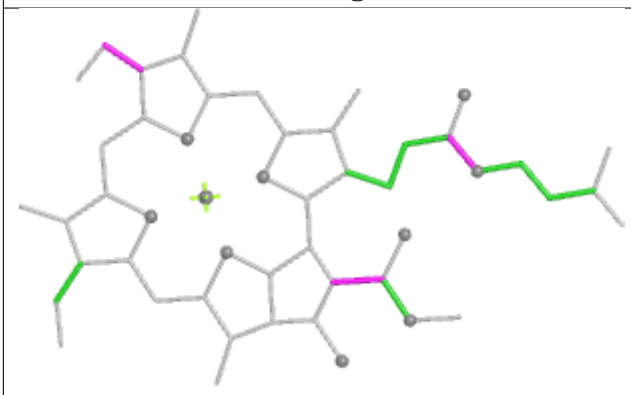

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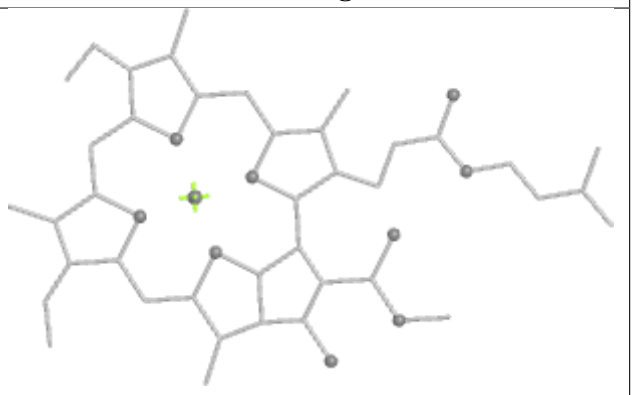
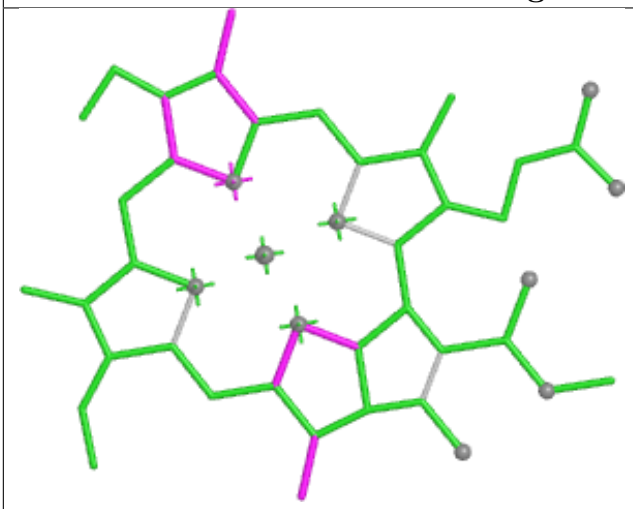


Rings

Ligand CLA b 512



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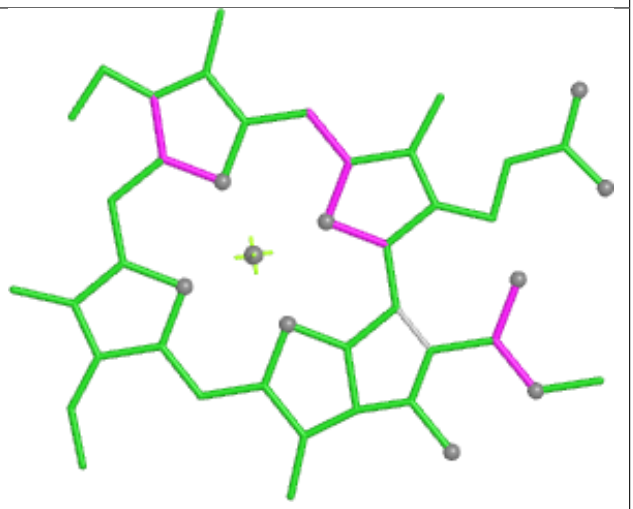

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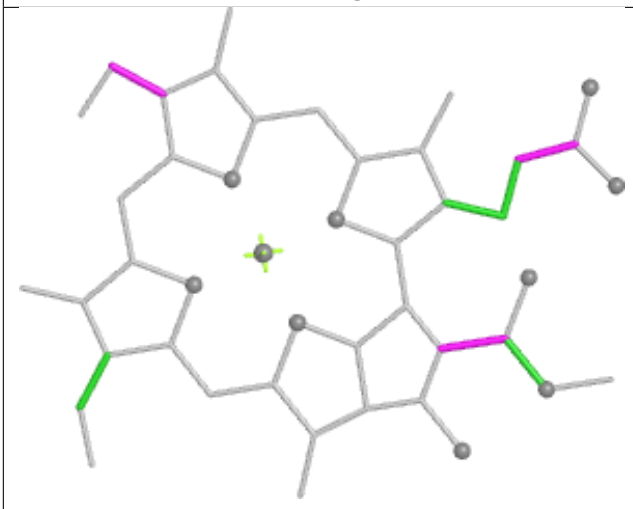
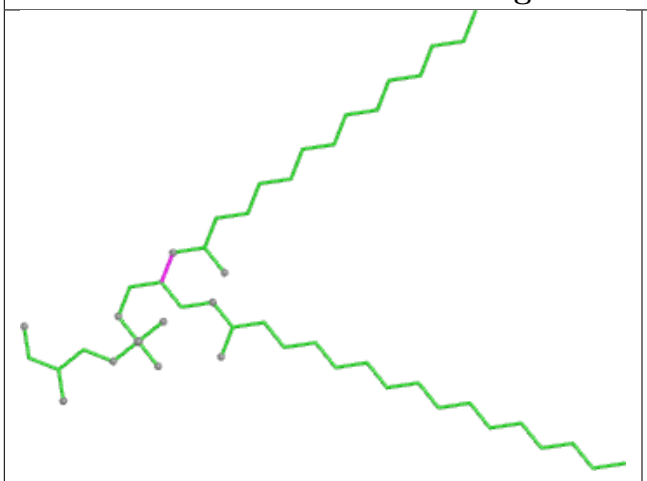


Torsions

Rings

Ligand LHG A 5007



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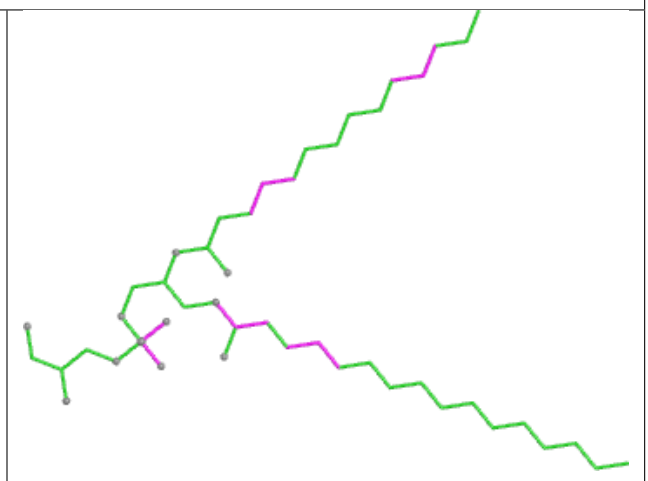

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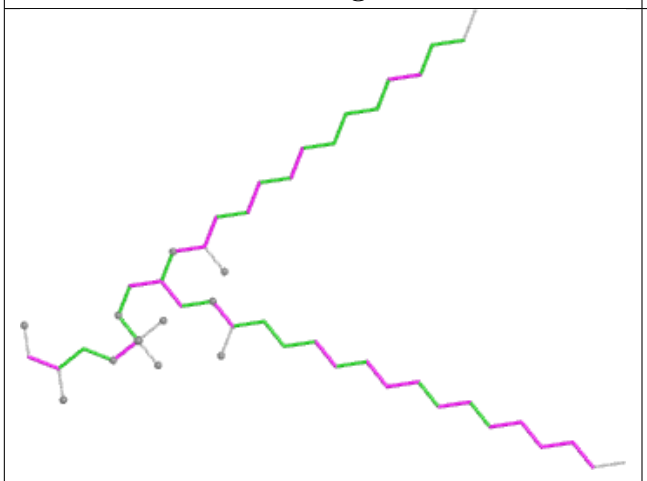

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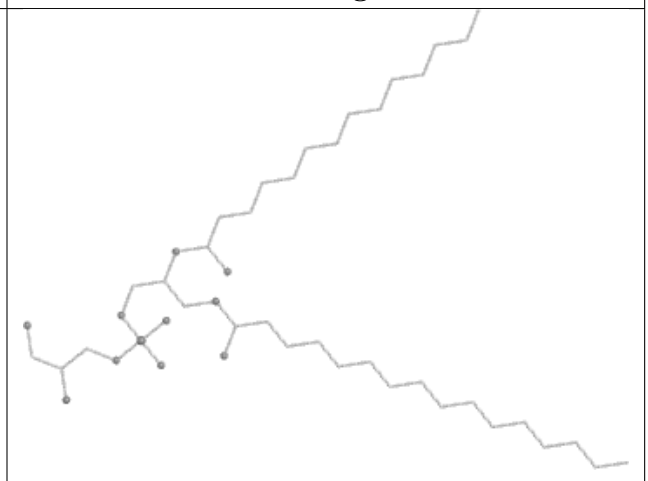
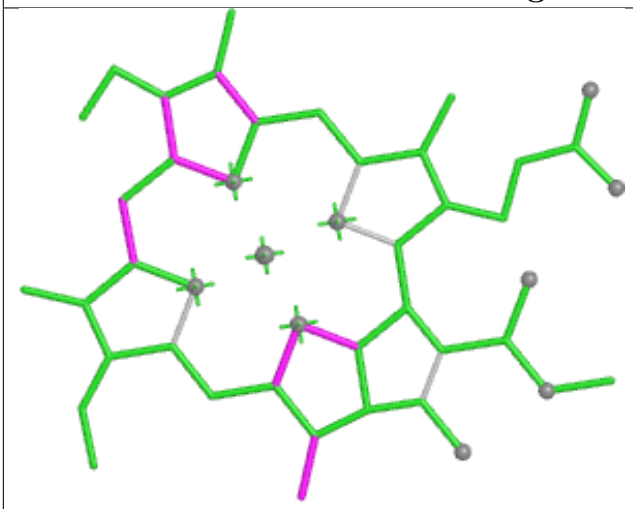


Rings

Ligand CLA b 504



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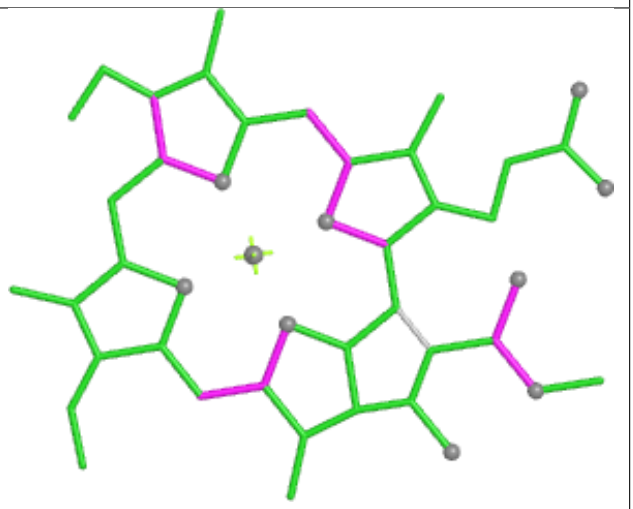

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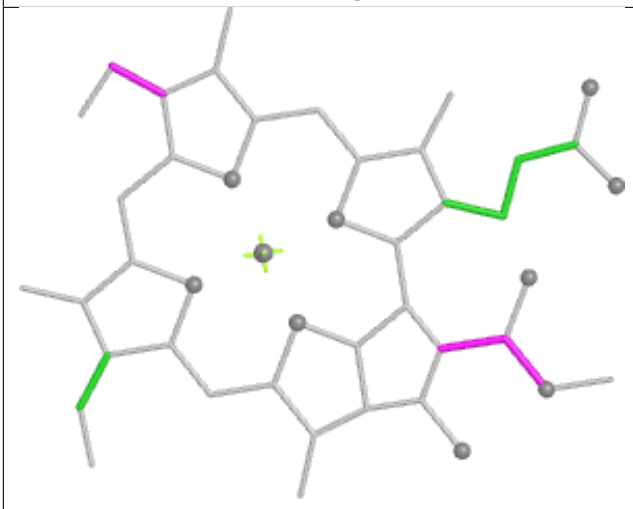
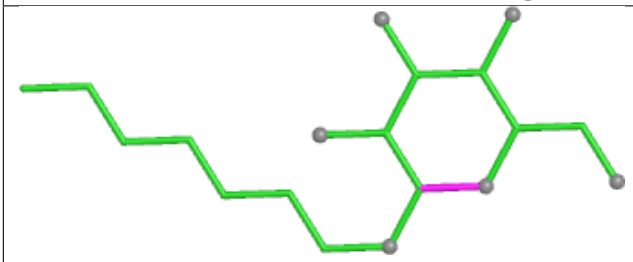


Torsions

Rings

Ligand LMU Y 902



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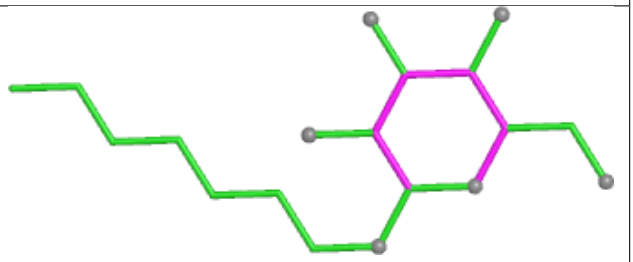

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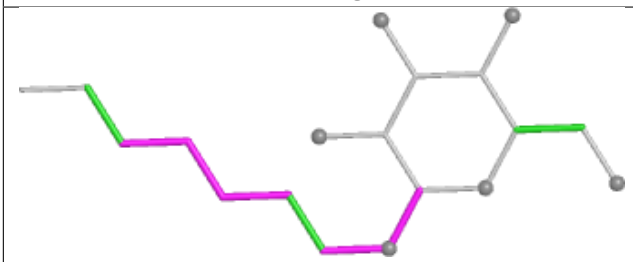

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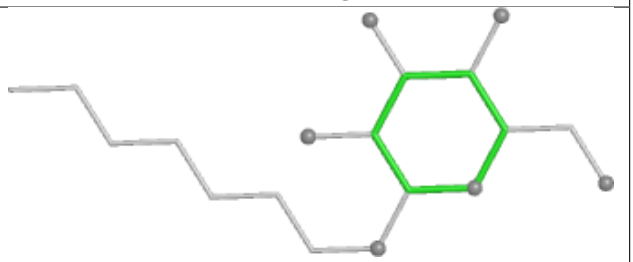
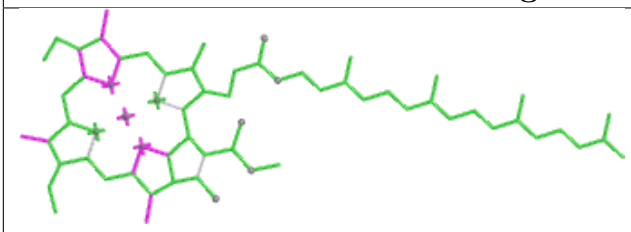


Rings

Ligand CLA e 1107



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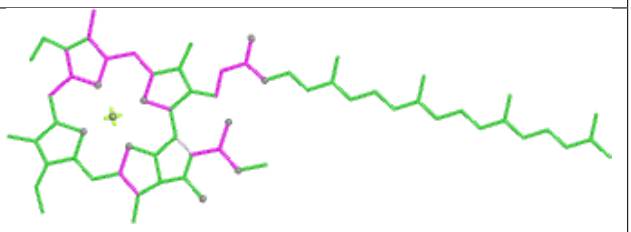

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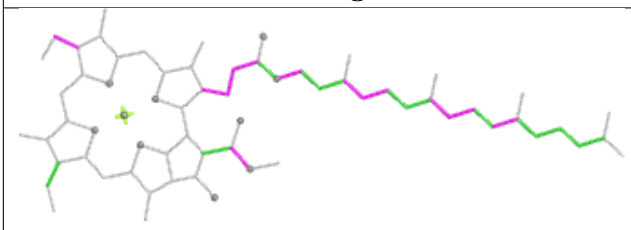

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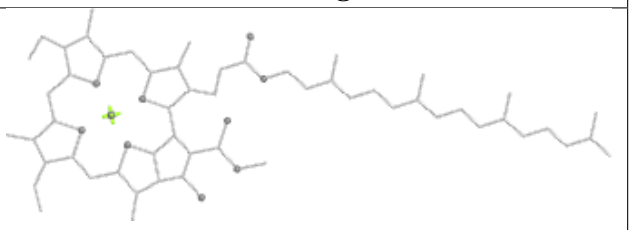

Rings

Ligand BCR 5 522

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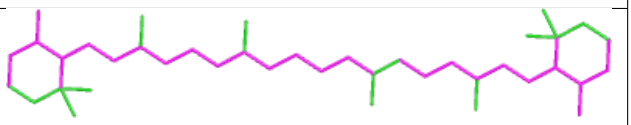

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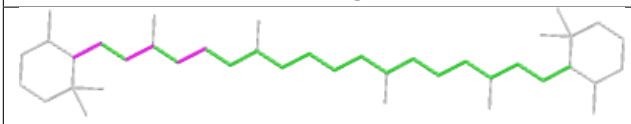

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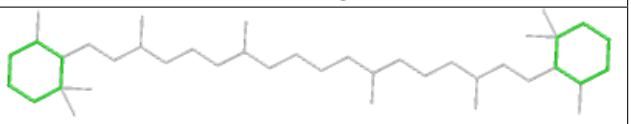
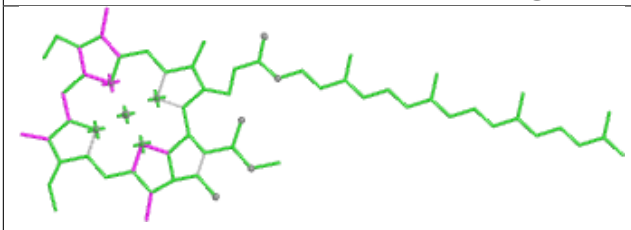


Rings

Ligand CLA 2 501



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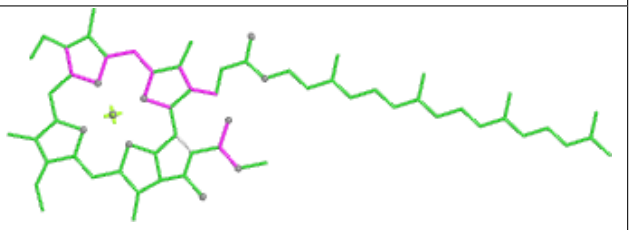
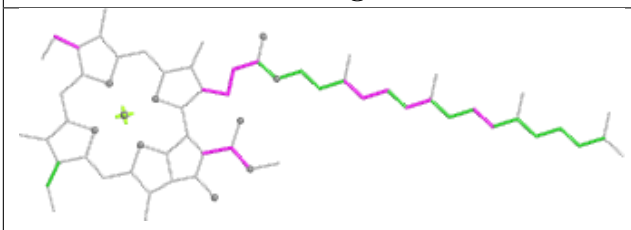
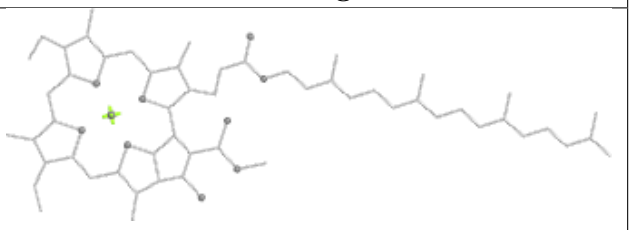


Bond angles

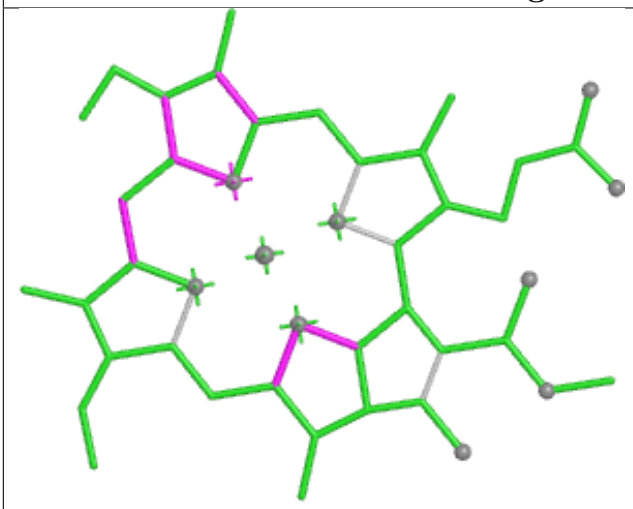


Torsions



Rings

Ligand CLA v 516



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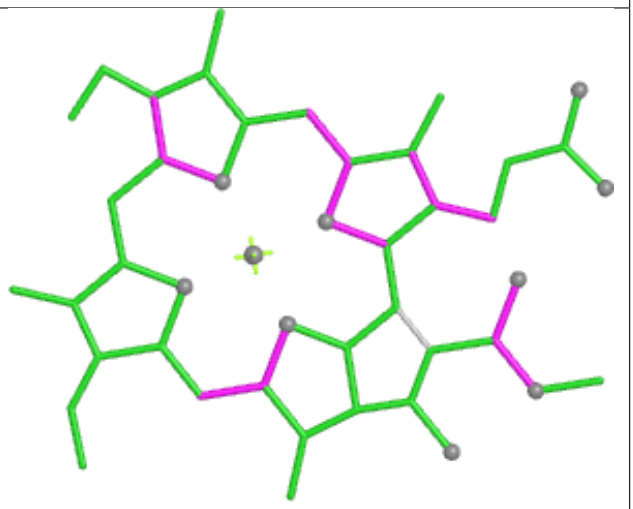
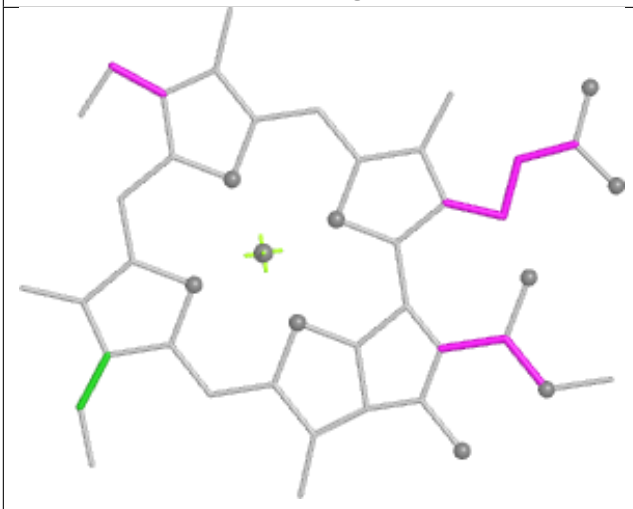


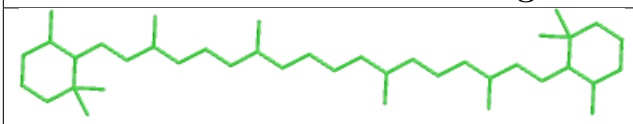
Bond angles



Torsions

Rings

Ligand BCR o 4021



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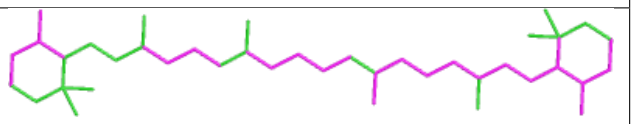
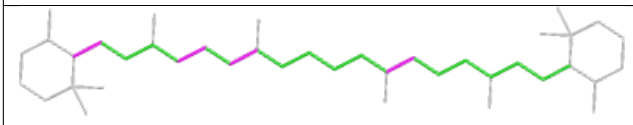
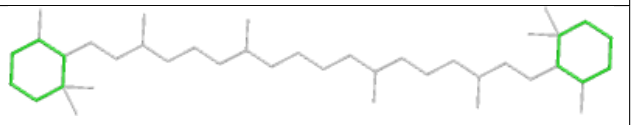


Bond angles

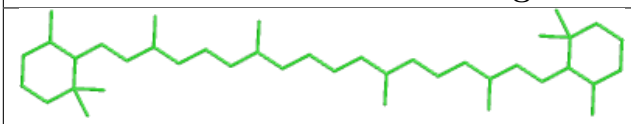


Torsions

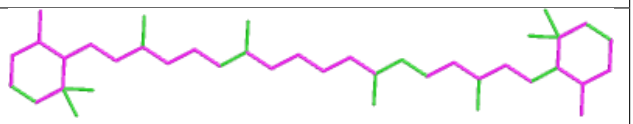


Rings

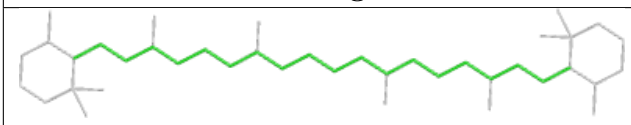
Ligand BCR A 4007



Bond lengths



Bond angles



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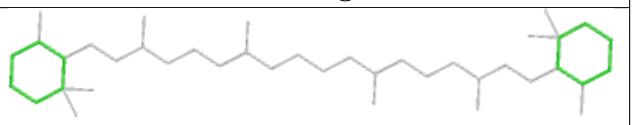
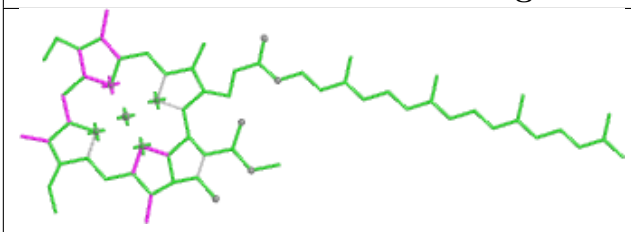


Rings

Ligand CLA B 1227



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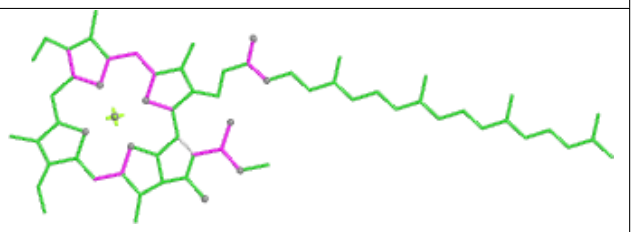
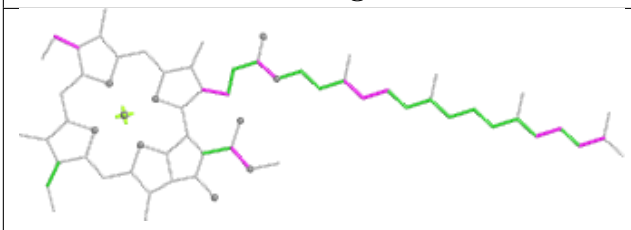


Bond angles



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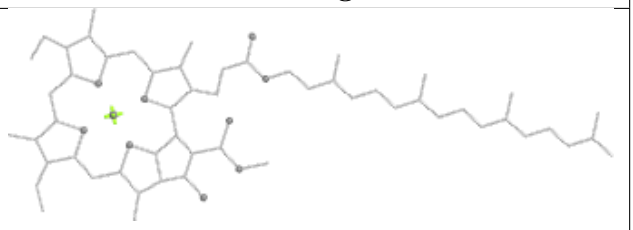
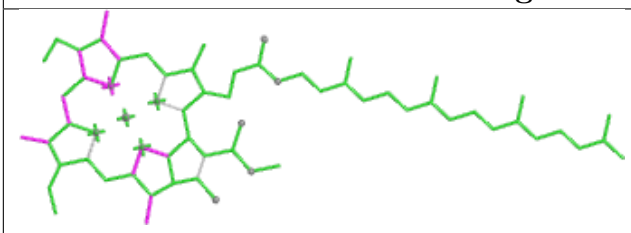


Rings

Ligand CLA B 1214



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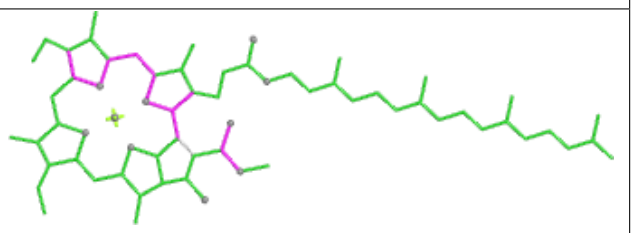
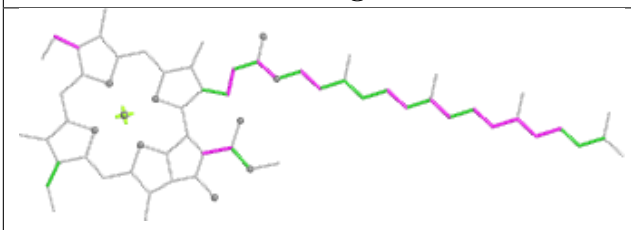


Bond angles



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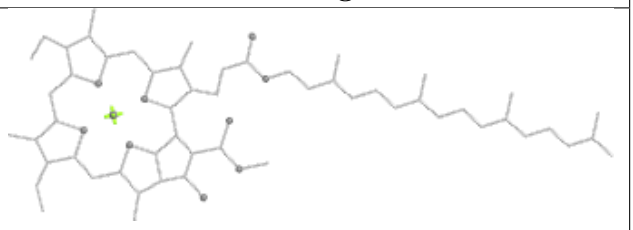
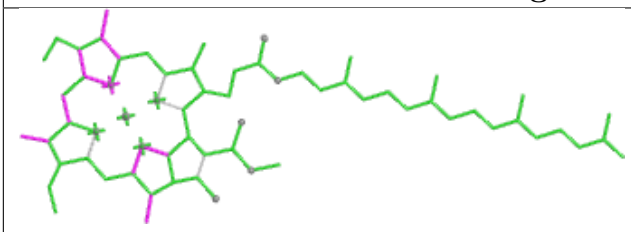


Rings

Ligand CLA r 509



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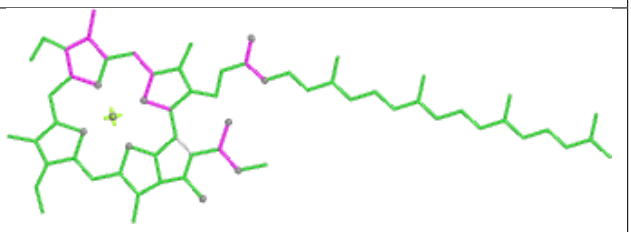

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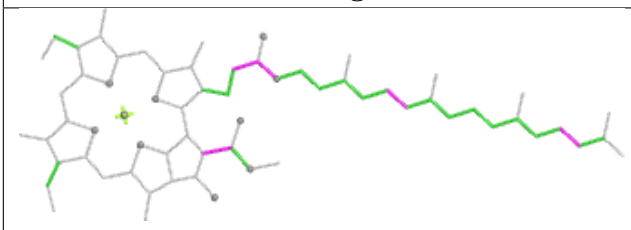

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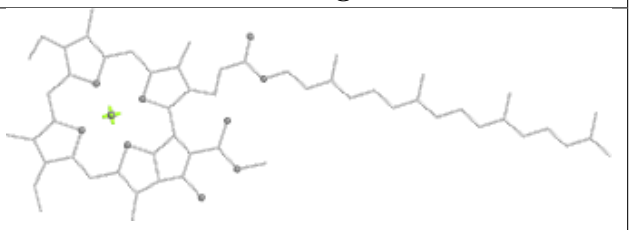
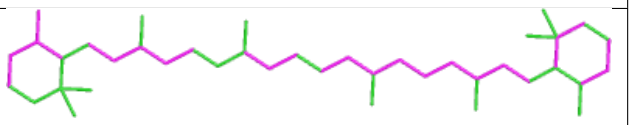


Rings

Ligand BCR 4 521

Bond lengths



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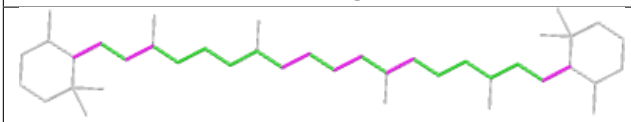

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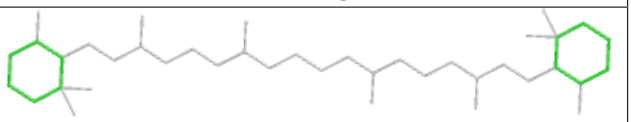
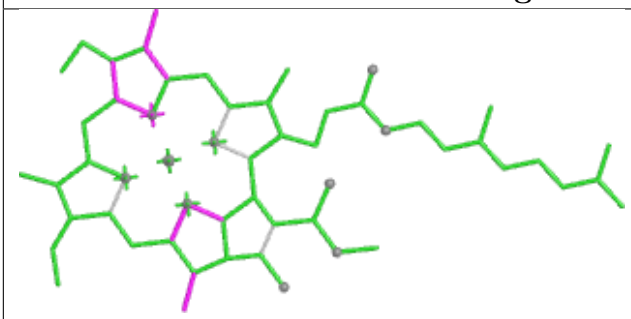


Rings

Ligand CLA H 1236



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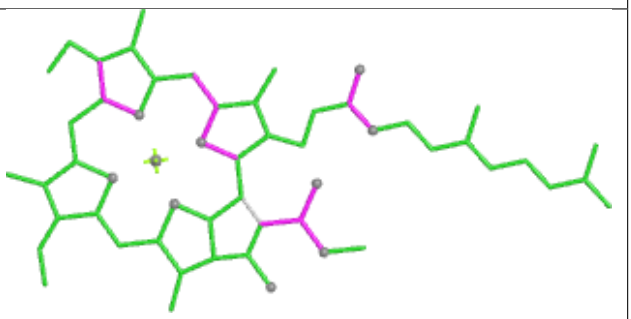
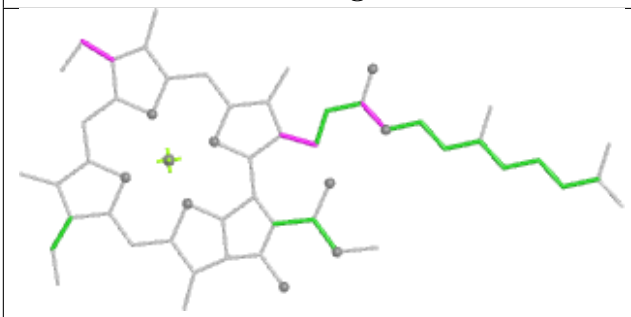


Bond angles



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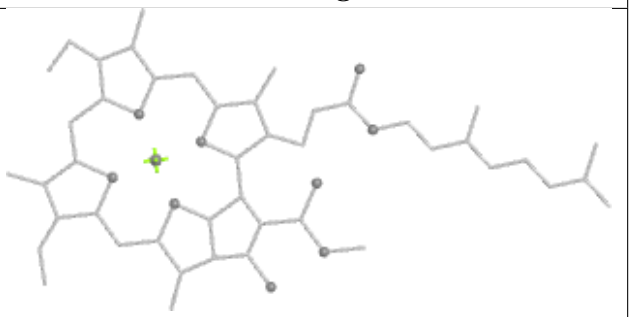
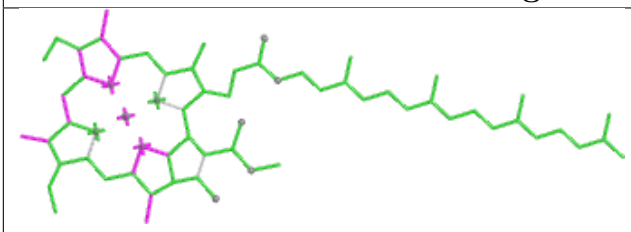


Rings

Ligand CLA f 1203



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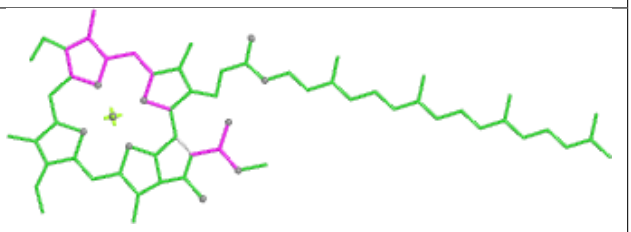

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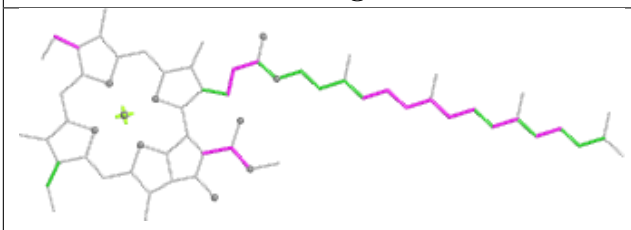

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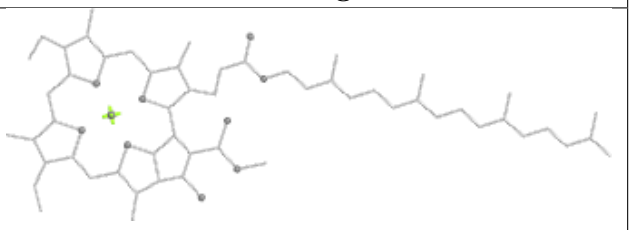
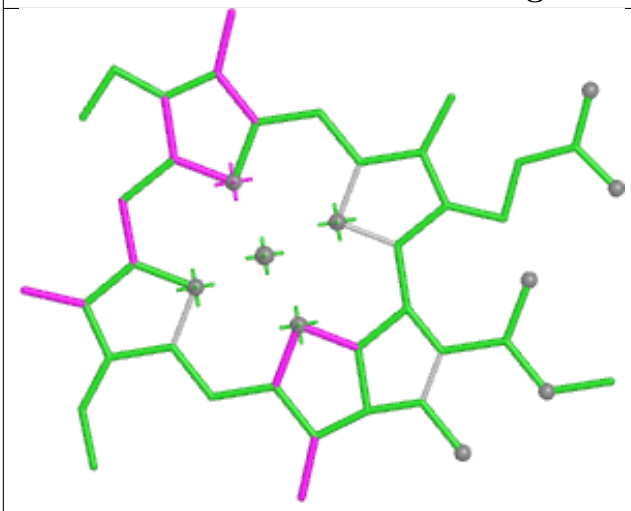


Rings

Ligand CLA Z 517



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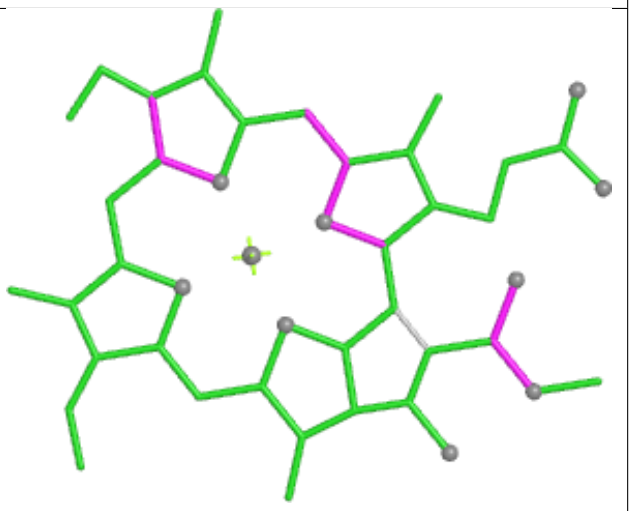

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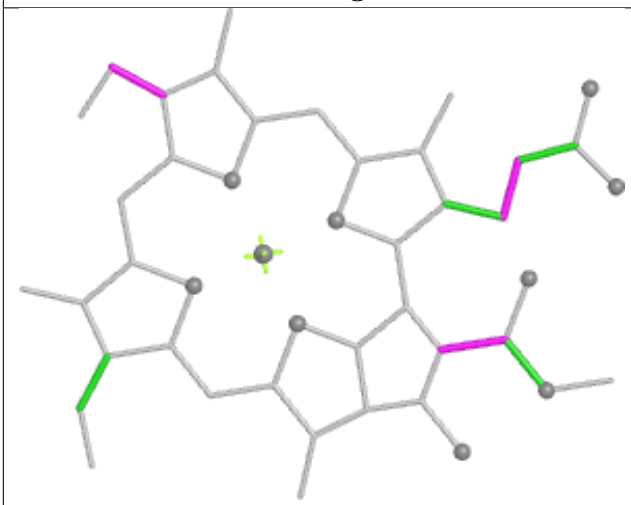

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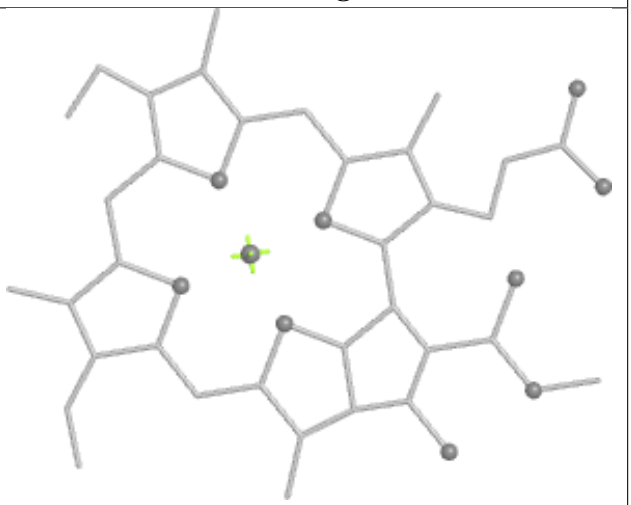
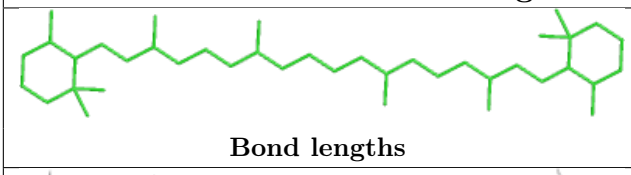


Rings

Ligand BCR L 4019



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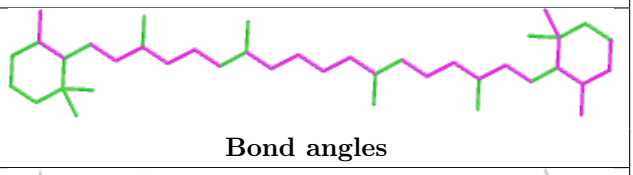

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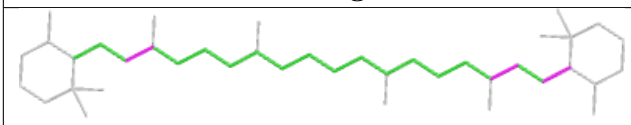

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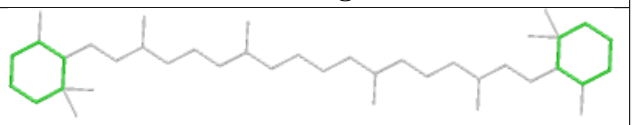
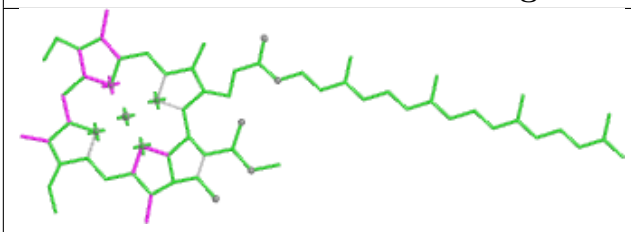


Rings

Ligand CLA e 1101



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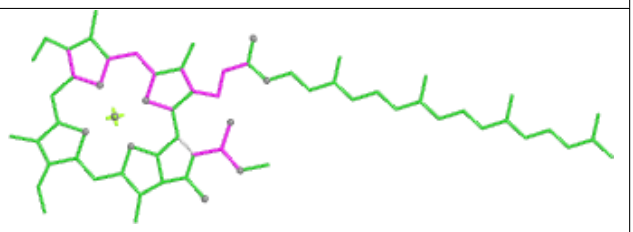

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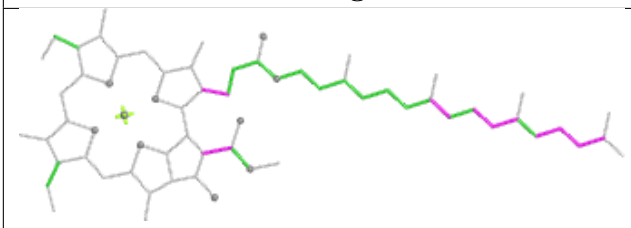

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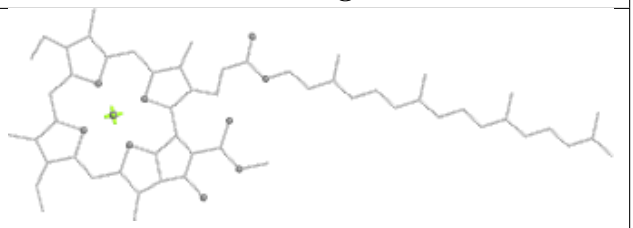
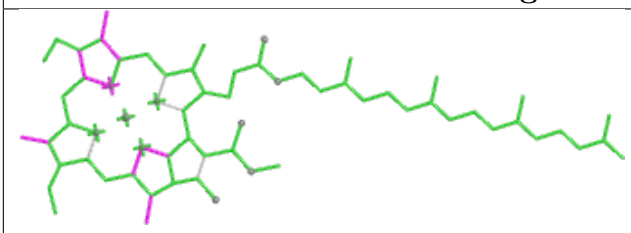


Rings

Ligand CLA e 1237



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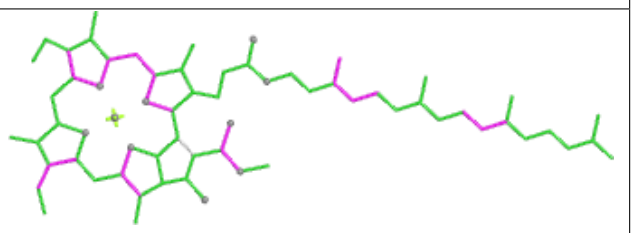
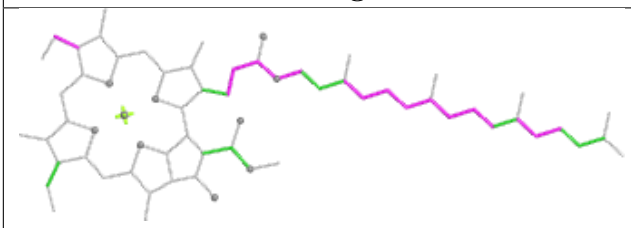


Bond angles



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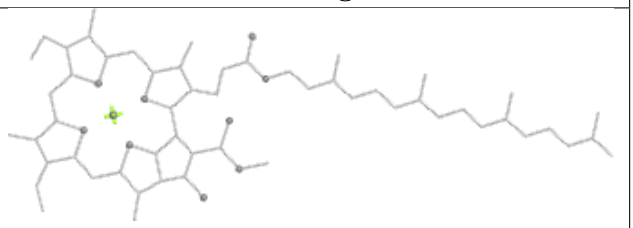
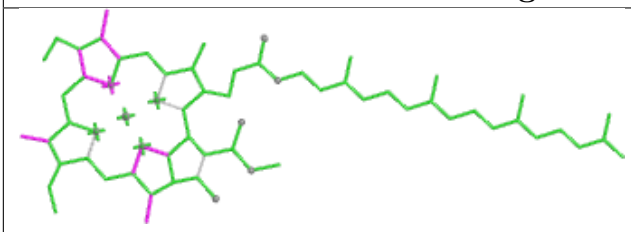
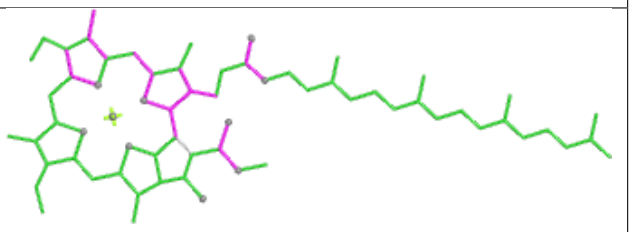
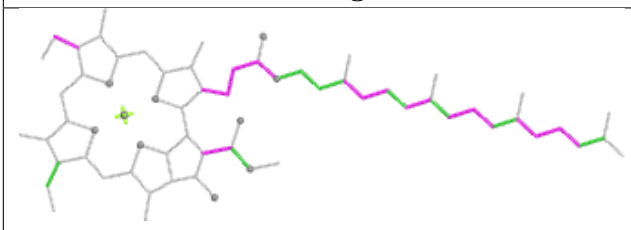
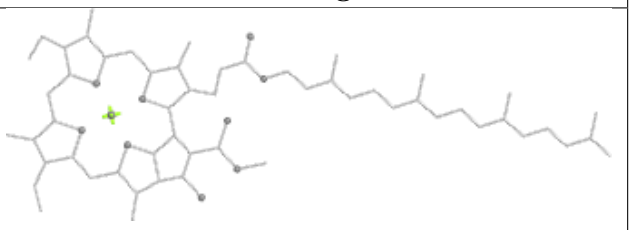


Rings

Ligand CLA n 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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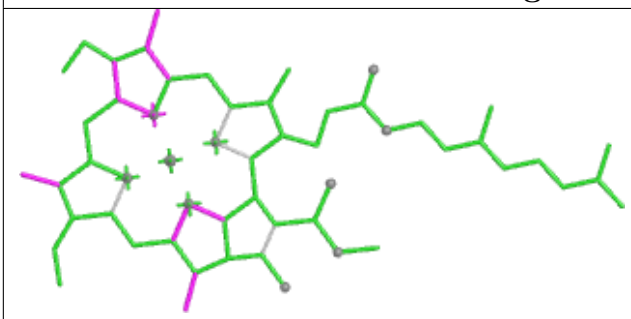
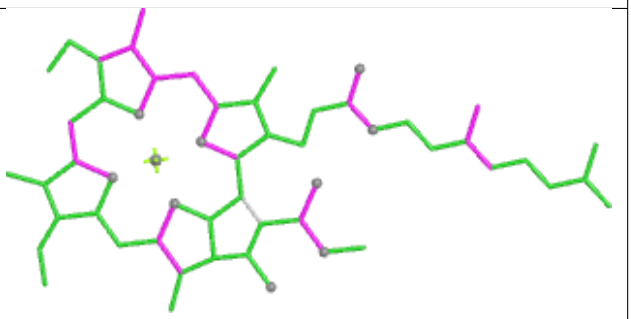
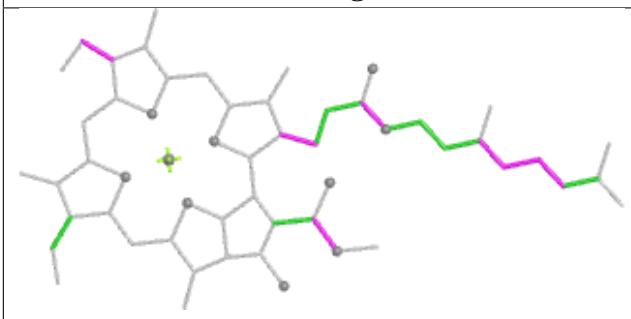
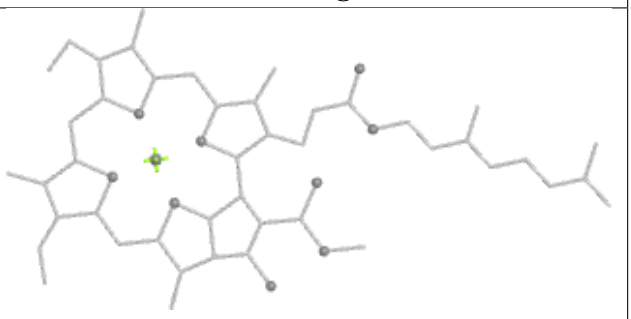
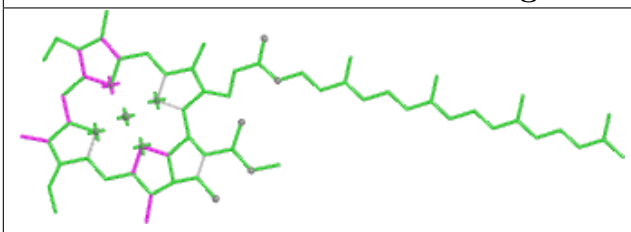
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA e 1127



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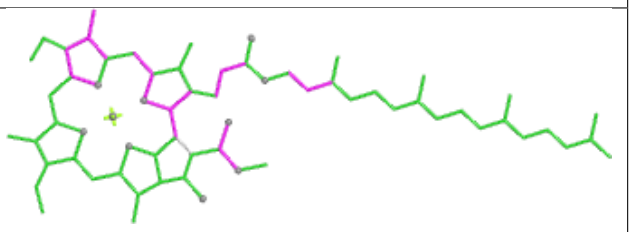

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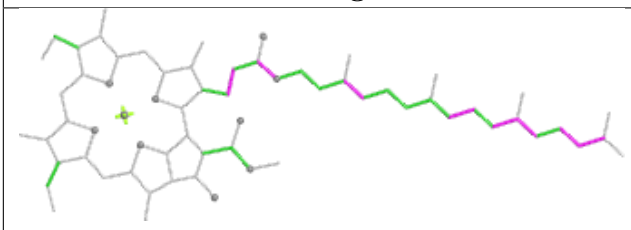

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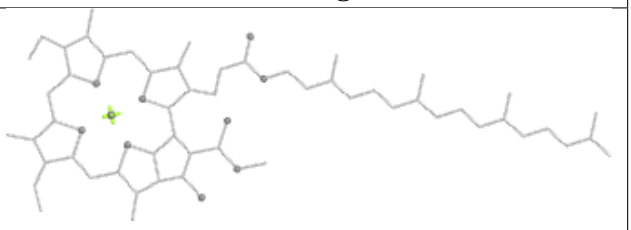
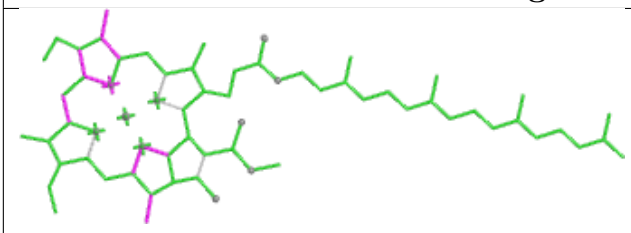


Rings

Ligand CLA 2 518



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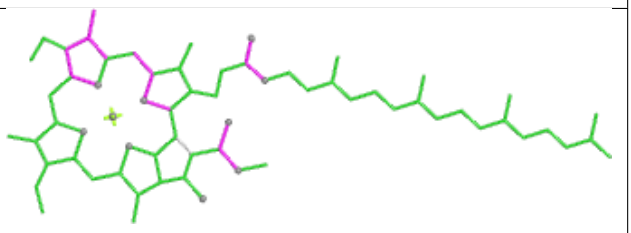

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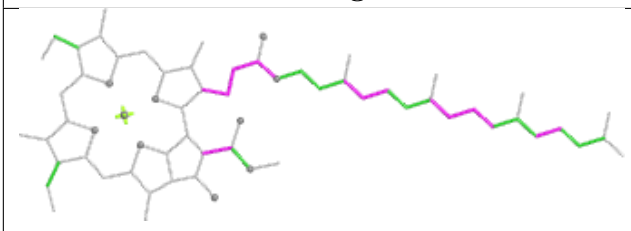

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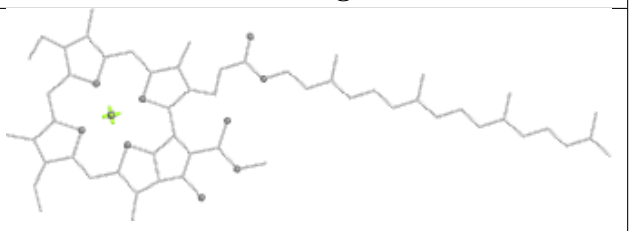

Rings

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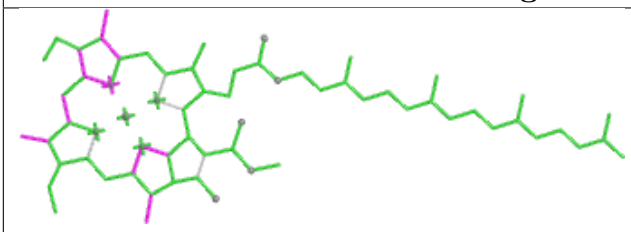

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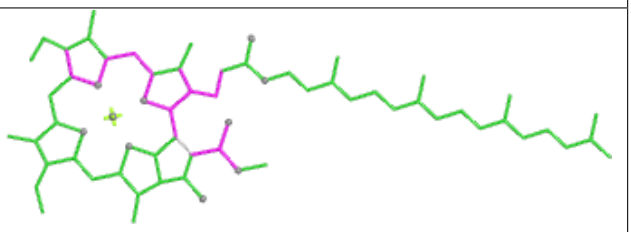

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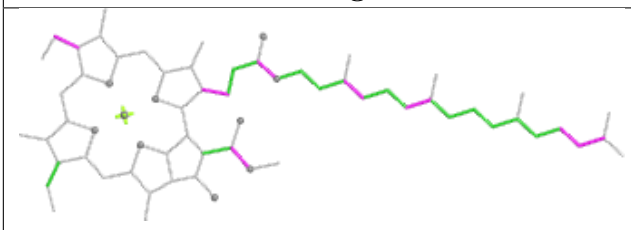

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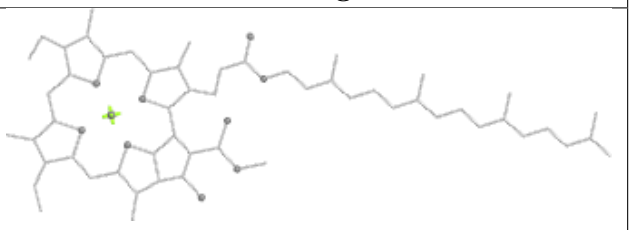

Rings

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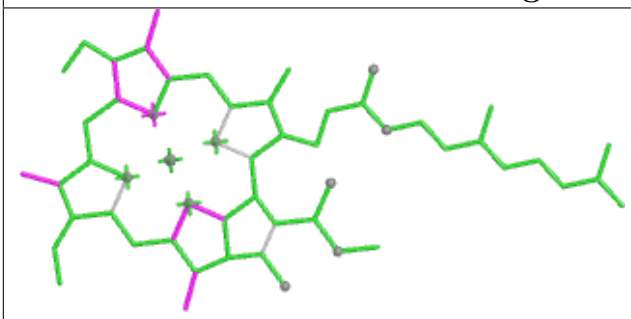

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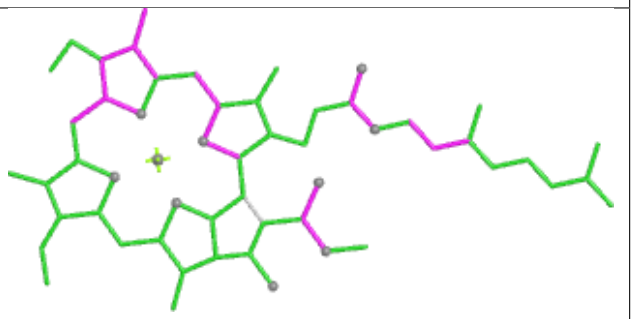

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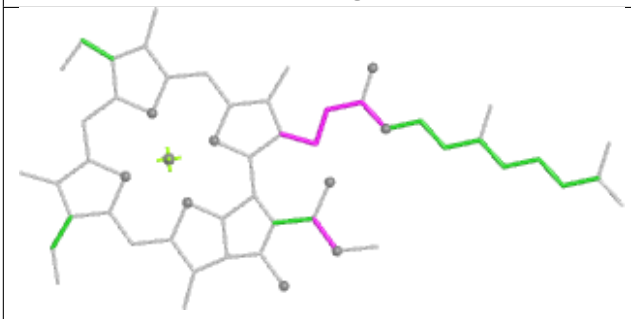

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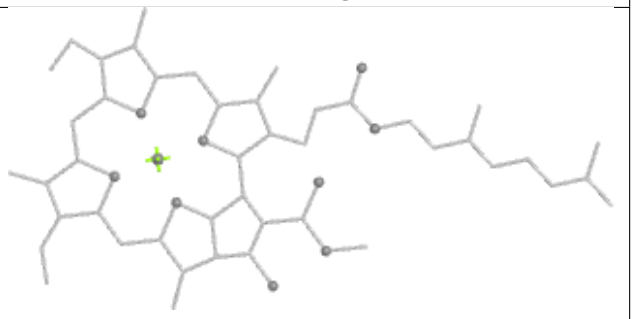

Rings

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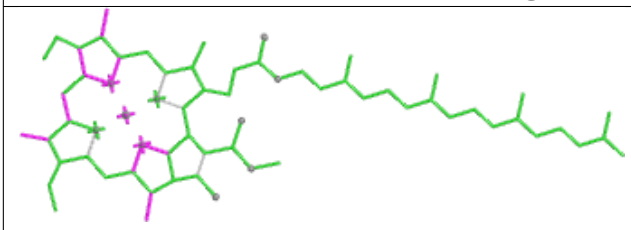

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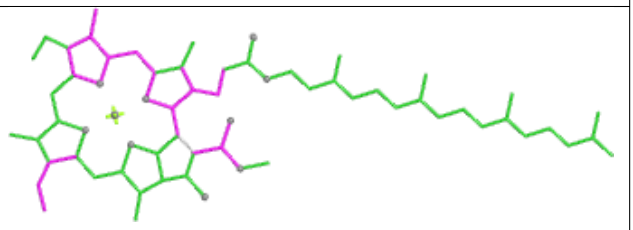

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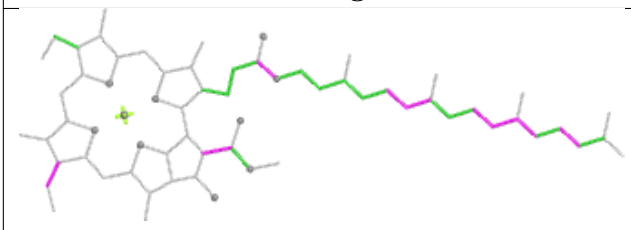

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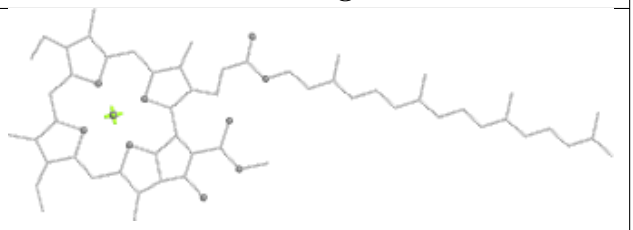
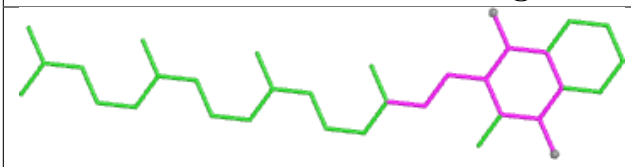


Rings

Ligand PQN A 2001



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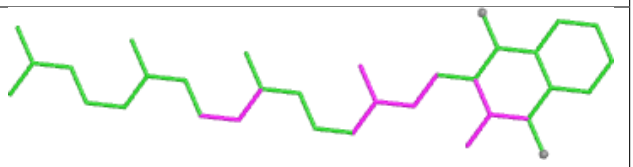

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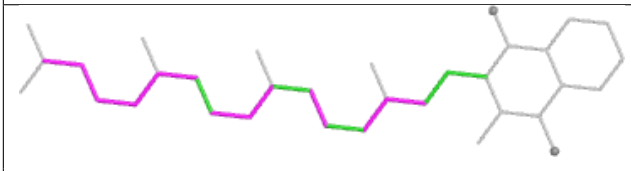

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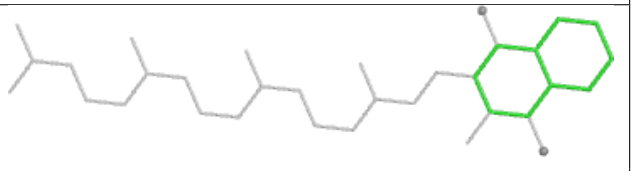
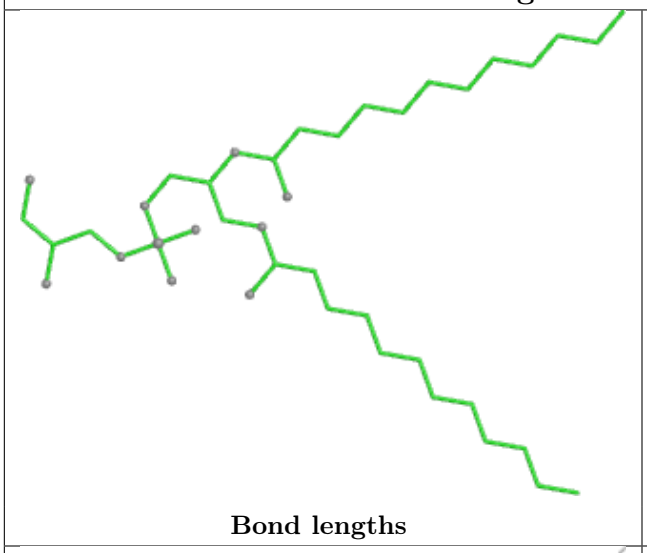


Rings

Ligand LHG L 5220



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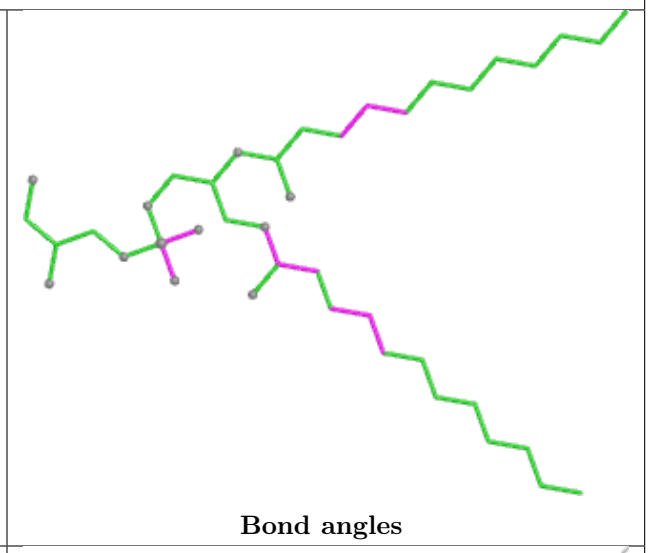

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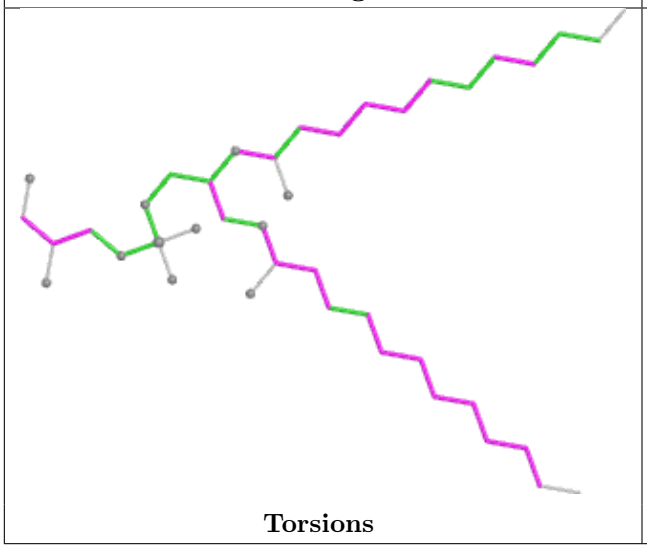

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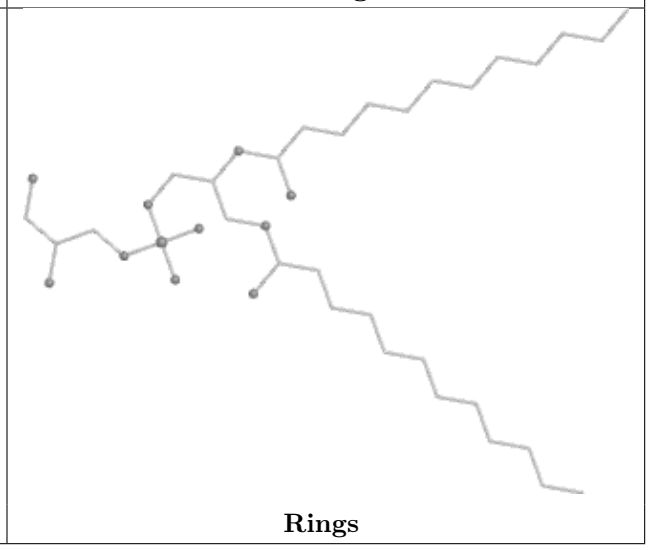
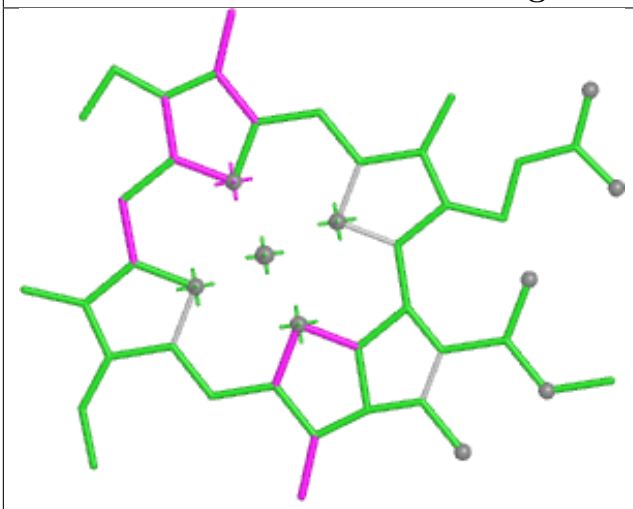


Rings

Ligand CLA a 504



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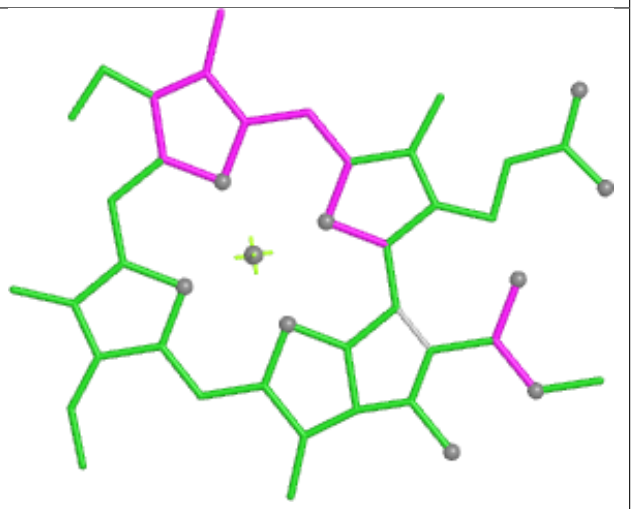

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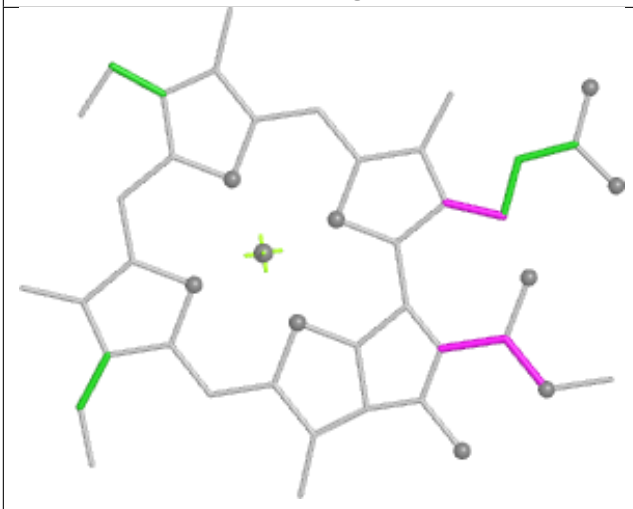

Torsions

Rings

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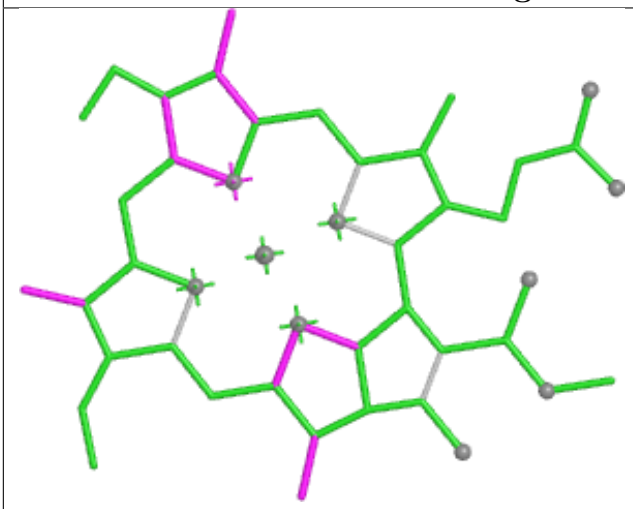

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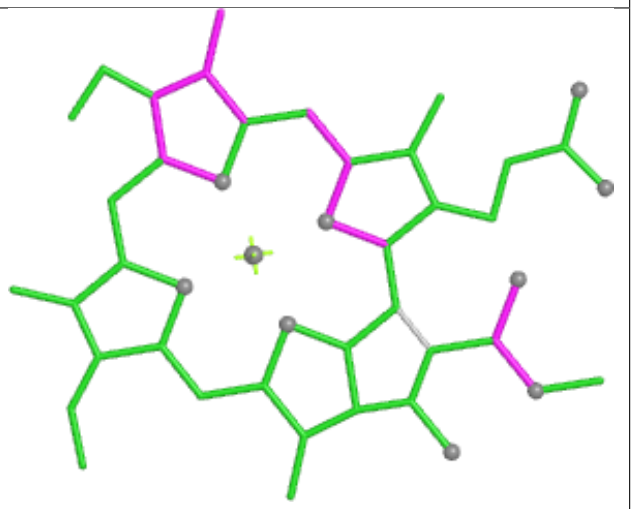

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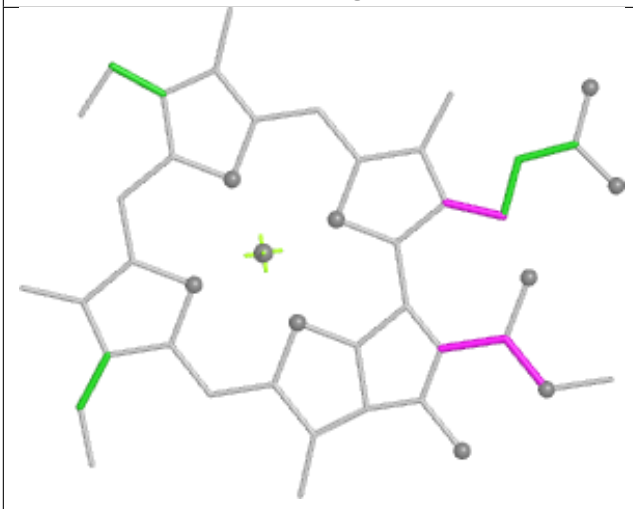

Torsions

Rings

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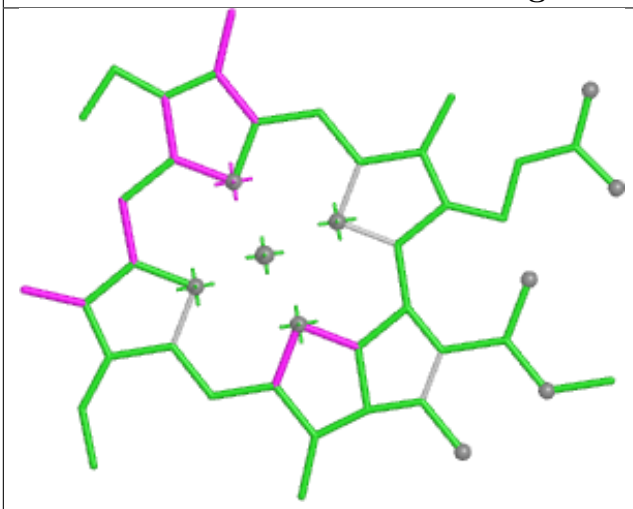

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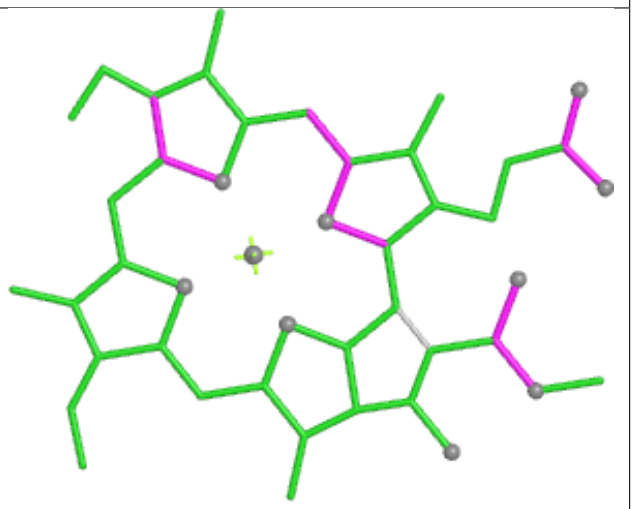

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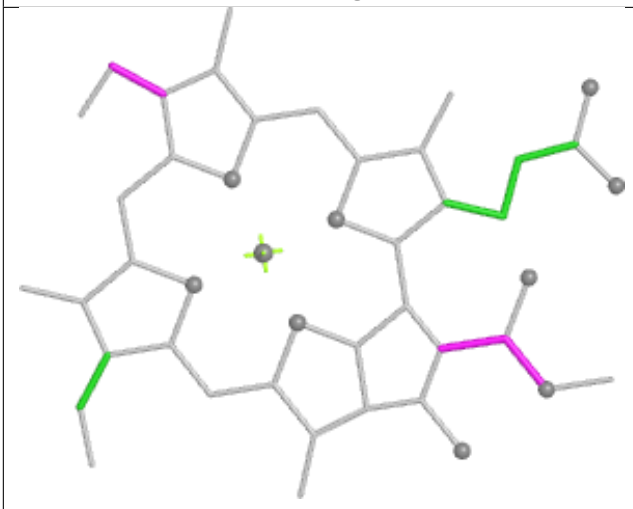

Torsions

Rings

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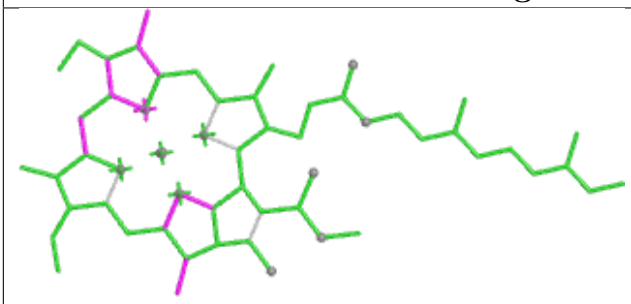
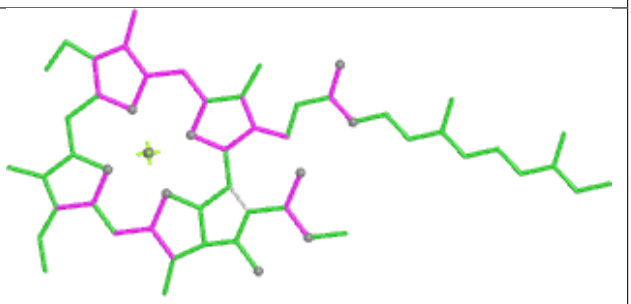
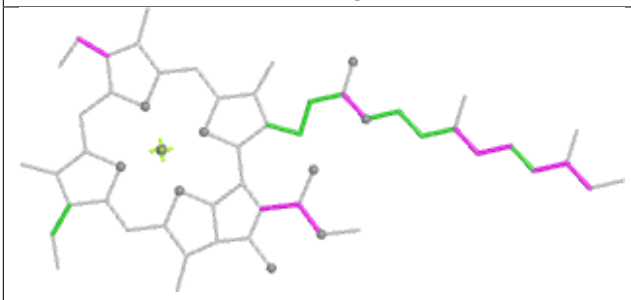
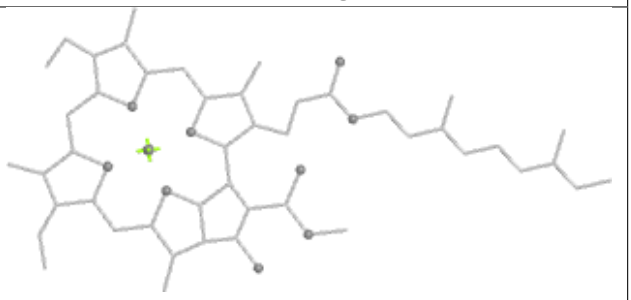
	
Bond lengths	Bond angles
	
Torsions	Rings

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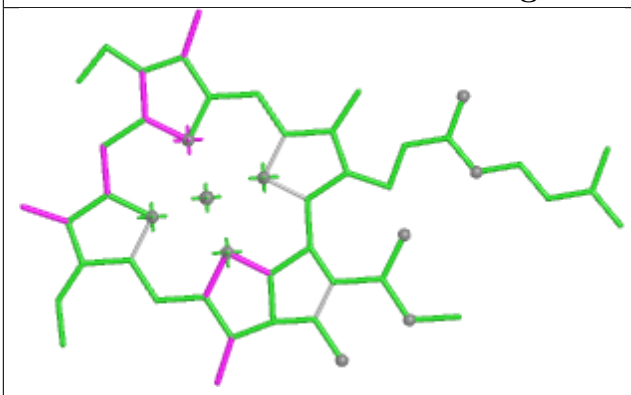	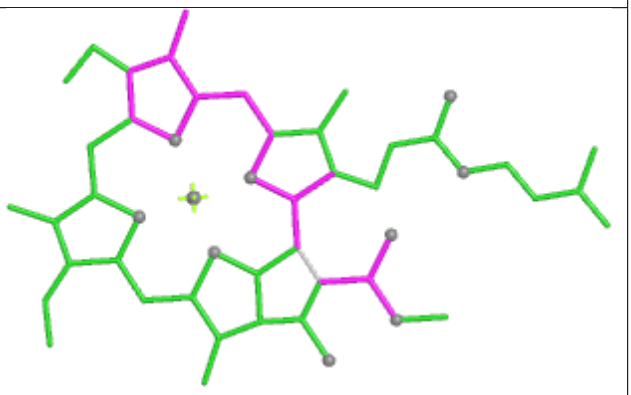
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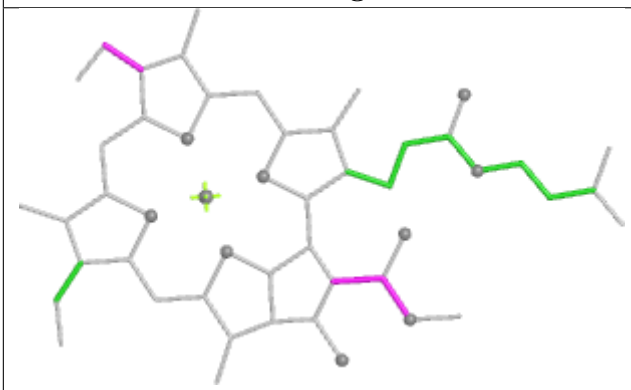
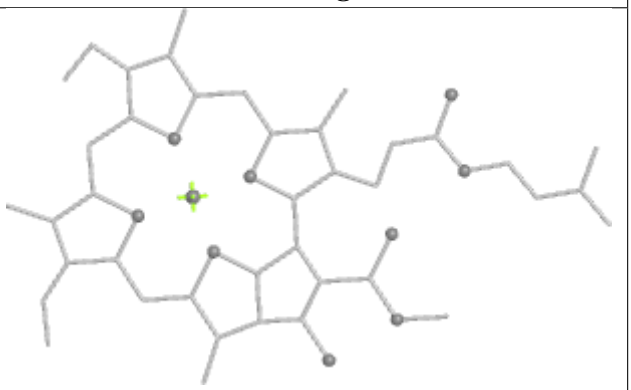
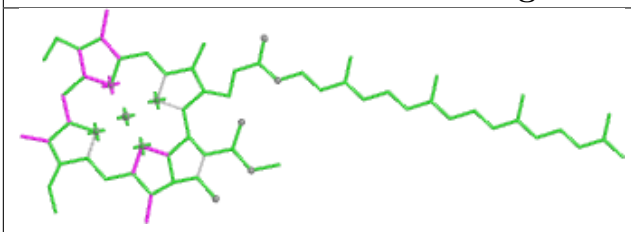
	
Torsions	Rings

Ligand CLA n 1502



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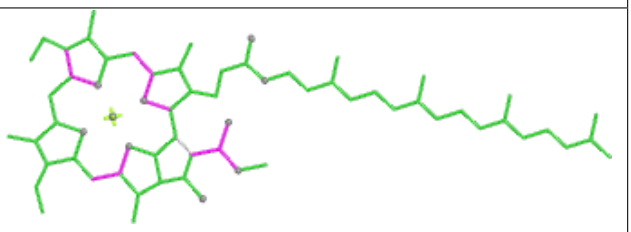
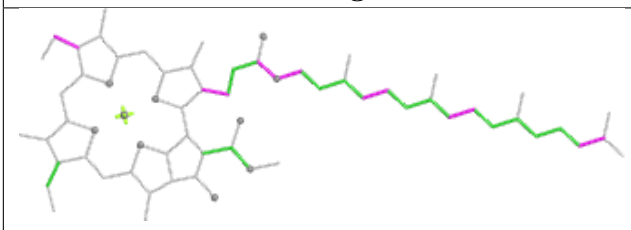


Bond angles



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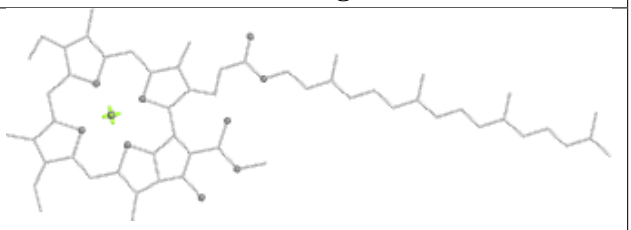
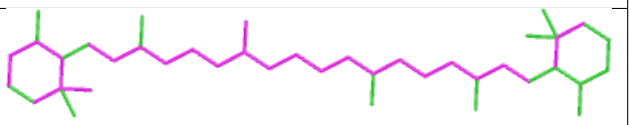


Rings

Ligand BCR J 4013

Bond lengths



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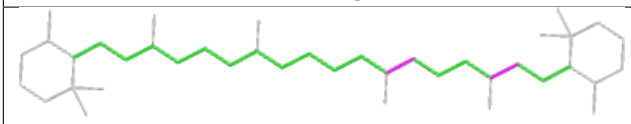
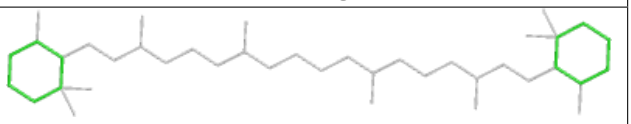
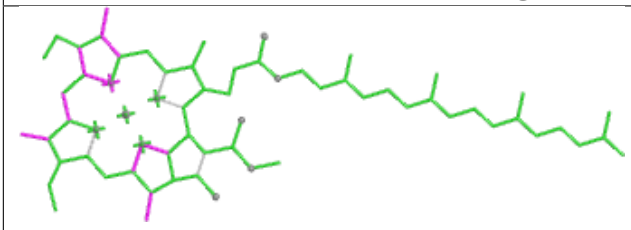


Torsions

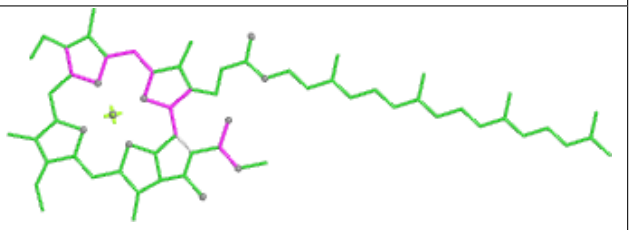


Rings

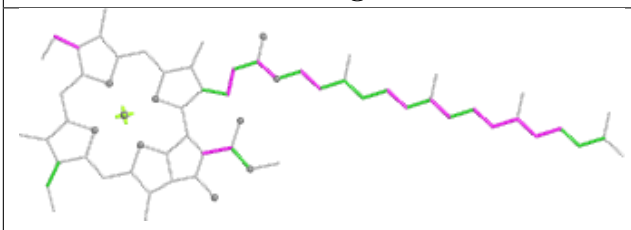
Ligand CLA H 1214



Bond lengths



Bond angles



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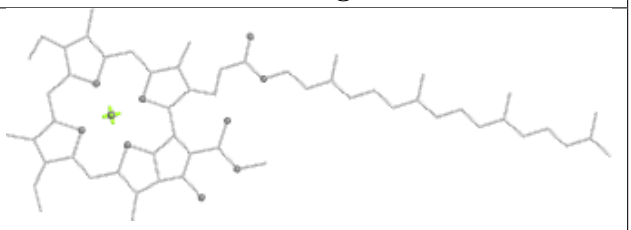
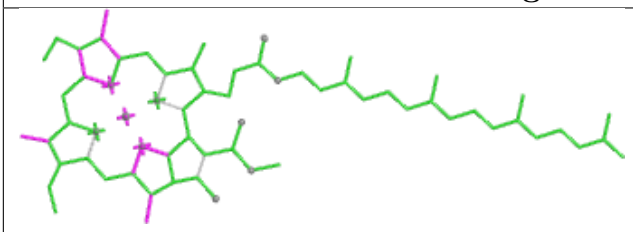


Rings

Ligand CLA f 1205



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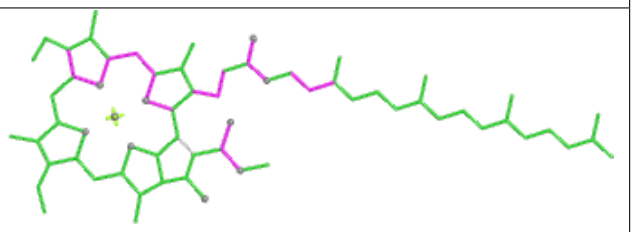

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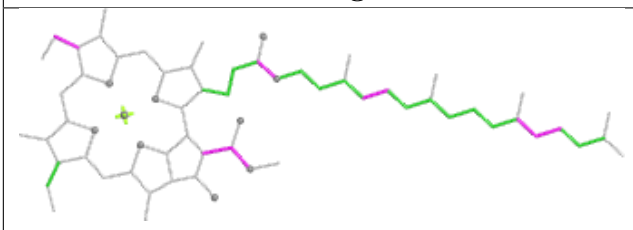

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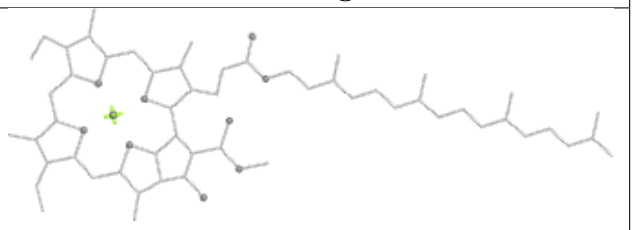
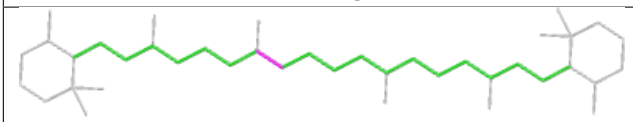


Rings

Ligand BCR j 4016

Bond lengths

Bond angles



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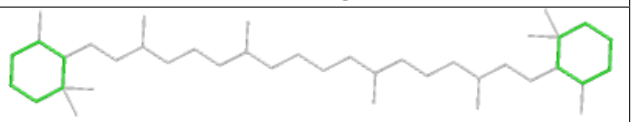
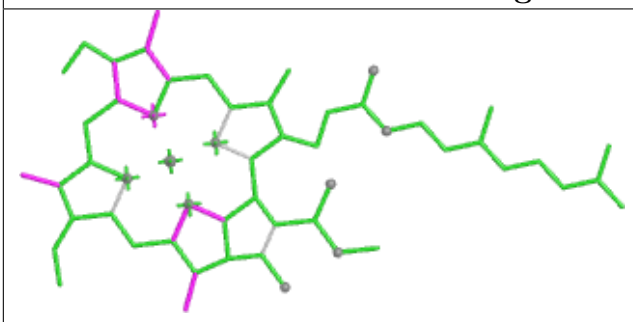


Rings

Ligand CLA H 1228



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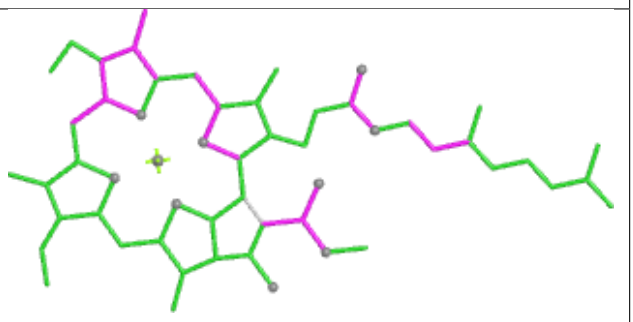
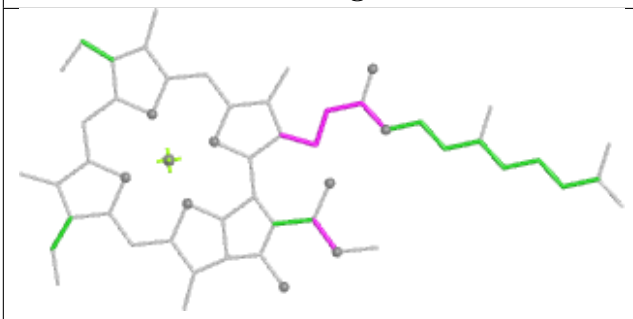


Bond angles



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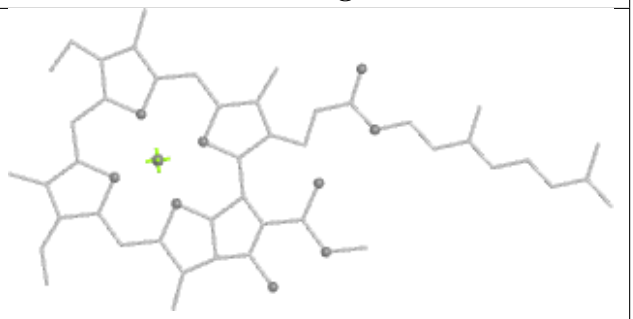
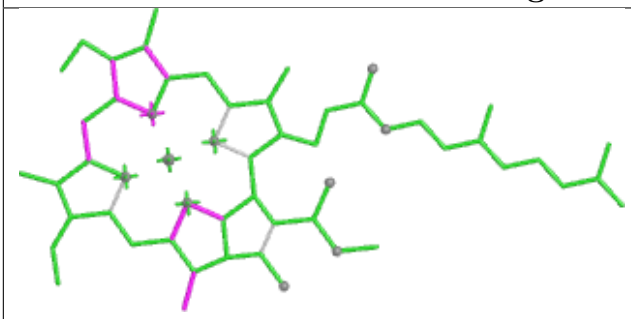


Rings

Ligand CLA b 503



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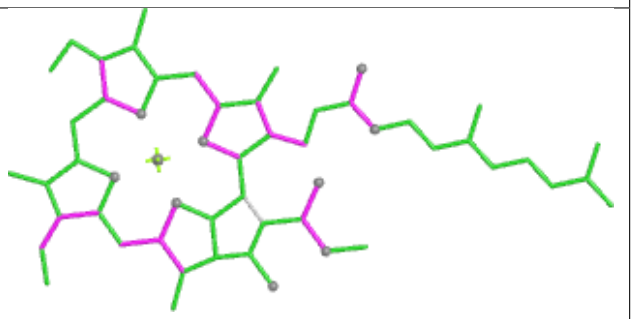
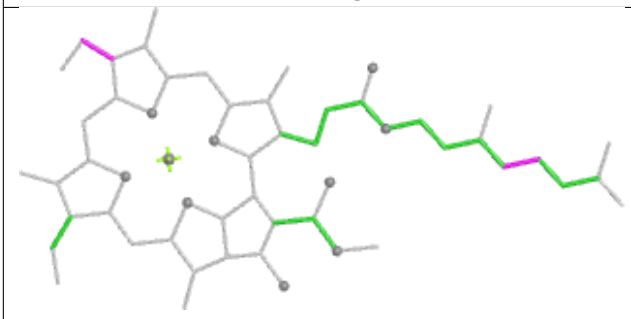


Bond angles



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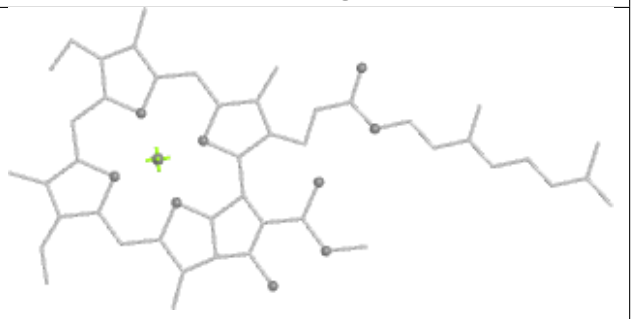
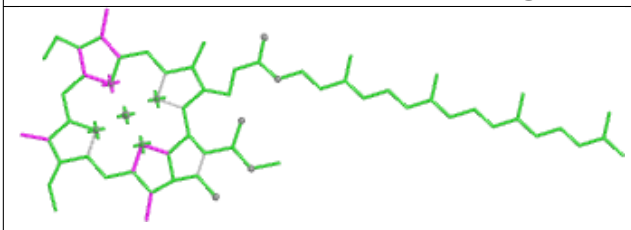


Rings

Ligand CLA e 1109



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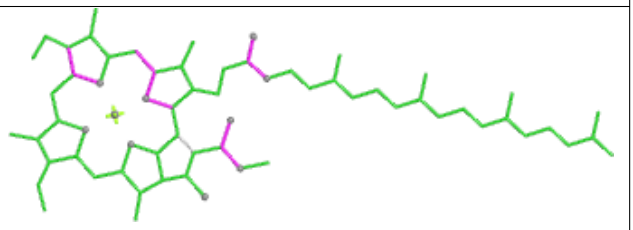
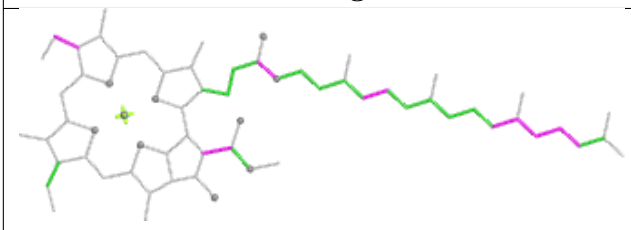


Bond angles



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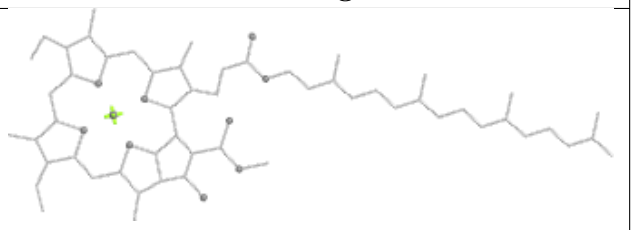
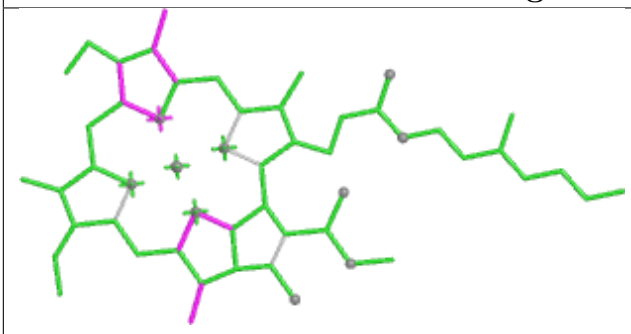


Rings

Ligand CLA Z 512



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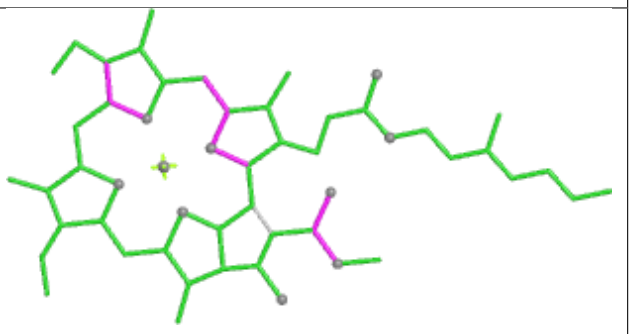

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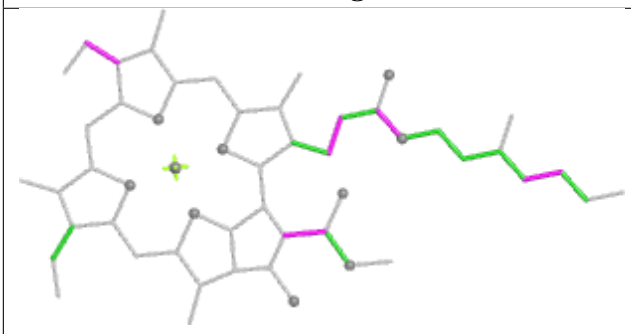

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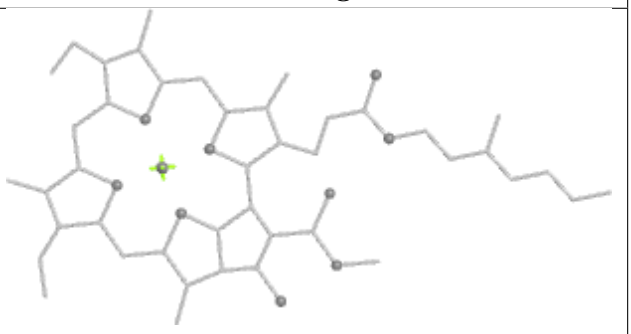

Rings

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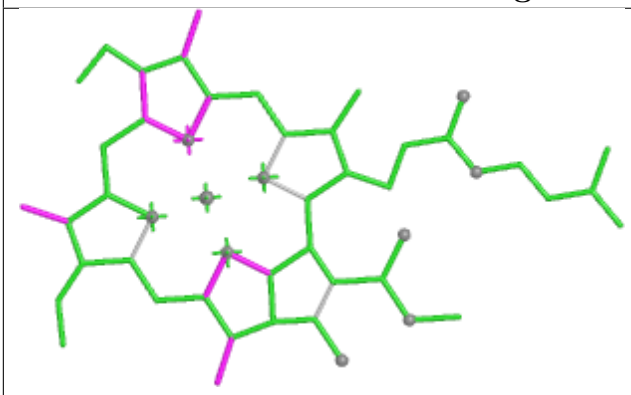

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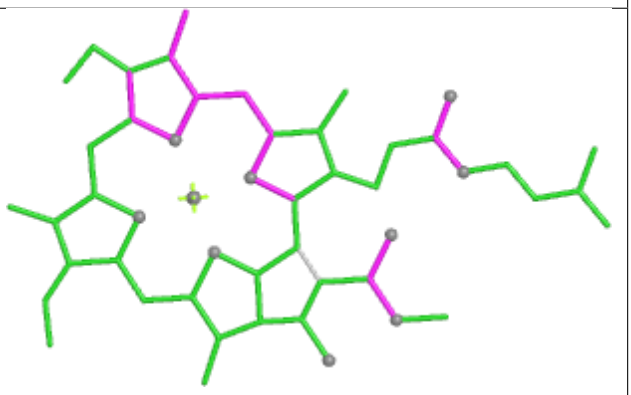

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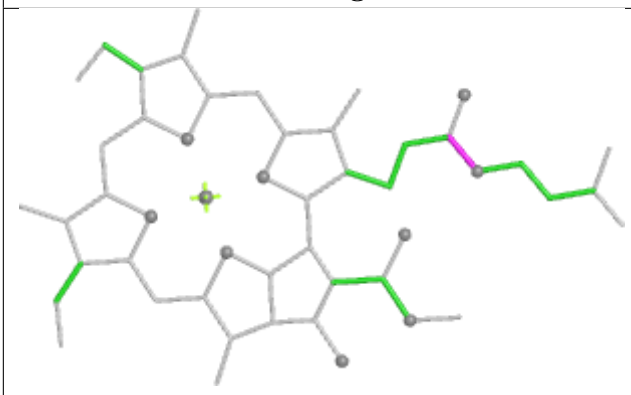

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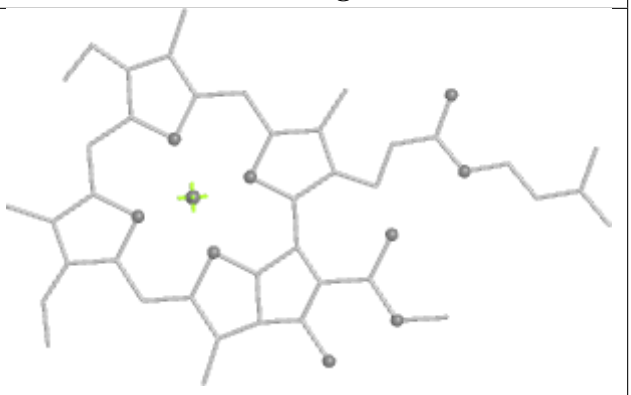

Rings

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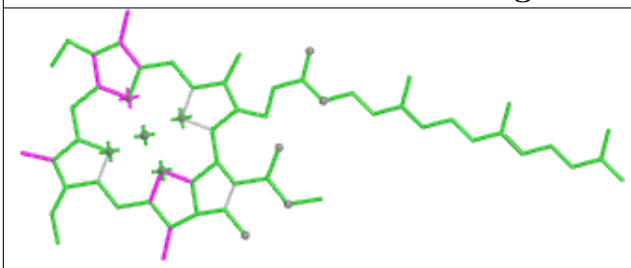

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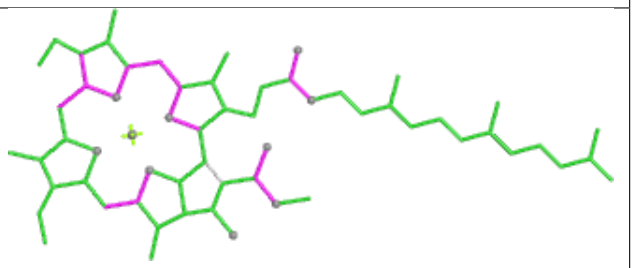

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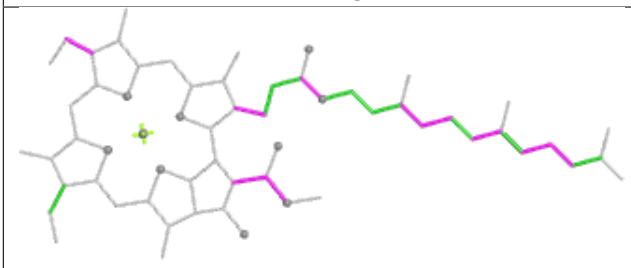

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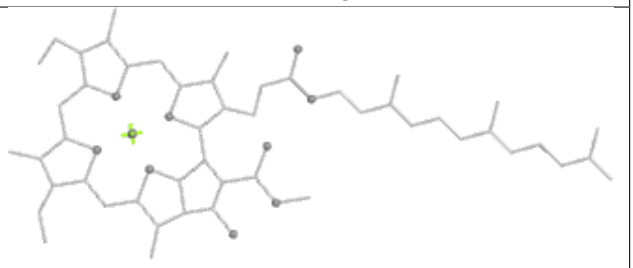
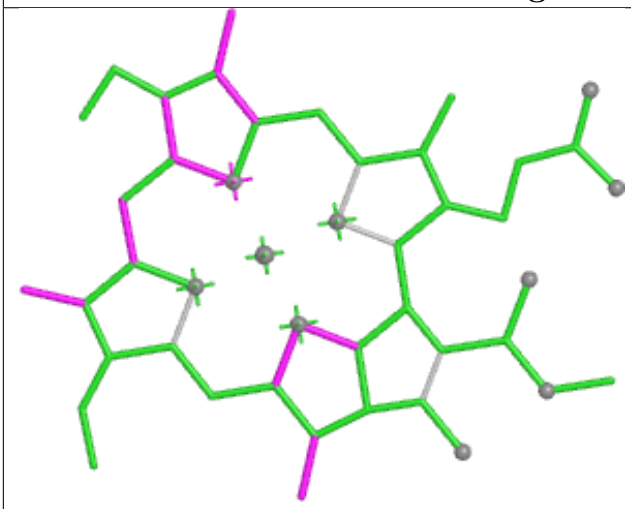


Rings

Ligand CLA 5 513



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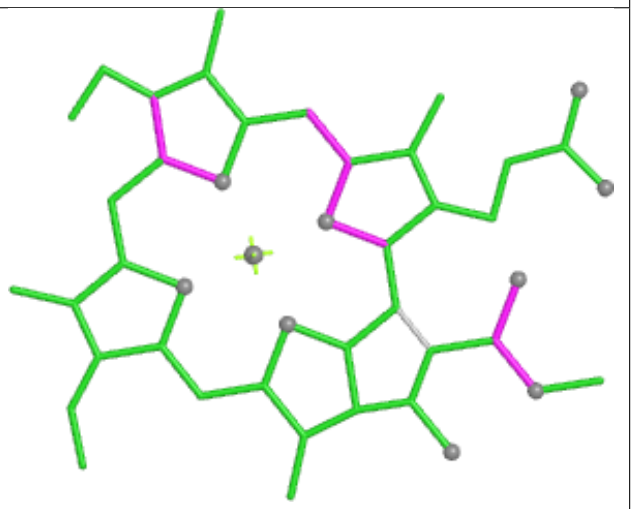
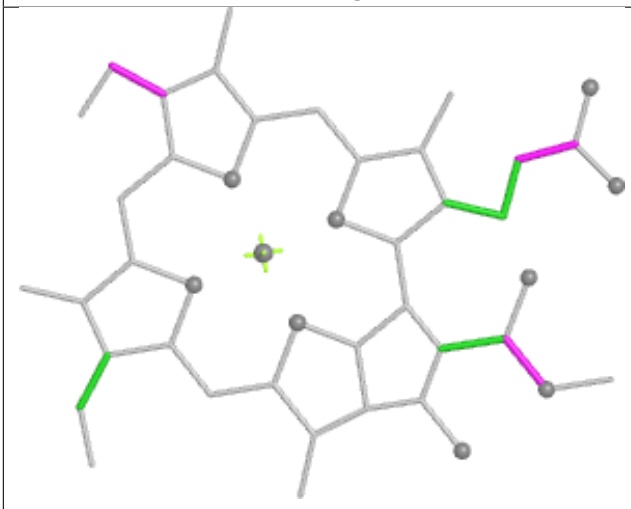


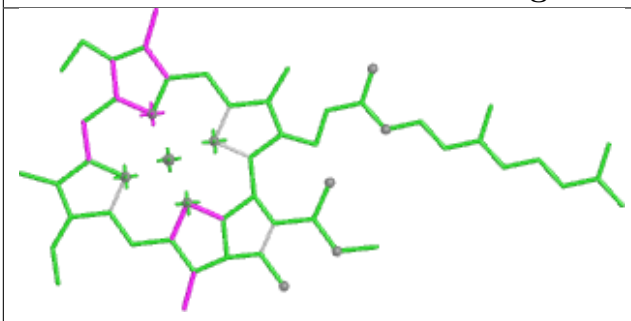
Bond angles



Torsions

Rings

Ligand CLA r 511



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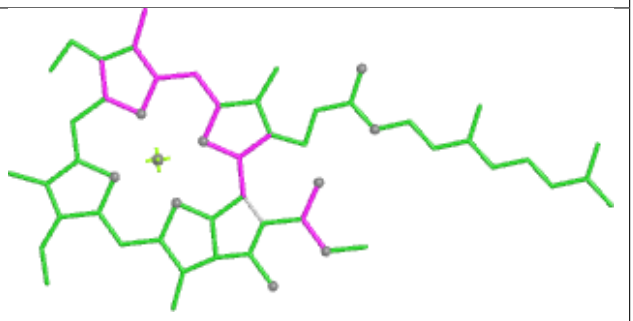
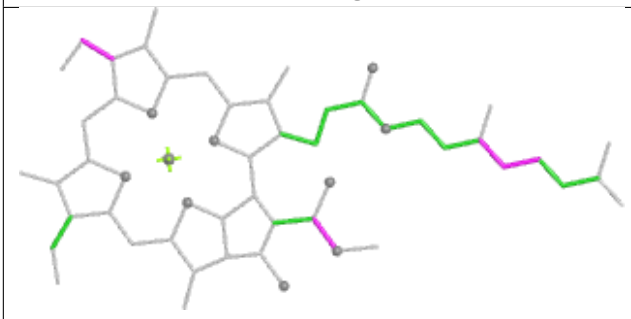
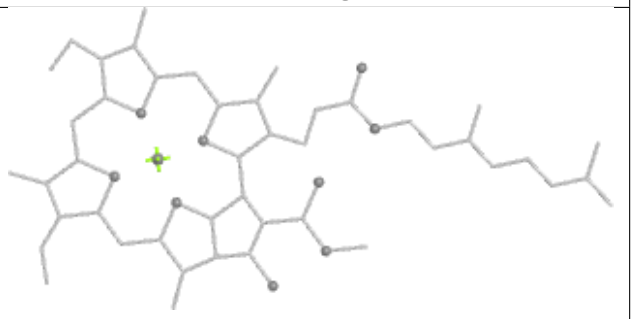


Bond angles

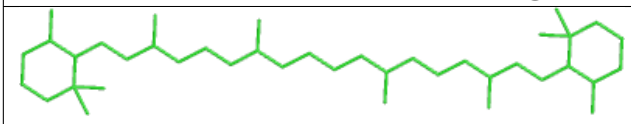


Torsions



Rings

Ligand BCR 2 522



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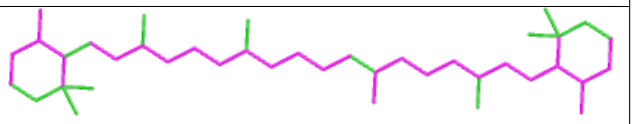
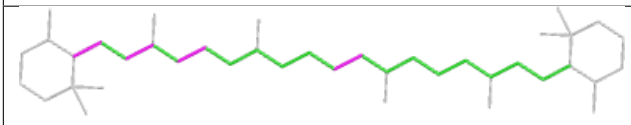


Bond angles



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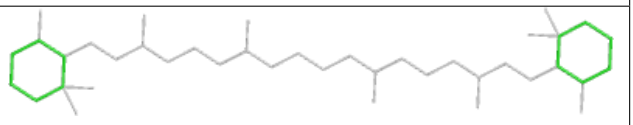
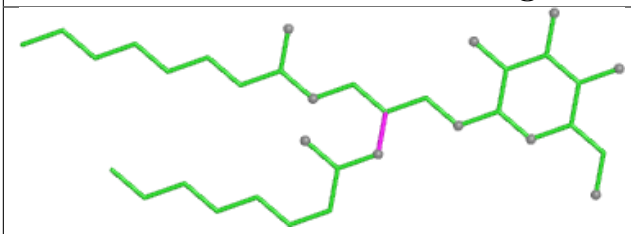


Rings

Ligand LMG l 5104



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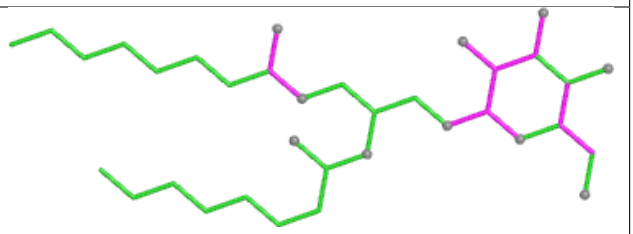
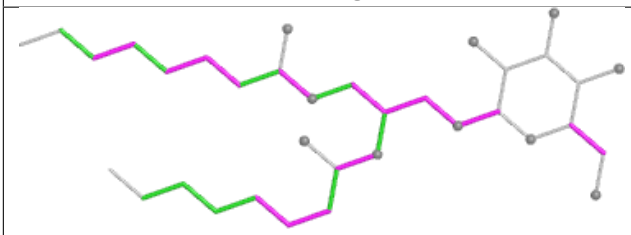


Bond angles



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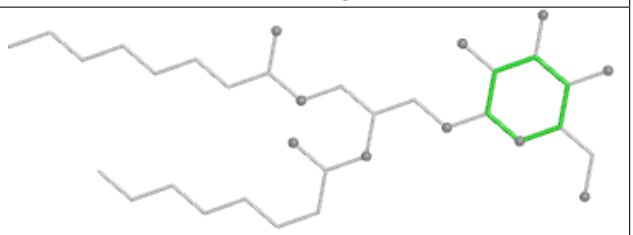
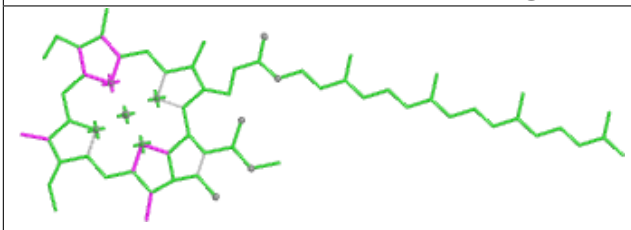
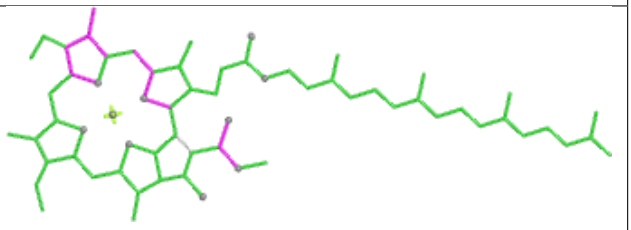
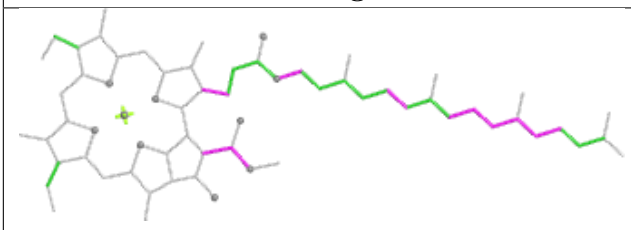
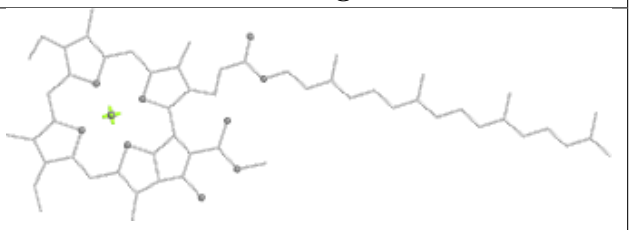
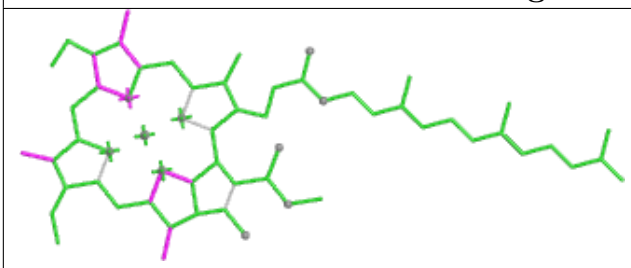
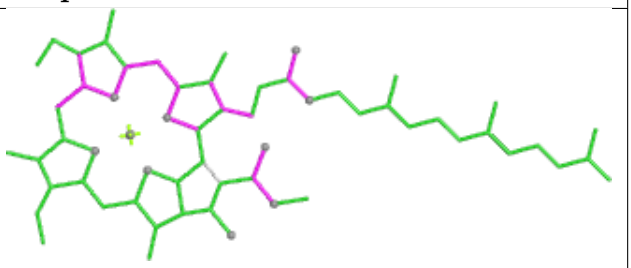
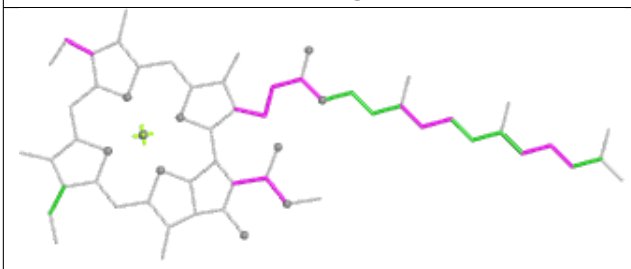
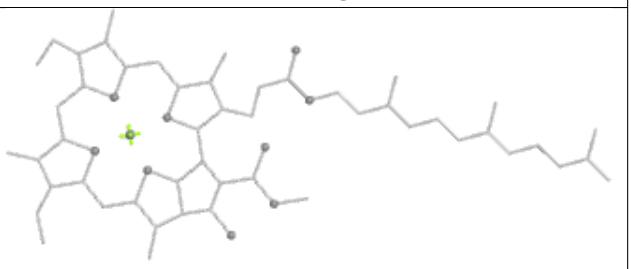
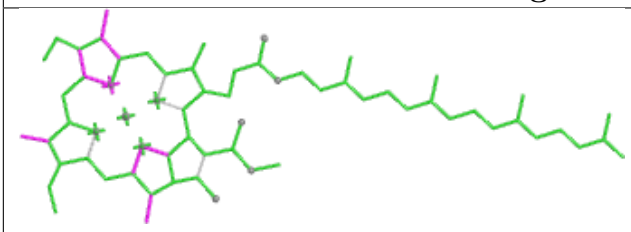


Rings

Ligand CLA f 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 507



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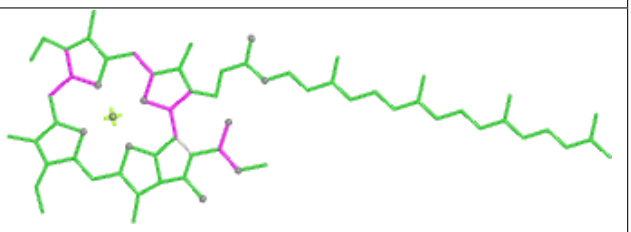

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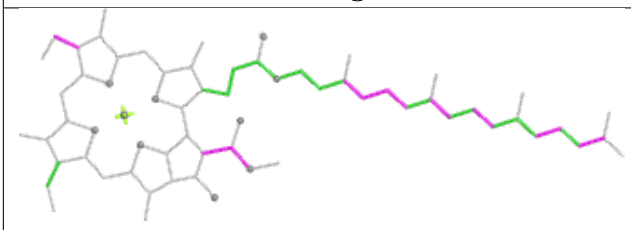
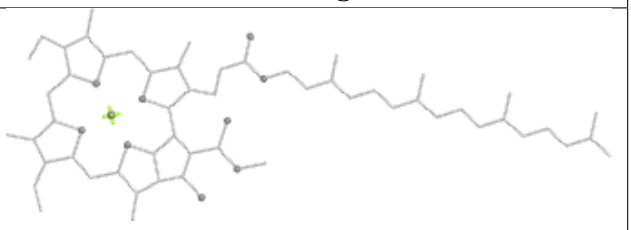
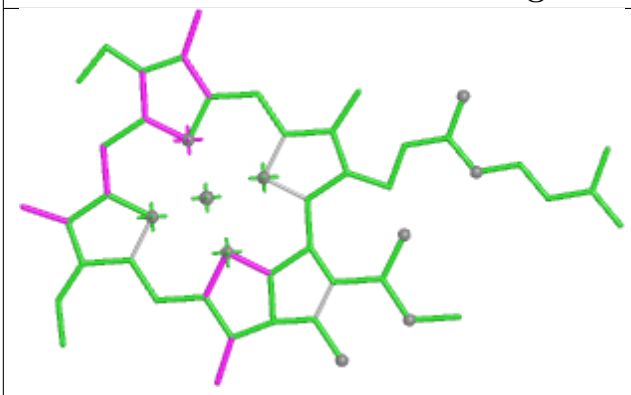


Torsions



Rings

Ligand CLA u 502



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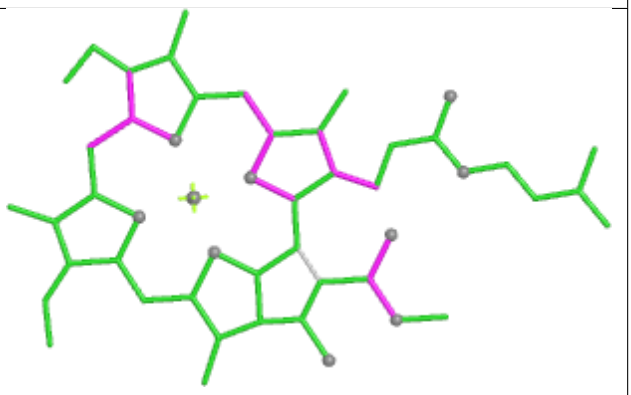
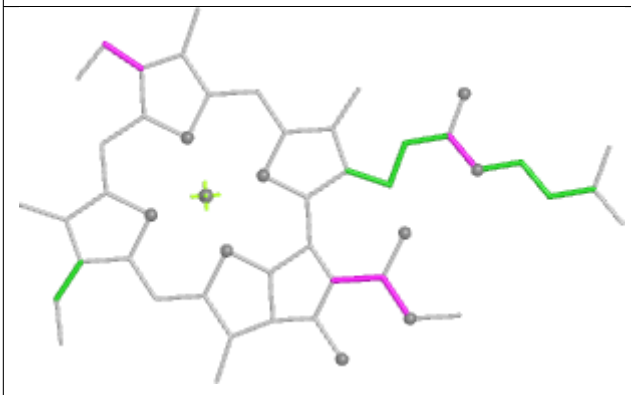


Bond angles



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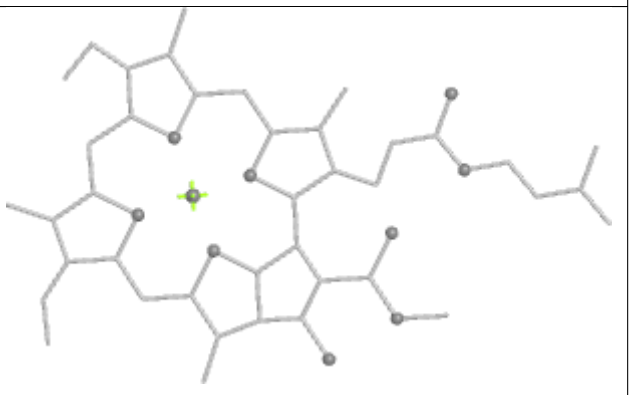
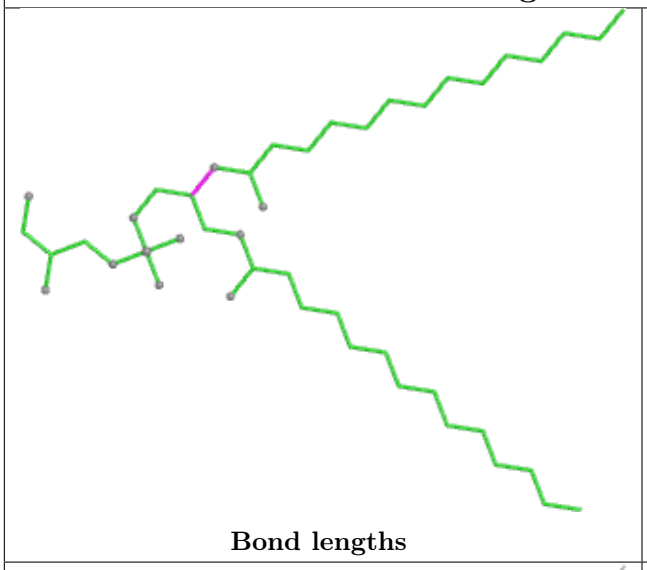


Rings

Ligand LHG e 5005



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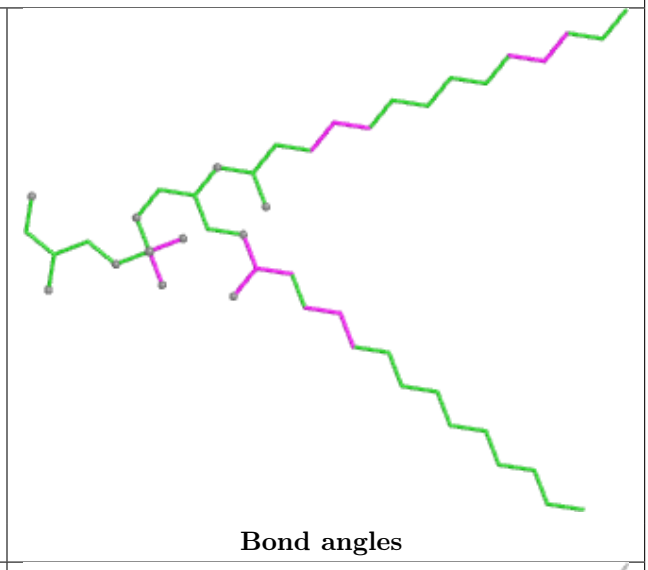
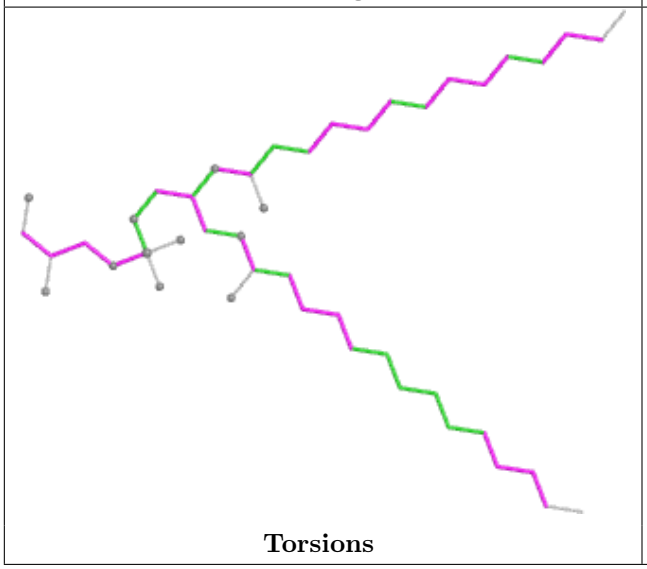


Bond angles



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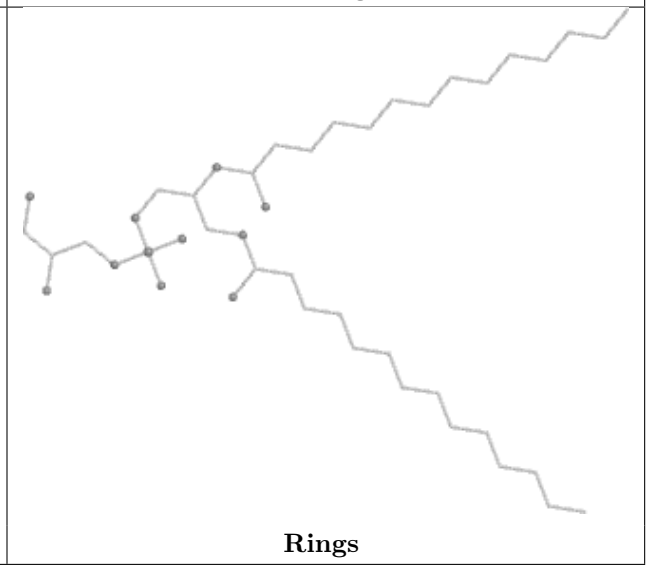
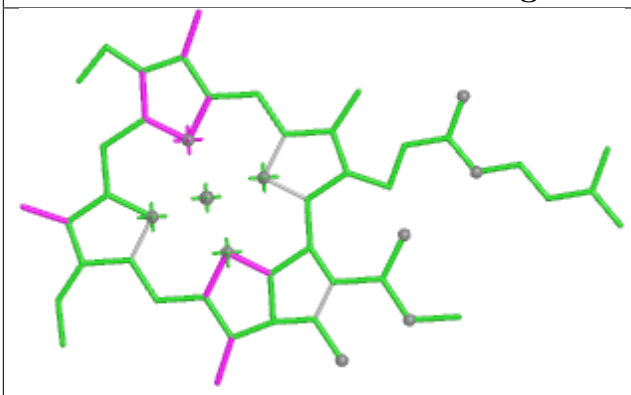


Rings

Ligand CLA e 1114



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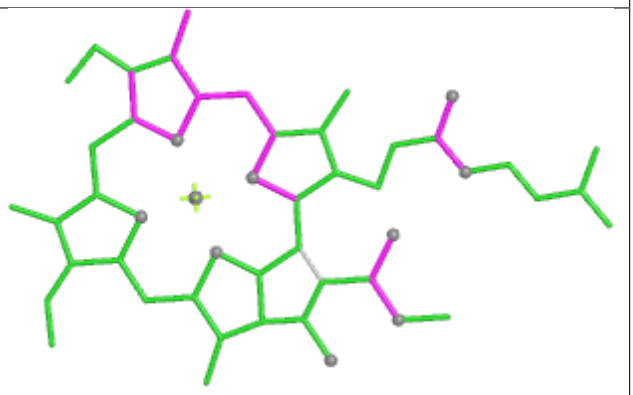

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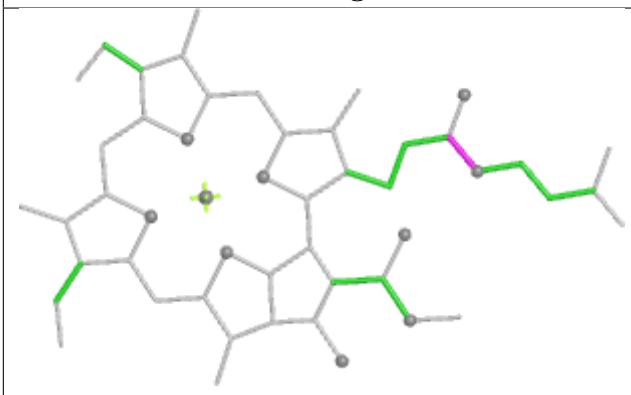

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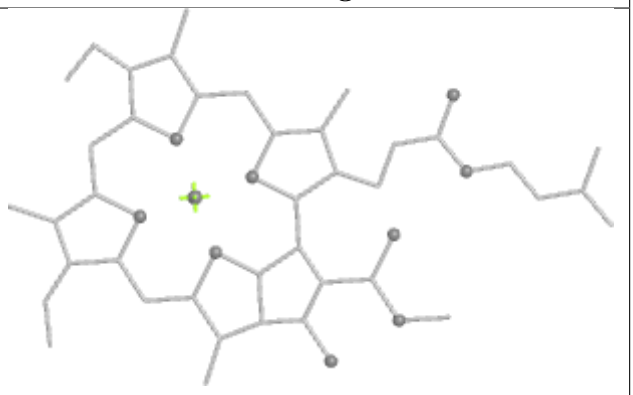
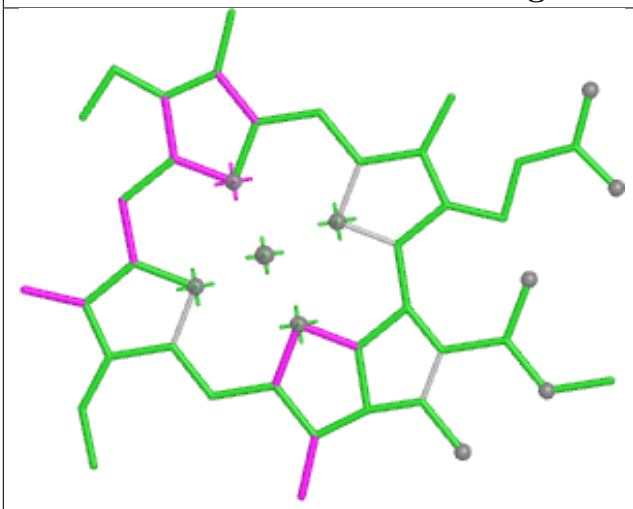


Rings

Ligand CLA v 517



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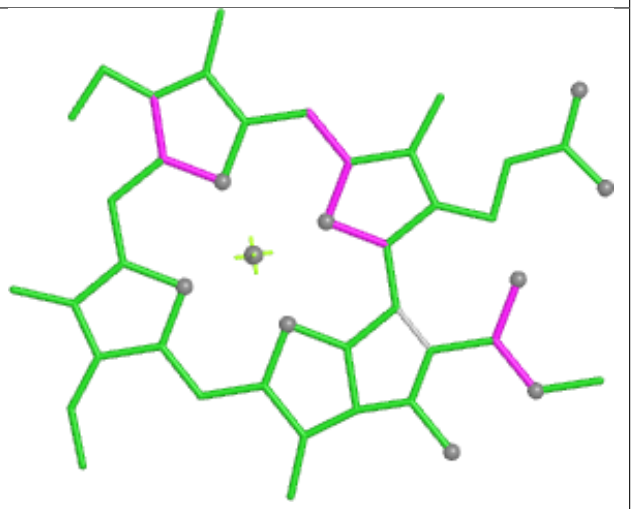
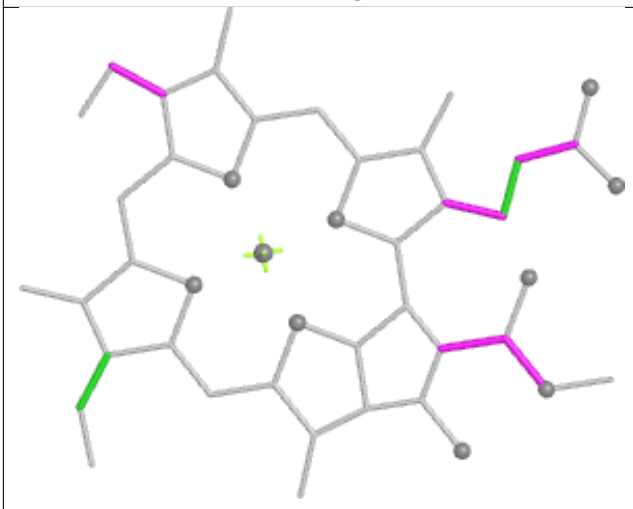


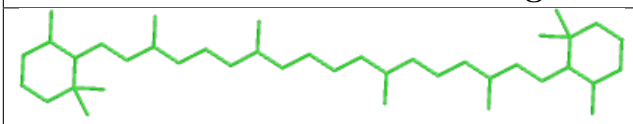
Bond angles



Torsions

Rings

Ligand BCR b 524



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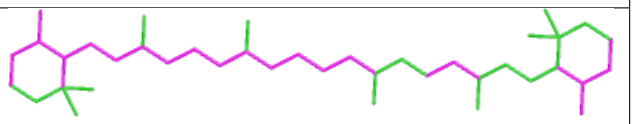

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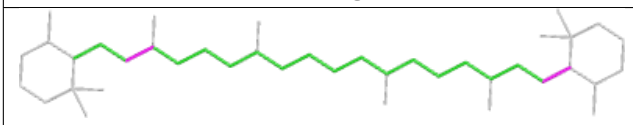

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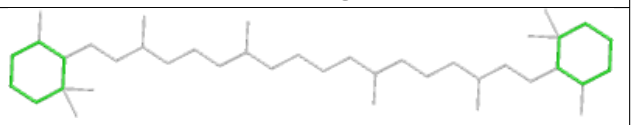
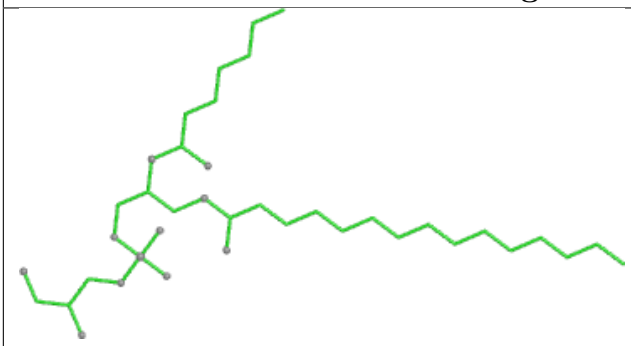


Rings

Ligand LHG f 1842



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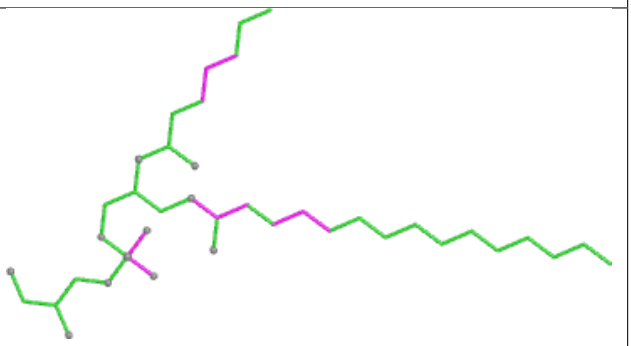

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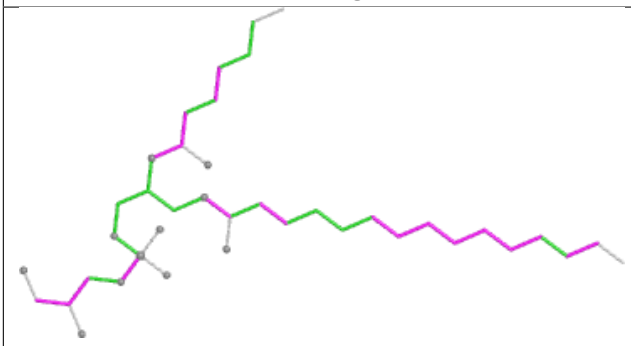

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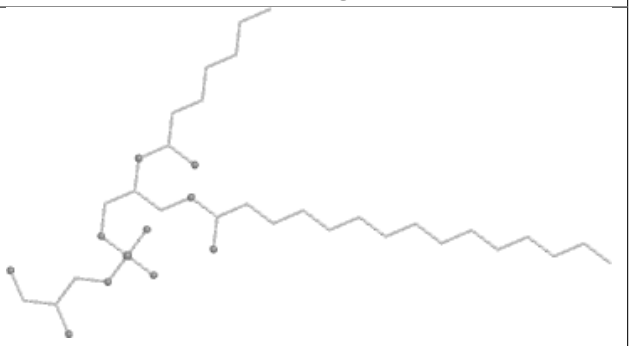
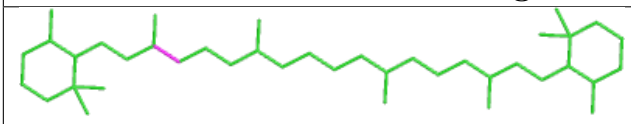


Rings

Ligand BCR A 4008



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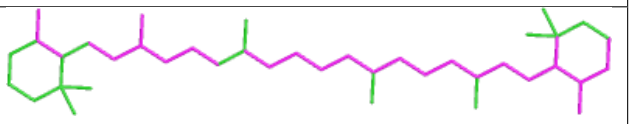
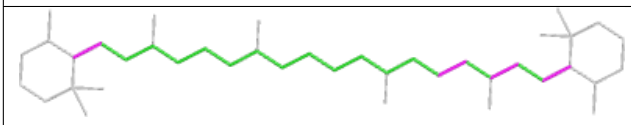


Bond angles



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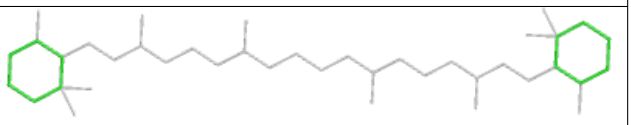
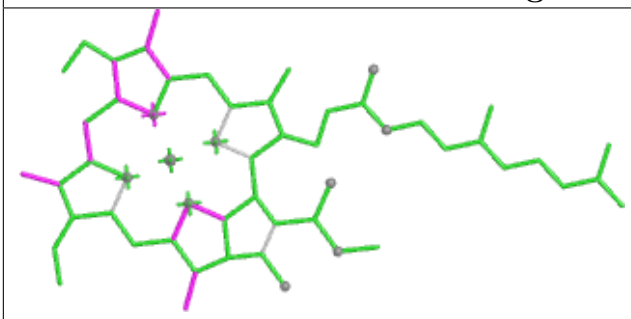


Rings

Ligand CLA Z 506



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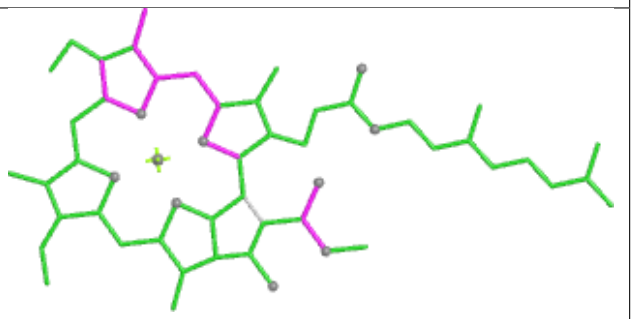
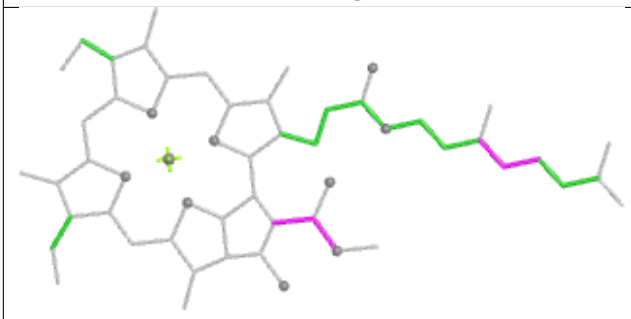


Bond angles



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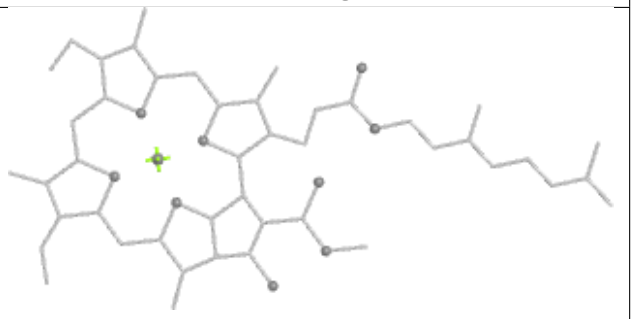
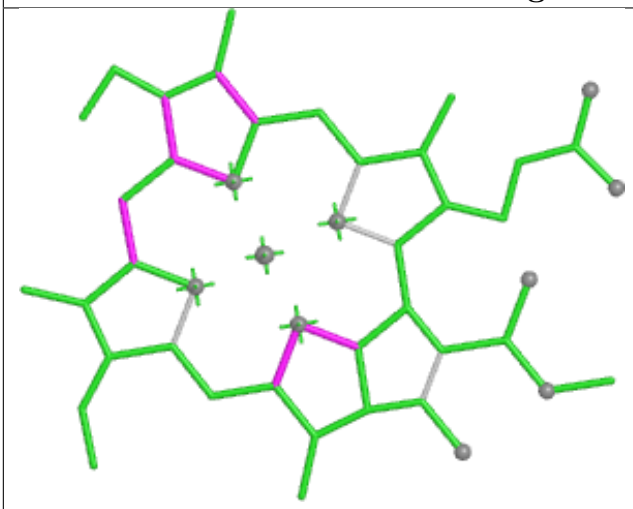


Rings

Ligand CLA v 513



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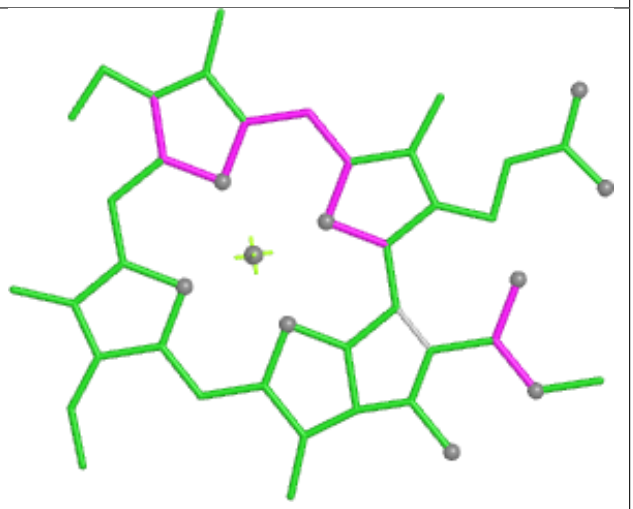
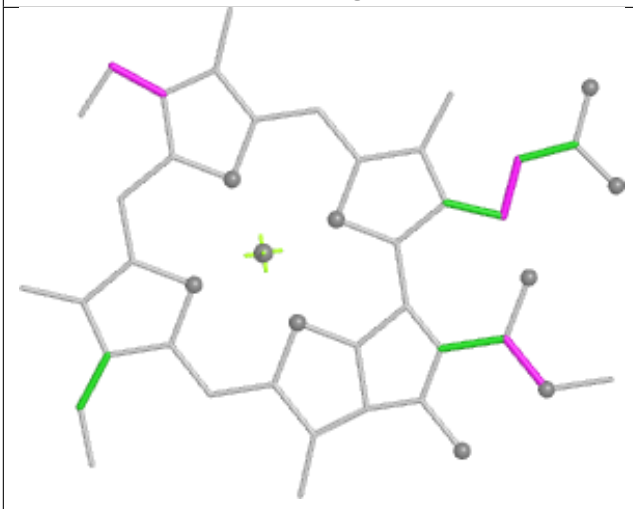


Bond angles



Torsions

Rings

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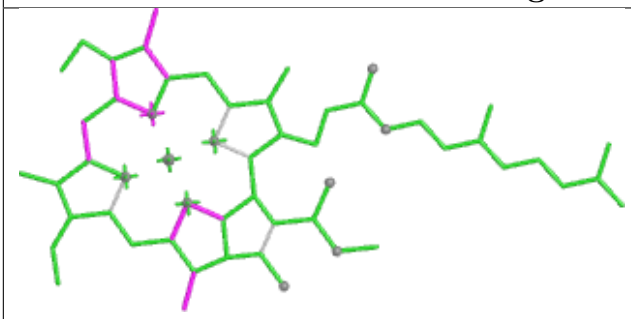

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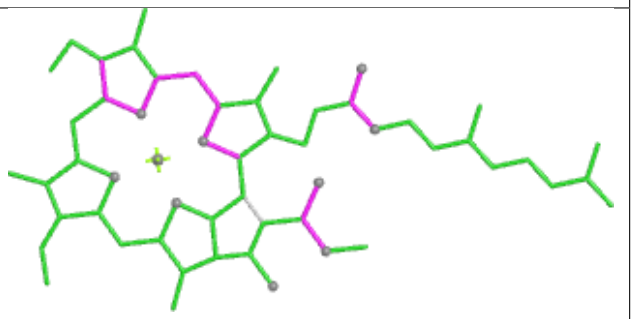
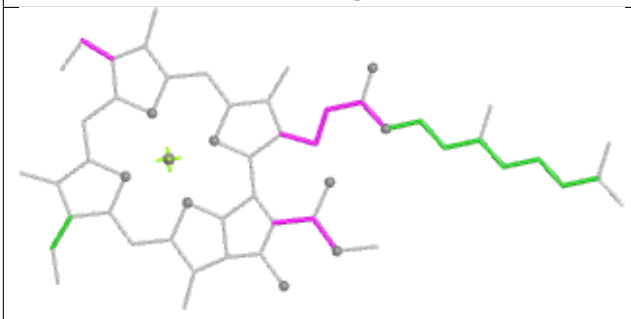
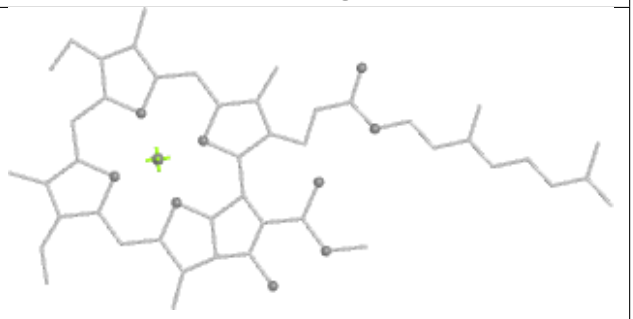


Bond angles

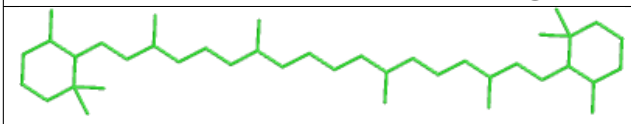


Torsions



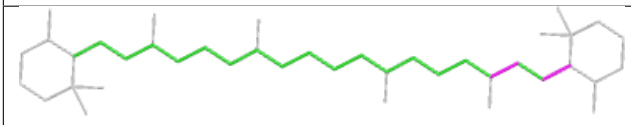
Rings

Ligand BCR 3 523

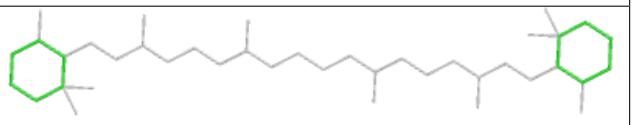


Bond lengths

Bond angles

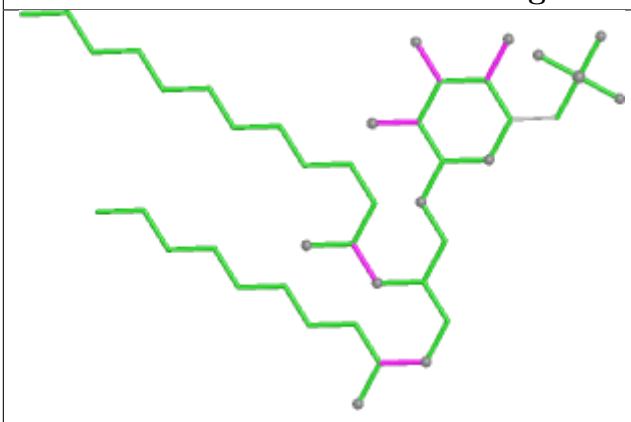


Torsions



Rings

Ligand SQD 3 822



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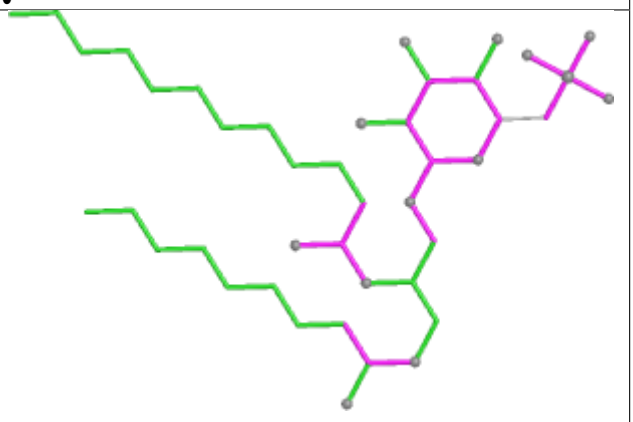

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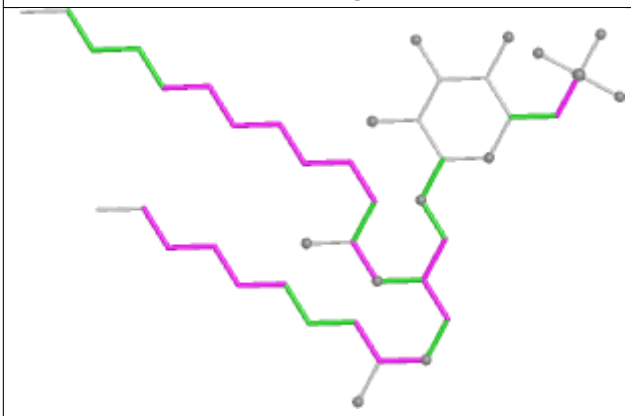
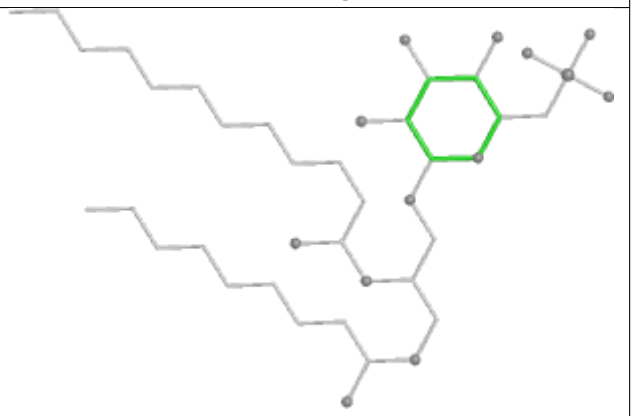
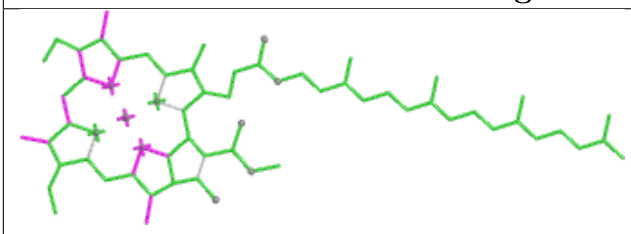


Torsions



Rings

Ligand CLA H 1012



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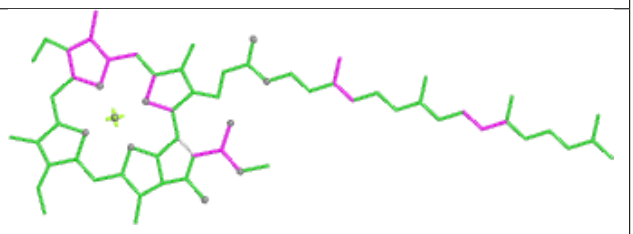

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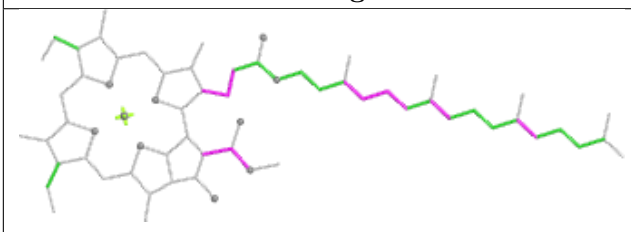

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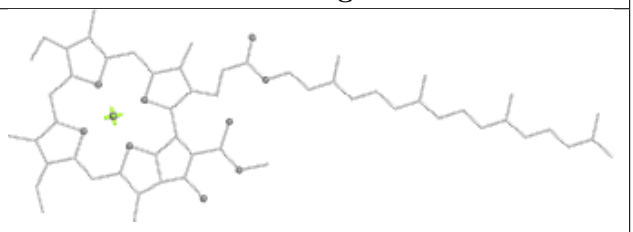
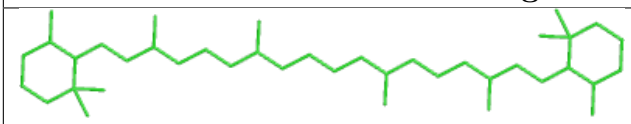


Rings

Ligand BCR l 4013



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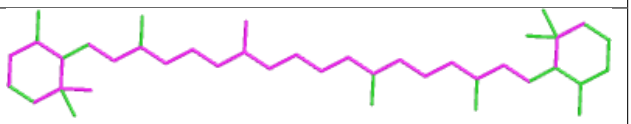

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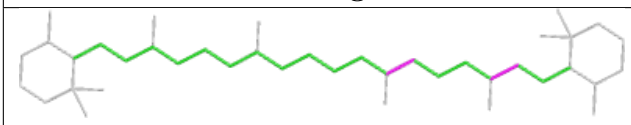

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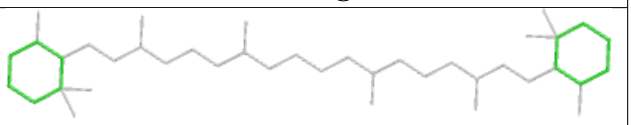
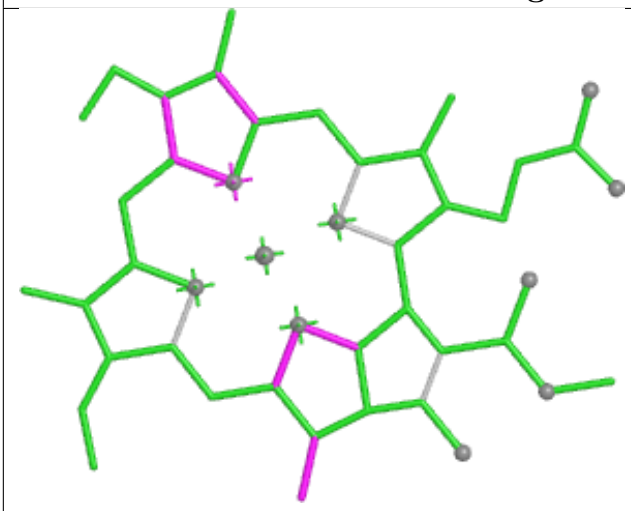


Rings

Ligand CLA b 507



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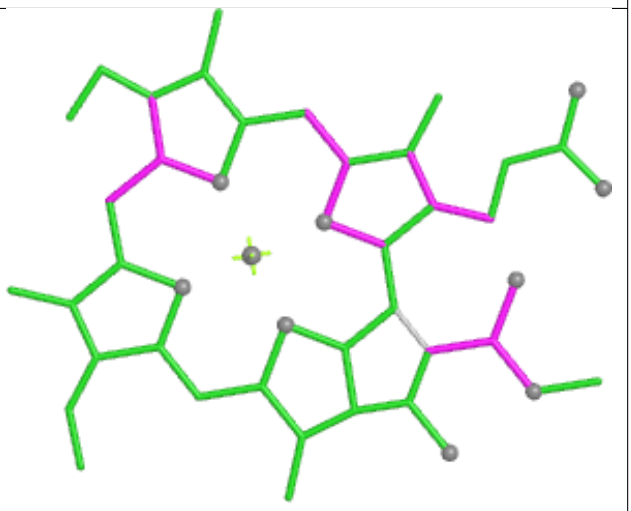

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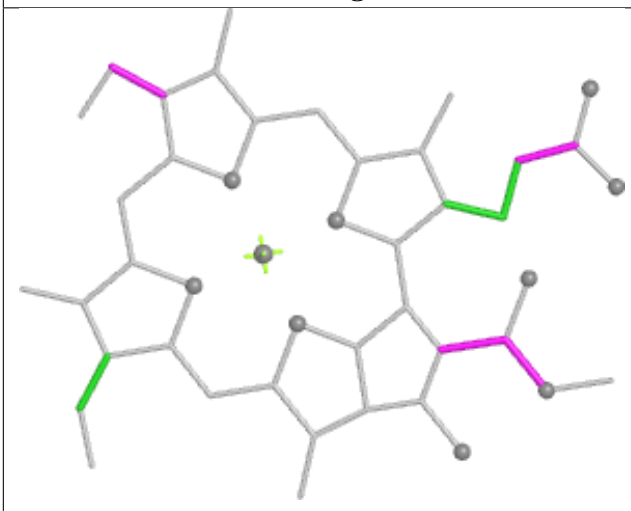

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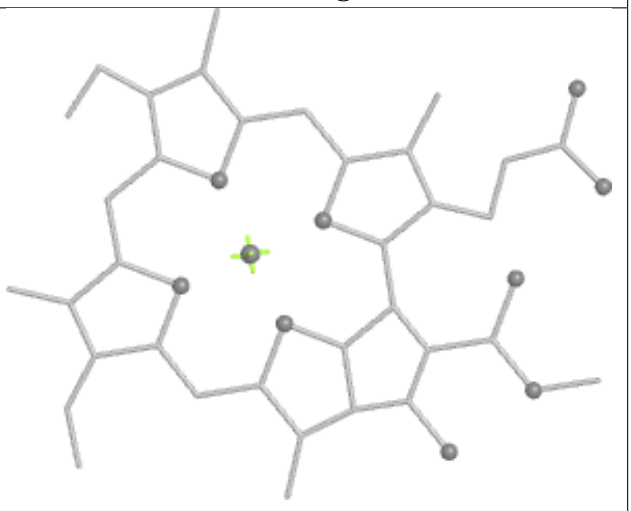
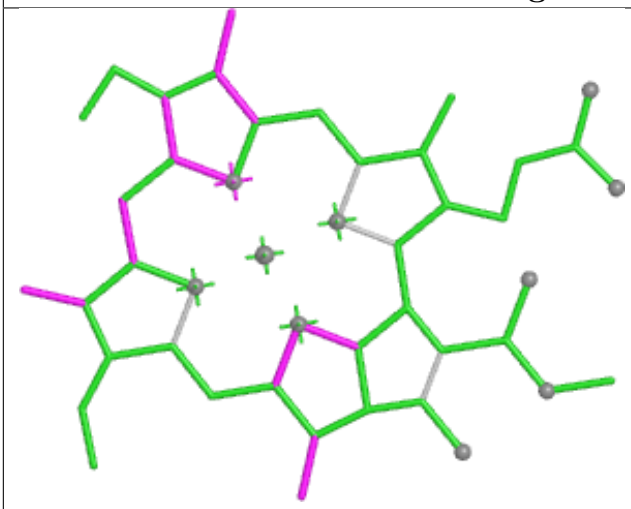


Rings

Ligand CLA 1 504



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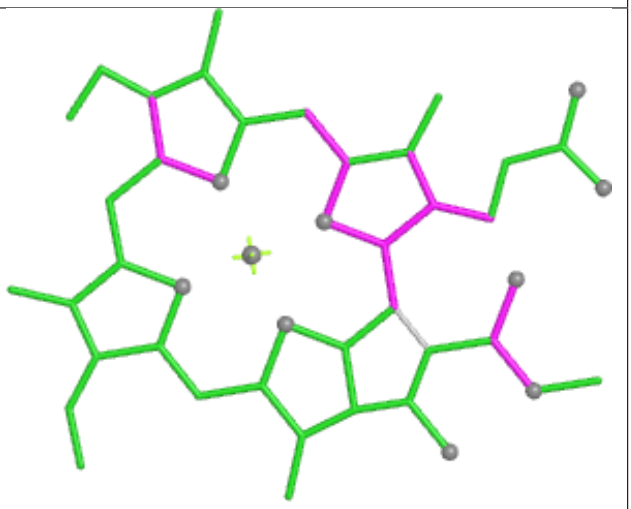

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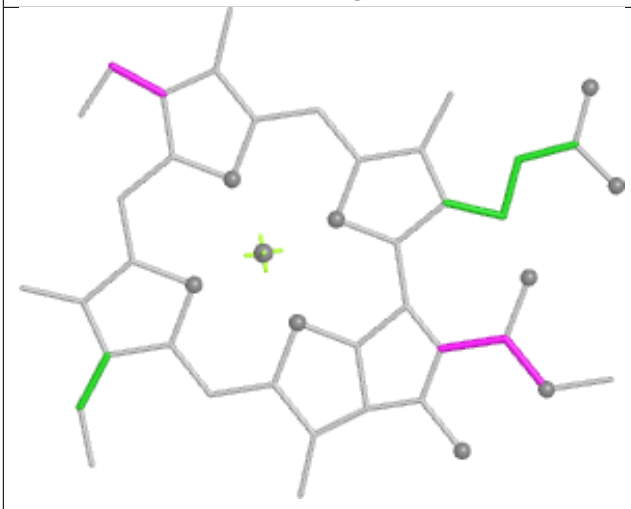

Torsions

Rings

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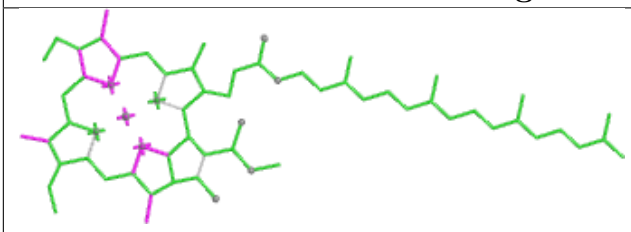

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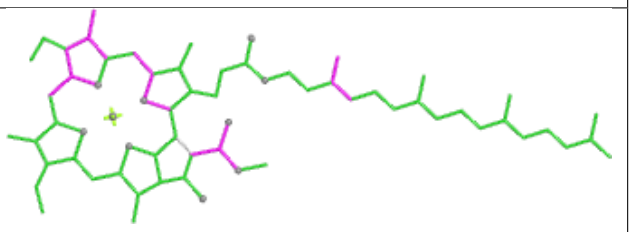

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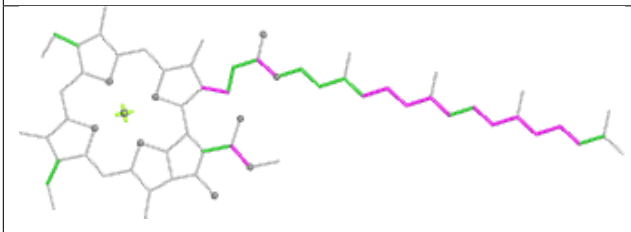

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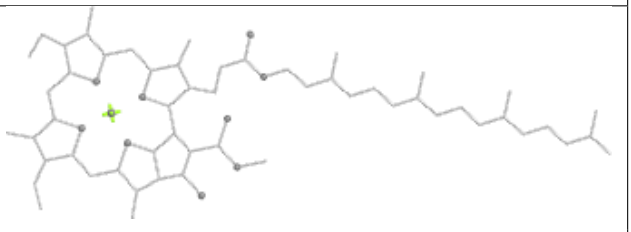
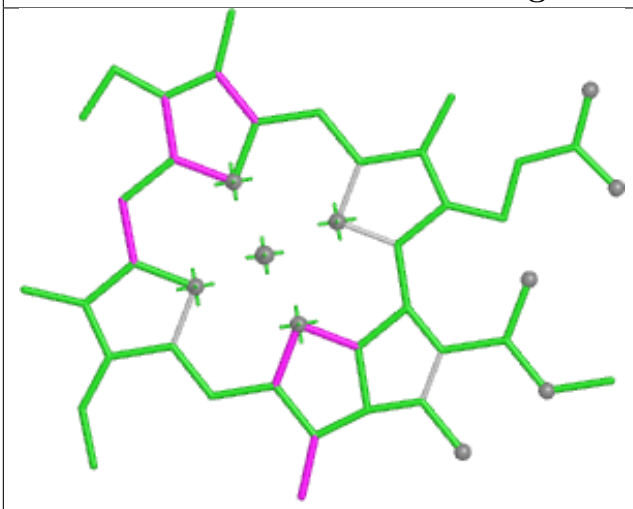


Rings

Ligand CLA 4 504



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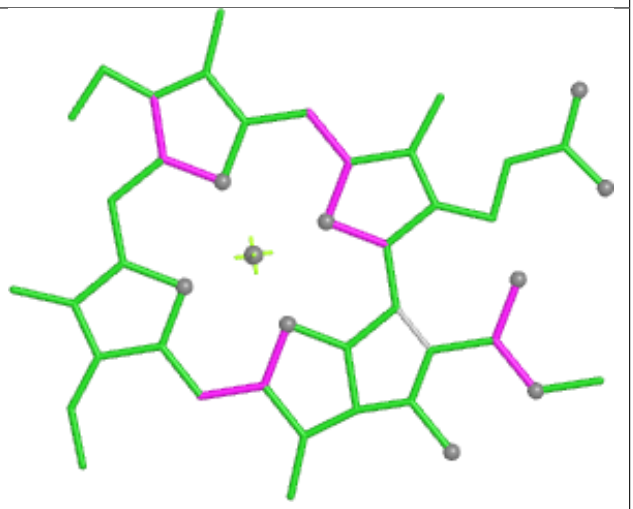

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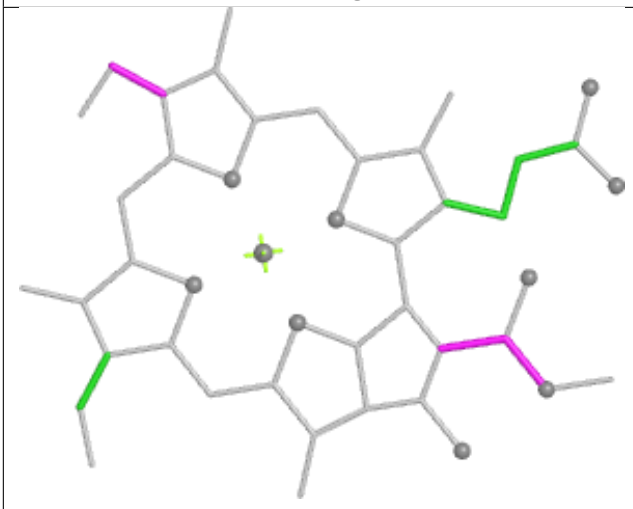

Torsions

Rings

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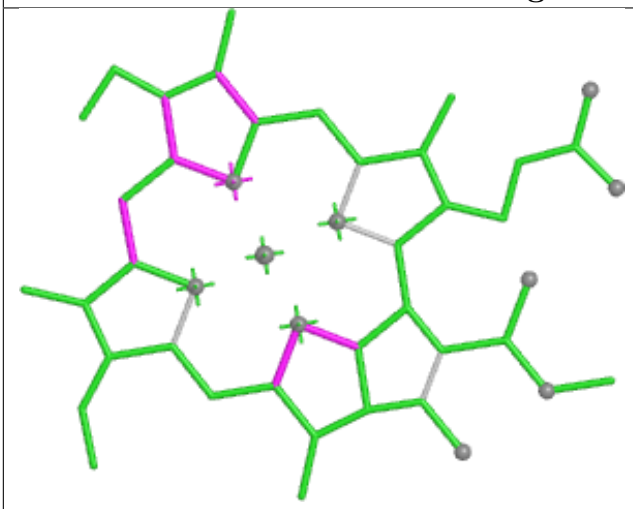

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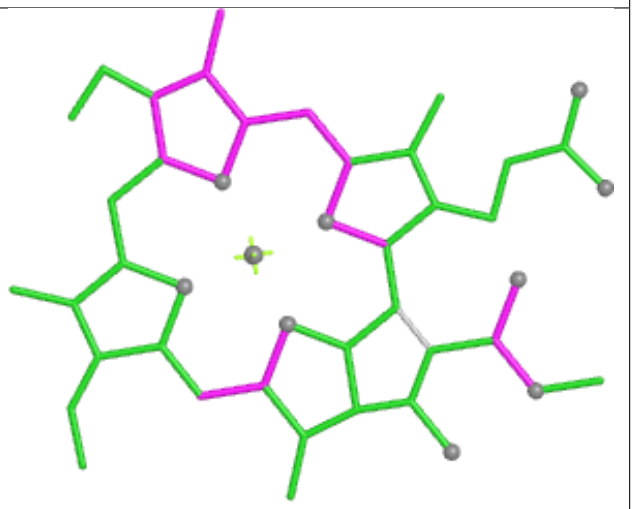

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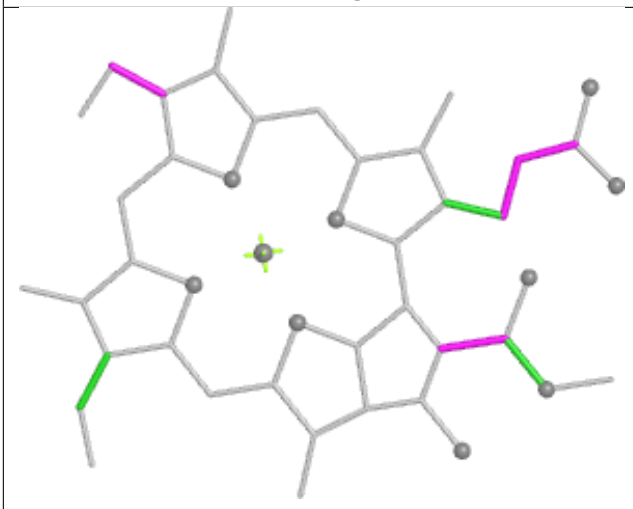

Torsions

Rings

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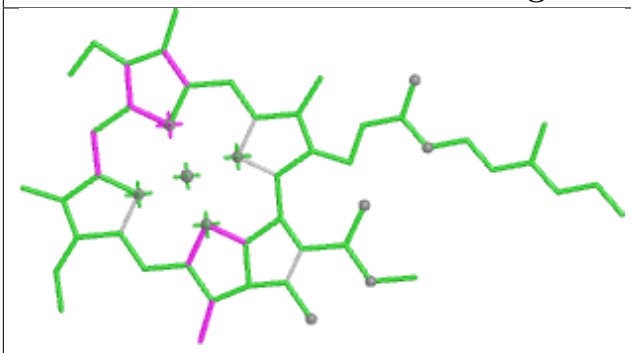
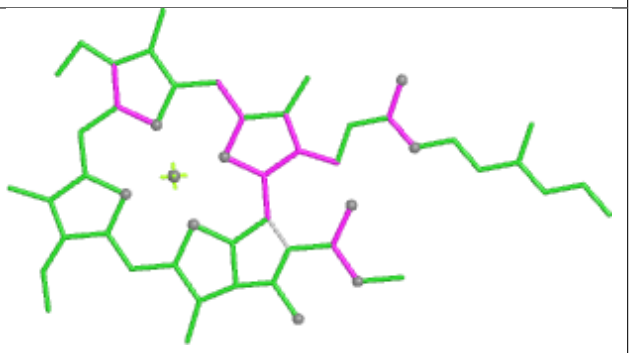
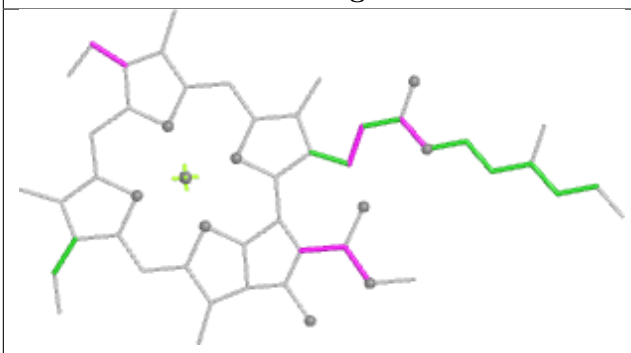
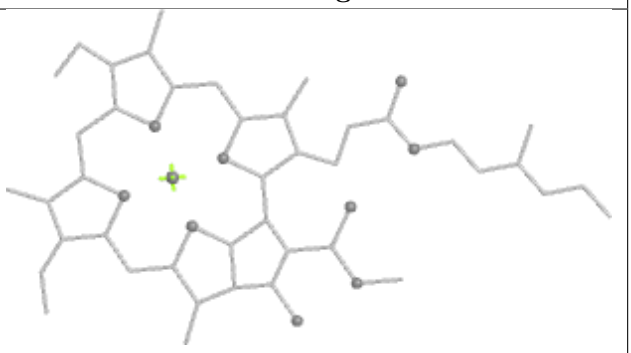
	
Bond lengths	Bond angles
	
Torsions	Rings

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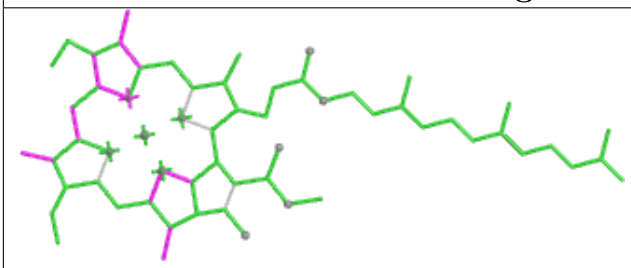	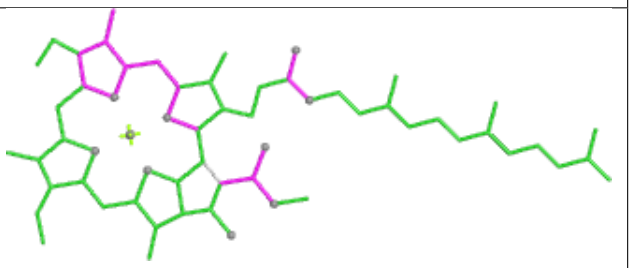
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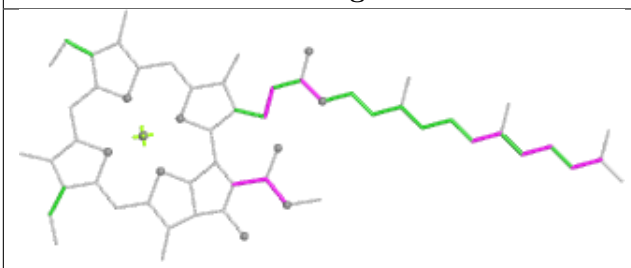
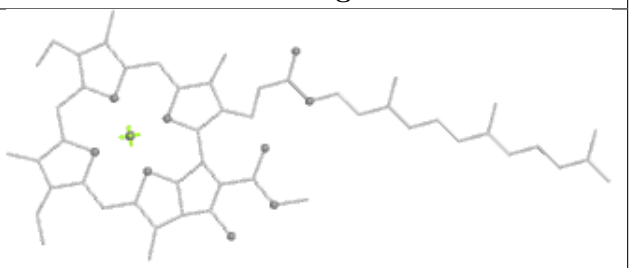
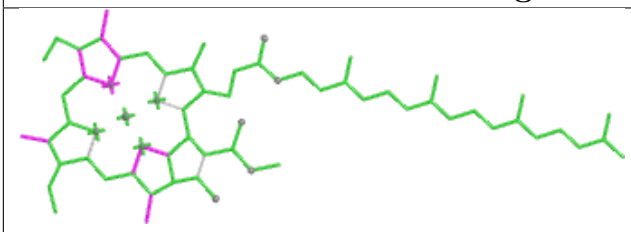
	
Torsions	Rings

Ligand CLA A 1104



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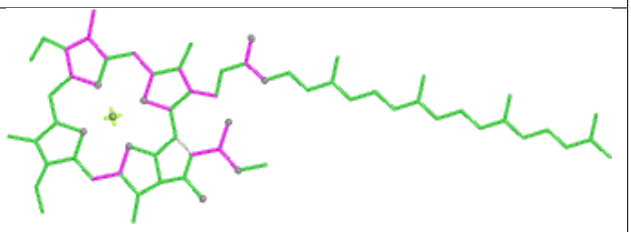

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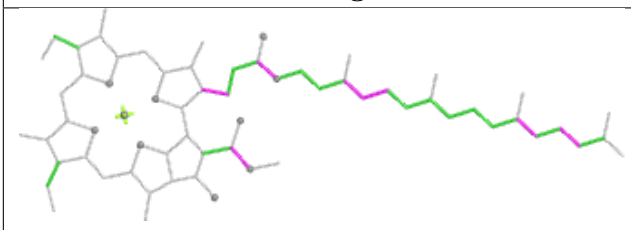
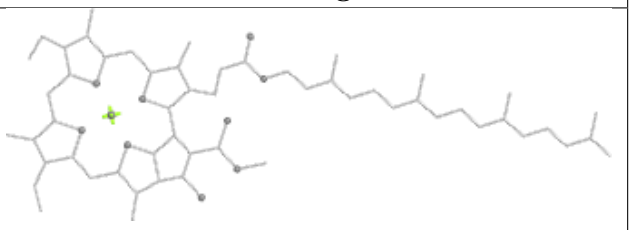
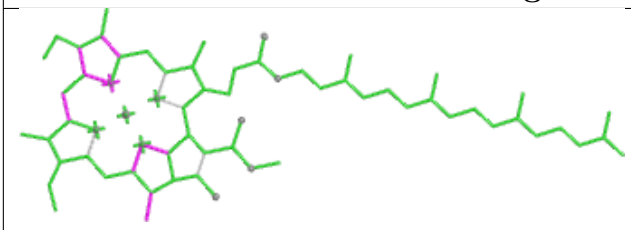


Torsions



Rings

Ligand CLA Y 505



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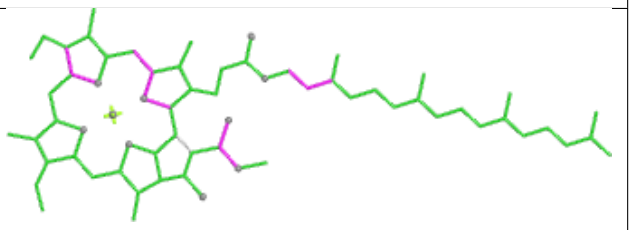
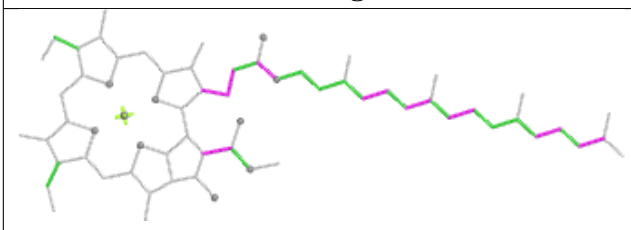


Bond angles



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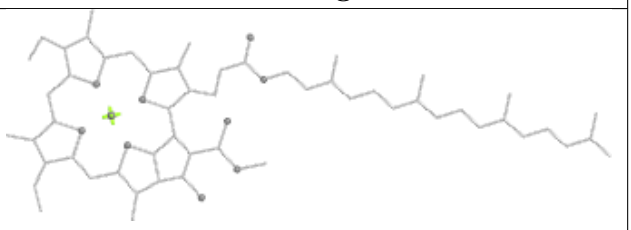
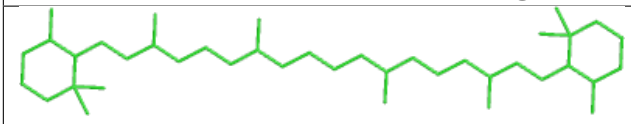


Rings

Ligand BCR B 4017



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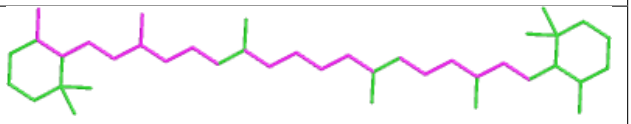
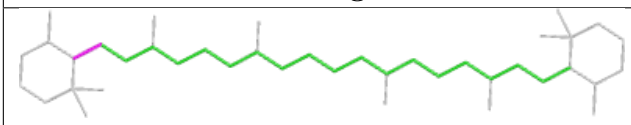


Bond angles



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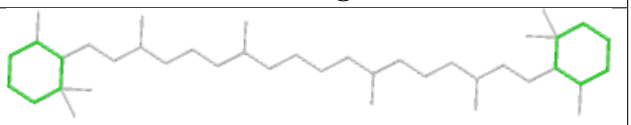
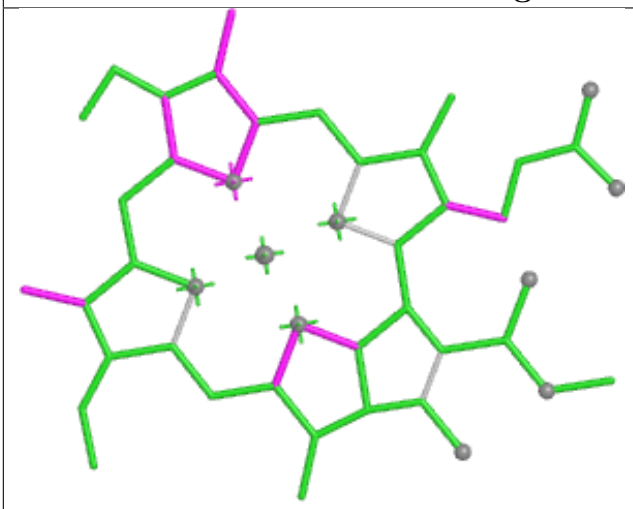


Rings

Ligand CLA G 1801



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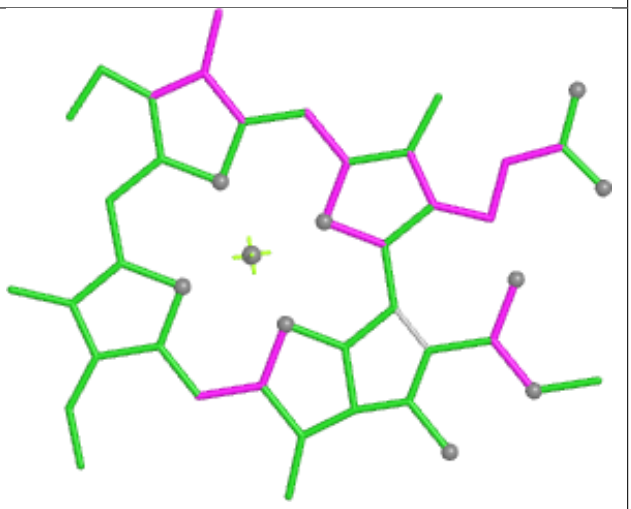
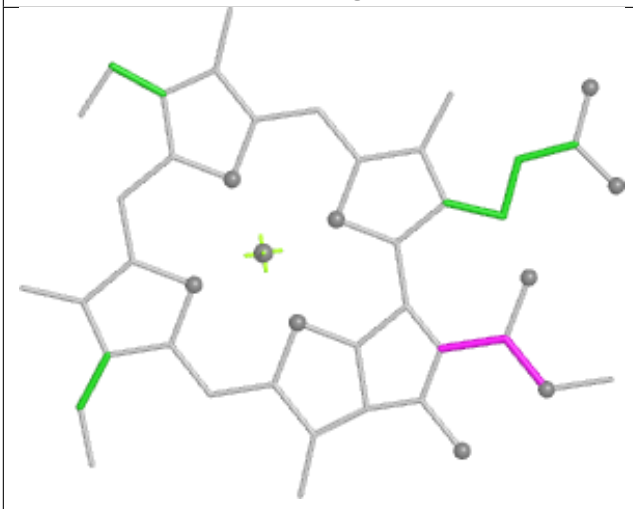


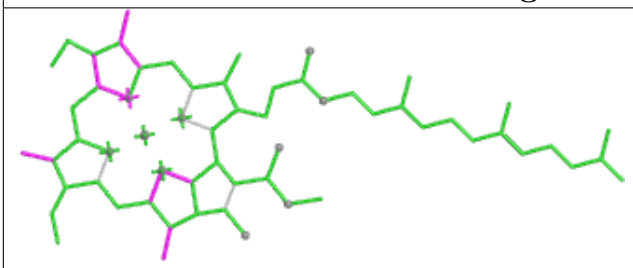
Bond angles



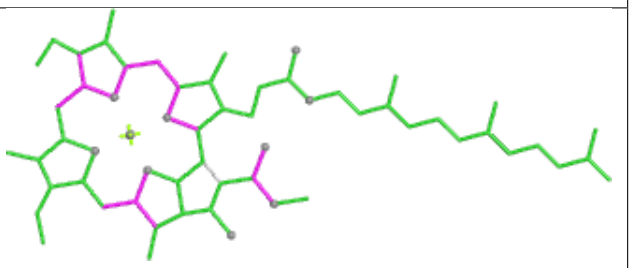
Torsions

Rings

Ligand CLA e 1122



Bond lengths



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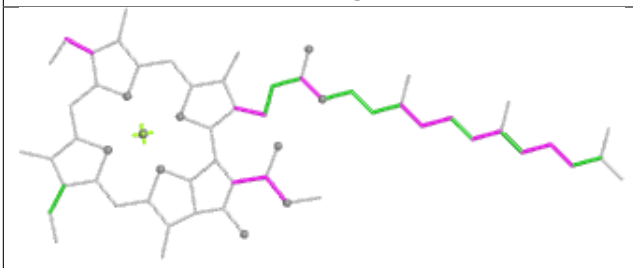

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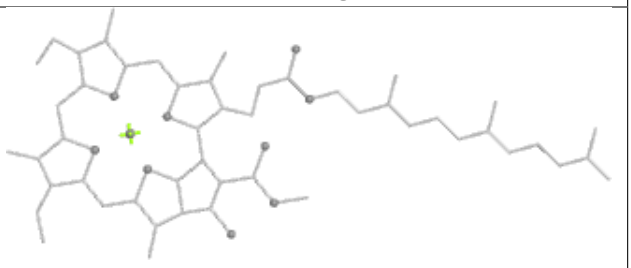
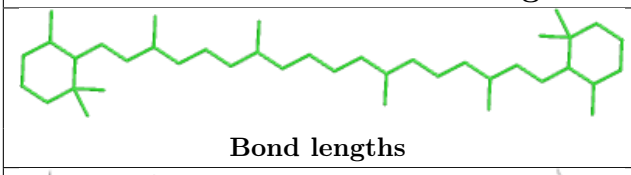


Rings

Ligand BCR Y 521



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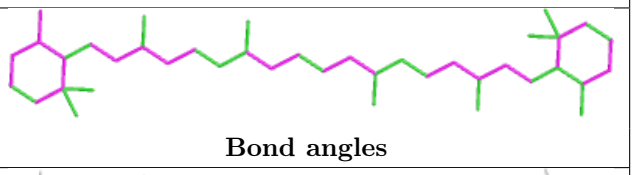

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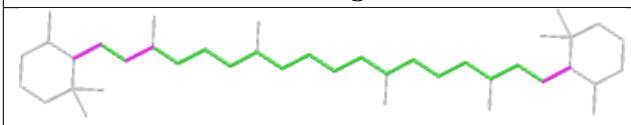

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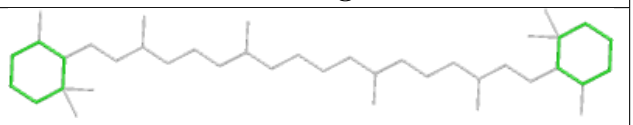
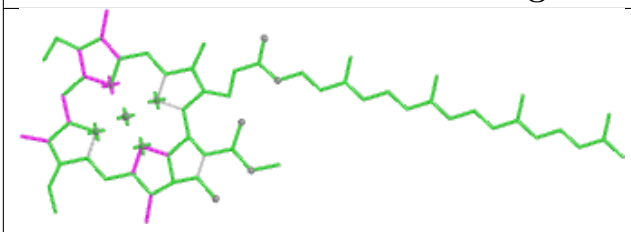


Rings

Ligand CLA 1 509



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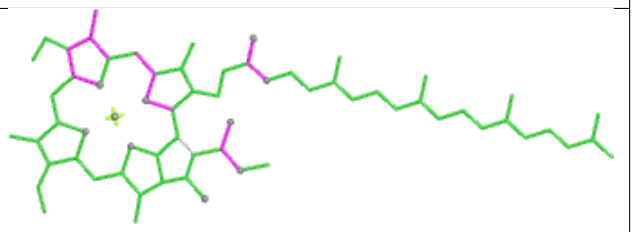

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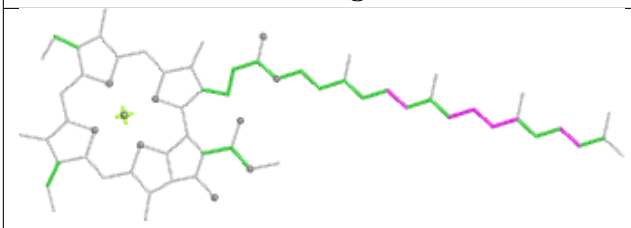

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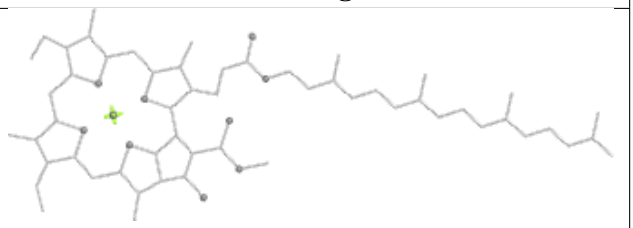

Rings

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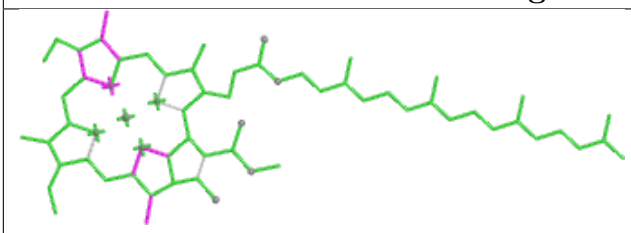

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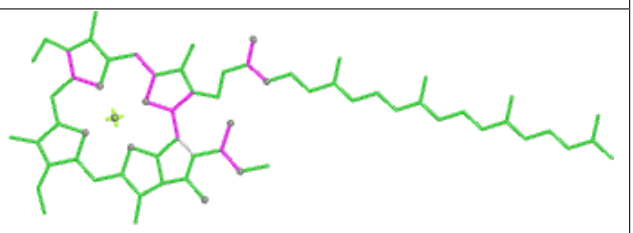

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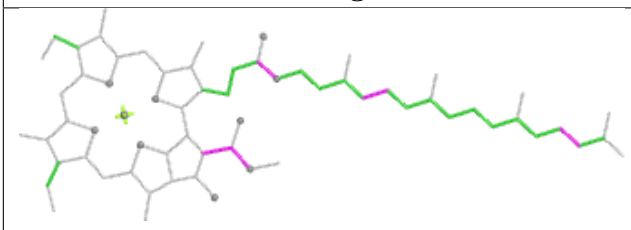

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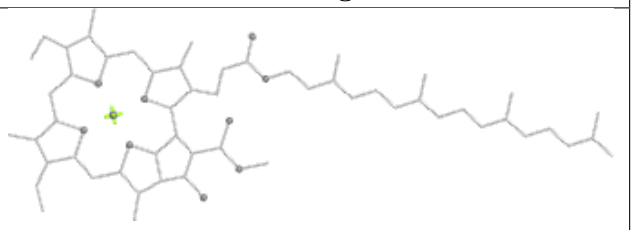
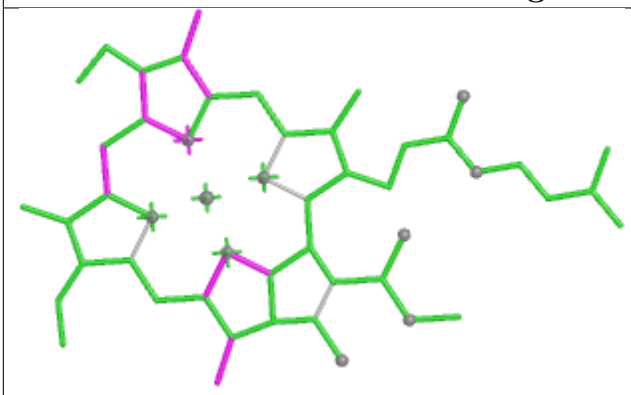


Rings

Ligand CLA b 502



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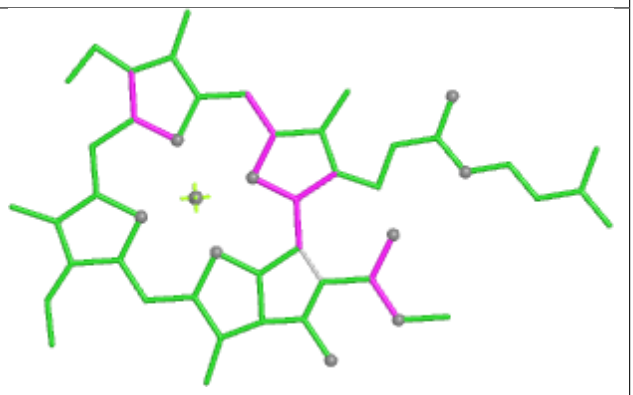

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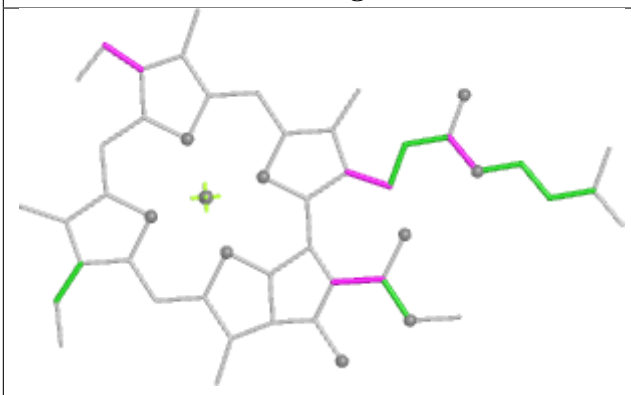

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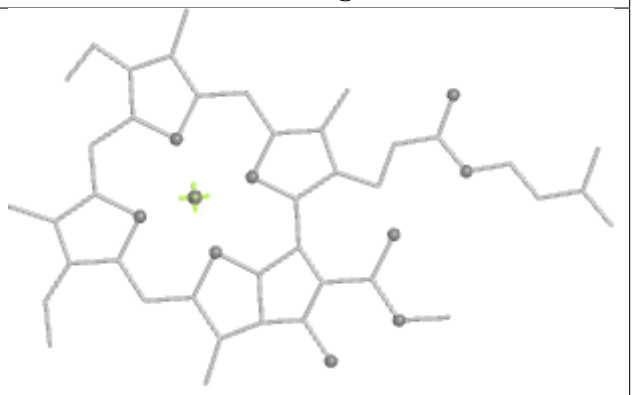

Rings

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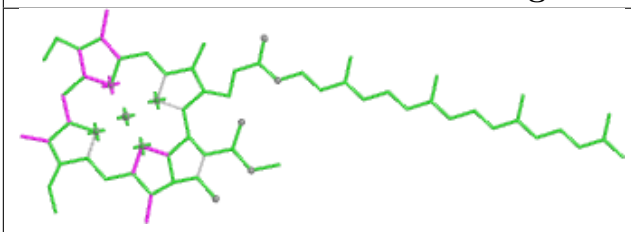

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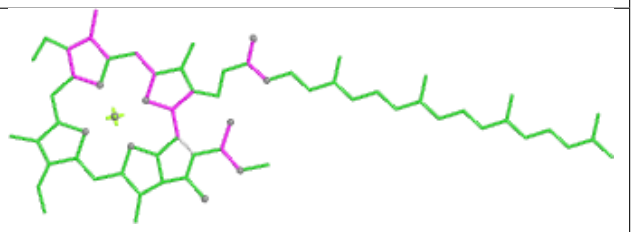

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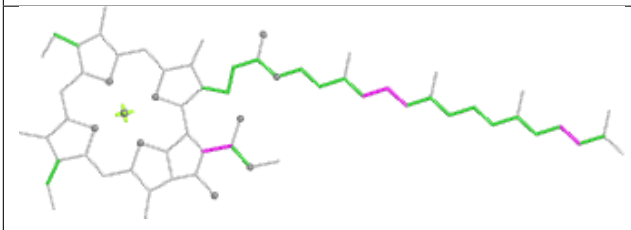

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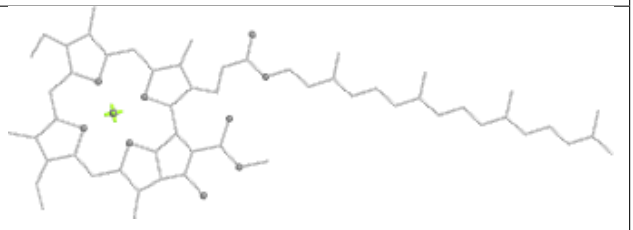
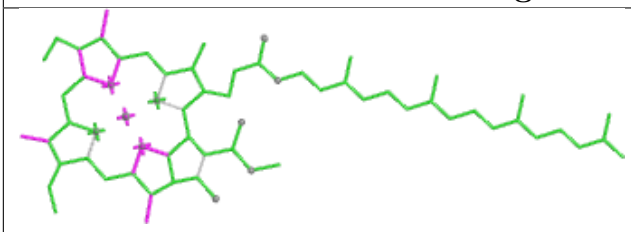


Rings

Ligand CLA A 1119



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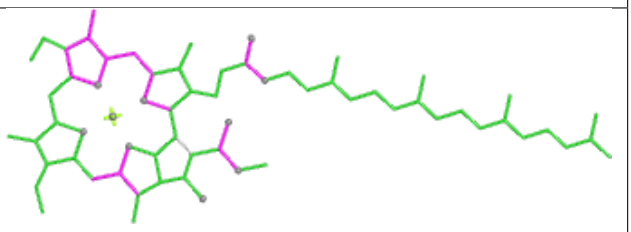

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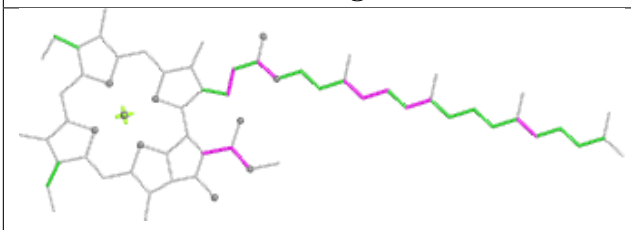

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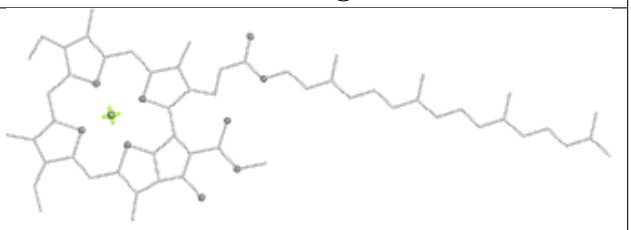

Rings

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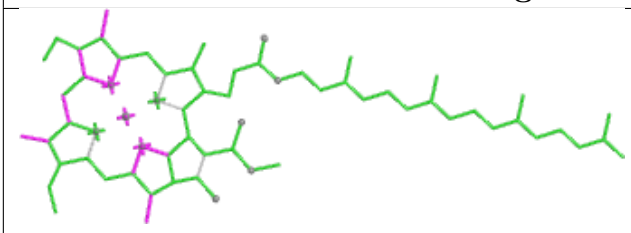

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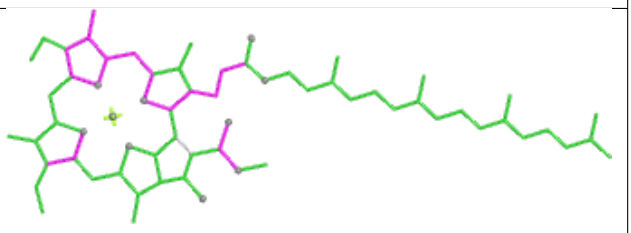

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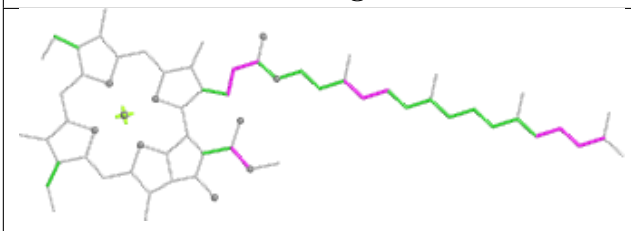

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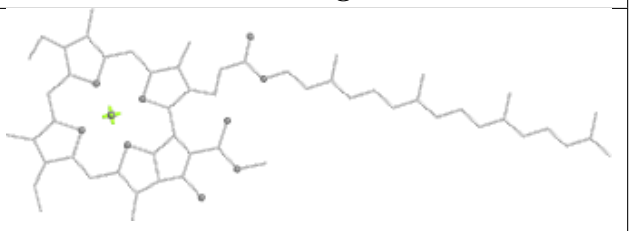
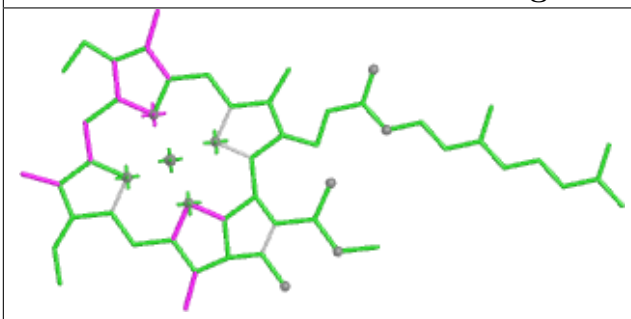


Rings

Ligand CLA r 508



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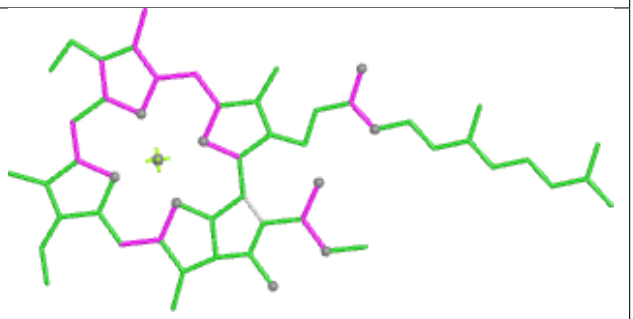

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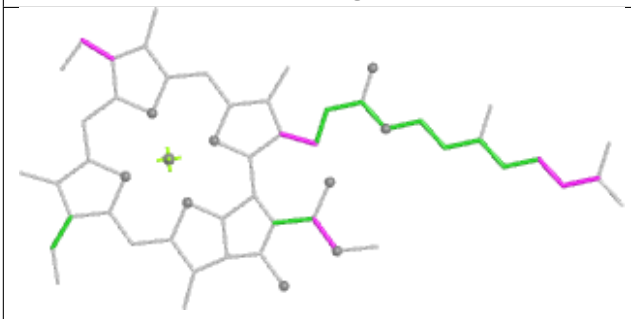

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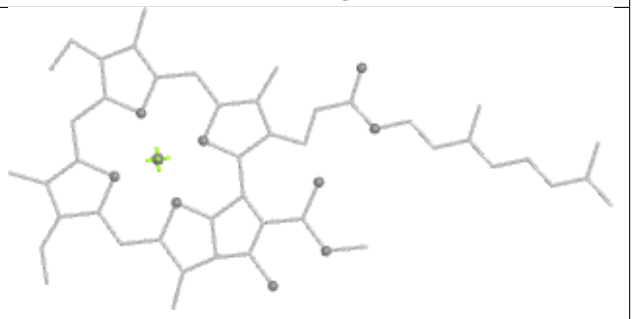

Rings

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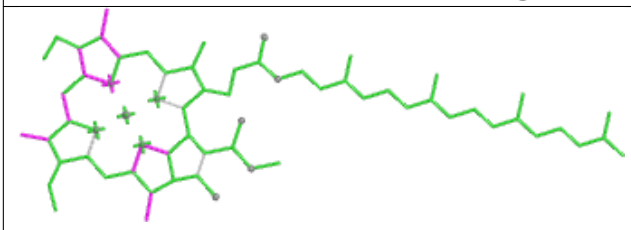

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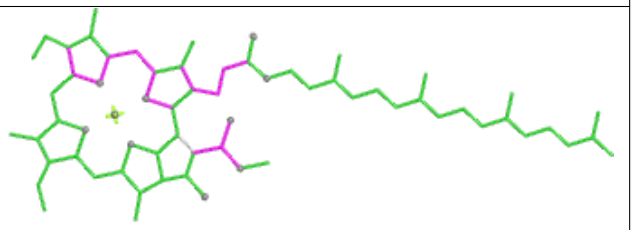

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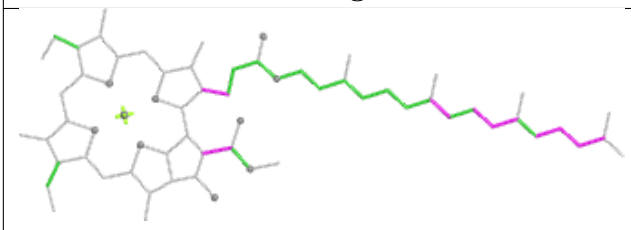

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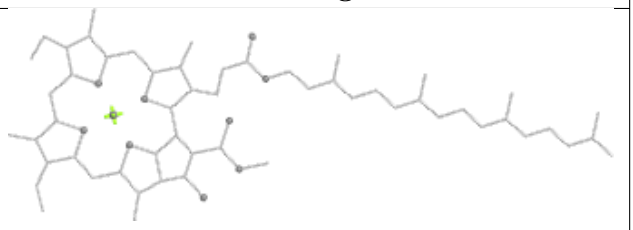
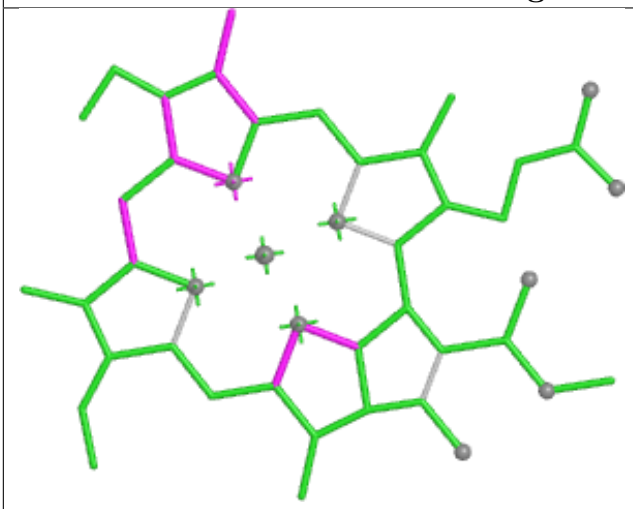


Rings

Ligand CLA d 510



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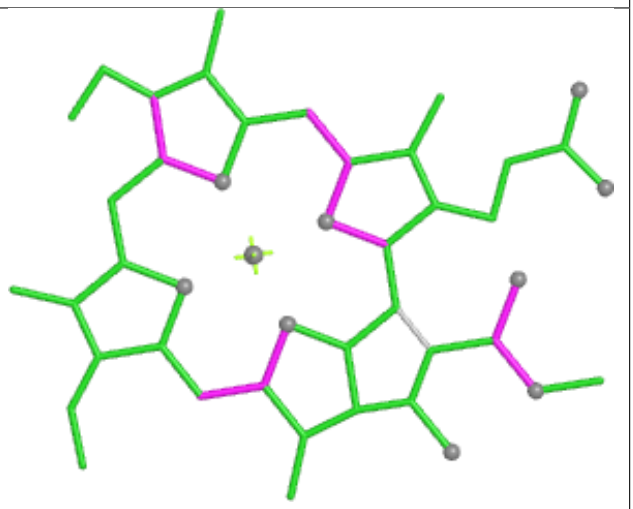

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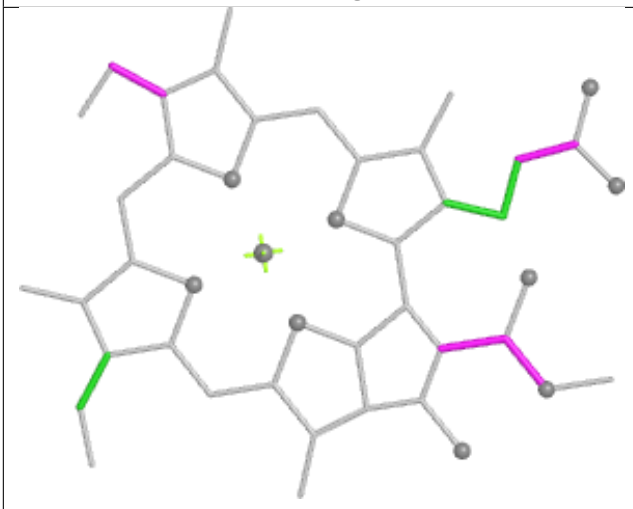

Torsions

Rings

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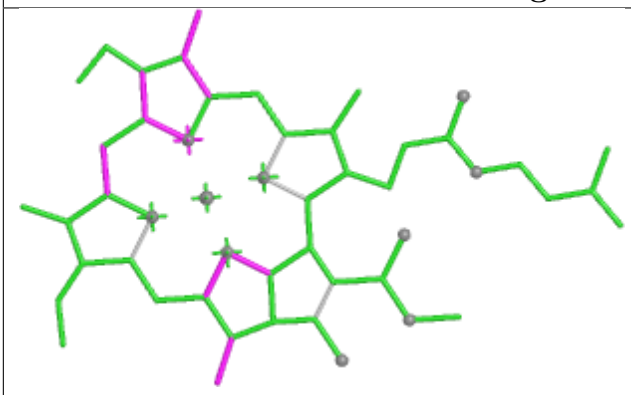

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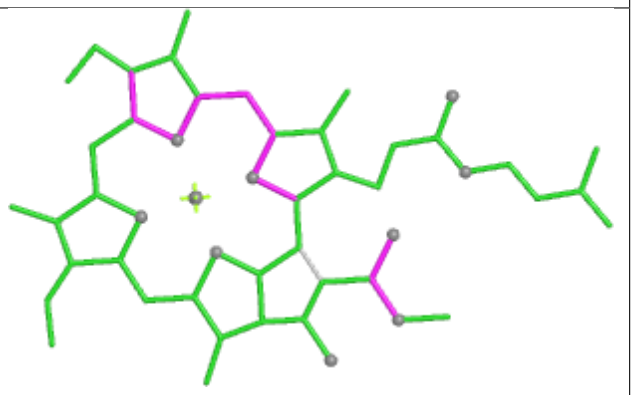

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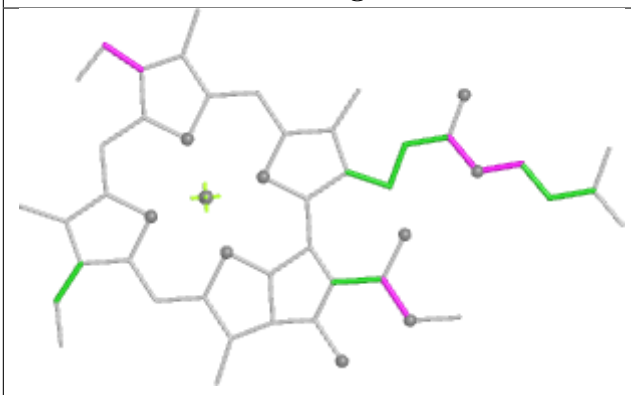

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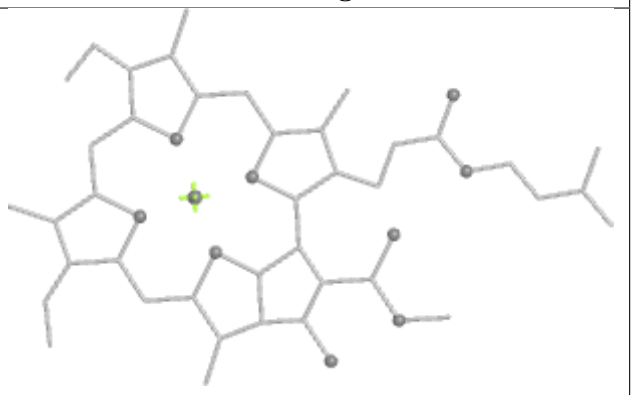
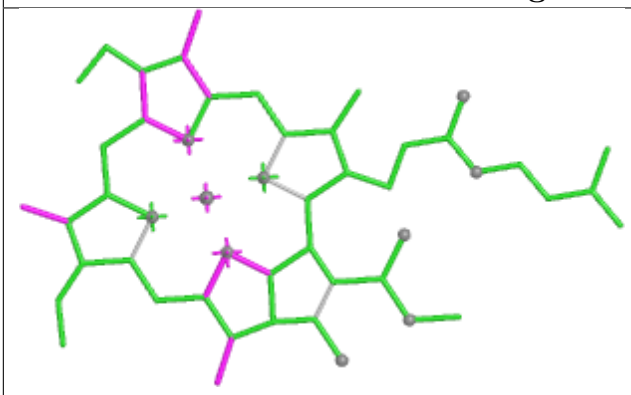
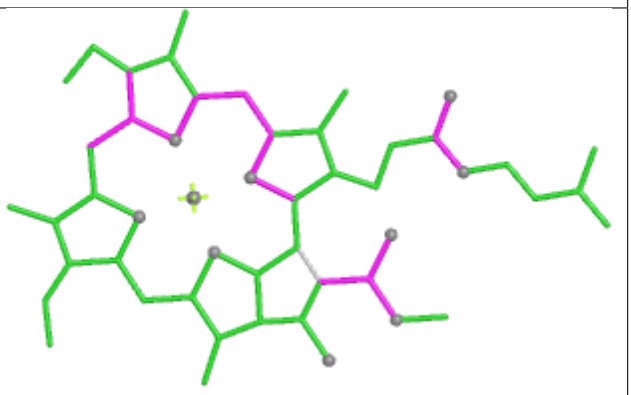
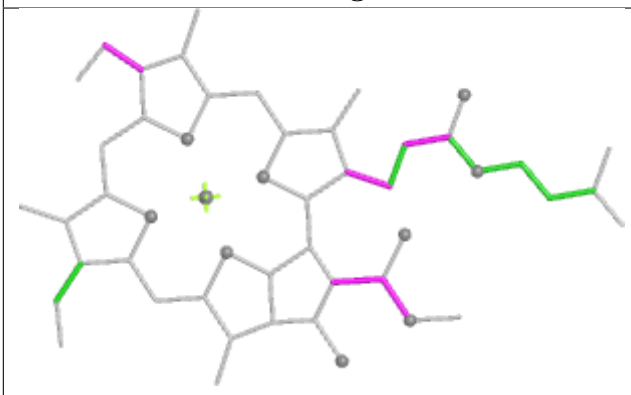
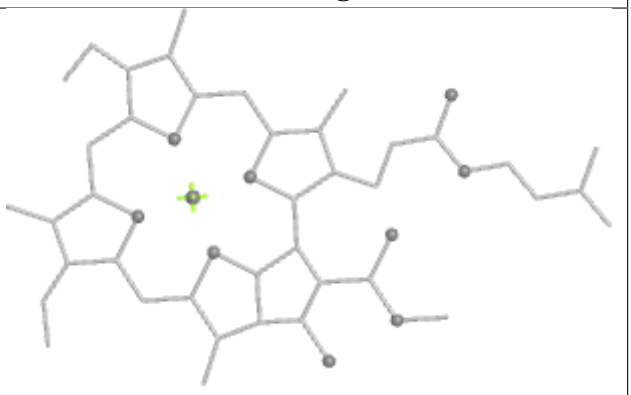


Rings

Ligand CLA 1 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

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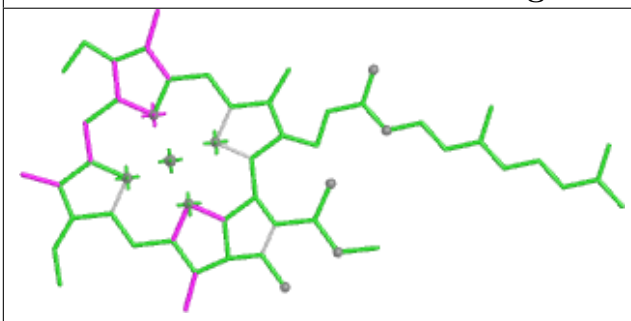
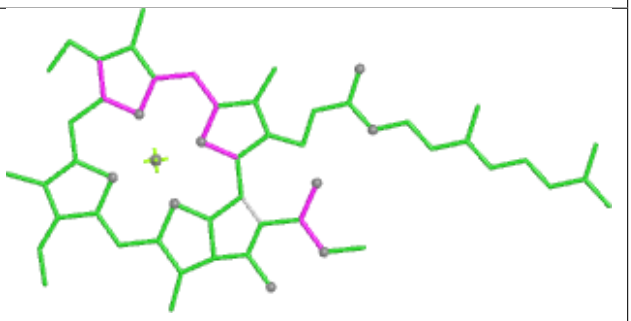
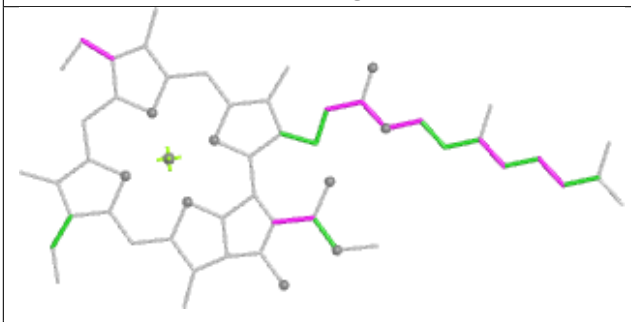
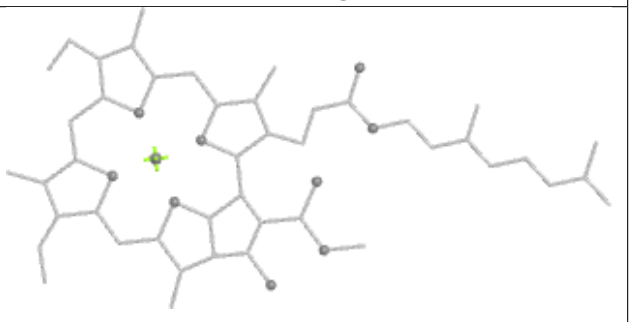
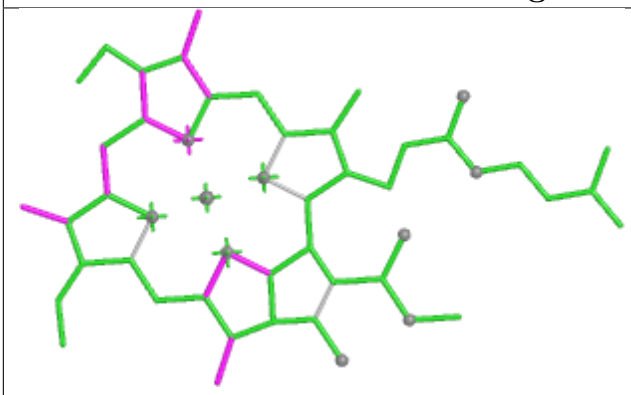
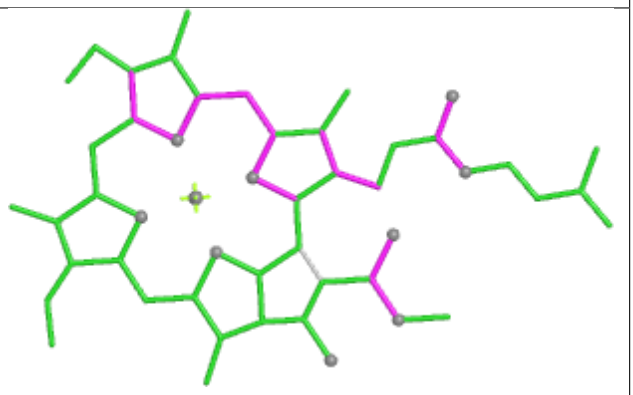
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 504



Bond lengths



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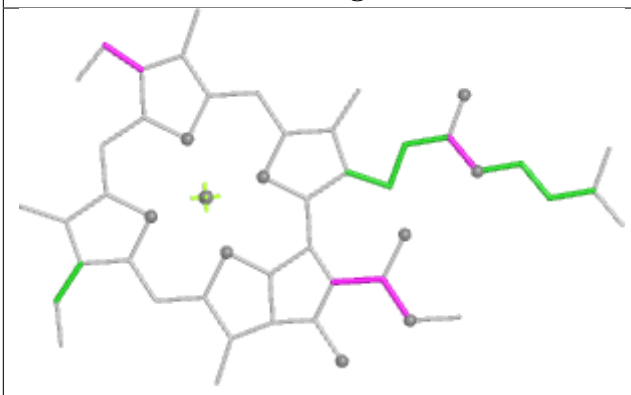
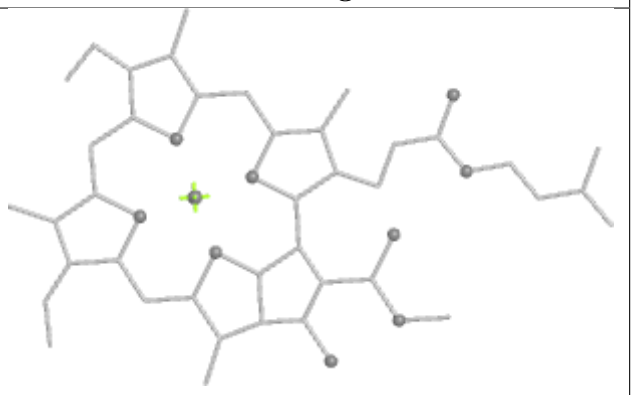
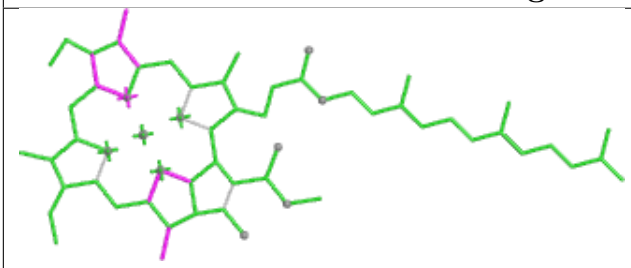


Torsions



Rings

Ligand CLA q 507



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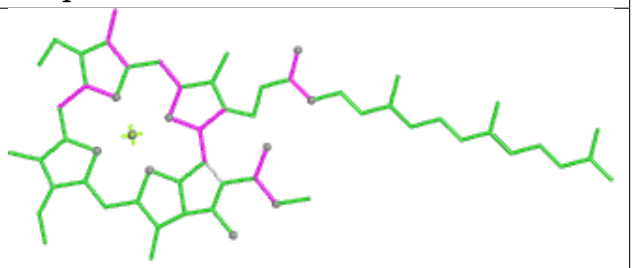
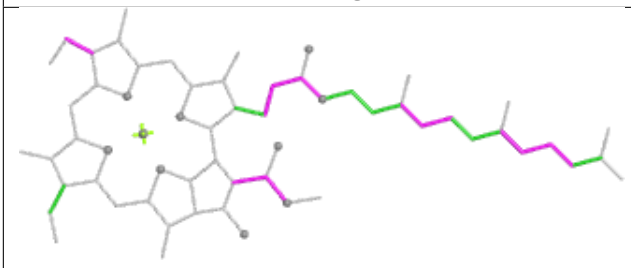


Bond angles



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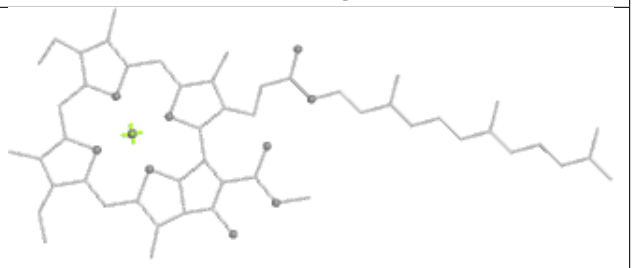
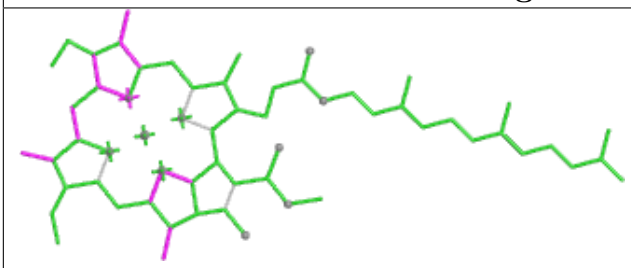
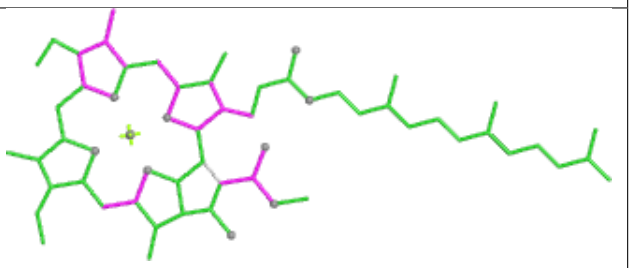
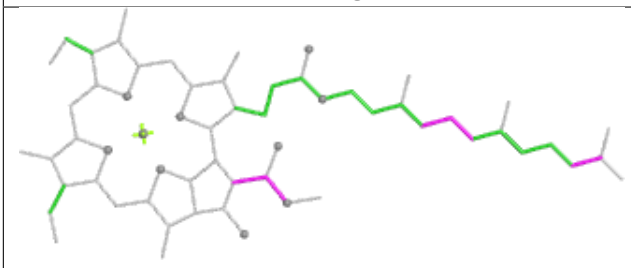
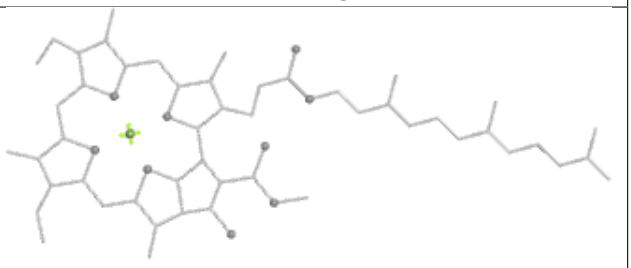
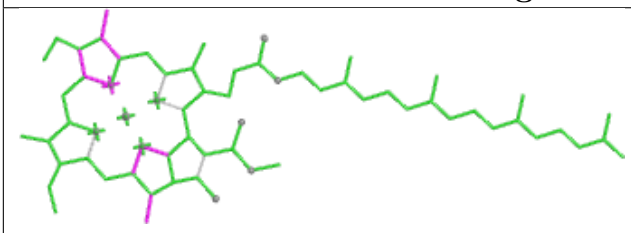
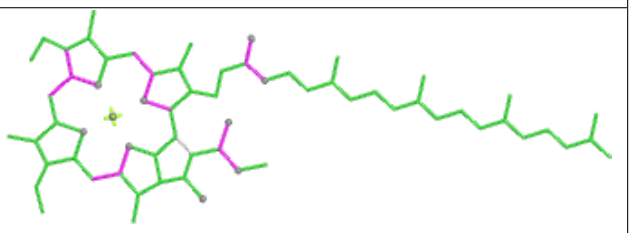
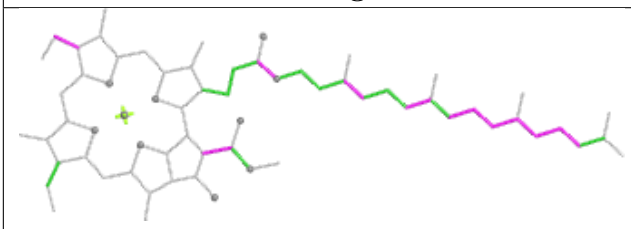
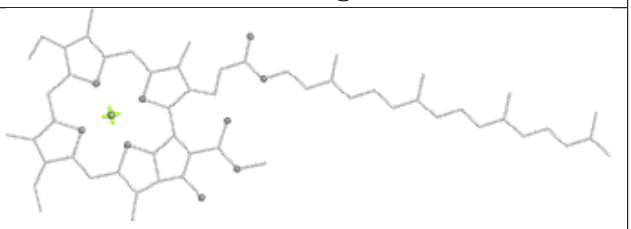
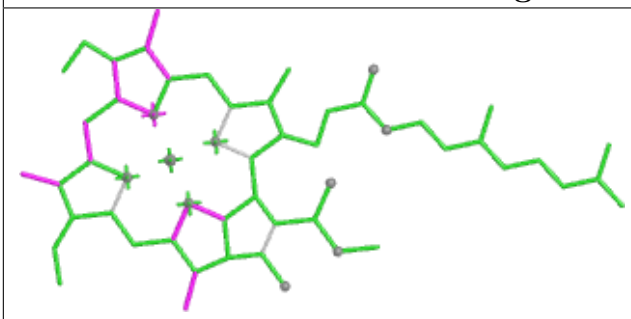


Rings

Ligand CLA B 1222	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1208	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA K 1401



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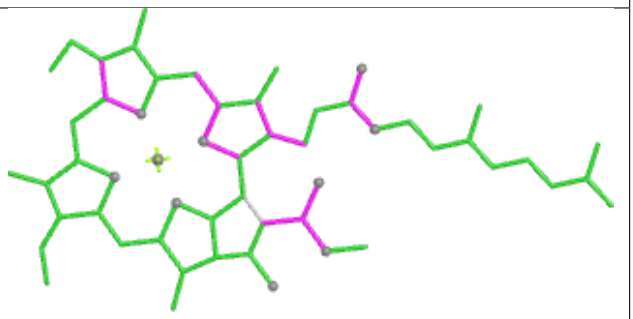

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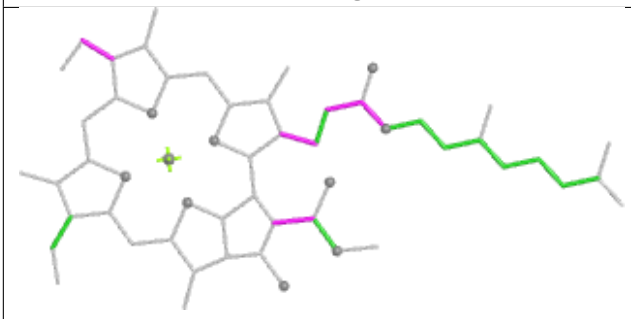
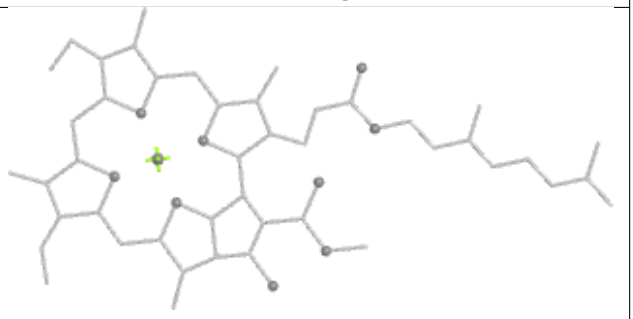
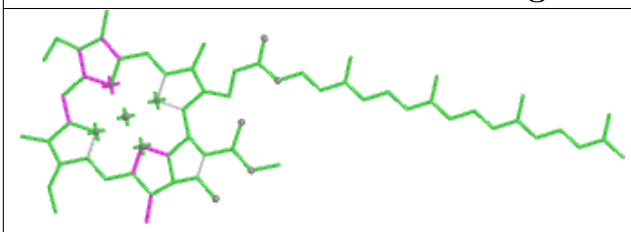


Torsions



Rings

Ligand CLA 3 510



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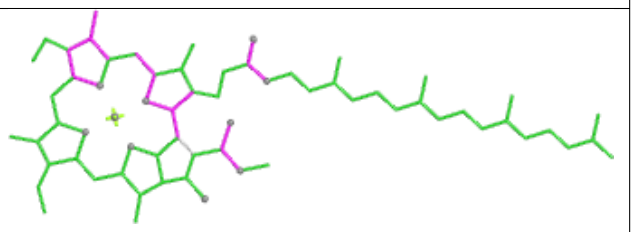
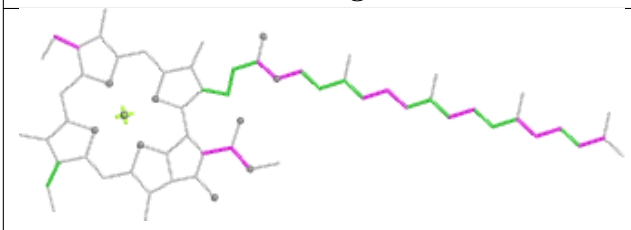


Bond angles



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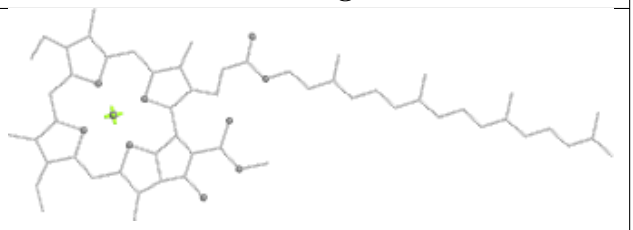
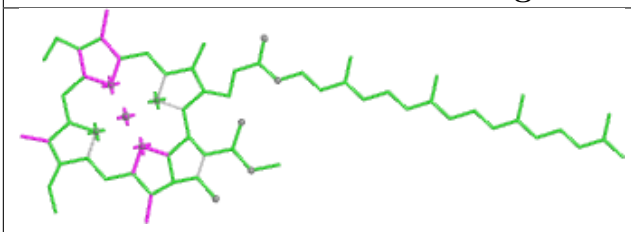


Rings

Ligand CLA H 1215



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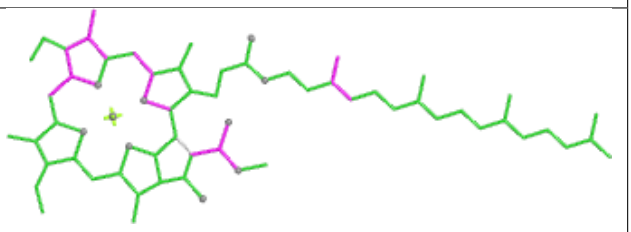

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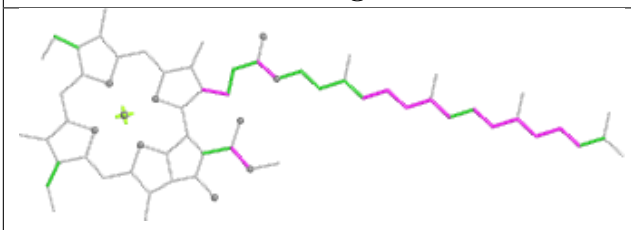

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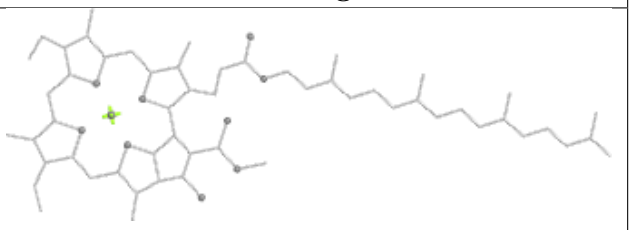
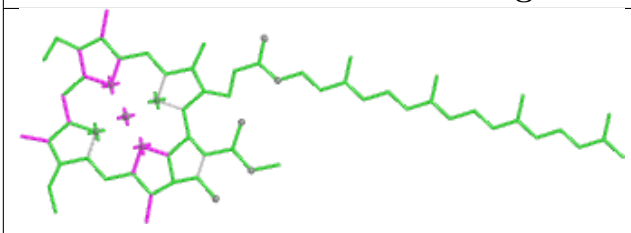


Rings

Ligand CLA B 1234



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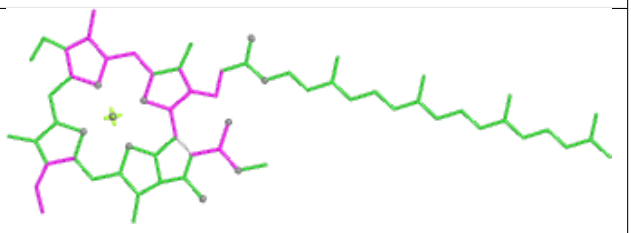
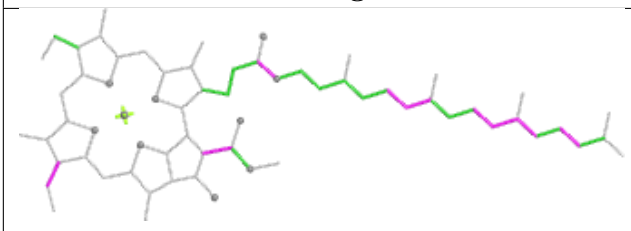


Bond angles



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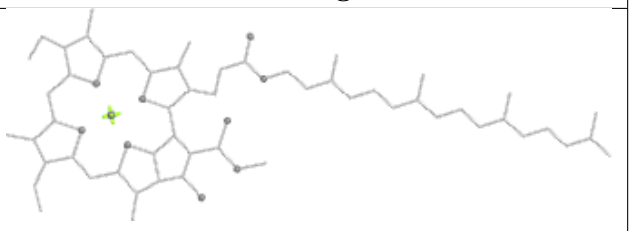
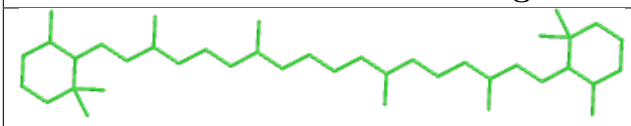


Rings

Ligand BCR A 4001



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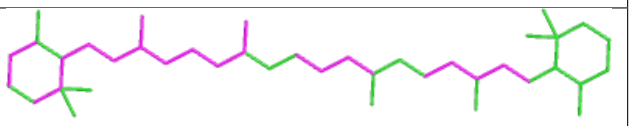

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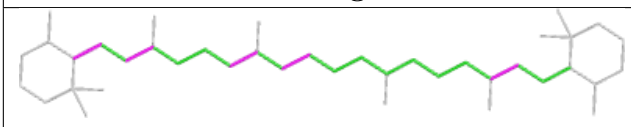

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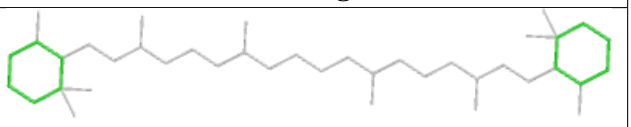
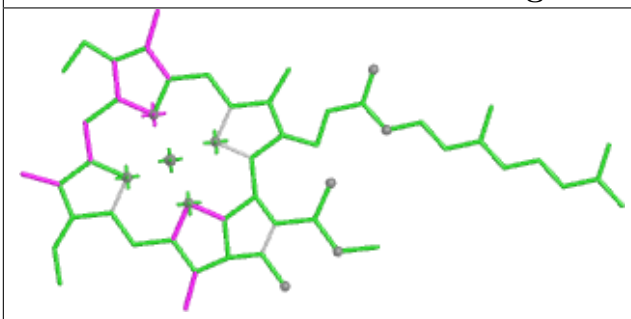
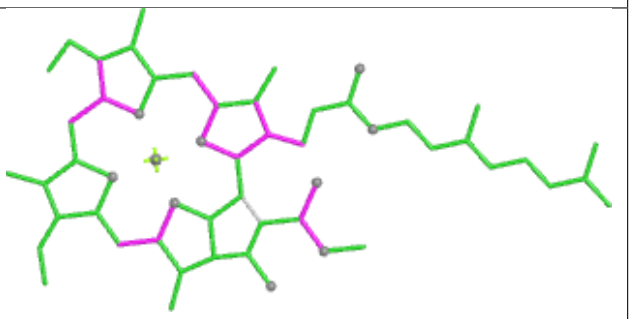
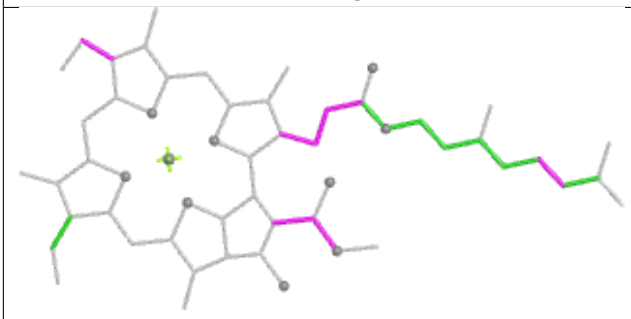
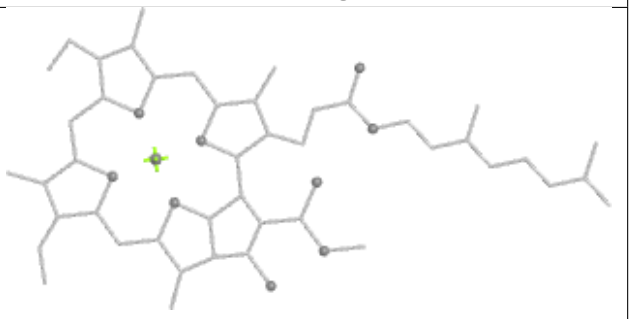
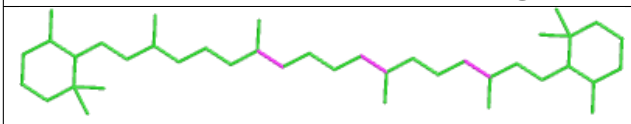
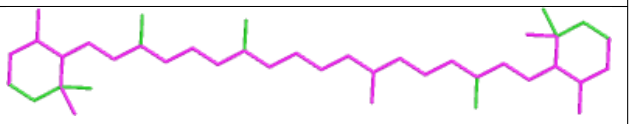
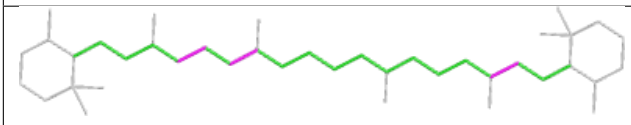
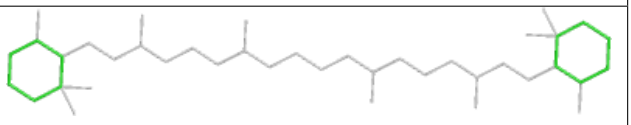
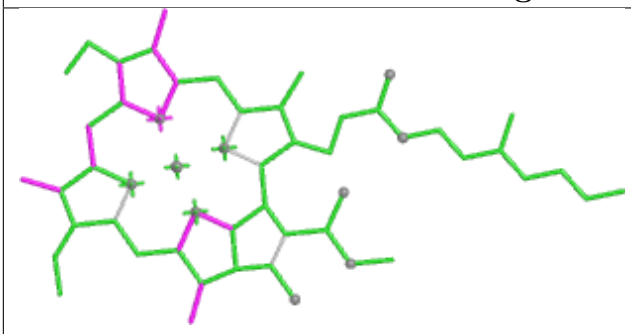


Rings

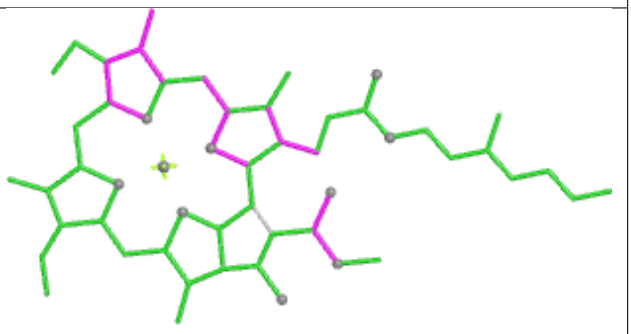
Ligand CLA Z 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4010	
	
Bond lengths	Bond angles
	
Torsions	Rings

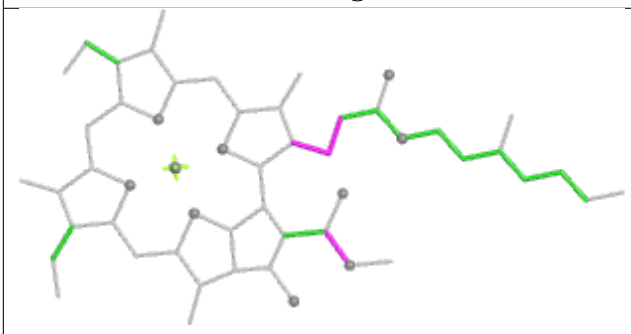
Ligand CLA A 1120



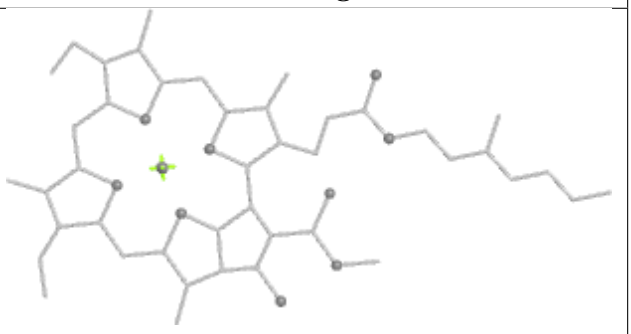
Bond lengths



Bond angles

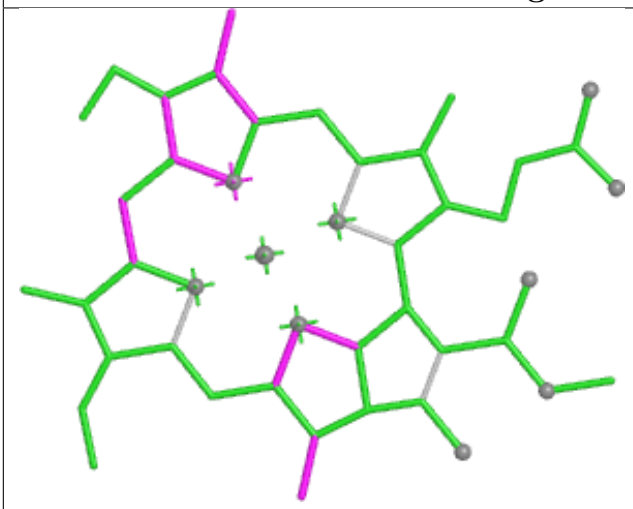


Torsions

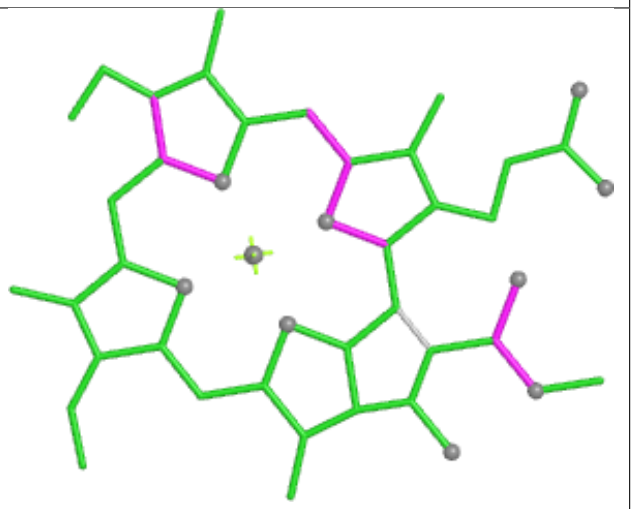


Rings

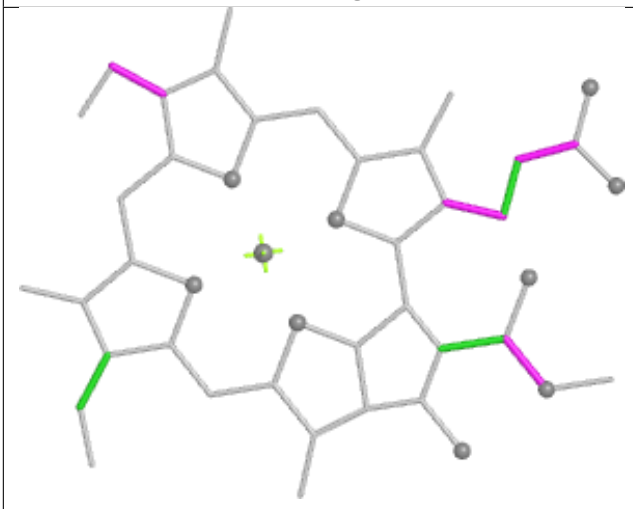
Ligand CLA v 512



Bond lengths



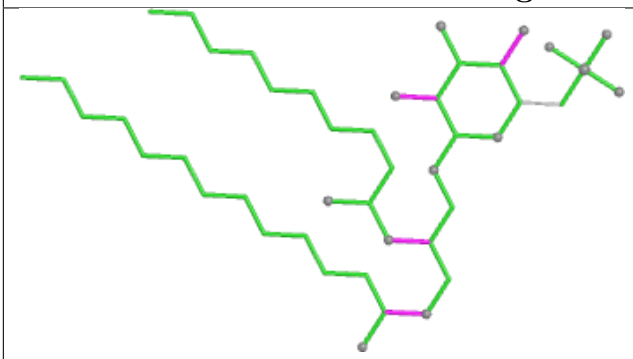
Bond angles



Torsions

Rings

Ligand SQD B 1852



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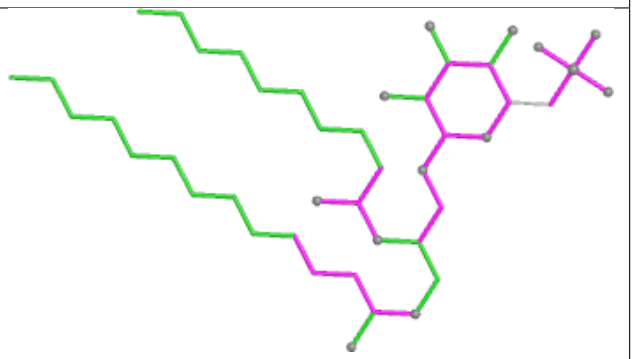

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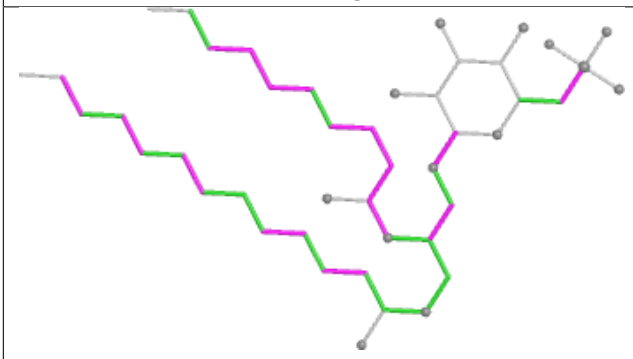

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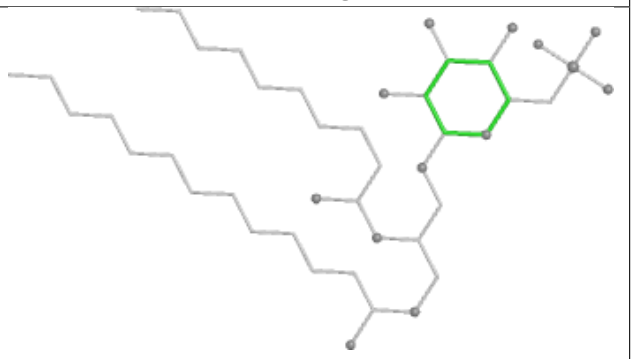
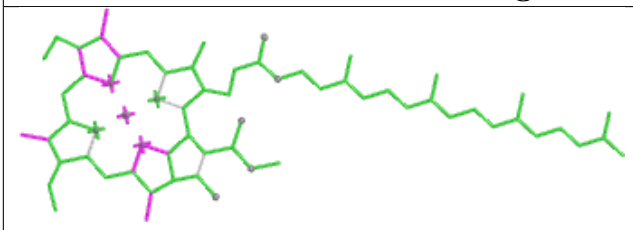


Rings

Ligand CLA A 1022



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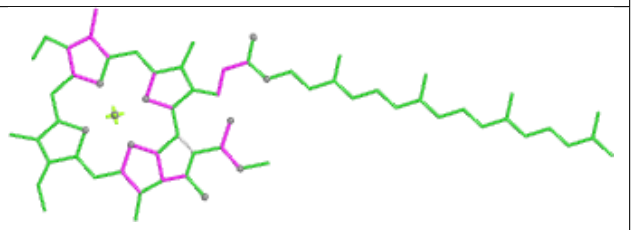

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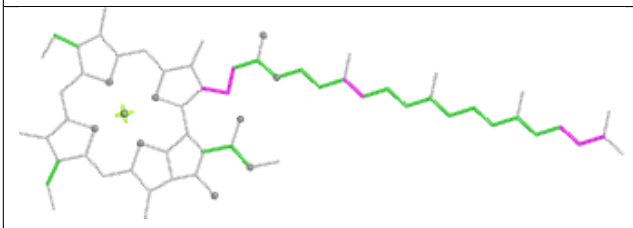

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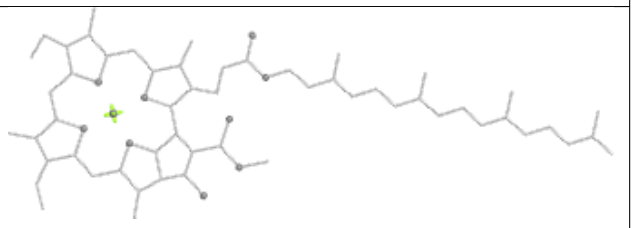

Rings

Ligand BCR 3 524

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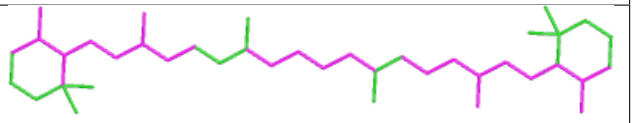

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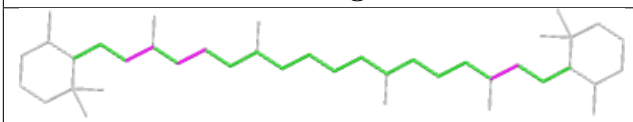

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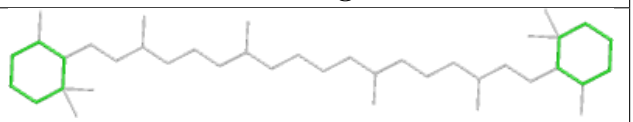
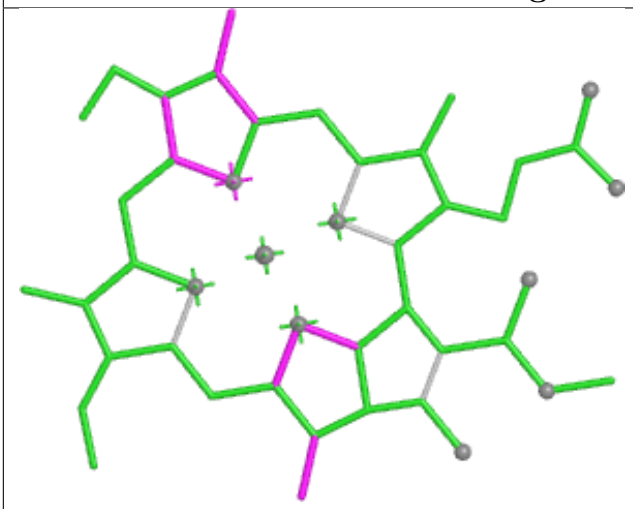


Rings

Ligand CLA c 507



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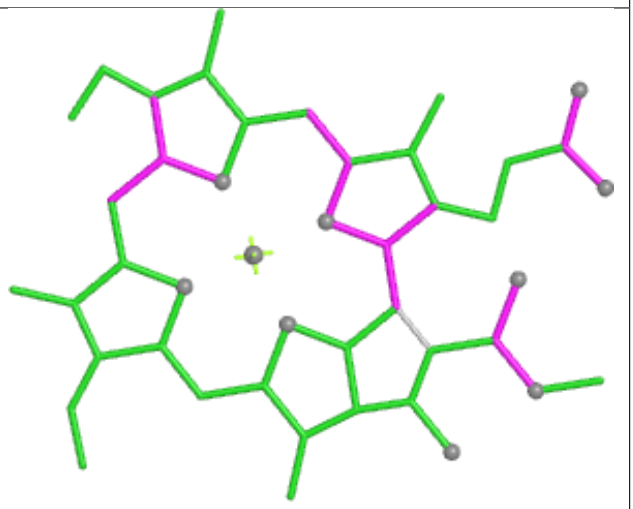

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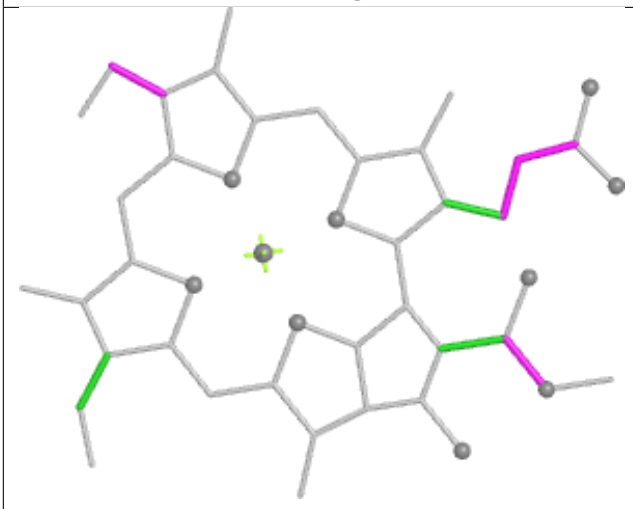
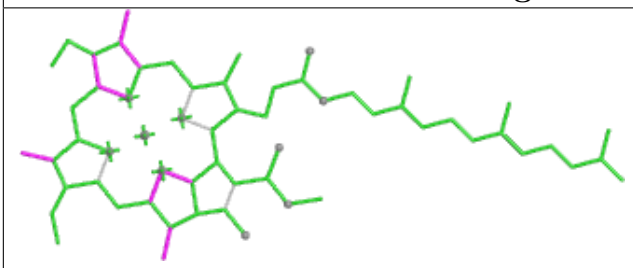


Torsions

Rings

Ligand CLA G 1136



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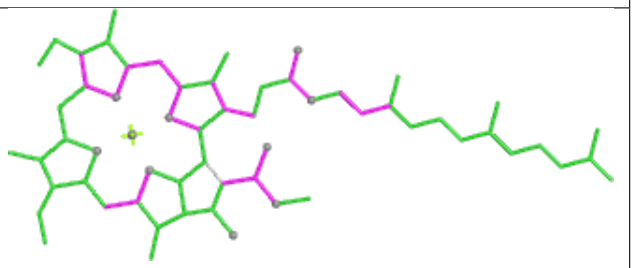

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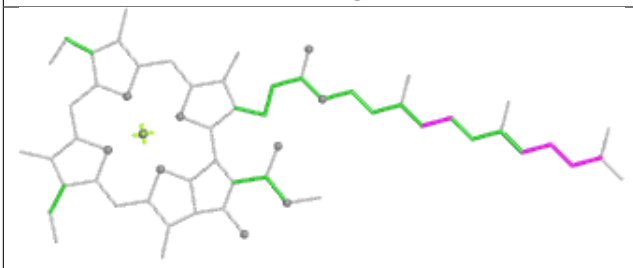

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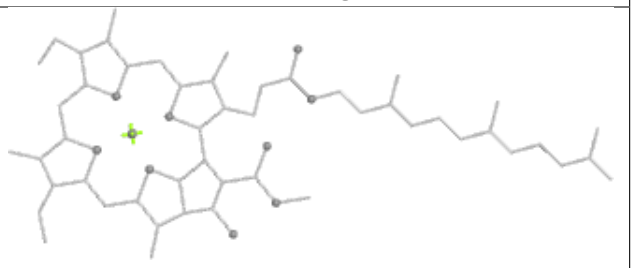

Rings

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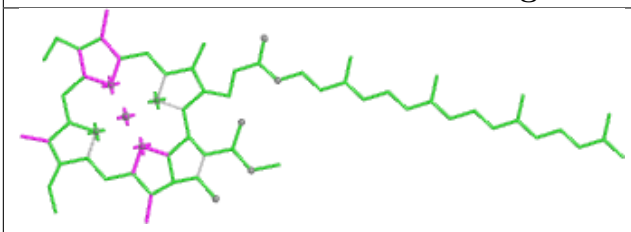

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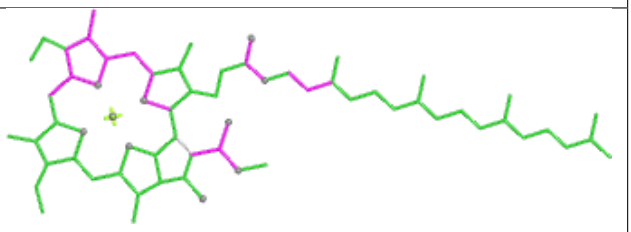

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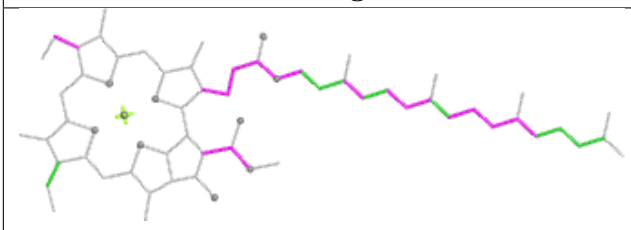

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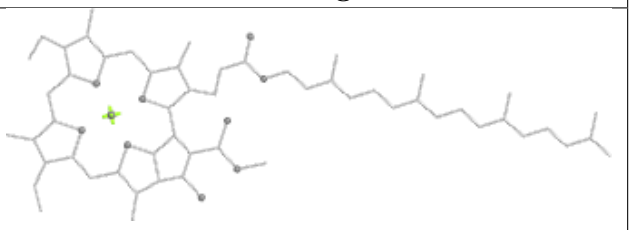

Rings

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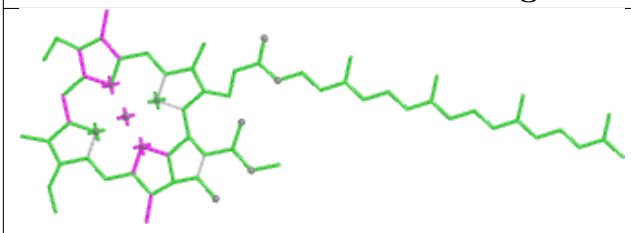

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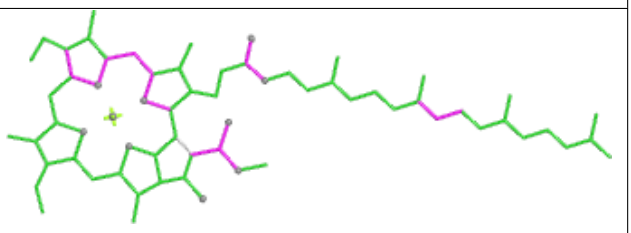

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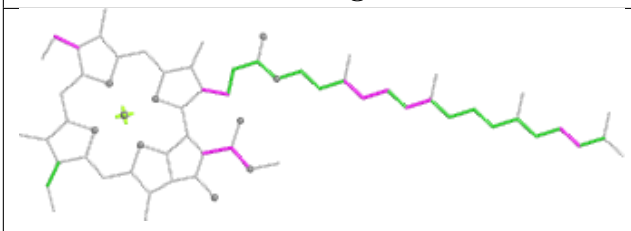

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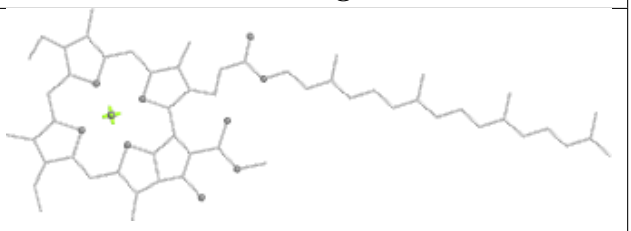
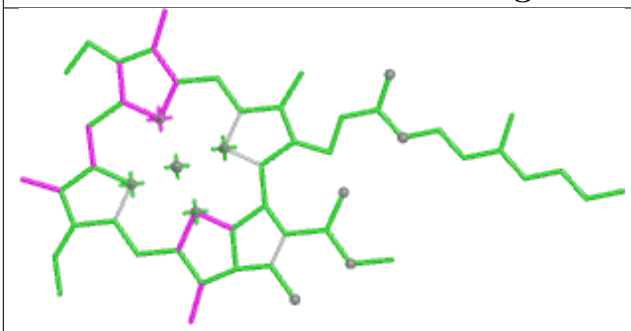


Rings

Ligand CLA G 1120



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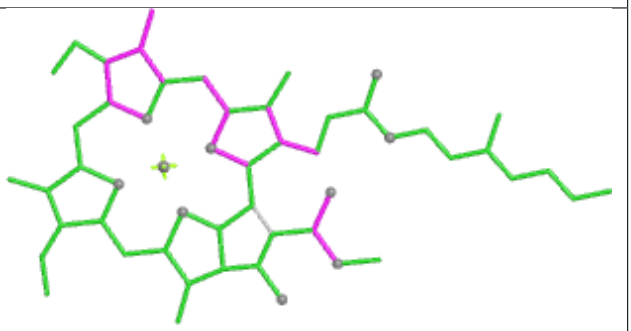

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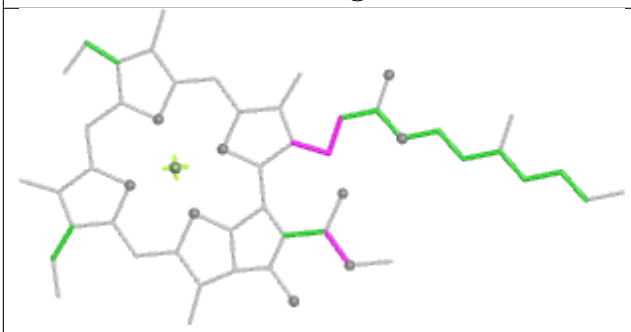

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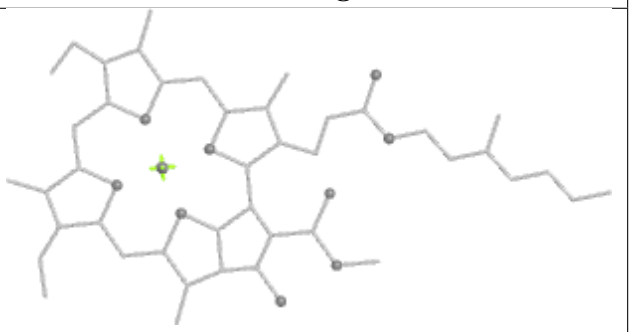

Rings

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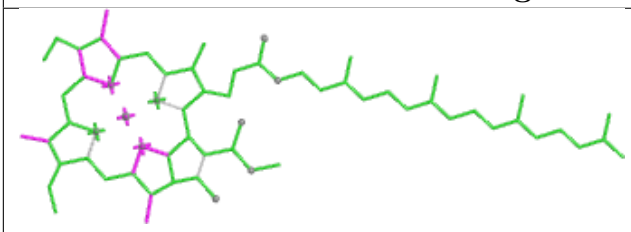

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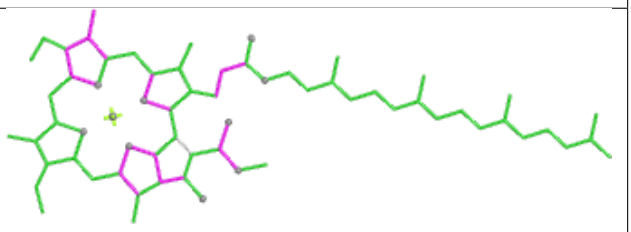

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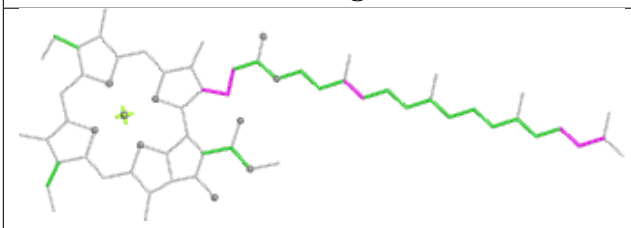

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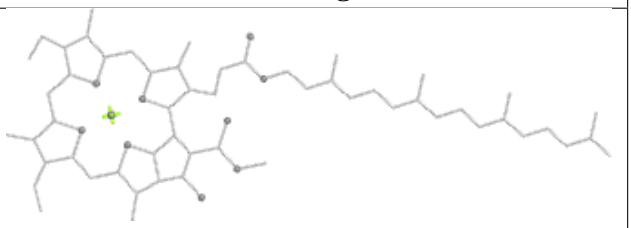

Rings

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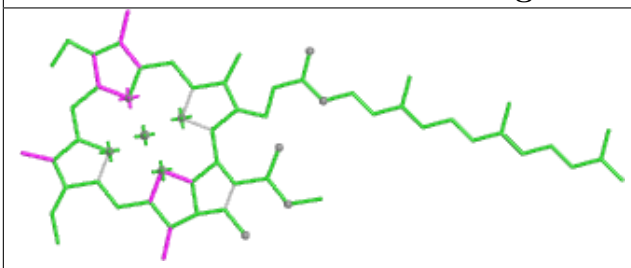
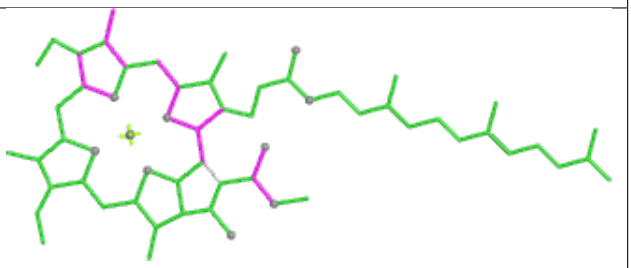
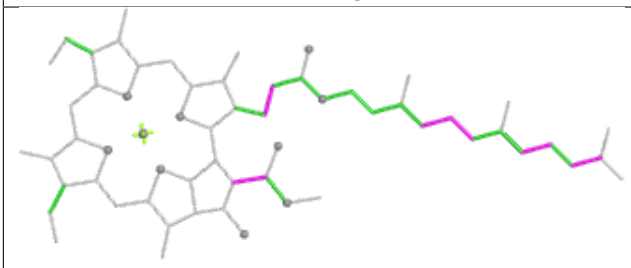
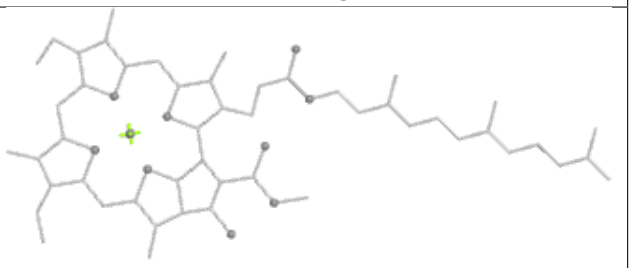
	
Bond lengths	Bond angles
	
Torsions	Rings

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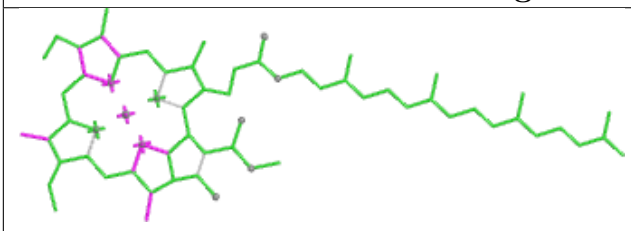
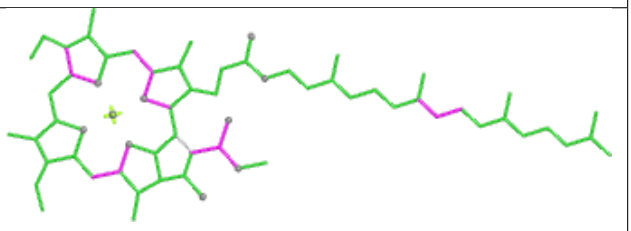
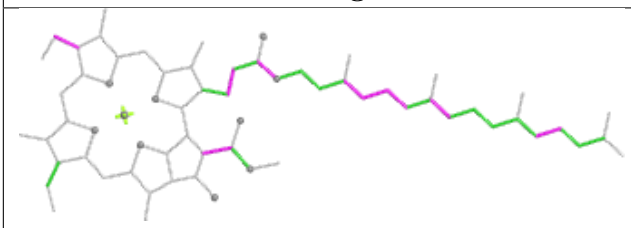
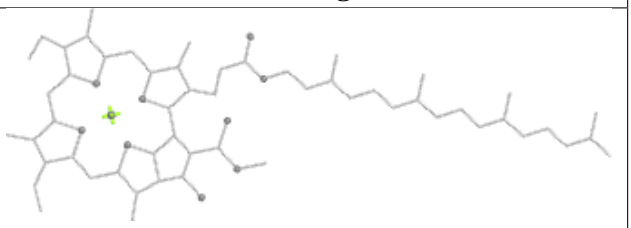
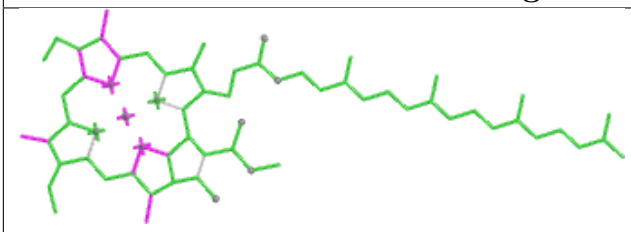
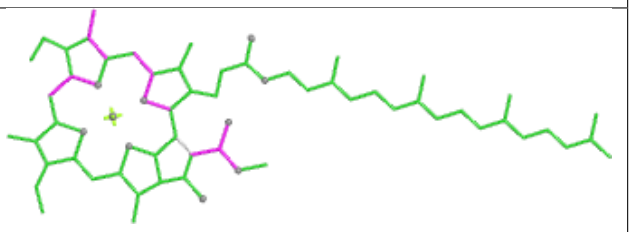
	
Bond lengths	Bond angles
	
Torsions	Rings

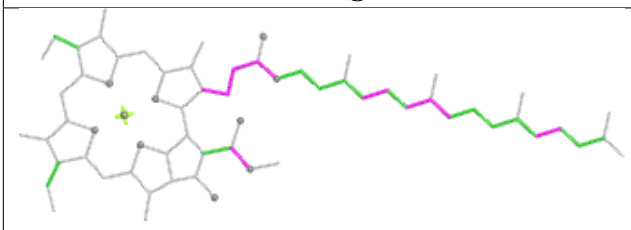
Ligand CLA f 1206



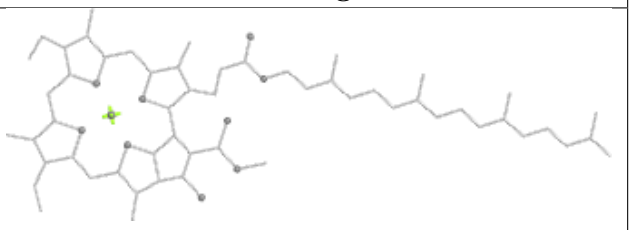
Bond lengths



Bond angles



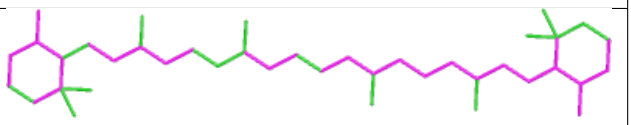
Torsions



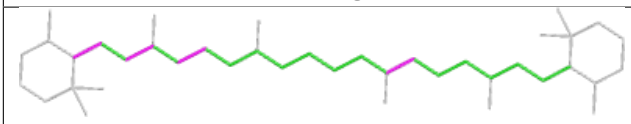
Rings

Ligand BCR c 521

Bond lengths



Bond angles



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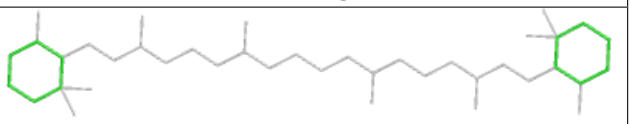
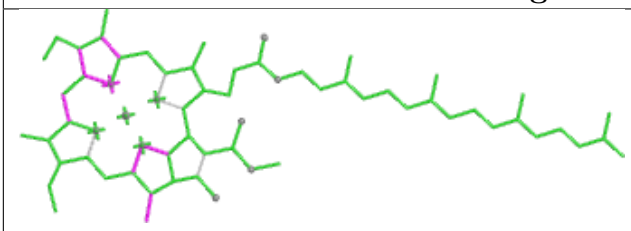
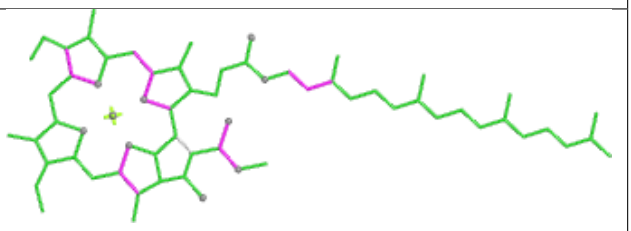


Rings

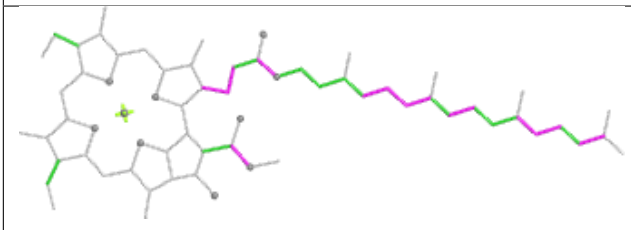
Ligand CLA r 505



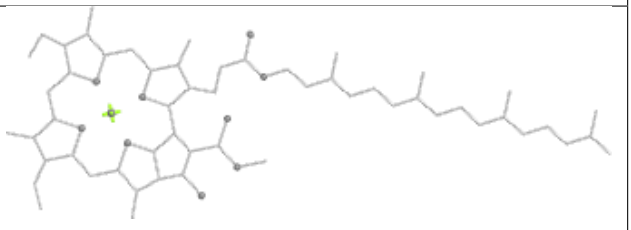
Bond lengths



Bond angles

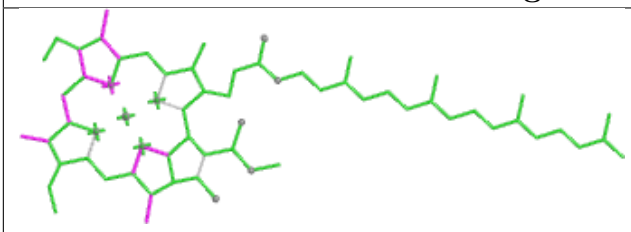


Torsions



Rings

Ligand CLA Y 501



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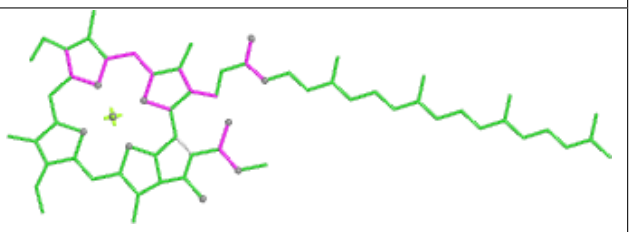

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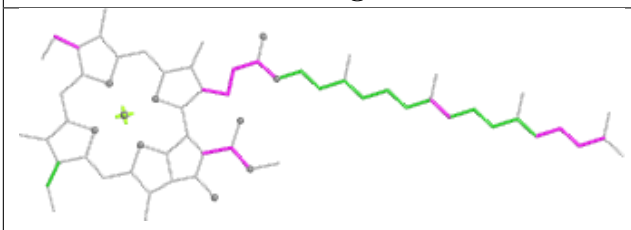

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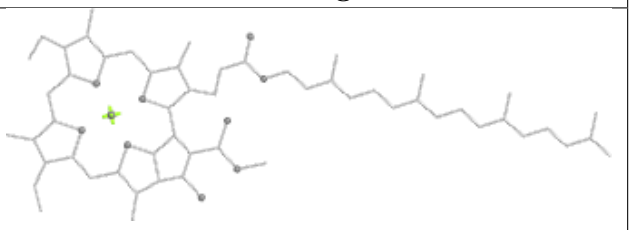
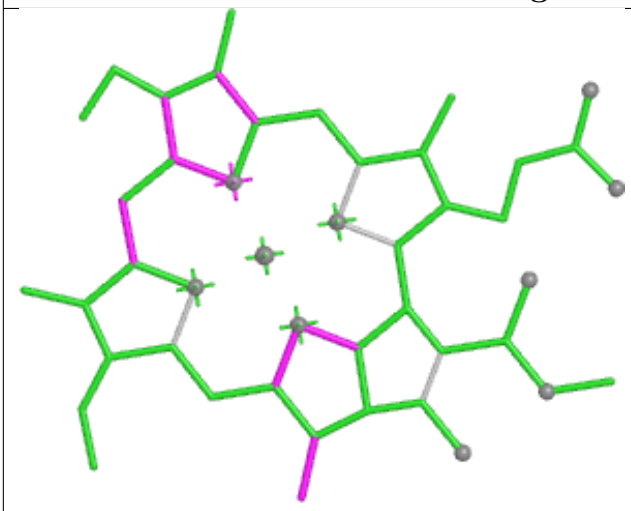


Rings

Ligand CLA t 504



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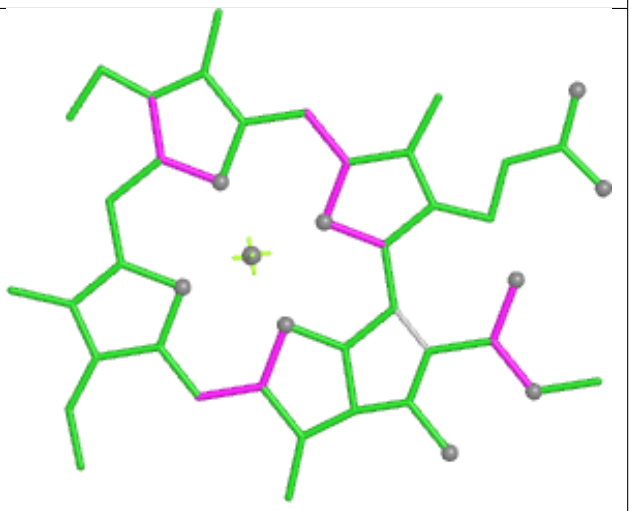

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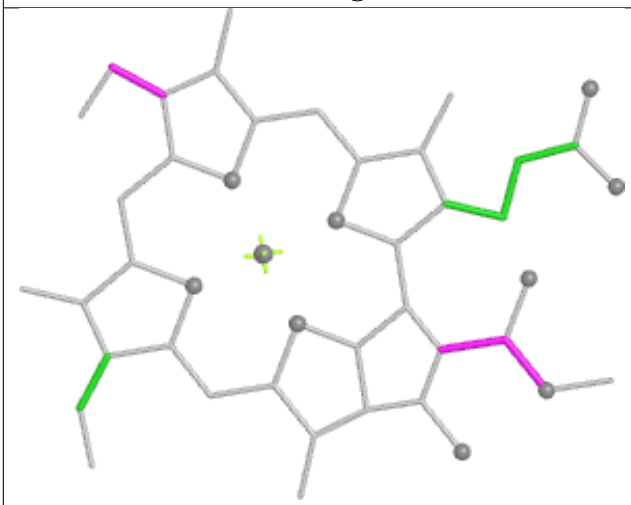

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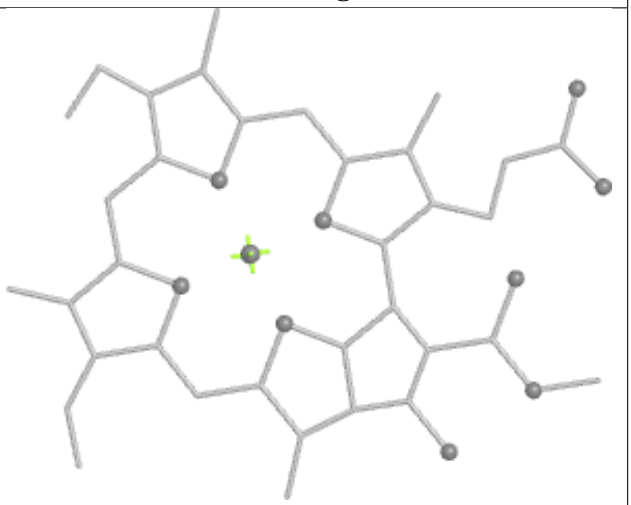
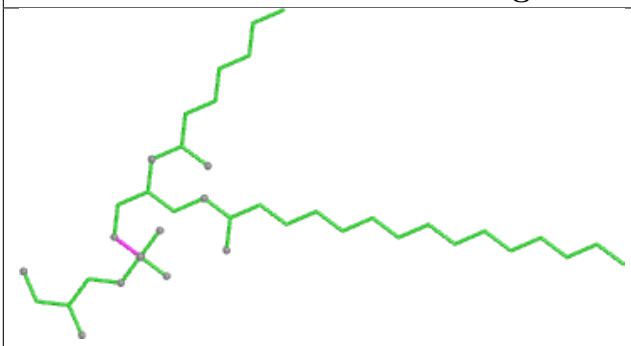


Rings

Ligand LHG G 5002



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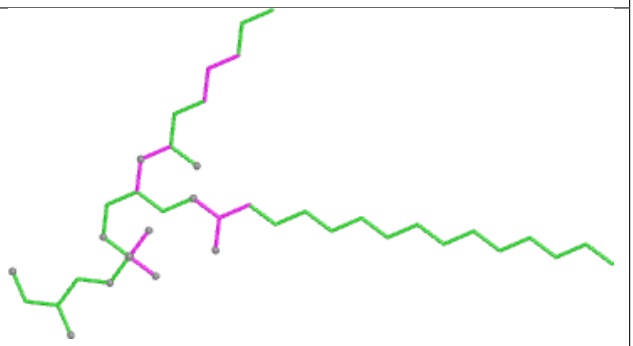

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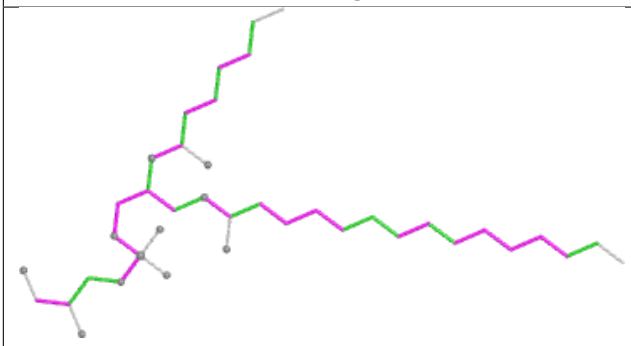

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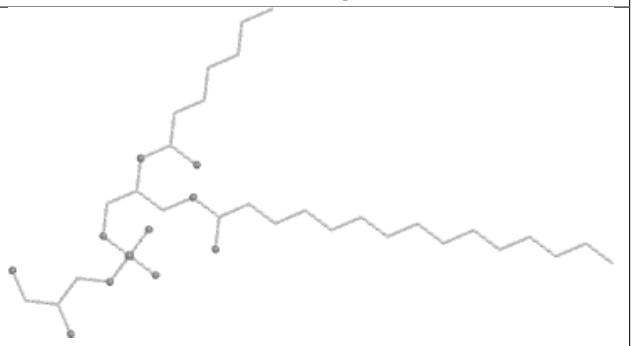

Rings

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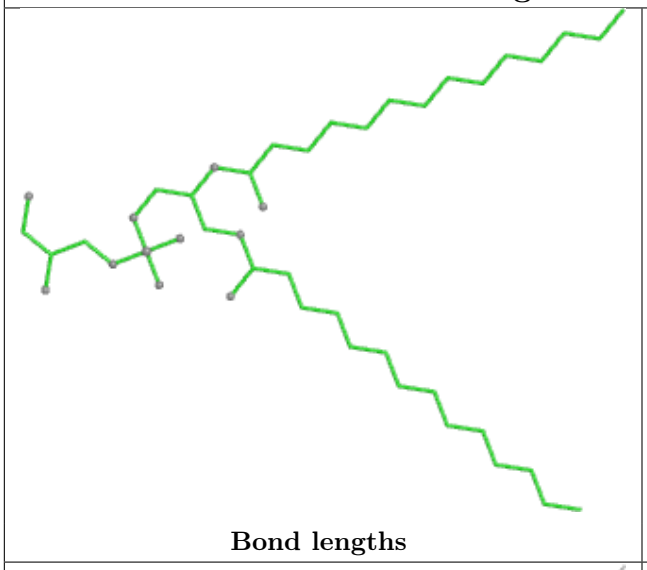

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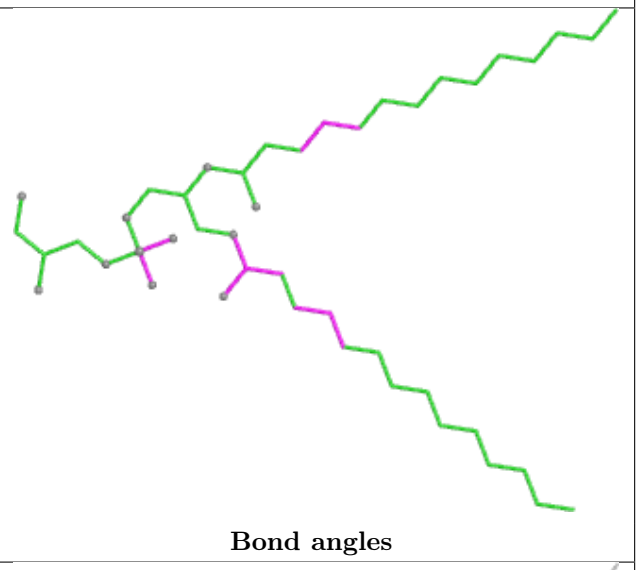

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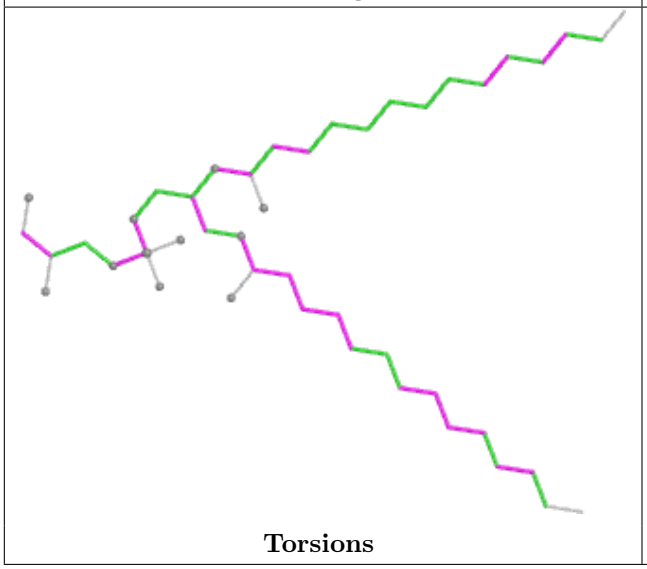

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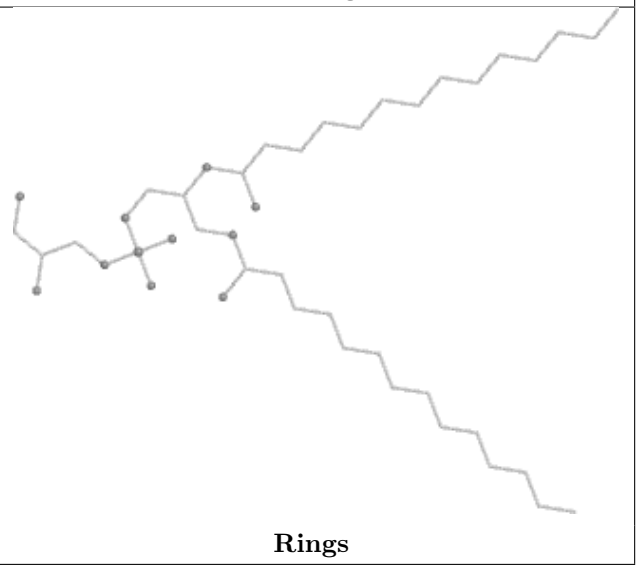
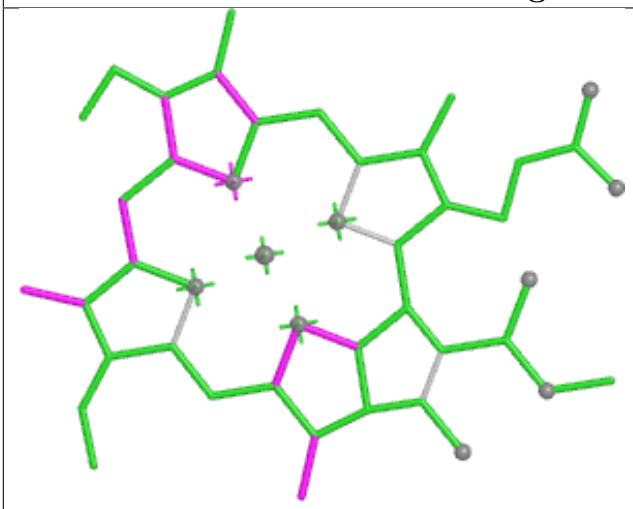


Rings

Ligand CLA 6 517



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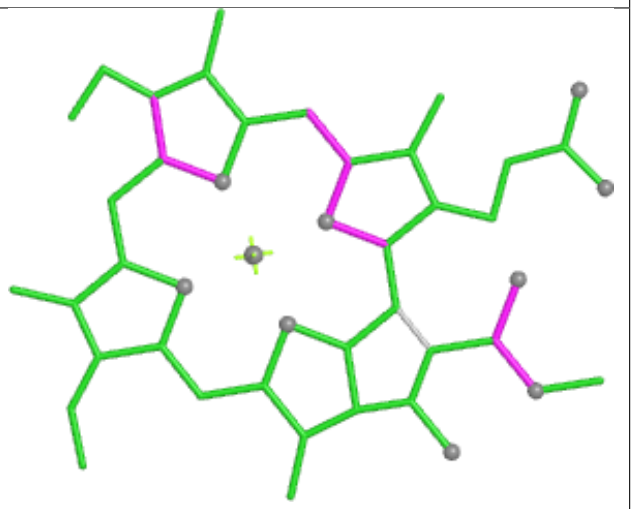

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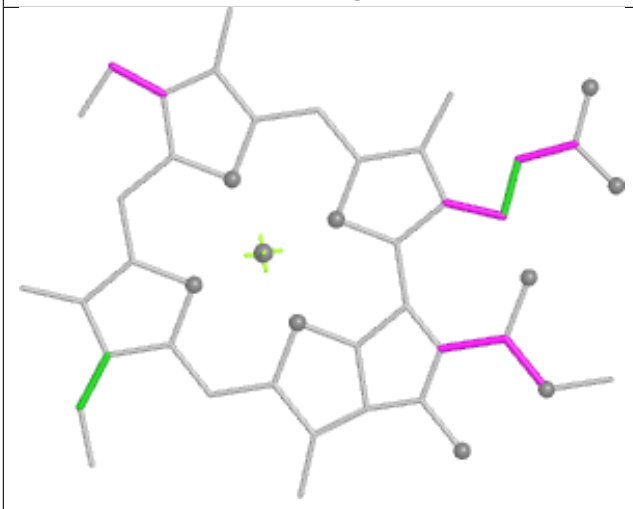
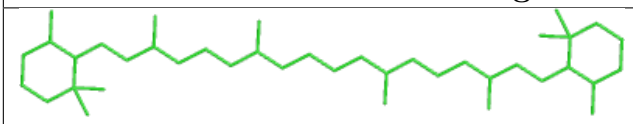


Torsions

Rings

Ligand BCR V 4022



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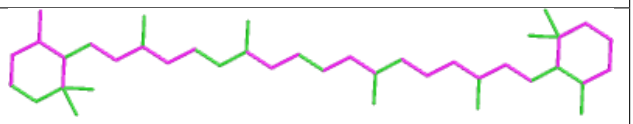

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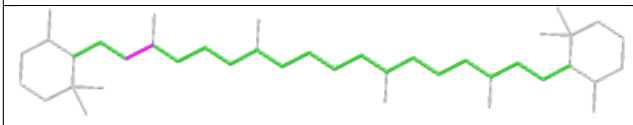

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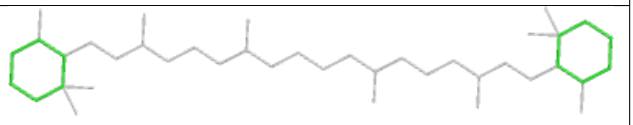
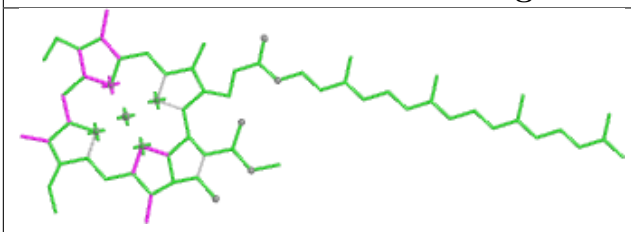


Rings

Ligand CLA B 1207



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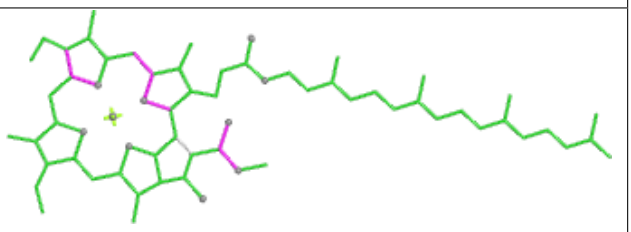

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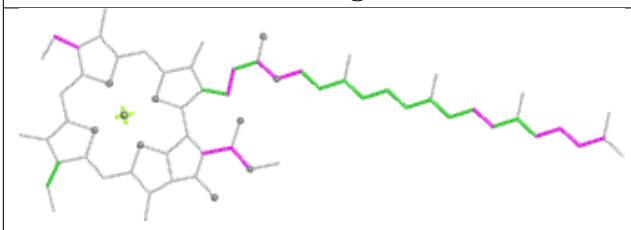

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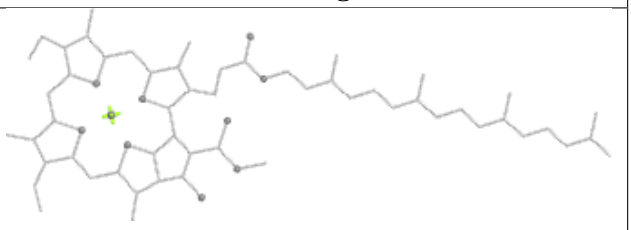
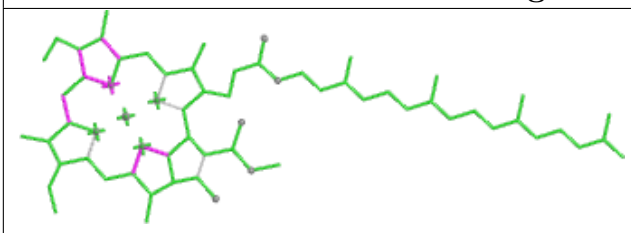


Rings

Ligand CLA q 510



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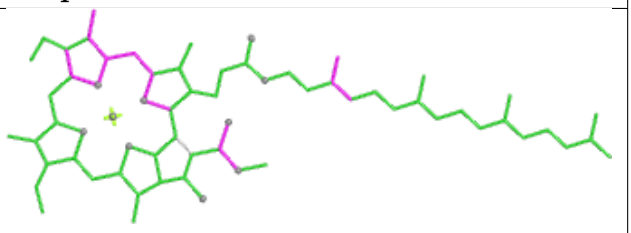
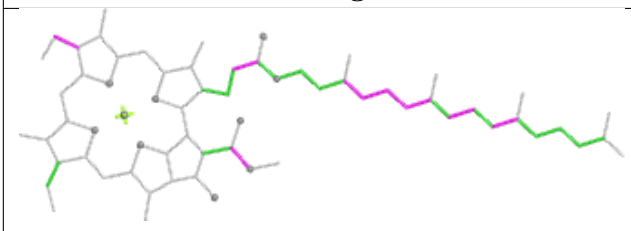


Bond angles



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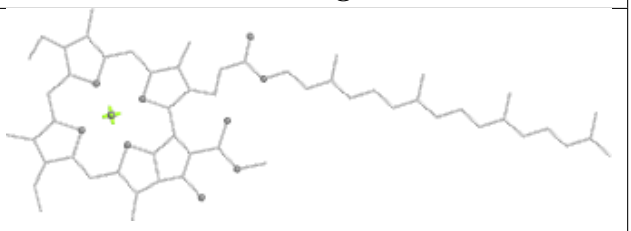
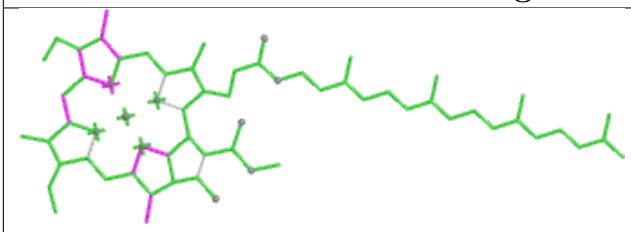


Rings

Ligand CLA H 1208



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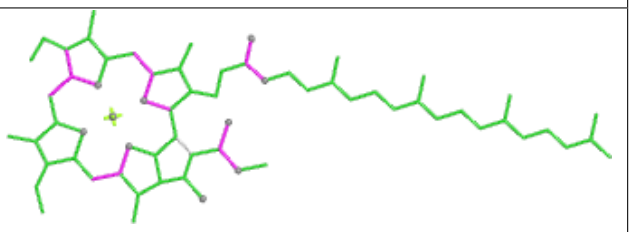

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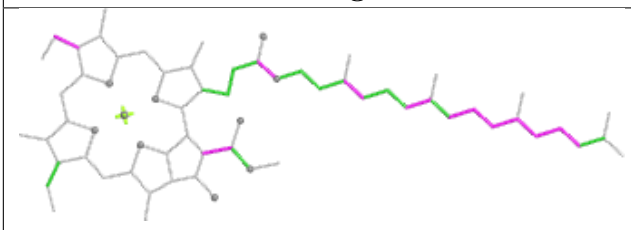

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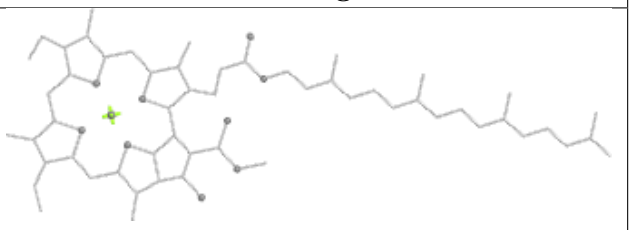
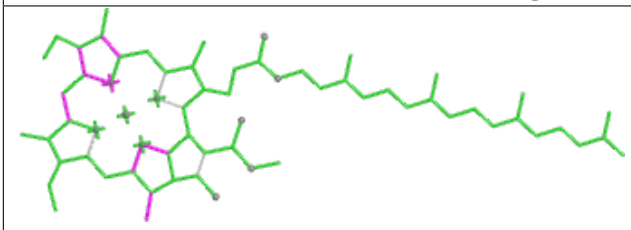
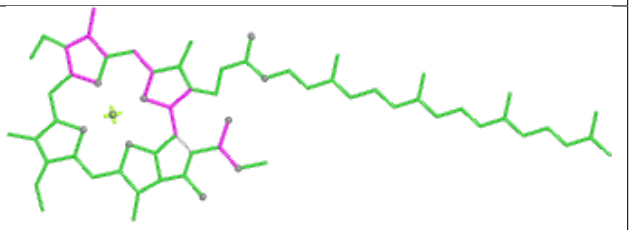
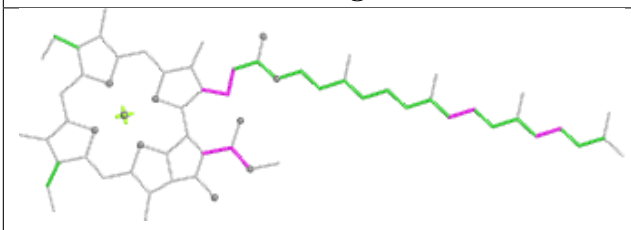
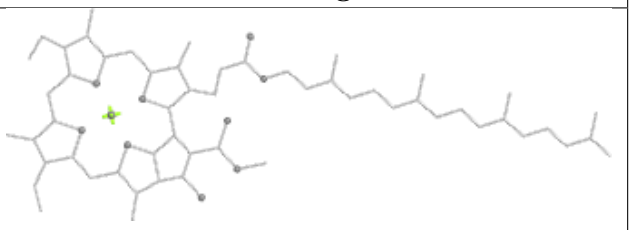


Rings

Ligand CLA Z 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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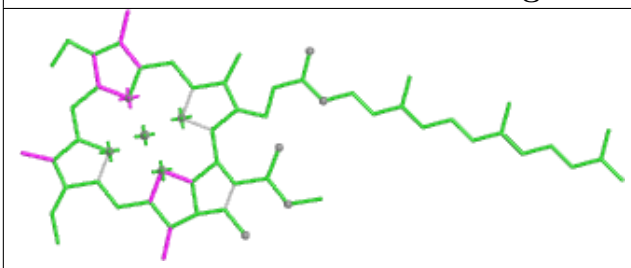
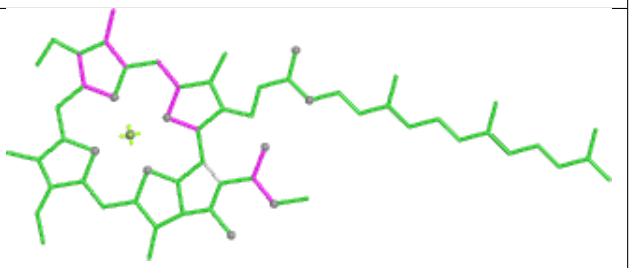
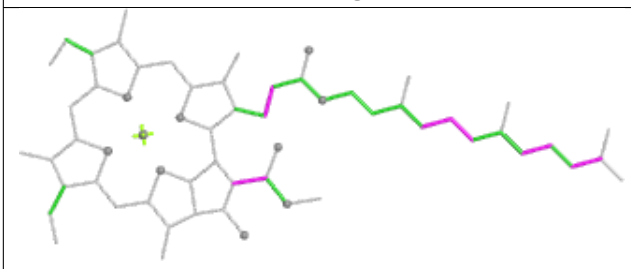
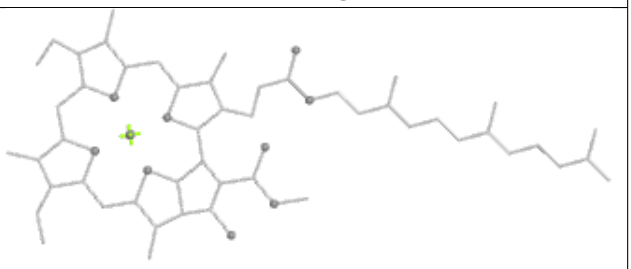
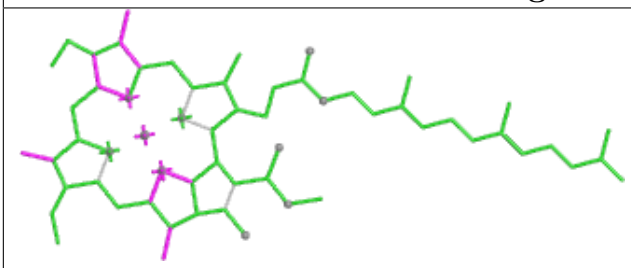
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 518



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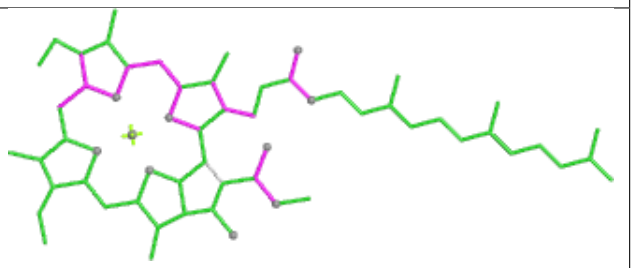
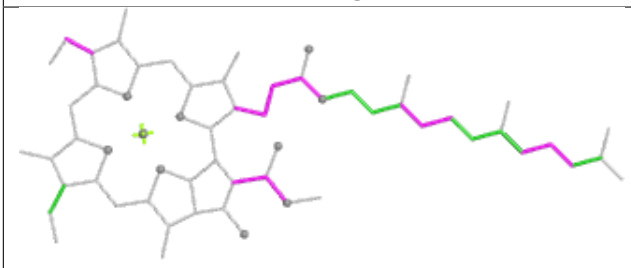


Bond angles



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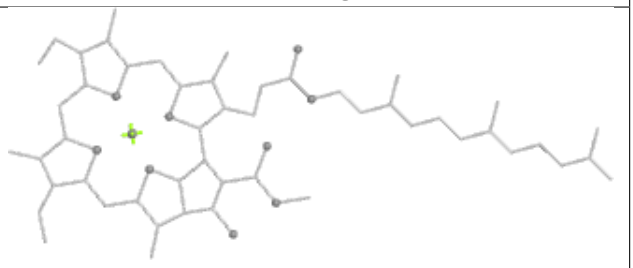
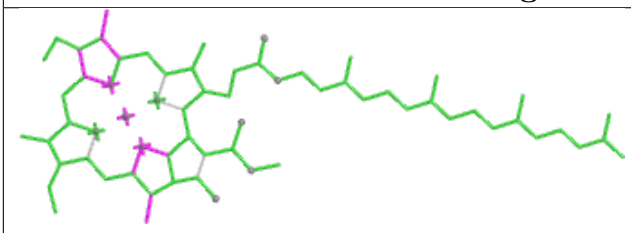


Rings

Ligand CLA e 1133



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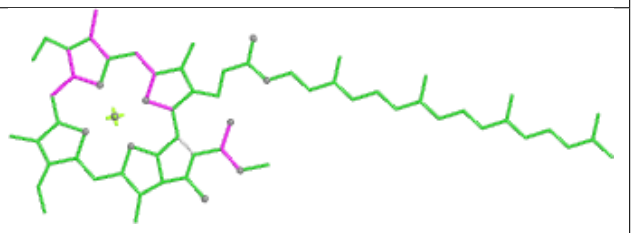
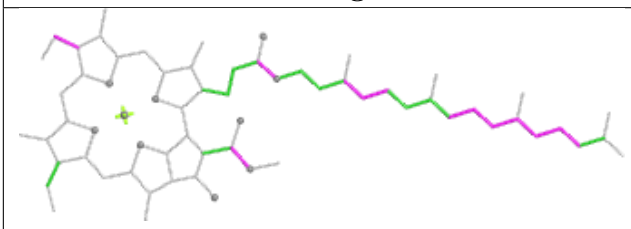
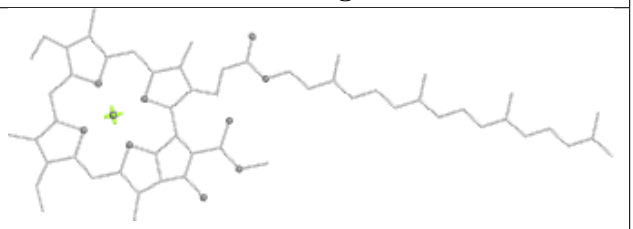


Bond angles



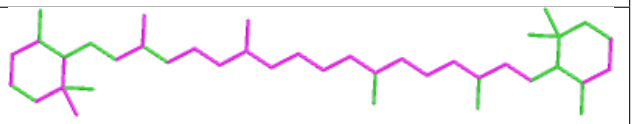
Torsions



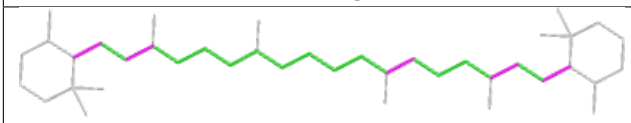
Rings

Ligand BCR f 4014

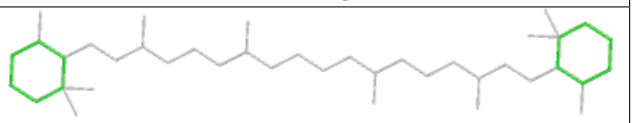
Bond lengths



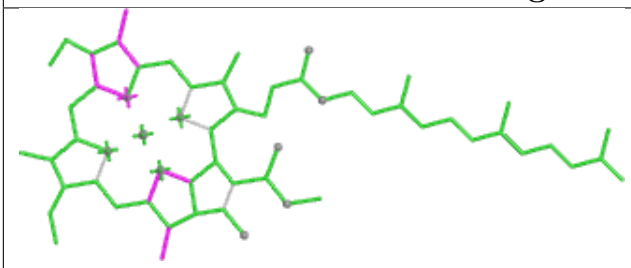
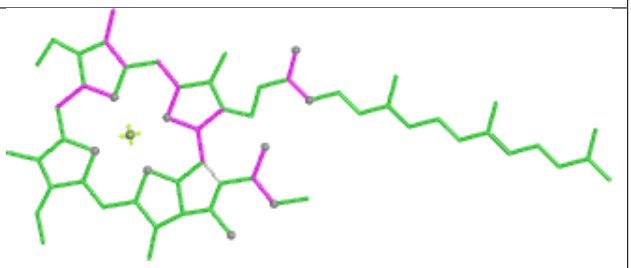
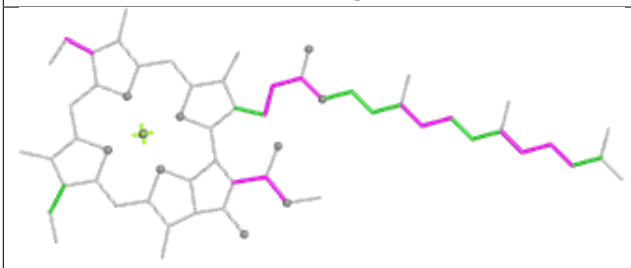
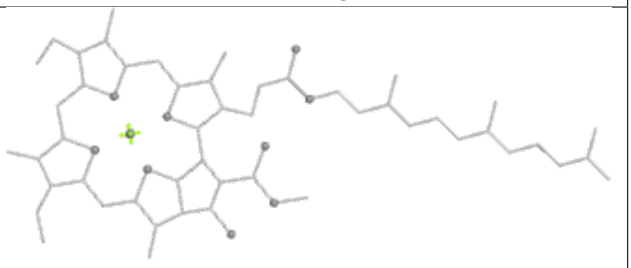
Bond angles

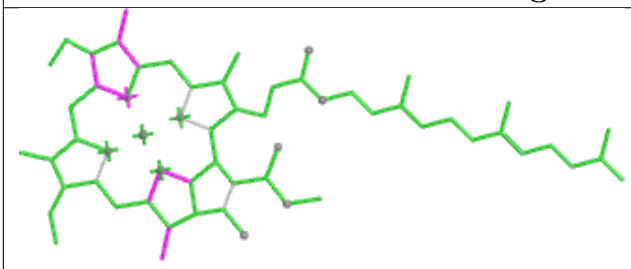
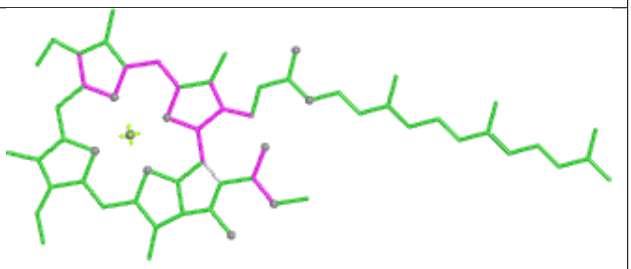
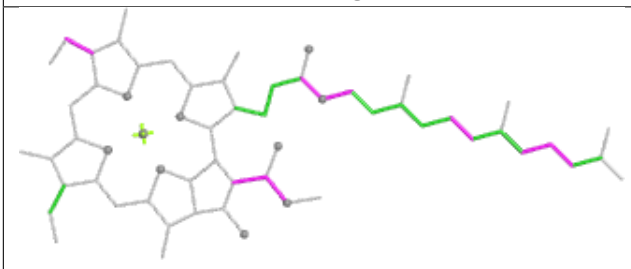
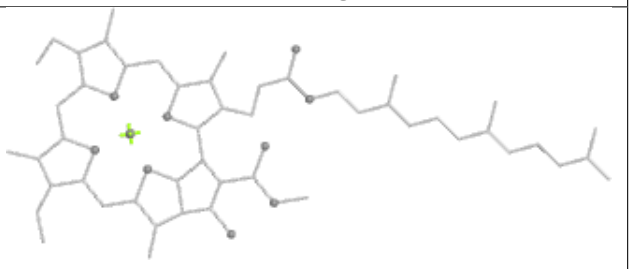


Torsions

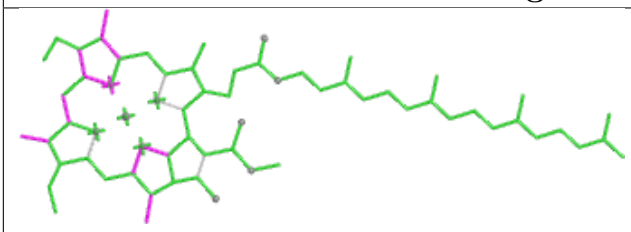


Rings

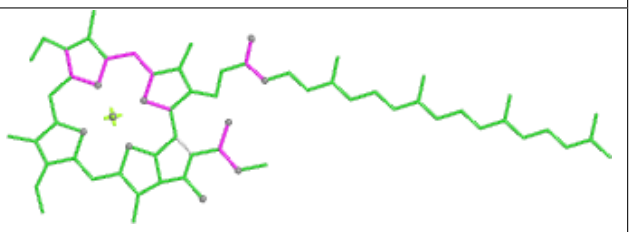
Ligand CLA 1 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

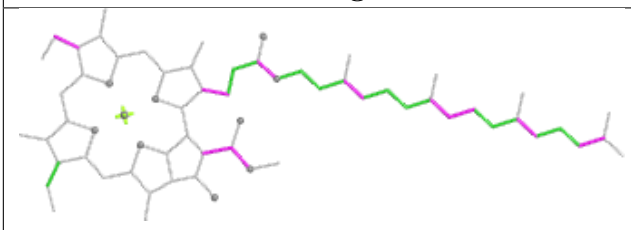
Ligand CLA Z 513



Bond lengths



Bond angles



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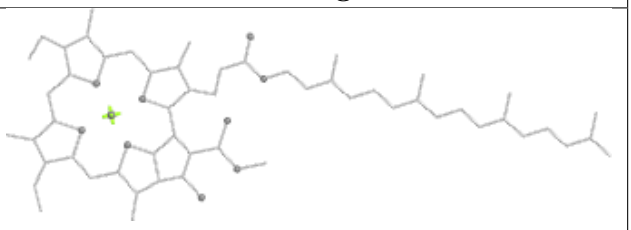
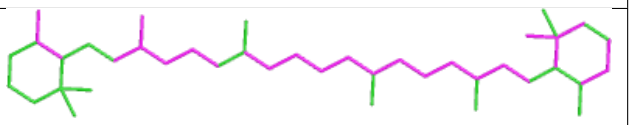


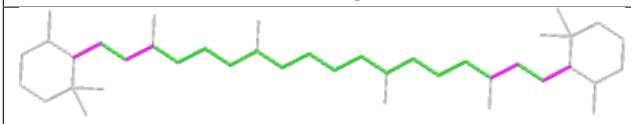
Rings

Ligand BCR B 4004

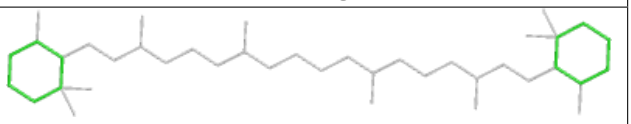
Bond lengths



Bond angles

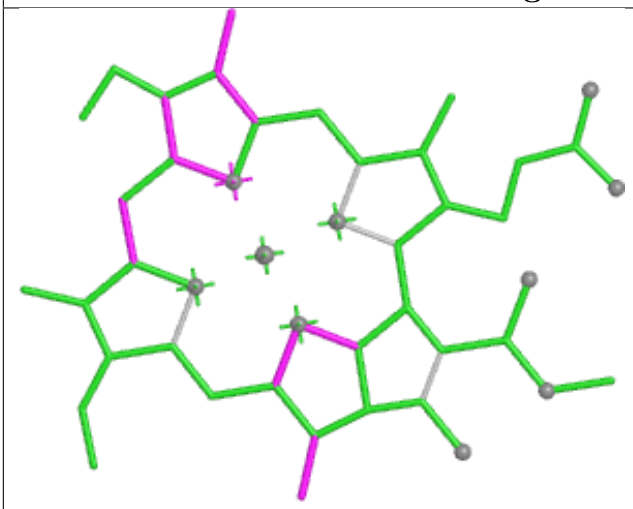


Torsions



Rings

Ligand CLA Y 516



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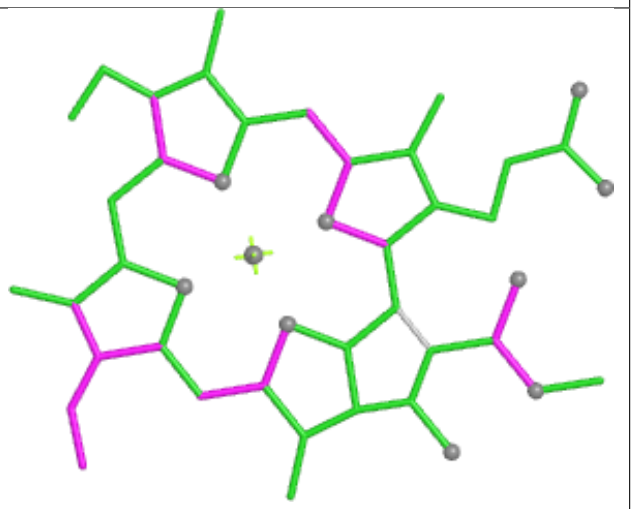
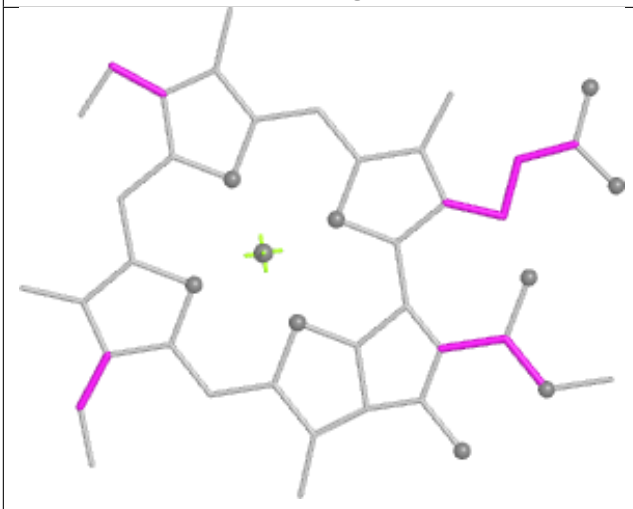


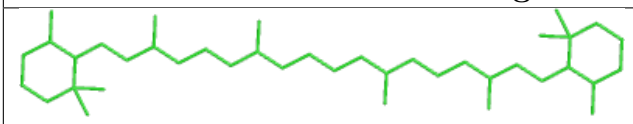
Bond angles



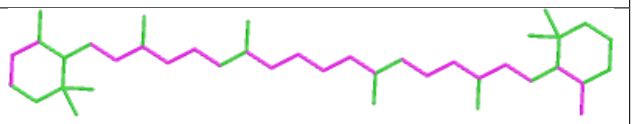
Torsions

Rings

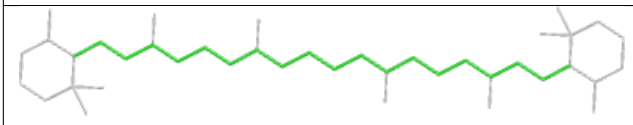
Ligand BCR A 4003



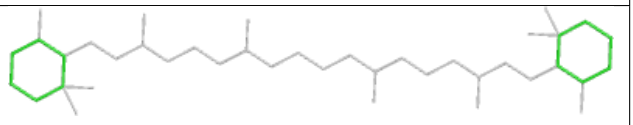
Bond lengths



Bond angles

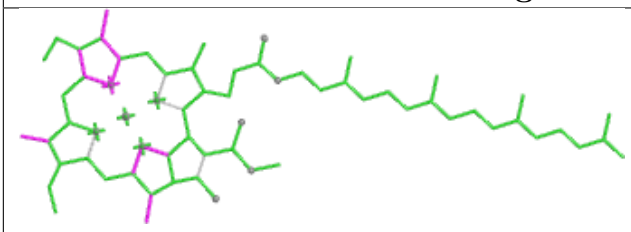


Torsions



Rings

Ligand CLA B 1235



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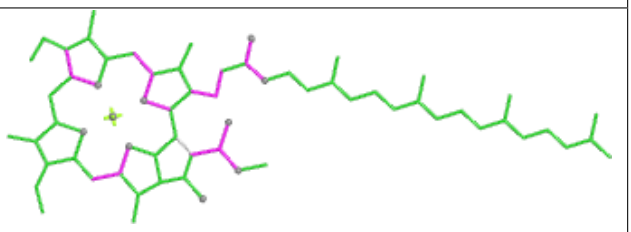
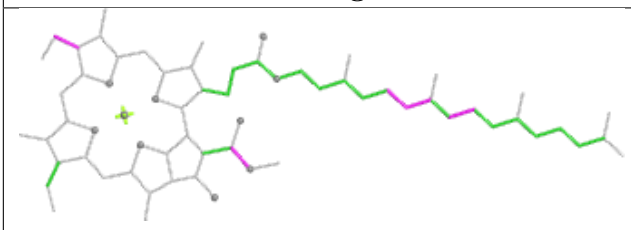


Bond angles



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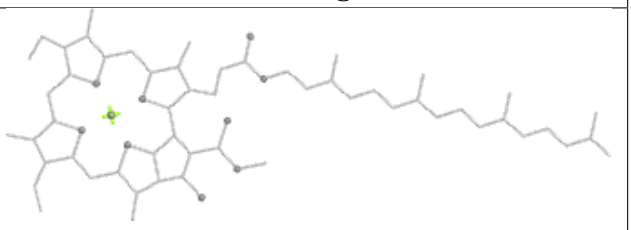
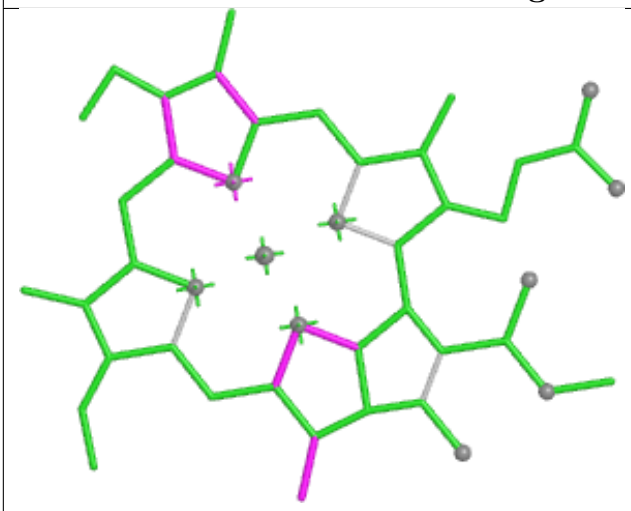


Rings

Ligand CLA 4 507



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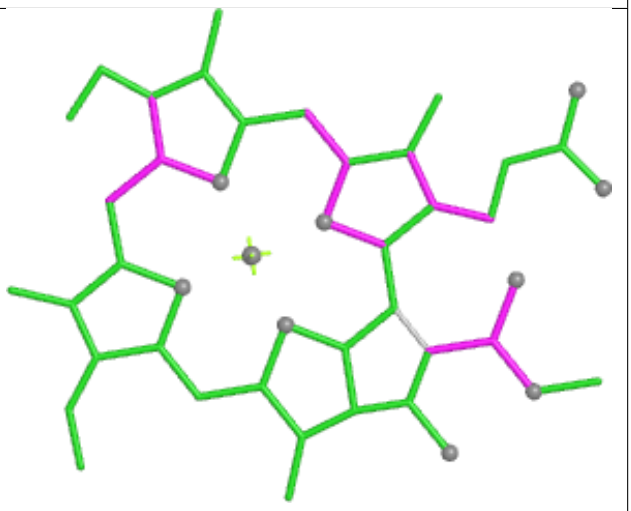
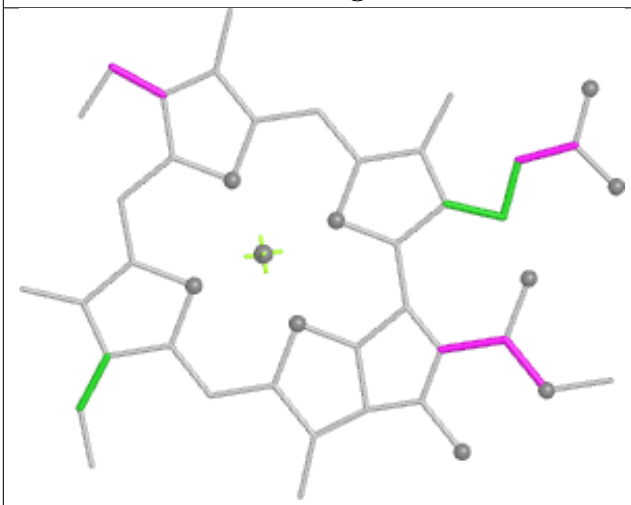


Bond angles



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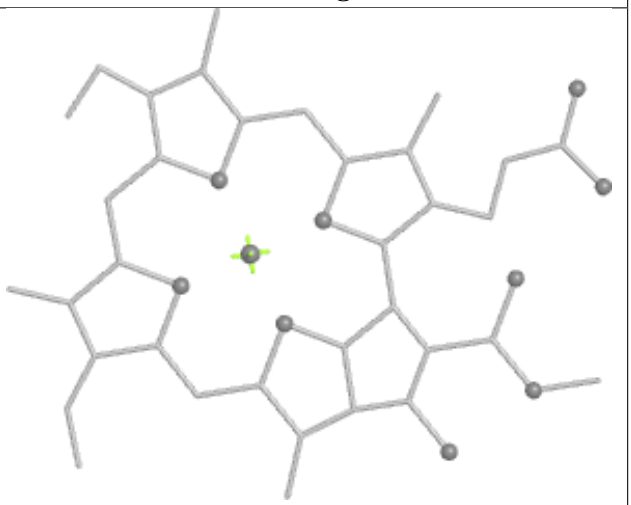
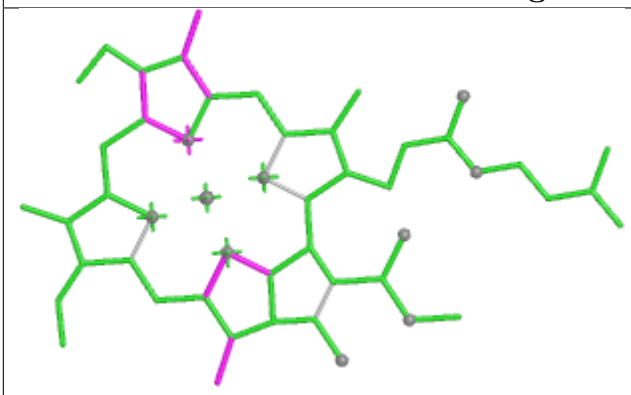


Rings

Ligand CLA 6 502



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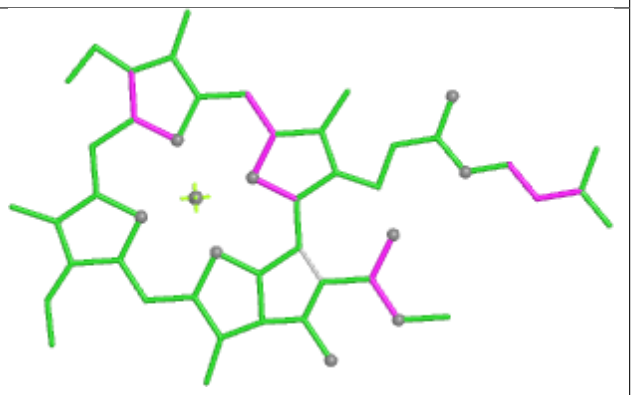
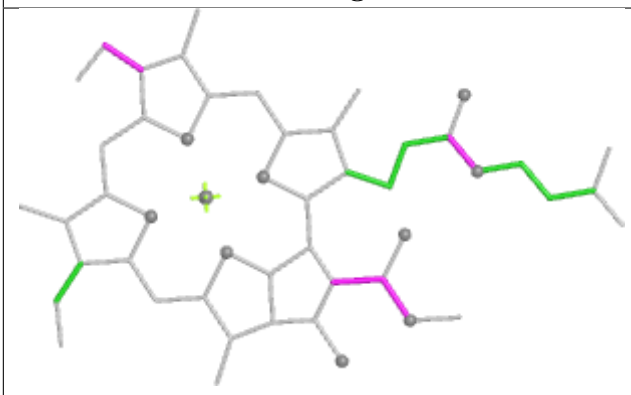


Bond angles



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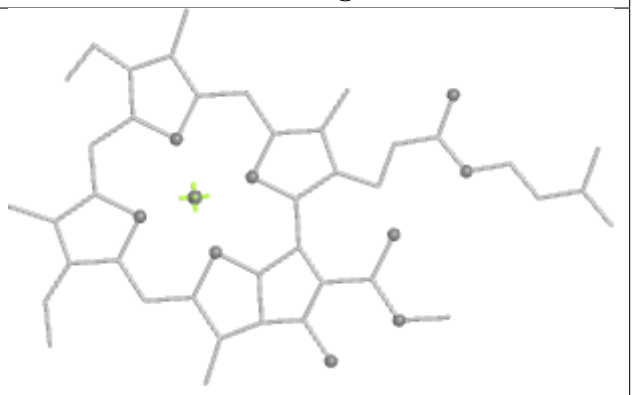
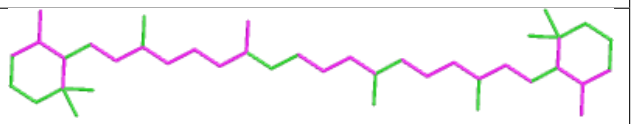


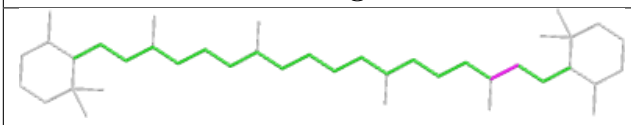
Rings

Ligand BCR I 4018

Bond lengths



Bond angles



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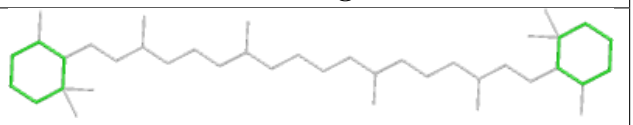
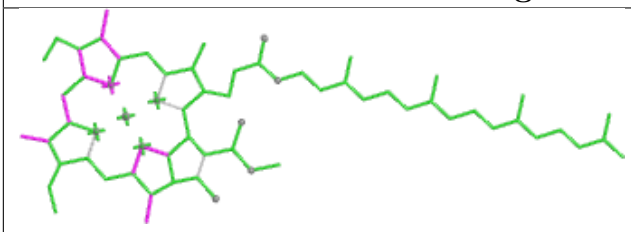


Rings

Ligand CLA A 1101



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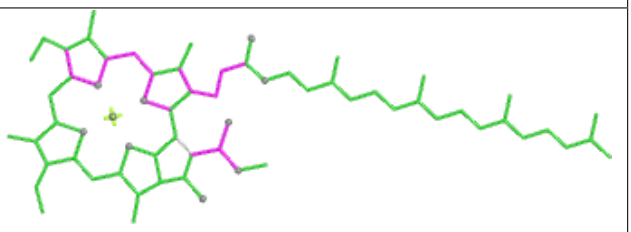
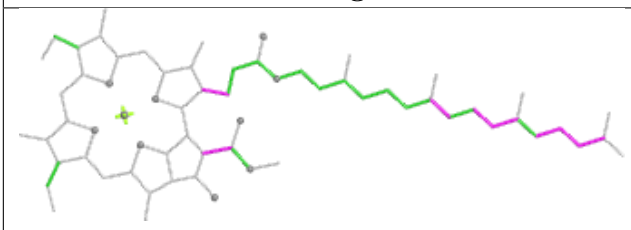
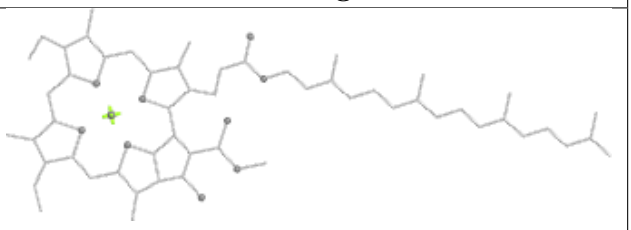


Bond angles

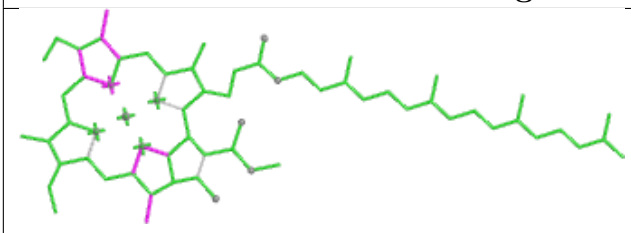


Torsions



Rings

Ligand CLA B 1219



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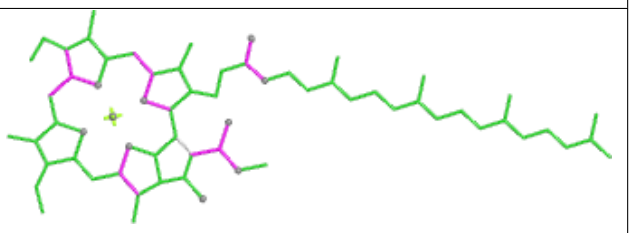
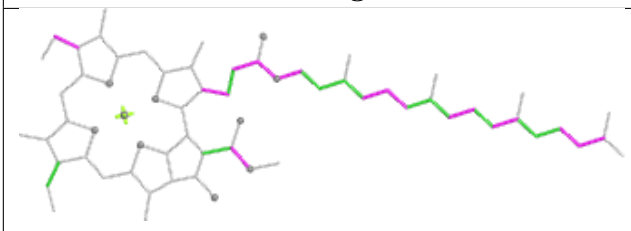
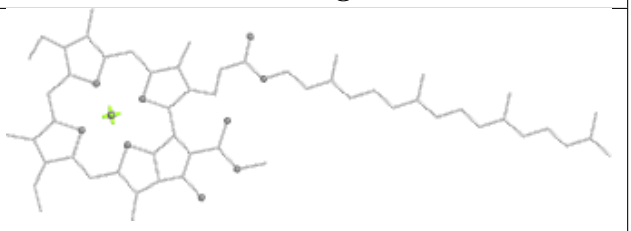


Bond angles

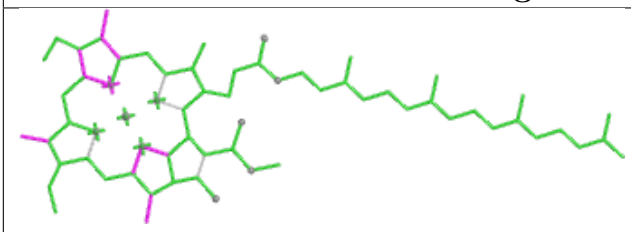


Torsions



Rings

Ligand CLA G 1109



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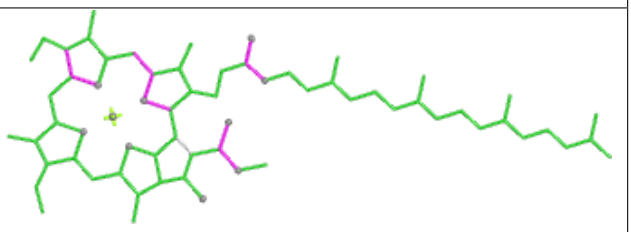
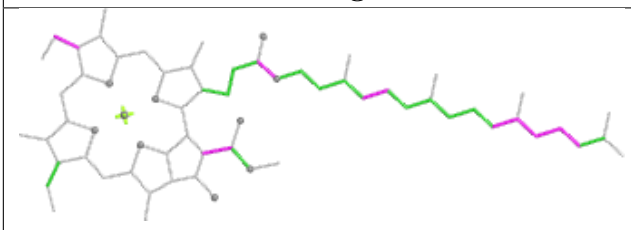
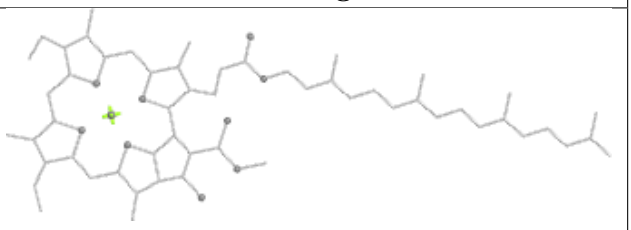


Bond angles

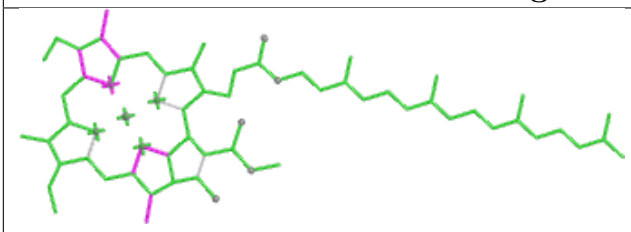


Torsions



Rings

Ligand CLA t 509



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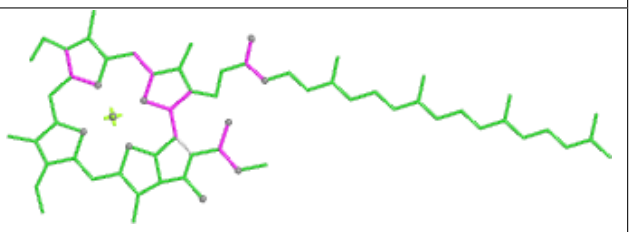

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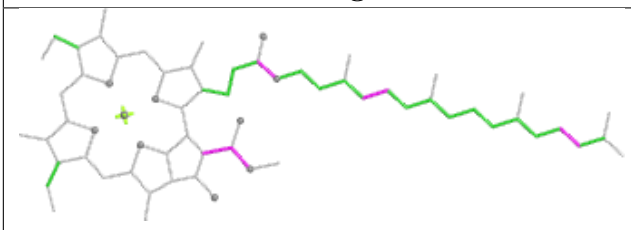

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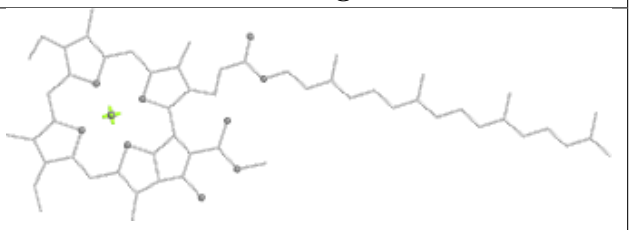

Rings

Ligand BCR 4 522

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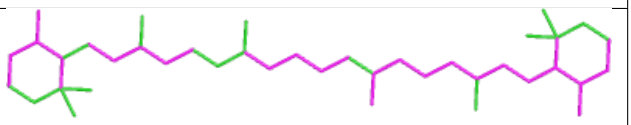

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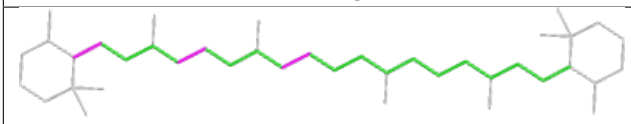

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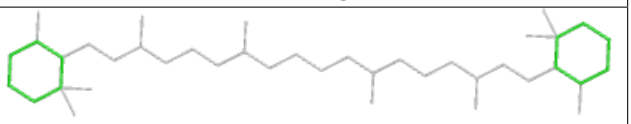
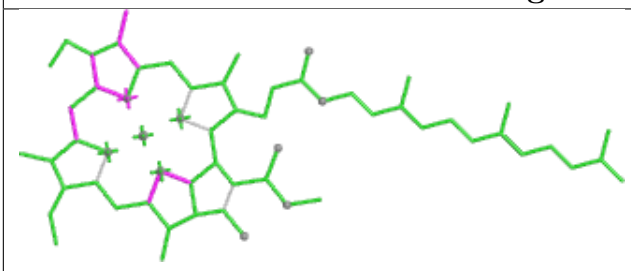


Rings

Ligand CLA b 501



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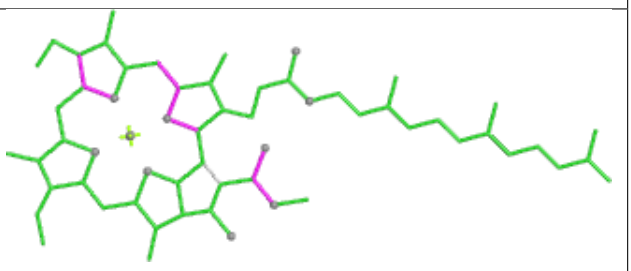

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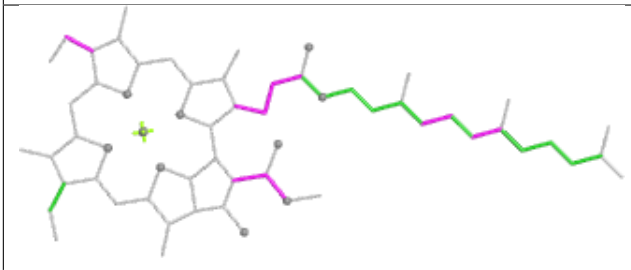

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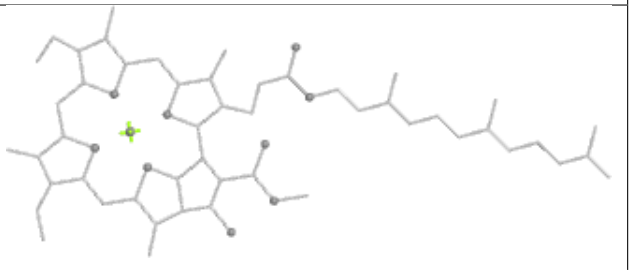
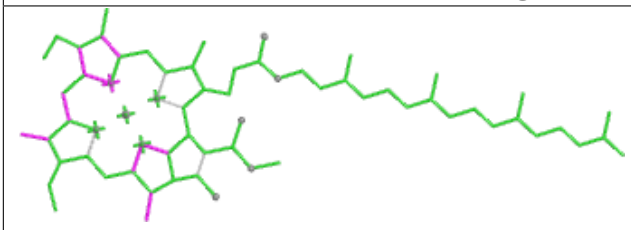


Rings

Ligand CLA G 1127



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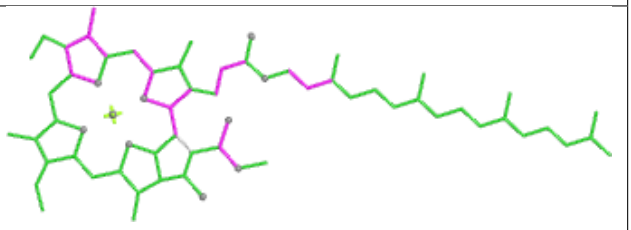
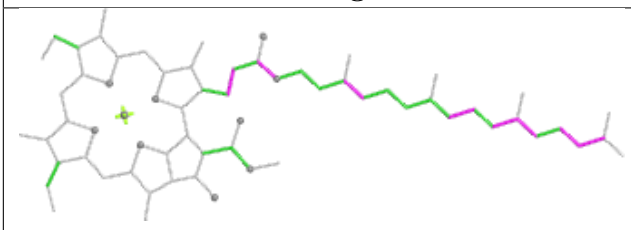


Bond angles



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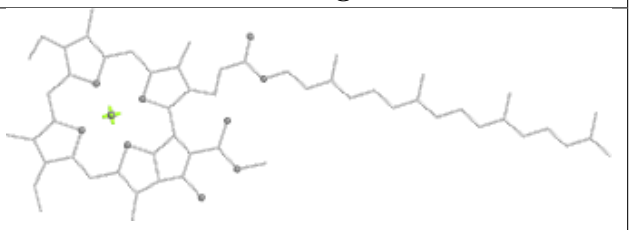

Rings

Ligand BCR J 4015

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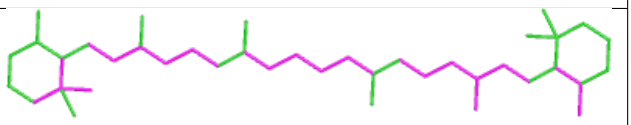

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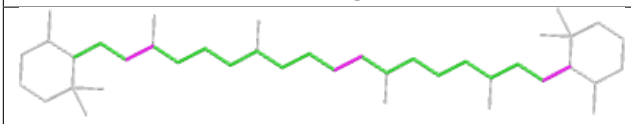

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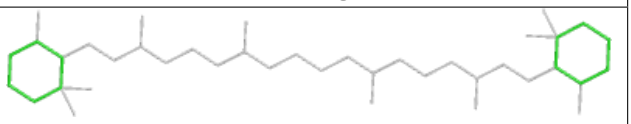
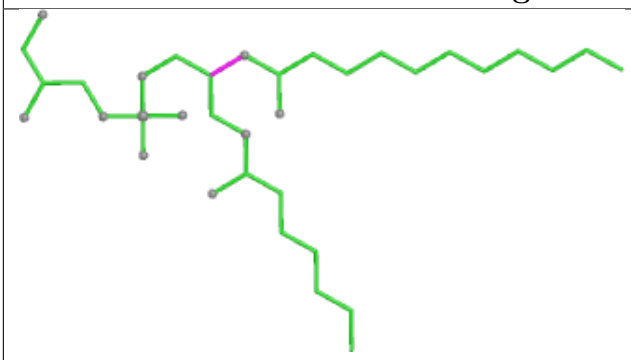


Rings

Ligand LHG G 5008



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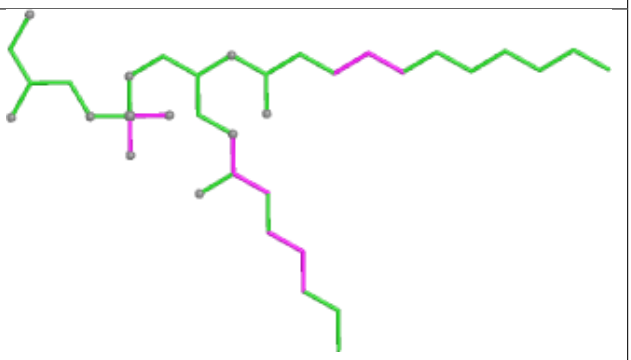

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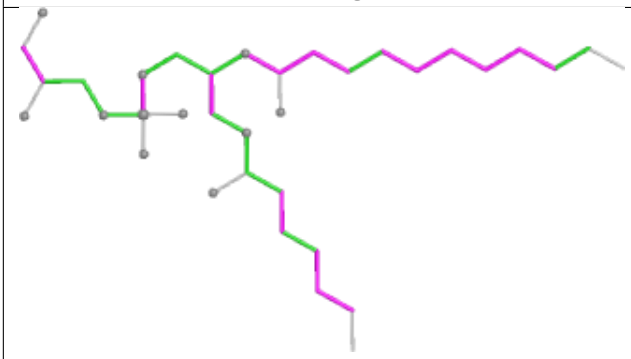

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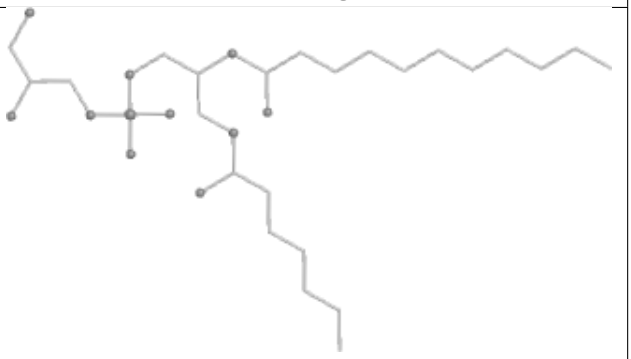
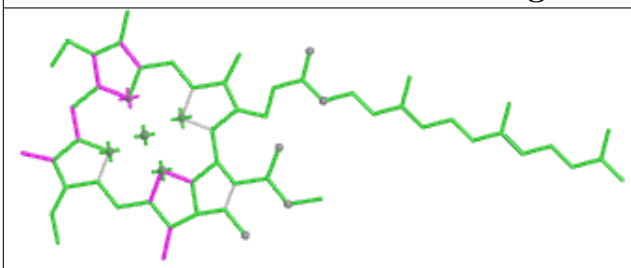


Rings

Ligand CLA v 501



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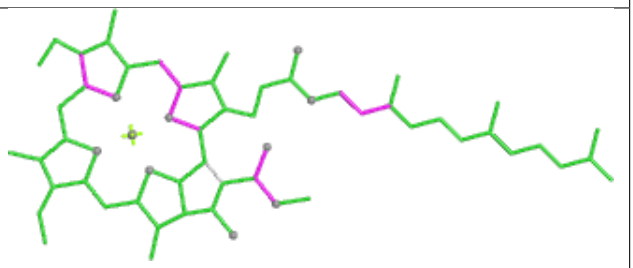

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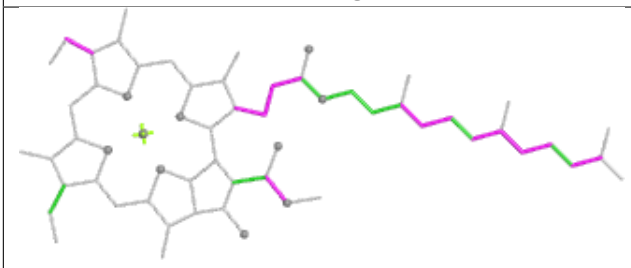

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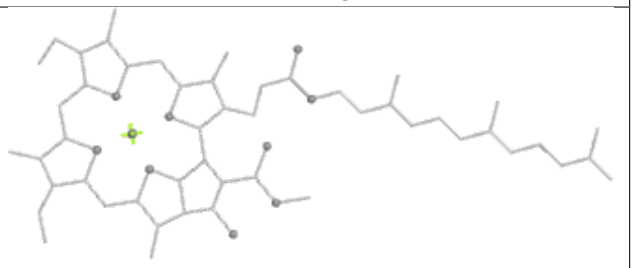

Rings

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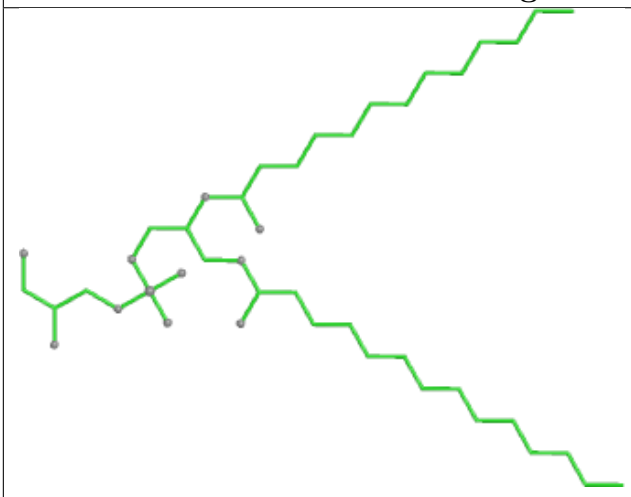

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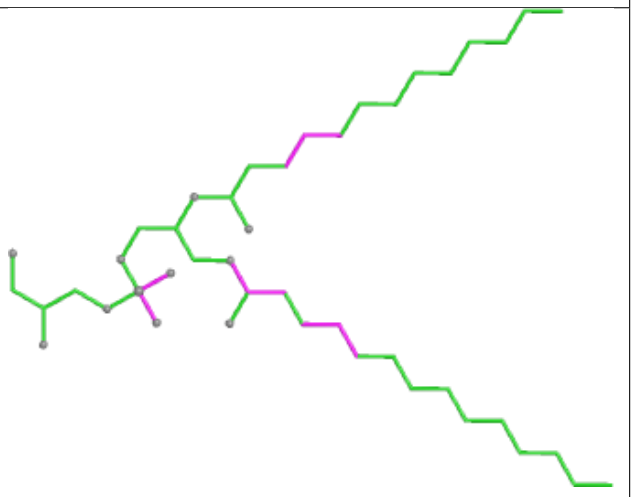

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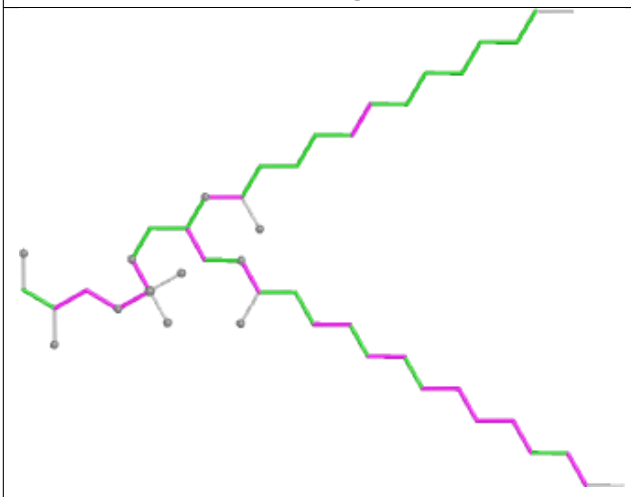

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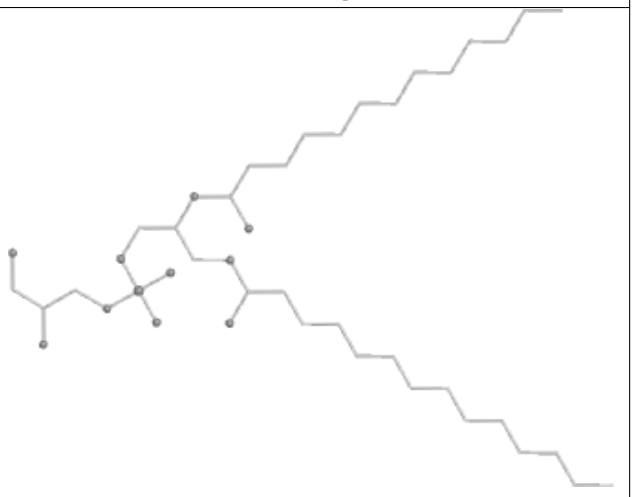
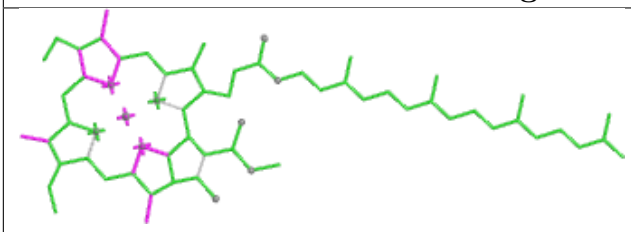


Rings

Ligand CLA e 1117



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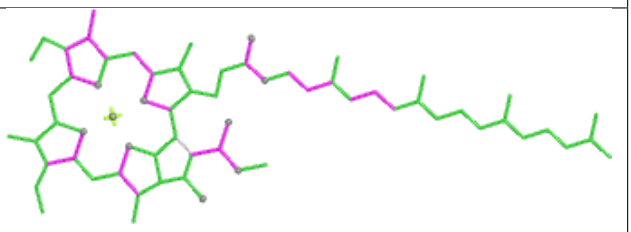

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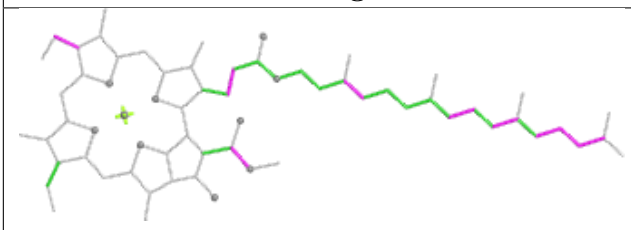

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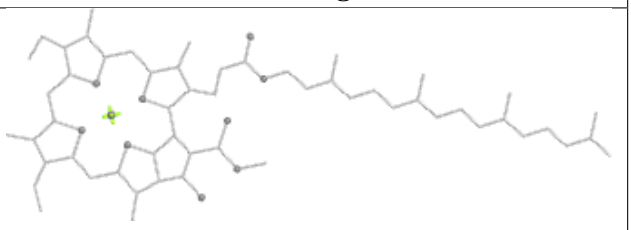
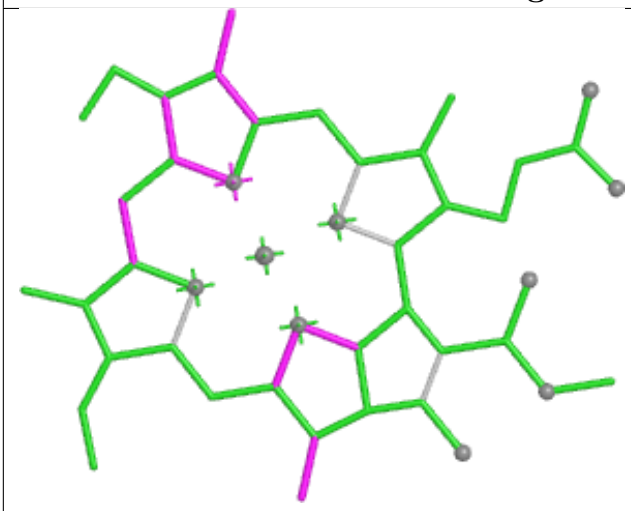


Rings

Ligand CLA u 510



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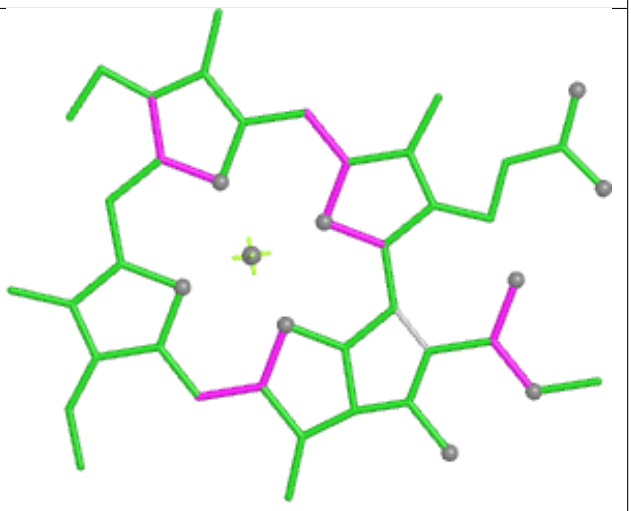

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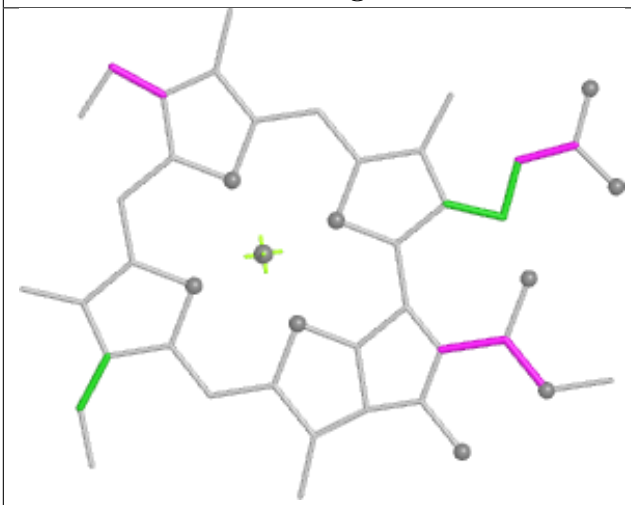

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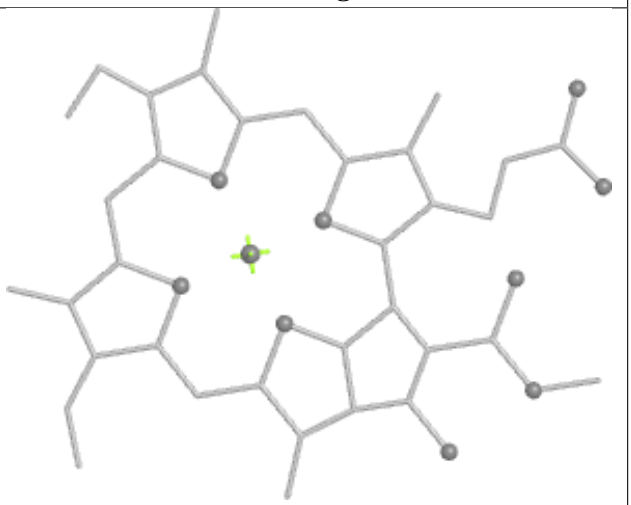
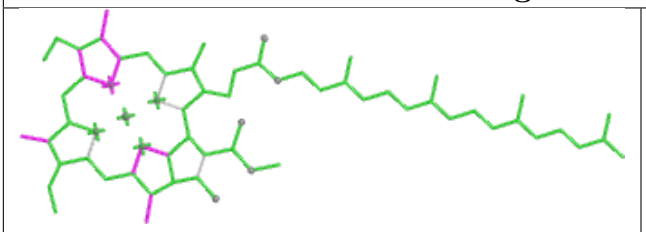


Rings

Ligand CLA G 1104



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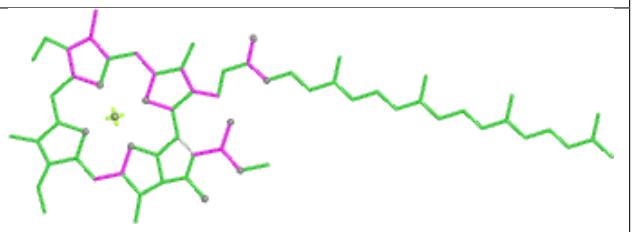

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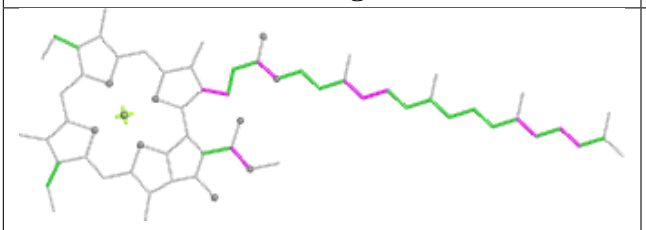

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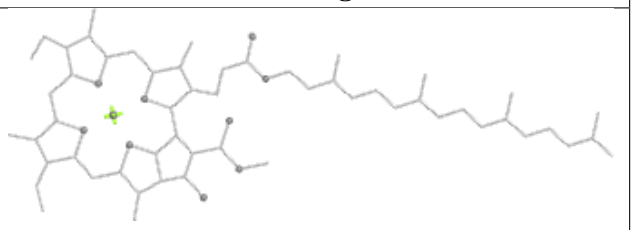
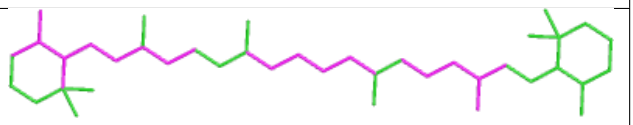


Rings

Ligand BCR 2 524

Bond lengths



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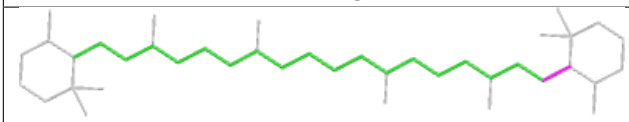

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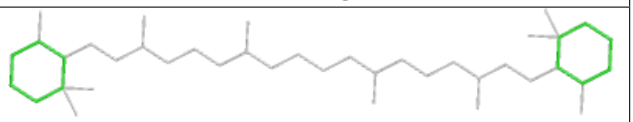
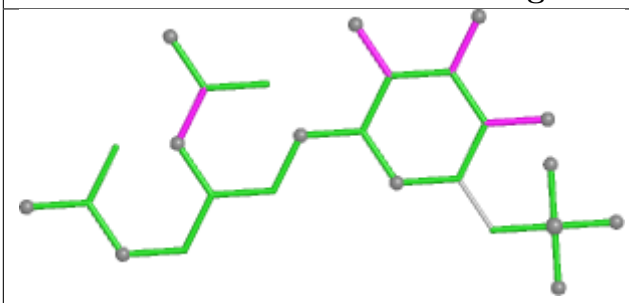


Rings

Ligand SQD d 822



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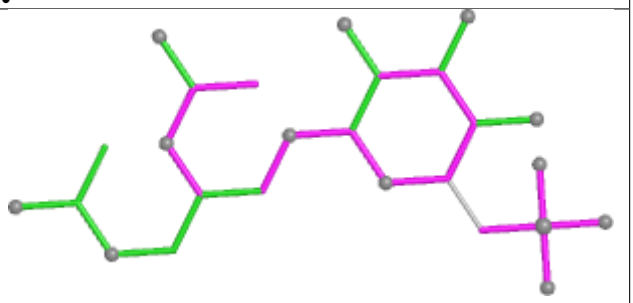
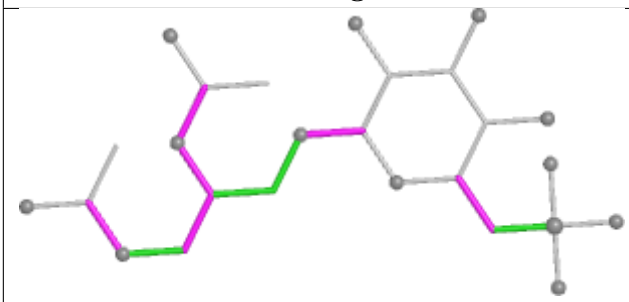


Bond angles



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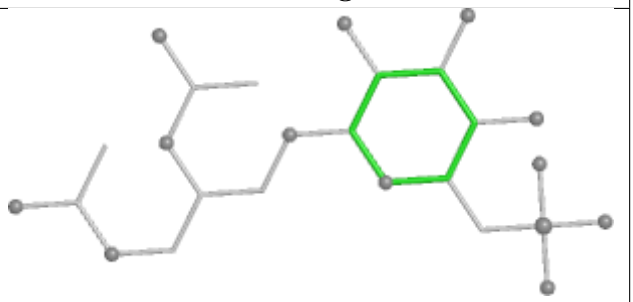
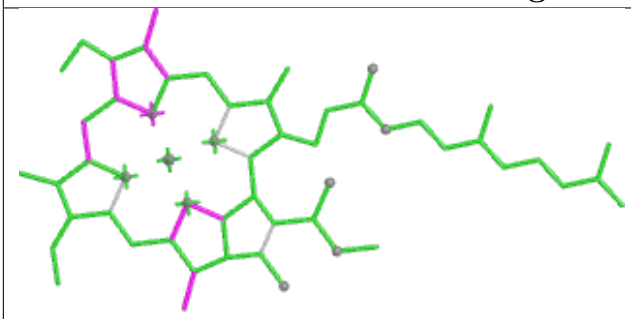
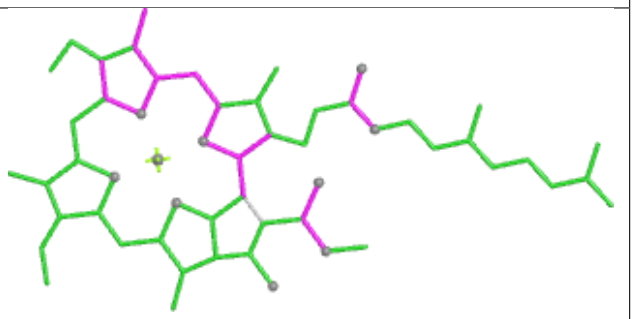


Rings

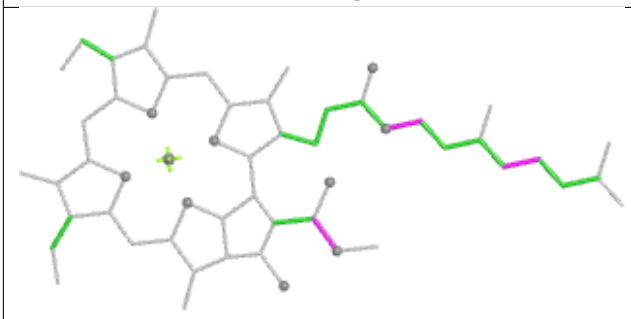
Ligand CLA 1 511



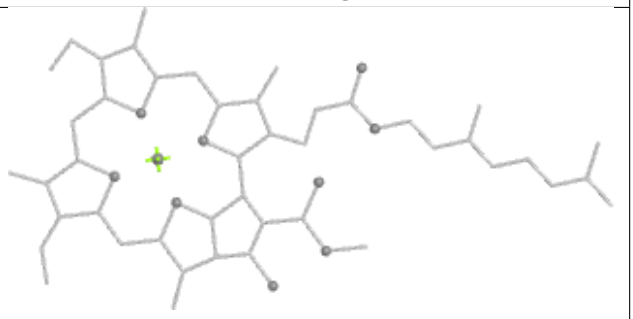
Bond lengths



Bond angles

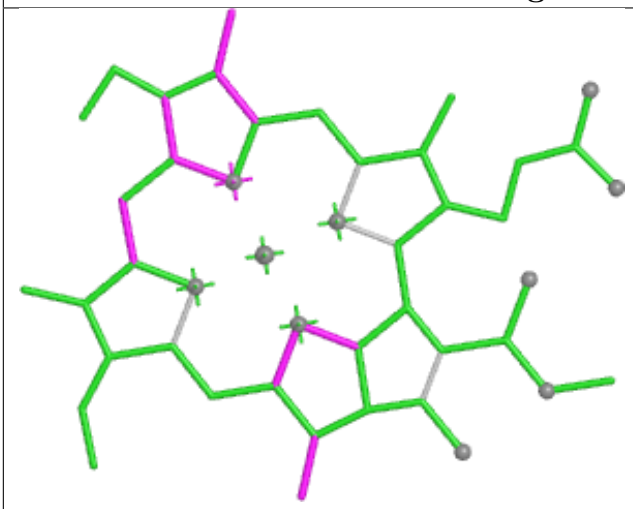


Torsions



Rings

Ligand CLA b 511



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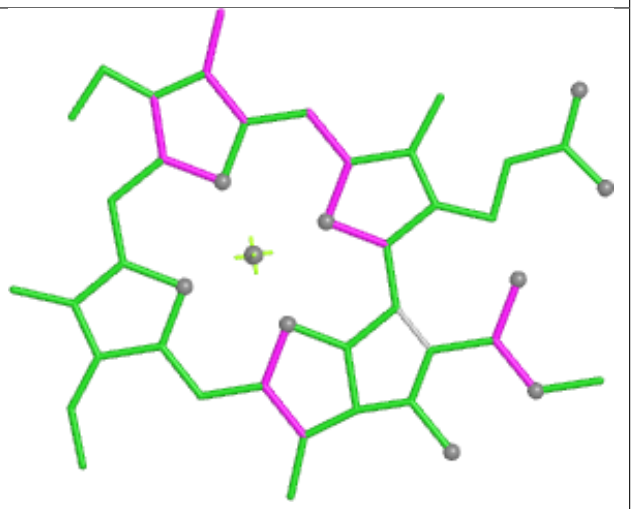
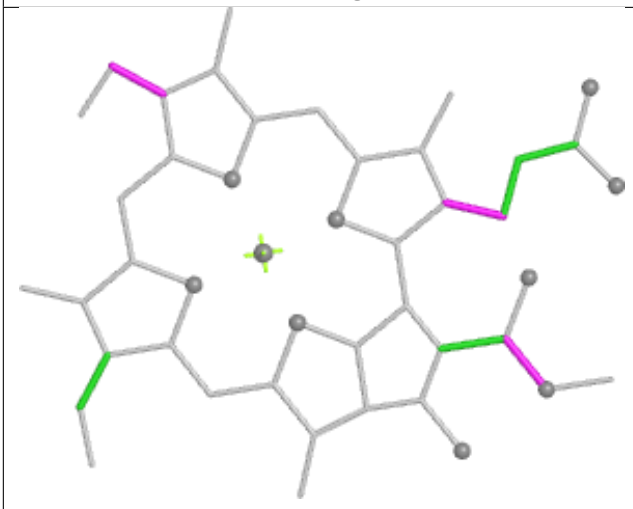


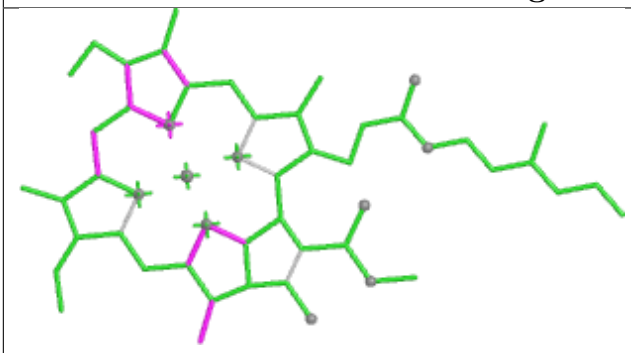
Bond angles



Torsions

Rings

Ligand CLA 6 503



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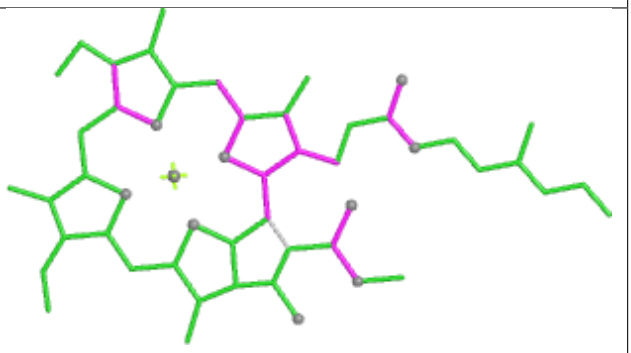

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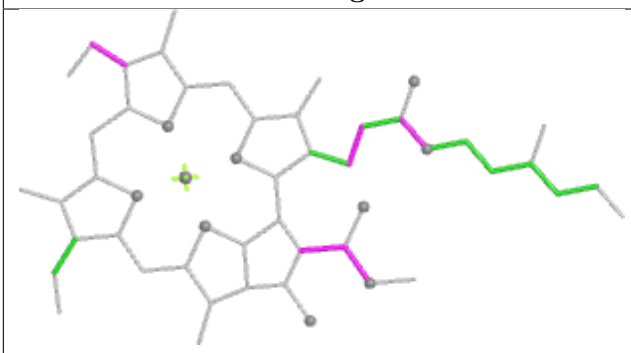

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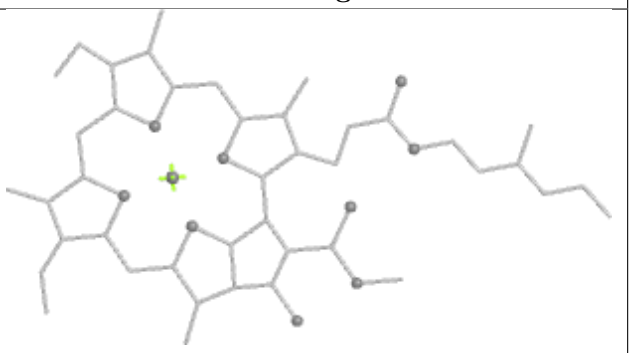
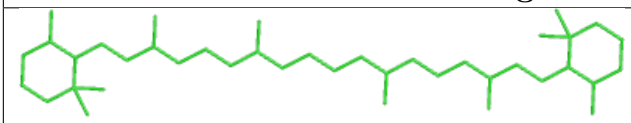


Rings

Ligand BCR n 4019



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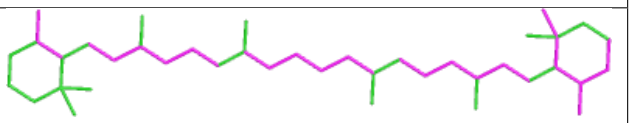
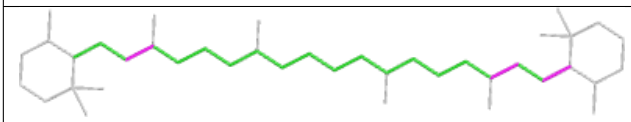


Bond angles



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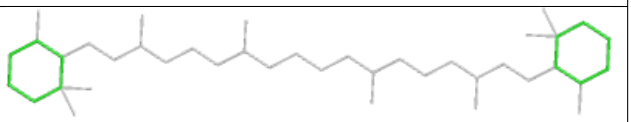
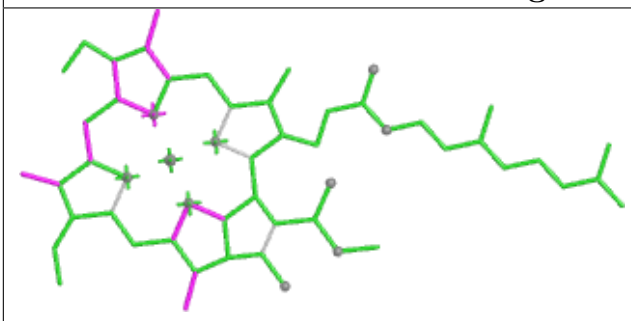


Rings

Ligand CLA 3 508



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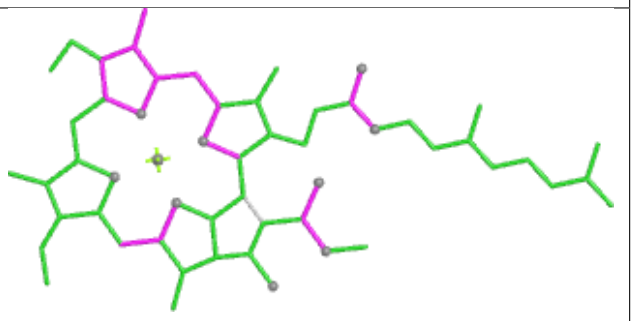

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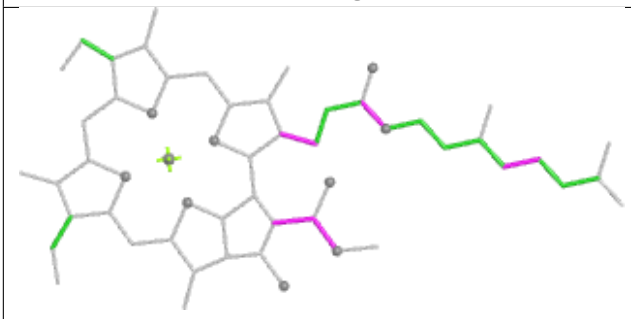

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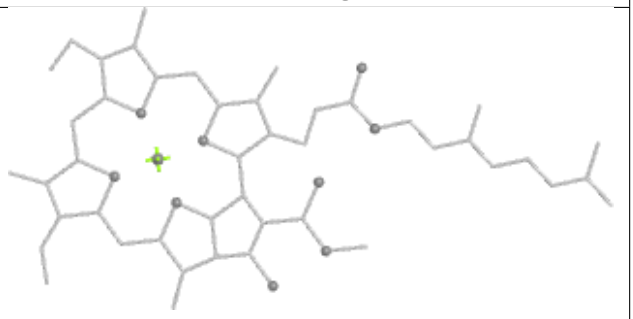
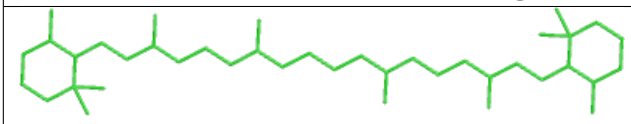


Rings

Ligand BCR m 4104



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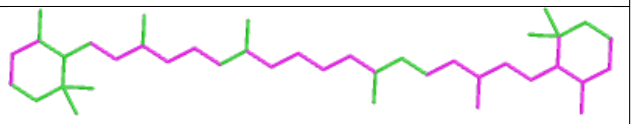

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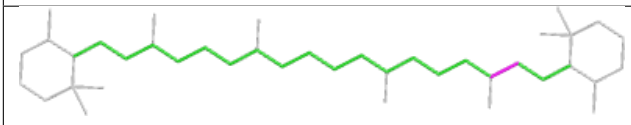

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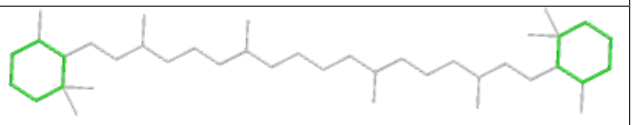
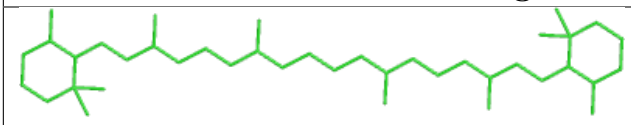


Rings

Ligand BCR B 4014



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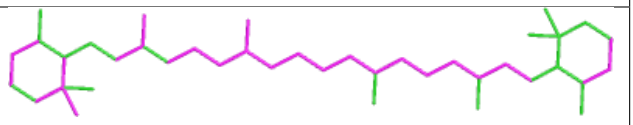

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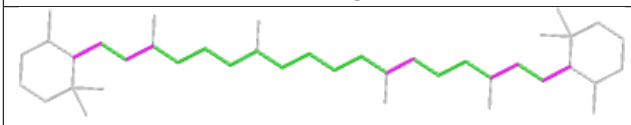

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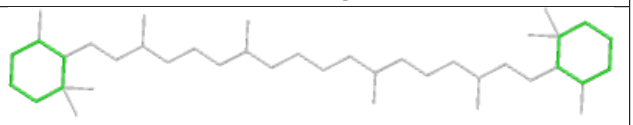
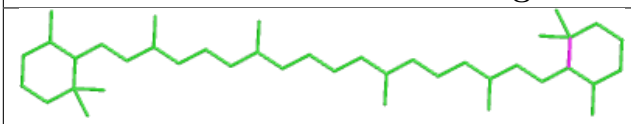


Rings

Ligand BCR A 4002



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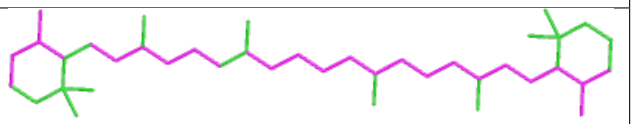

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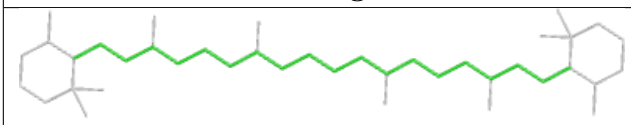

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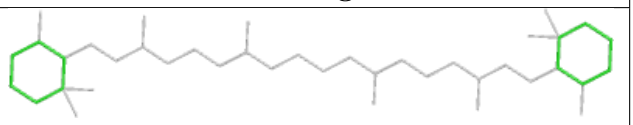
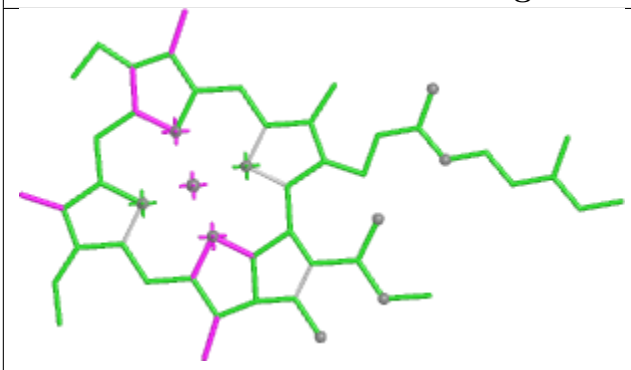


Rings

Ligand CLA G 1129



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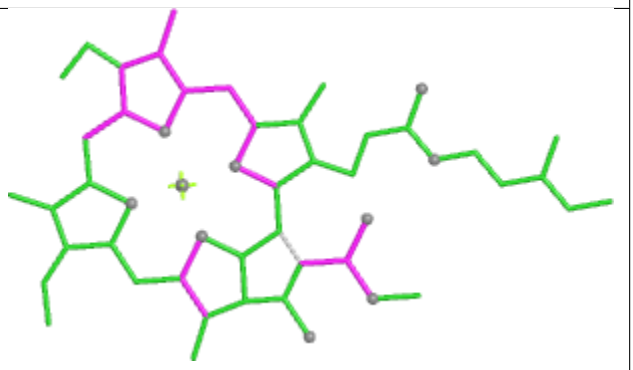
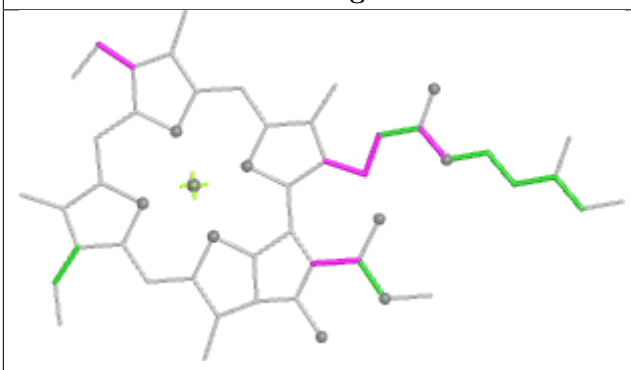


Bond angles



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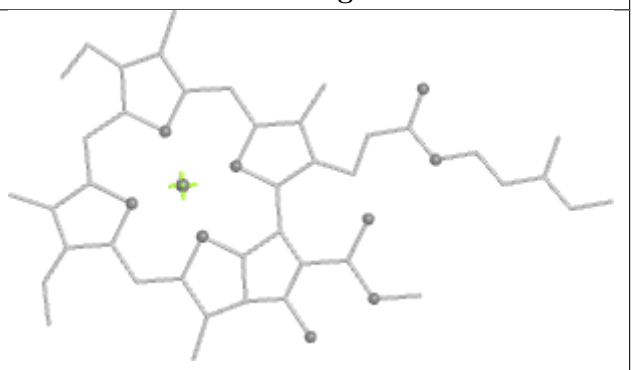
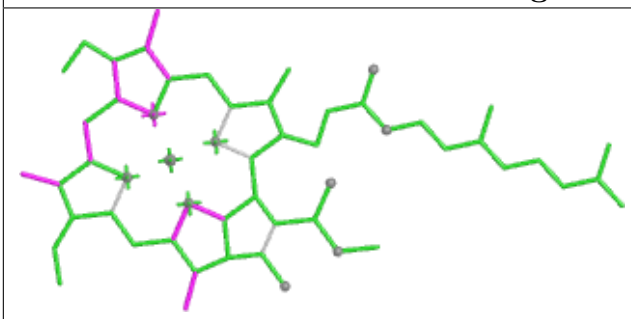


Rings

Ligand CLA t 519



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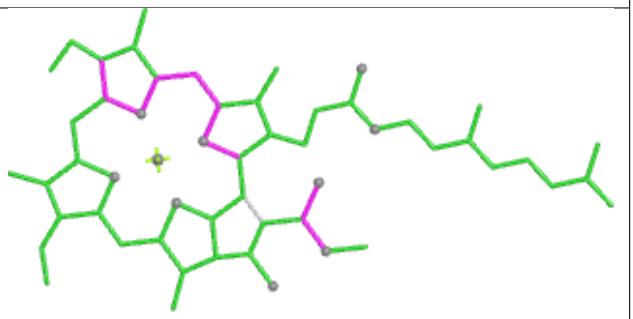

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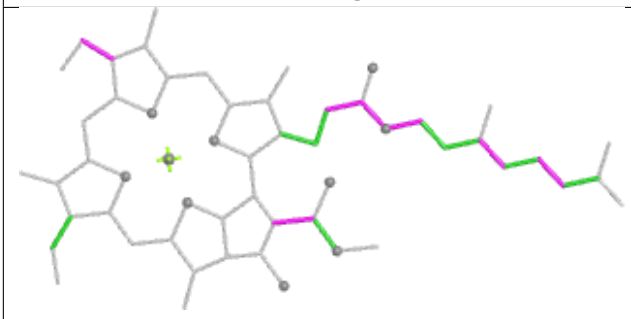

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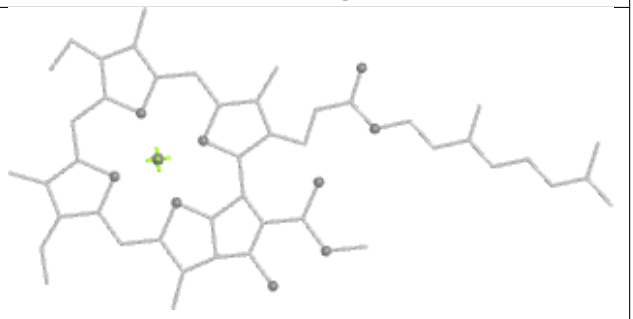
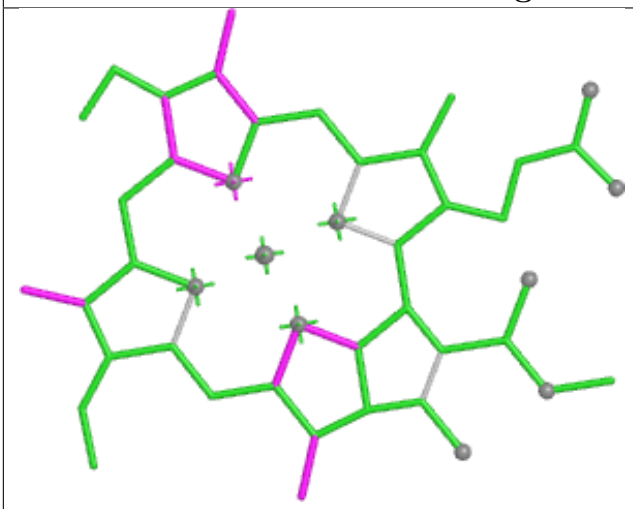


Rings

Ligand CLA A 1113



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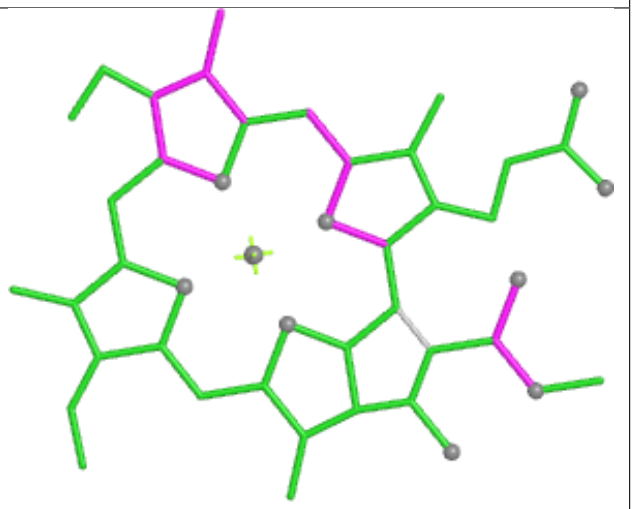

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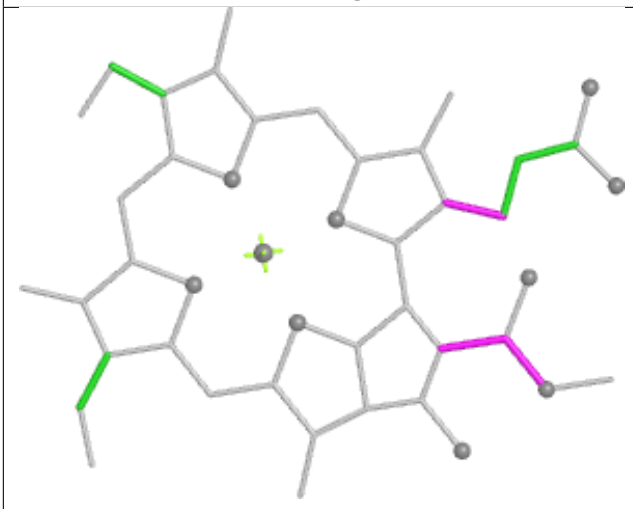
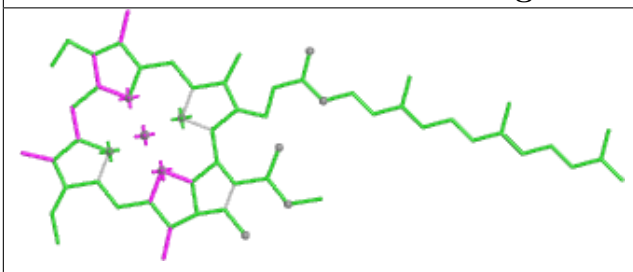


Torsions

Rings

Ligand CLA B 1216



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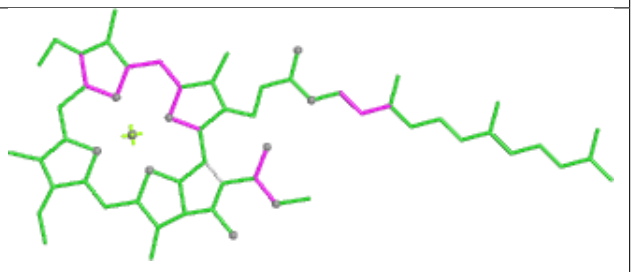

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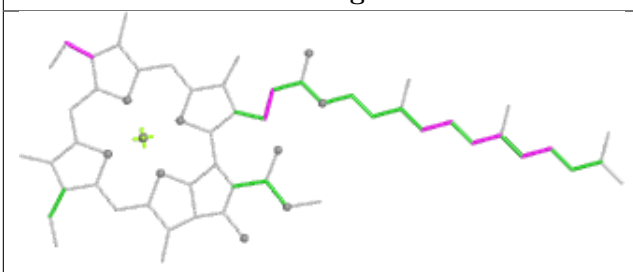

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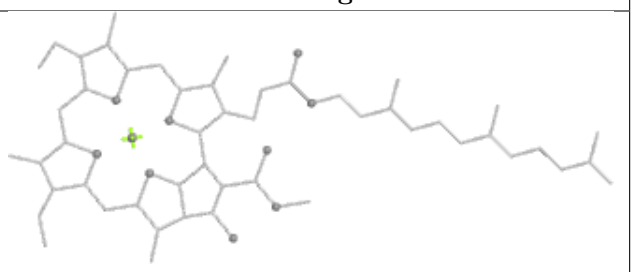
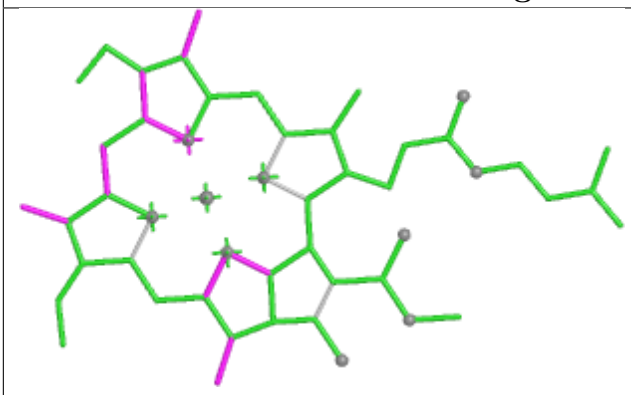


Rings

Ligand CLA G 1112



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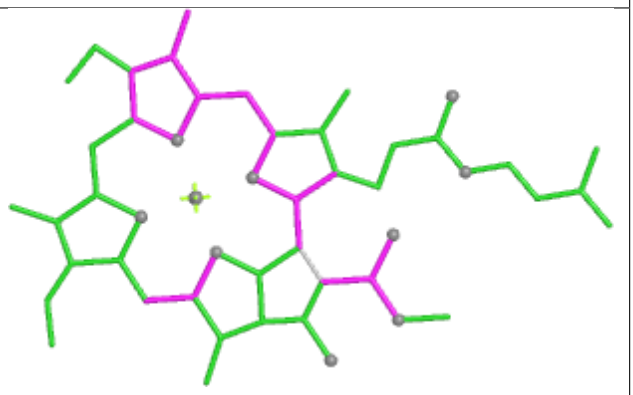
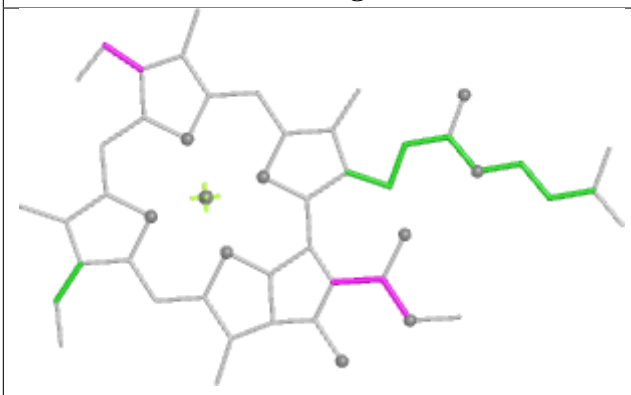


Bond angles



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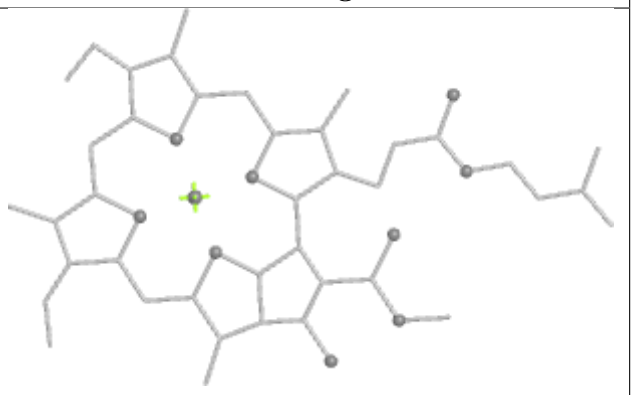
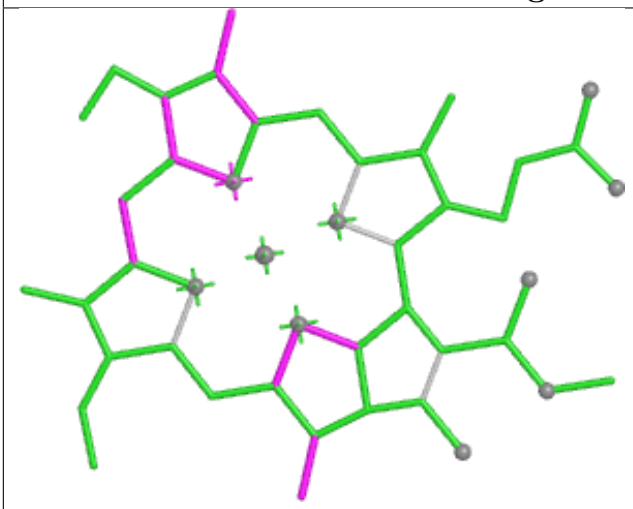


Rings

Ligand CLA v 510



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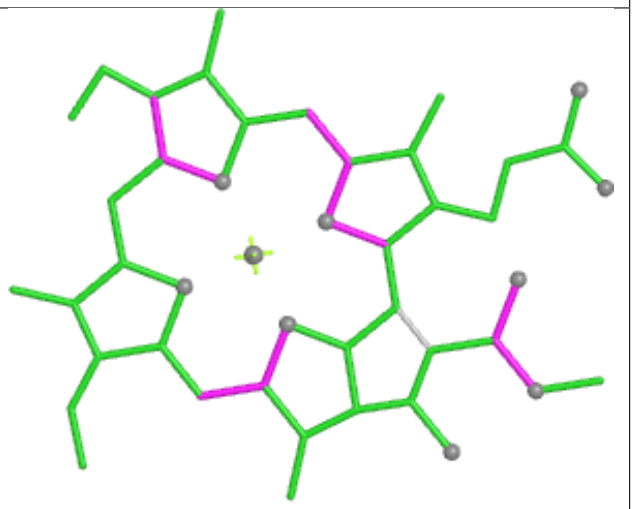
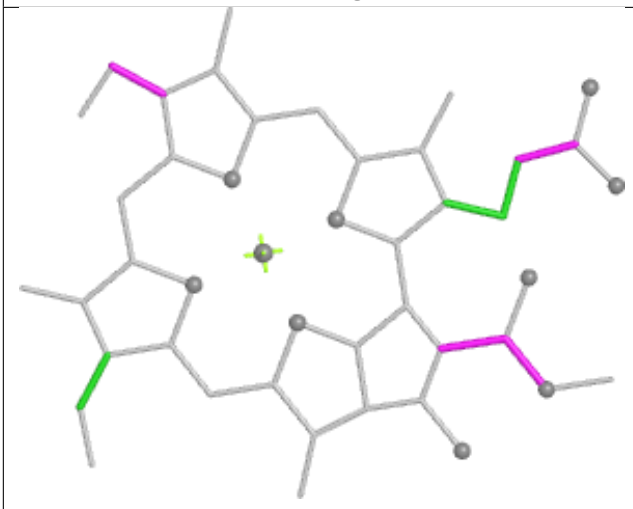


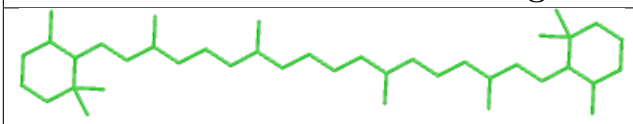
Bond angles



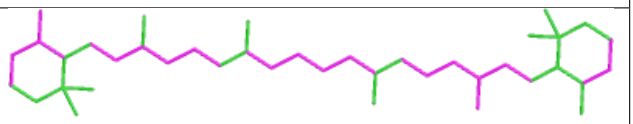
Torsions

Rings

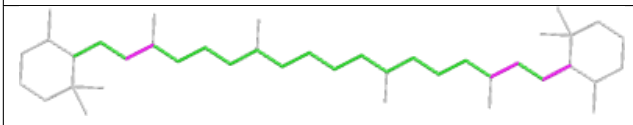
Ligand BCR r 523



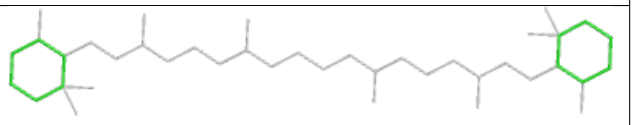
Bond lengths



Bond angles

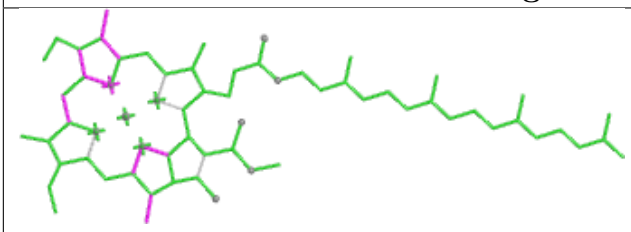


Torsions



Rings

Ligand CLA j 1301



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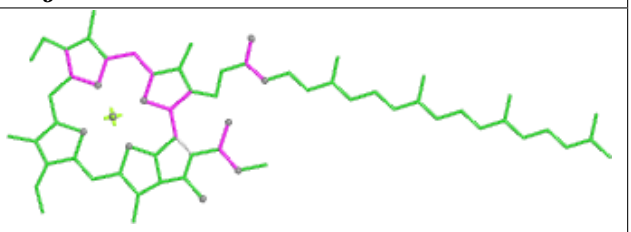
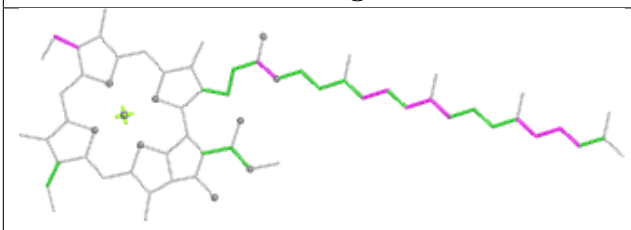


Bond angles



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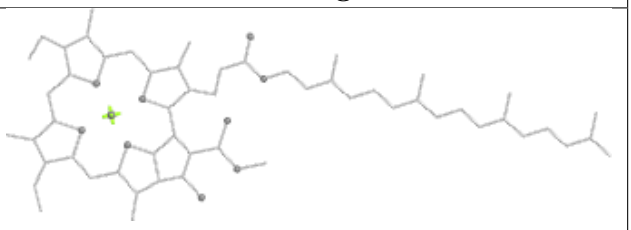
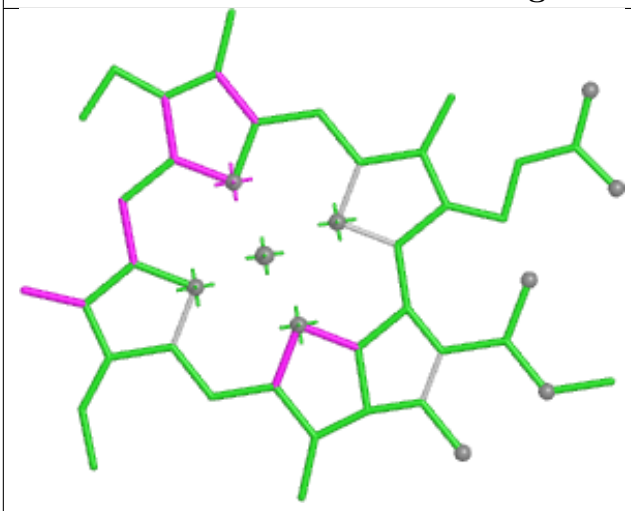


Rings

Ligand CLA 4 517



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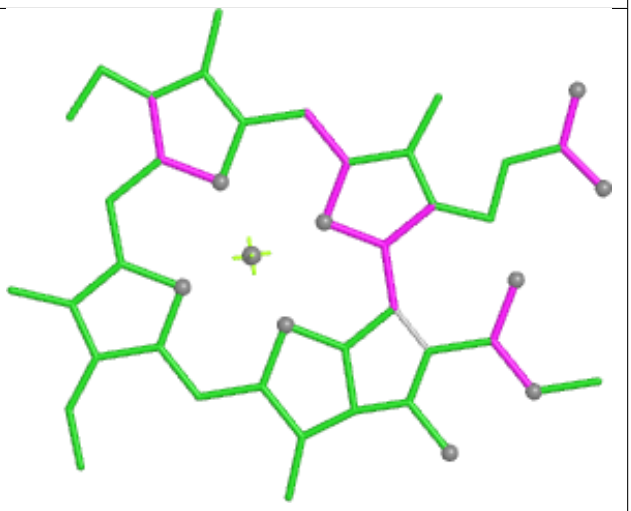
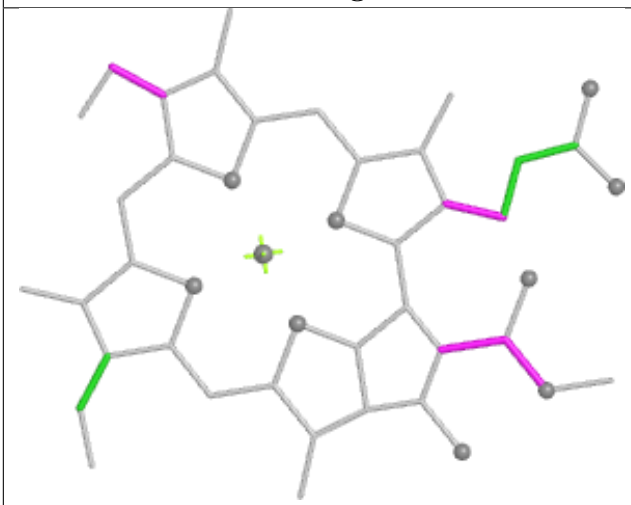


Bond angles



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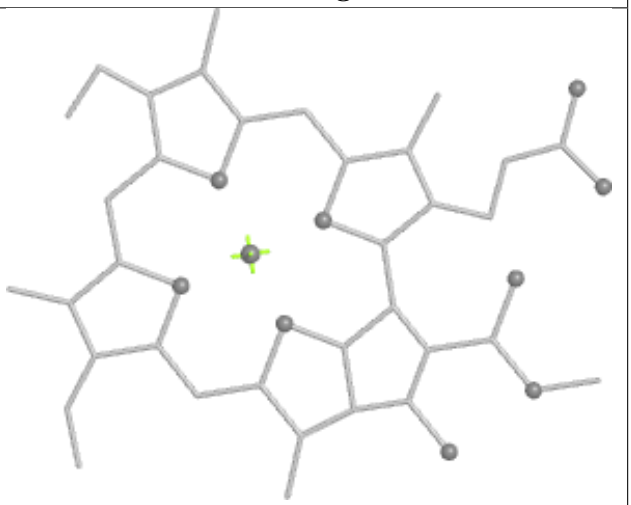
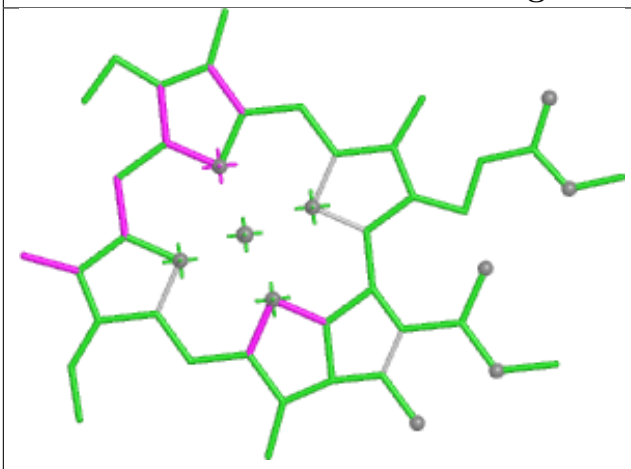


Rings

Ligand CLA v 519



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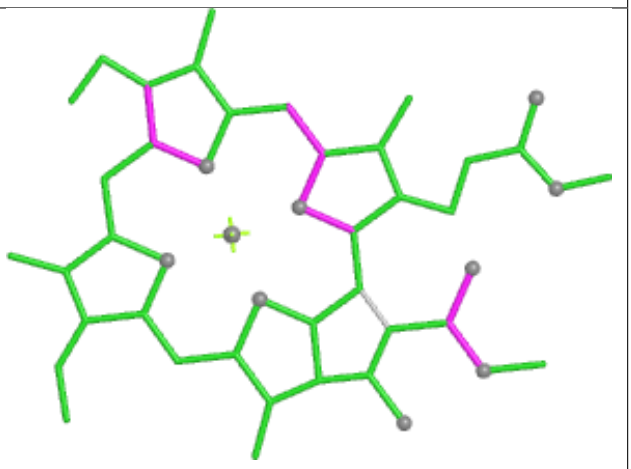
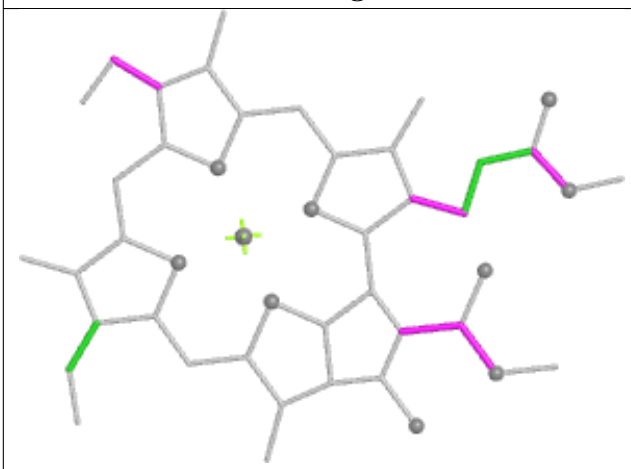


Bond angles



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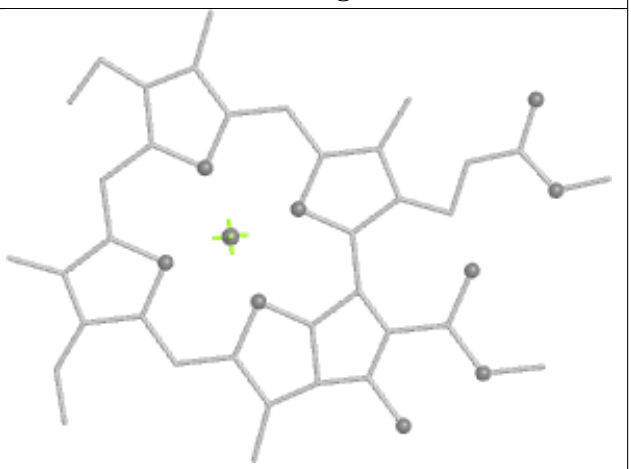
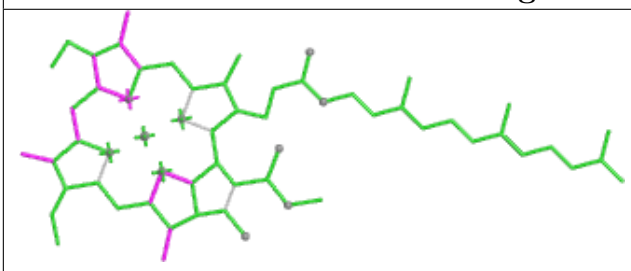


Rings

Ligand CLA n 1503



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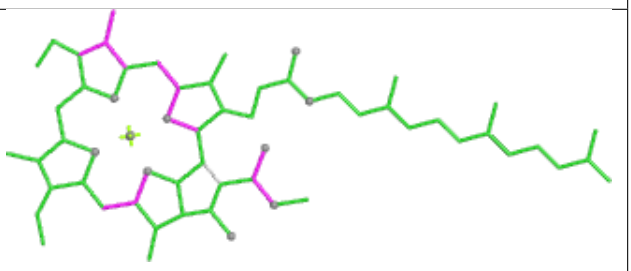
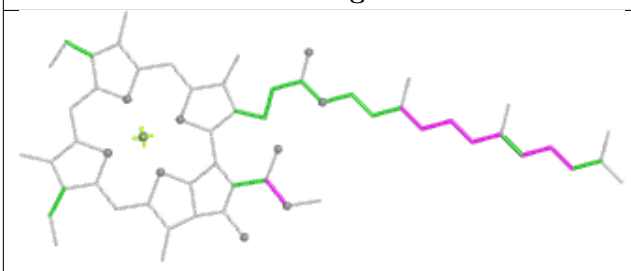


Bond angles



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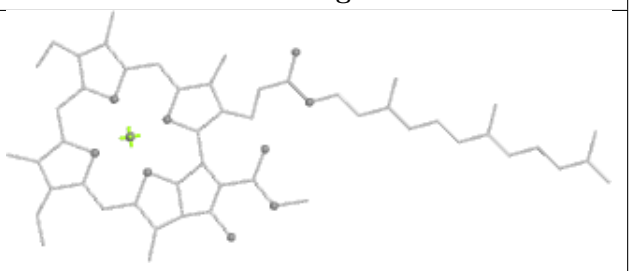
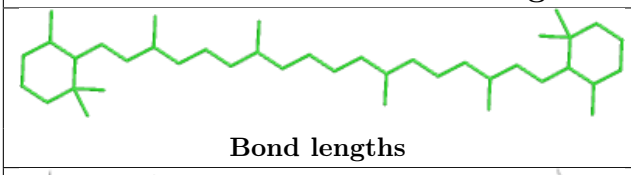


Rings

Ligand BCR r 521



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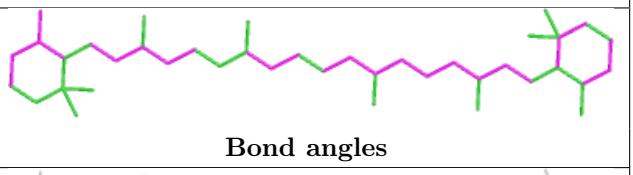

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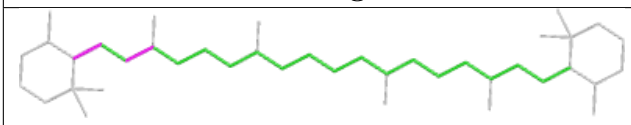

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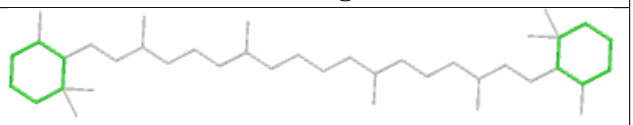
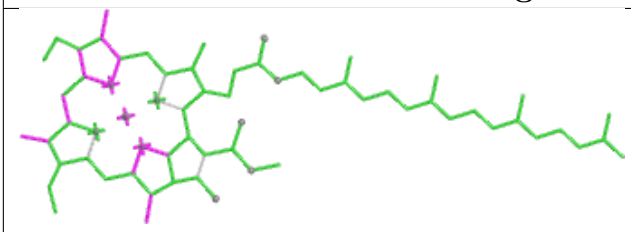


Rings

Ligand CLA B 1203



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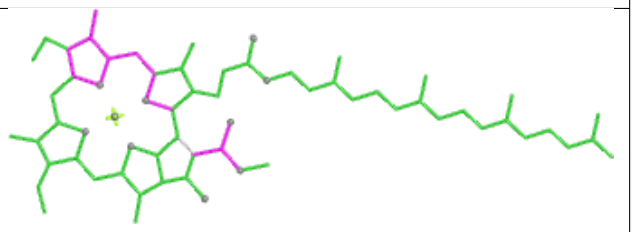
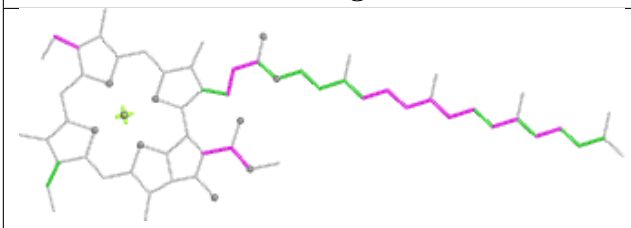


Bond angles



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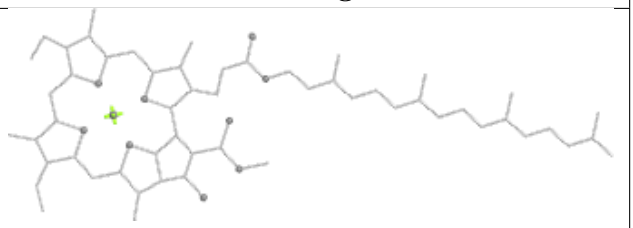
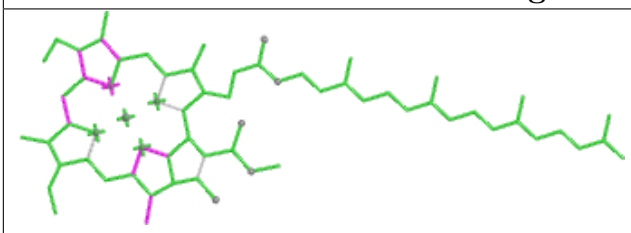


Rings

Ligand CLA 2 503



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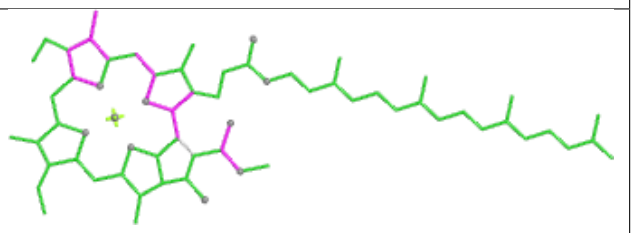

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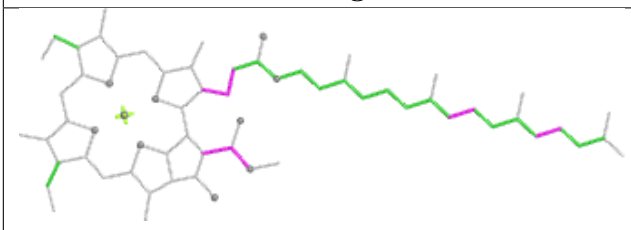

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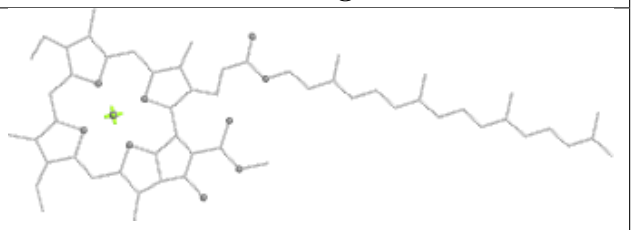
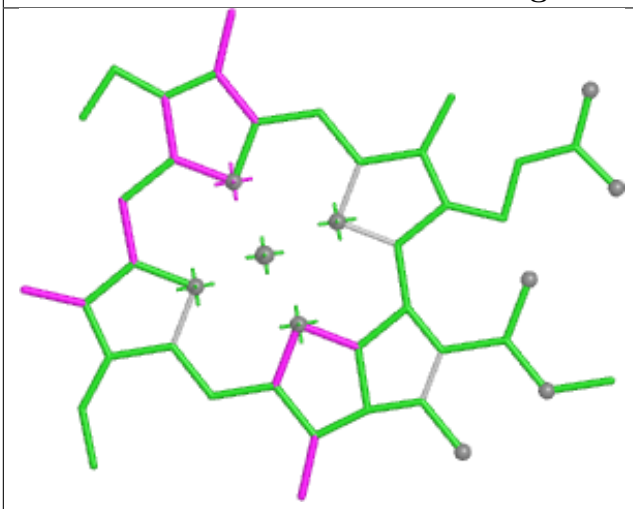


Rings

Ligand CLA r 517



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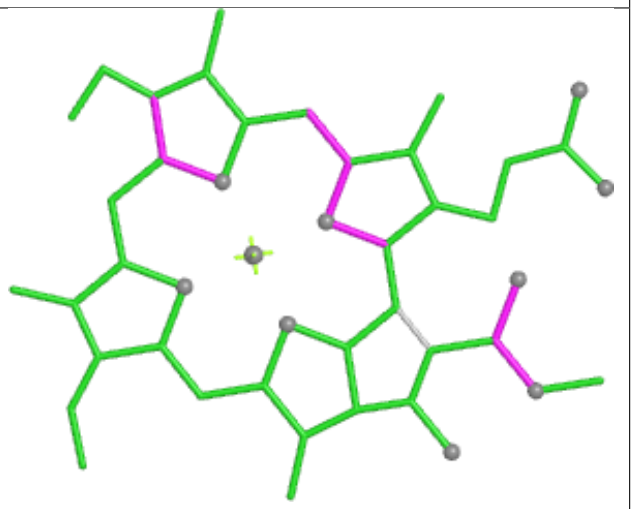
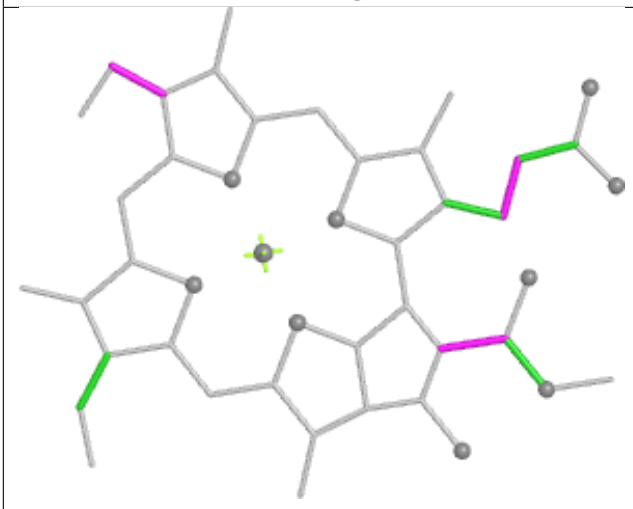


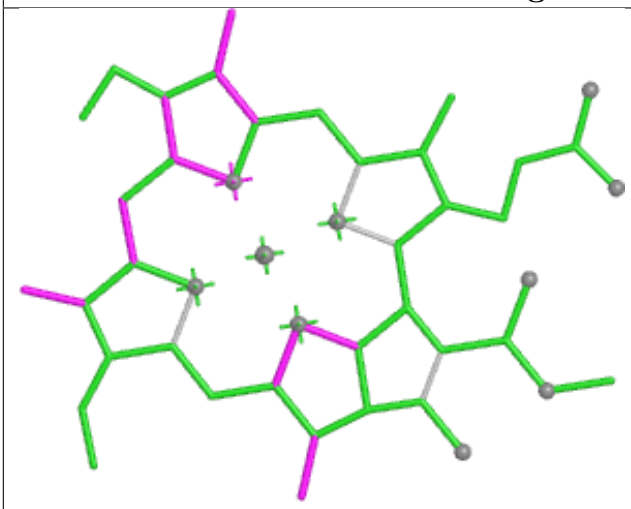
Bond angles



Torsions

Rings

Ligand CLA v 506



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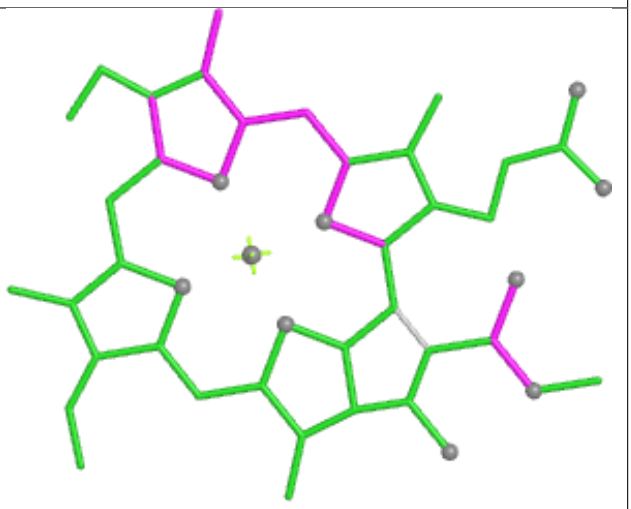

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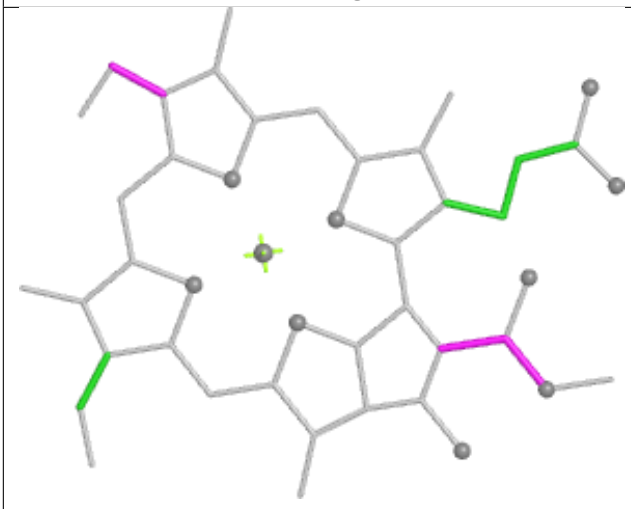
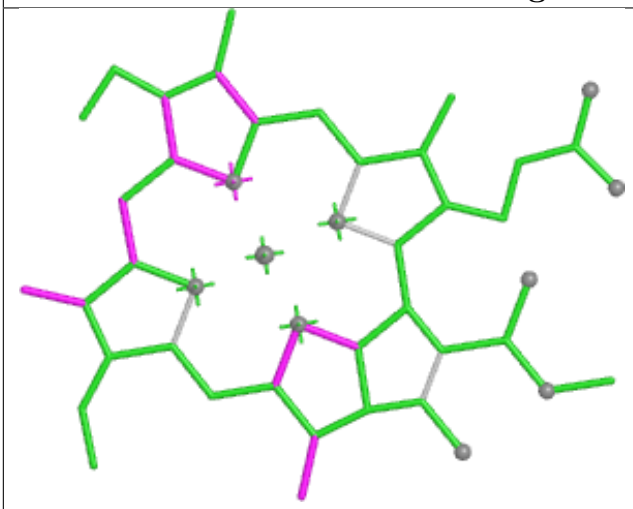


Torsions

Rings

Ligand CLA 4 513



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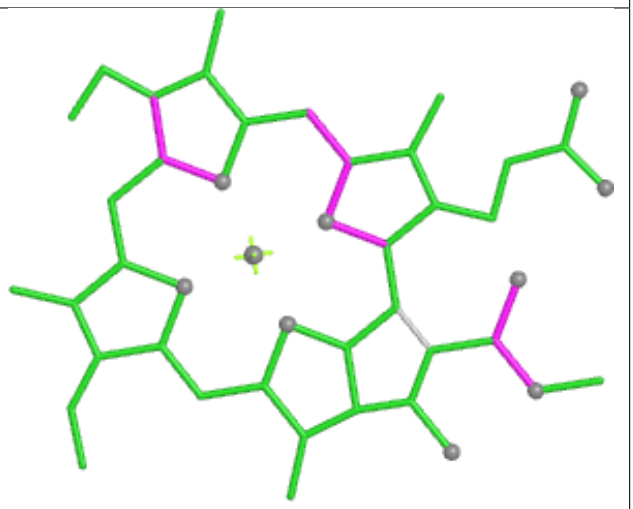

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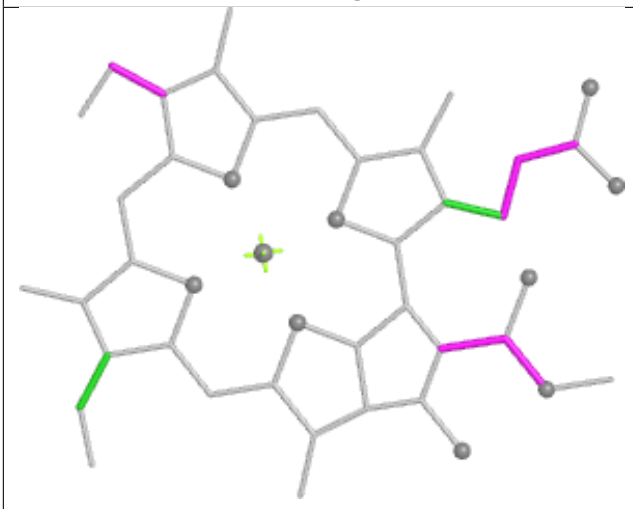
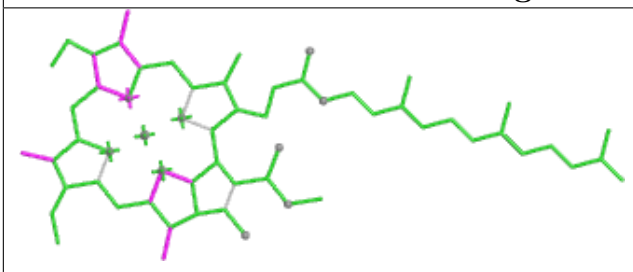


Torsions

Rings

Ligand CLA H 1218



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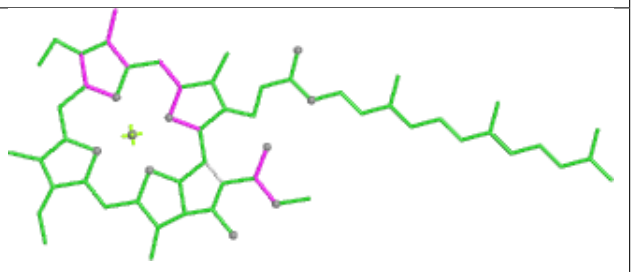

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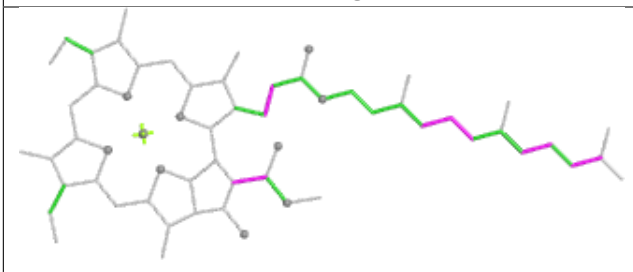
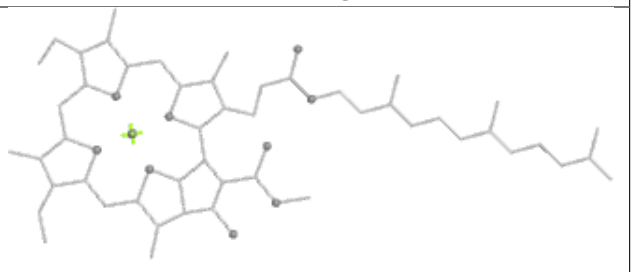
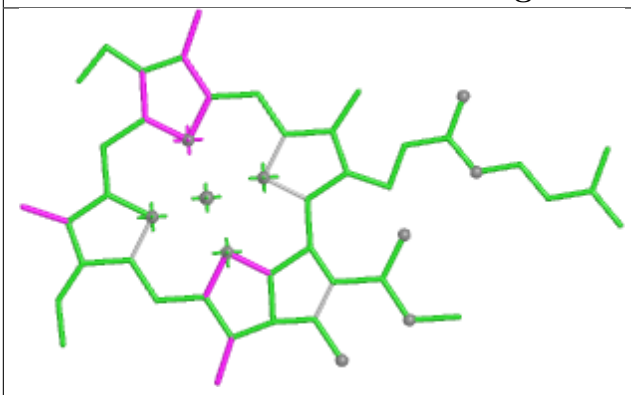


Torsions



Rings

Ligand CLA A 1114



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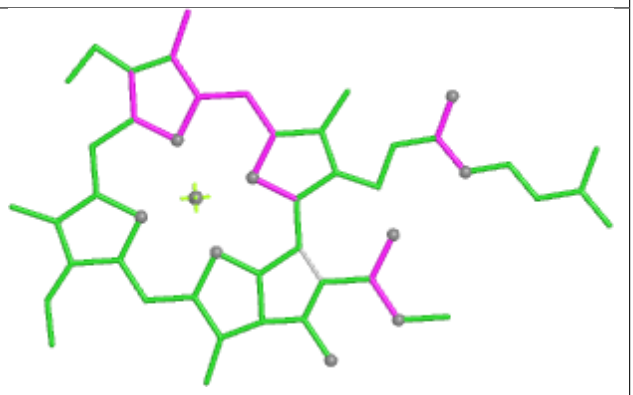
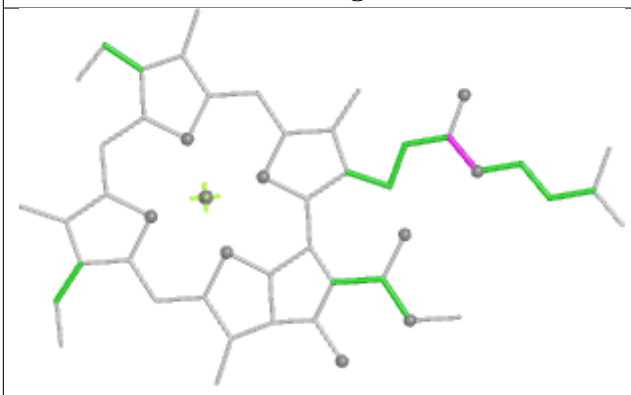


Bond angles



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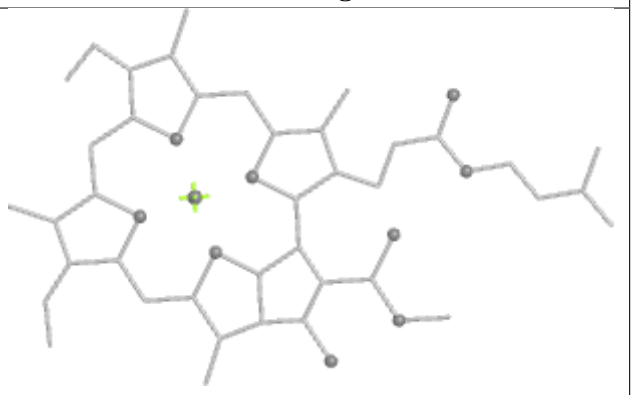
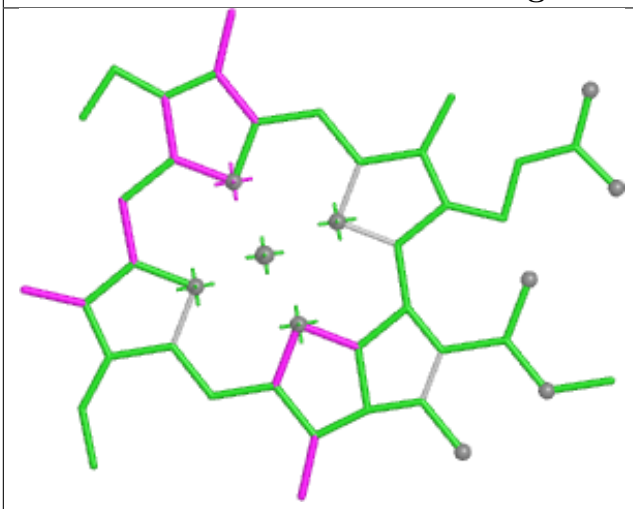


Rings

Ligand CLA v 508



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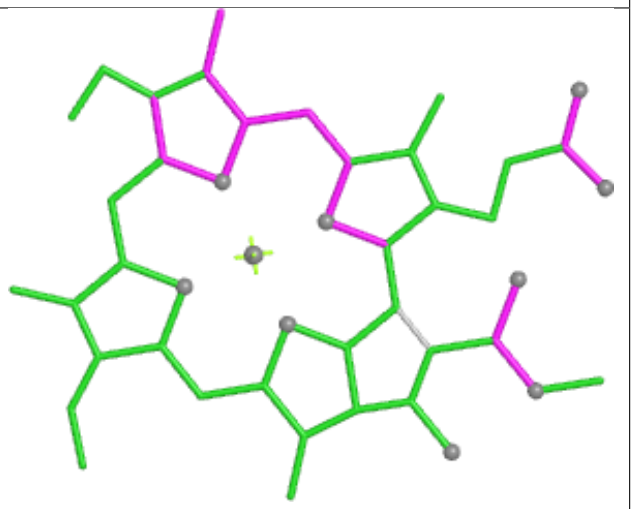
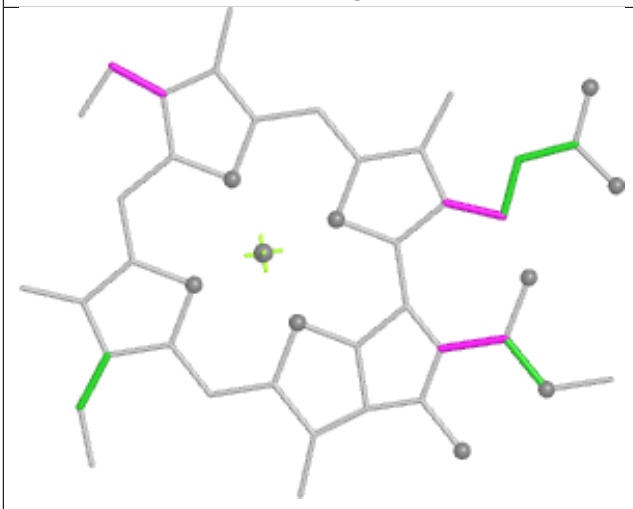


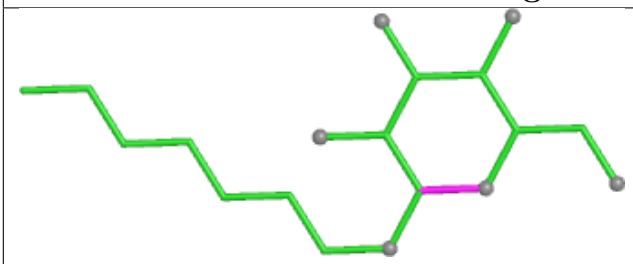
Bond angles



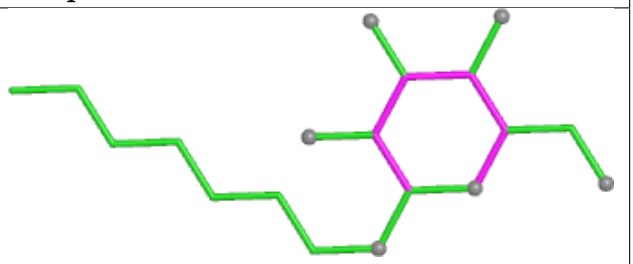
Torsions

Rings

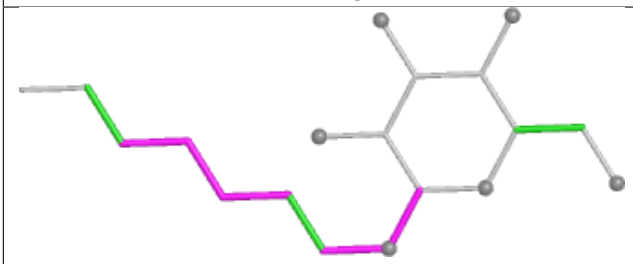
Ligand LMU q 902



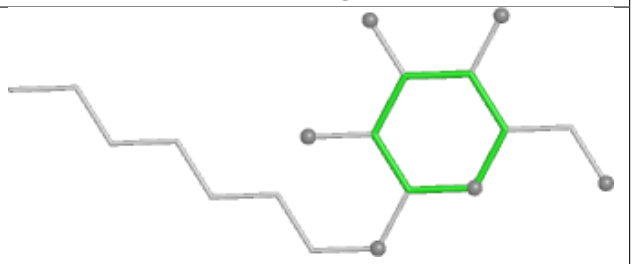
Bond lengths



Bond angles

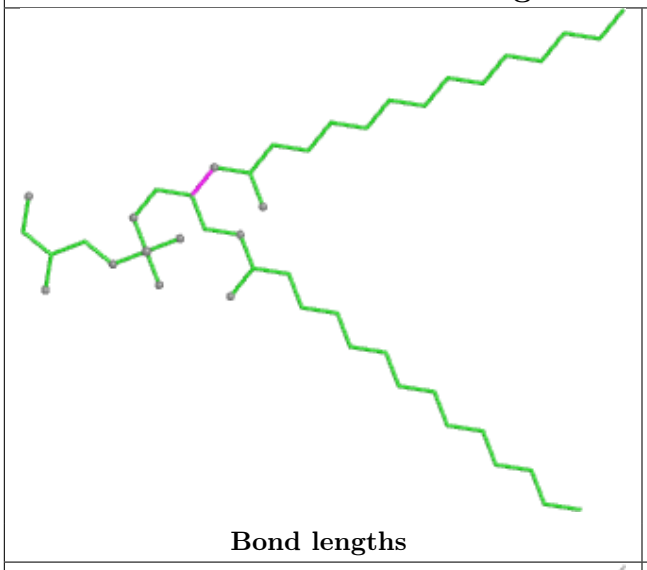


Torsions



Rings

Ligand LHG G 5005



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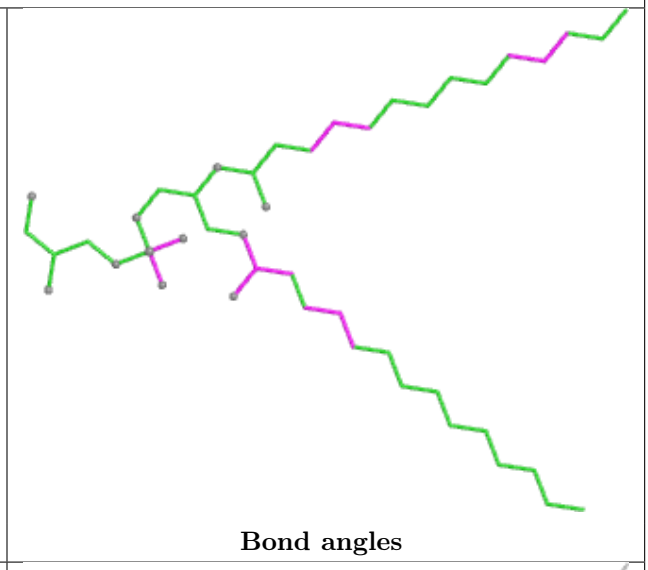

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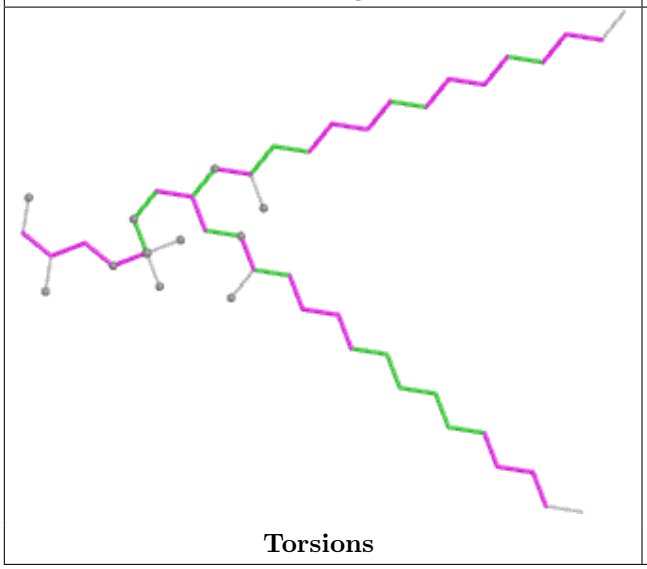

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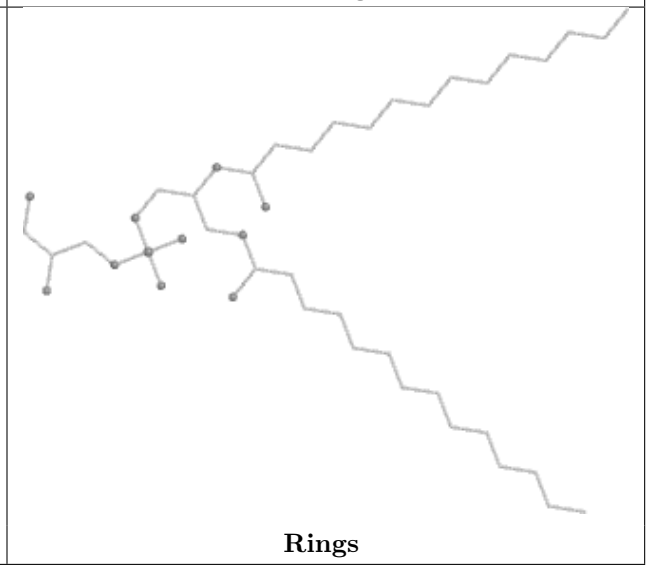
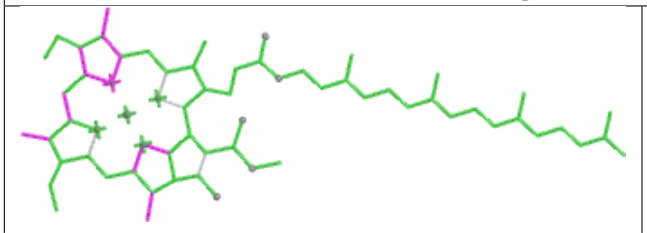


Rings

Ligand CLA B 1213



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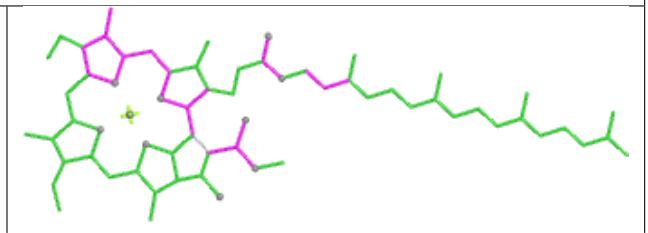
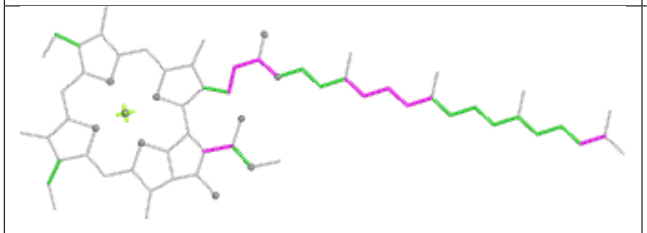


Bond angles



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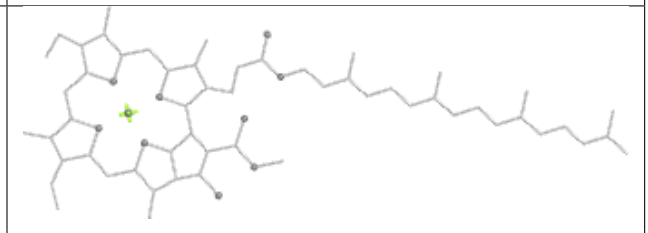
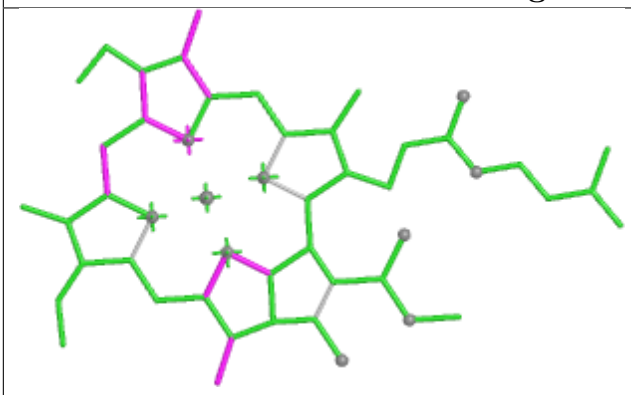


Rings

Ligand CLA a 511



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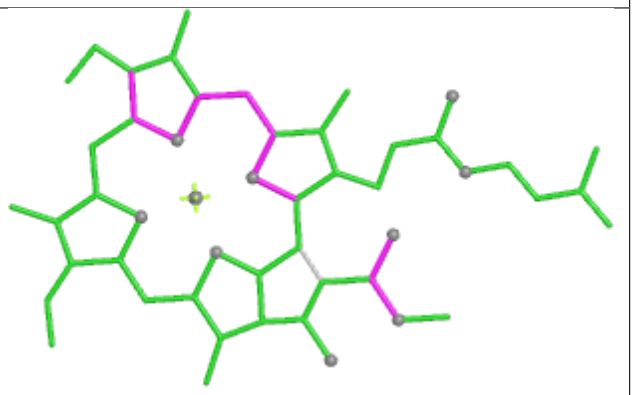
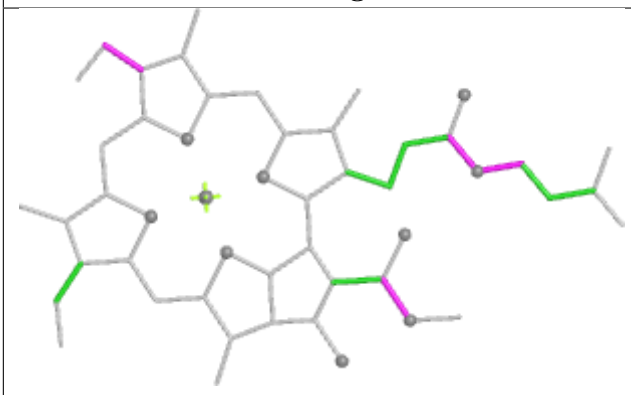


Bond angles



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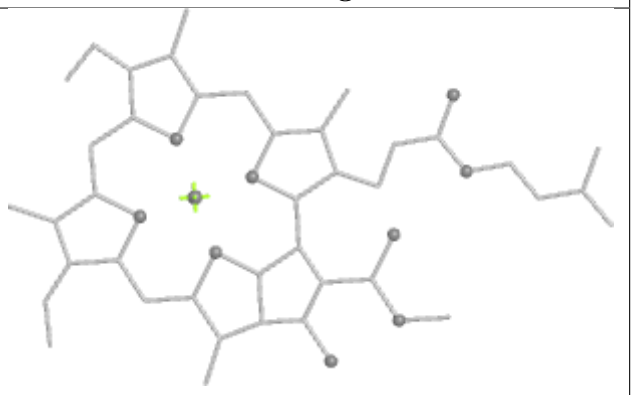
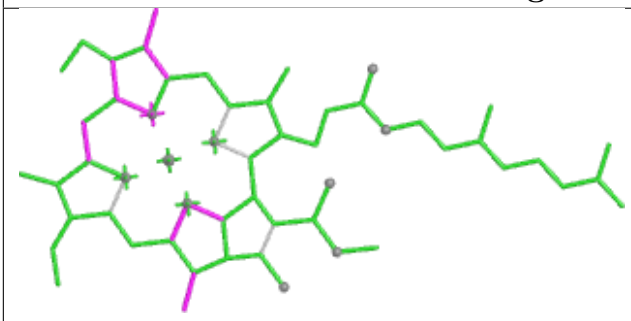


Rings

Ligand CLA u 518



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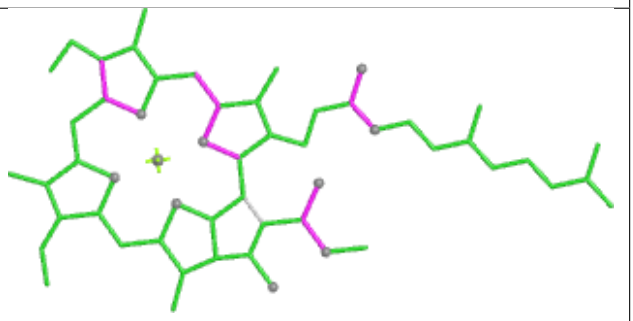

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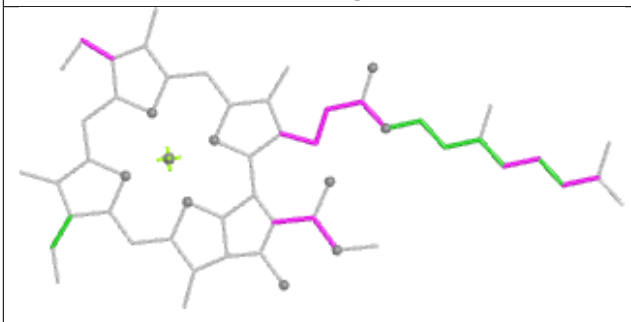

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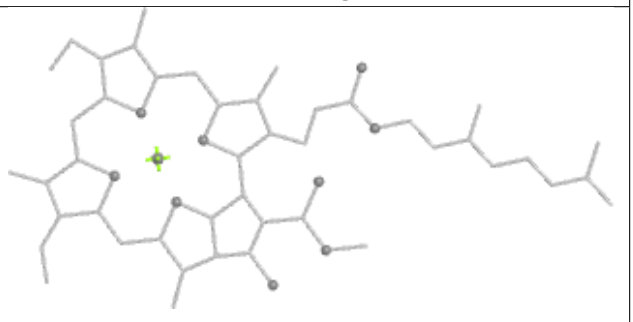
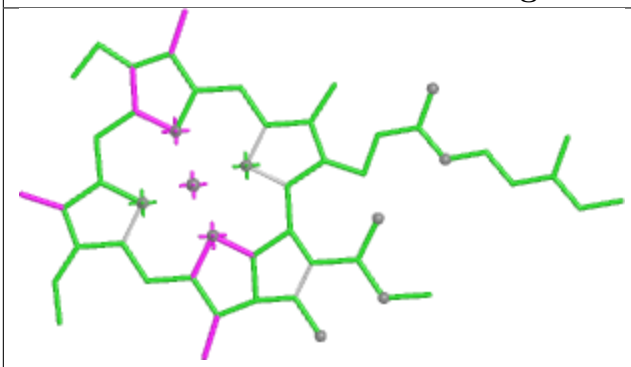


Rings

Ligand CLA e 1129



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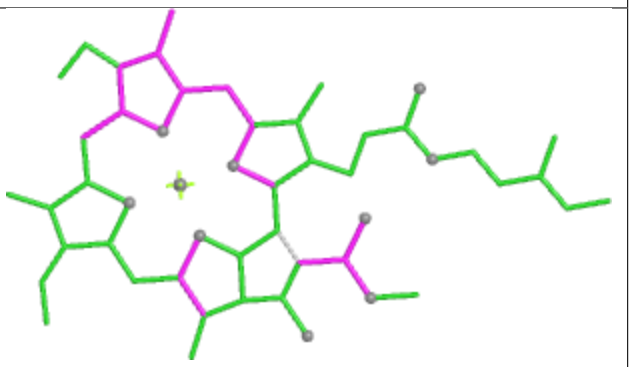
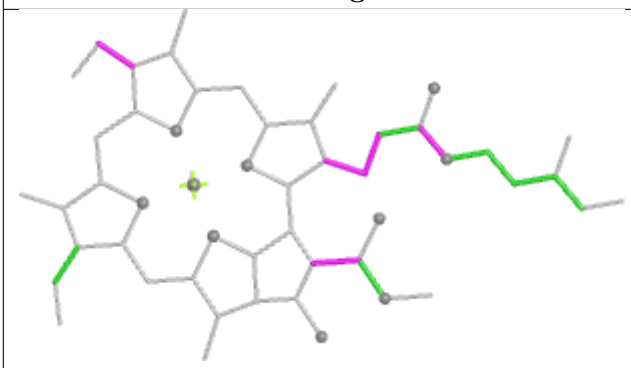


Bond angles



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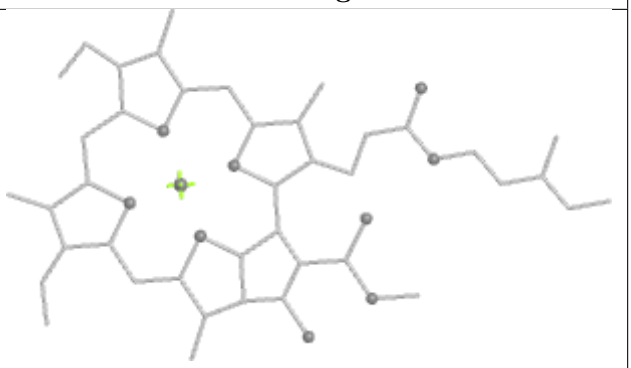
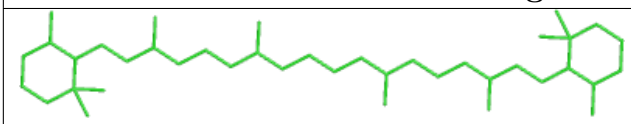


Rings

Ligand BCR v 522



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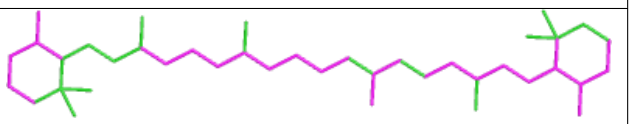
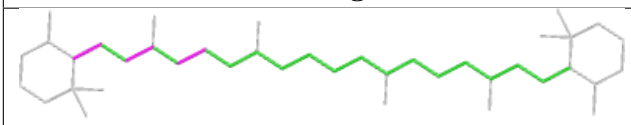


Bond angles



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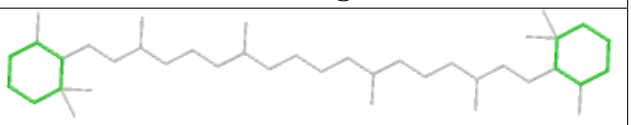
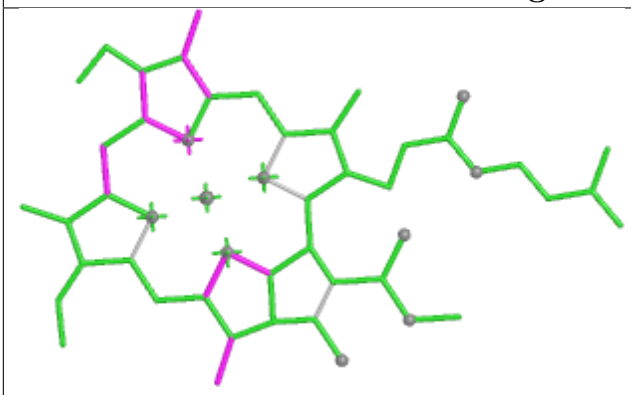


Rings

Ligand CLA 4 502



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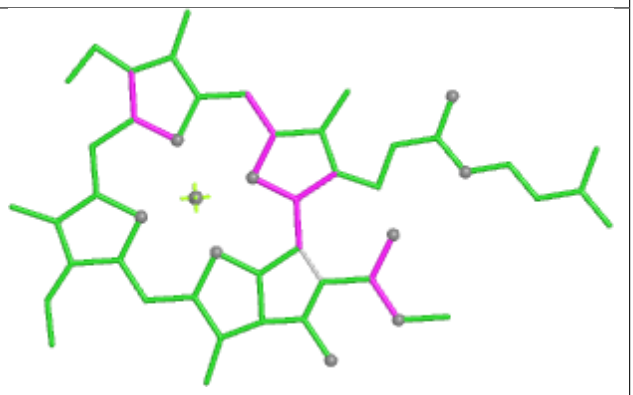

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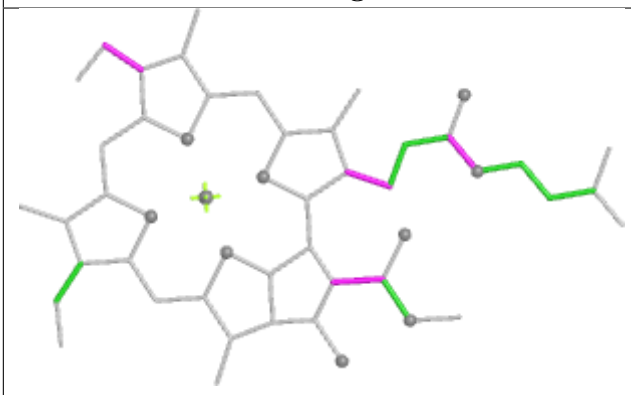

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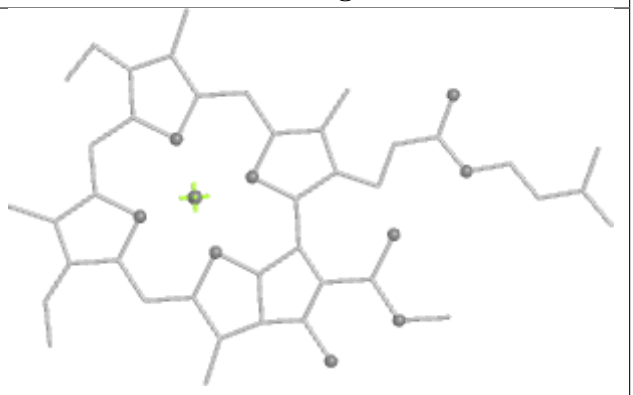
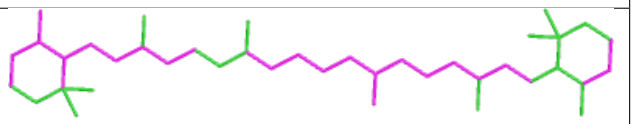


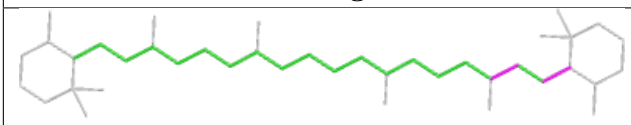
Rings

Ligand BCR s 523

Bond lengths



Bond angles



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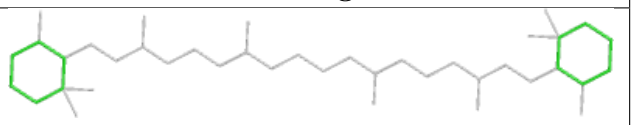
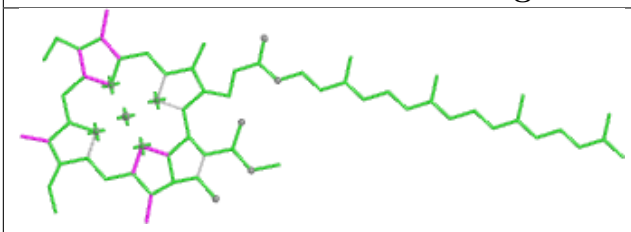


Rings

Ligand CLA G 1103



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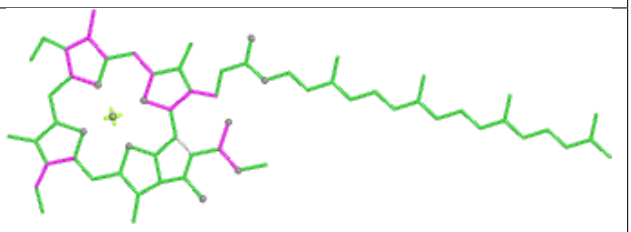
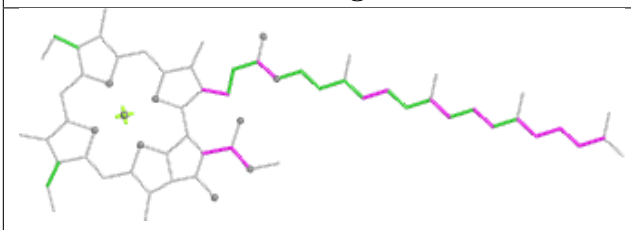


Bond angles



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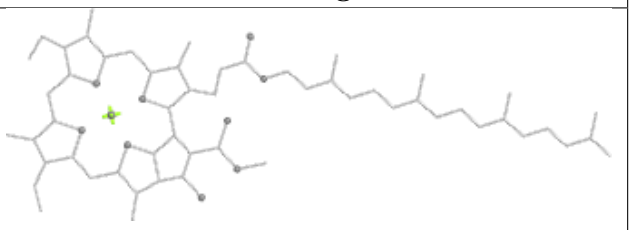
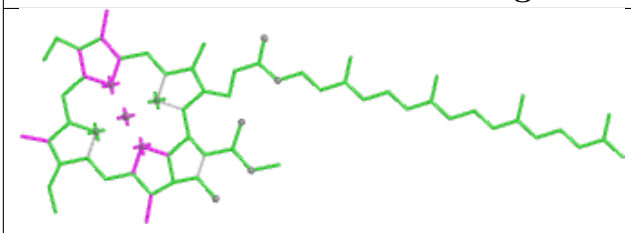


Rings

Ligand CLA G 1117



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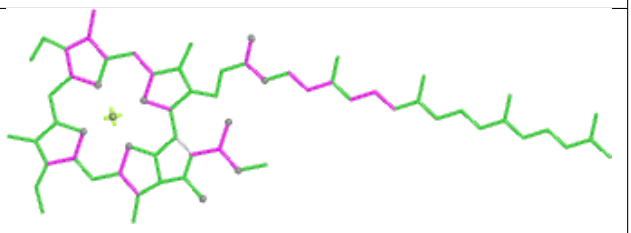
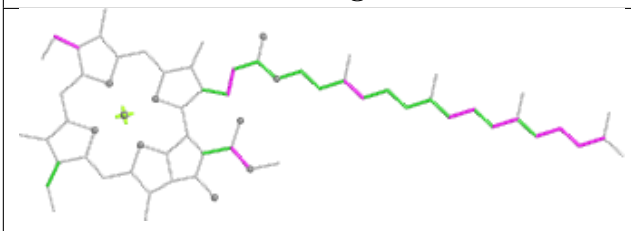


Bond angles



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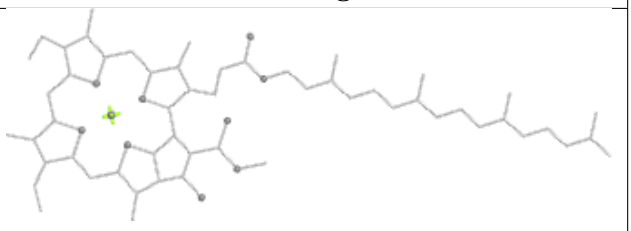
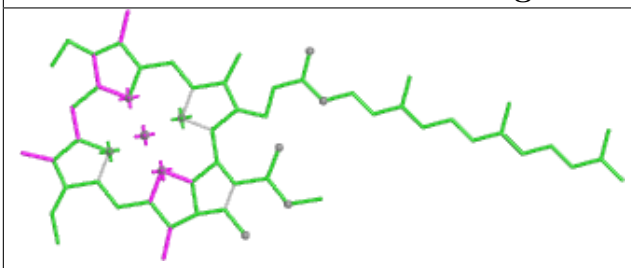
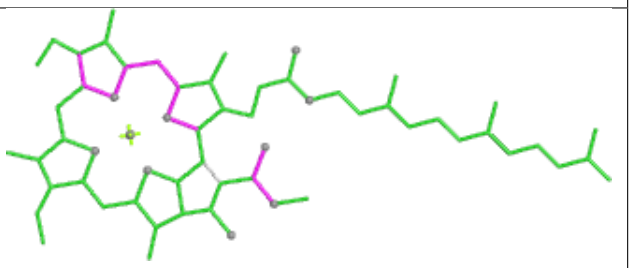
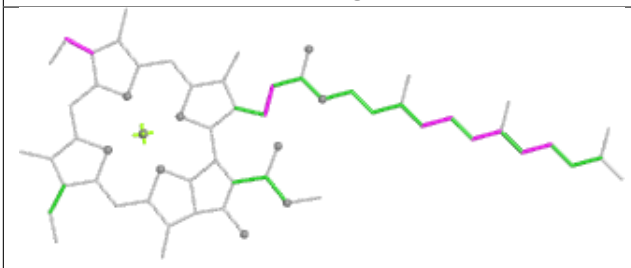
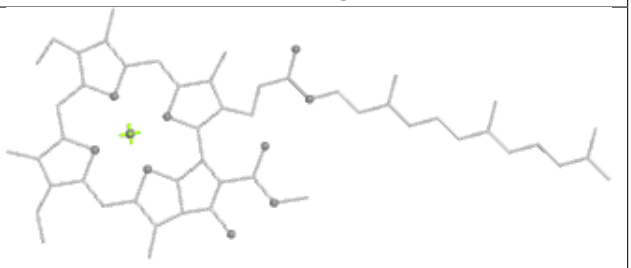
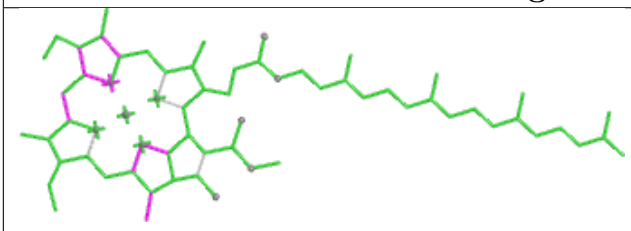
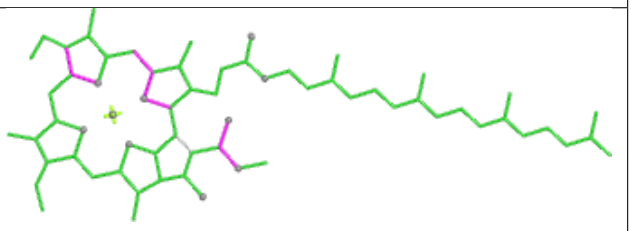
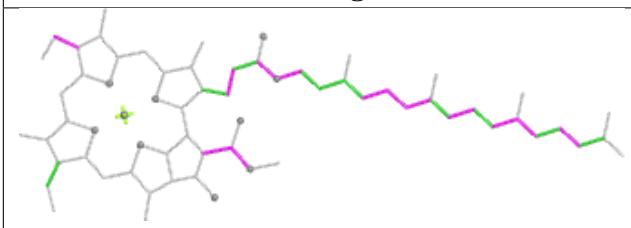
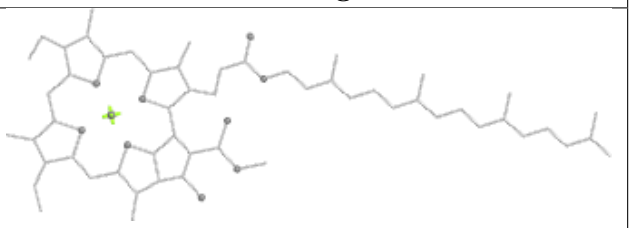
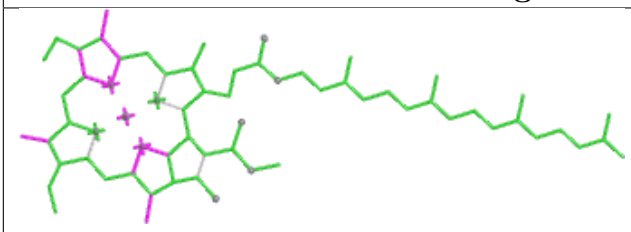


Rings

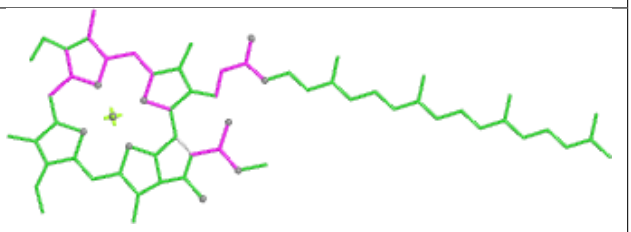
Ligand CLA H 1216	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

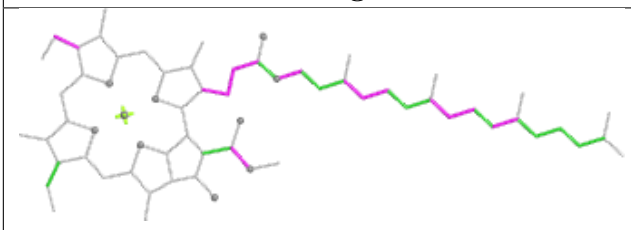
Ligand CLA G 1107



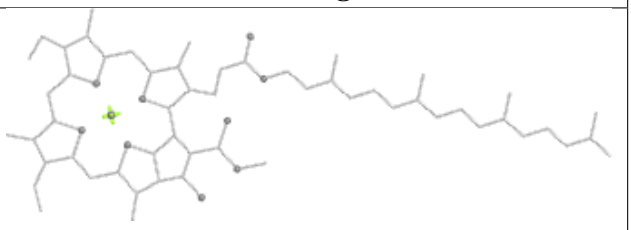
Bond lengths



Bond angles

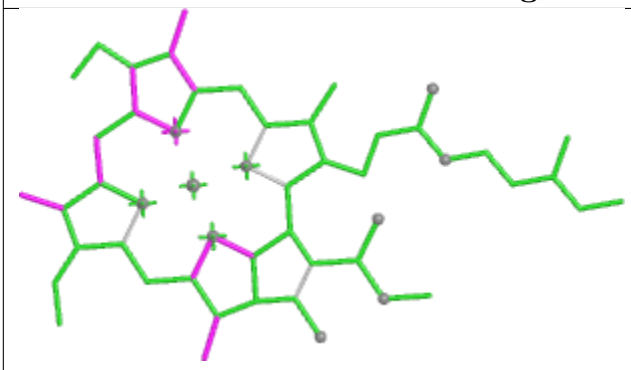


Torsions



Rings

Ligand CLA e 1110



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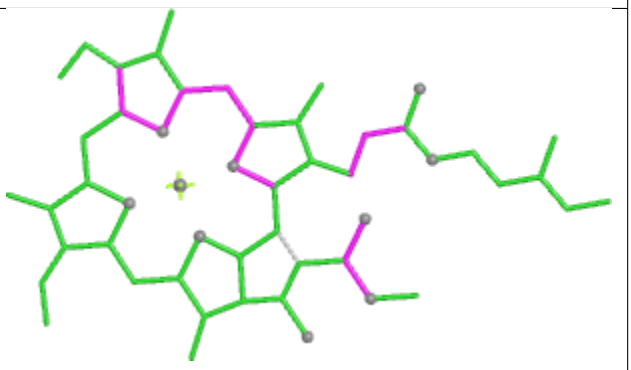

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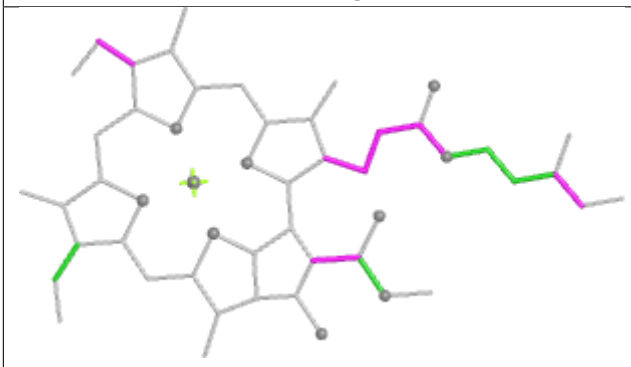

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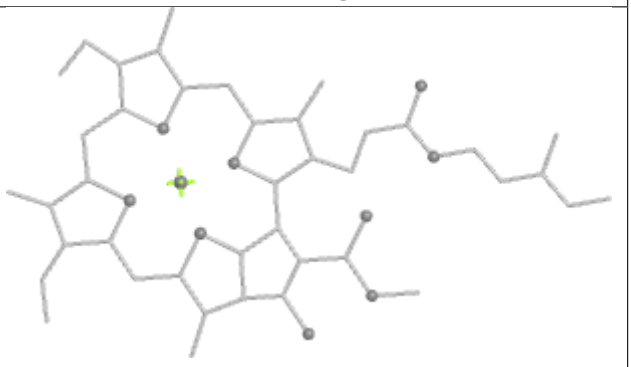
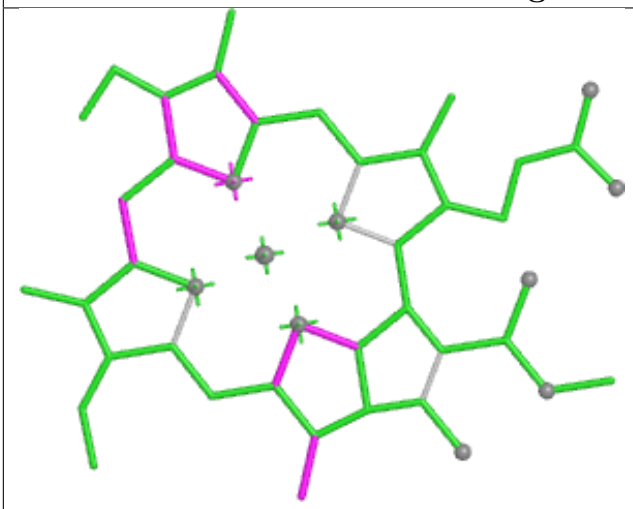


Rings

Ligand CLA 3 516



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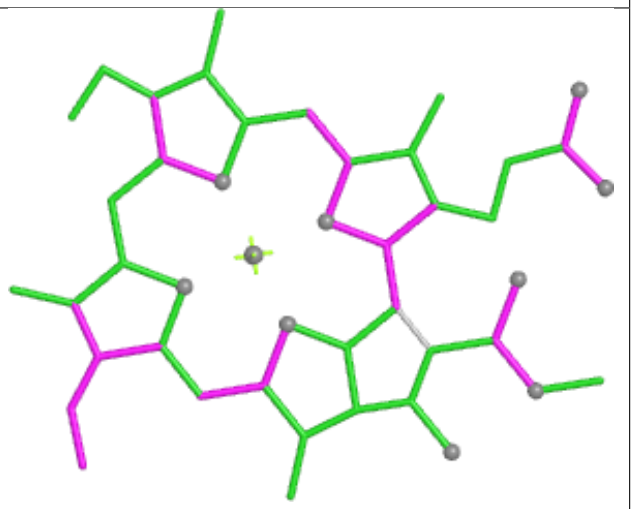
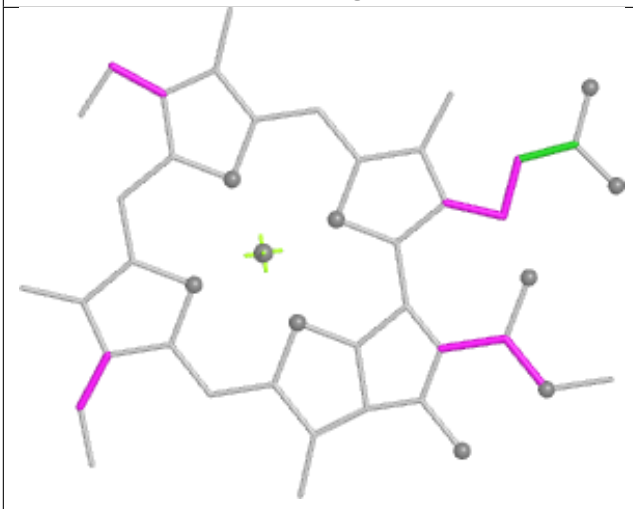


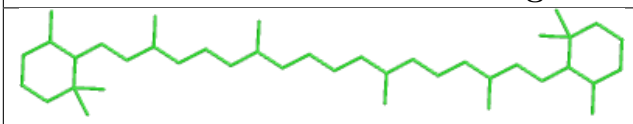
Bond angles



Torsions

Rings

Ligand BCR 2 521



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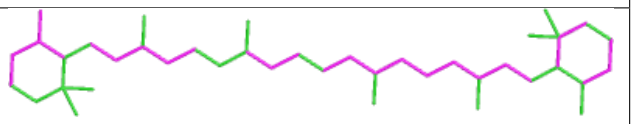

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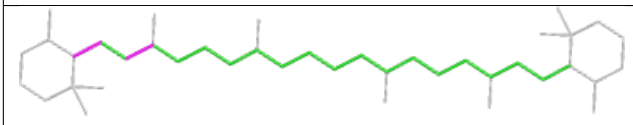

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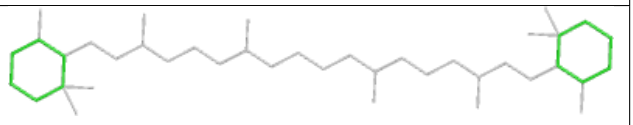
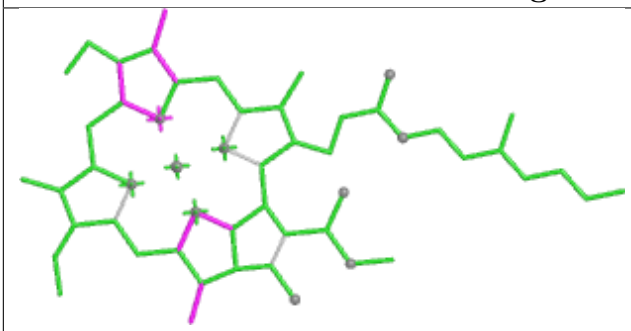


Rings

Ligand CLA r 512



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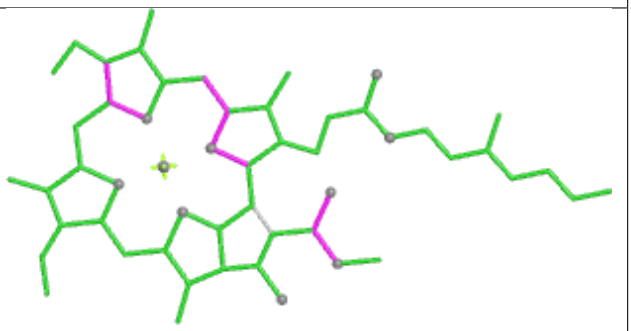
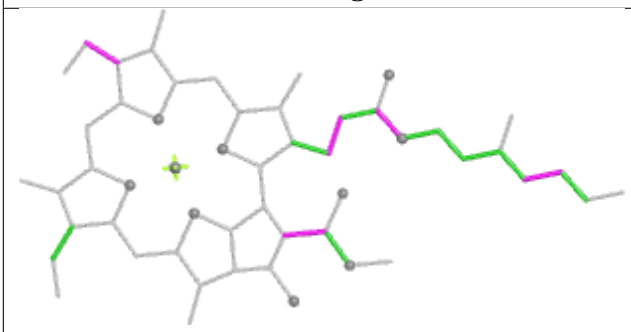


Bond angles



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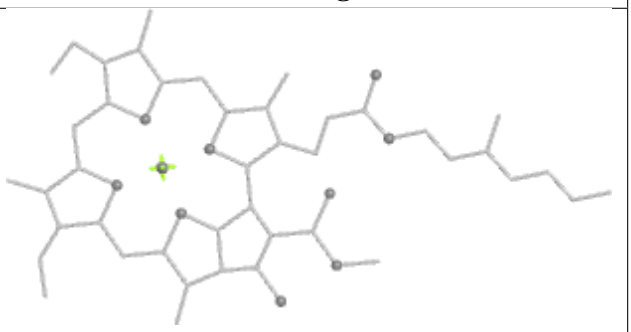
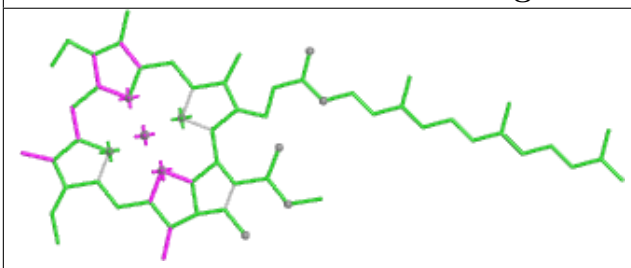


Rings

Ligand CLA G 1116



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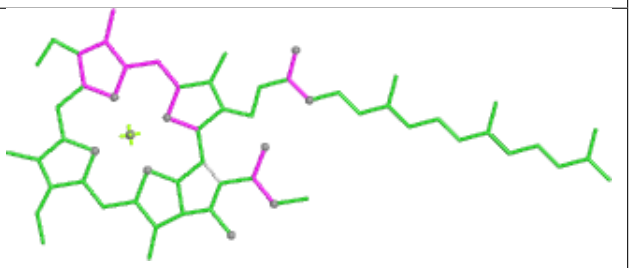

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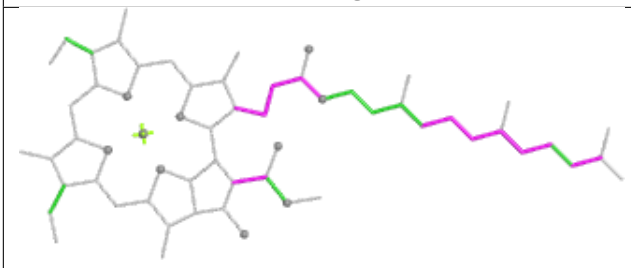

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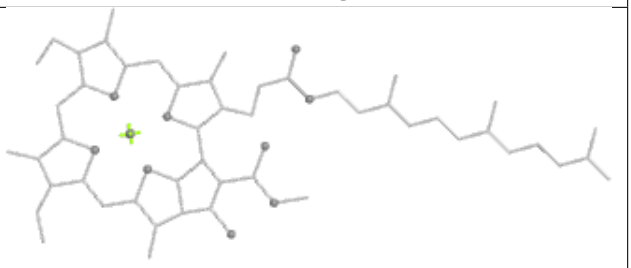
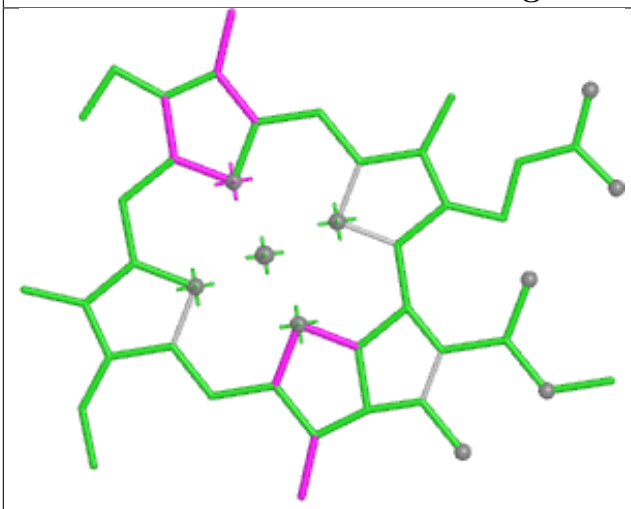


Rings

Ligand CLA j 1302



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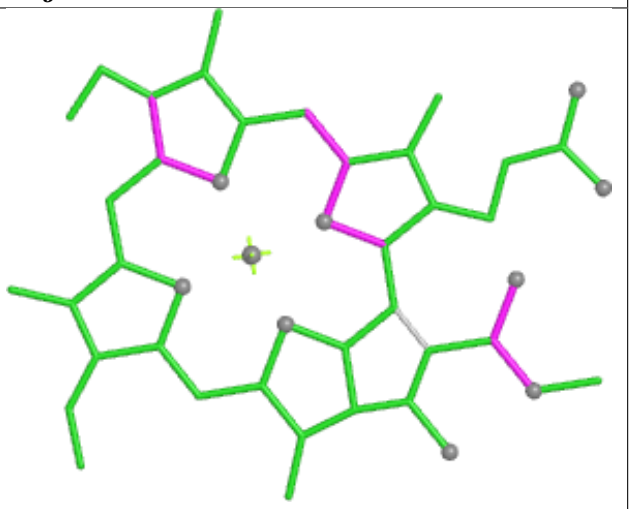

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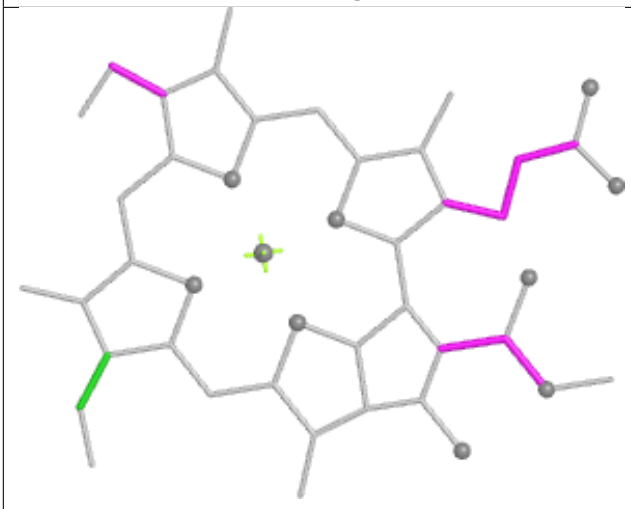
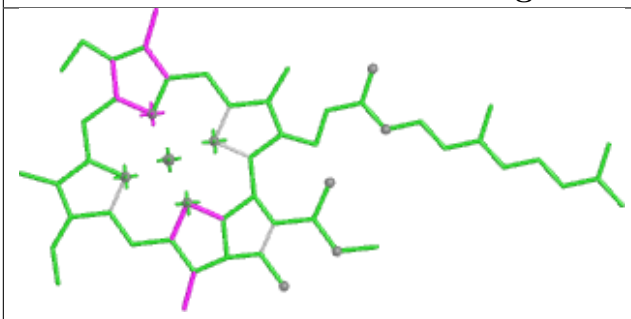


Torsions

Rings

Ligand CLA B 1236



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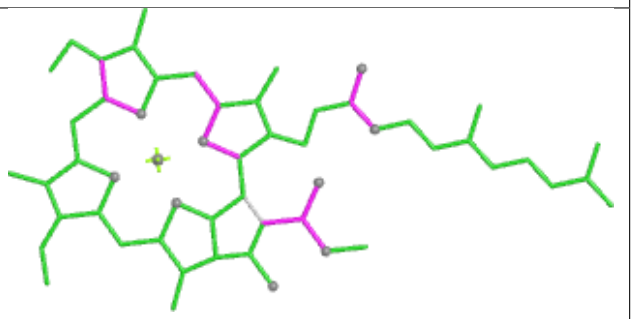

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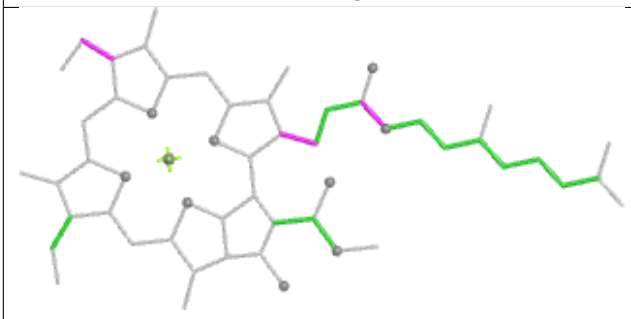

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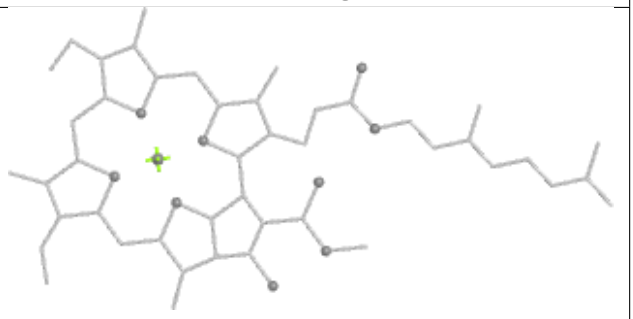
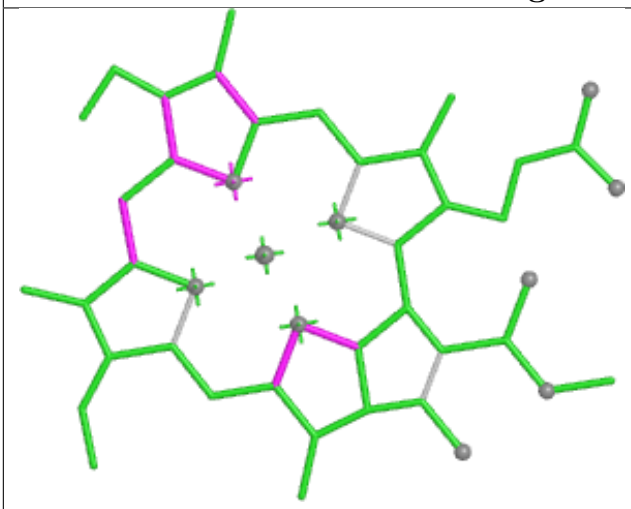


Rings

Ligand CLA 6 504



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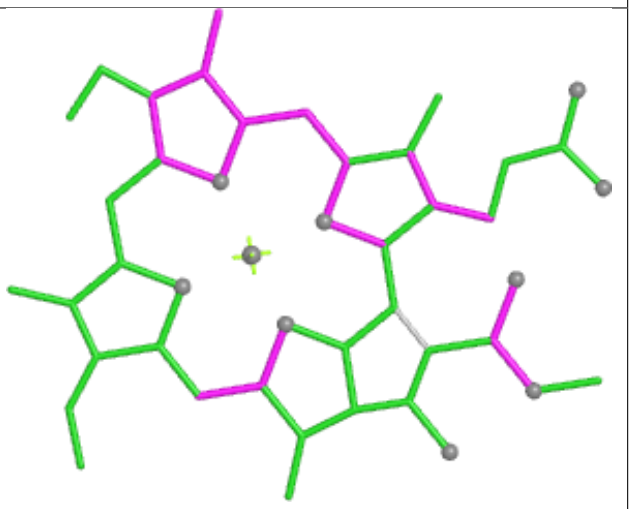

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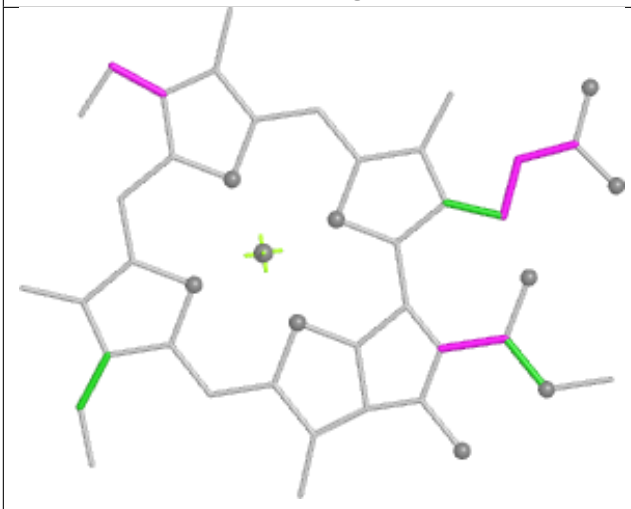
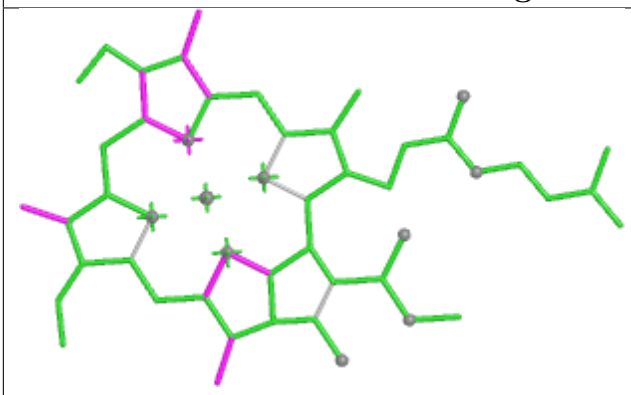


Torsions

Rings

Ligand CLA U 1103



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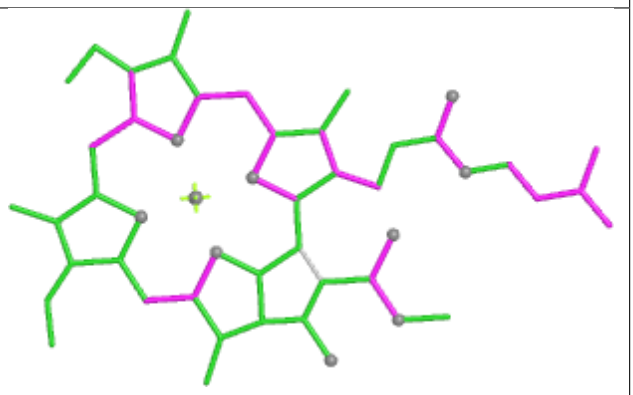

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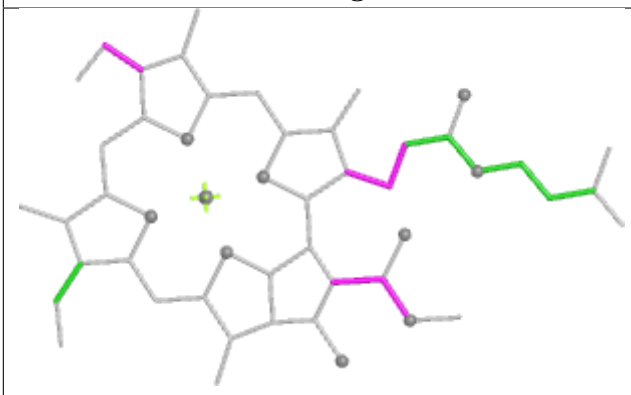

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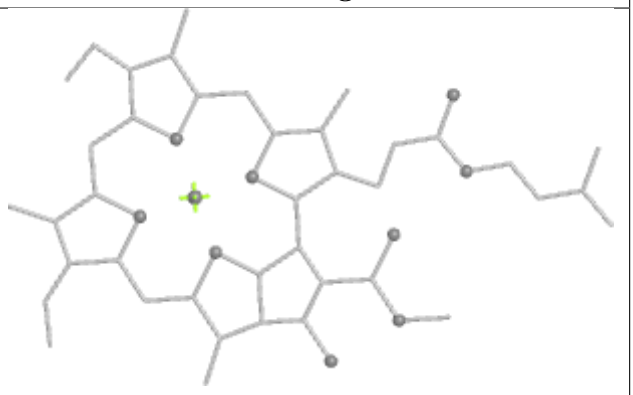
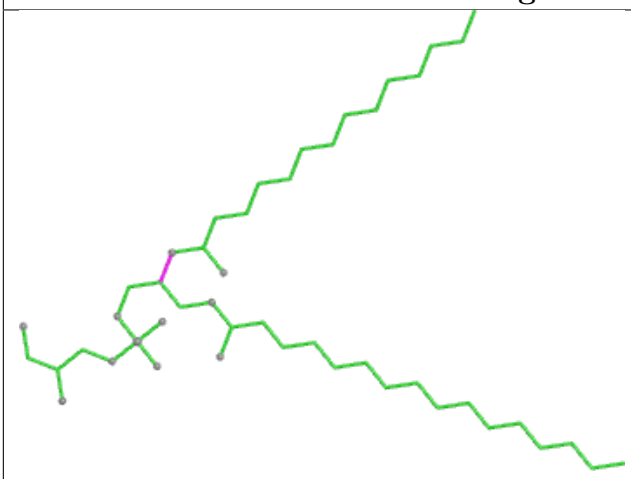


Rings

Ligand LHG e 5007



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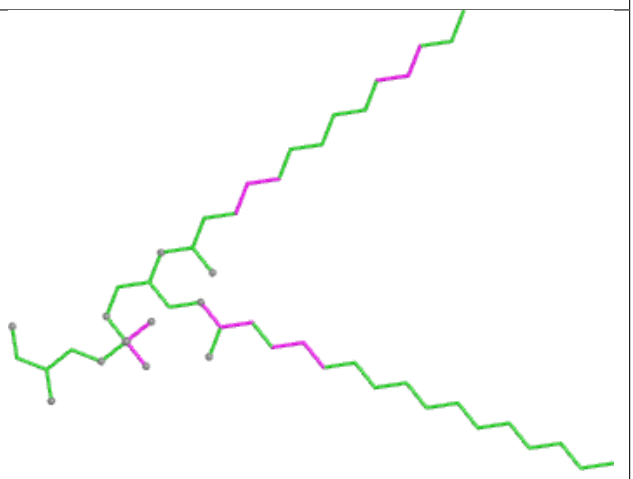
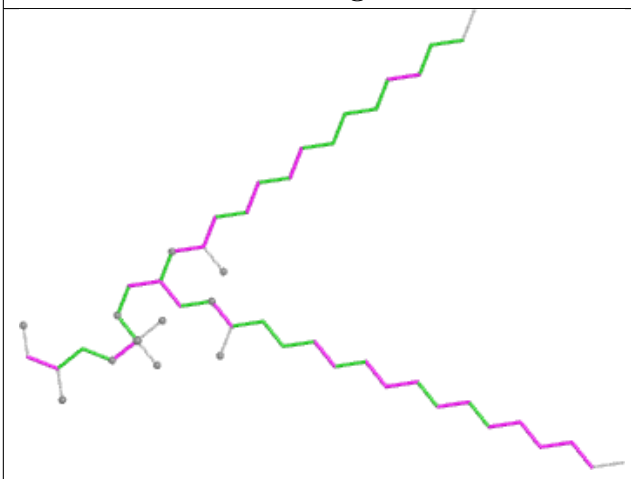


Bond angles



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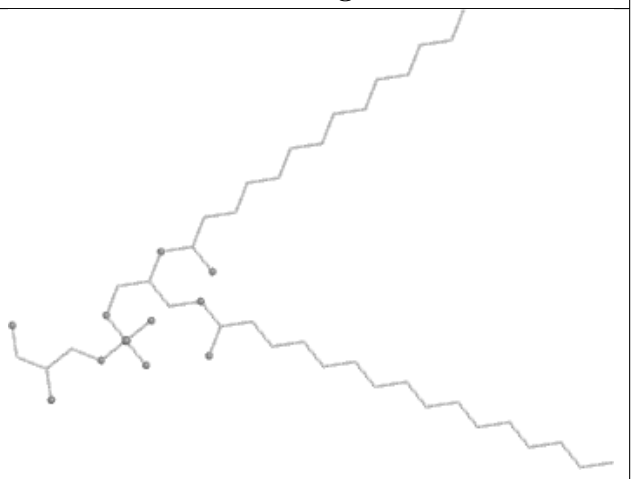
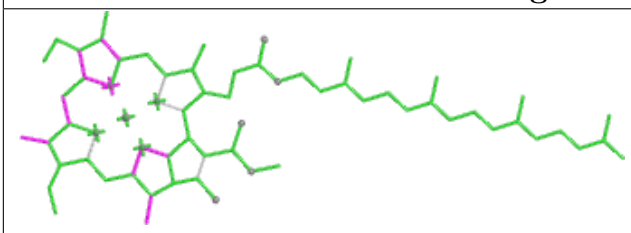


Rings

Ligand CLA r 503



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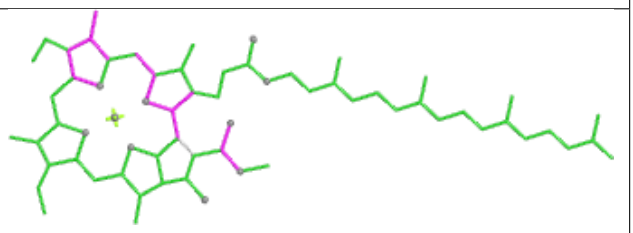
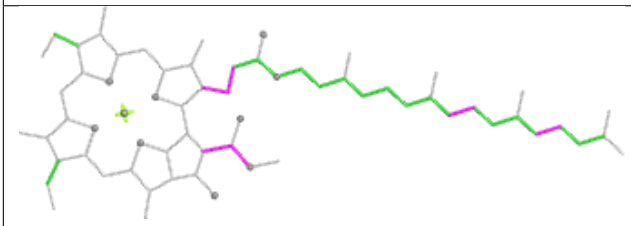


Bond angles



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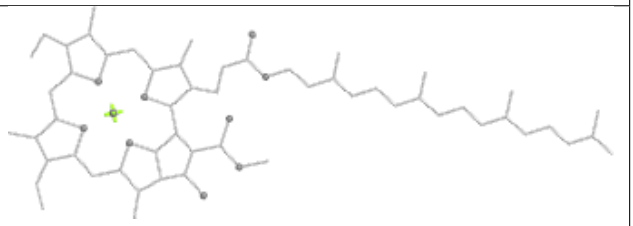
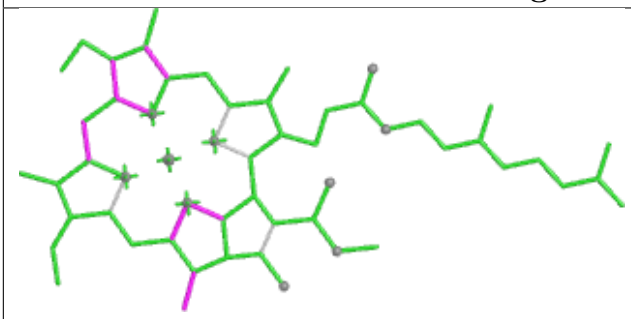


Rings

Ligand CLA t 503



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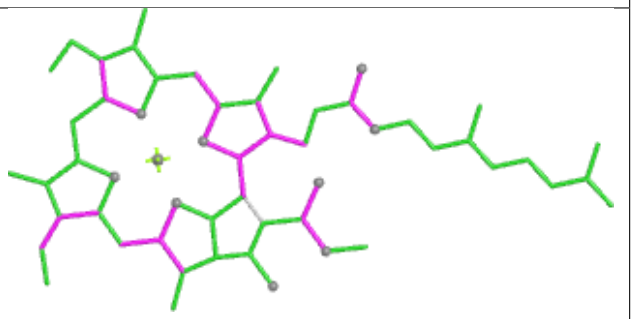
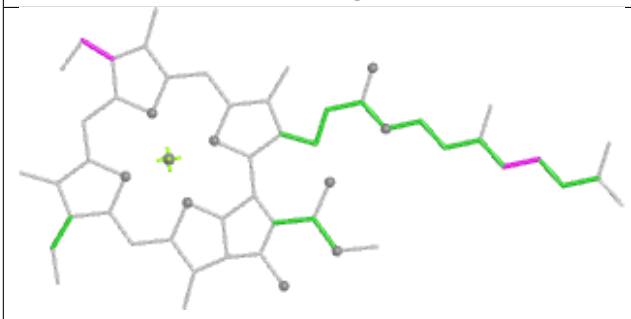


Bond angles



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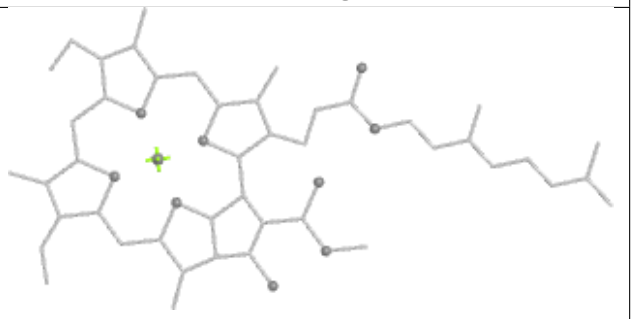
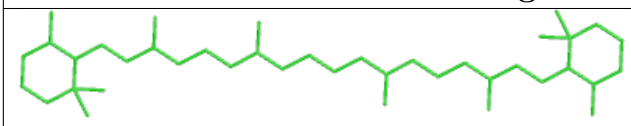


Rings

Ligand BCR e 4003



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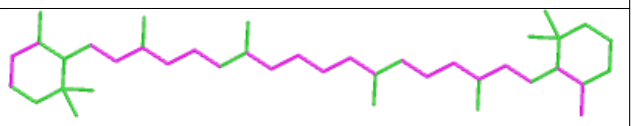
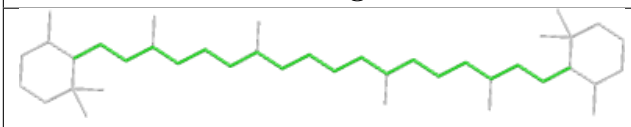


Bond angles



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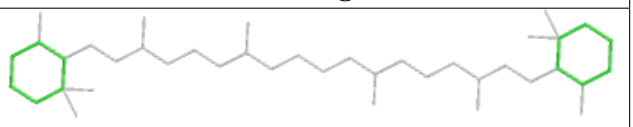
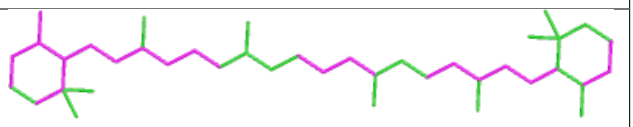


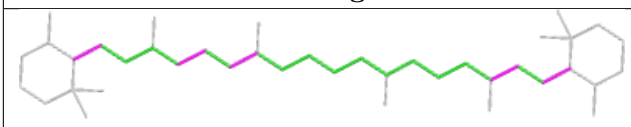
Rings

Ligand BCR J 4012

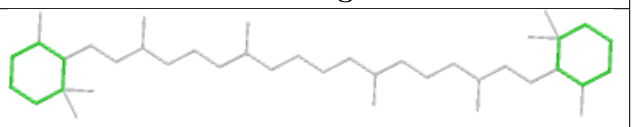
Bond lengths



Bond angles

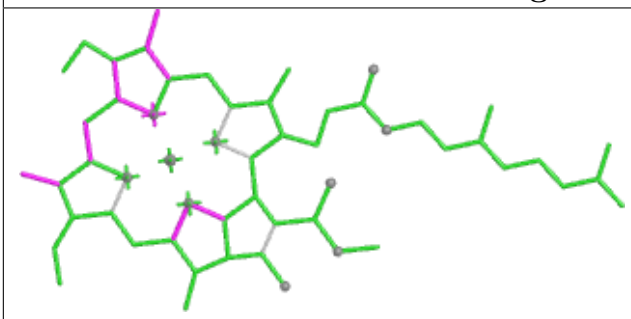


Torsions

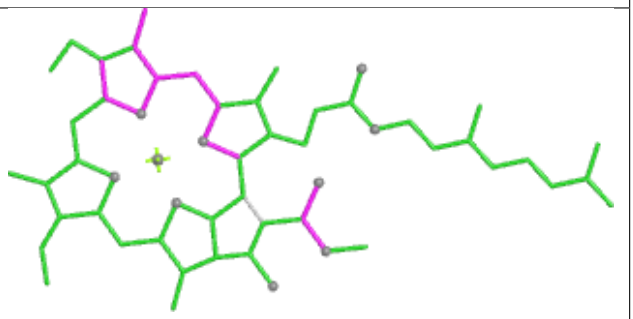


Rings

Ligand CLA r 506



Bond lengths



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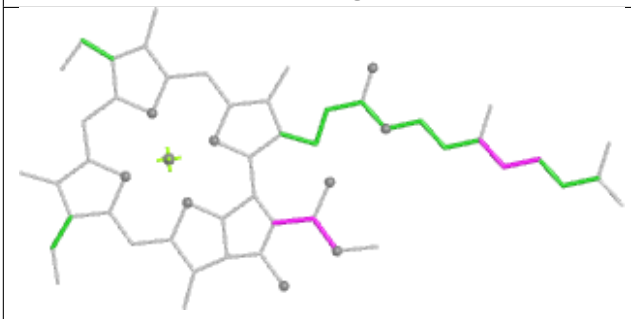

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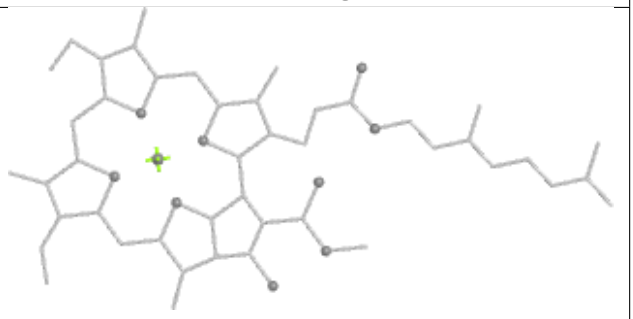
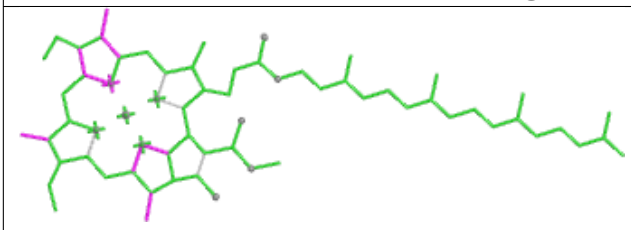


Rings

Ligand CLA f 1210



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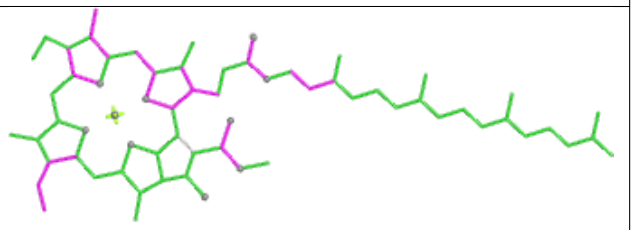
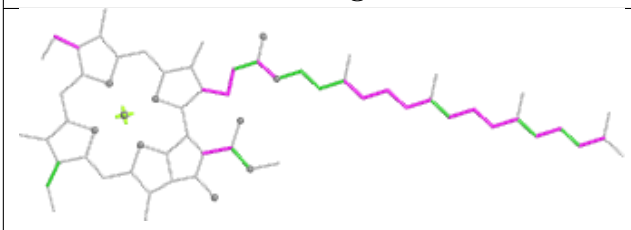


Bond angles



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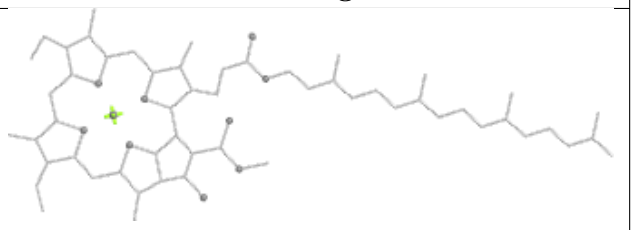
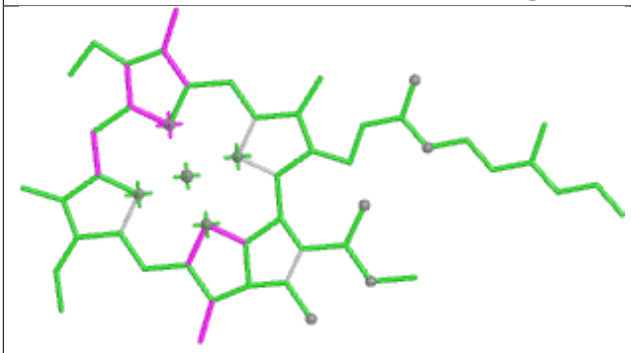


Rings

Ligand CLA Y 512



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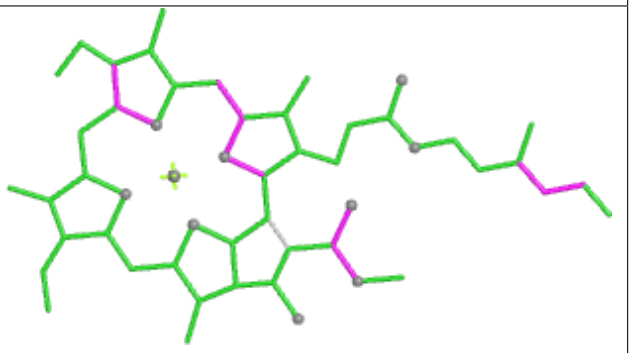
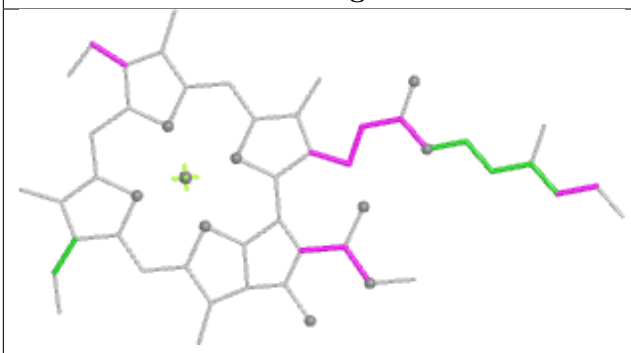


Bond angles



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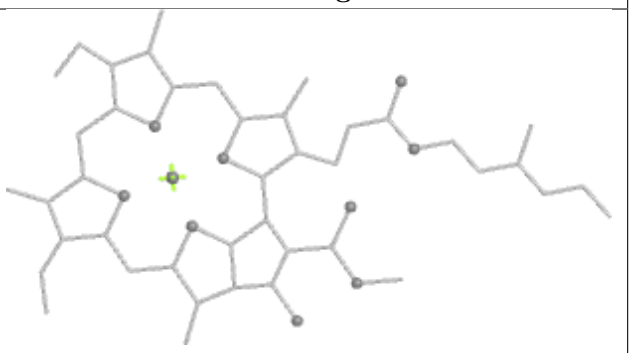
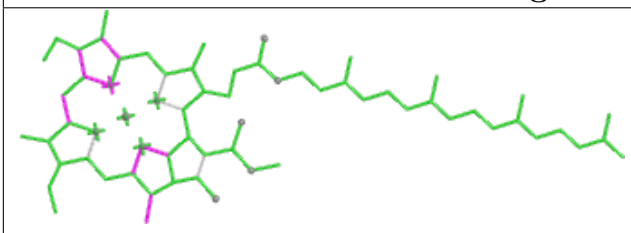


Rings

Ligand CLA s 510



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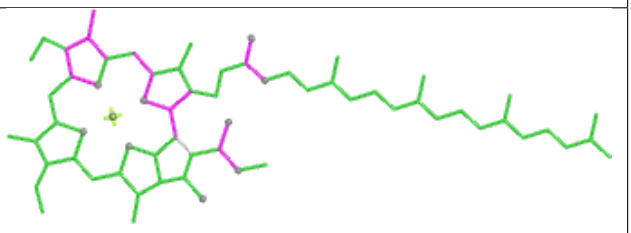

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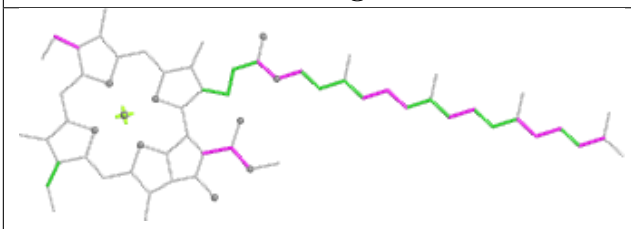

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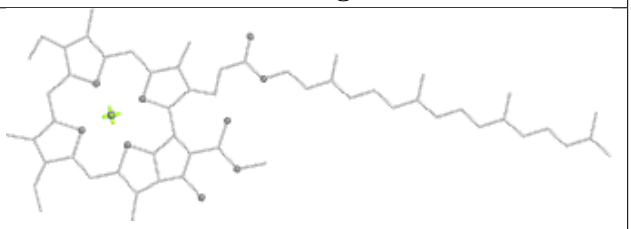
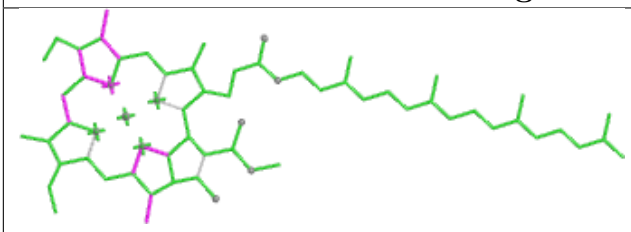


Rings

Ligand CLA B 1240



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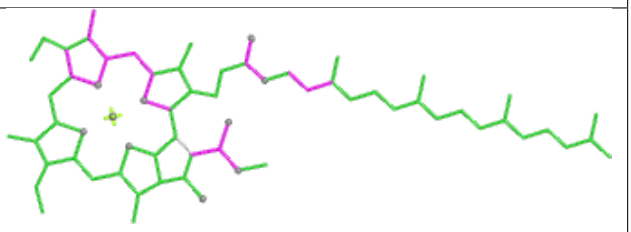

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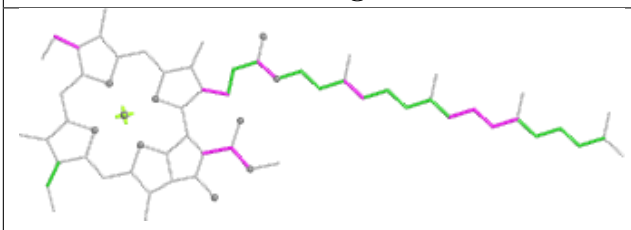

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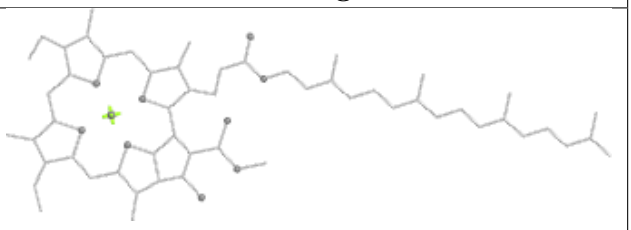
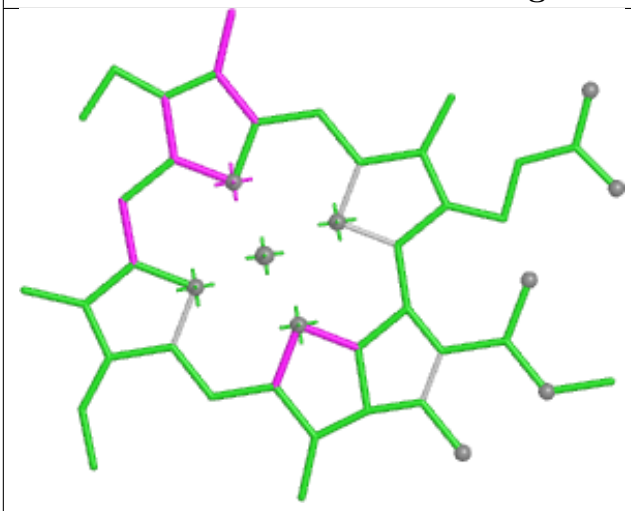


Rings

Ligand CLA 5 504



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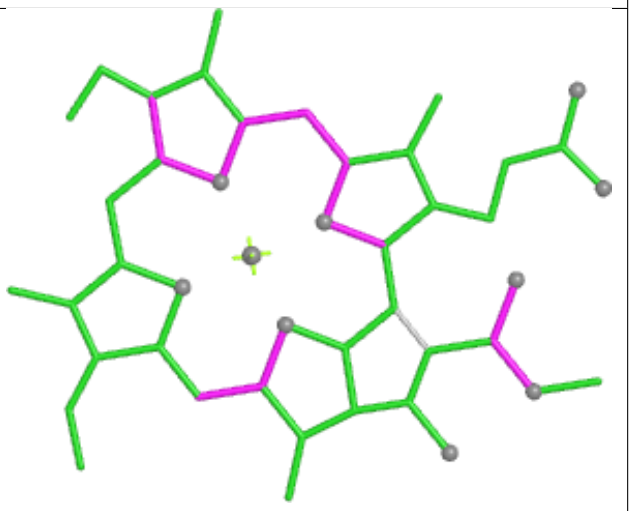

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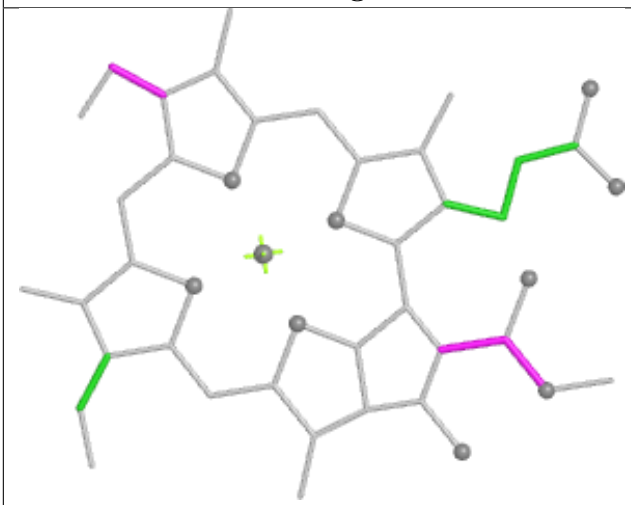

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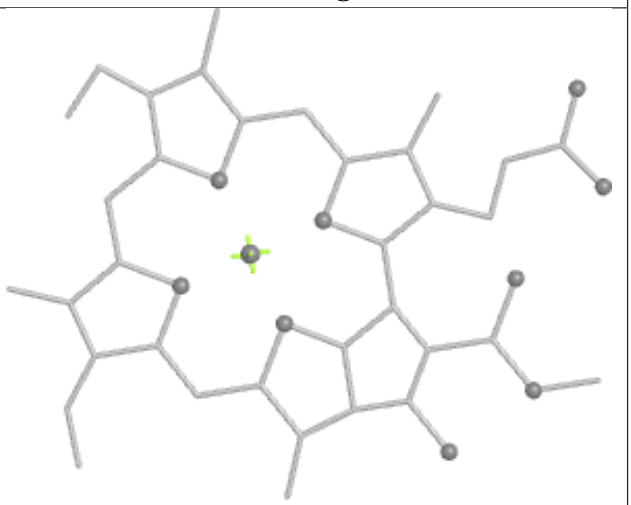
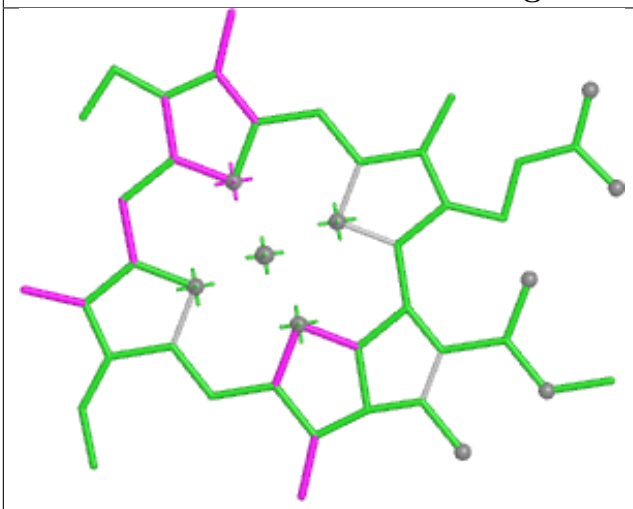


Rings

Ligand CLA Y 504



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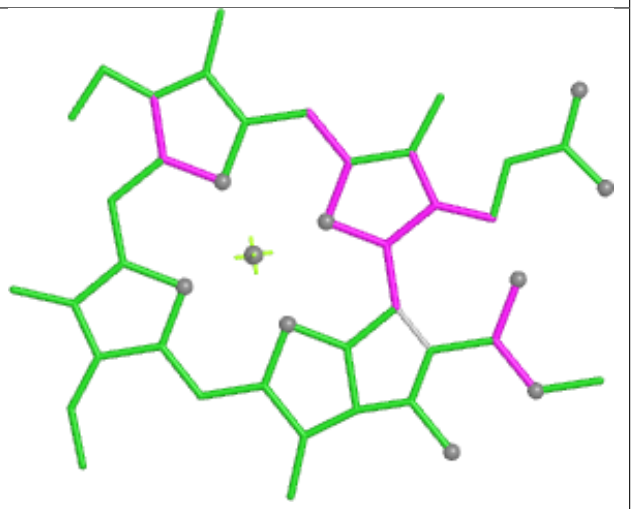

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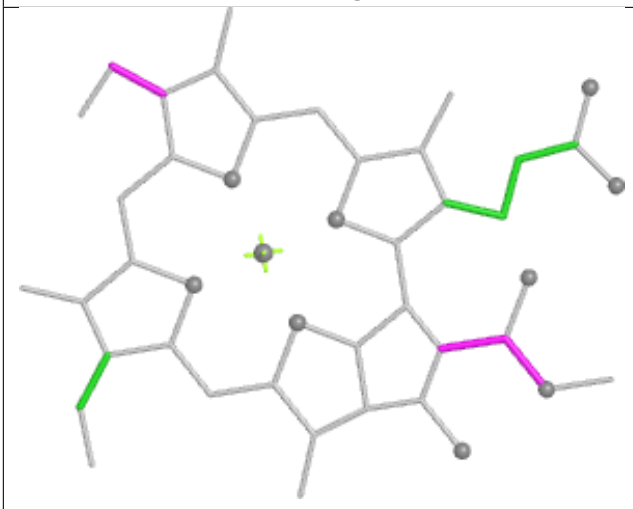
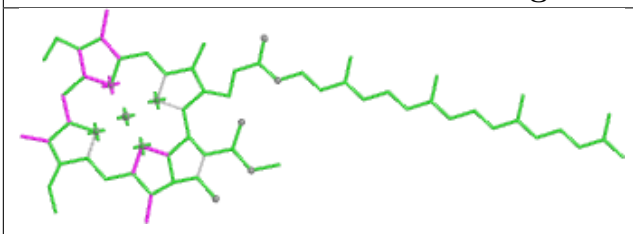


Torsions

Rings

Ligand CLA r 513



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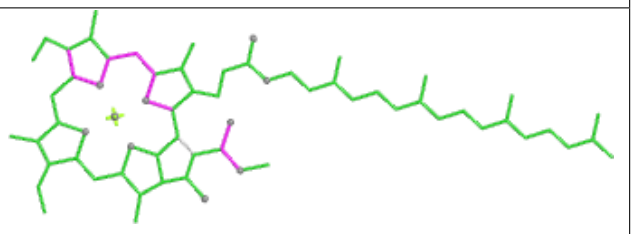

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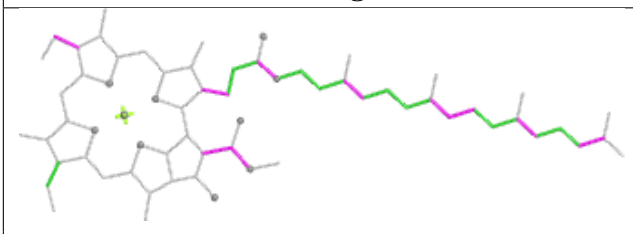
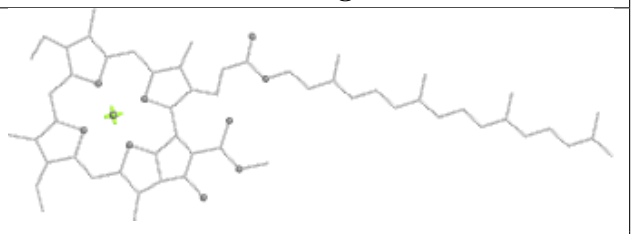
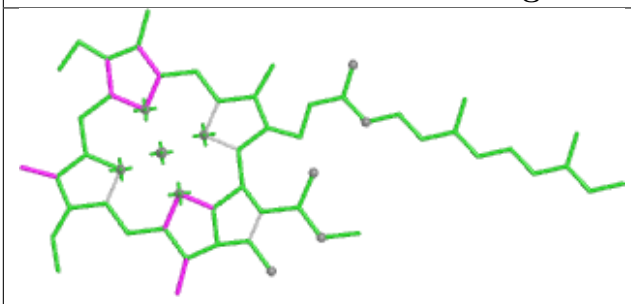
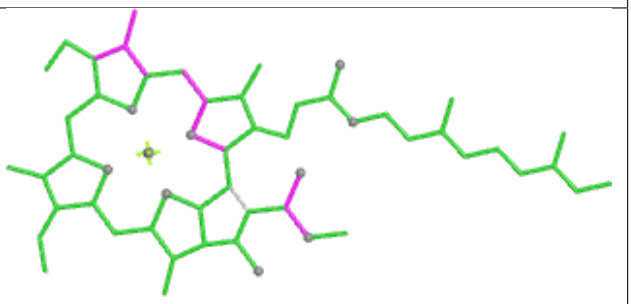
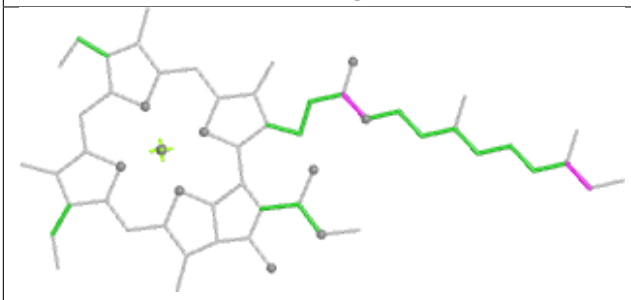
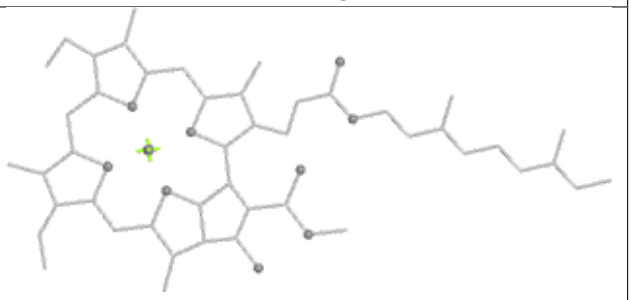
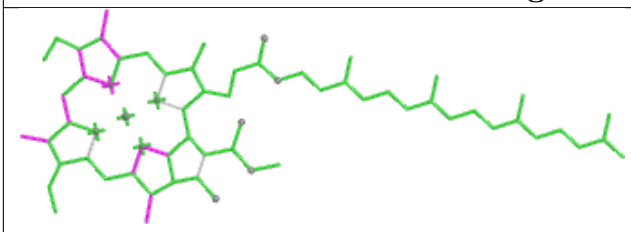
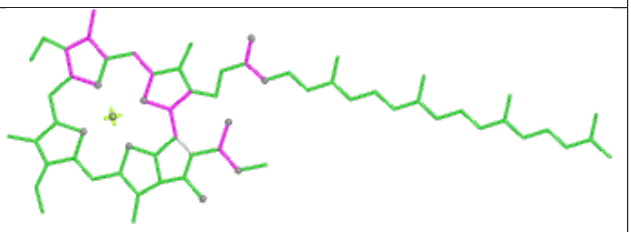


Torsions



Rings

Ligand CLA f 1211	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 509	
	
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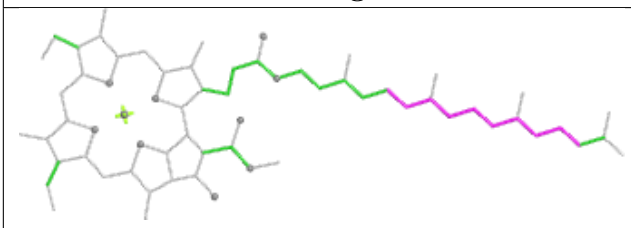
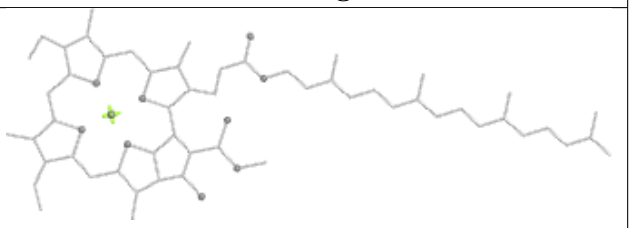
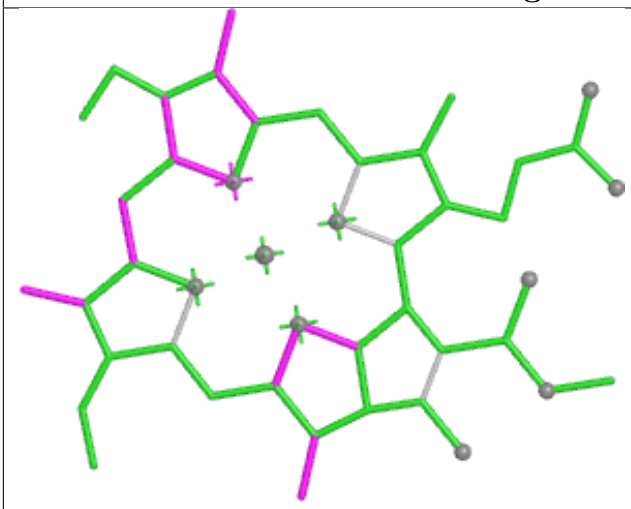
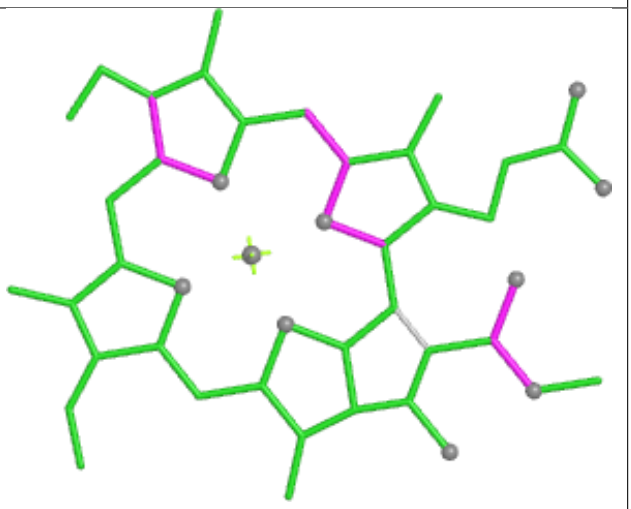
	
Torsions	Rings

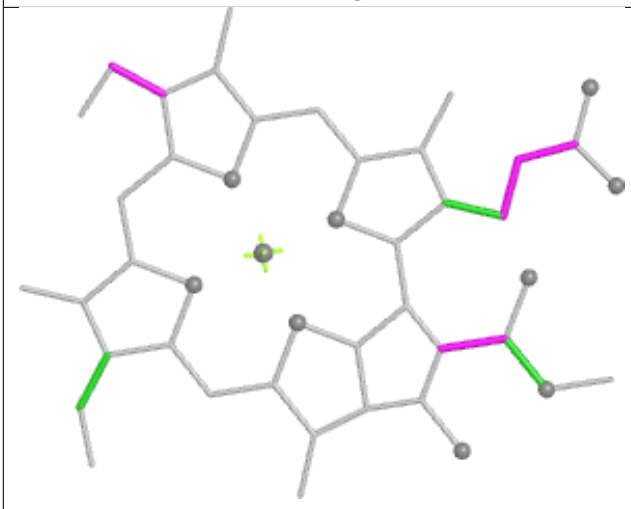
Ligand CLA Y 517



Bond lengths



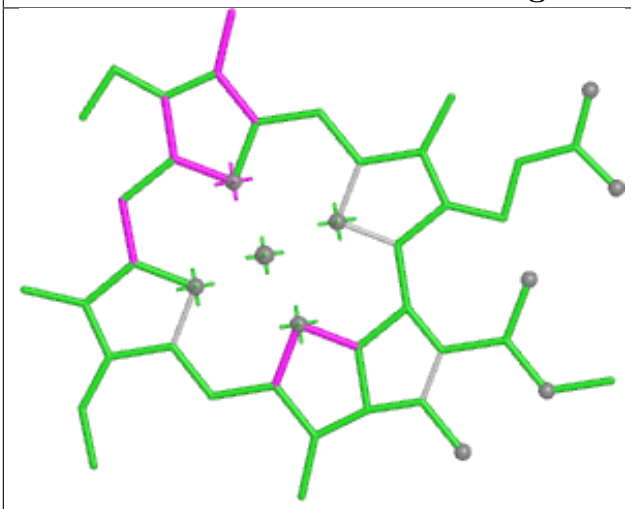
Bond angles



Torsions

Rings

Ligand CLA 6 506



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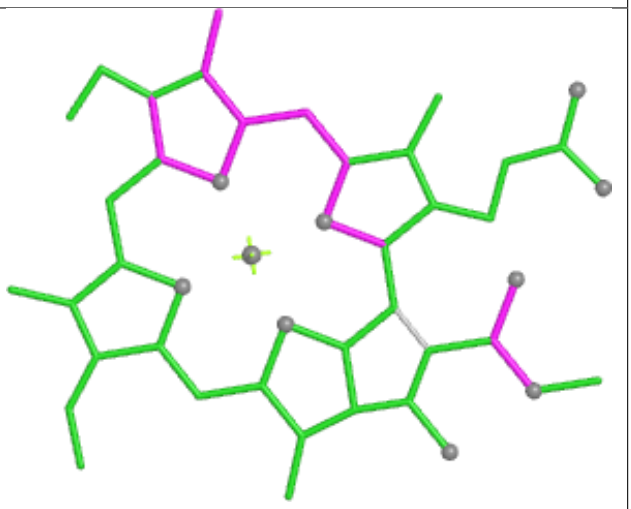
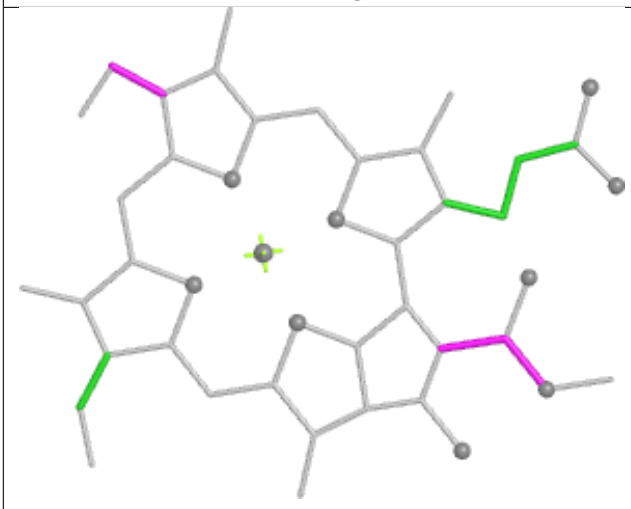


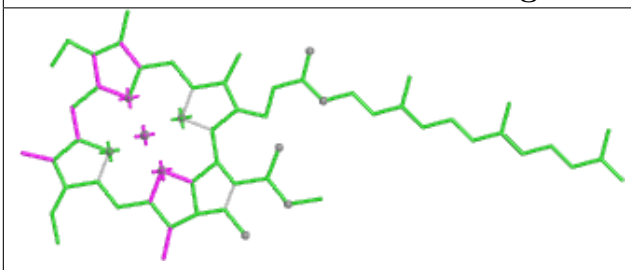
Bond angles



Torsions

Rings

Ligand CLA e 1116



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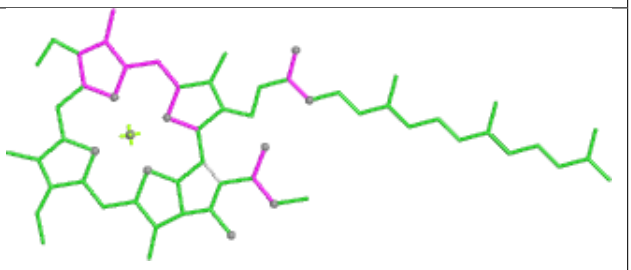
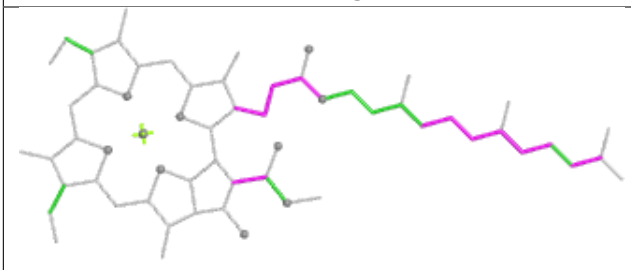
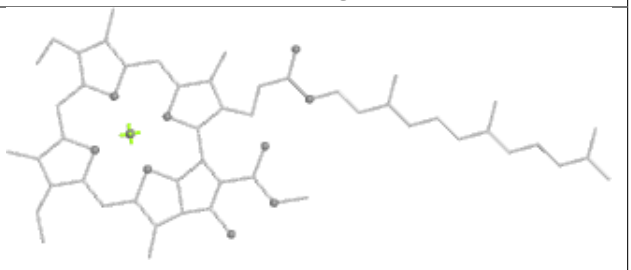


Bond angles

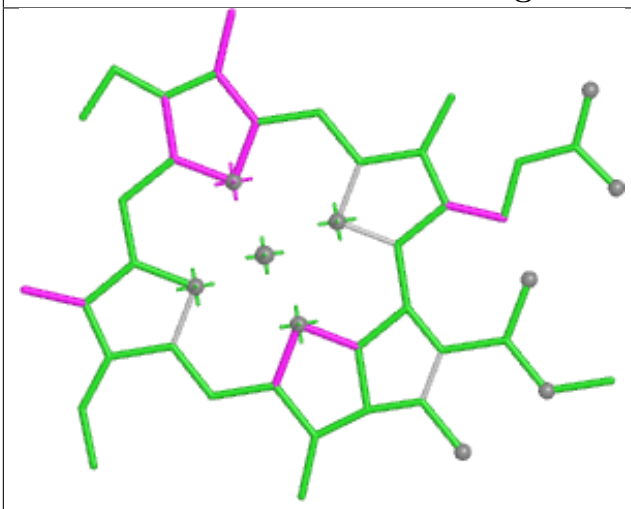


Torsions

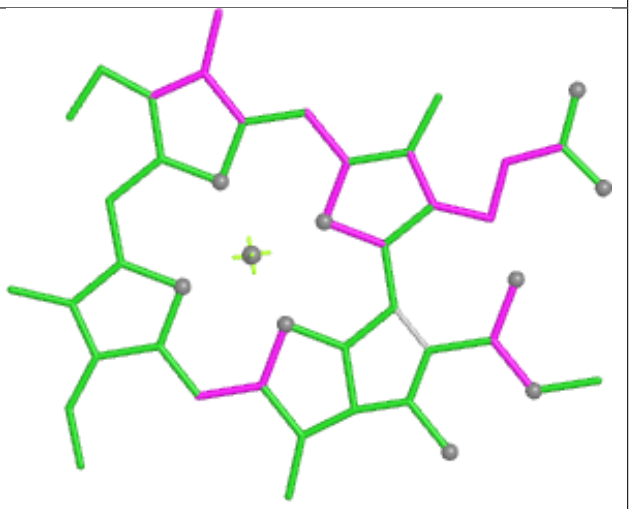


Rings

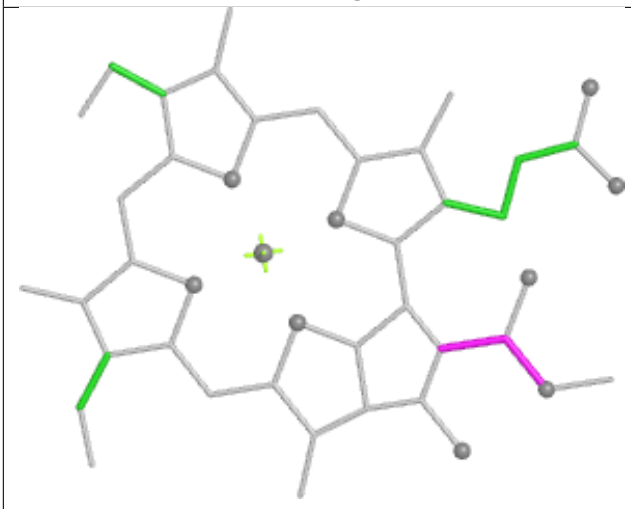
Ligand CLA A 1801



Bond lengths



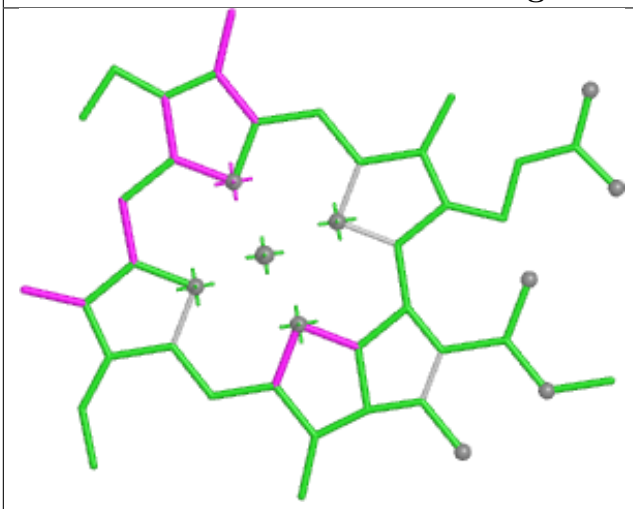
Bond angles



Torsions

Rings

Ligand CLA d 506



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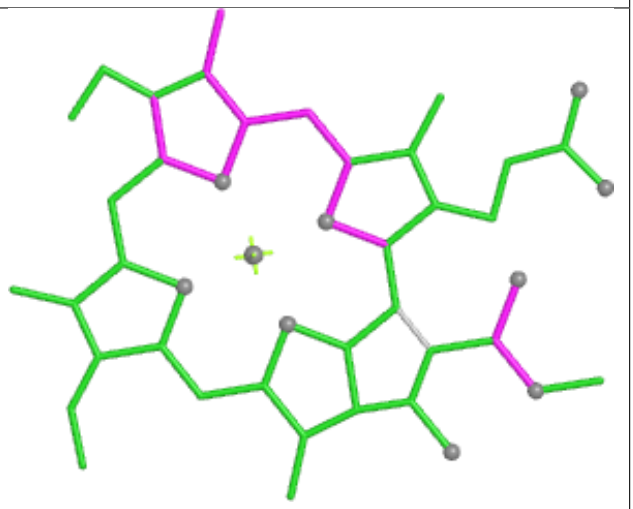
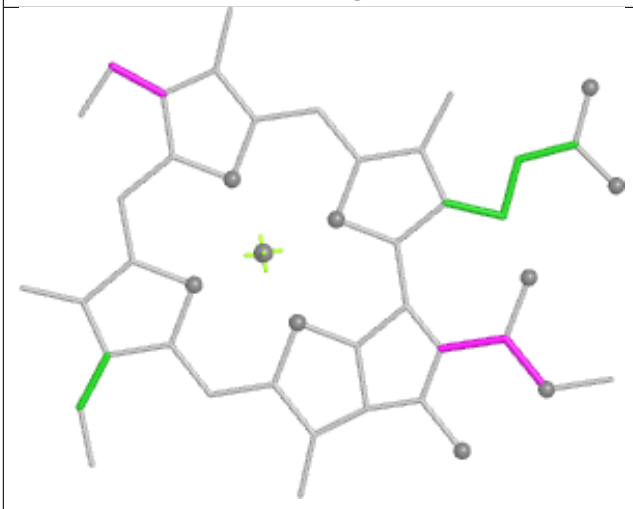


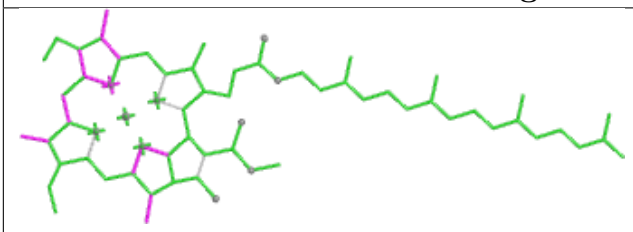
Bond angles



Torsions

Rings

Ligand CLA e 1111



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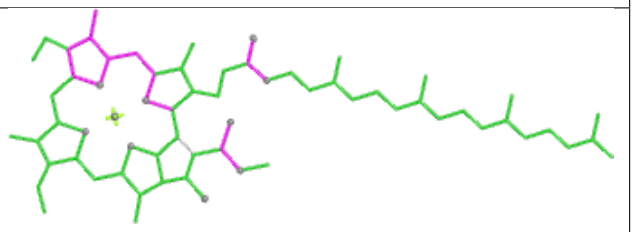
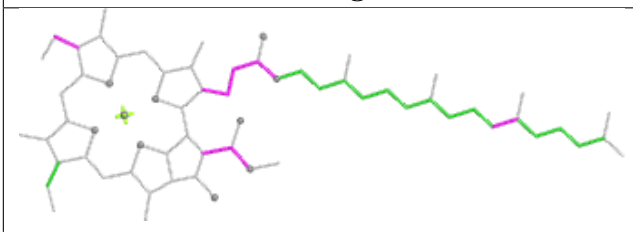


Bond angles



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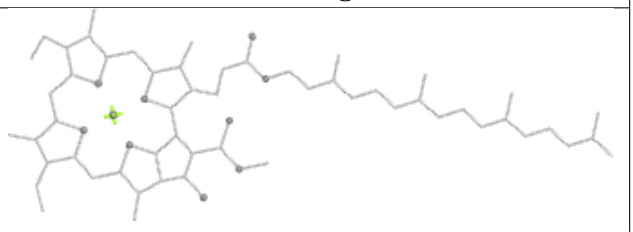
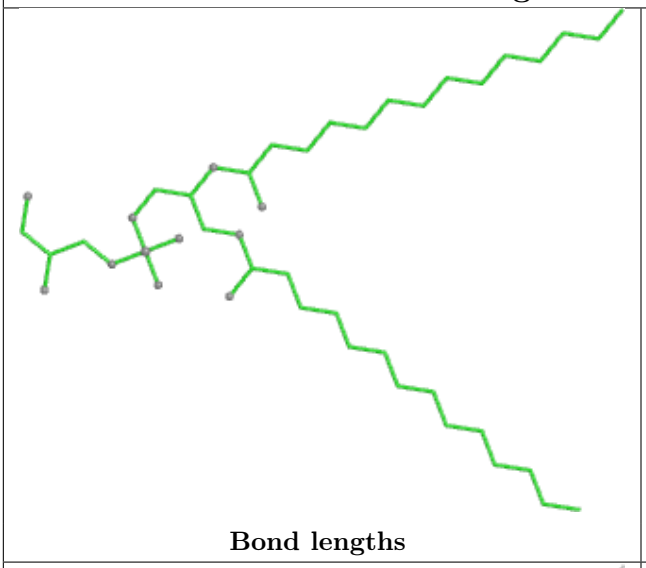


Rings

Ligand LHG A 5006



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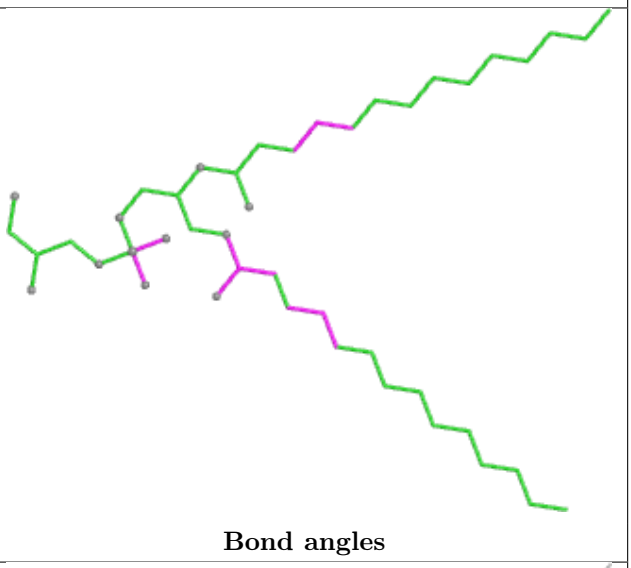
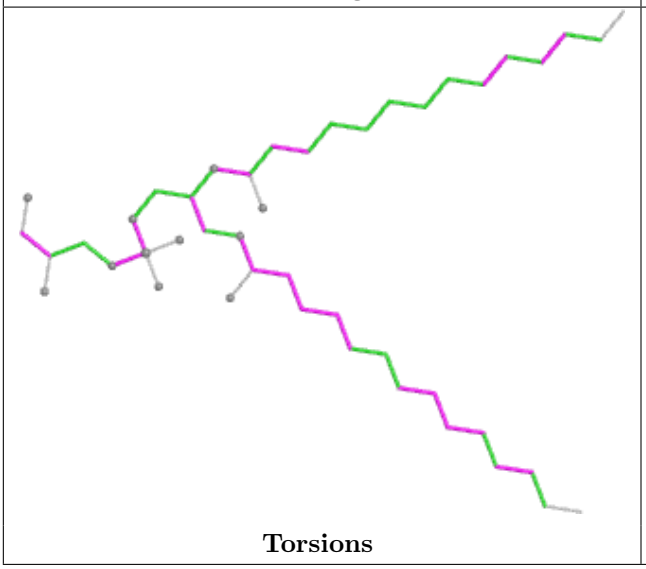


Bond angles



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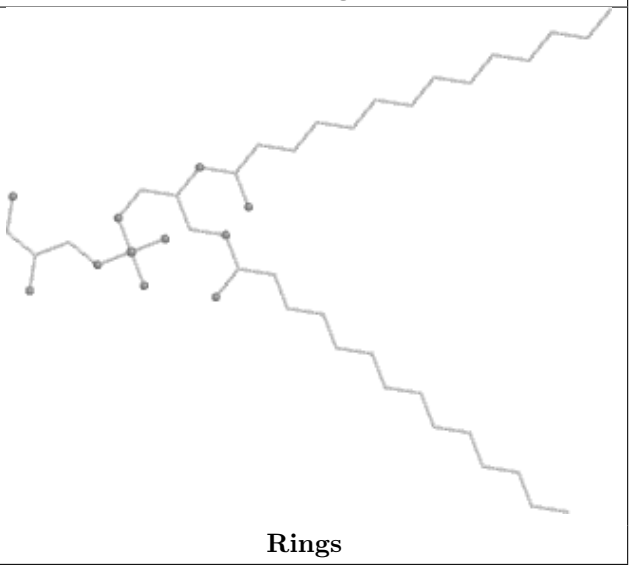
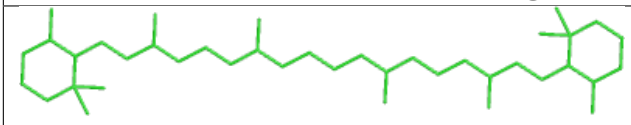


Rings

Ligand BCR Z 522



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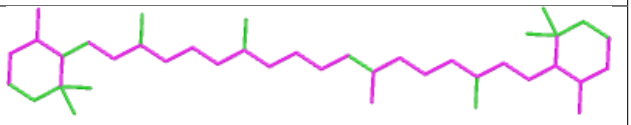

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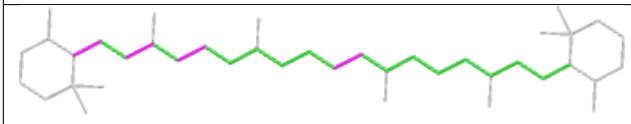

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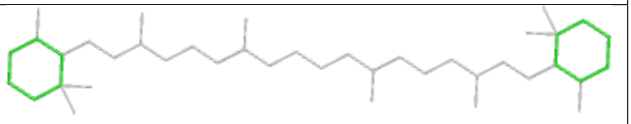
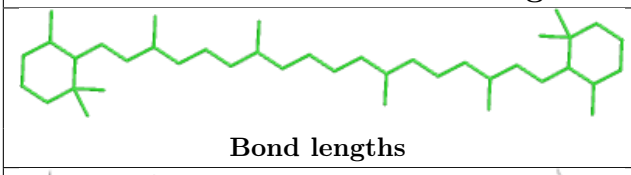


Rings

Ligand BCR q 523



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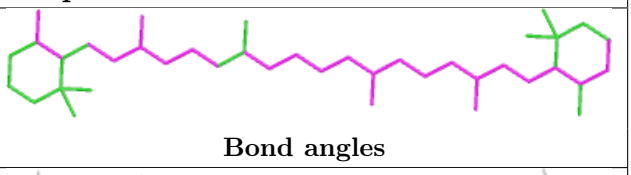

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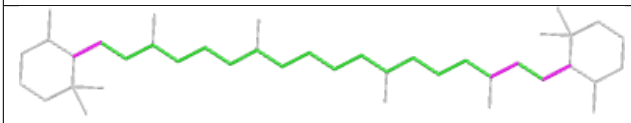

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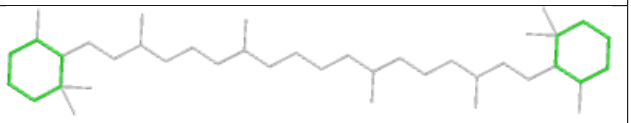
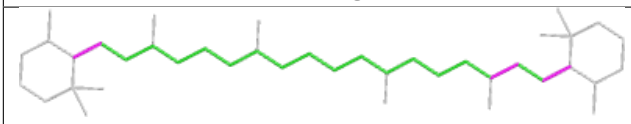


Rings

Ligand BCR Y 523

Bond lengths

Bond angles



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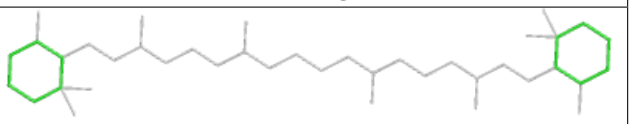
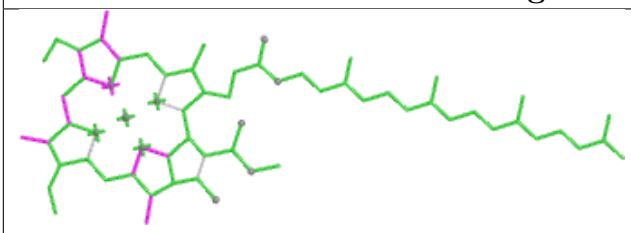


Rings

Ligand CLA q 509



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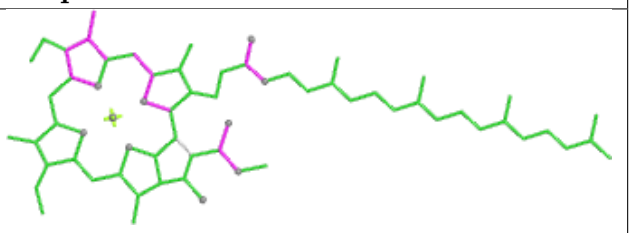
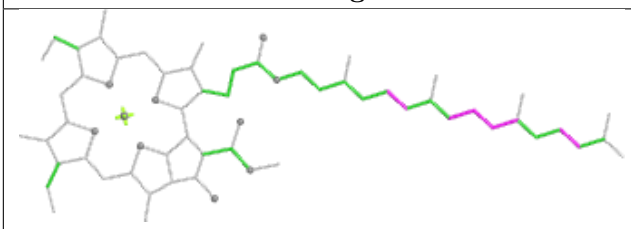


Bond angles



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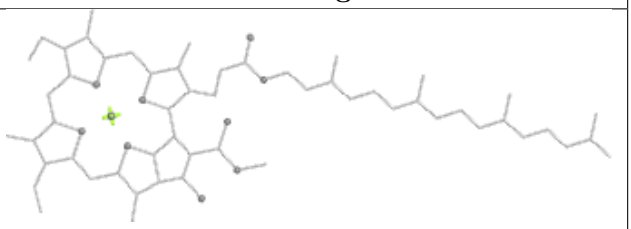
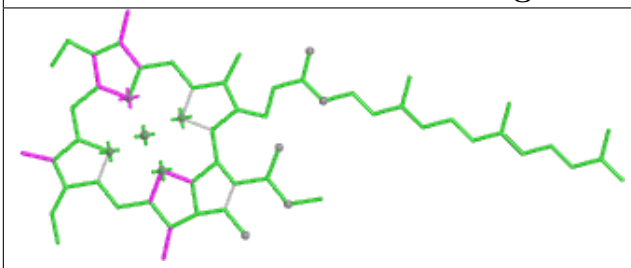
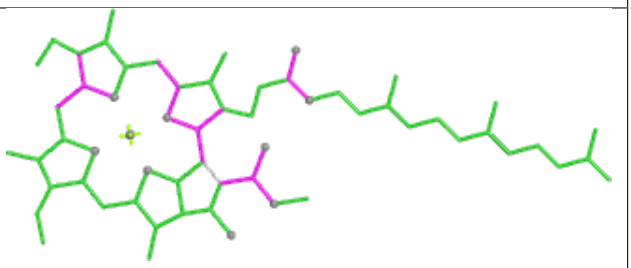
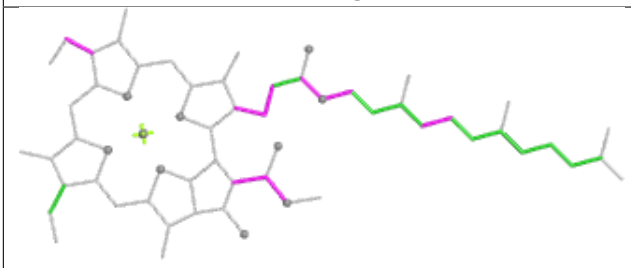
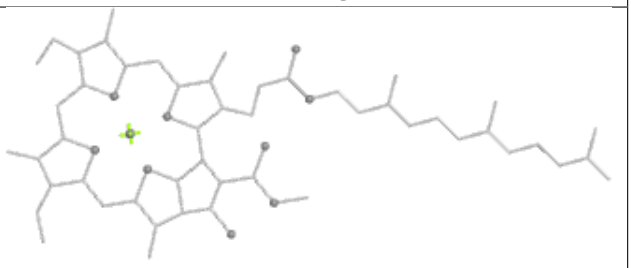


Rings

Ligand CLA G 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

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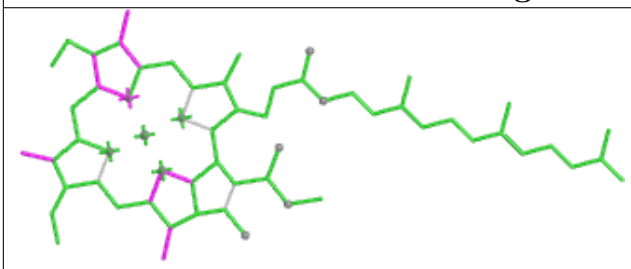
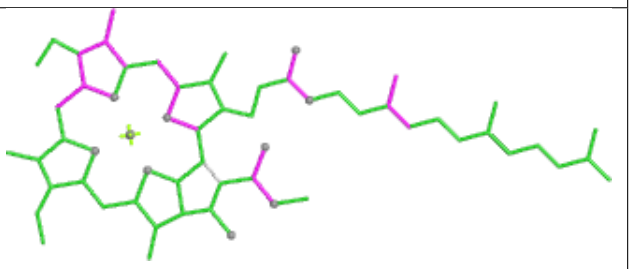
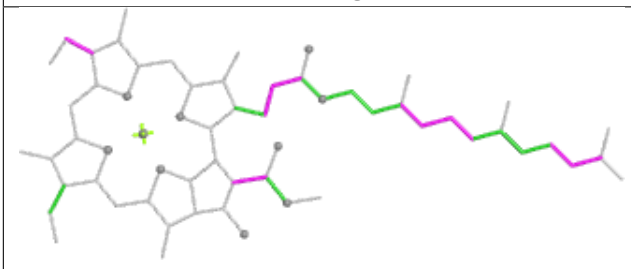
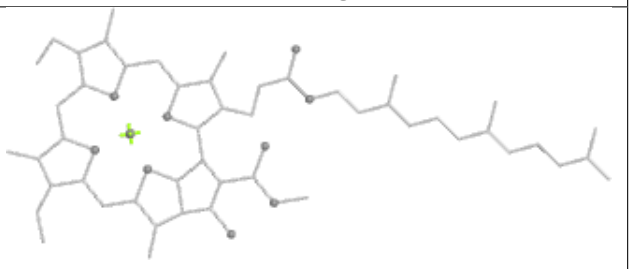
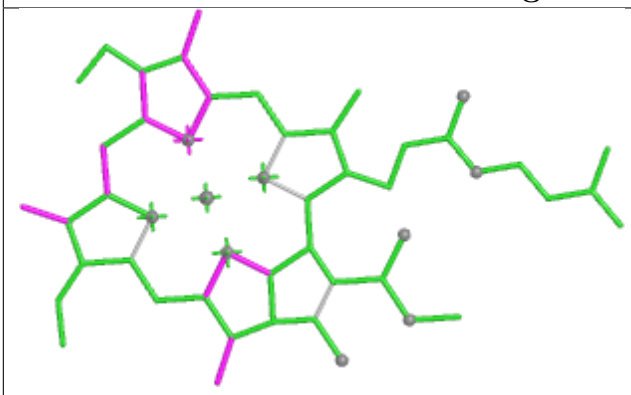
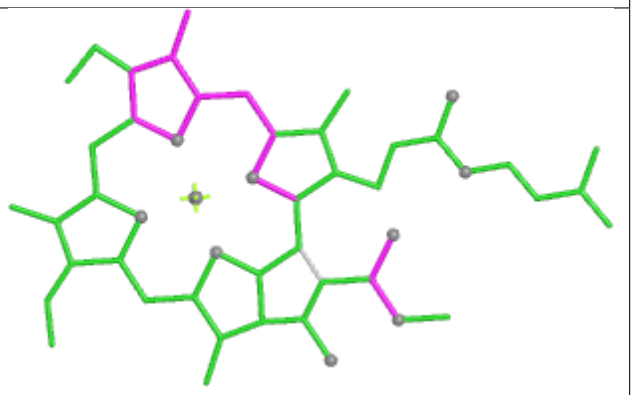
	
Bond lengths	Bond angles
	
Torsions	Rings

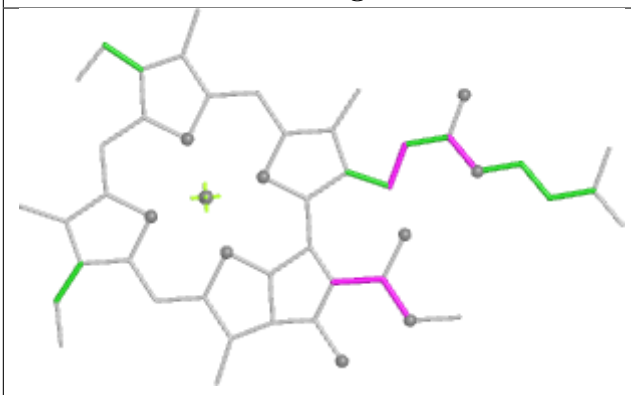
Ligand CLA f 1232



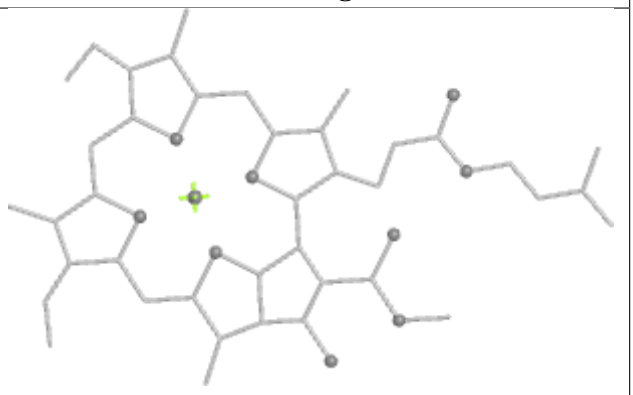
Bond lengths



Bond angles

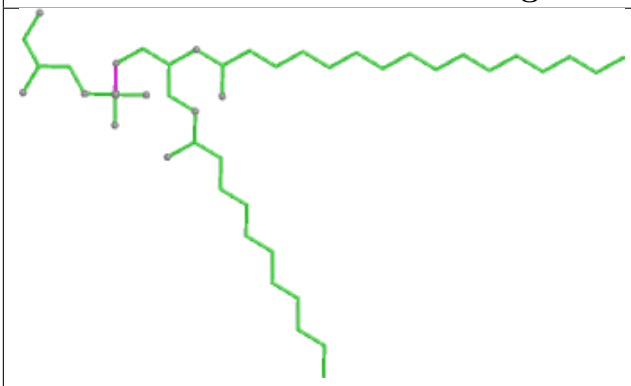


Torsions



Rings

Ligand LHG f 1855



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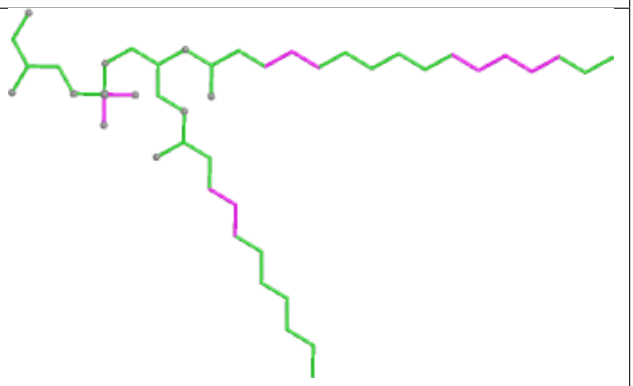
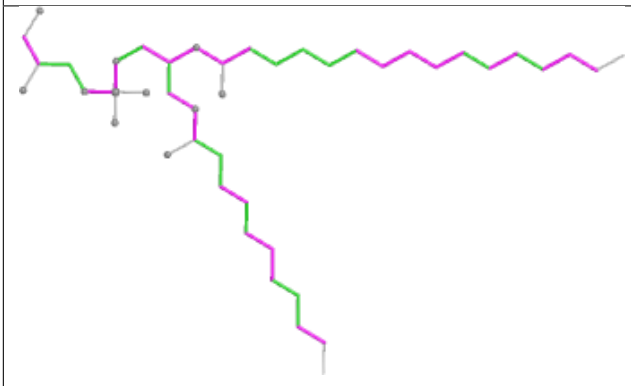


Bond angles



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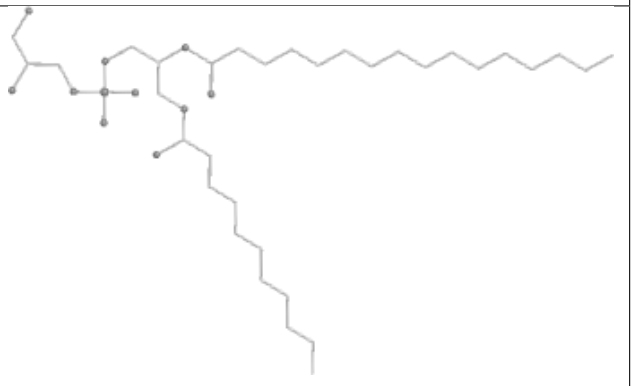
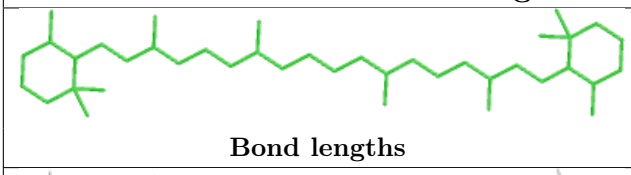


Rings

Ligand BCR B 4006



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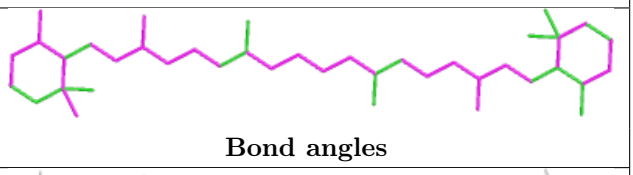
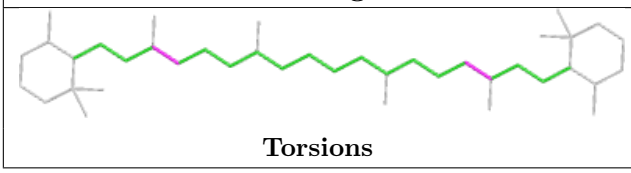
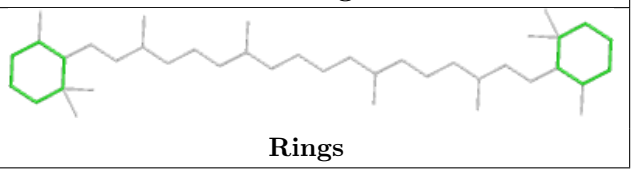


Bond angles

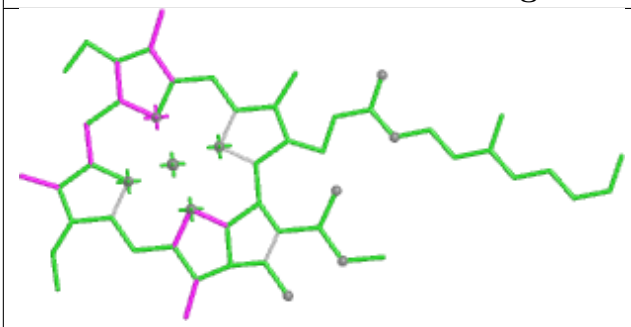


Torsions

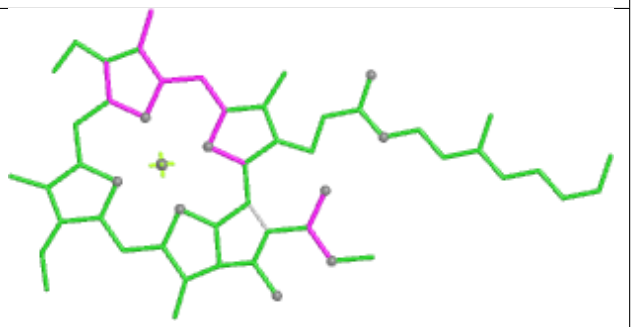


Rings

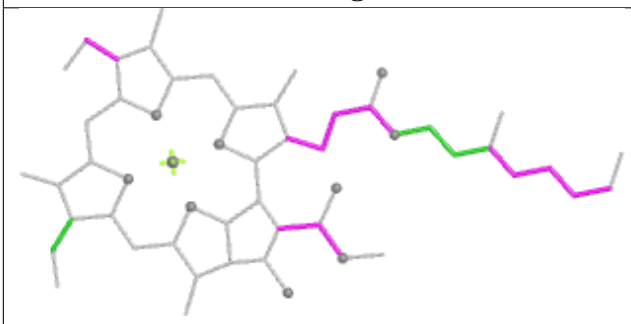
Ligand CLA e 1108



Bond lengths



Bond angles



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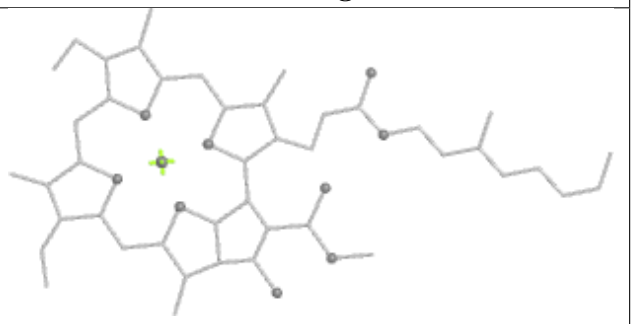
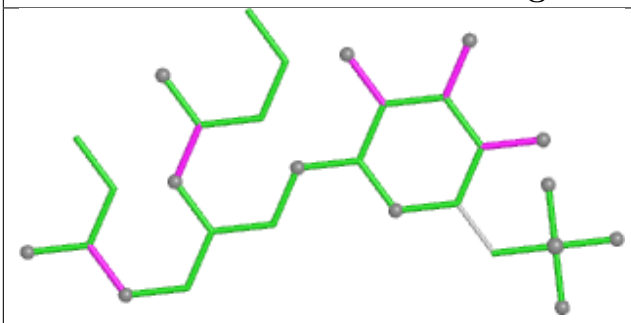
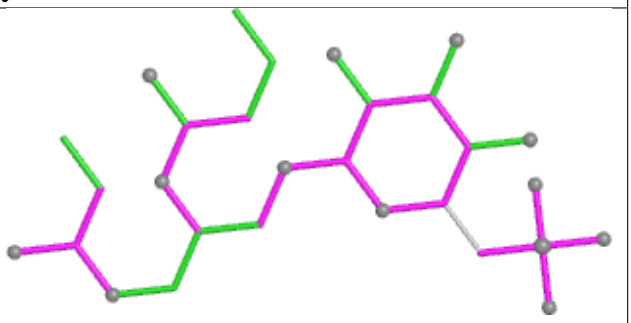


Rings

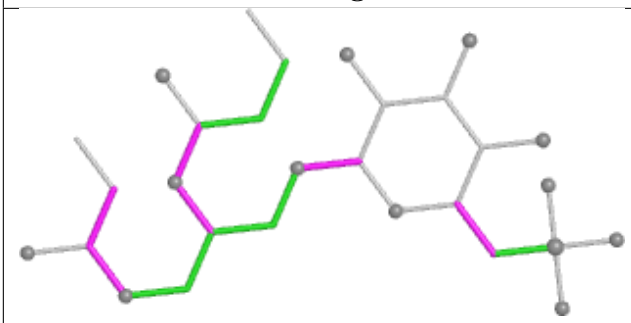
Ligand SQD 5 822



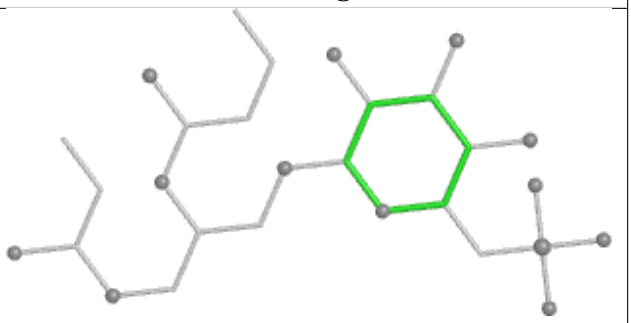
Bond lengths



Bond angles

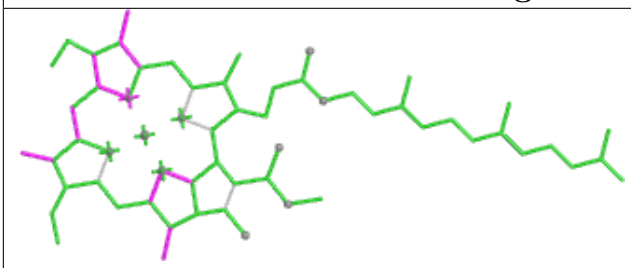


Torsions



Rings

Ligand CLA H 1222



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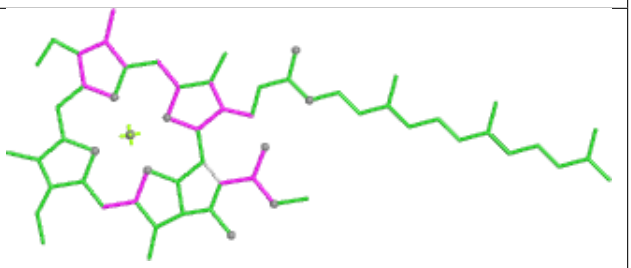

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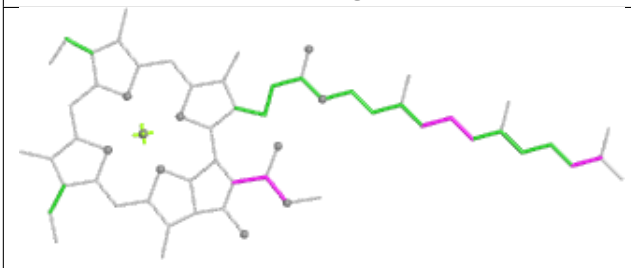

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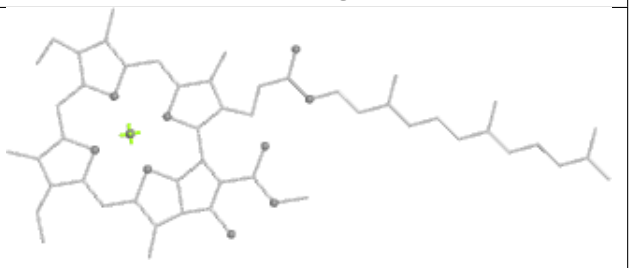
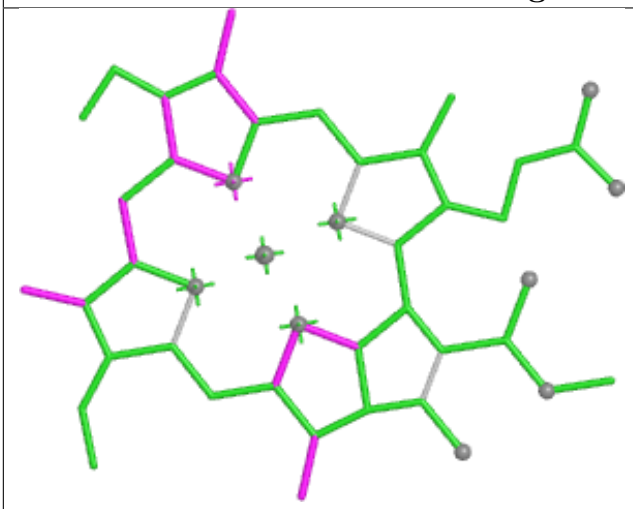


Rings

Ligand CLA 3 517



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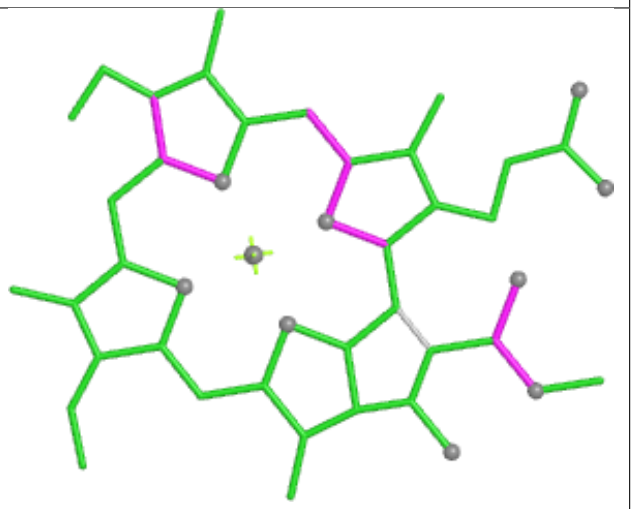
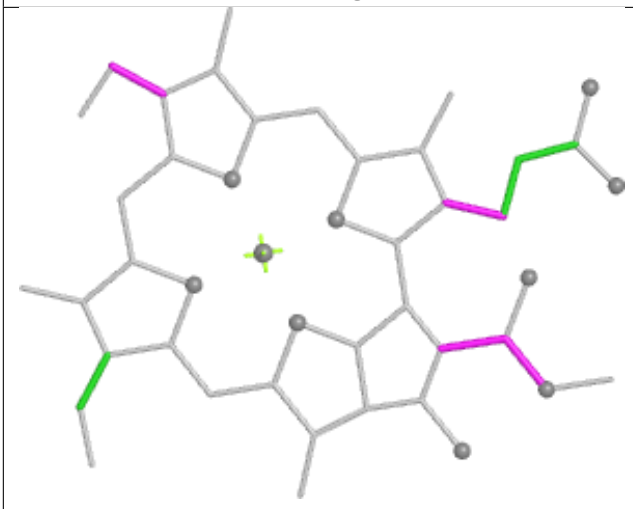


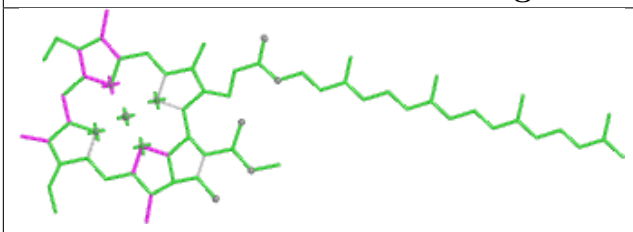
Bond angles



Torsions

Rings

Ligand CLA G 1125



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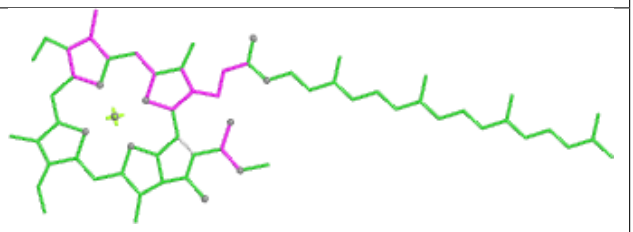

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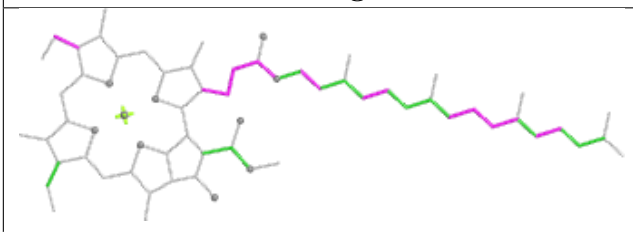
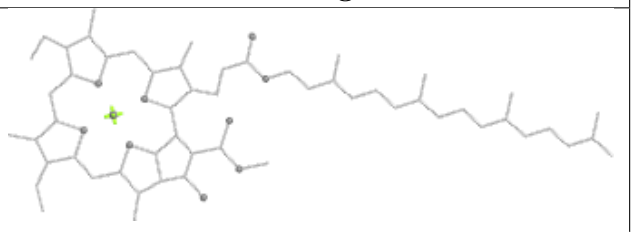
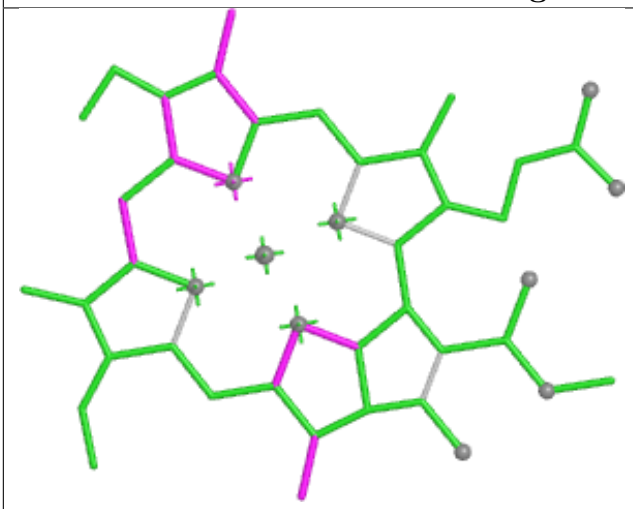


Torsions



Rings

Ligand CLA c 512



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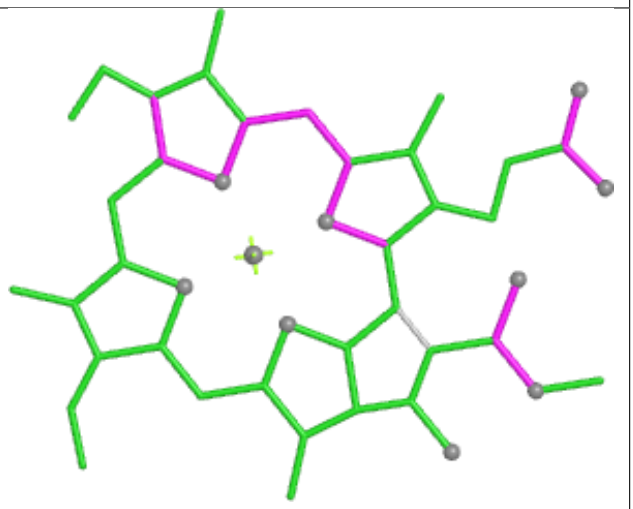
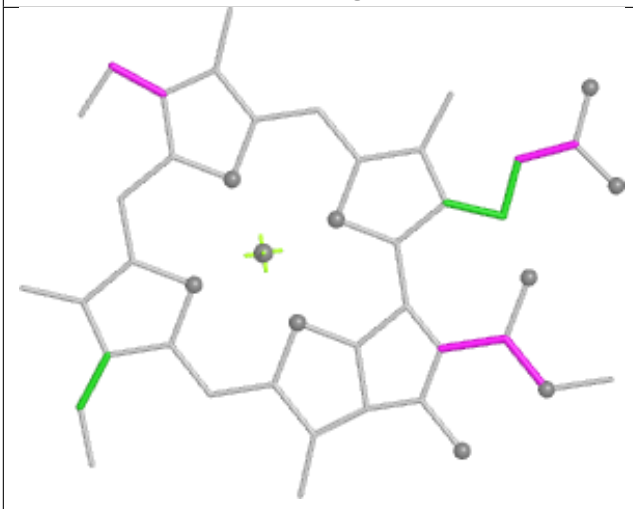


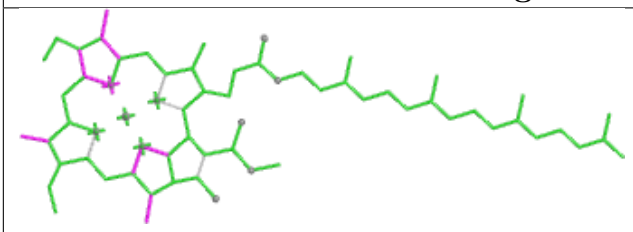
Bond angles



Torsions

Rings

Ligand CLA H 1235



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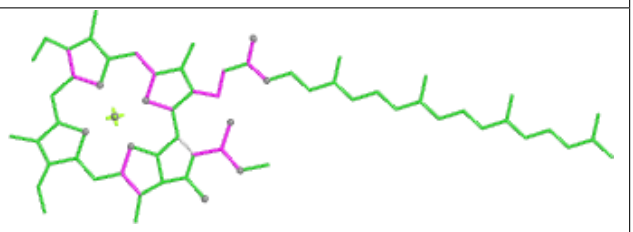
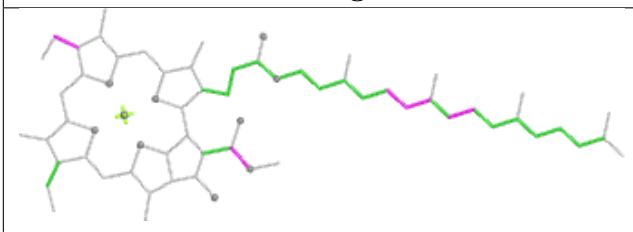


Bond angles



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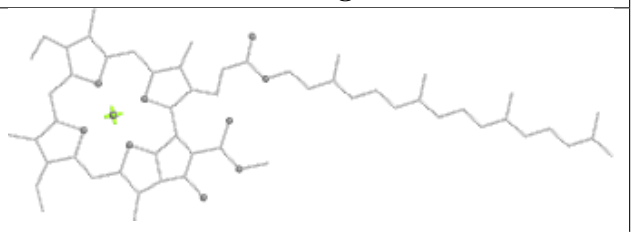
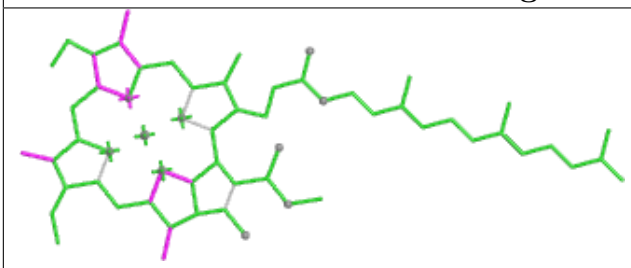


Rings

Ligand CLA e 1115



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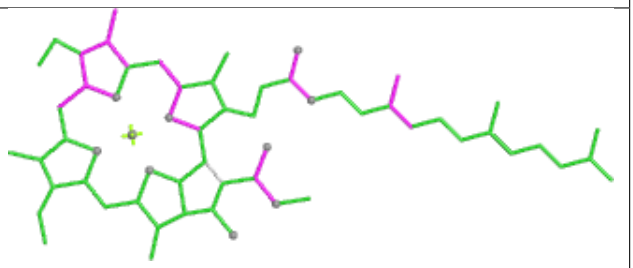
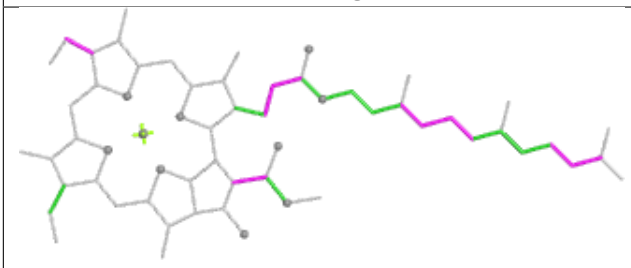


Bond angles



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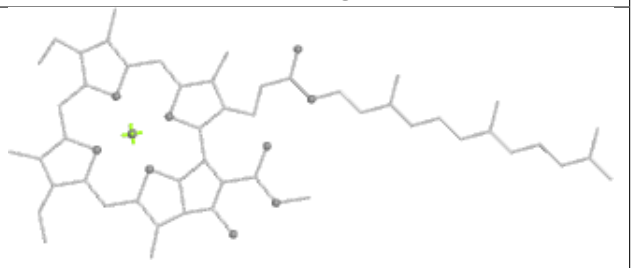
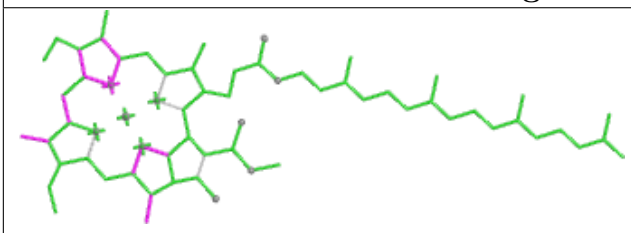


Rings

Ligand CLA f 1229



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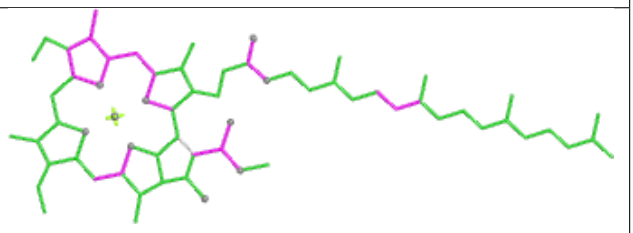

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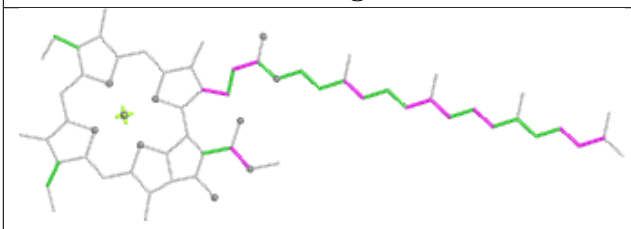

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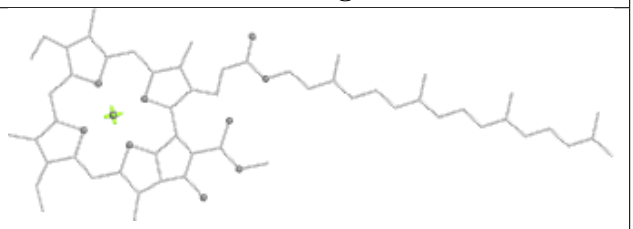
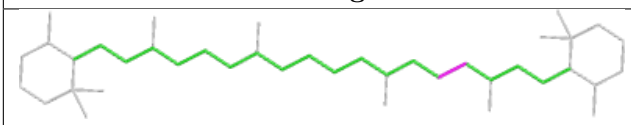


Rings

Ligand BCR B 4009

Bond lengths

Bond angles



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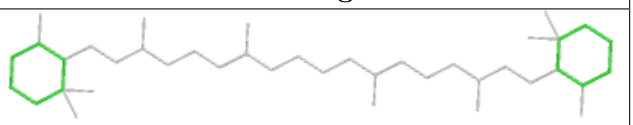
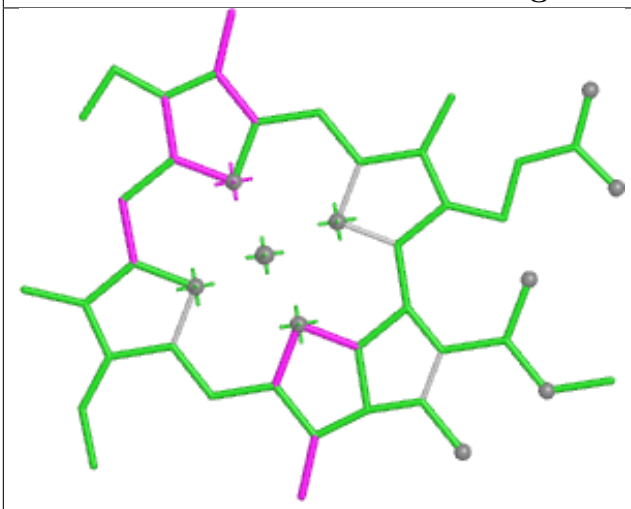


Rings

Ligand CLA t 511



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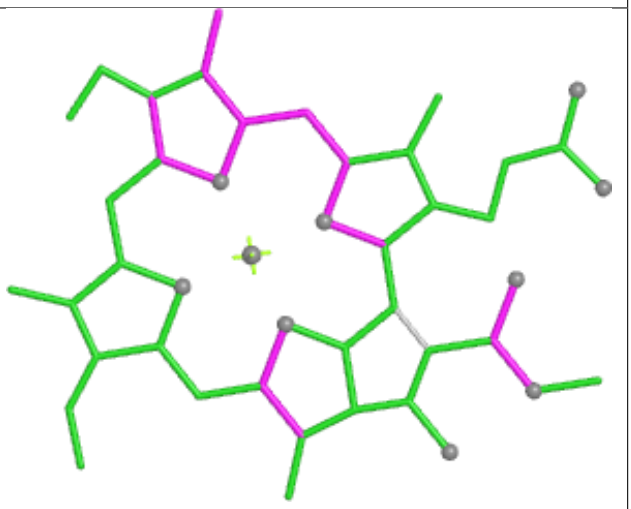
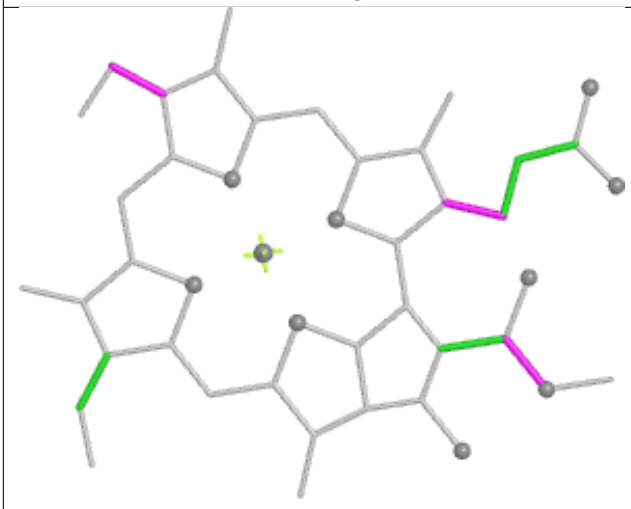


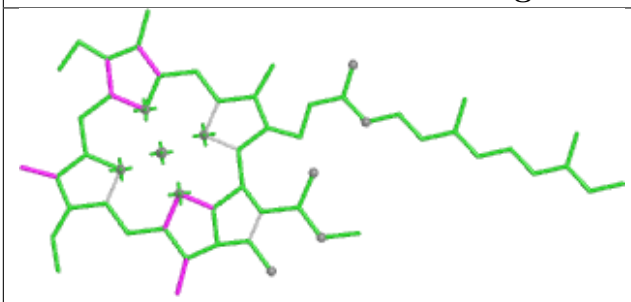
Bond angles



Torsions

Rings

Ligand CLA H 1211



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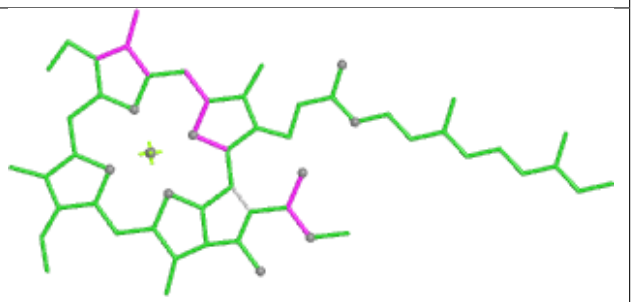
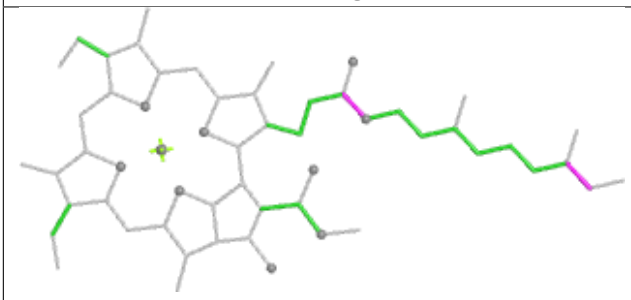
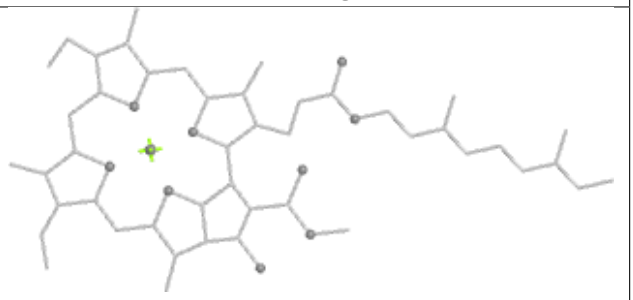


Bond angles

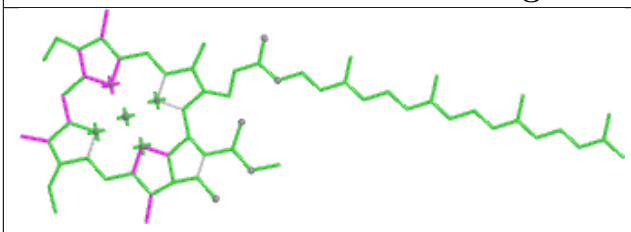


Torsions



Rings

Ligand CLA f 1238



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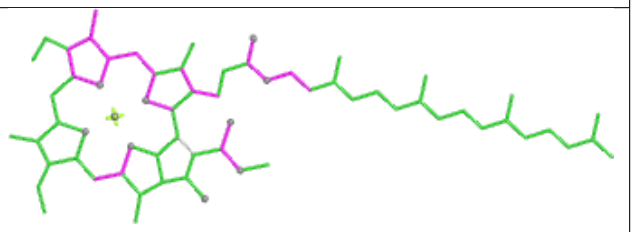

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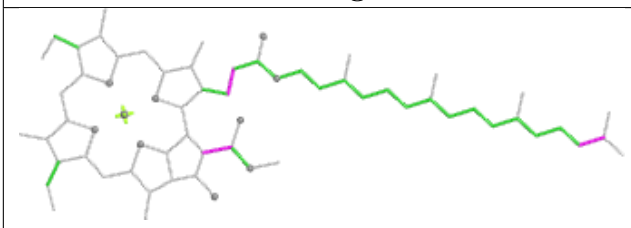

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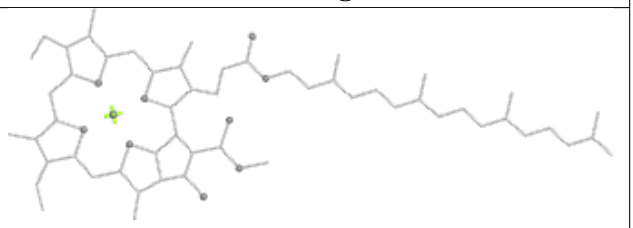
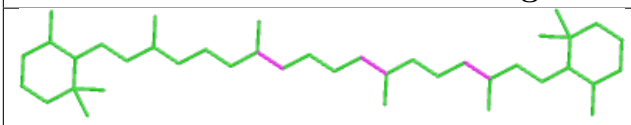


Rings

Ligand BCR f 4010



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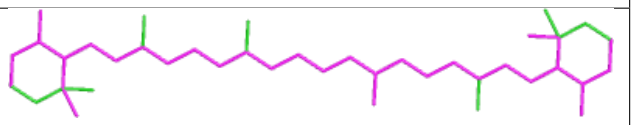
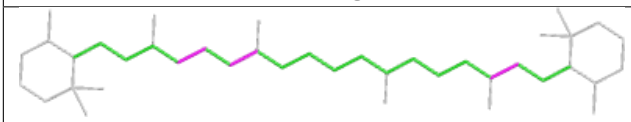


Bond angles



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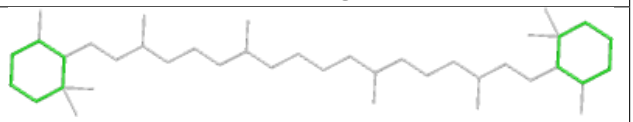
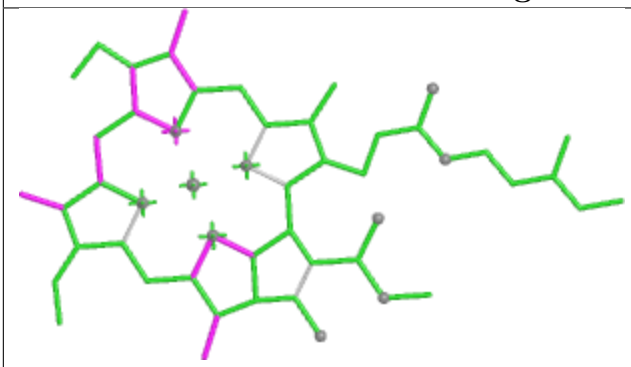


Rings

Ligand CLA G 1110



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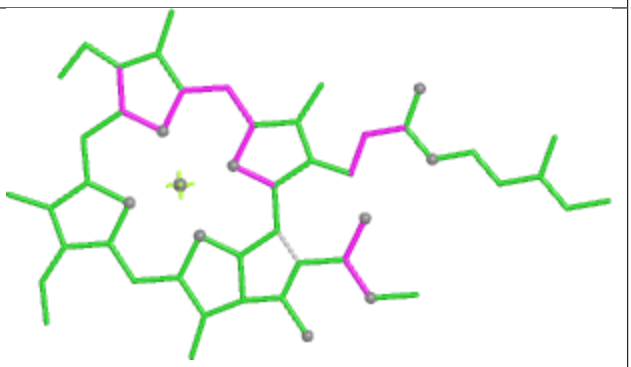
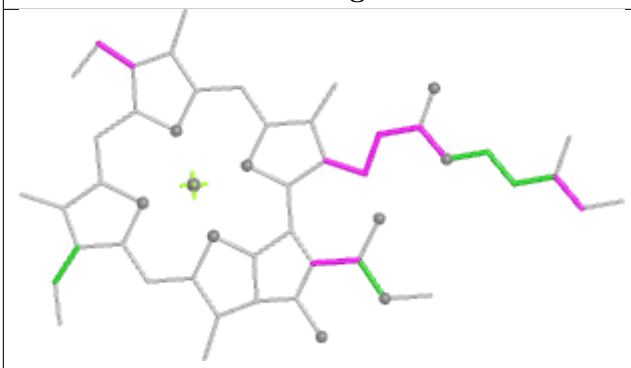


Bond angles



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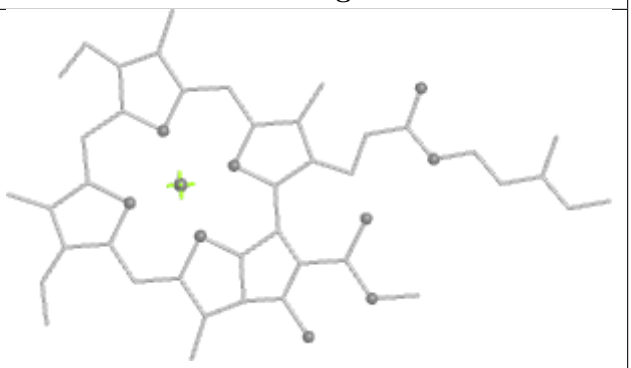
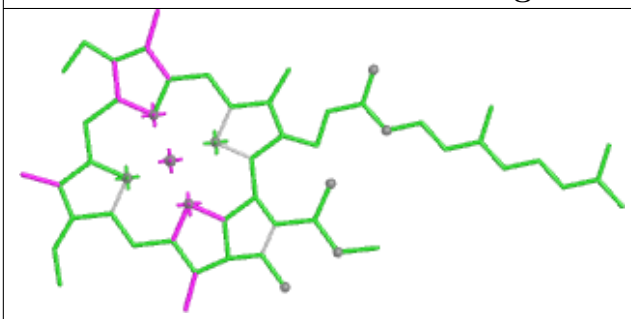


Rings

Ligand CLA G 1121



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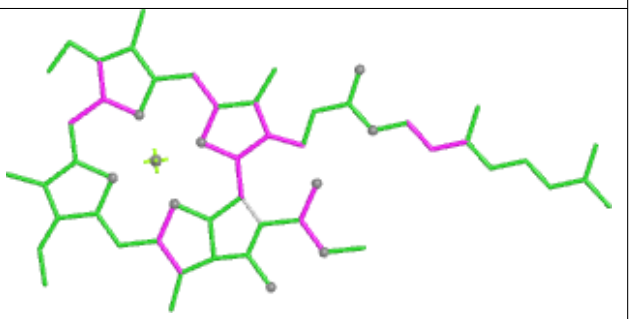
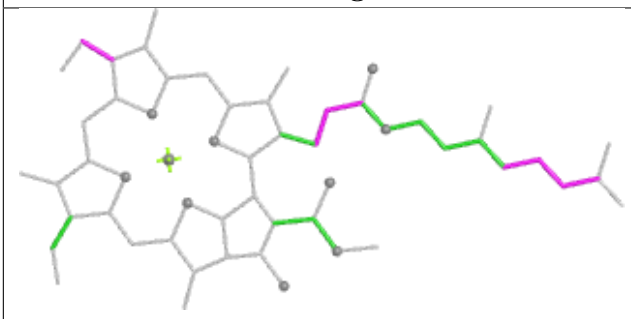
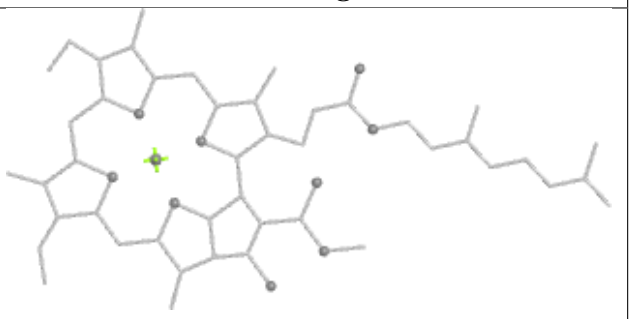


Bond angles

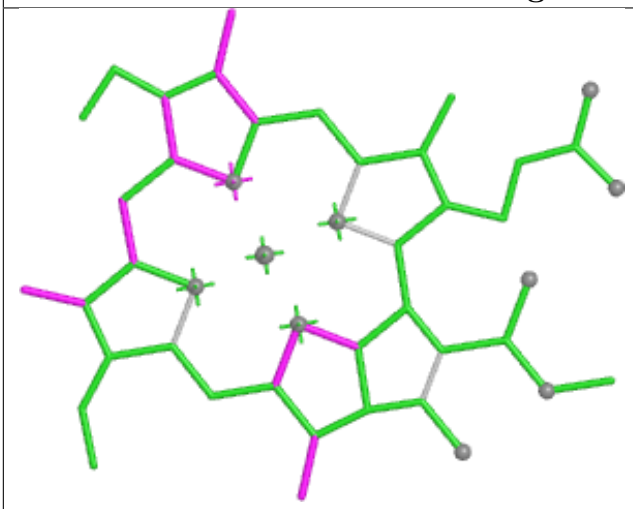


Torsions



Rings

Ligand CLA d 508



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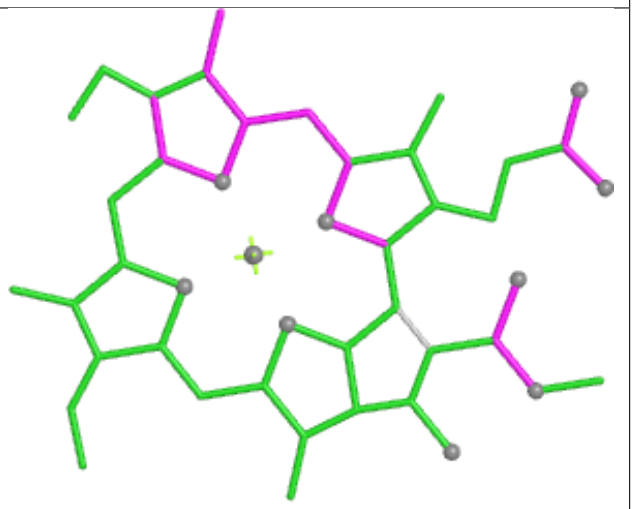
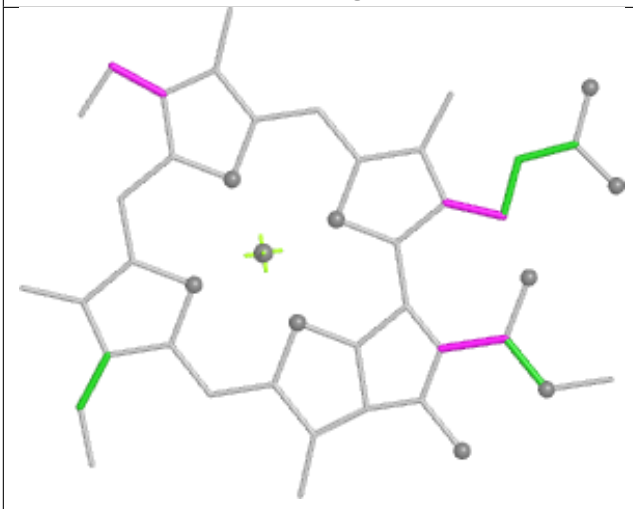


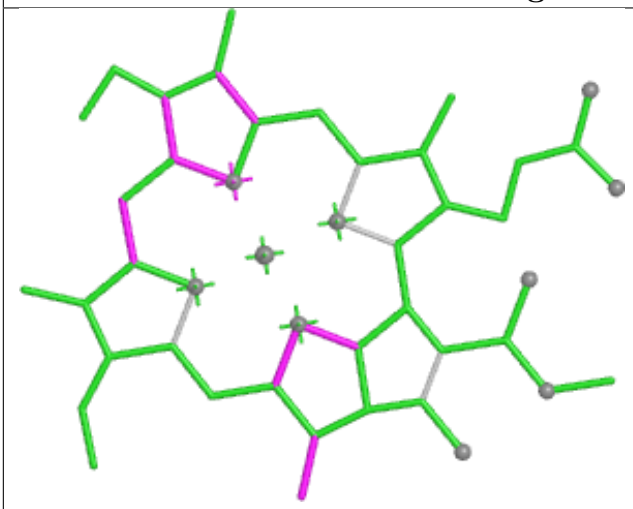
Bond angles



Torsions

Rings

Ligand CLA d 516



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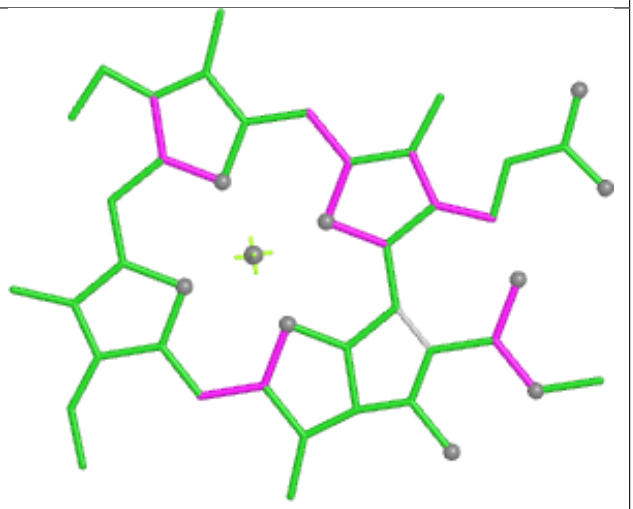
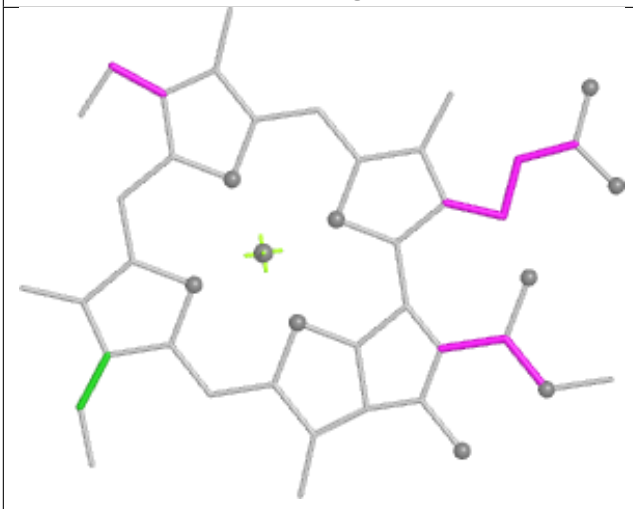


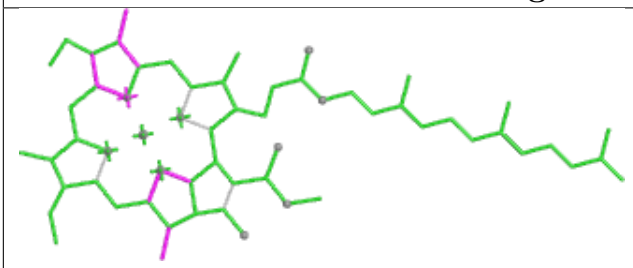
Bond angles



Torsions

Rings

Ligand CLA 1 502



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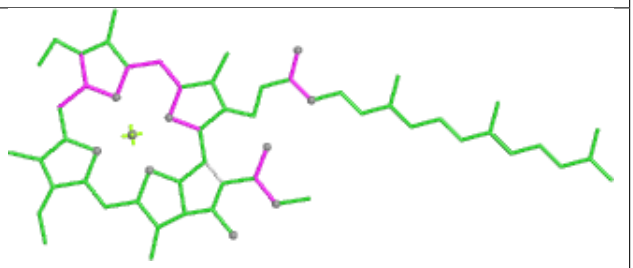
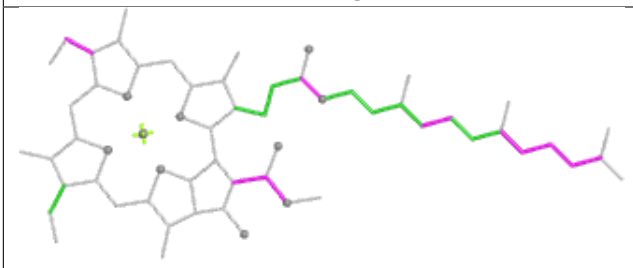
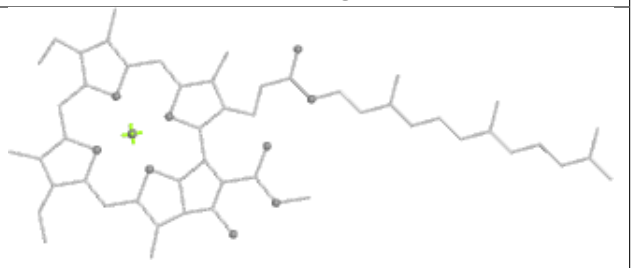


Bond angles

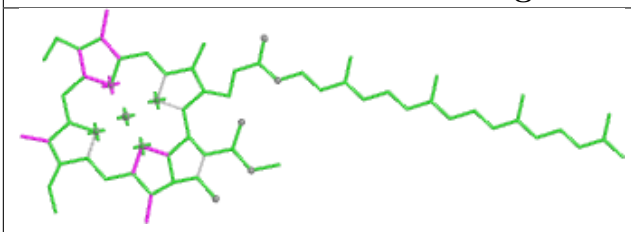


Torsions



Rings

Ligand CLA A 1237



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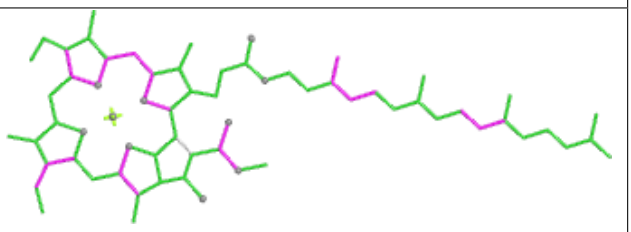
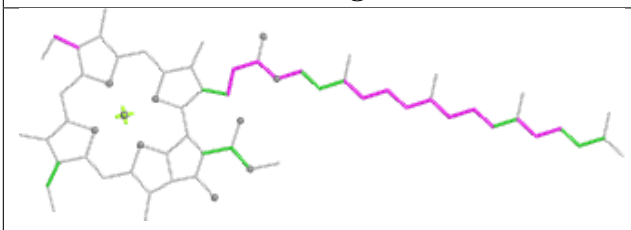


Bond angles



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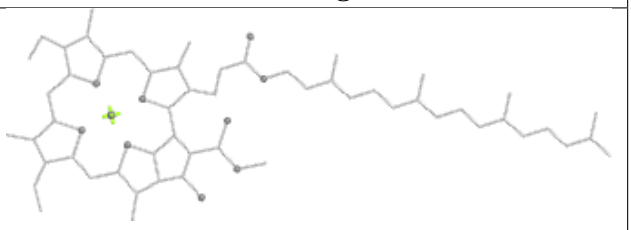
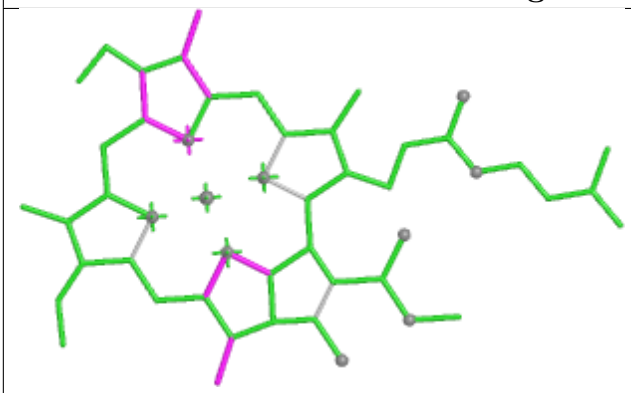


Rings

Ligand CLA d 502



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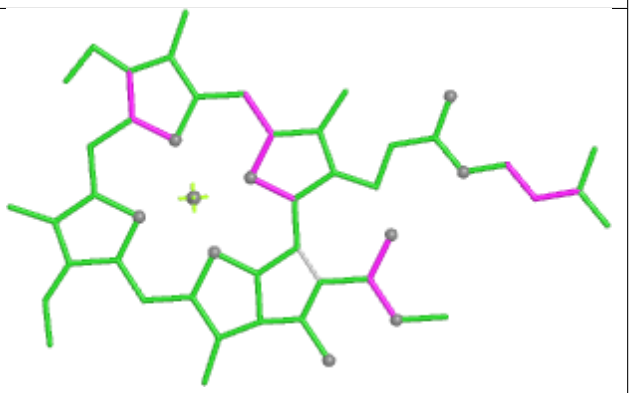

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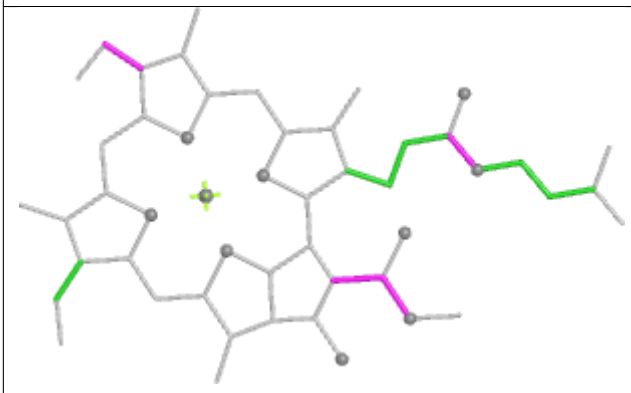

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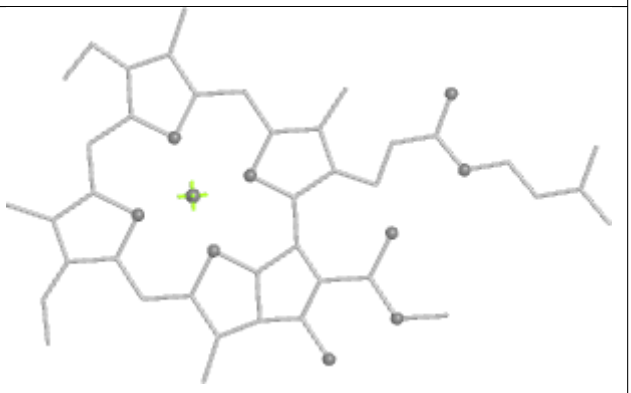
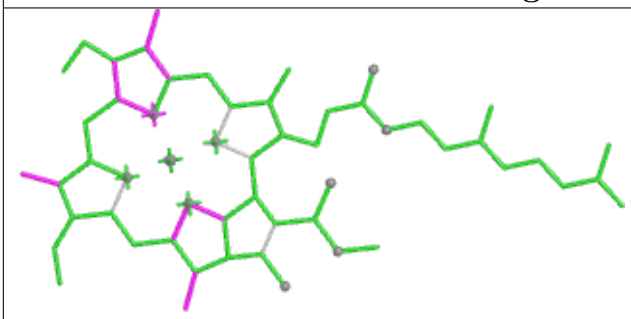


Rings

Ligand CLA f 1212



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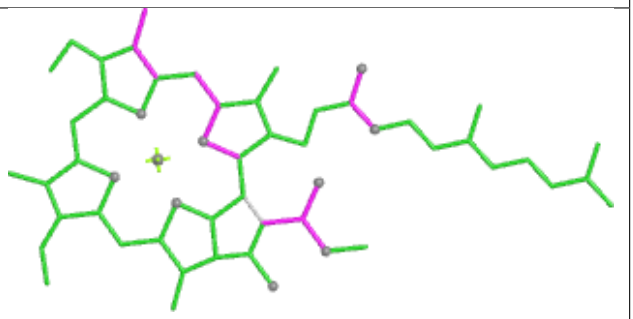
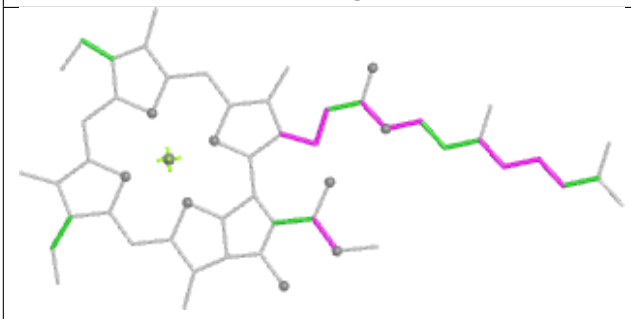


Bond angles



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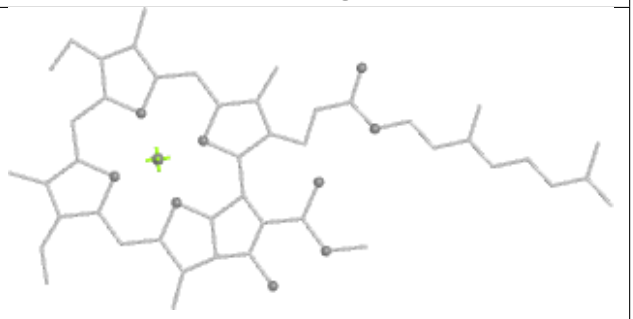
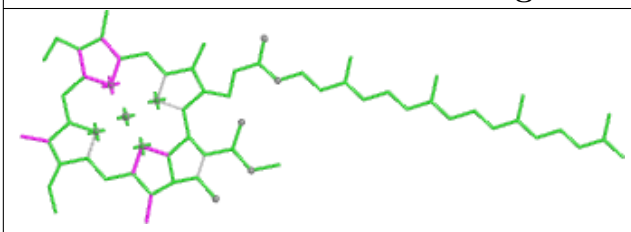


Rings

Ligand CLA B 1223



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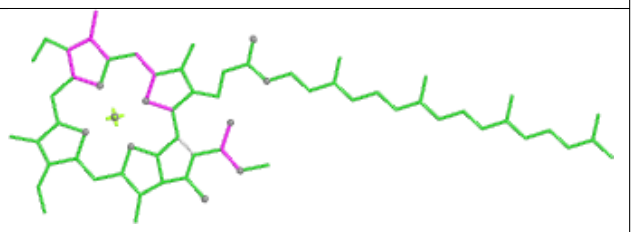
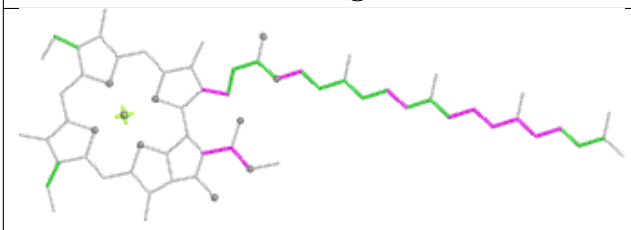


Bond angles



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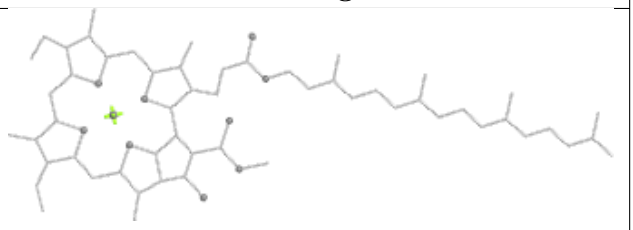
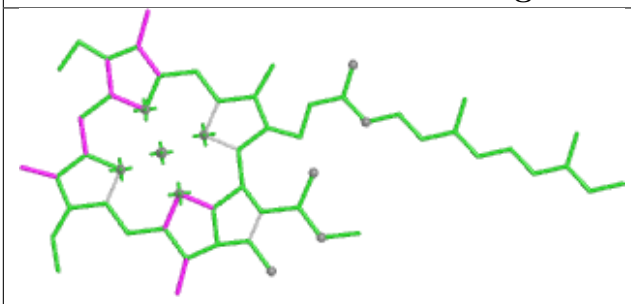


Rings

Ligand CLA A 1134



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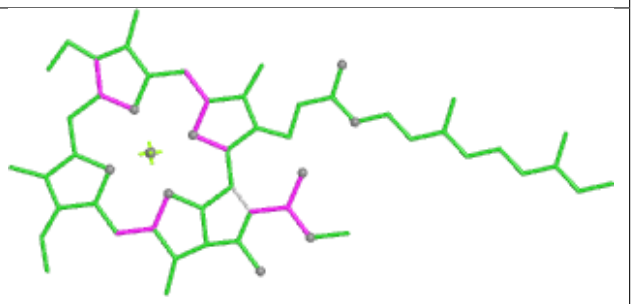
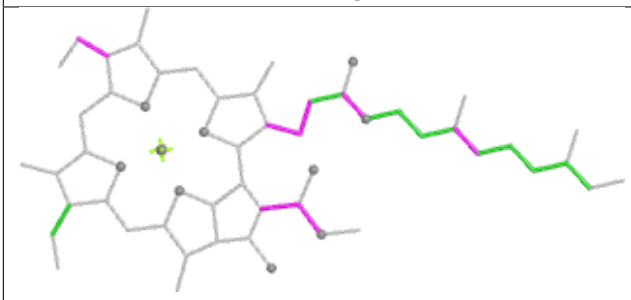
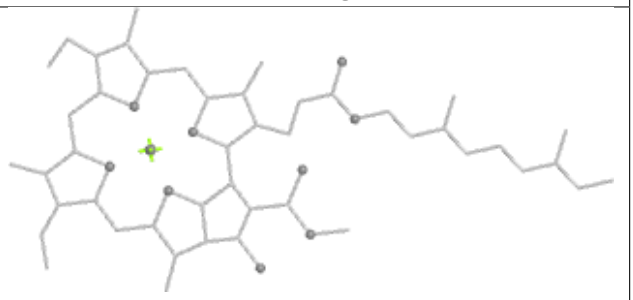


Bond angles

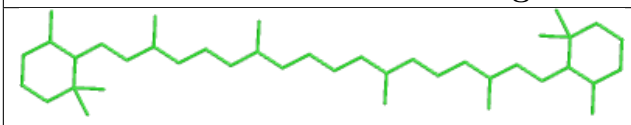


Torsions



Rings

Ligand BCR G 4011



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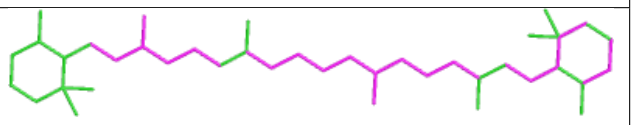
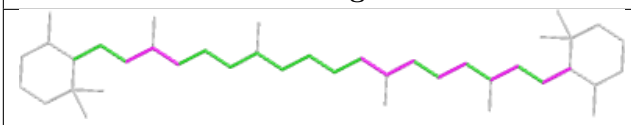
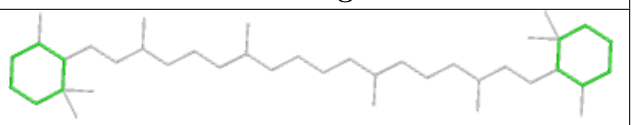


Bond angles



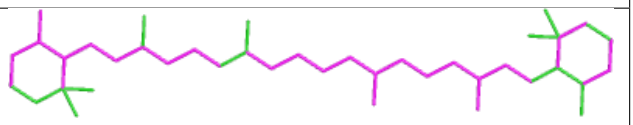
Torsions



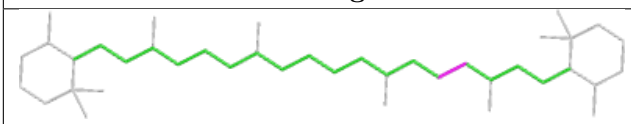
Rings

Ligand BCR H 4009

Bond lengths



Bond angles



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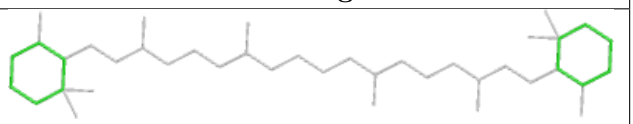
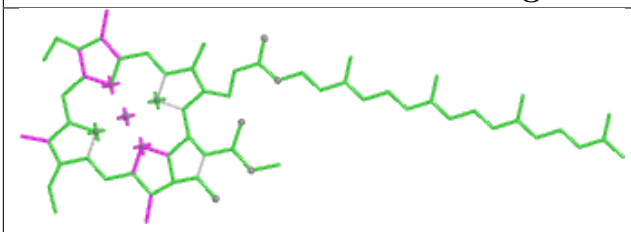


Rings

Ligand CLA f 1021



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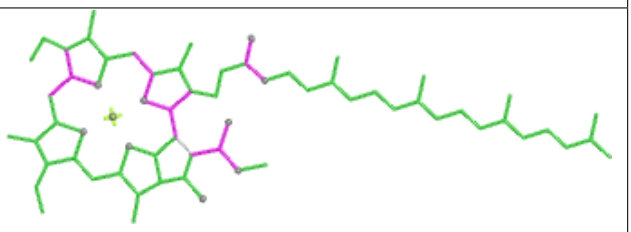
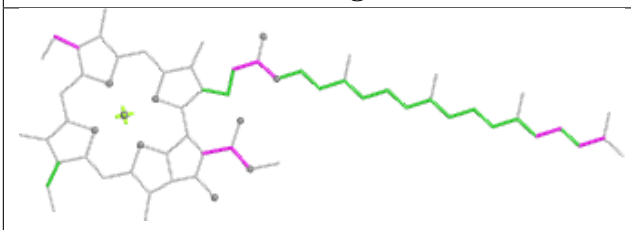


Bond angles



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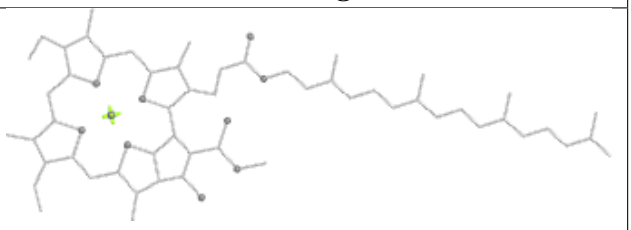
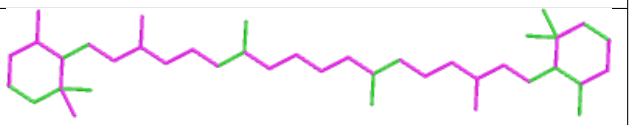


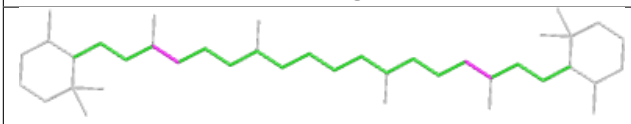
Rings

Ligand BCR f 4006

Bond lengths



Bond angles



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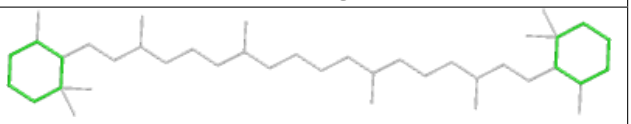
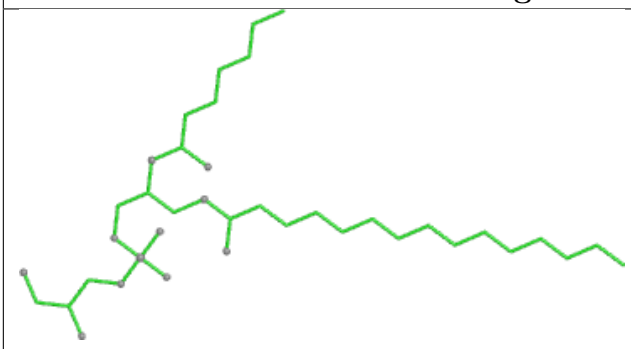
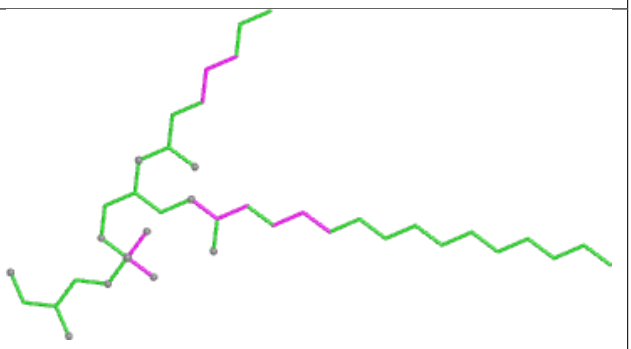


Rings

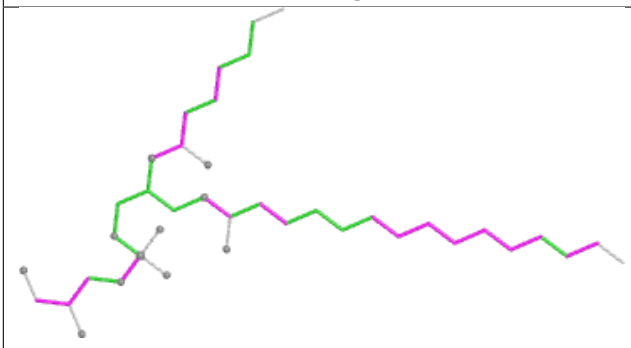
Ligand LHG B 1842



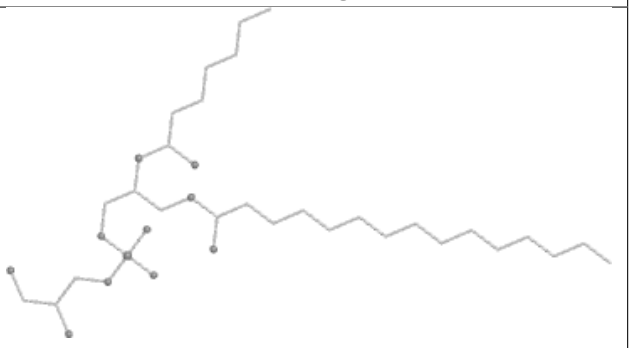
Bond lengths



Bond angles

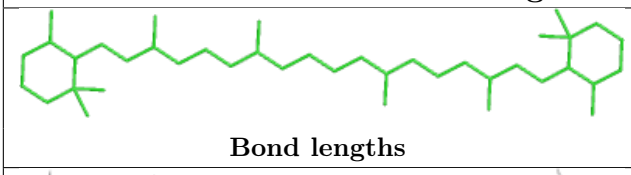


Torsions

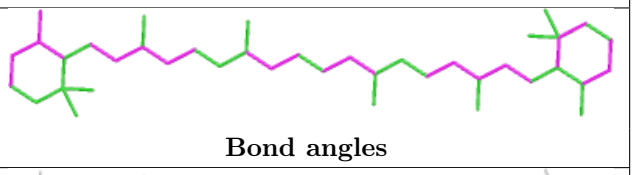


Rings

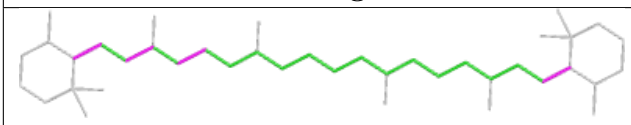
Ligand BCR 3 521



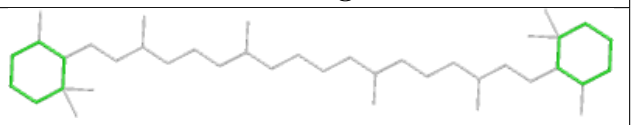
Bond lengths



Bond angles

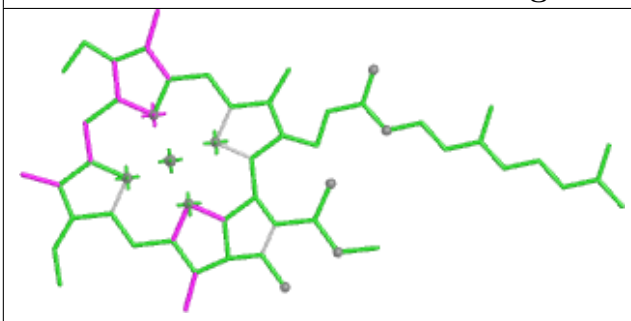


Torsions



Rings

Ligand CLA s 508



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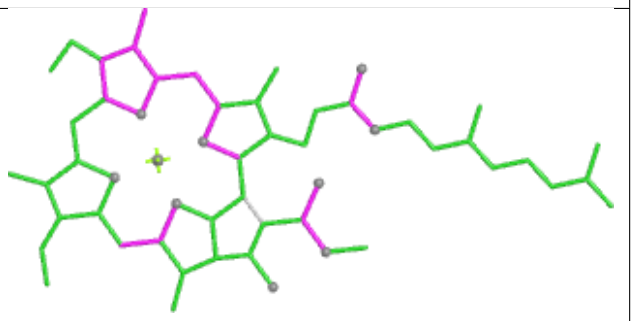

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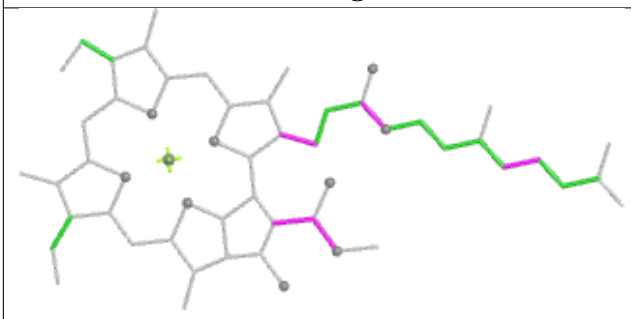

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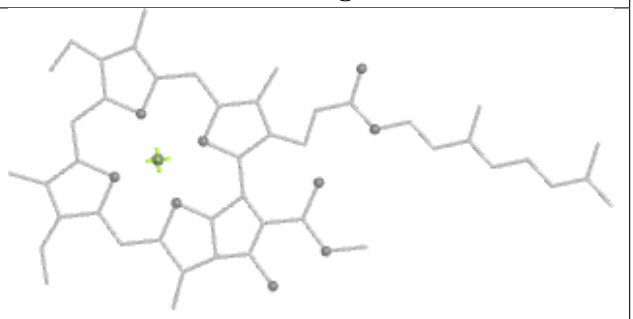
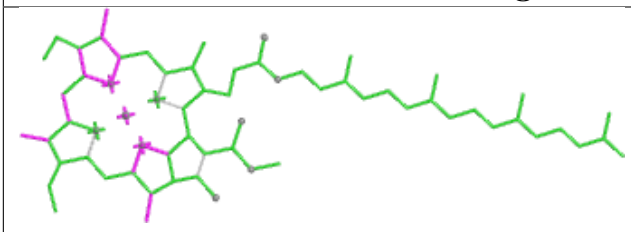


Rings

Ligand CLA H 1203



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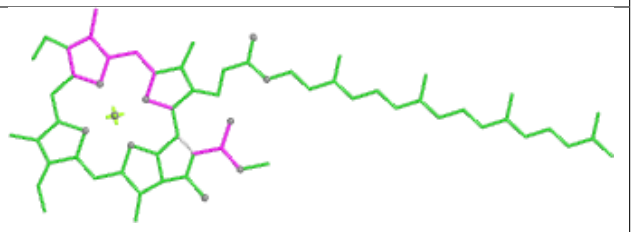

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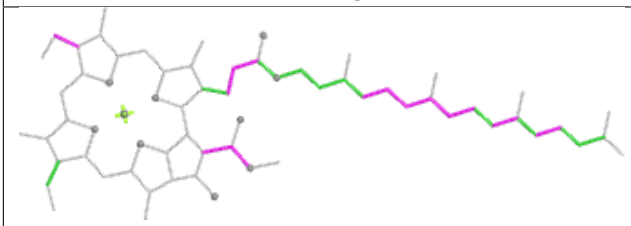

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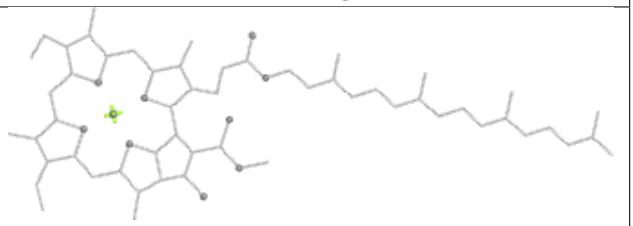

Rings

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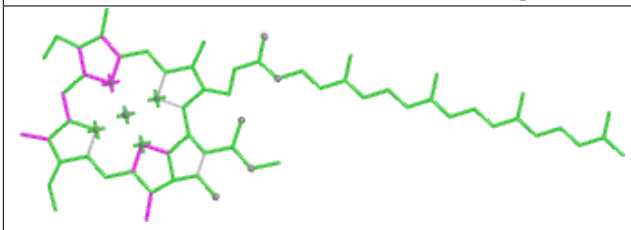

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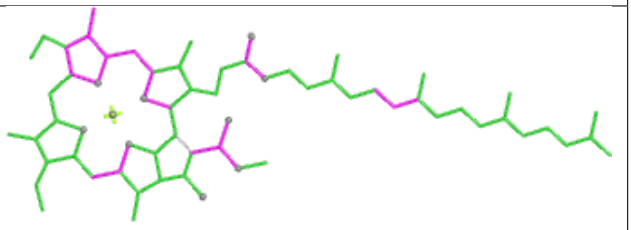
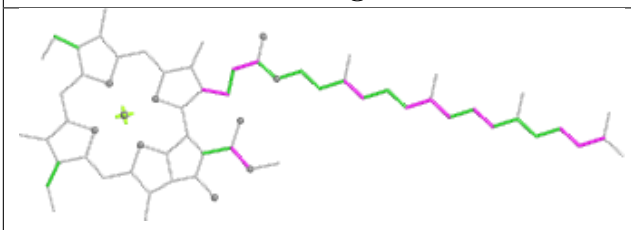


Bond angles



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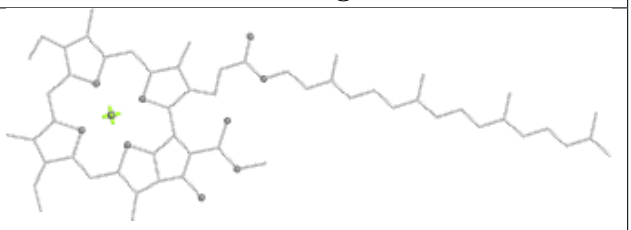
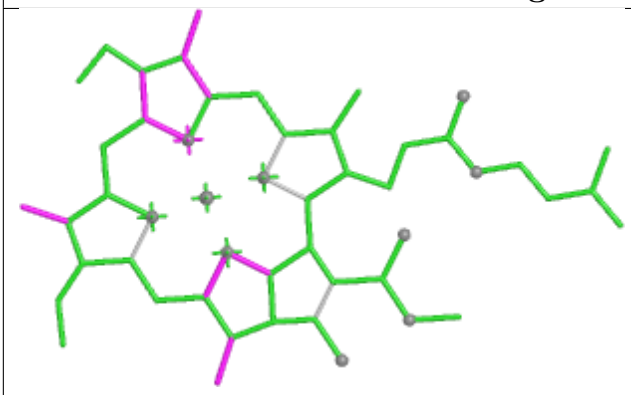


Rings

Ligand CLA a 506



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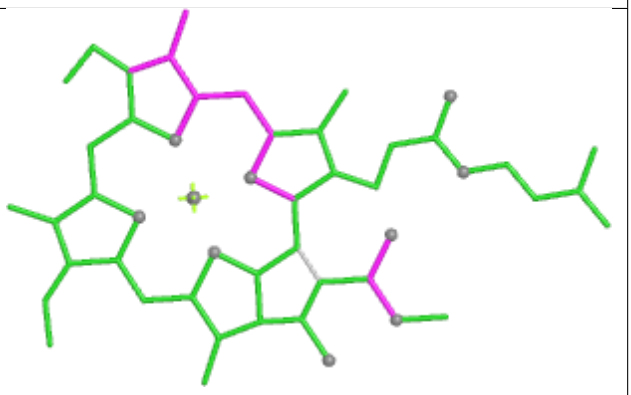

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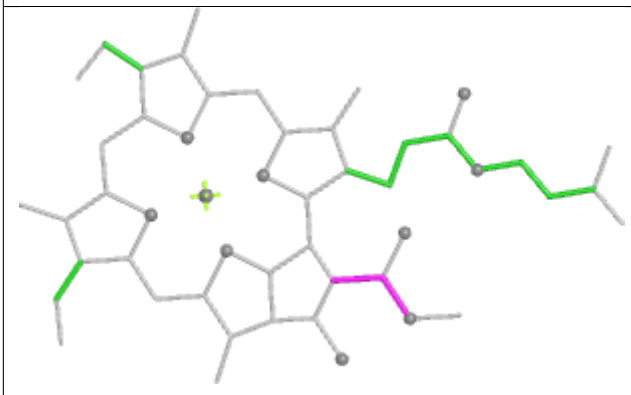

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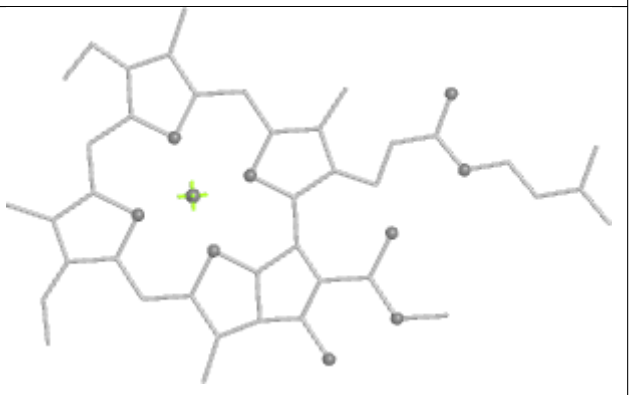

Rings

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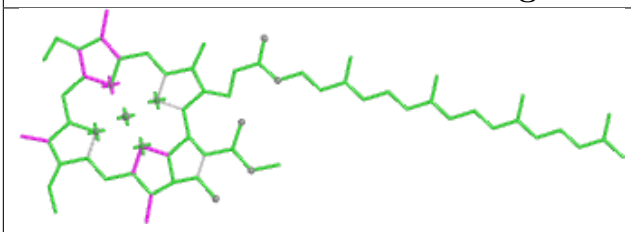

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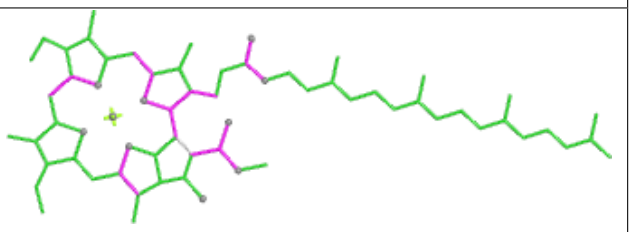

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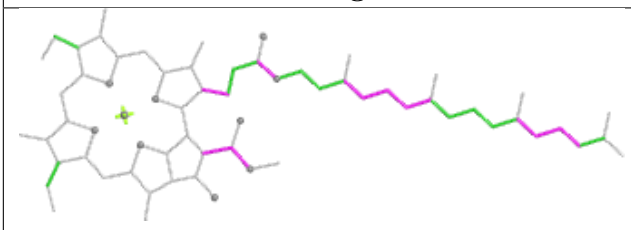

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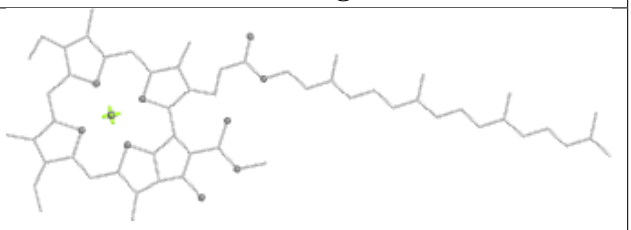
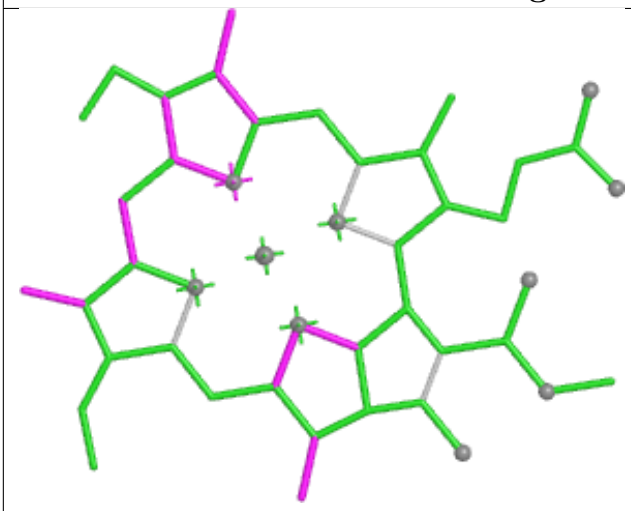


Rings

Ligand CLA c 513



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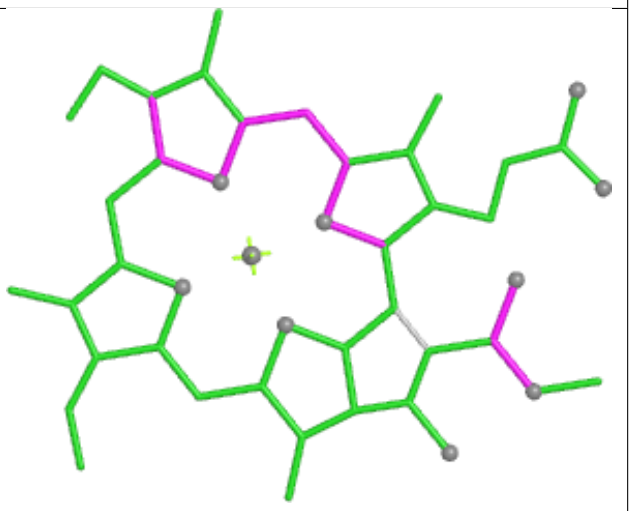
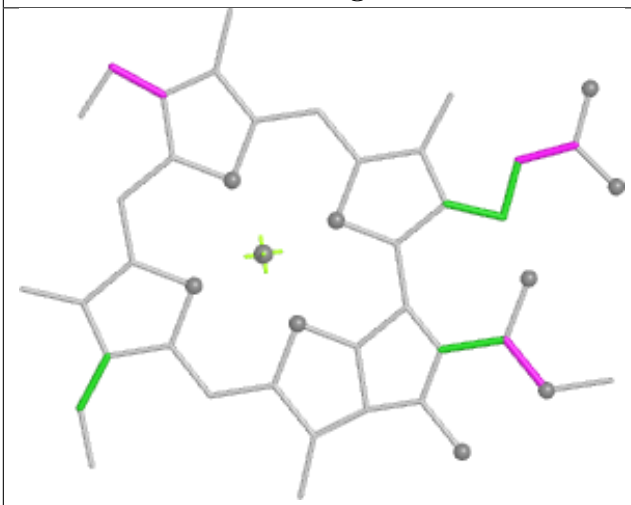


Bond angles



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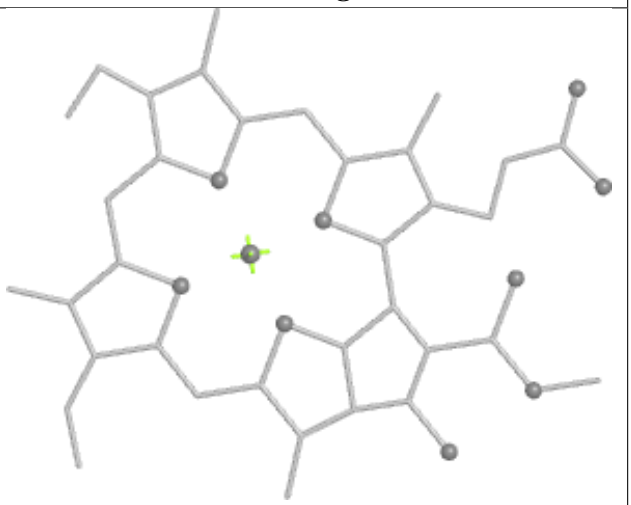
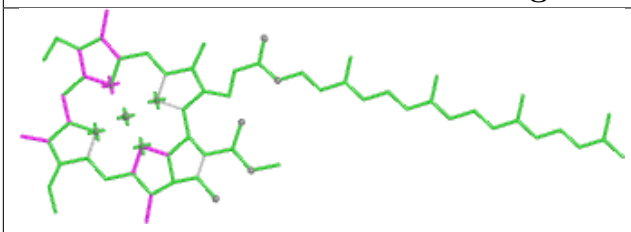


Rings

Ligand CLA r 501



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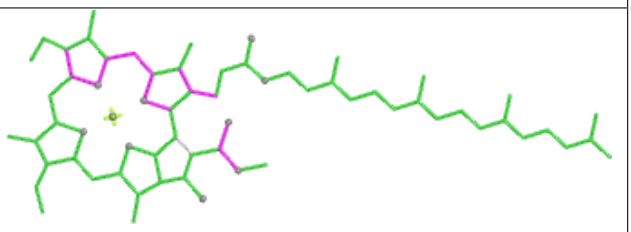

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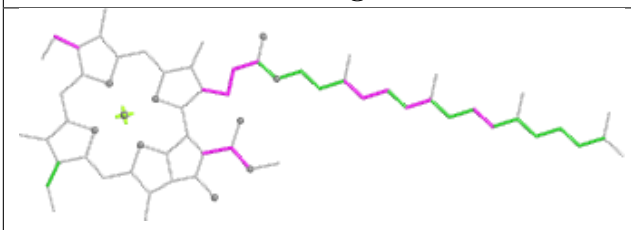

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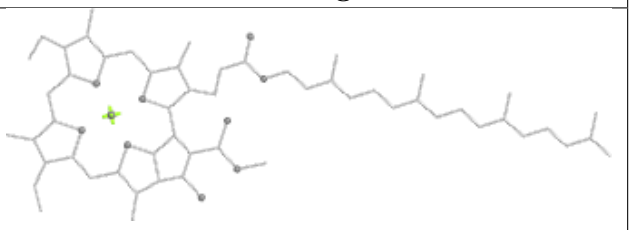
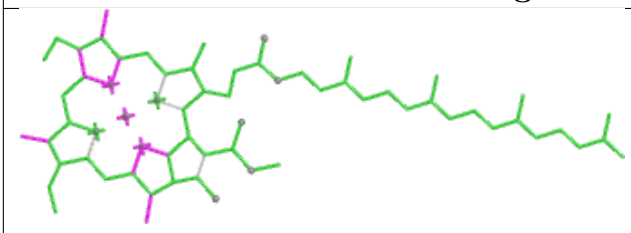


Rings

Ligand CLA G 1128



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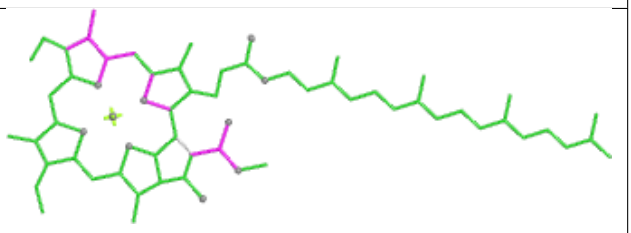
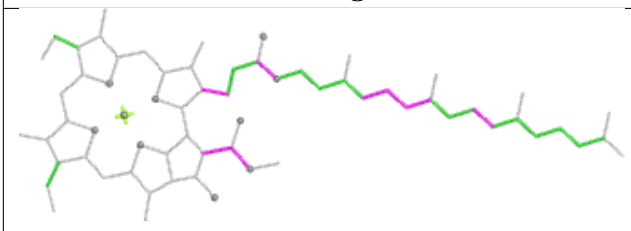


Bond angles



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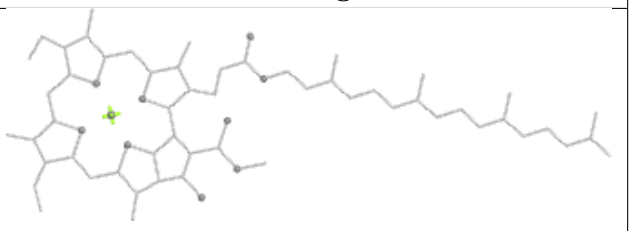
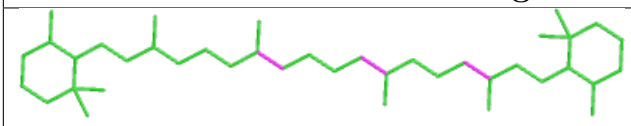


Rings

Ligand BCR H 4010



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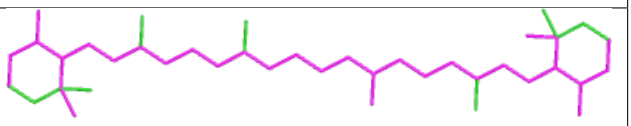

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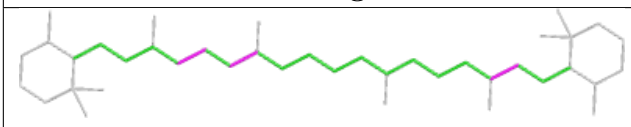

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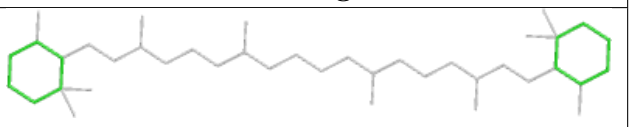
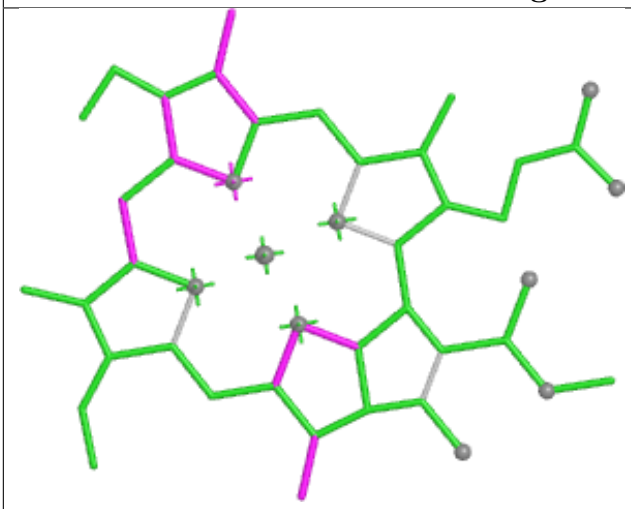


Rings

Ligand CLA t 506



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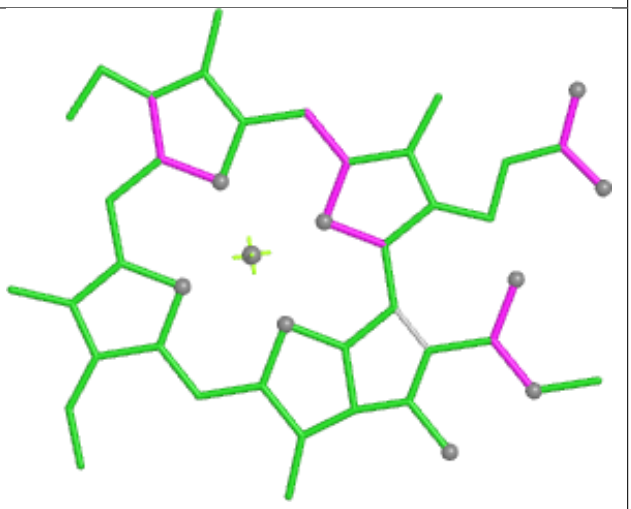
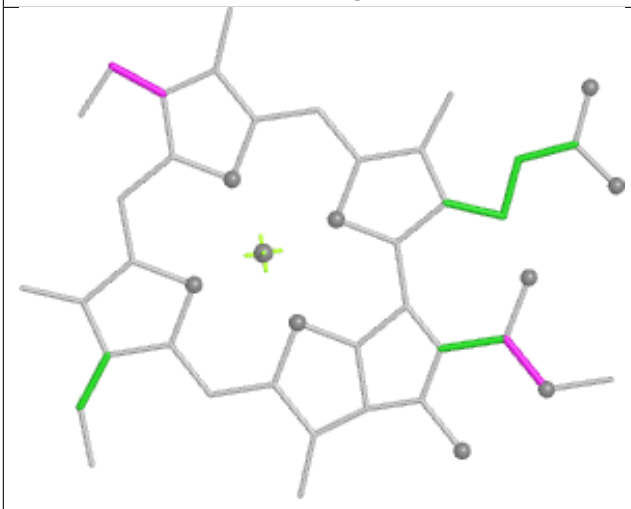


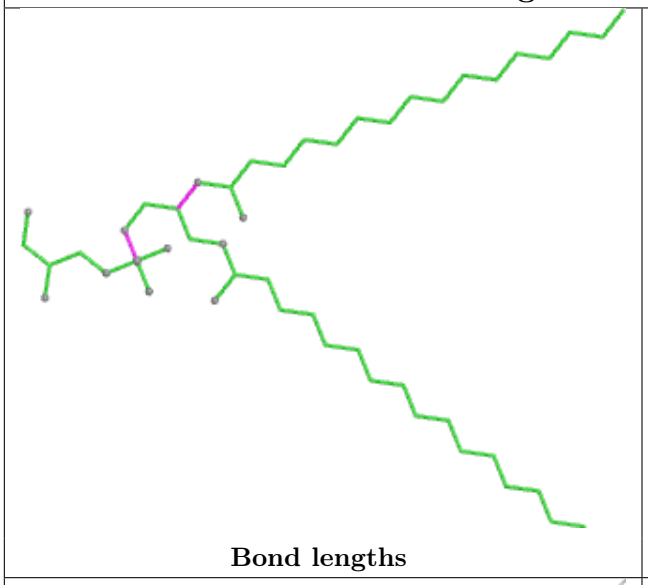
Bond angles



Torsions

Rings

Ligand LHG n 5221



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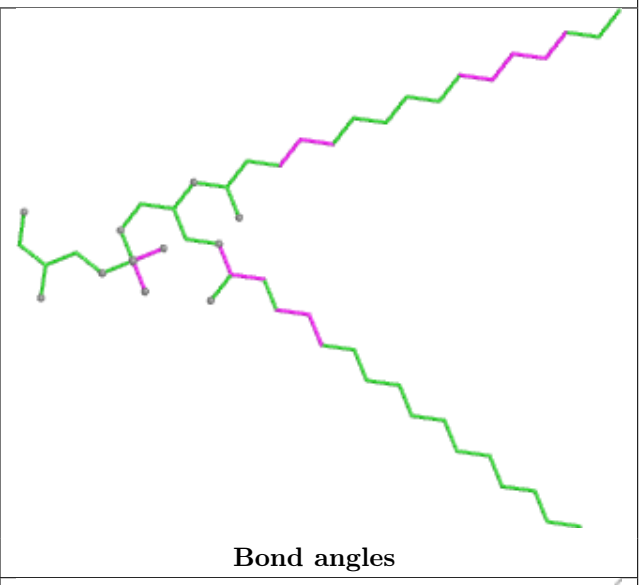
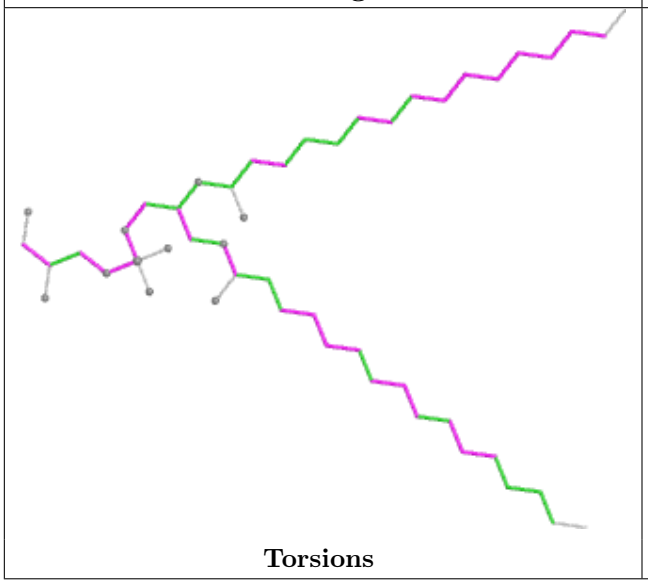
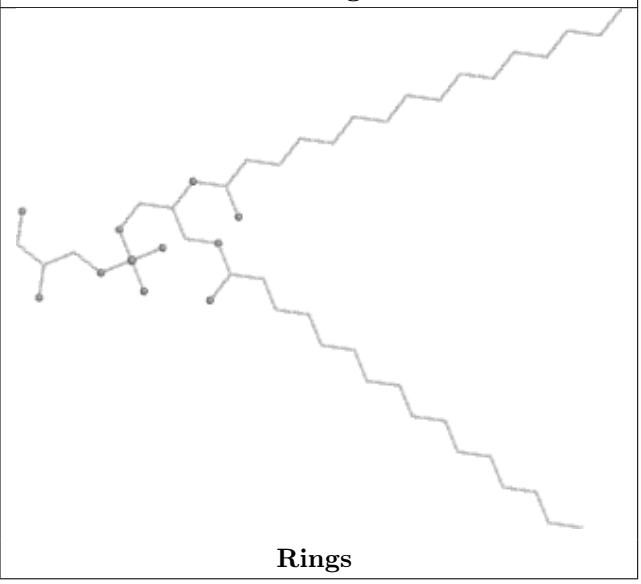


Bond angles

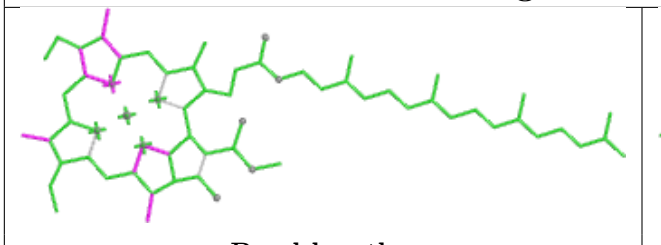


Torsions



Rings

Ligand CLA B 1210



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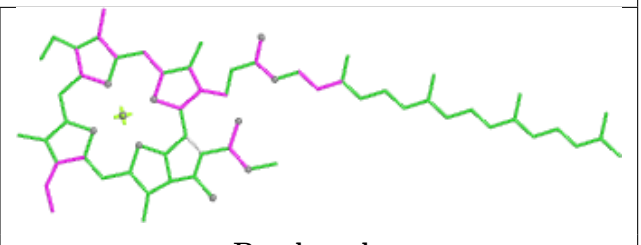
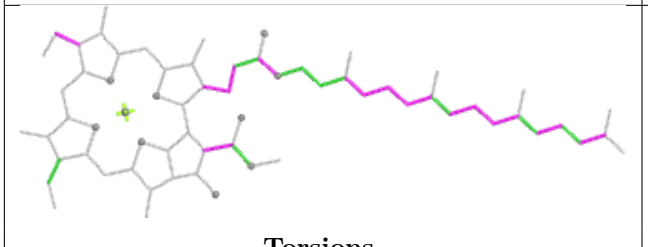


Bond angles



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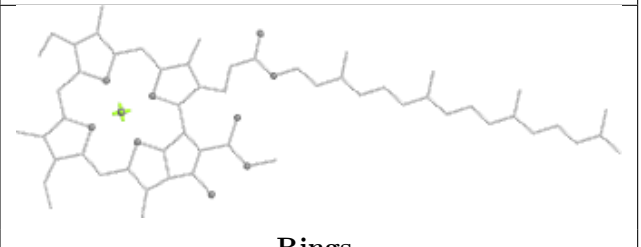
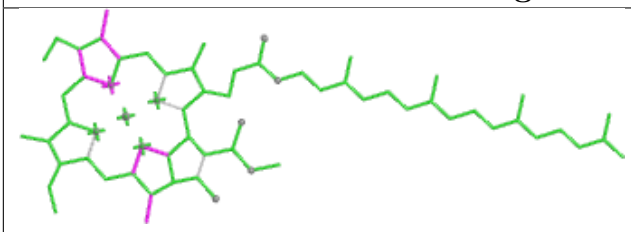


Rings

Ligand CLA H 1219



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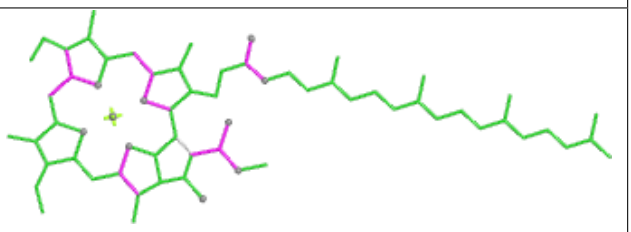
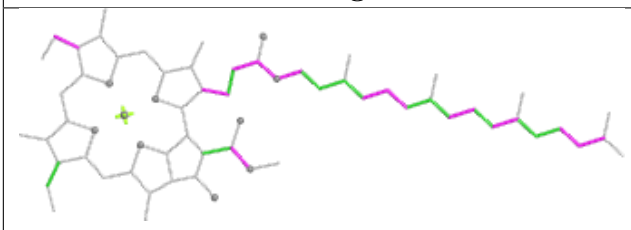
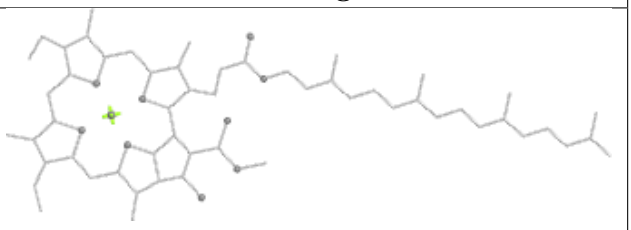


Bond angles

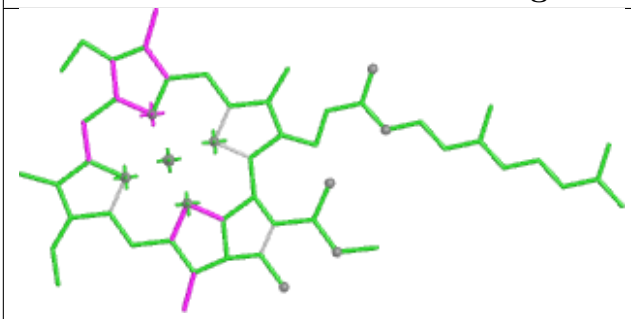


Torsions



Rings

Ligand CLA t 518



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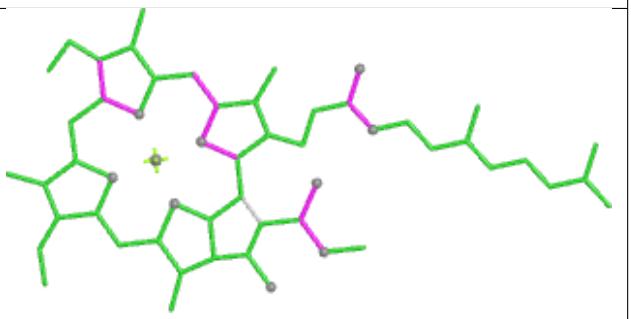

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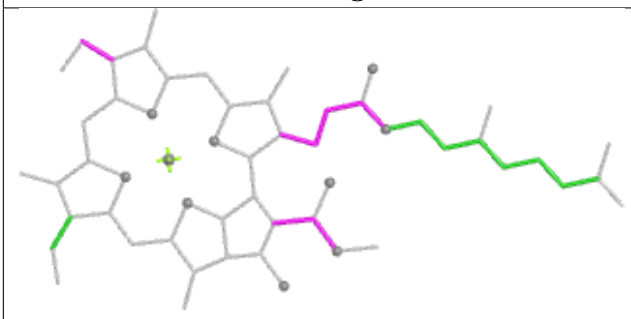

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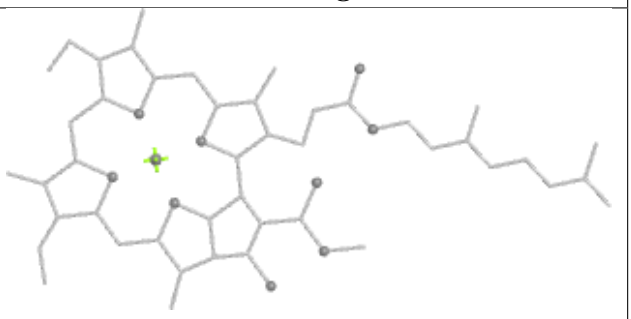
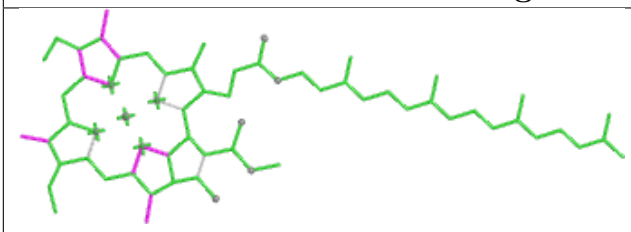


Rings

Ligand CLA A 1103



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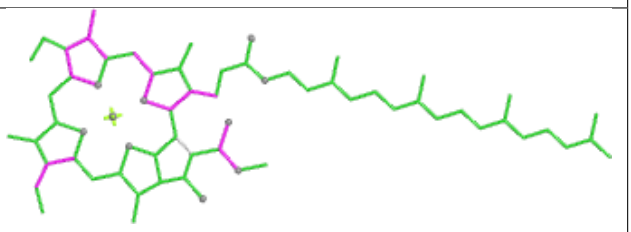

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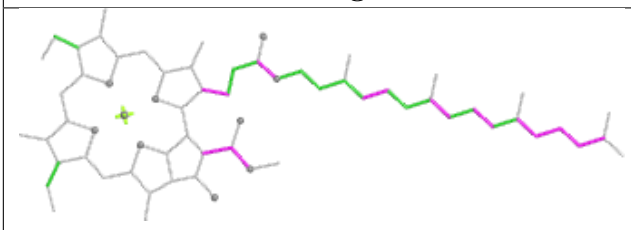

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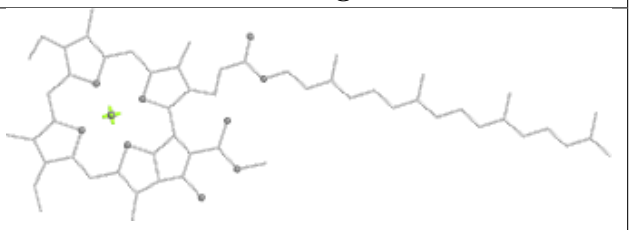

Rings

Ligand BCR 5 524

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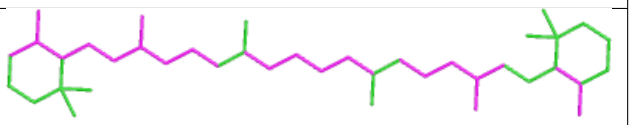
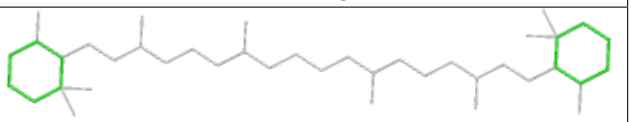


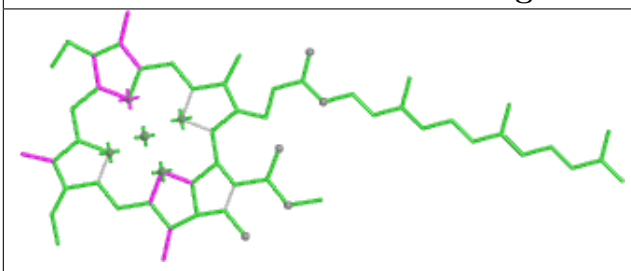
Bond angles

Torsions



Rings

Ligand CLA B 1224



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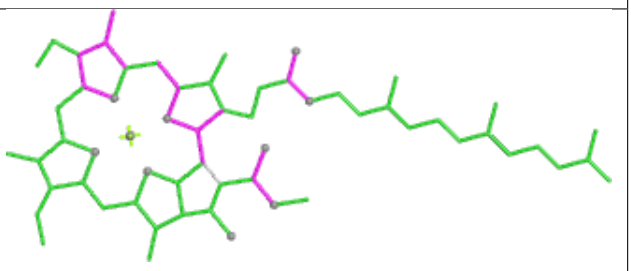

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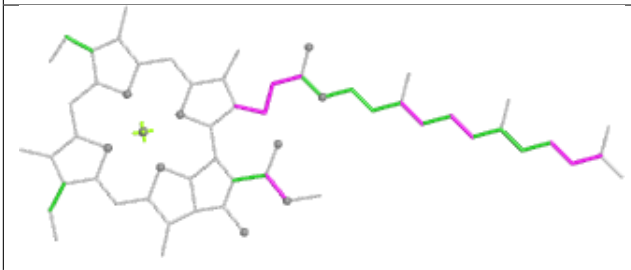

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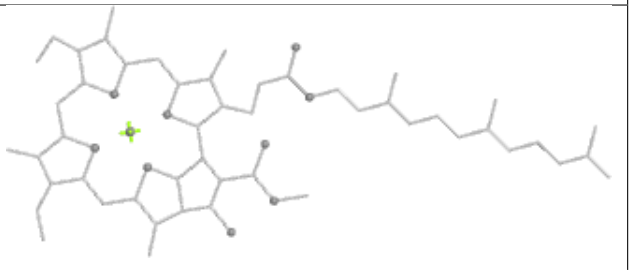
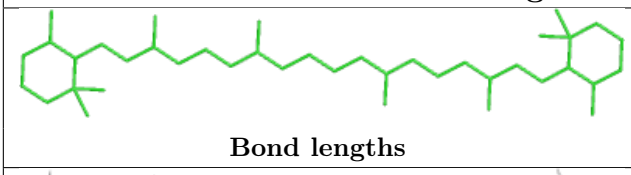


Rings

Ligand BCR 2 523



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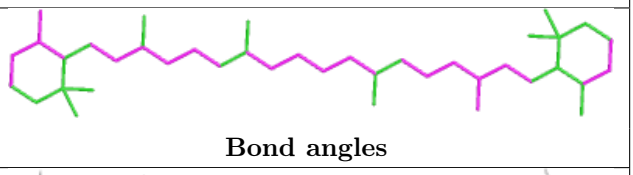

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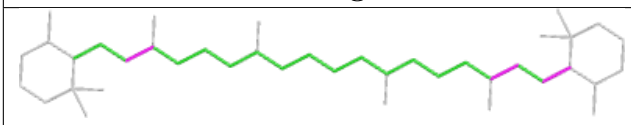

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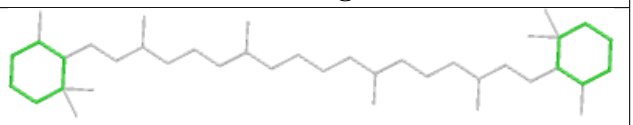
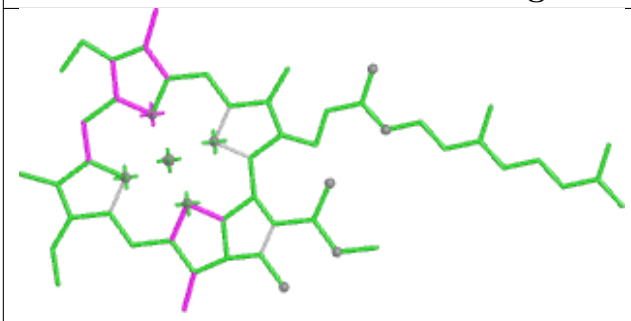


Rings

Ligand CLA q 511



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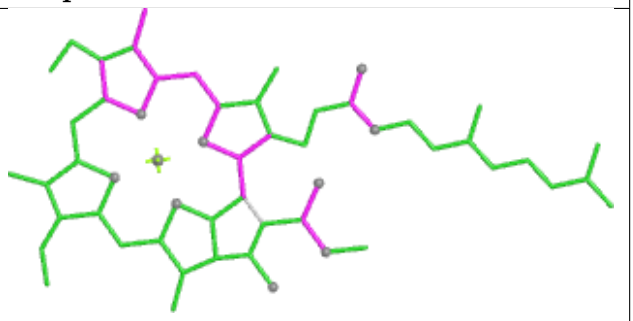

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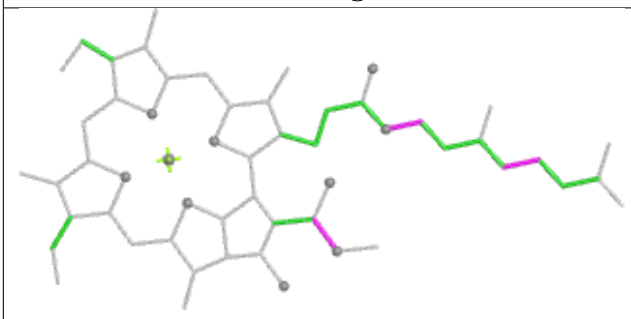

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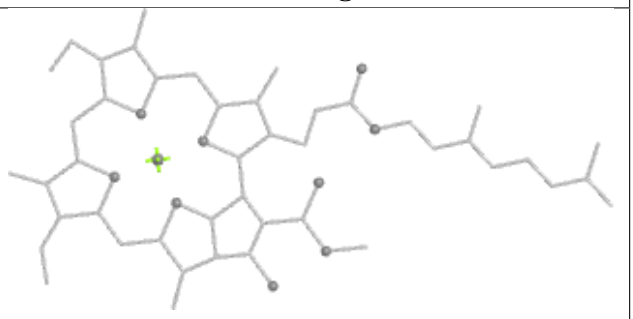
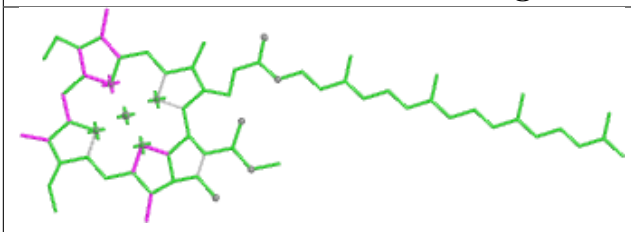


Rings

Ligand CLA G 1130



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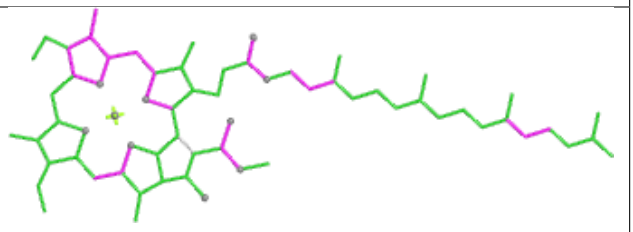

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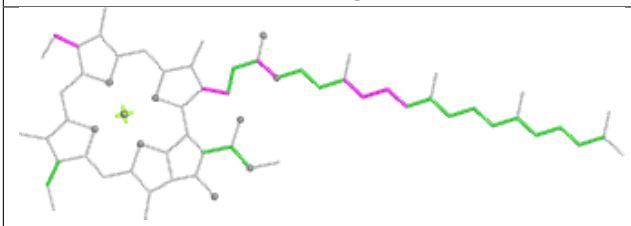

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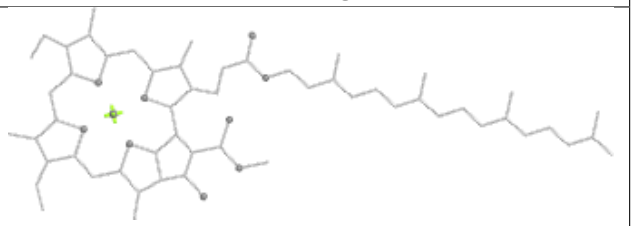
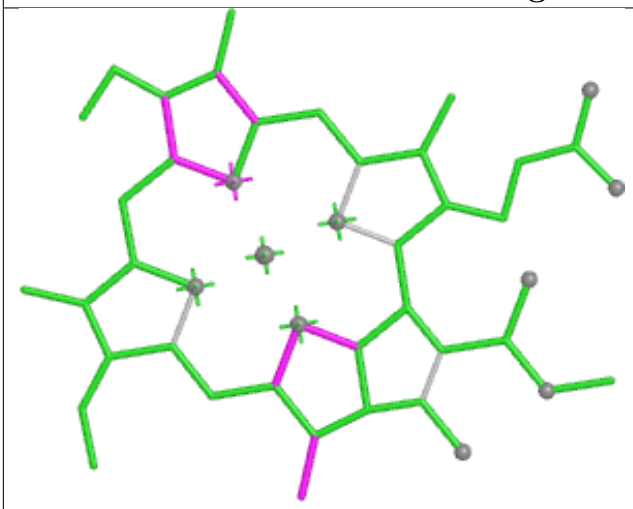


Rings

Ligand CLA 5 507



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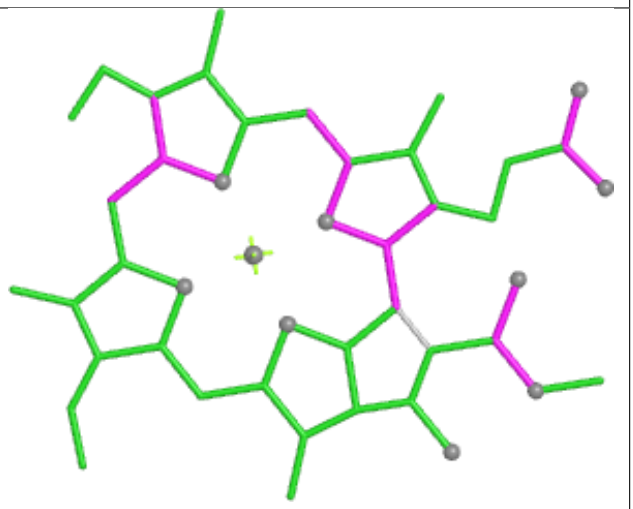

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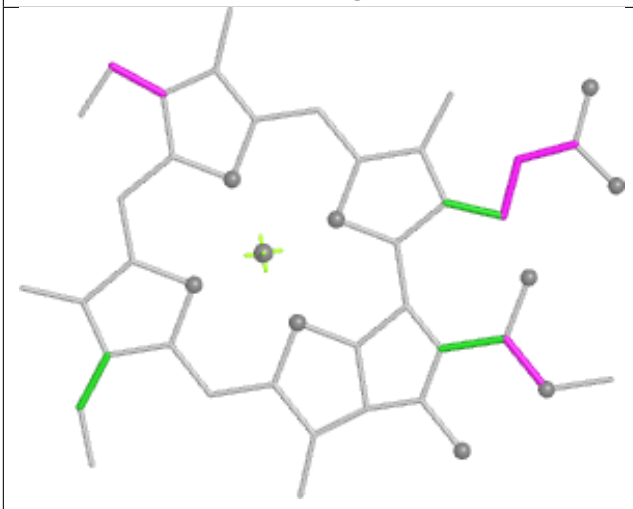
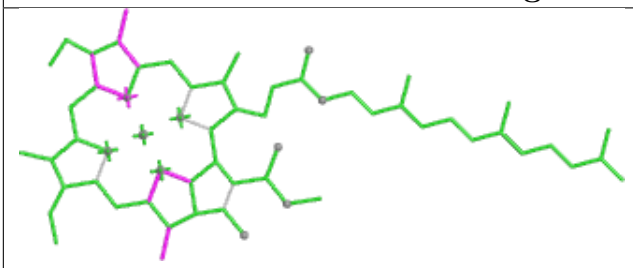


Torsions

Rings

Ligand CLA Y 507



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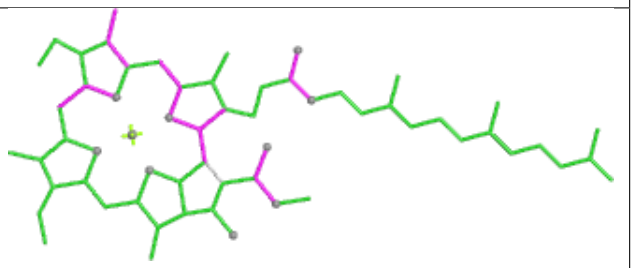

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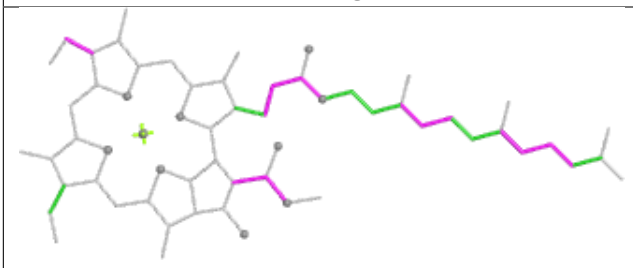

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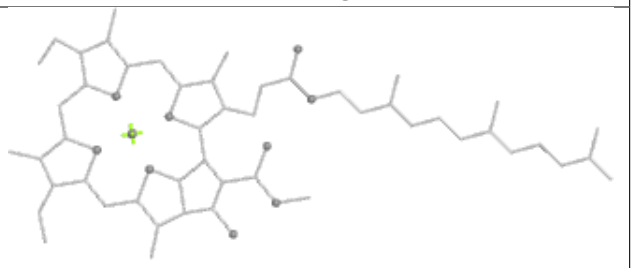
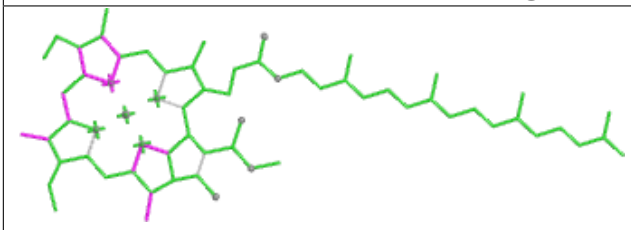


Rings

Ligand CLA f 1202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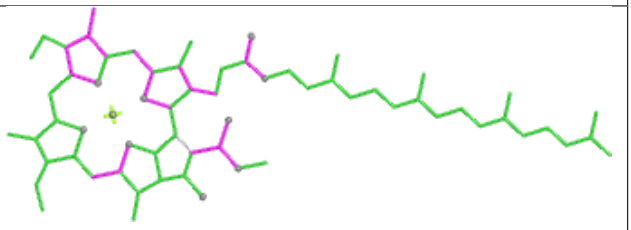
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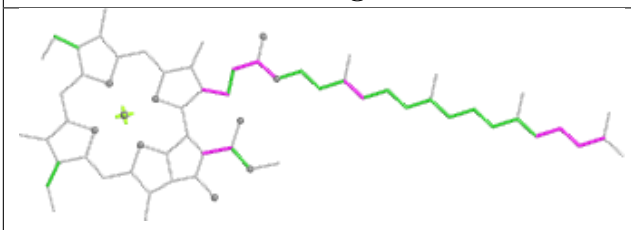
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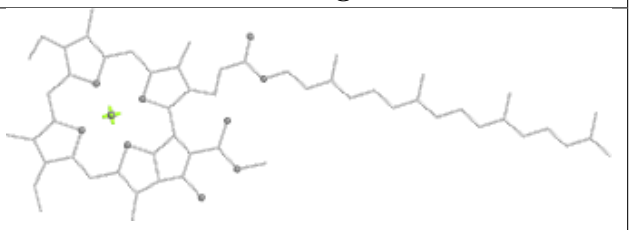
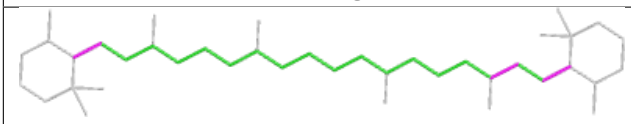

Rings

Ligand BCR 1 523

Bond lengths

Bond angles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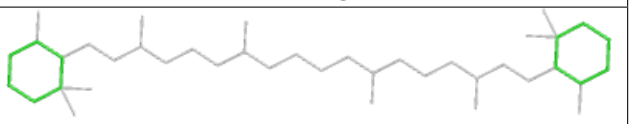
Rings

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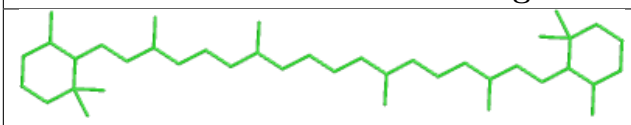
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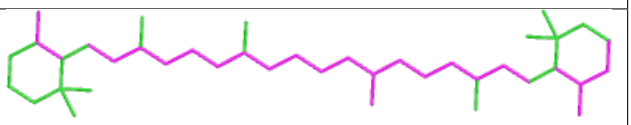
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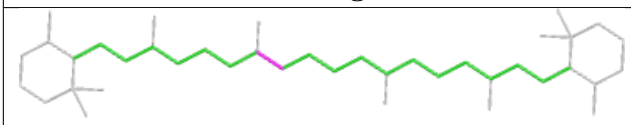
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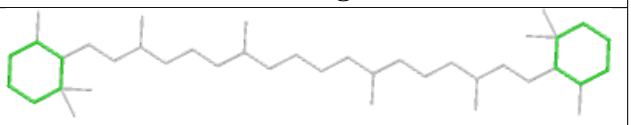
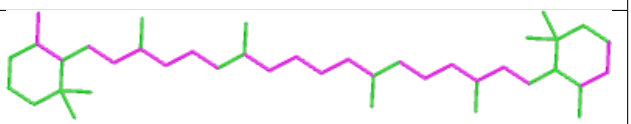

Rings

Ligand BCR b 523

Bond lengths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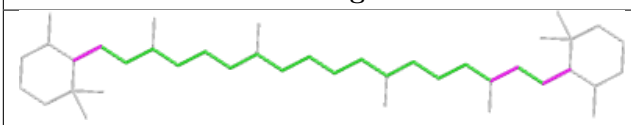
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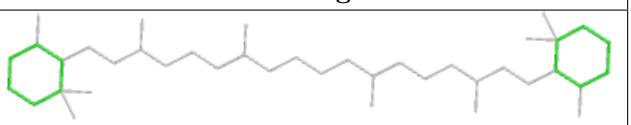
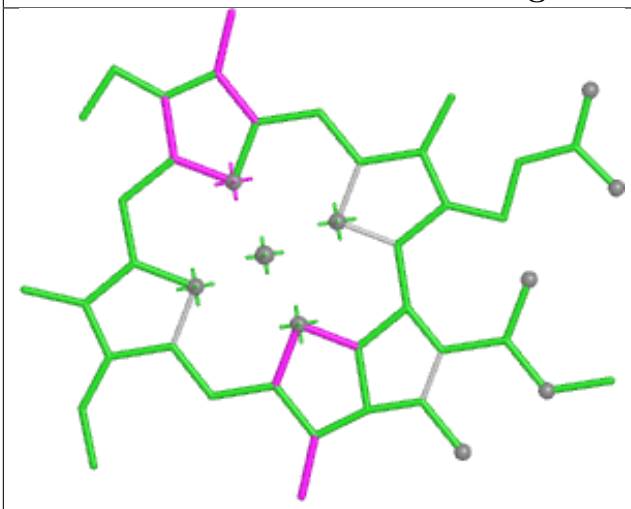

Rings

Ligand CLA 4 512



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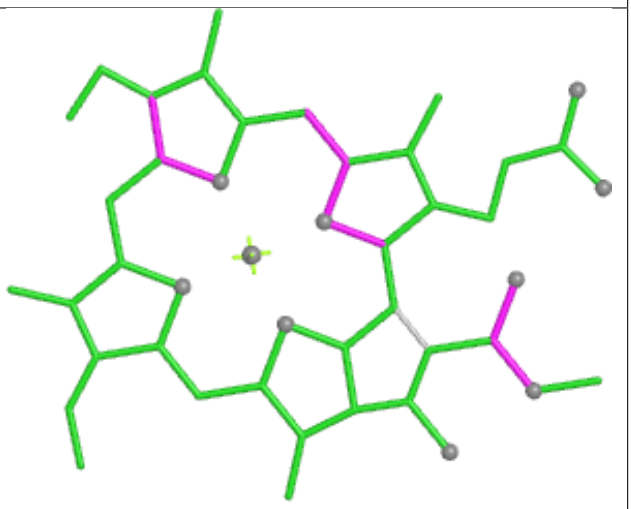
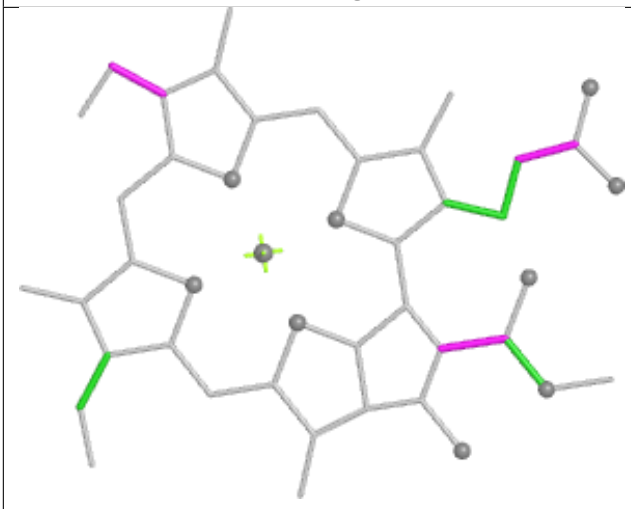


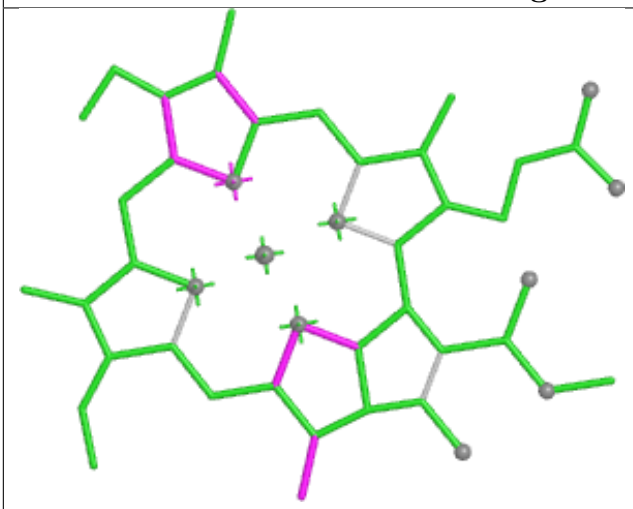
Bond angles



Torsions

Rings

Ligand CLA t 507



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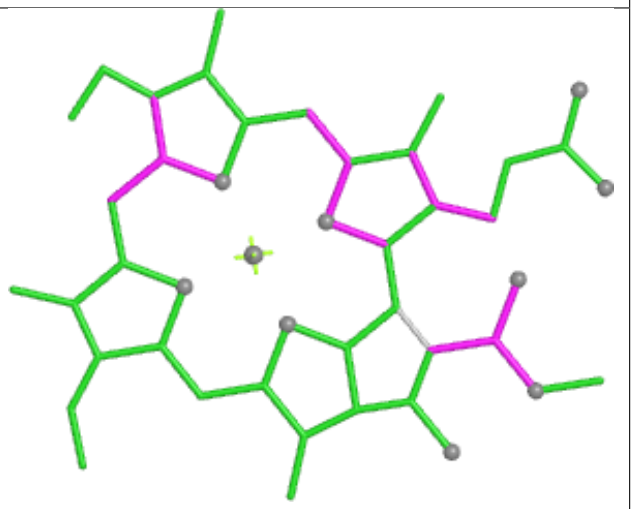
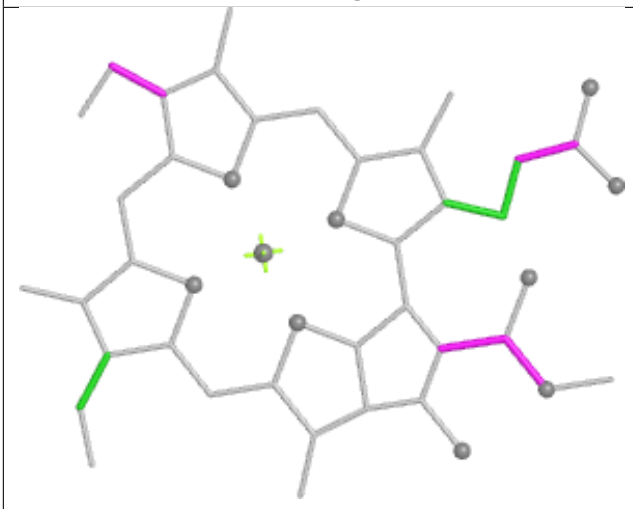


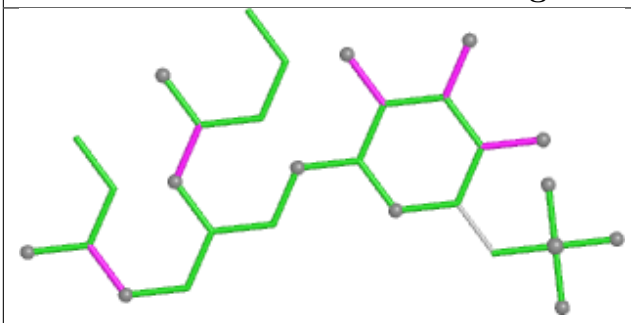
Bond angles



Torsions

Rings

Ligand SQD c 822



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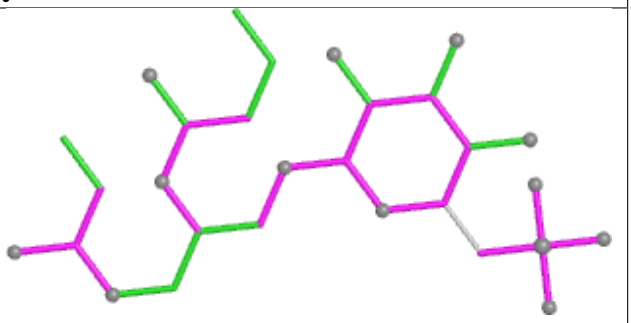

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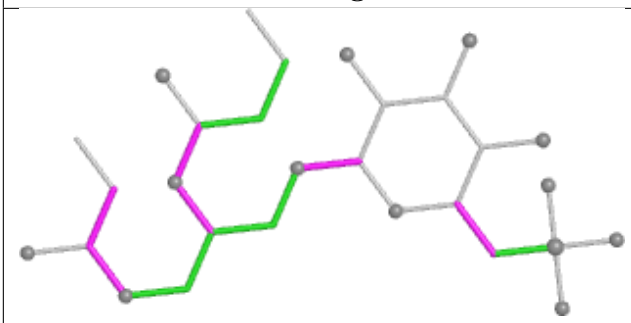

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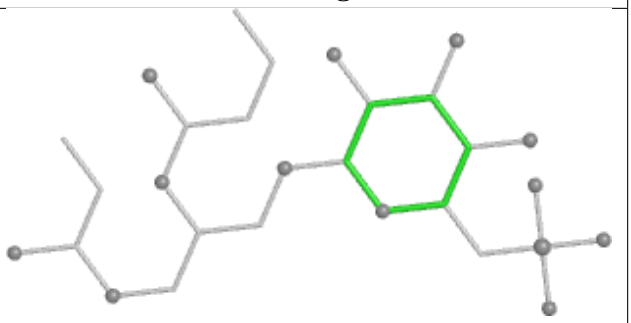

Rings

Ligand BCR d 524

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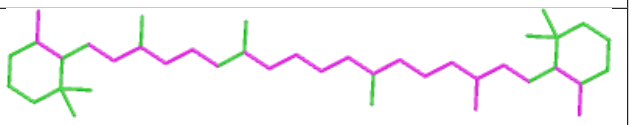

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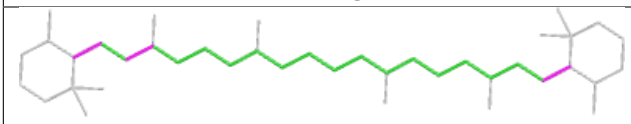

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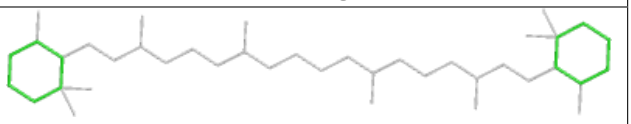
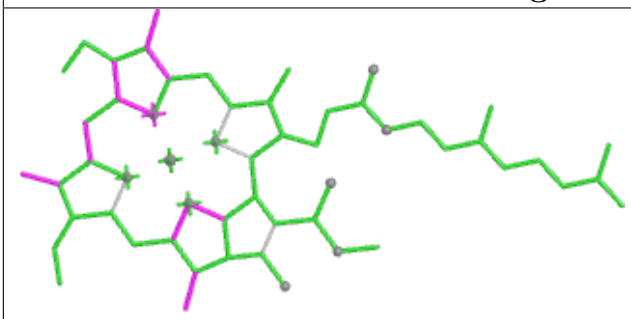


Rings

Ligand CLA s 518



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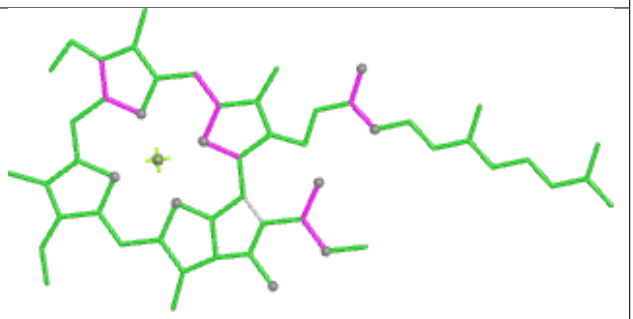

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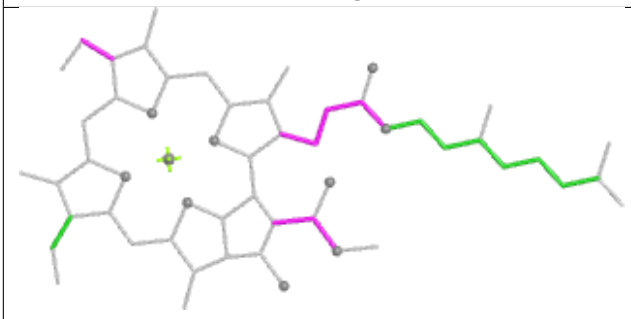

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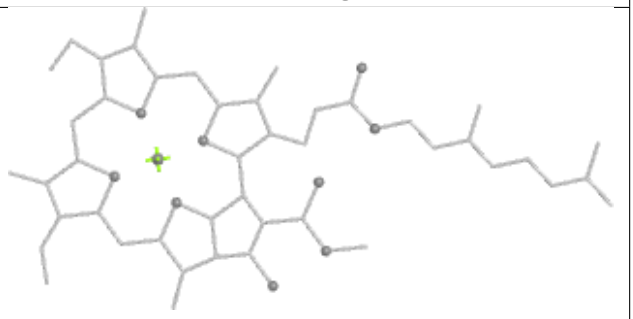
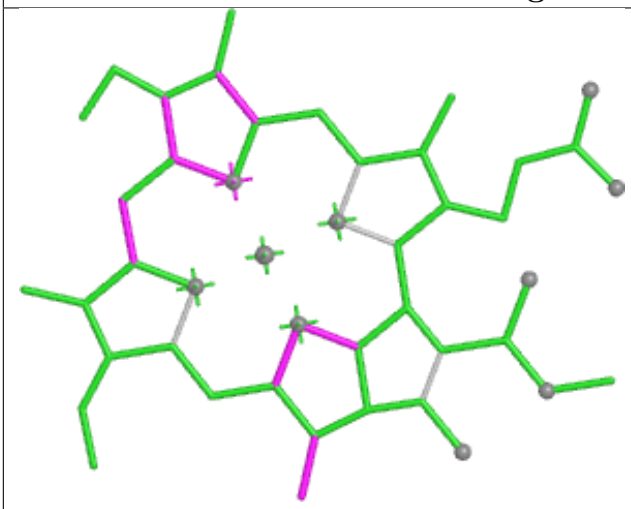


Rings

Ligand CLA b 516



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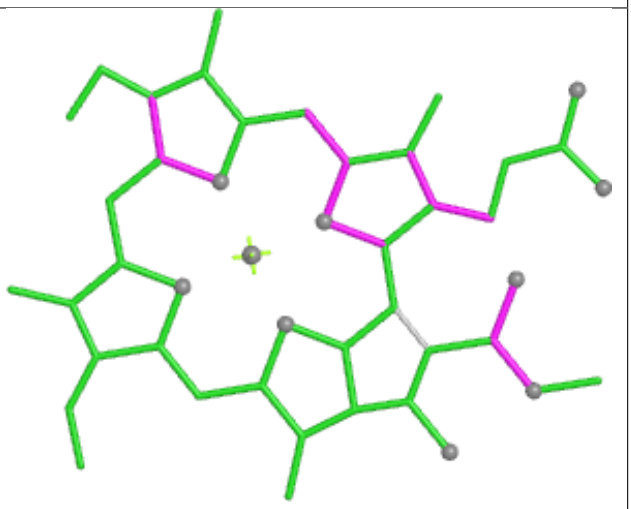

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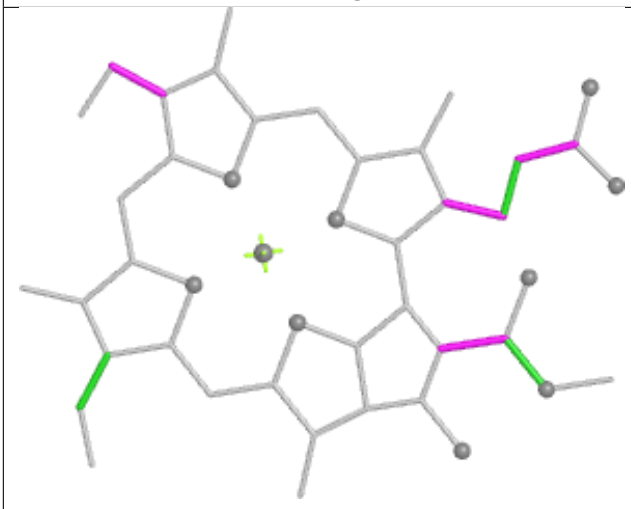
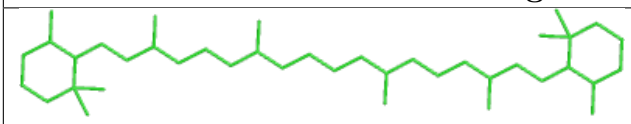


Torsions

Rings

Ligand BCR v 523



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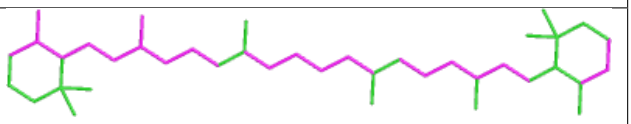

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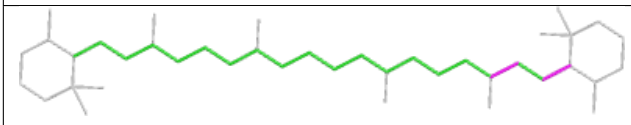

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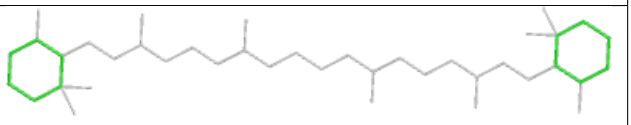
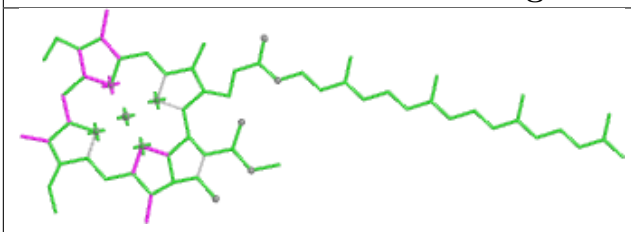


Rings

Ligand CLA Z 509



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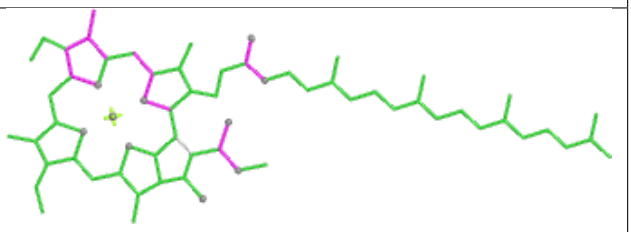

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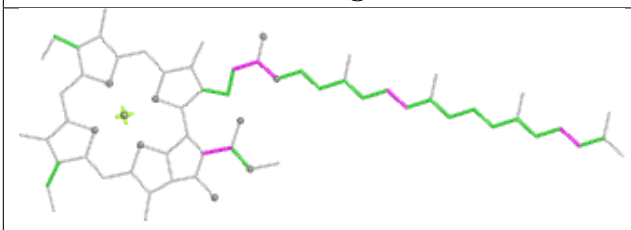

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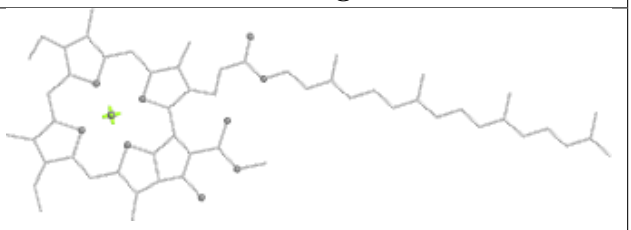
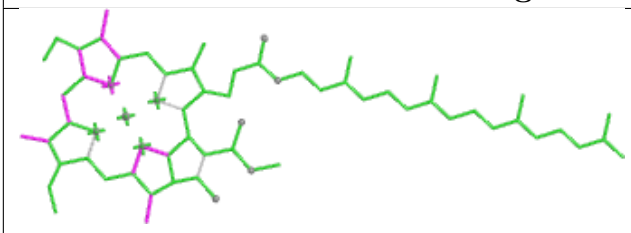


Rings

Ligand CLA A 1126



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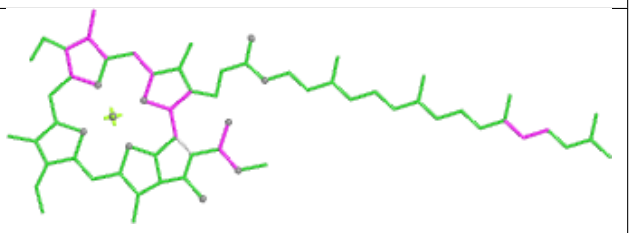

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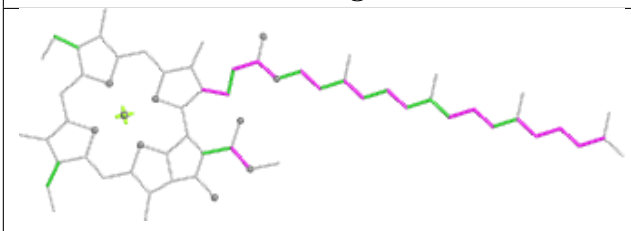

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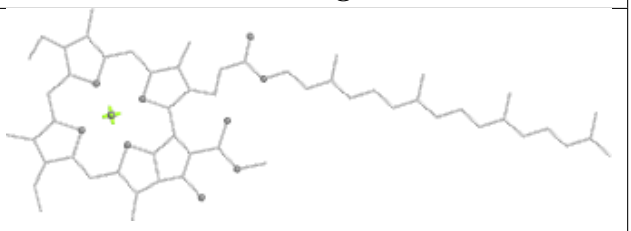

Rings

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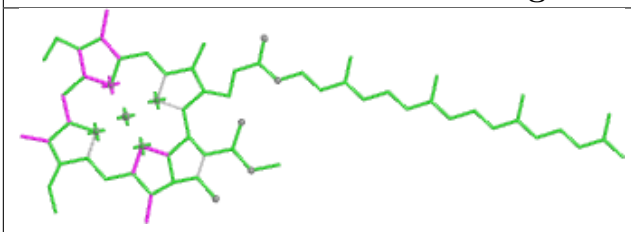

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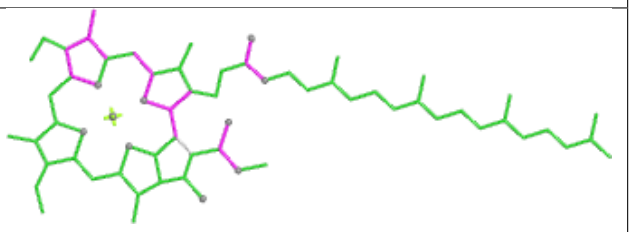

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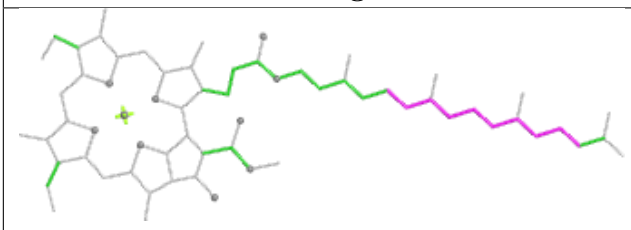

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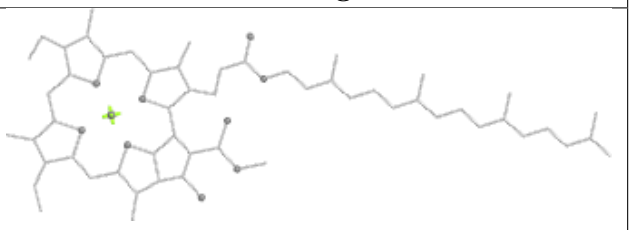

Rings

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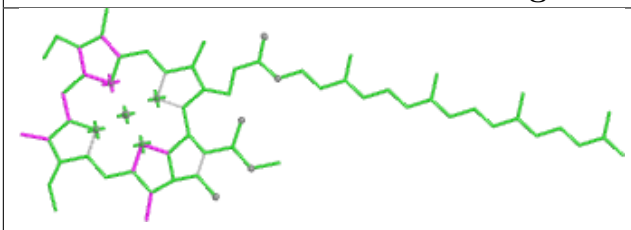

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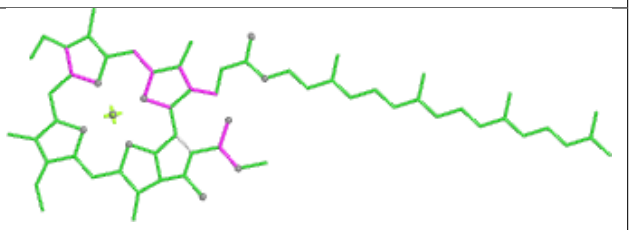

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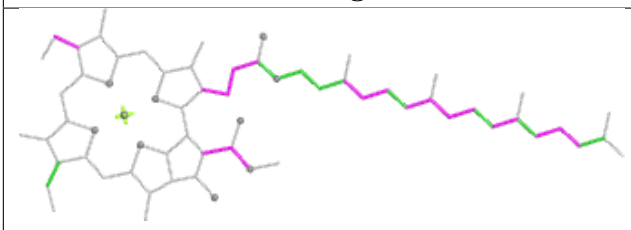

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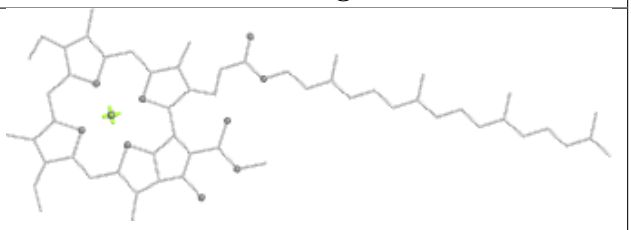

Rings

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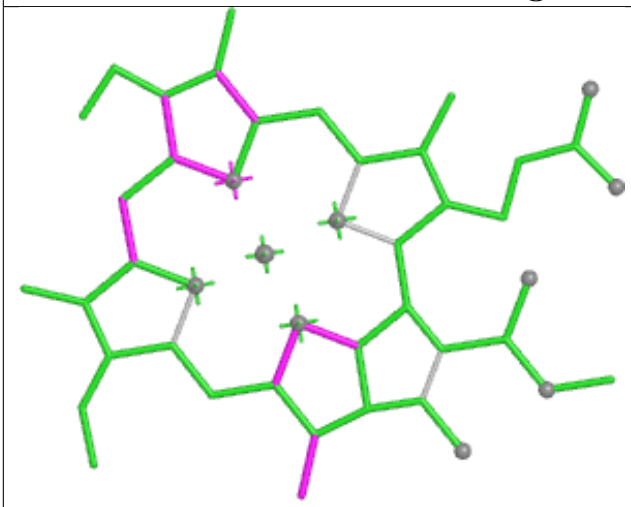

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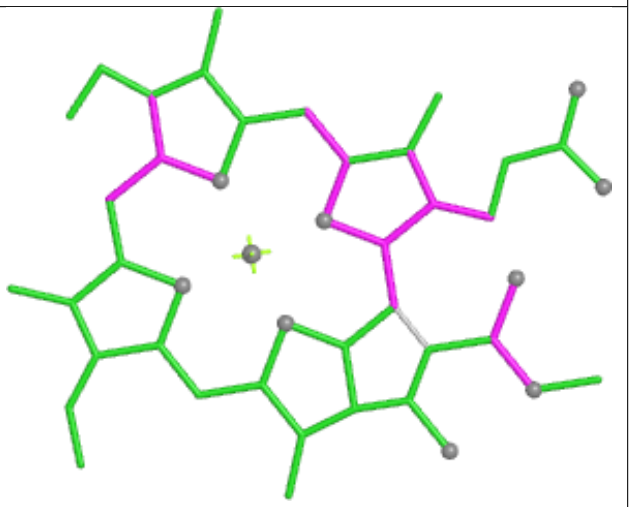

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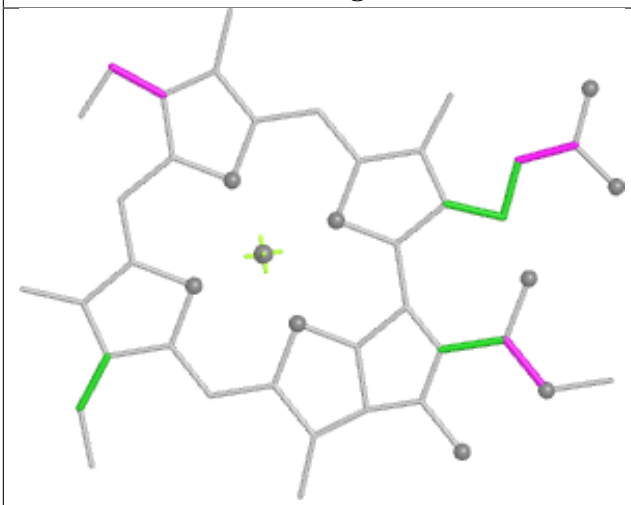

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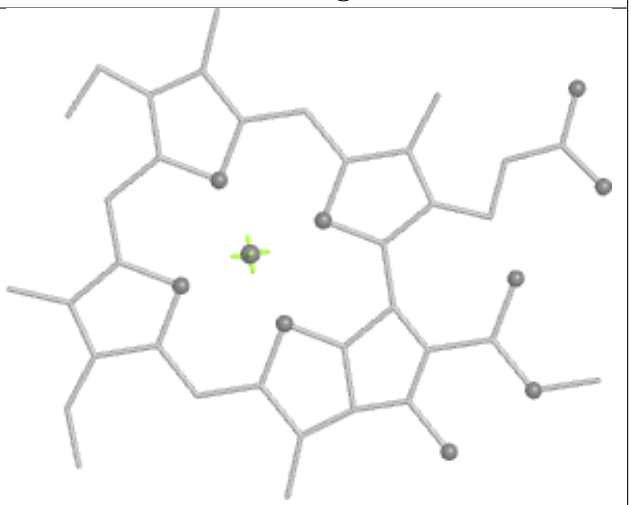
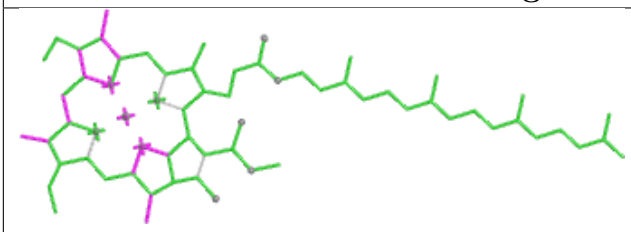


Rings

Ligand CLA f 1225



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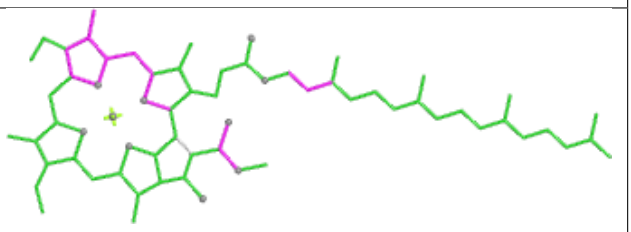

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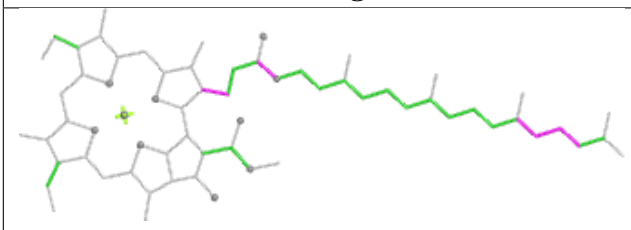

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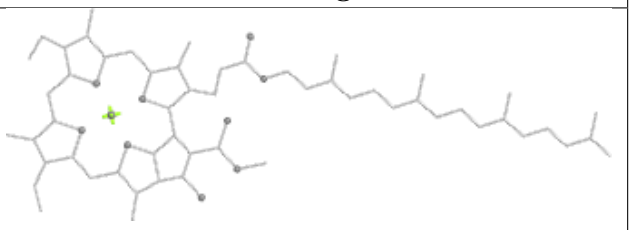
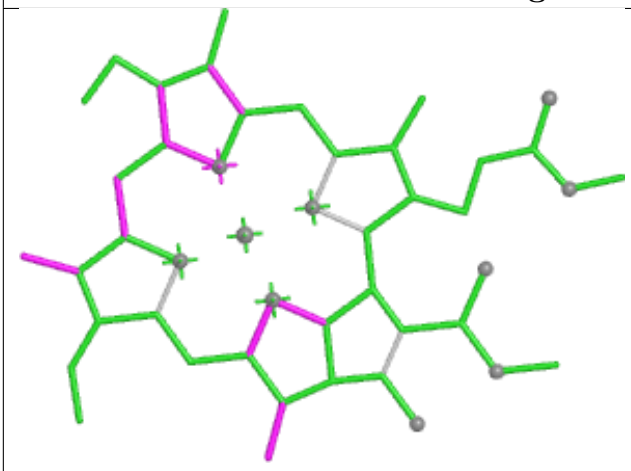


Rings

Ligand CLA 5 519



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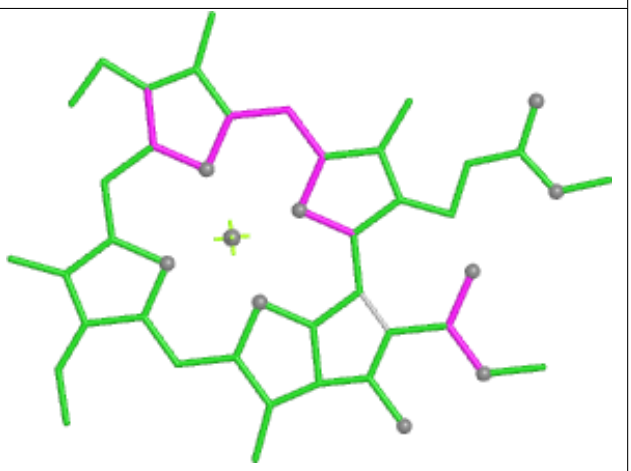
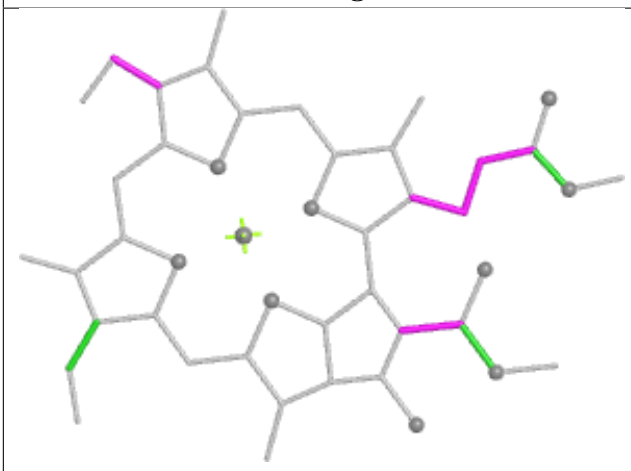


Bond angles



Torsions

Rings

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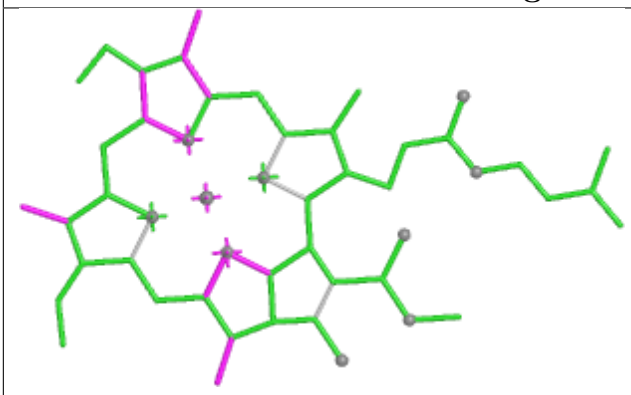

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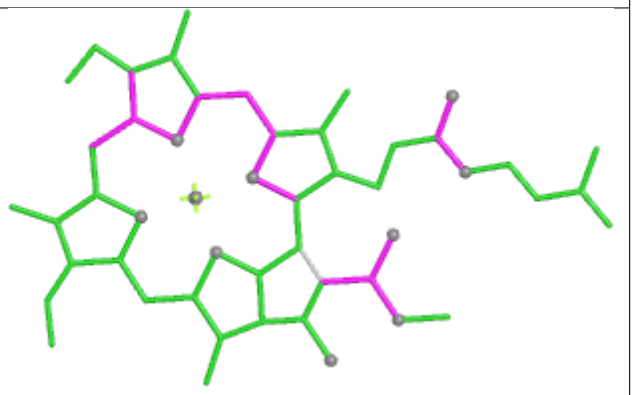
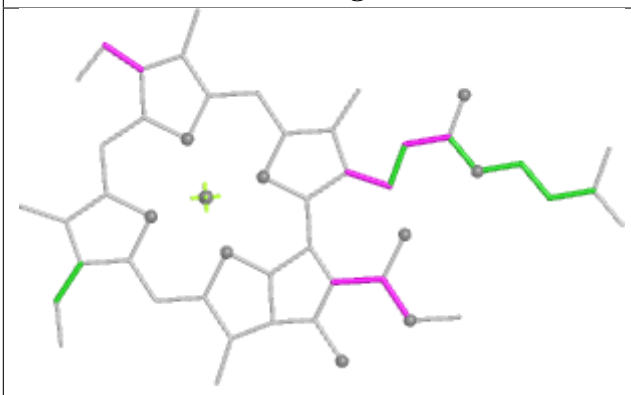
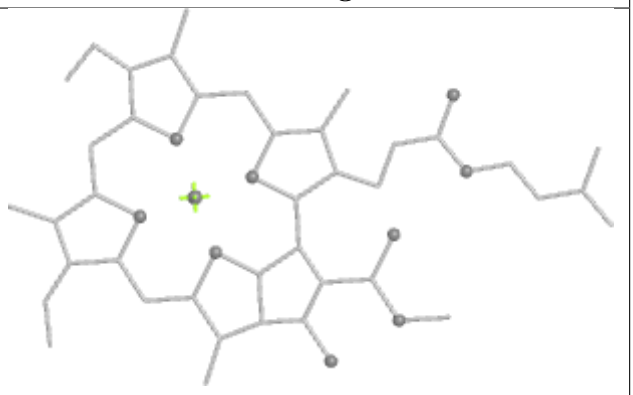


Bond angles

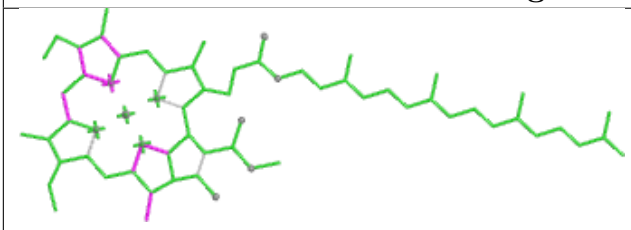


Torsions



Rings

Ligand CLA d 505



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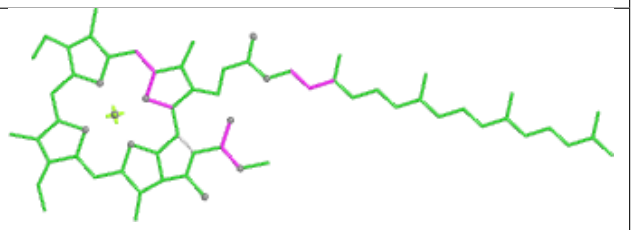
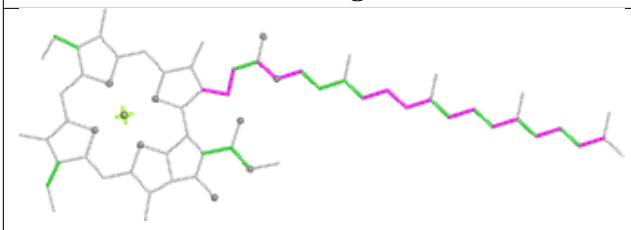
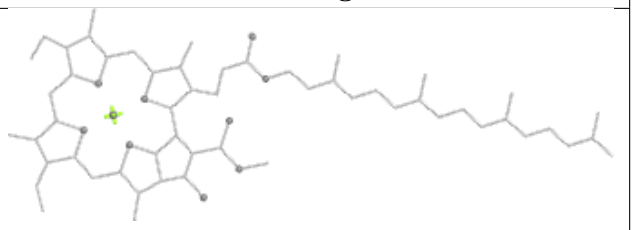


Bond angles

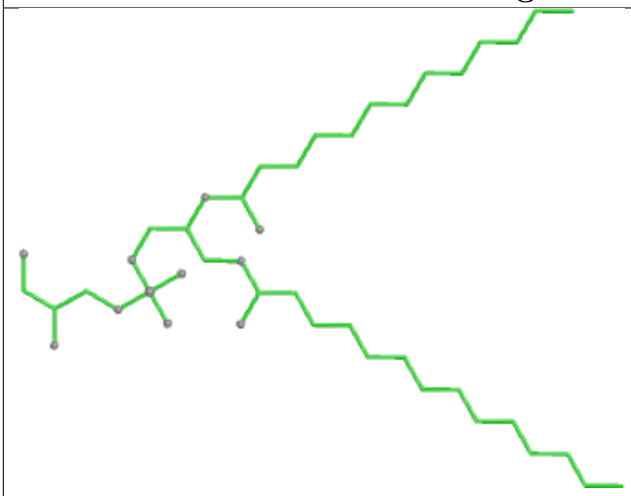


Torsions



Rings

Ligand LHG k 5001



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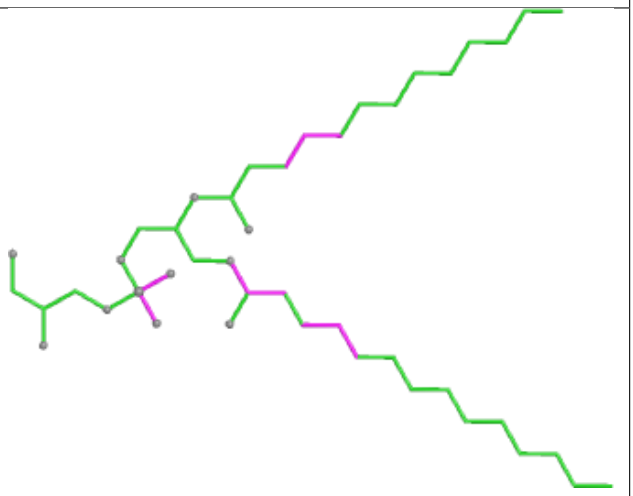
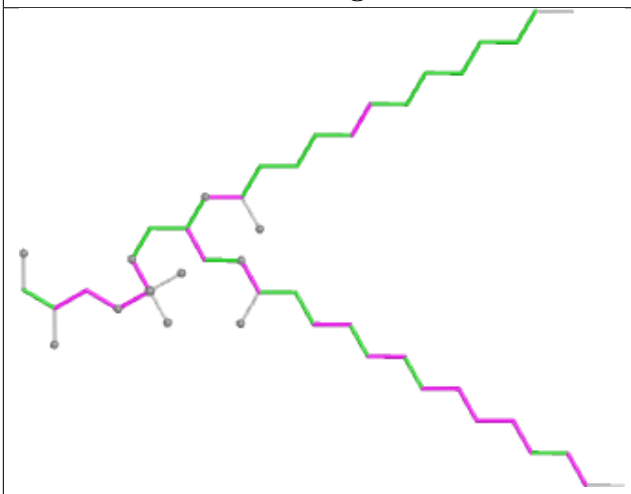


Bond angles



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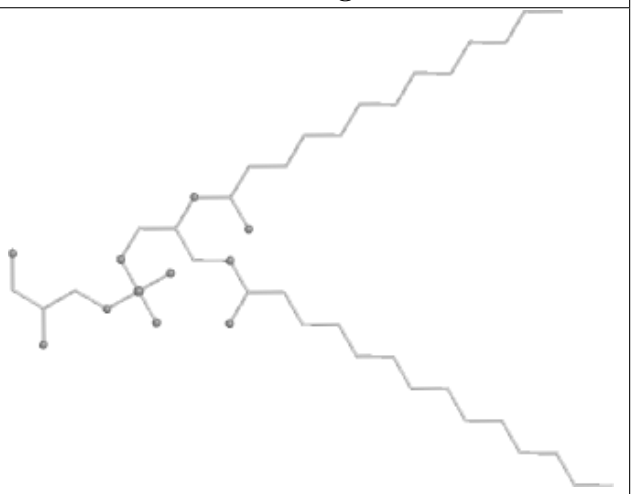
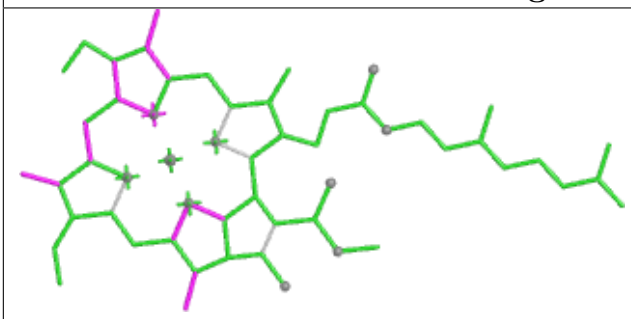


Rings

Ligand CLA 4 519



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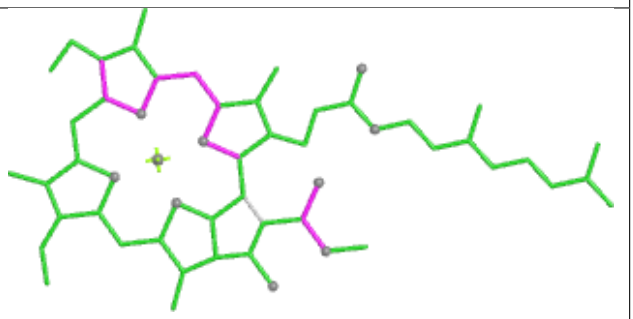

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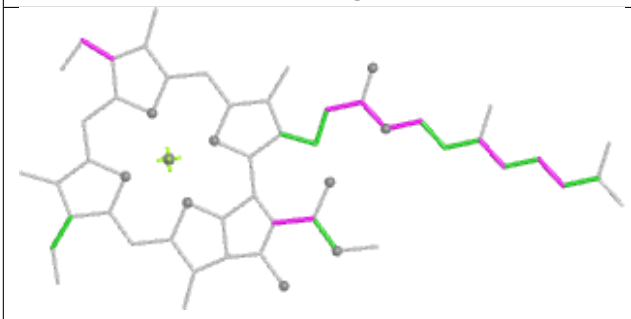

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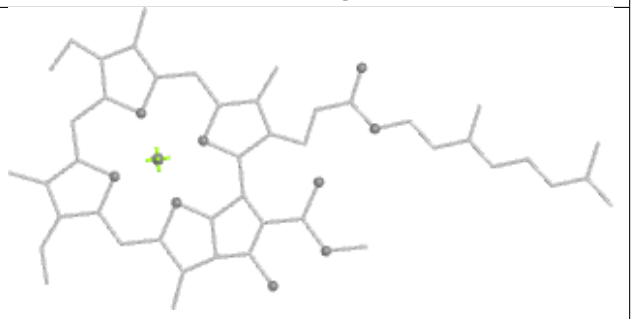
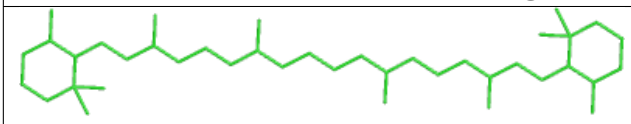


Rings

Ligand BCR Y 524



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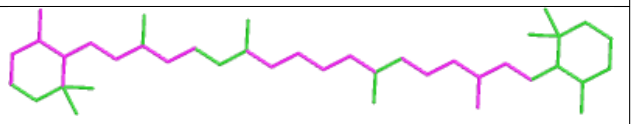

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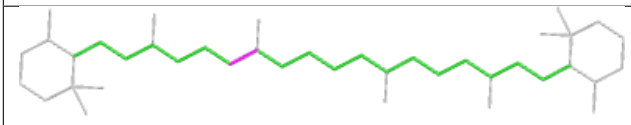

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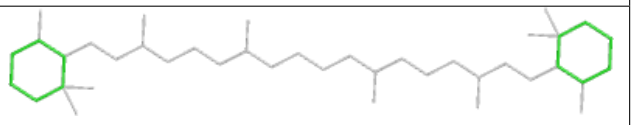
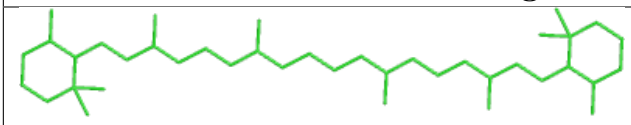


Rings

Ligand BCR f 4017



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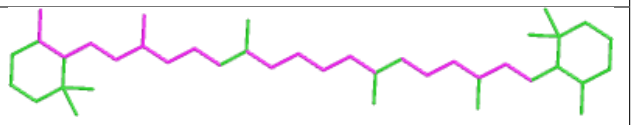
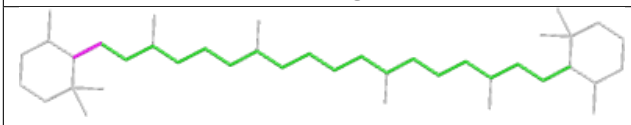


Bond angles



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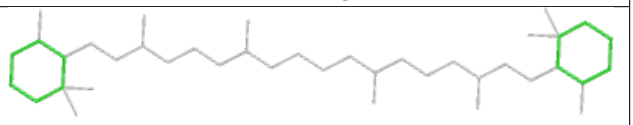
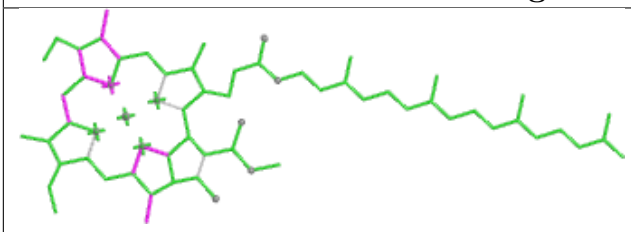


Rings

Ligand CLA 3 503



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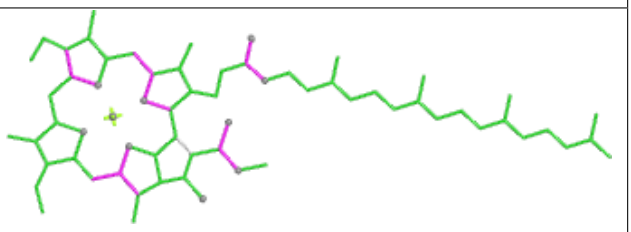

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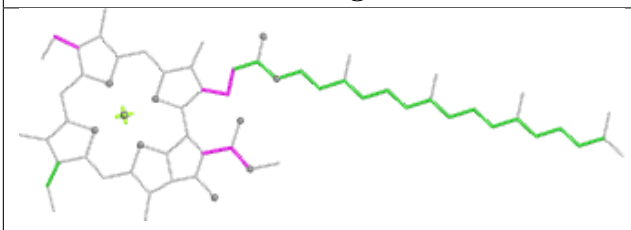

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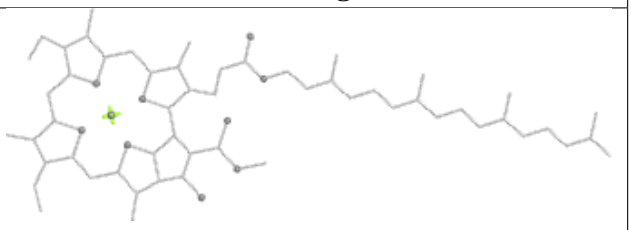
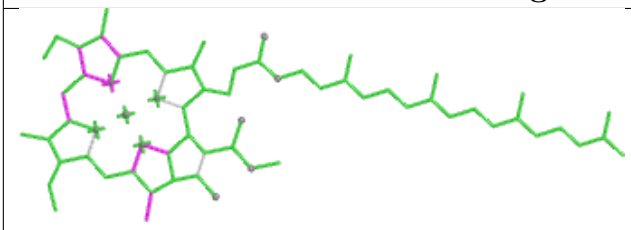


Rings

Ligand CLA s 505



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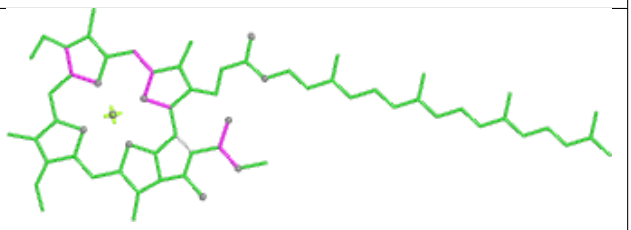

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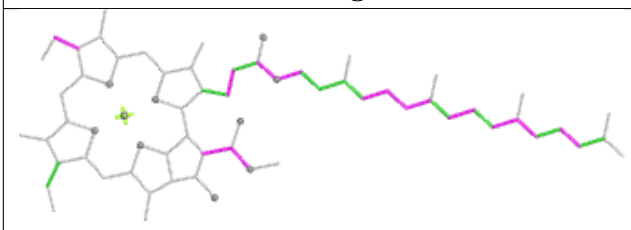

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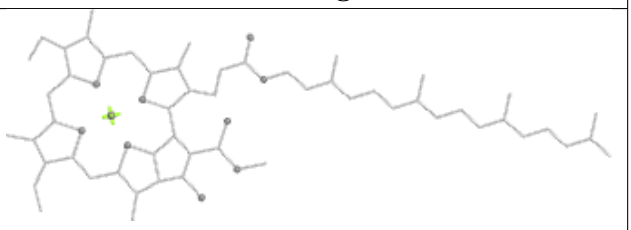
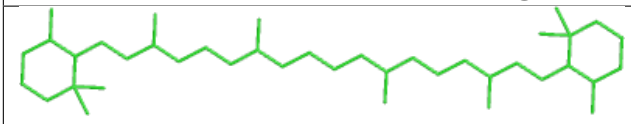


Rings

Ligand BCR L 4020



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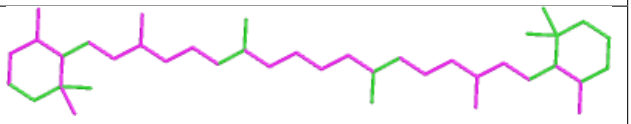

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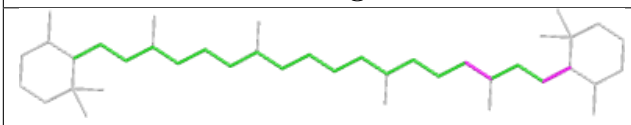

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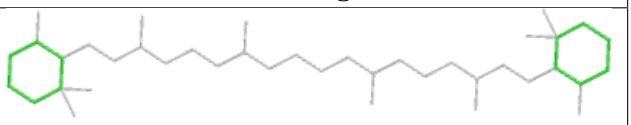
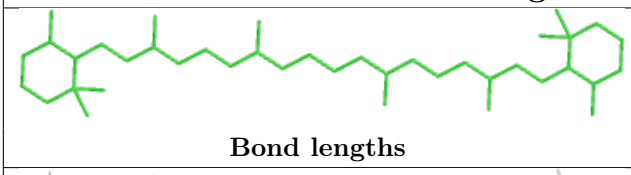


Rings

Ligand BCR s 521



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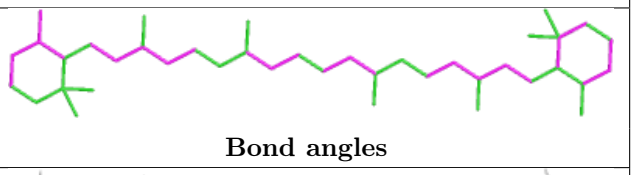
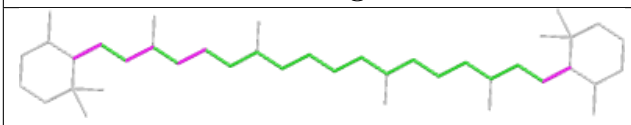


Bond angles



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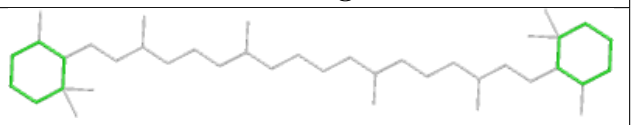
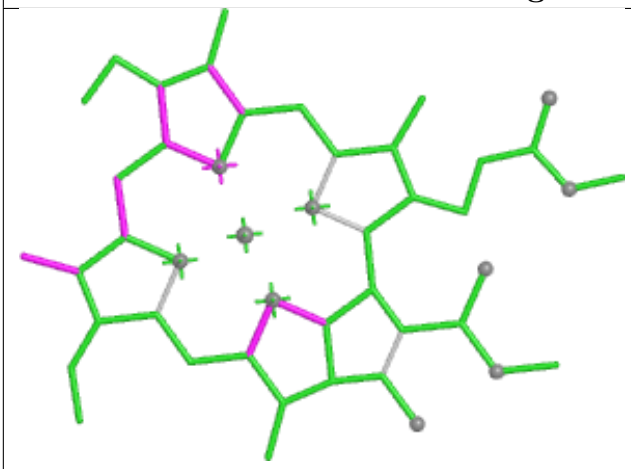


Rings

Ligand CLA d 519



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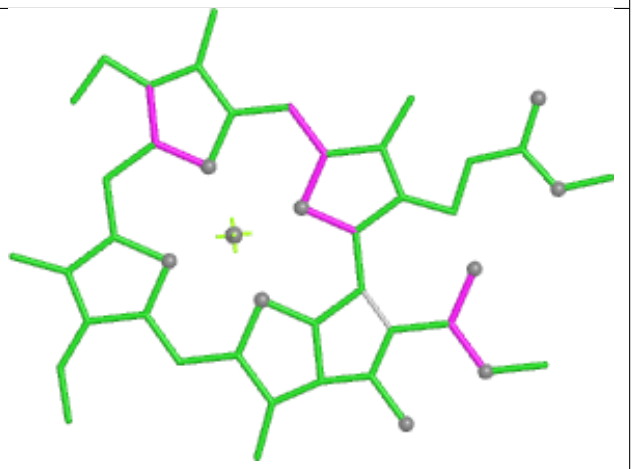
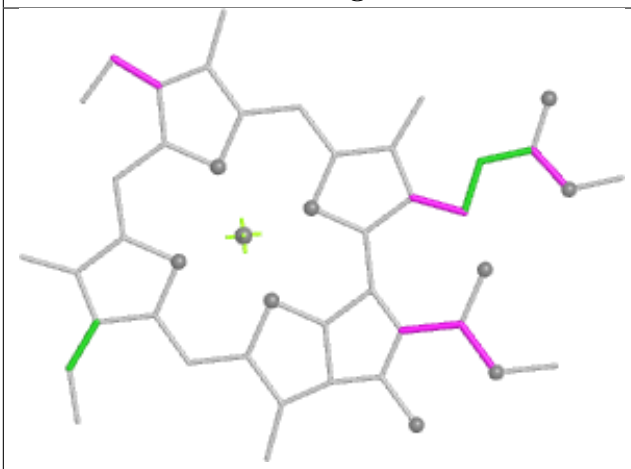


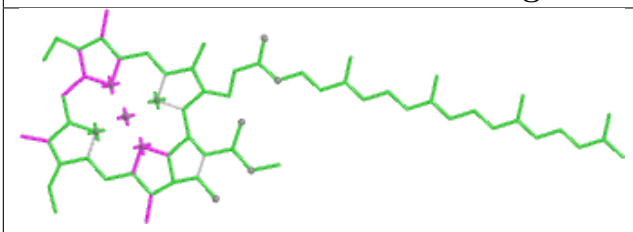
Bond angles



Torsions

Rings

Ligand CLA f 1226



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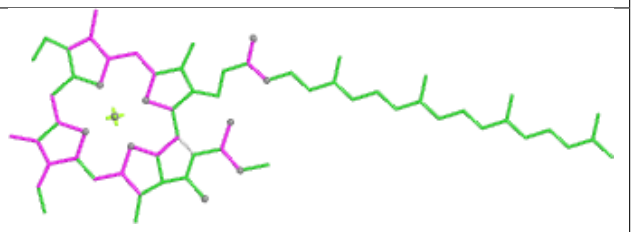
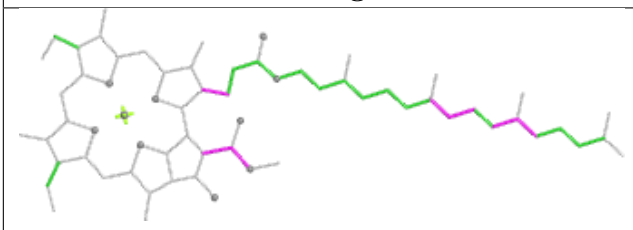


Bond angles



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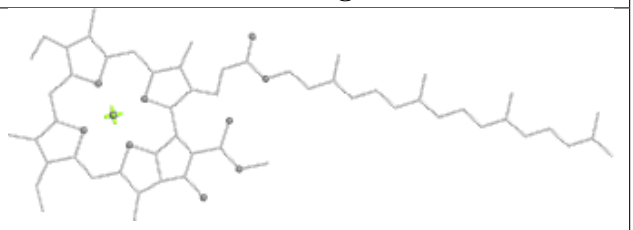
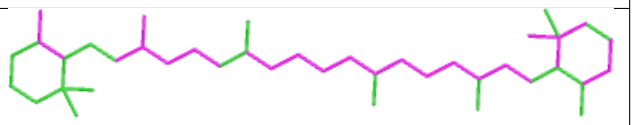


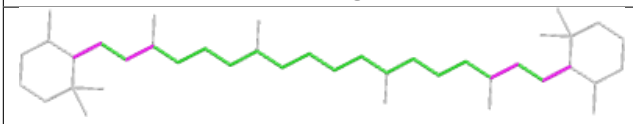
Rings

Ligand BCR H 4004

Bond lengths



Bond angles



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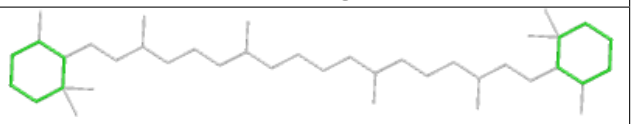
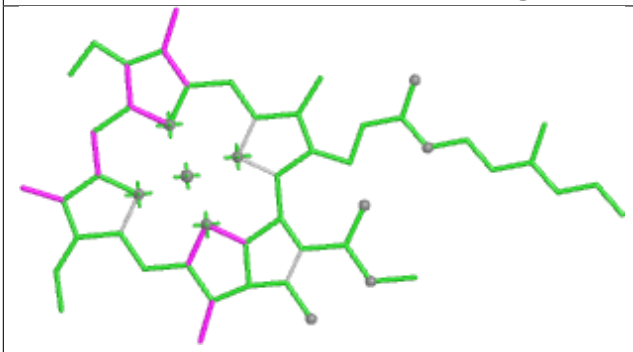


Rings

Ligand CLA H 1209



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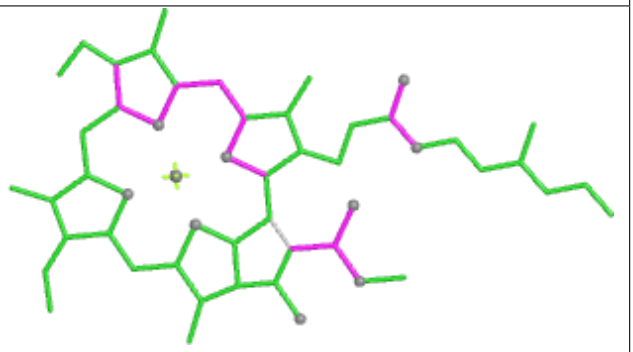
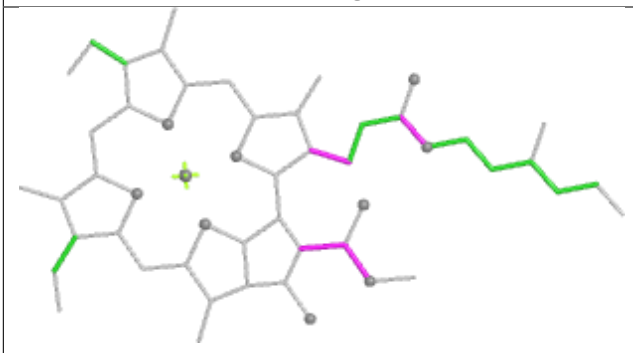


Bond angles



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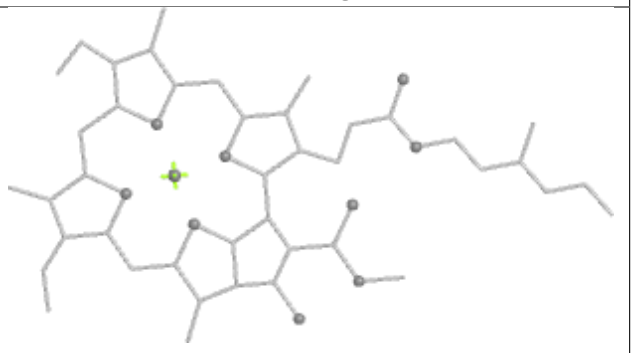
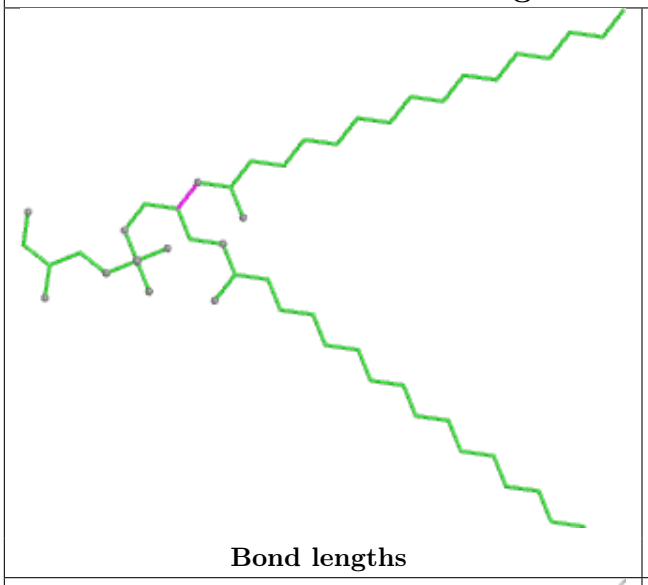


Rings

Ligand LHG G 5009



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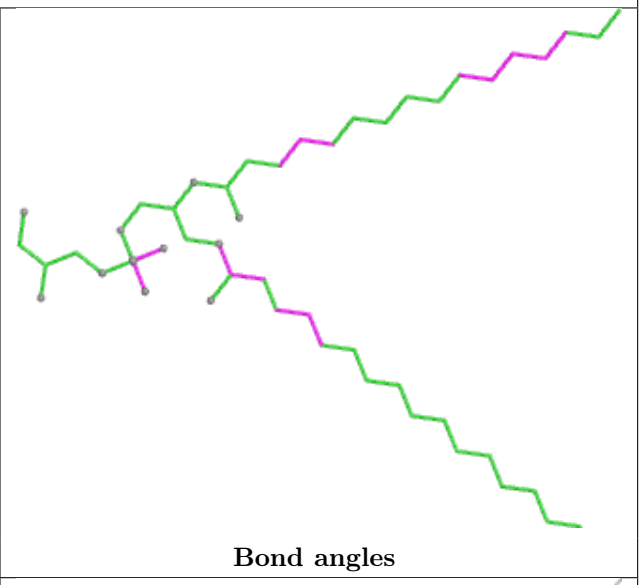
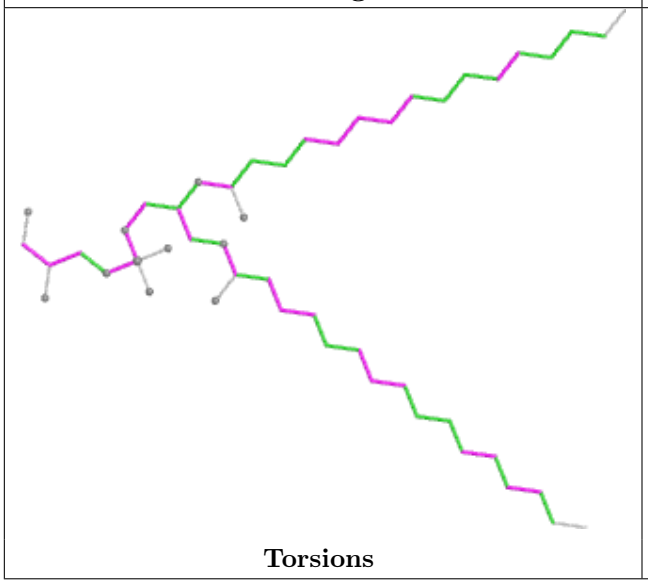


Bond angles



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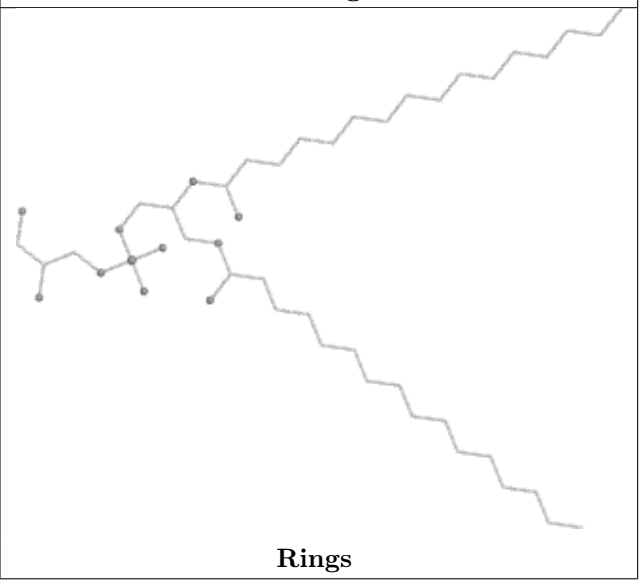
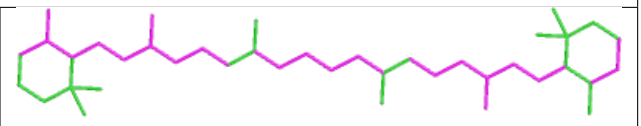


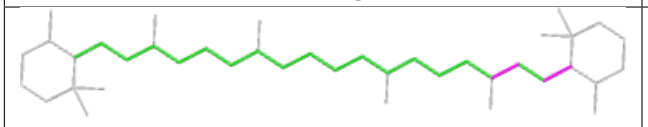
Rings

Ligand BCR c 523

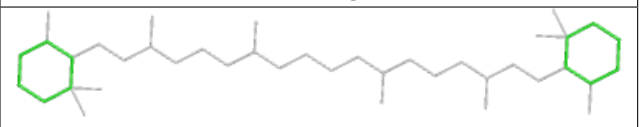
Bond lengths



Bond angles

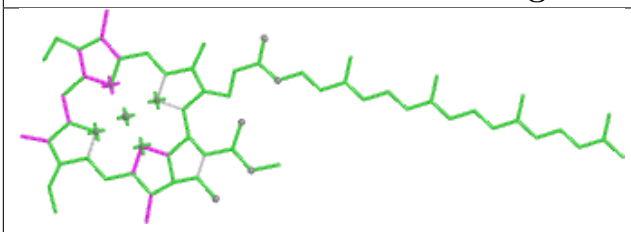


Torsions



Rings

Ligand CLA 2 513



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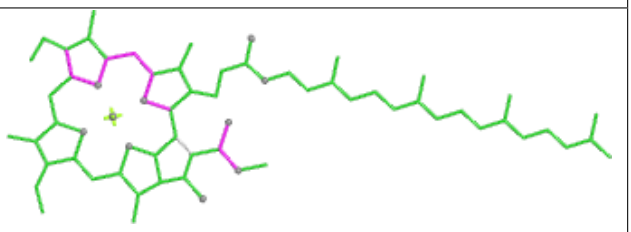
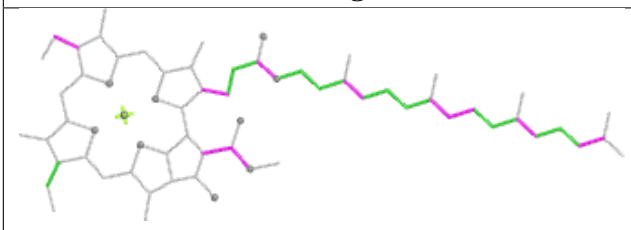


Bond angles



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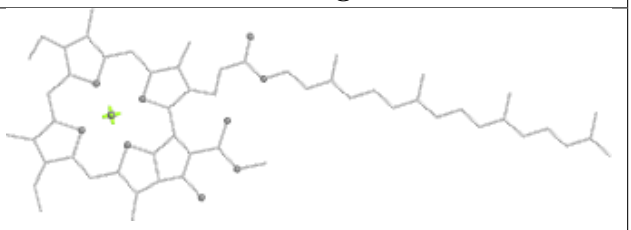
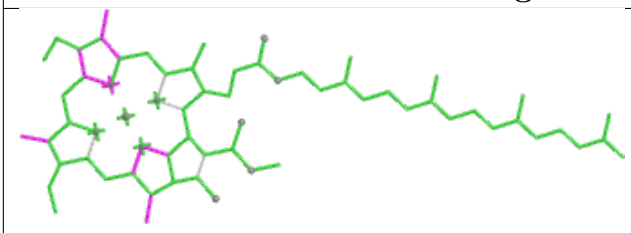


Rings

Ligand CLA A 1131



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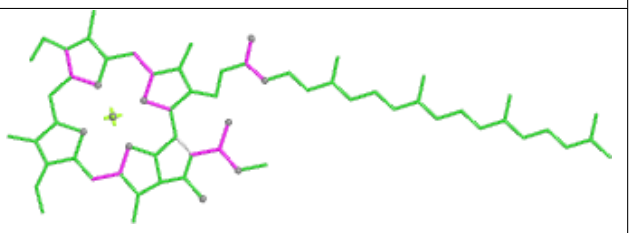

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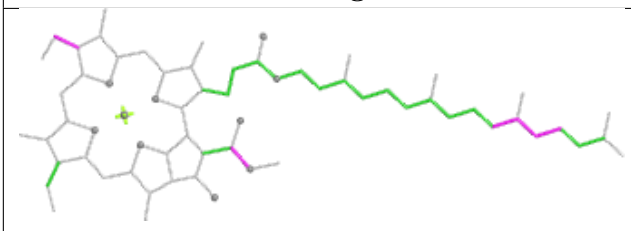

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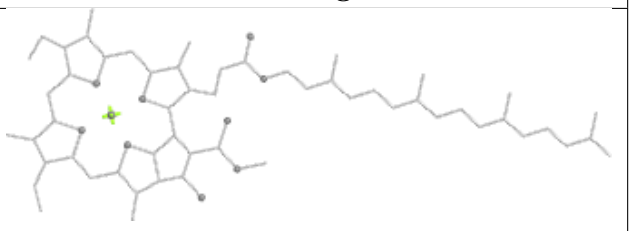
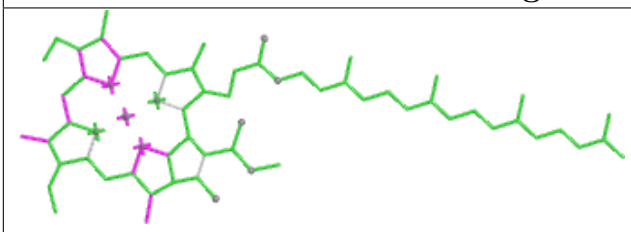


Rings

Ligand CLA f 1023



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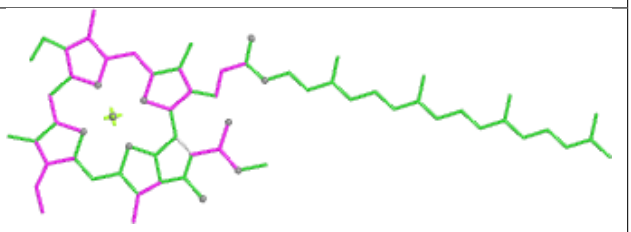

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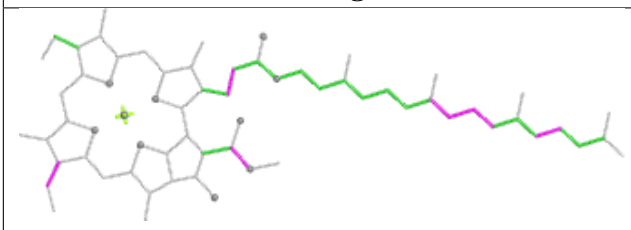

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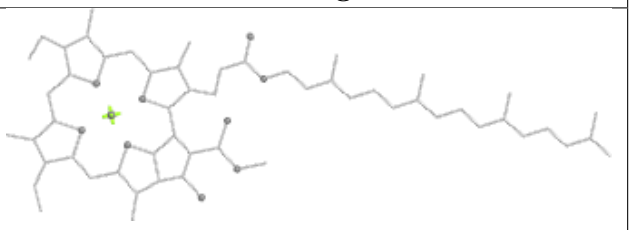
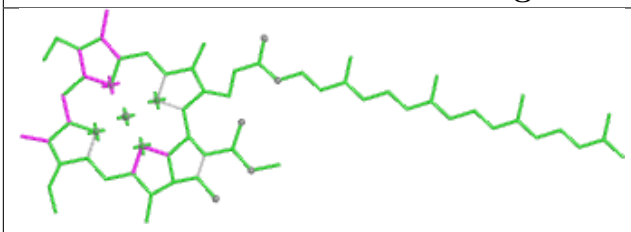


Rings

Ligand CLA G 1102



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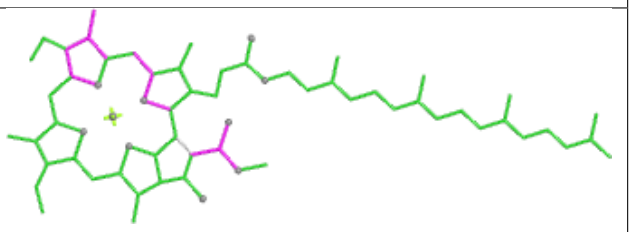
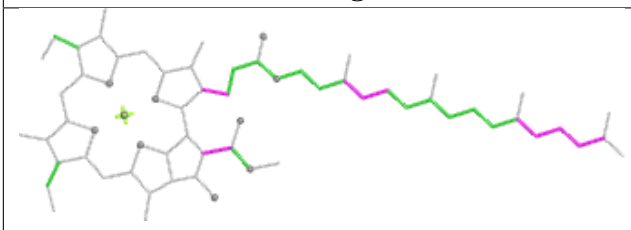


Bond angles



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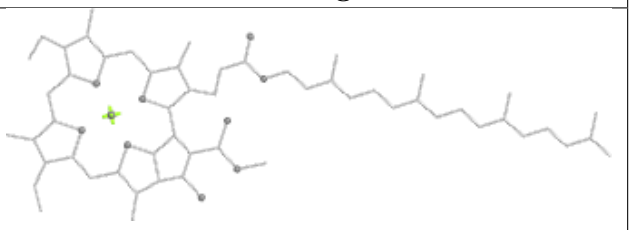
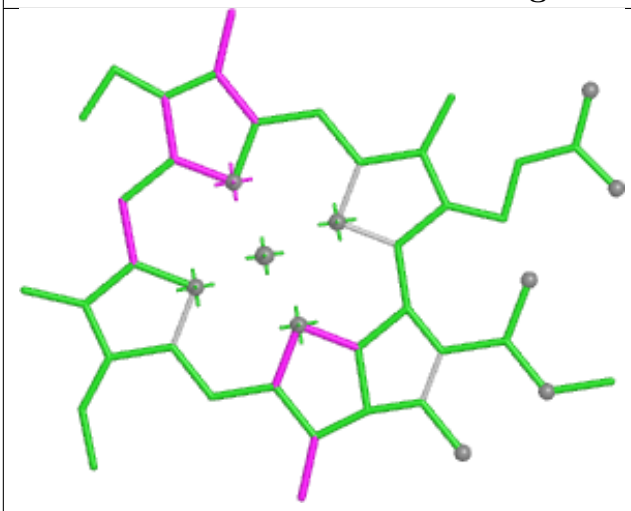


Rings

Ligand CLA c 516



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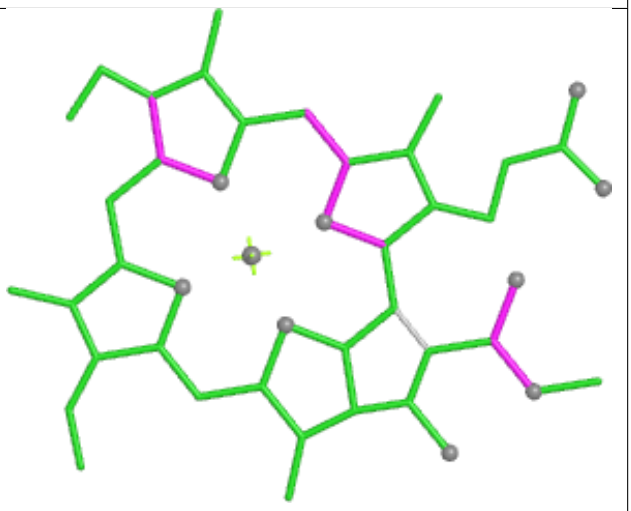

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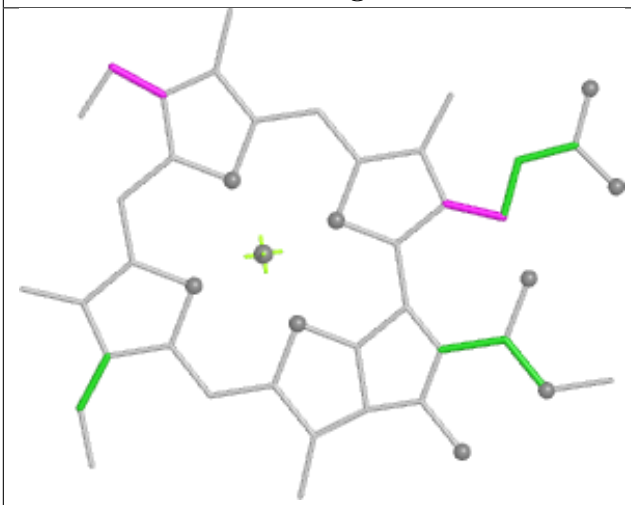

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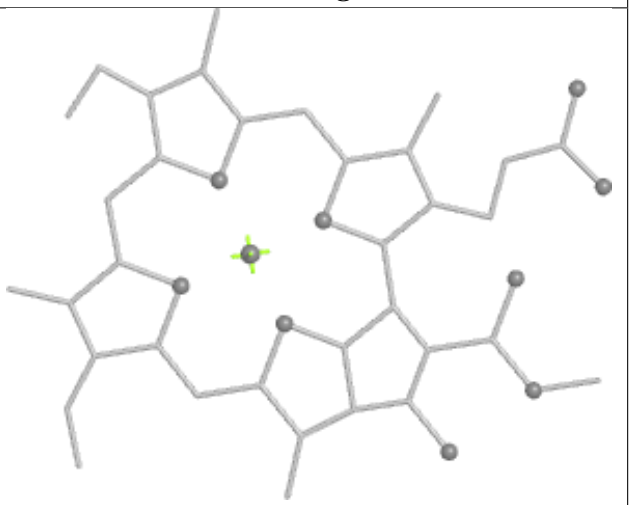
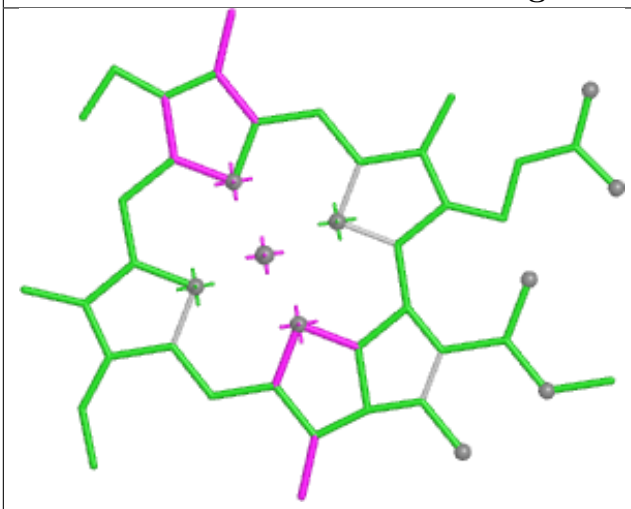


Rings

Ligand CLA 3 512



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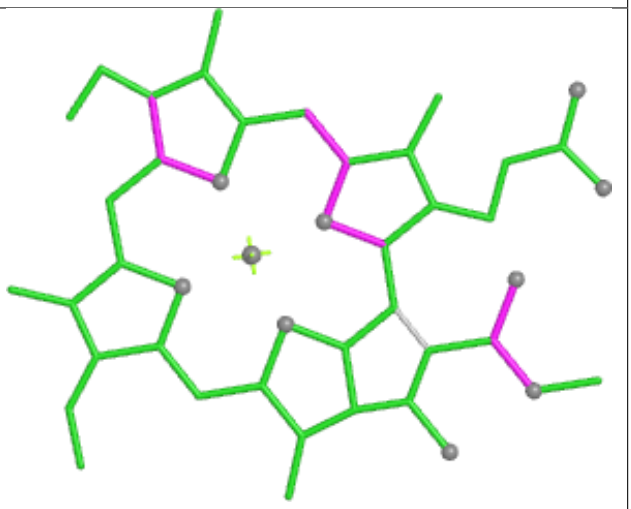
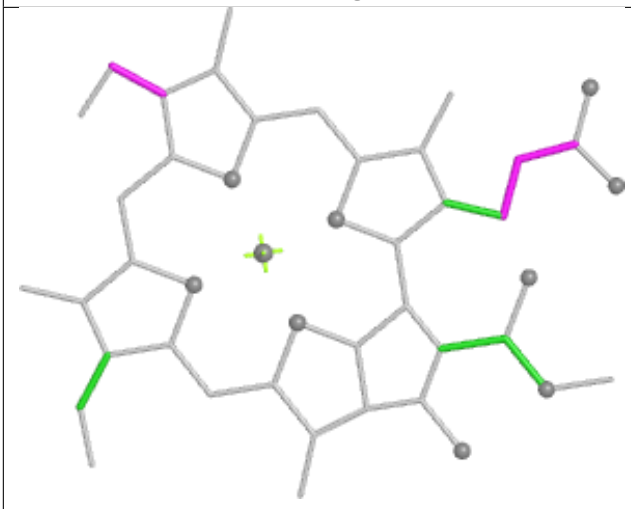


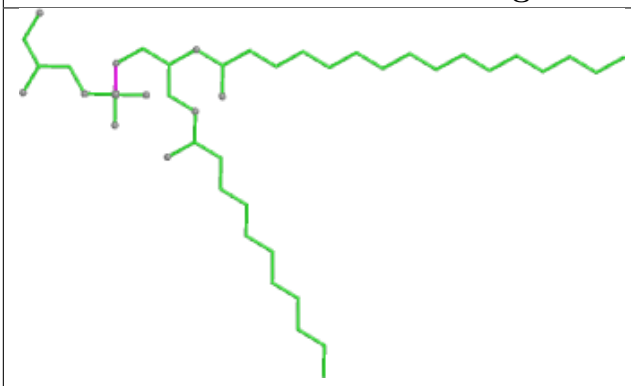
Bond angles



Torsions

Rings

Ligand LHG H 1855



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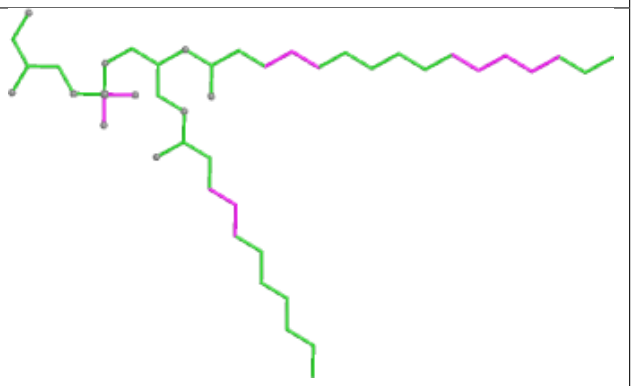

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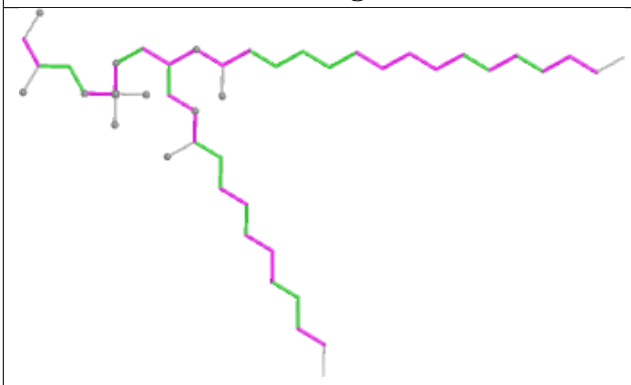
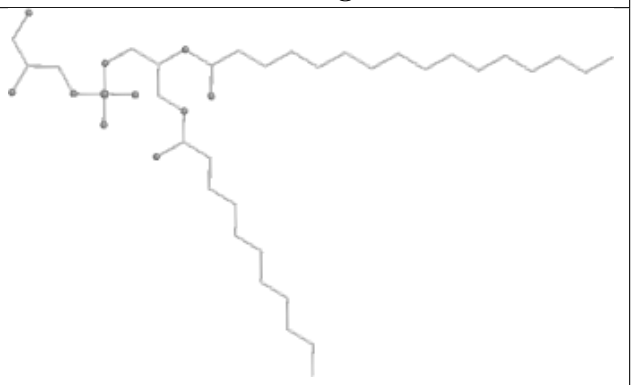
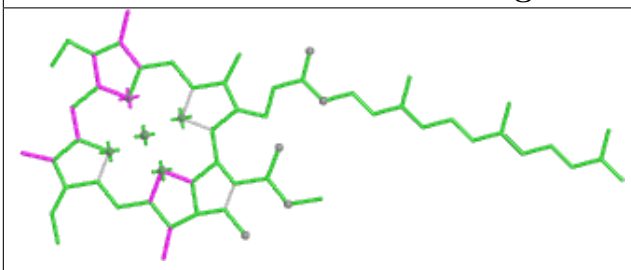


Torsions



Rings

Ligand CLA V 1503



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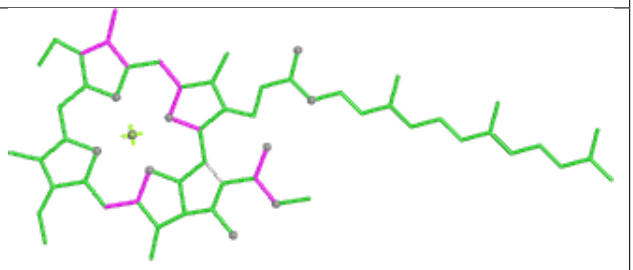
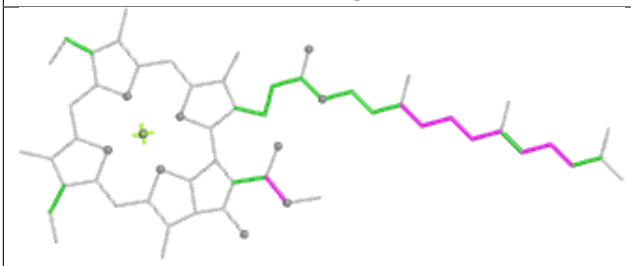
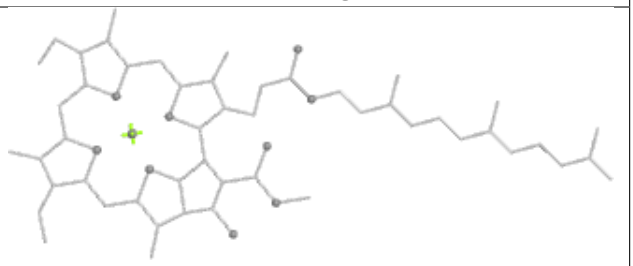


Bond angles

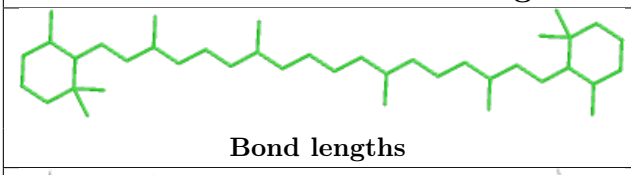


Torsions



Rings

Ligand BCR T 4015



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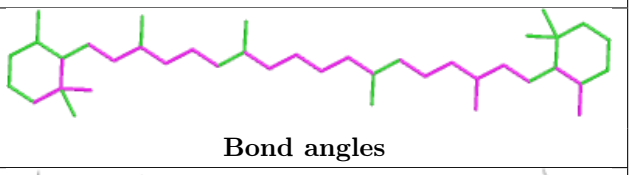

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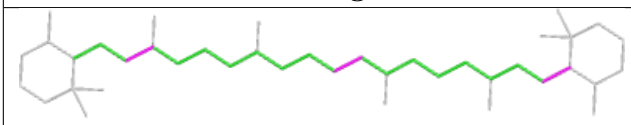

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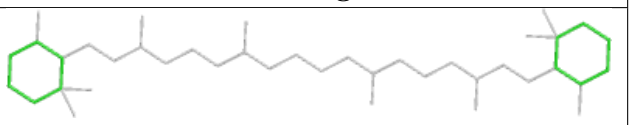
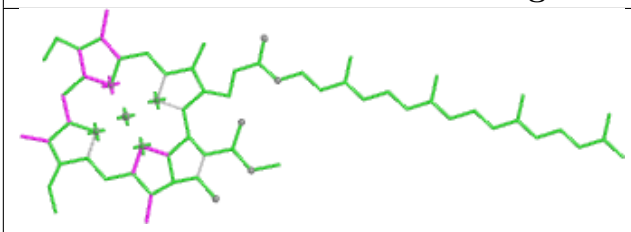


Rings

Ligand CLA 3 509



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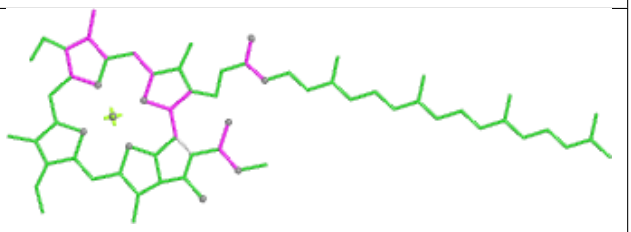

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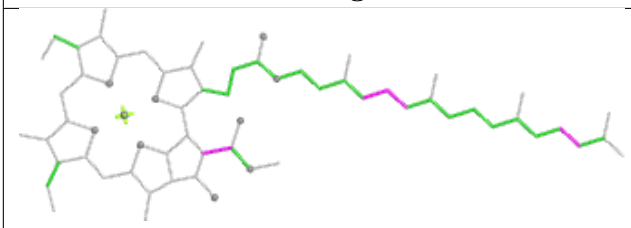

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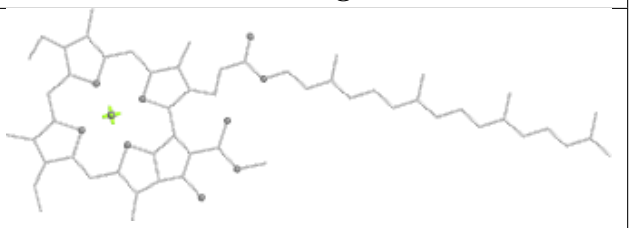
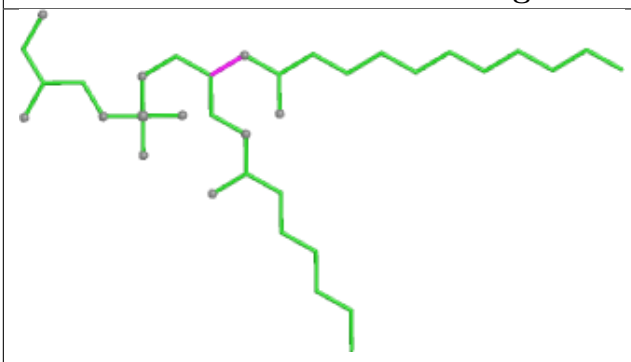


Rings

Ligand LHG A 5008



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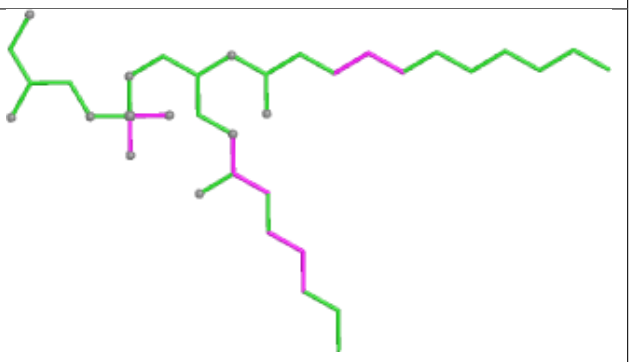

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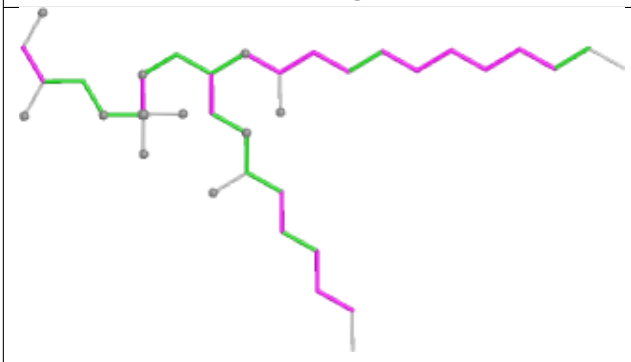

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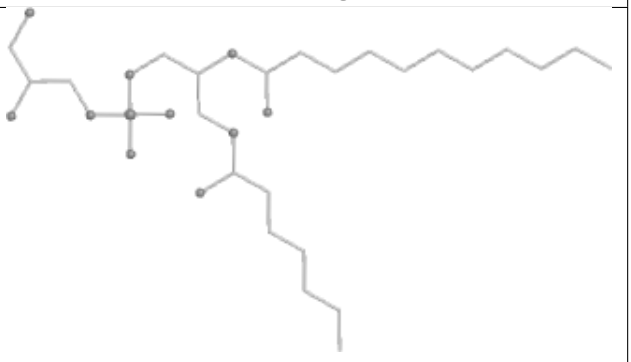
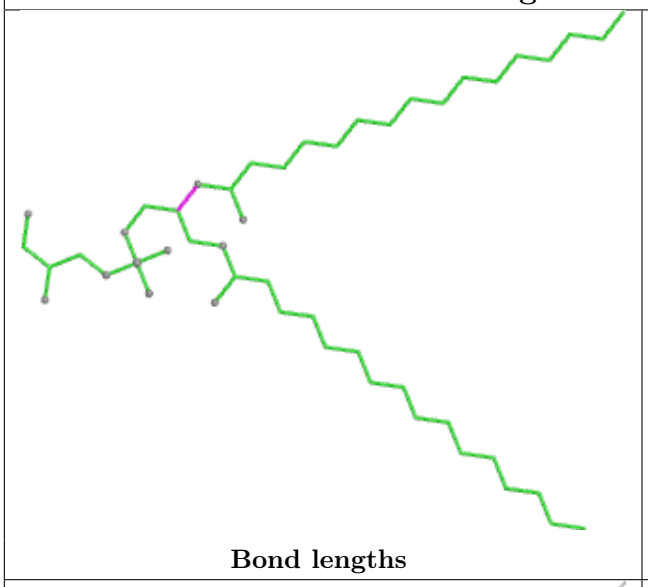


Rings

Ligand LHG e 5001



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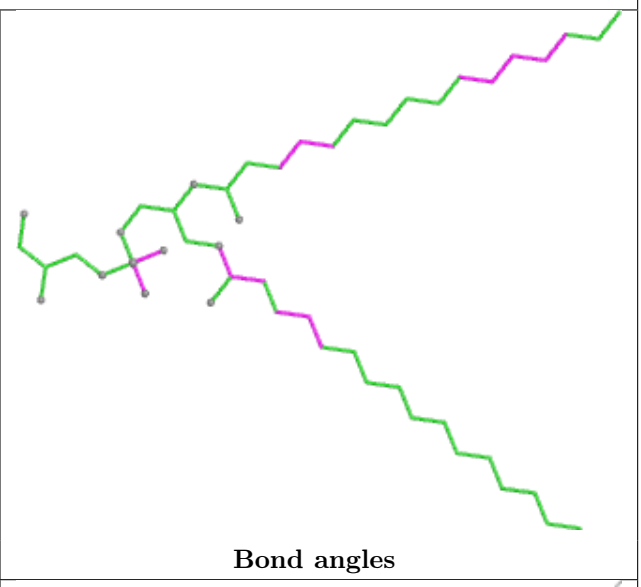
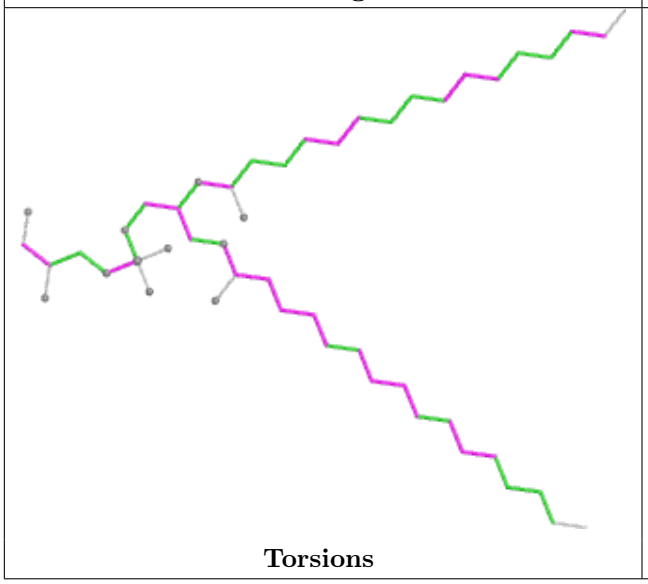


Bond angles



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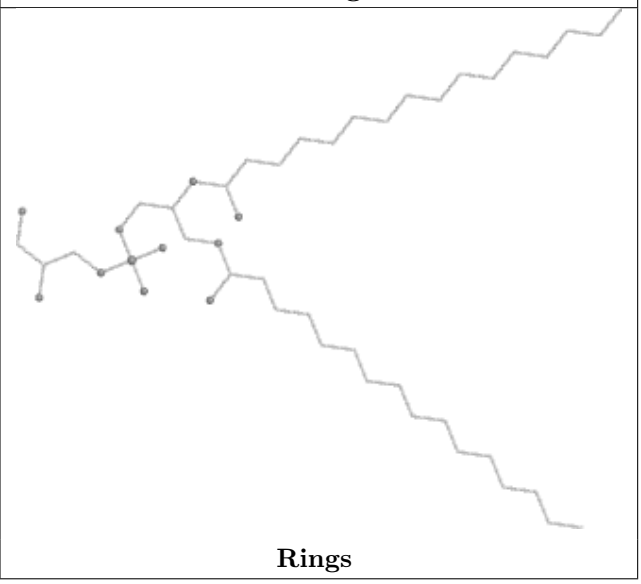
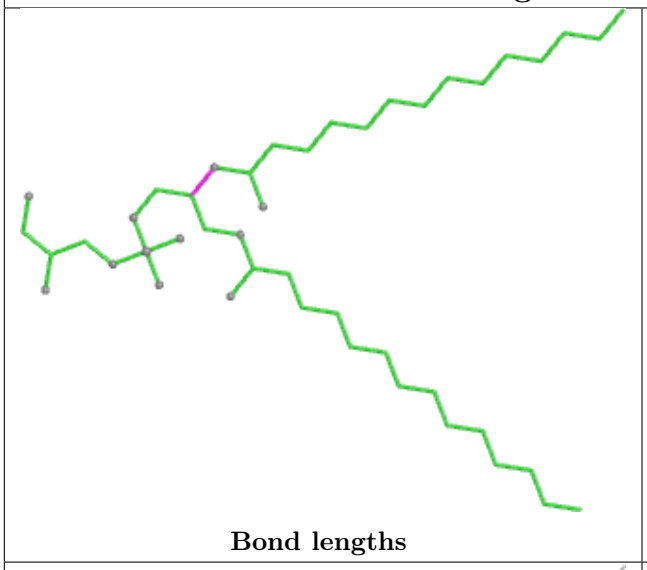


Rings

Ligand LHG A 5005



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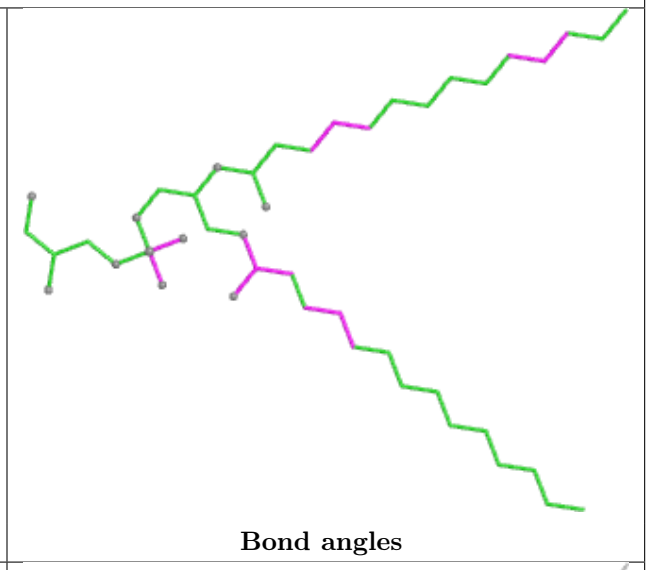
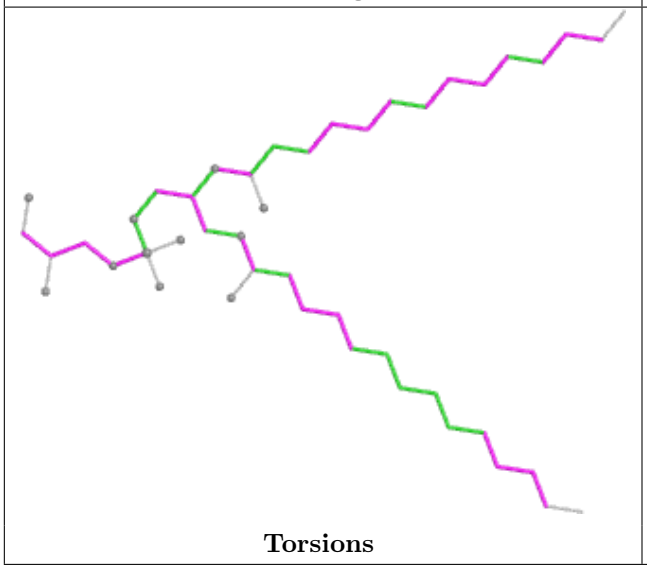
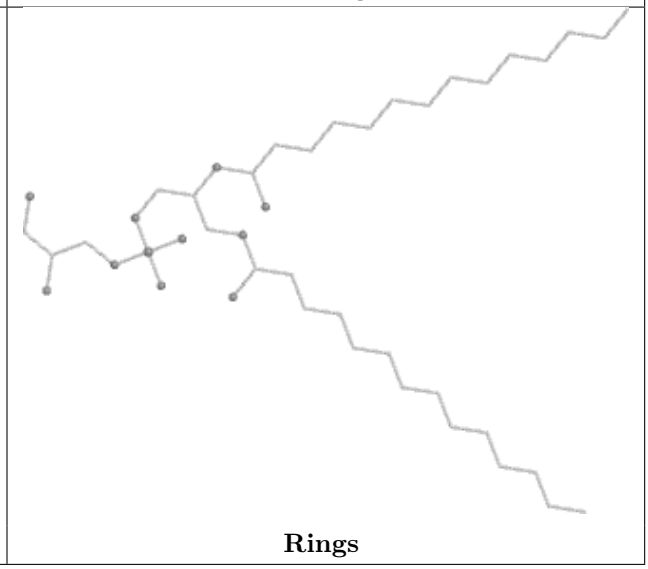


Bond angles

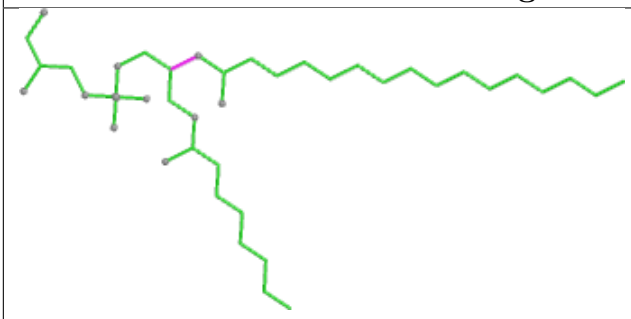


Torsions

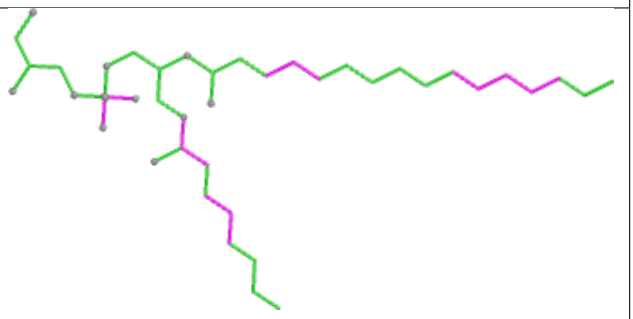


Rings

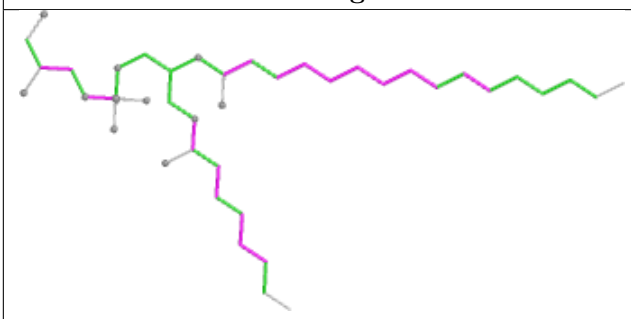
Ligand LHG e 5003



Bond lengths



Bond angles



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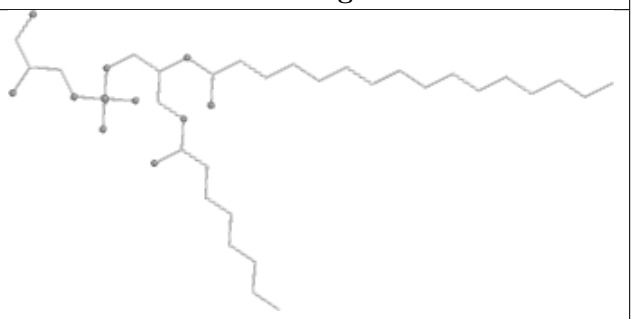
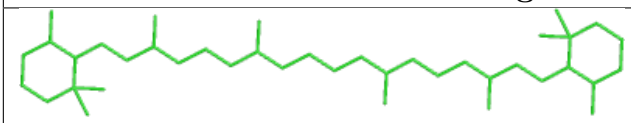


Rings

Ligand BCR n 4219



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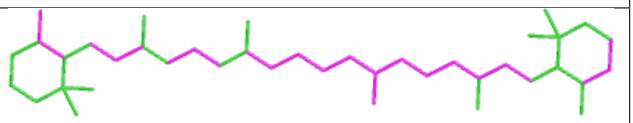
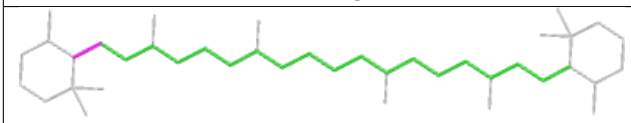


Bond angles



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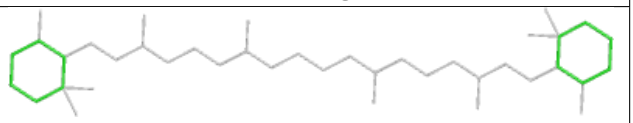
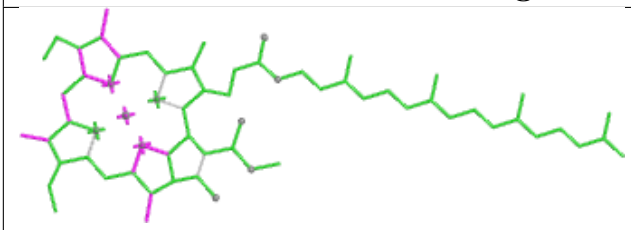


Rings

Ligand CLA A 1132



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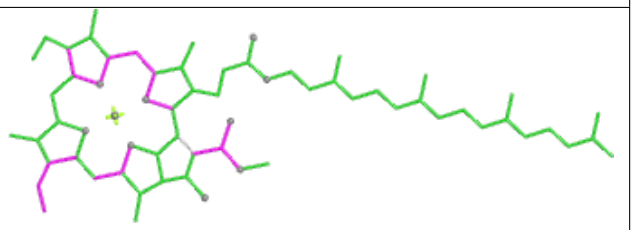
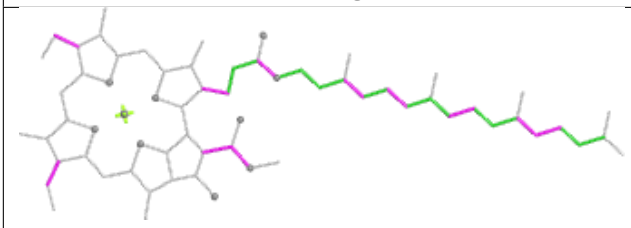


Bond angles



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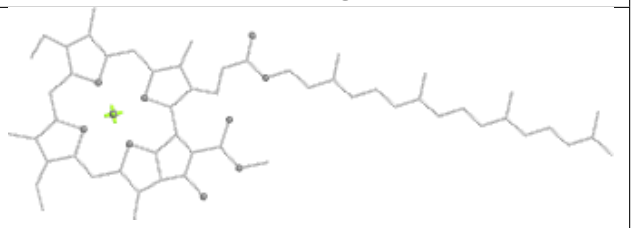
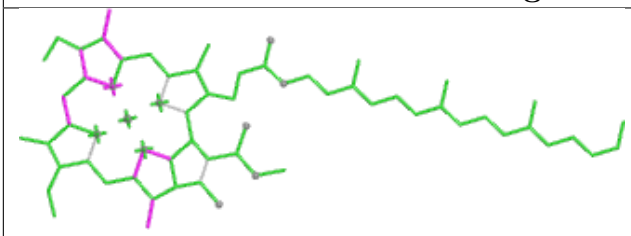
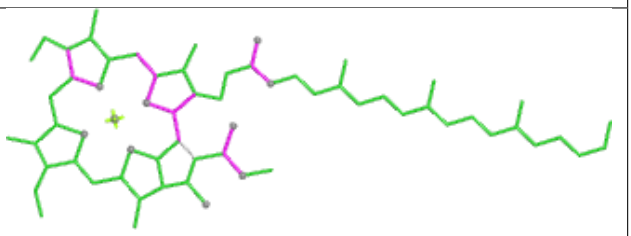
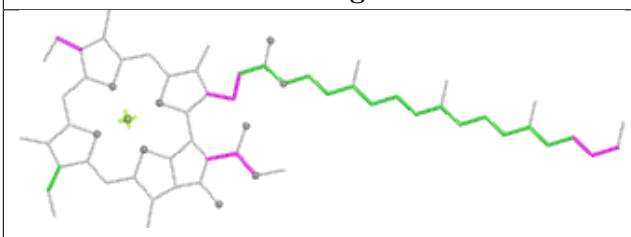
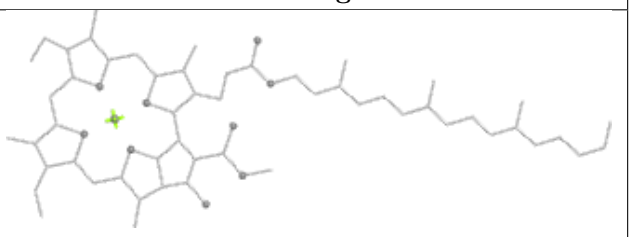


Rings

Ligand CLA Y 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

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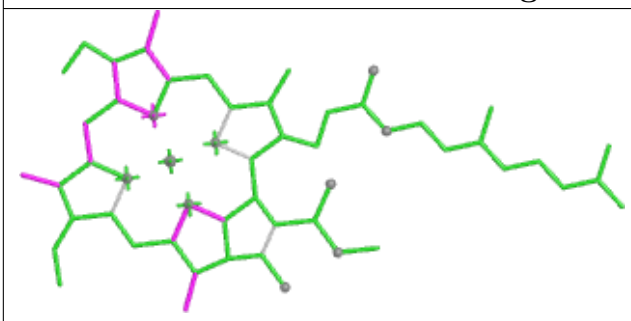
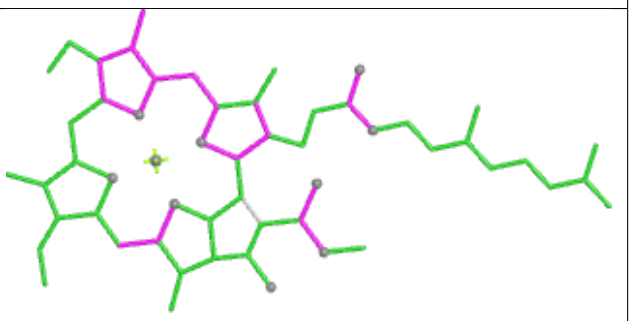
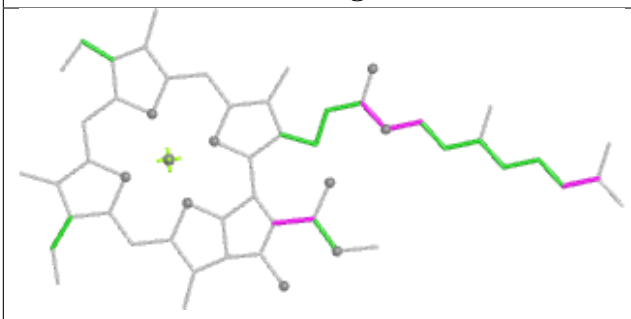
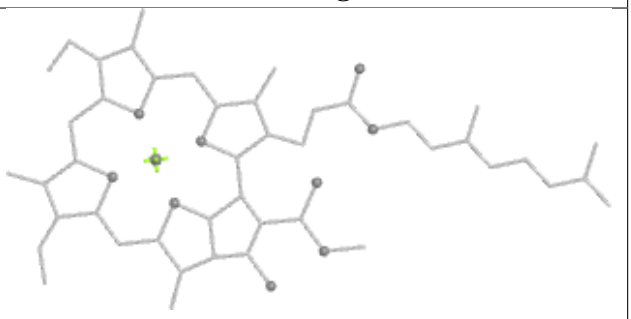
	
Bond lengths	Bond angles
	
Torsions	Rings

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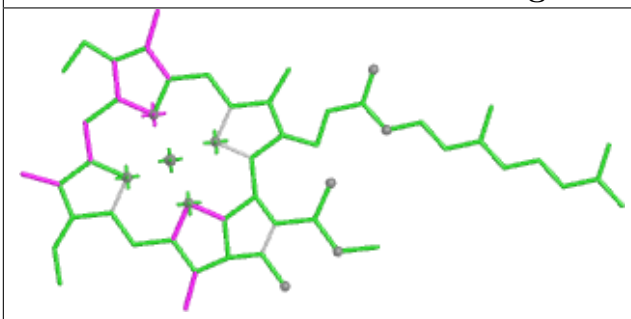
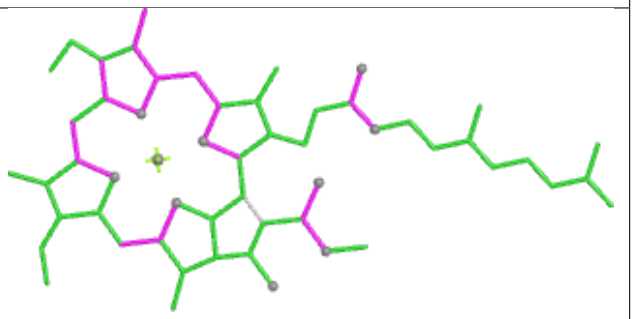
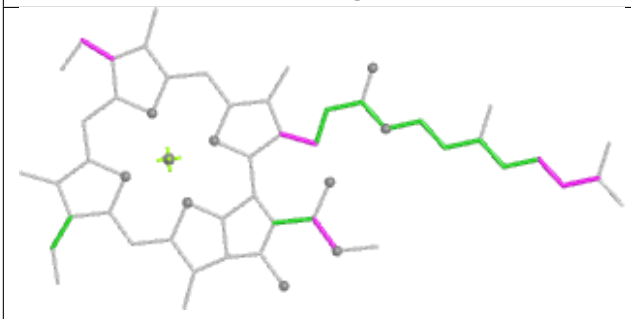


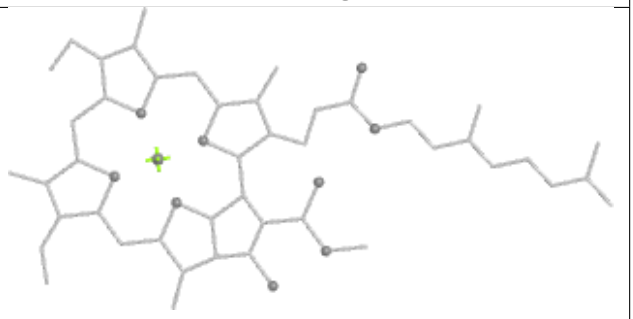
Bond lengths



Bond angles

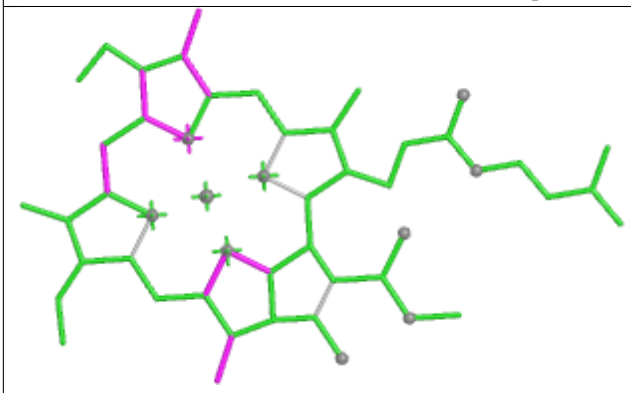


Torsions



Rings

Ligand CLA Z 504



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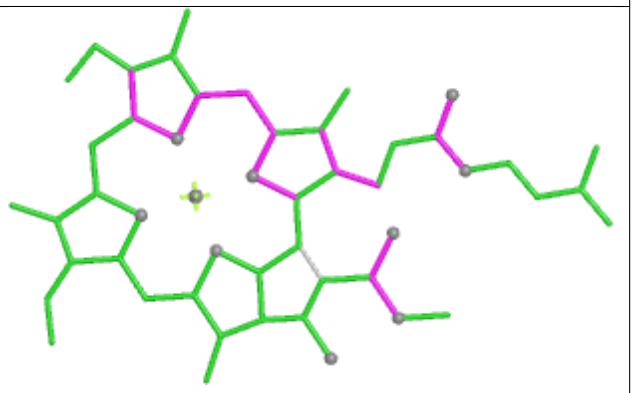

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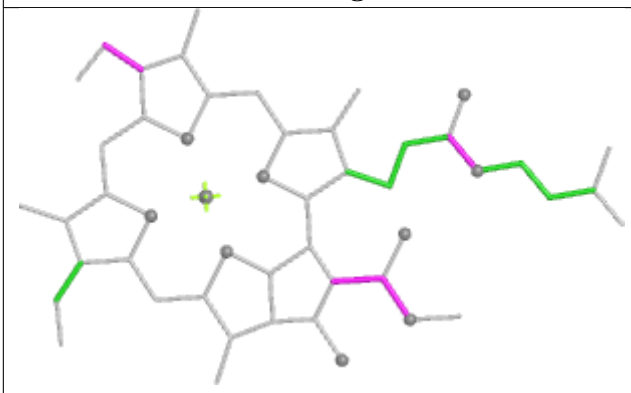

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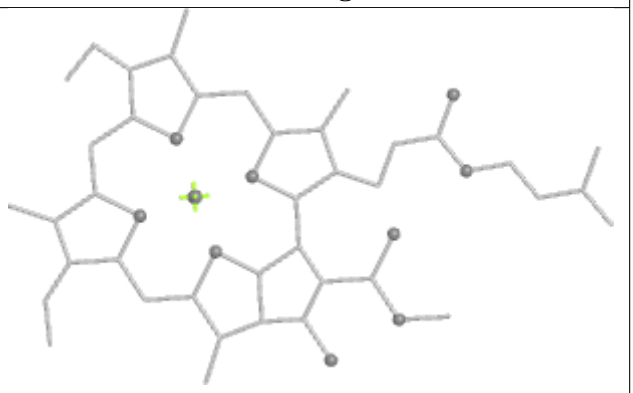
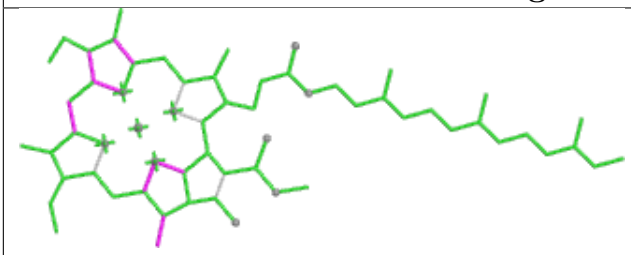
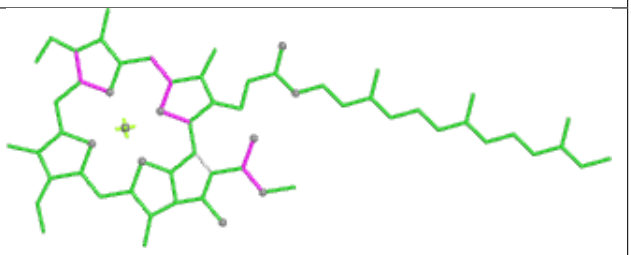
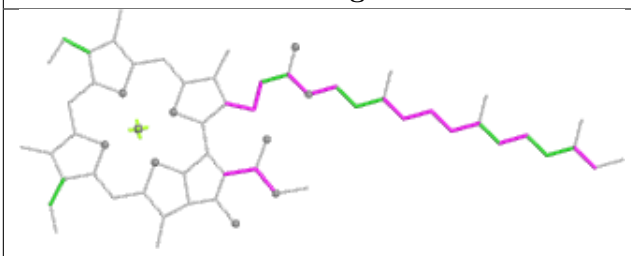
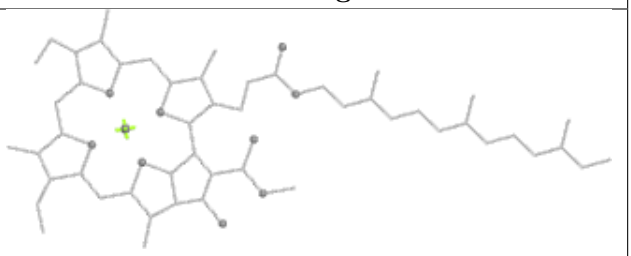


Rings

Ligand CLA 5 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

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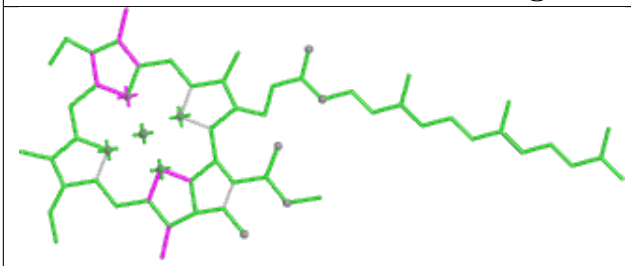
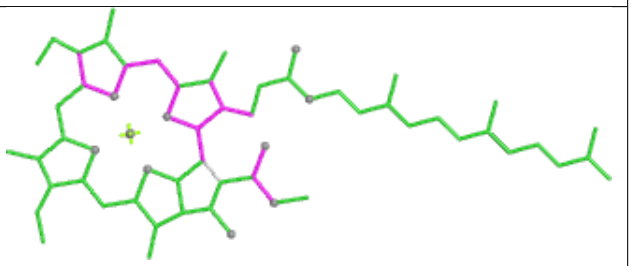
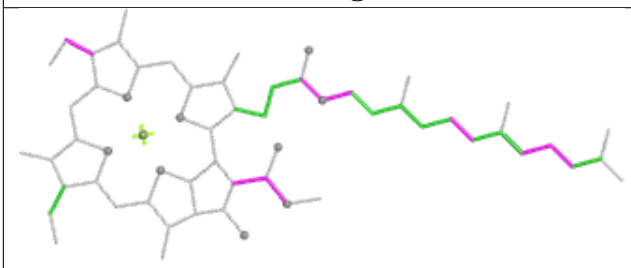
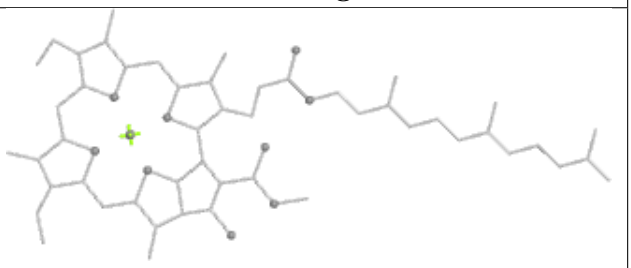
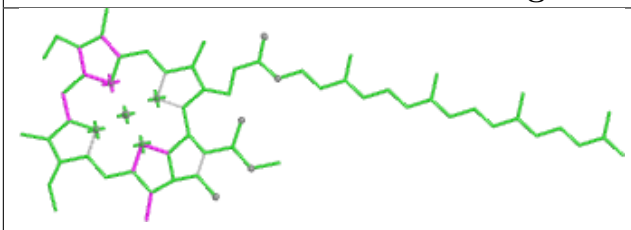
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 505



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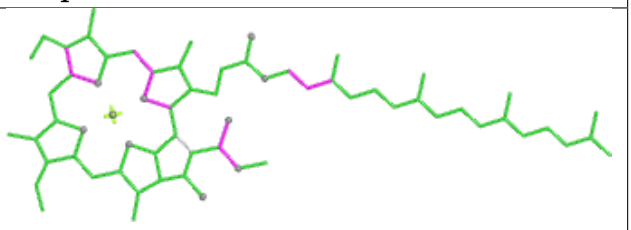
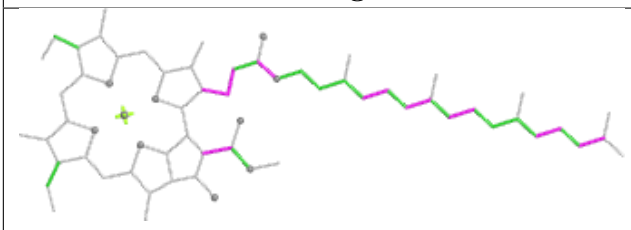
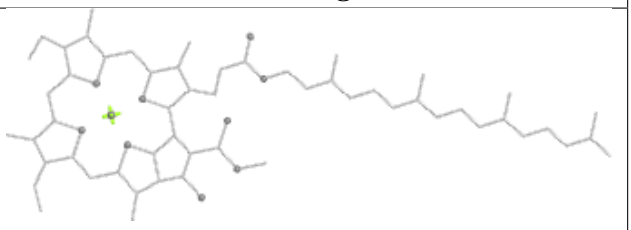


Bond angles

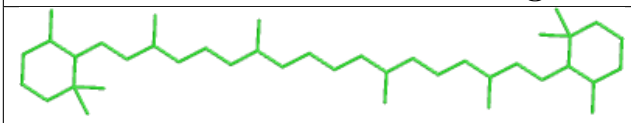


Torsions



Rings

Ligand BCR 5 521



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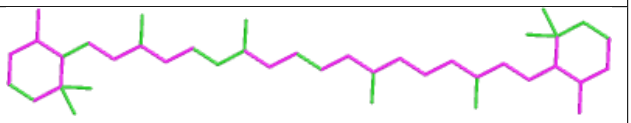
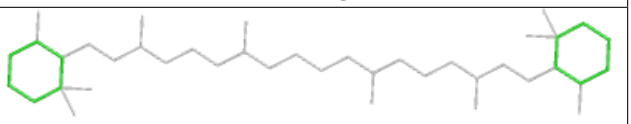


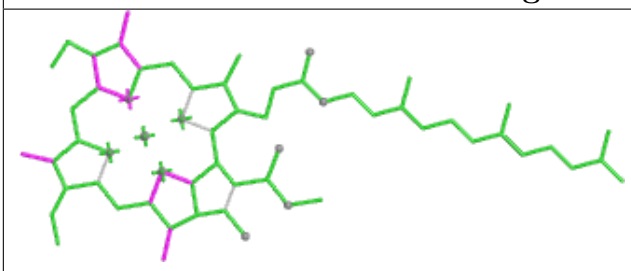
Bond angles

Torsions

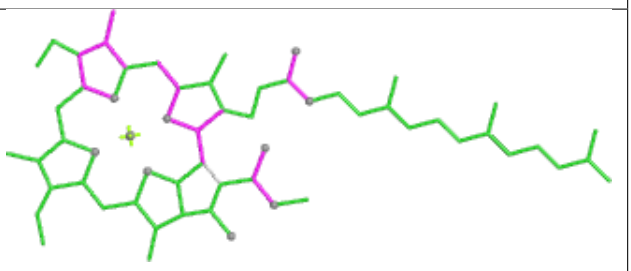


Rings

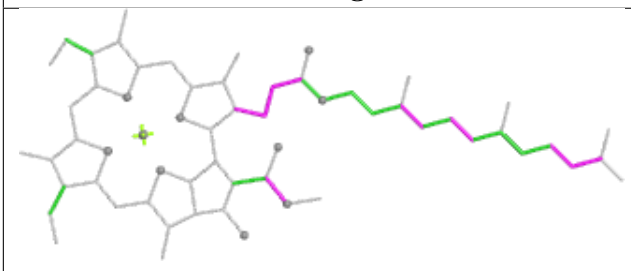
Ligand CLA f 1224



Bond lengths



Bond angles



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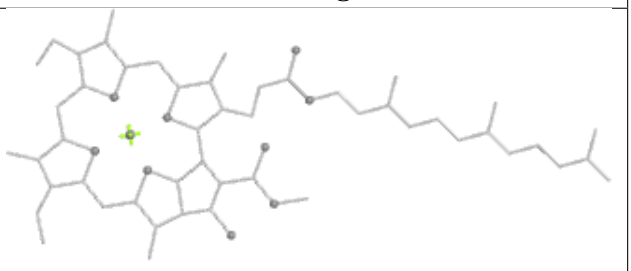
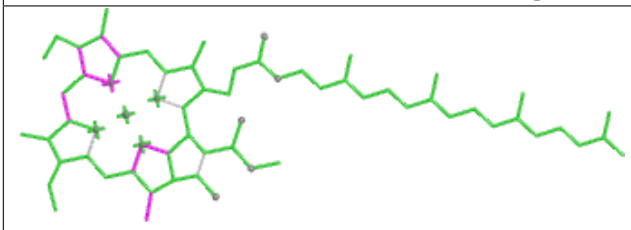
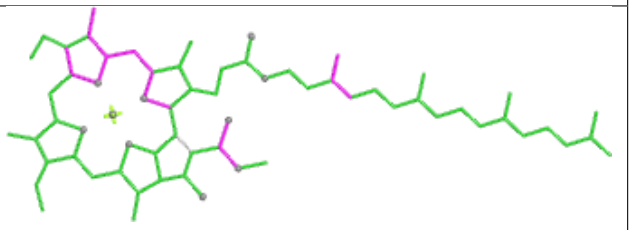


Rings

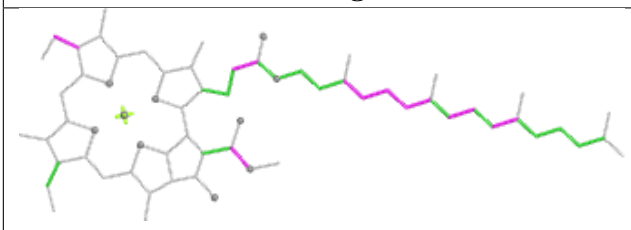
Ligand CLA 1 510



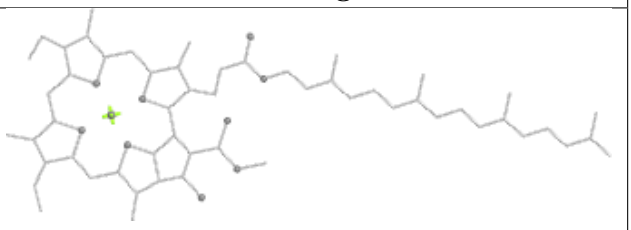
Bond lengths



Bond angles



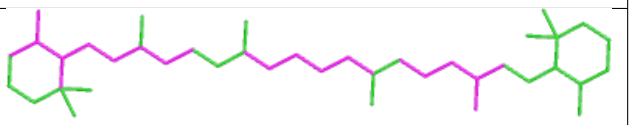
Torsions



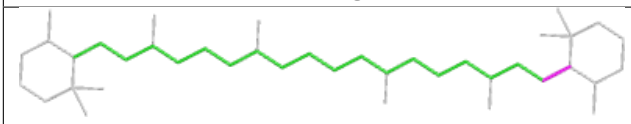
Rings

Ligand BCR r 524

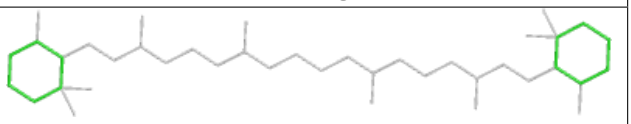
Bond lengths



Bond angles

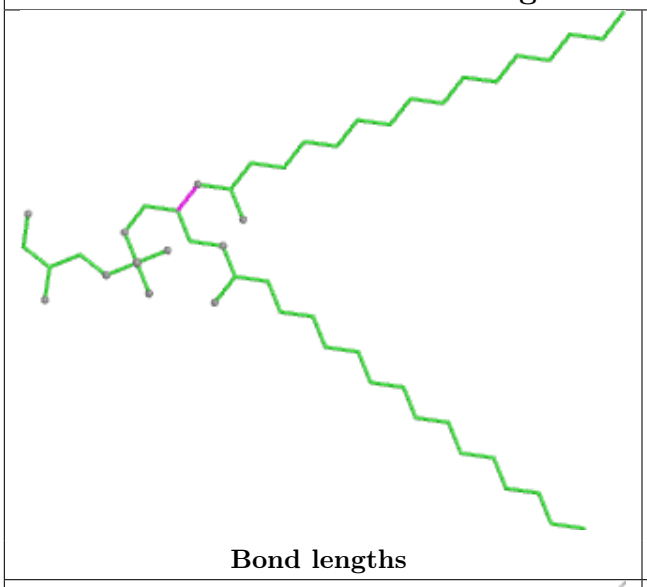


Torsions



Rings

Ligand LHG e 5009



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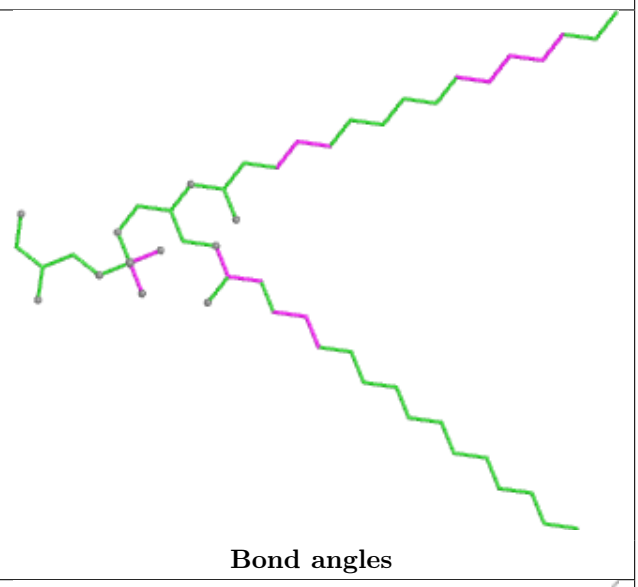
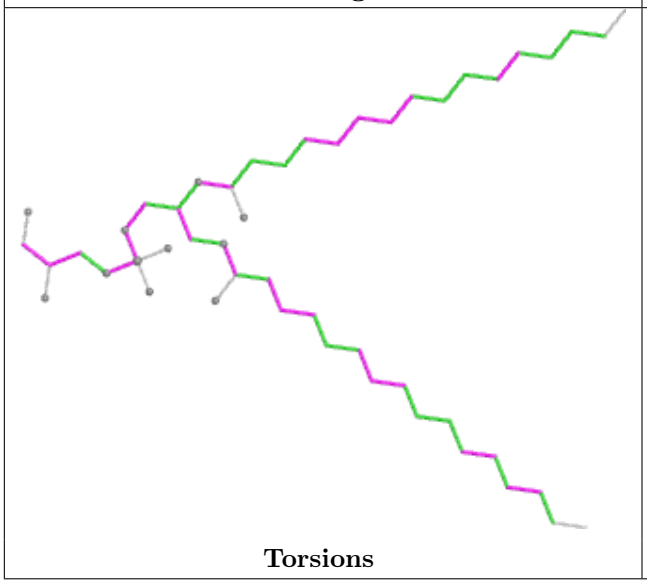


Bond angles



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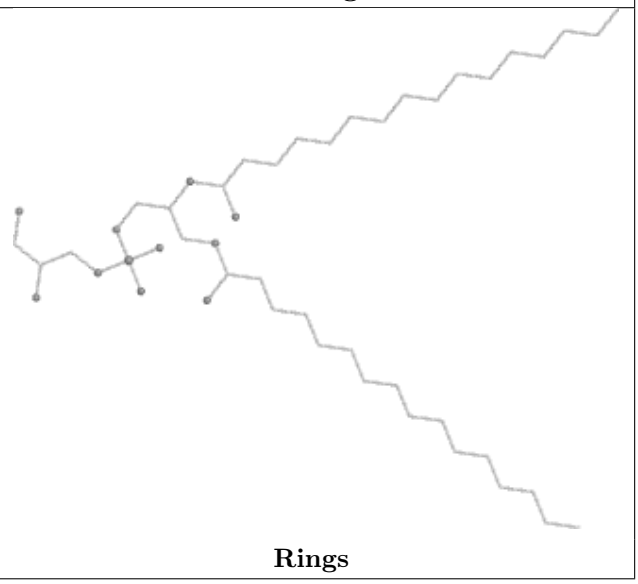
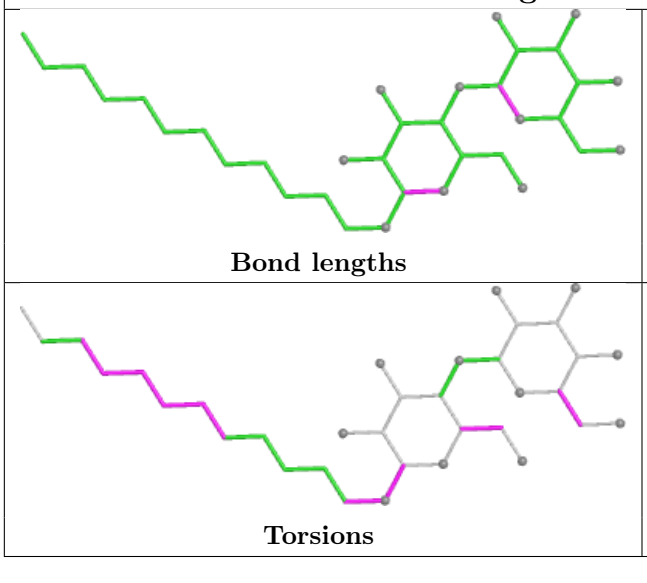


Rings

Ligand LMU f 1843



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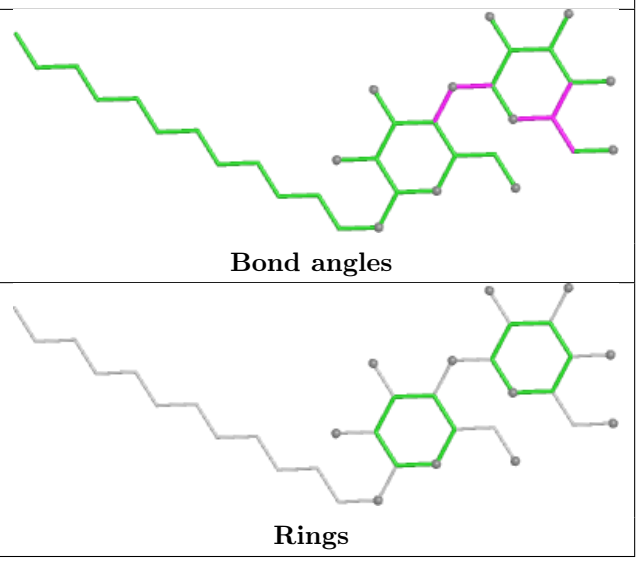
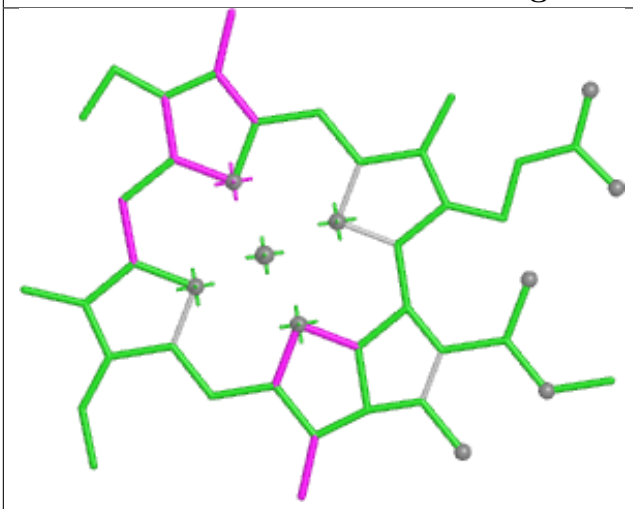


Bond angles

Torsions

Rings

Ligand CLA s 504



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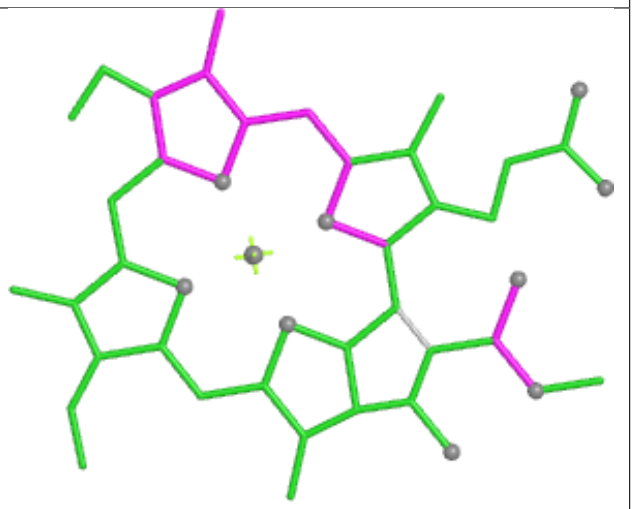
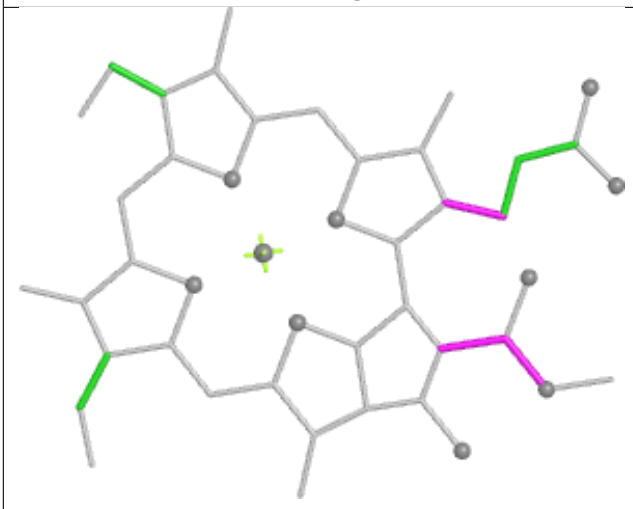


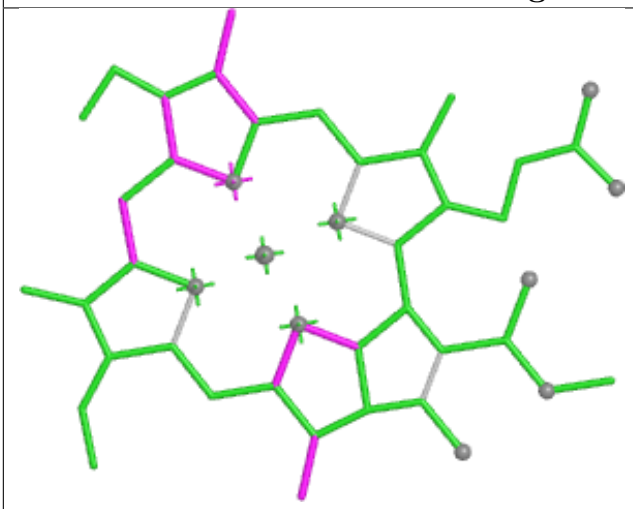
Bond angles



Torsions

Rings

Ligand CLA 1 516



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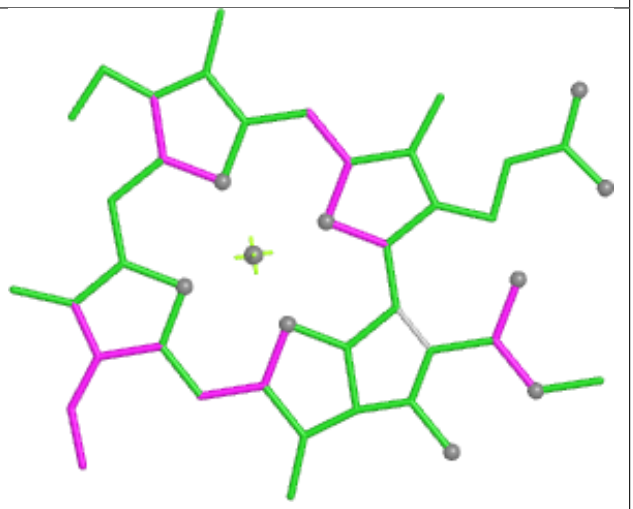

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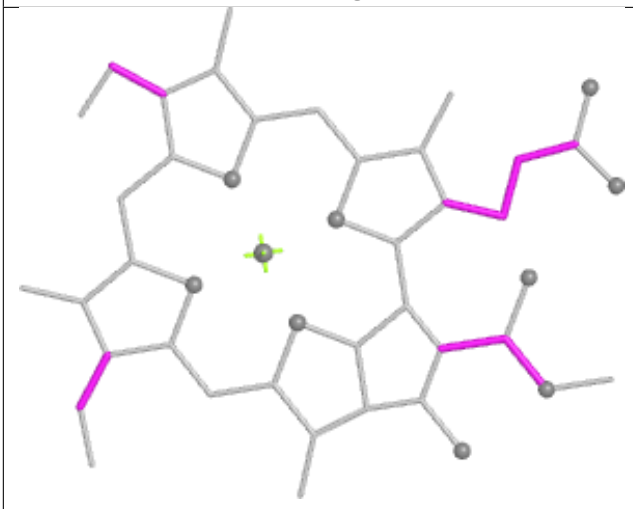
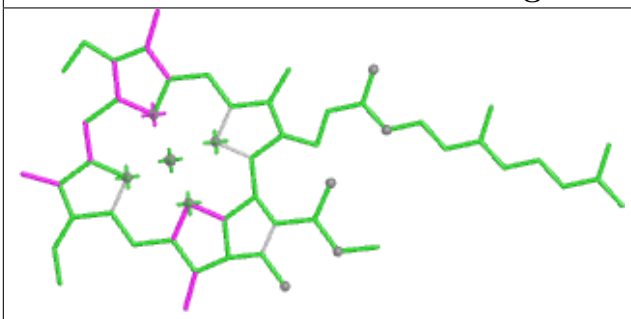


Torsions

Rings

Ligand CLA Y 513



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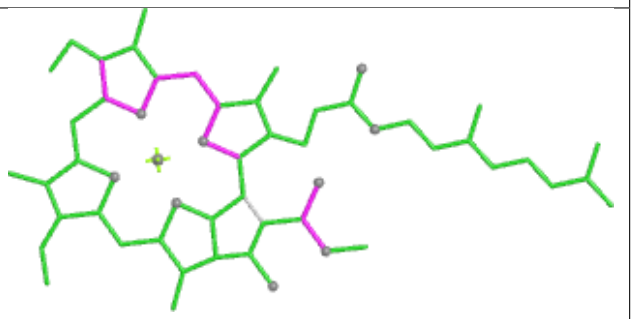
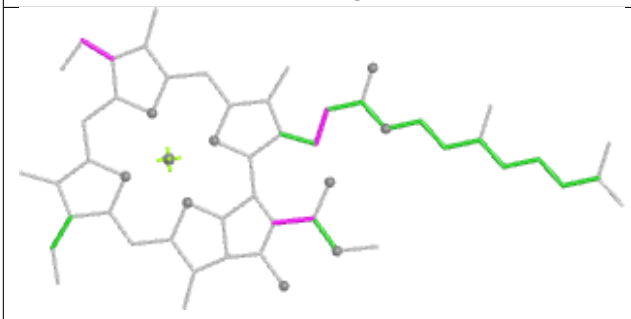
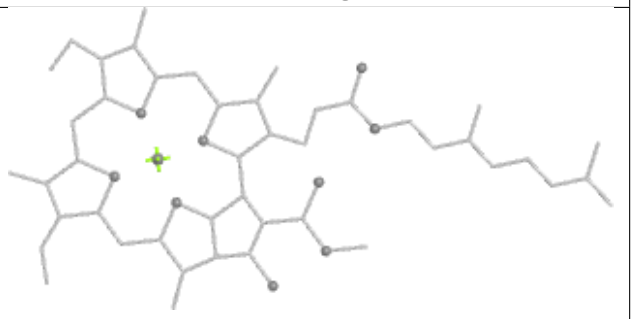


Bond angles

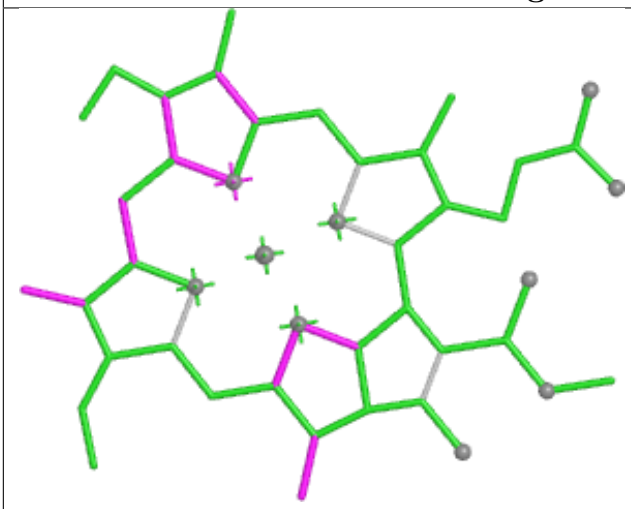


Torsions



Rings

Ligand CLA b 513



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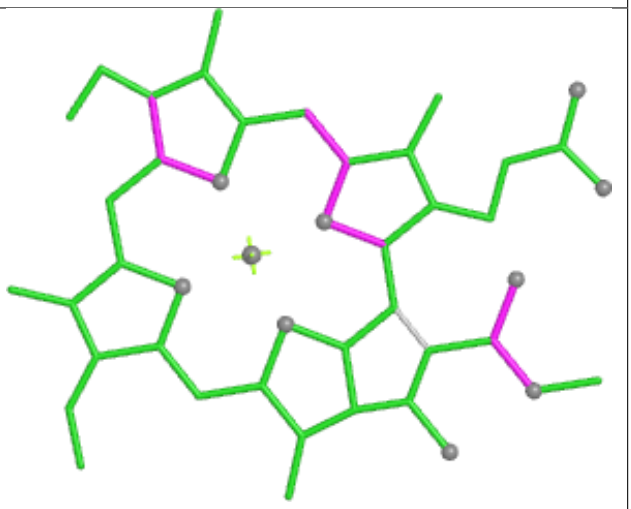
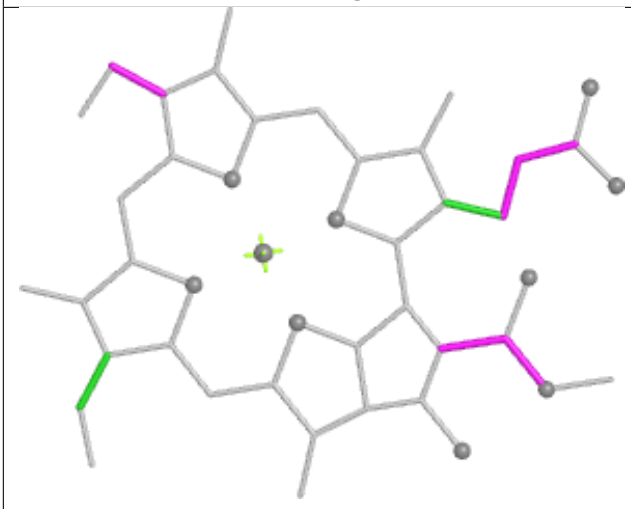


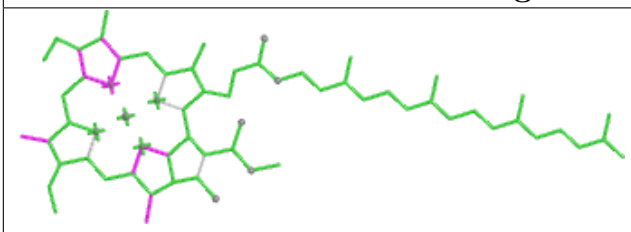
Bond angles



Torsions

Rings

Ligand CLA G 1123



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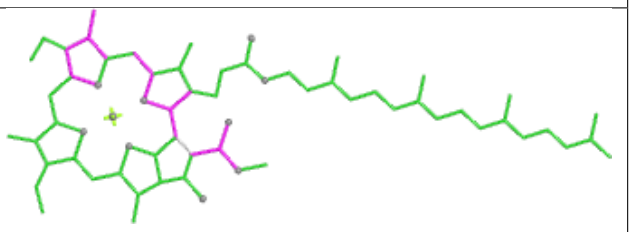

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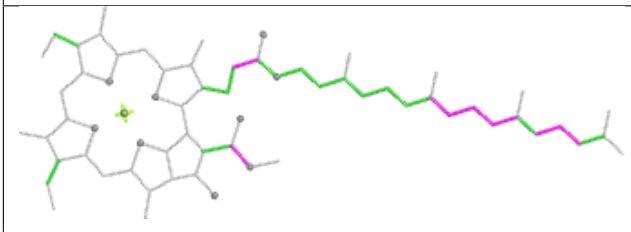
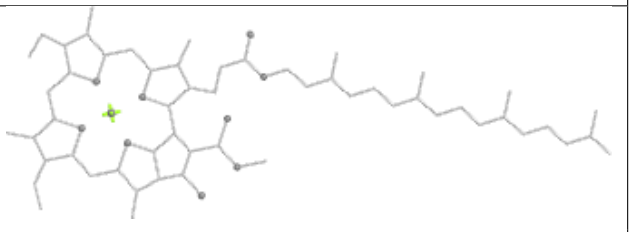
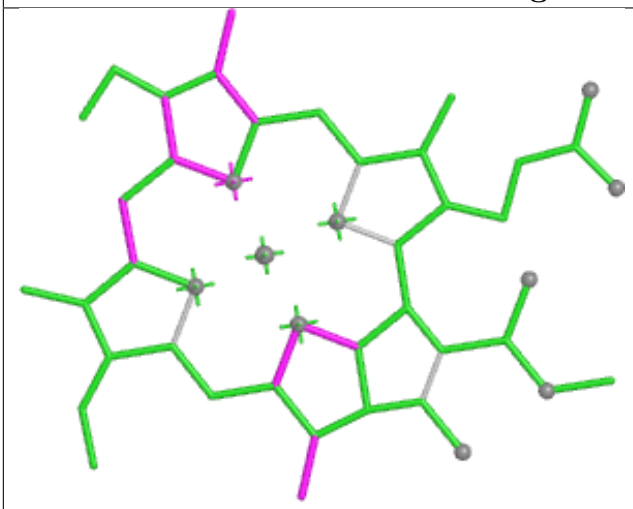


Torsions



Rings

Ligand CLA r 516



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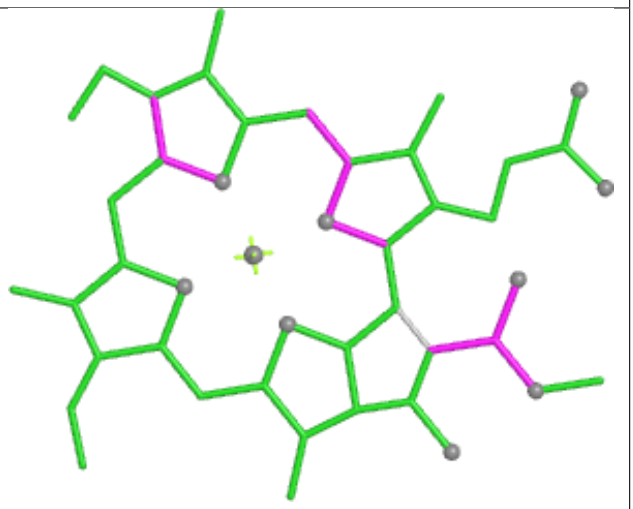

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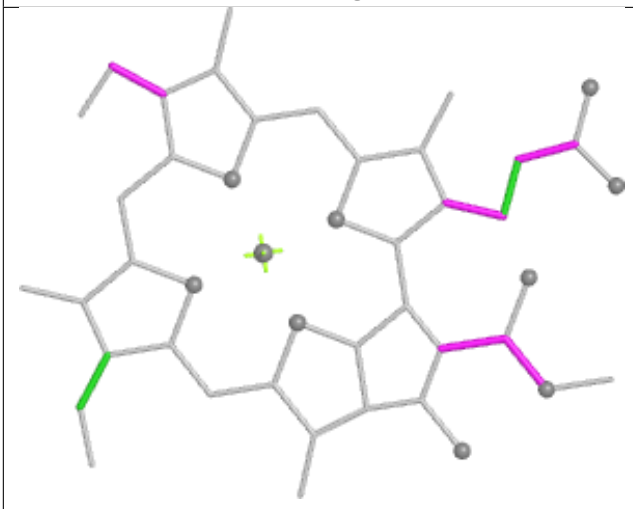
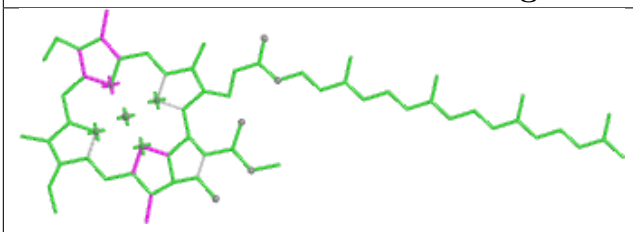


Torsions

Rings

Ligand CLA e 1011



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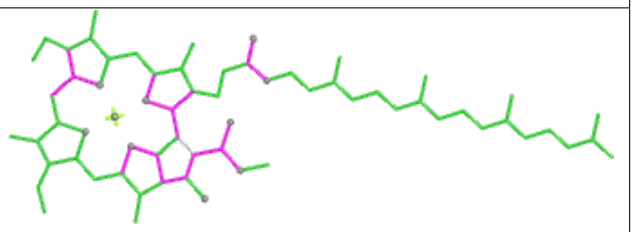
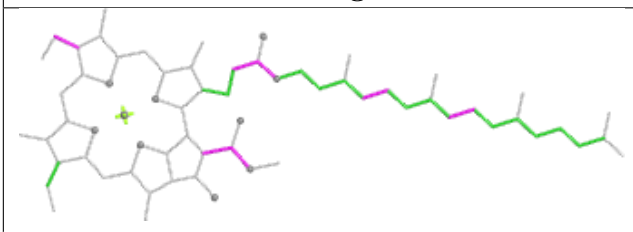
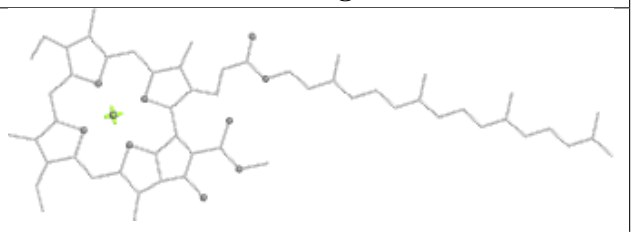


Bond angles

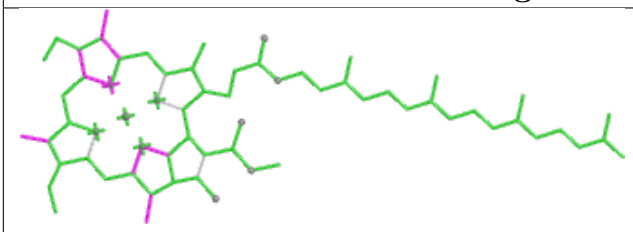


Torsions



Rings

Ligand CLA G 1237



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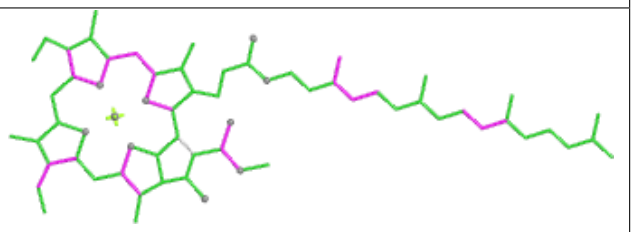

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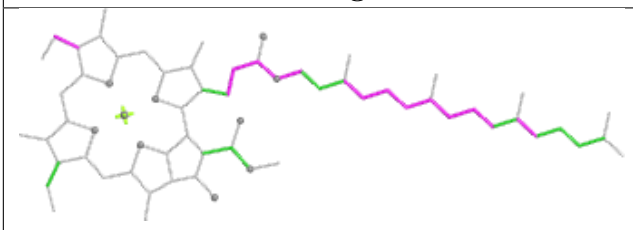

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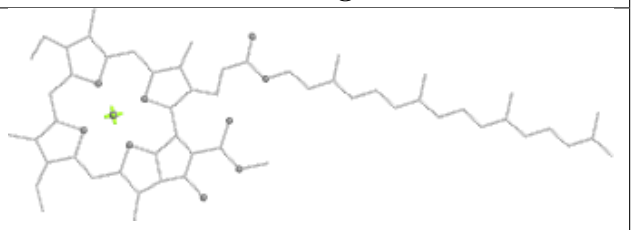
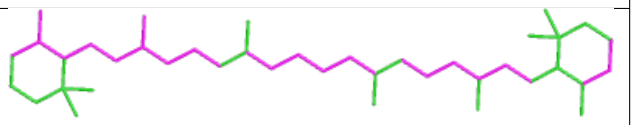


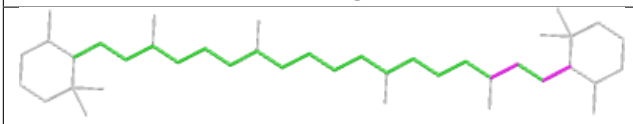
Rings

Ligand BCR 6 523

Bond lengths



Bond angles



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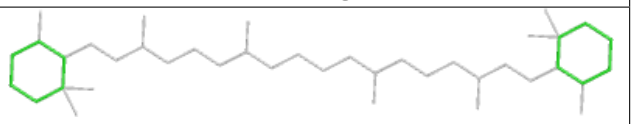
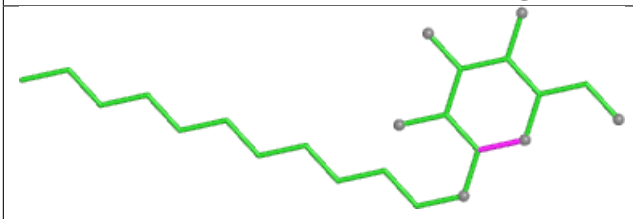


Rings

Ligand LMU e 1849



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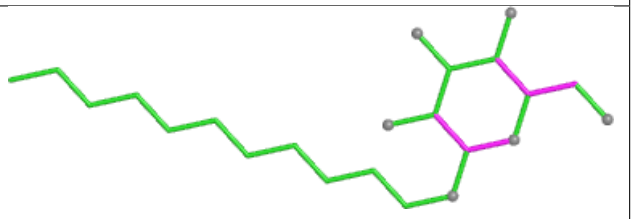
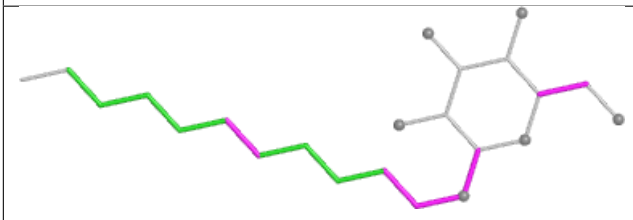


Bond angles



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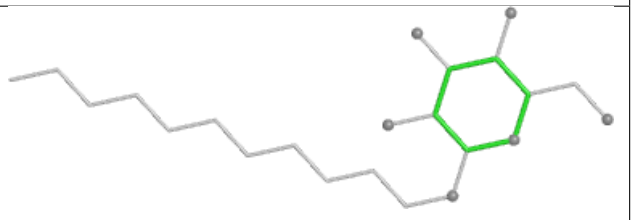
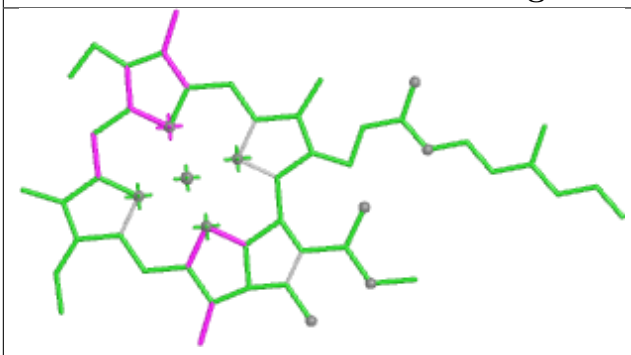


Rings

Ligand CLA q 512



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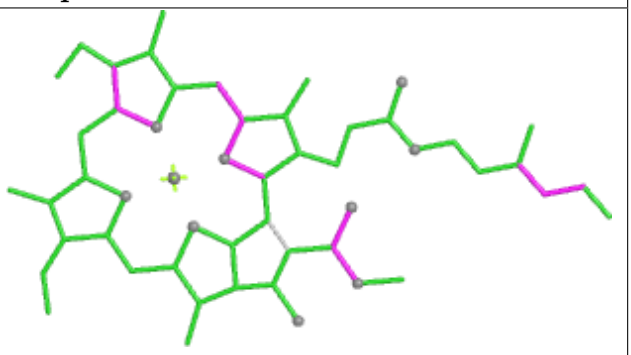
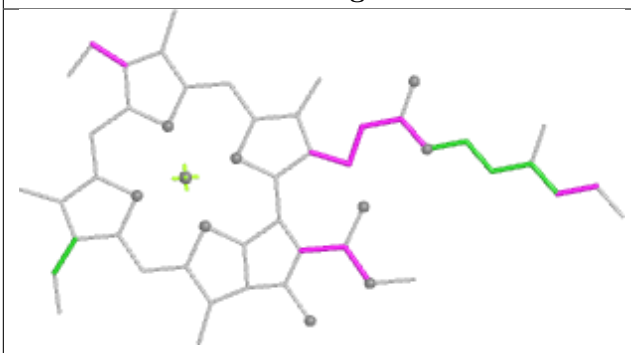


Bond angles



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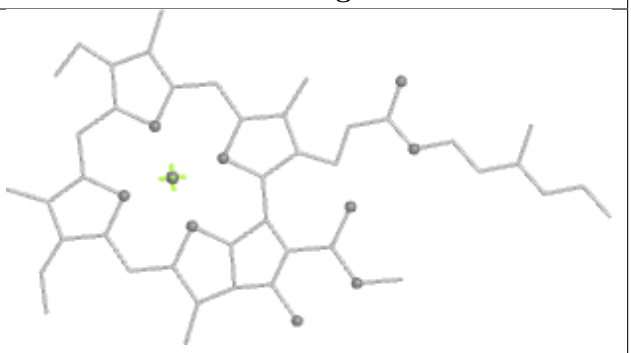
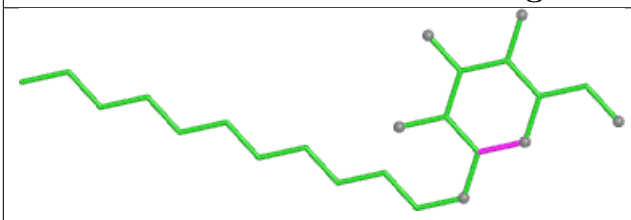
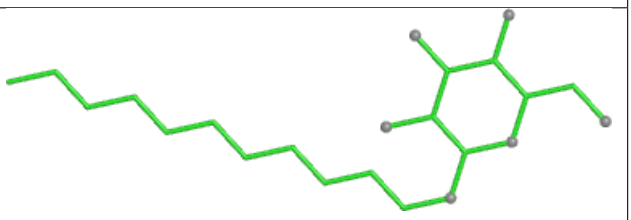


Rings

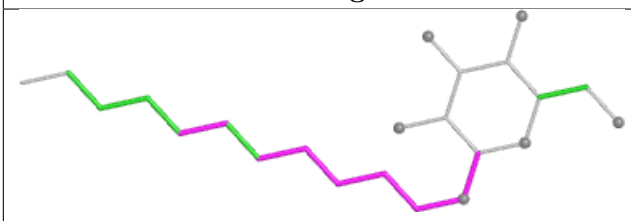
Ligand LMU r 901



Bond lengths



Bond angles



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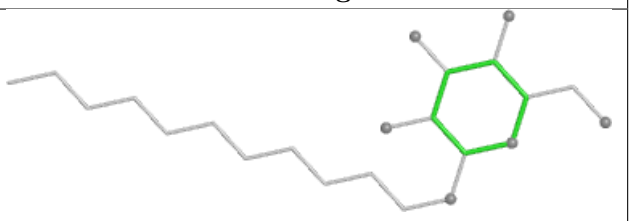
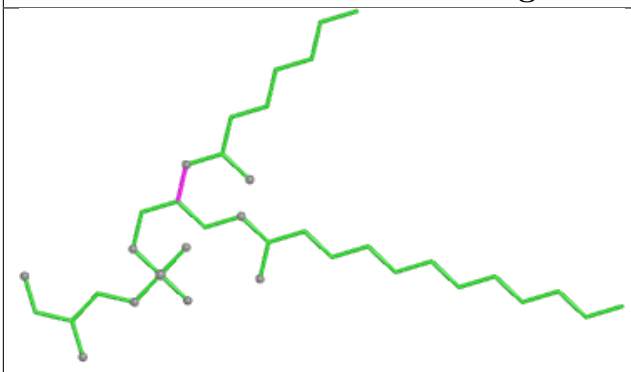
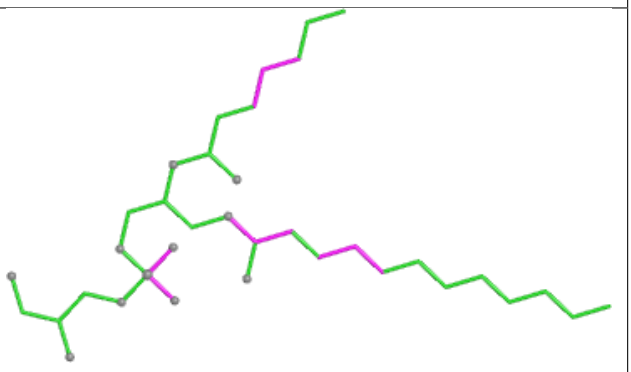


Rings

Ligand LHG e 5004



Bond lengths



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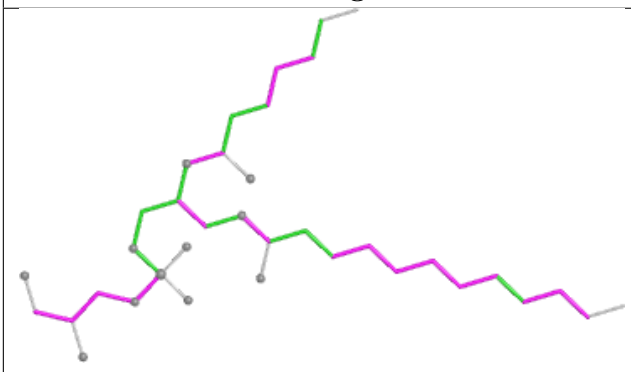
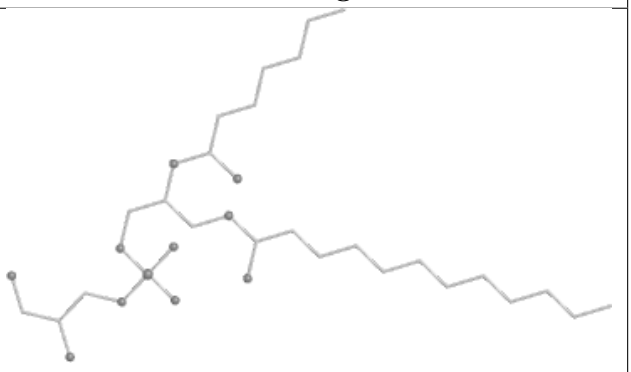
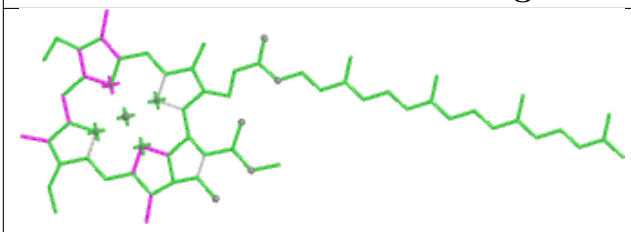


Torsions



Rings

Ligand CLA G 1140



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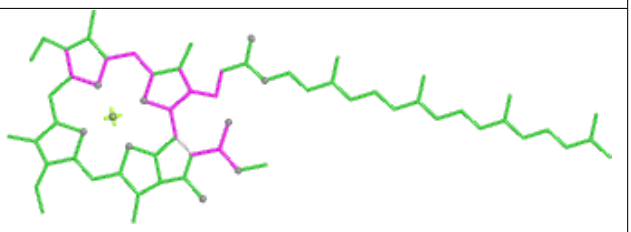

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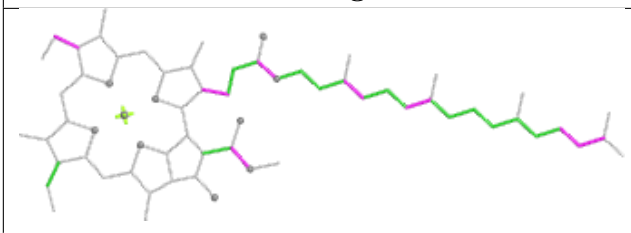

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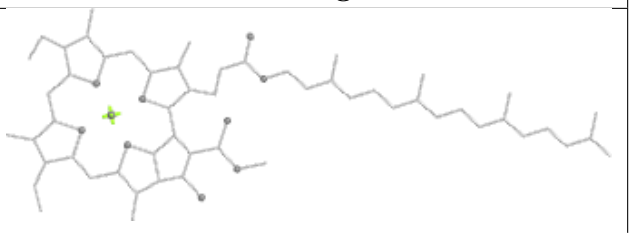
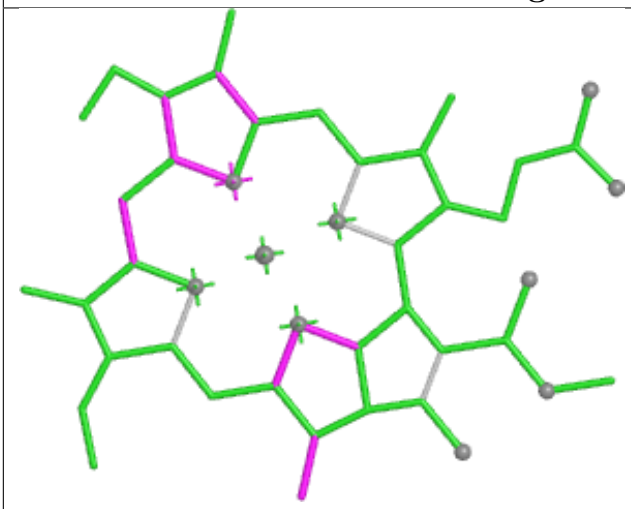


Rings

Ligand CLA 6 516



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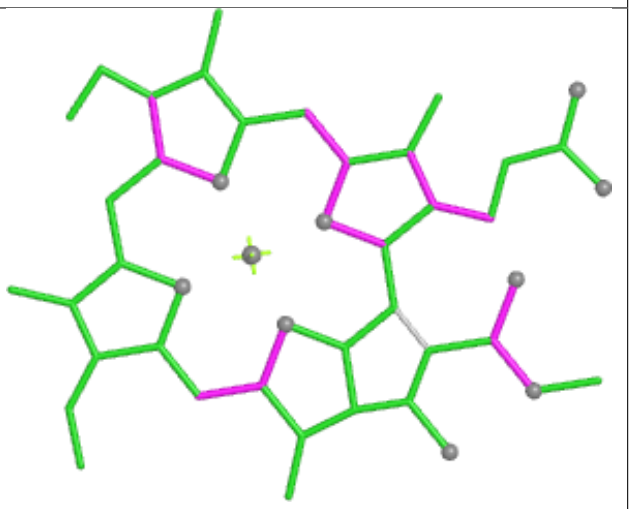

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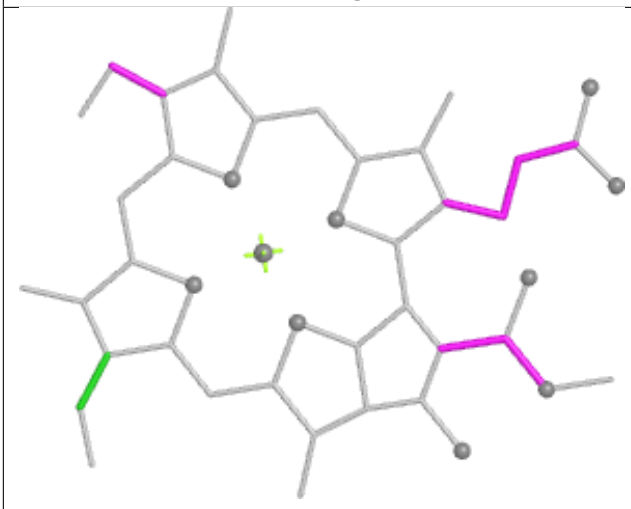
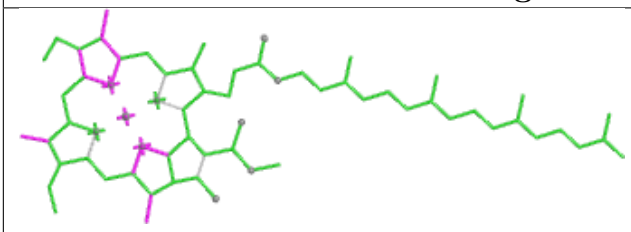


Torsions

Rings

Ligand CLA H 1206



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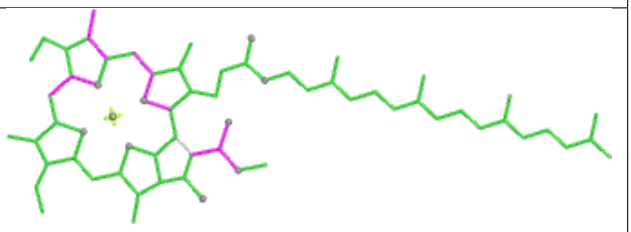

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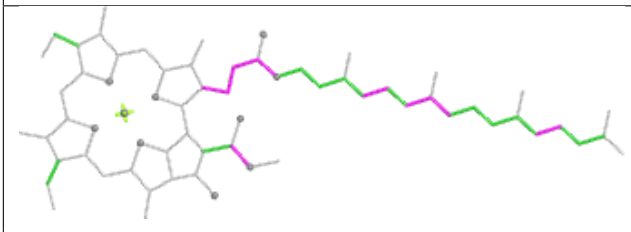

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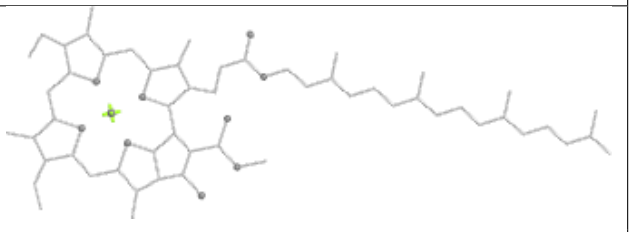
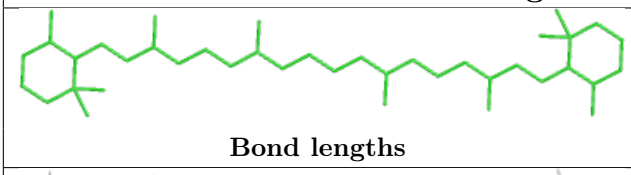


Rings

Ligand BCR q 521



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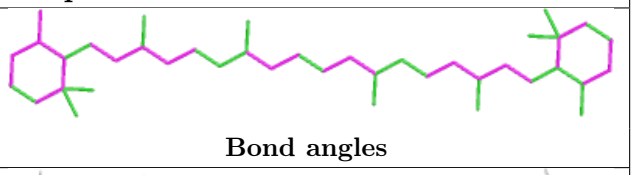

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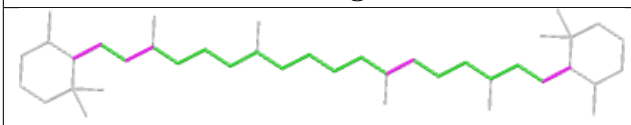

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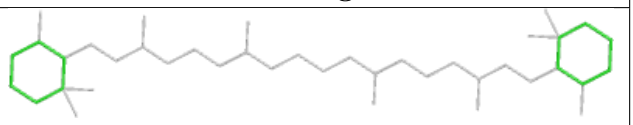

Rings

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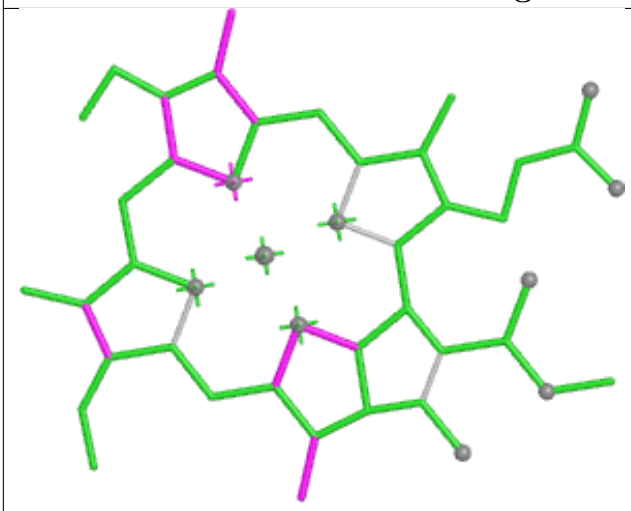

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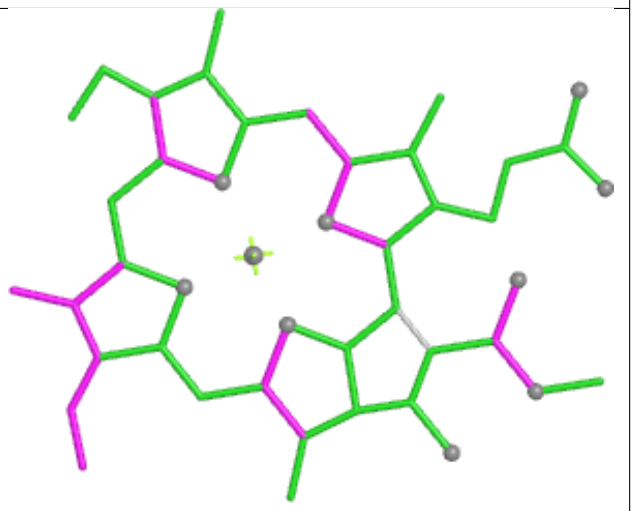

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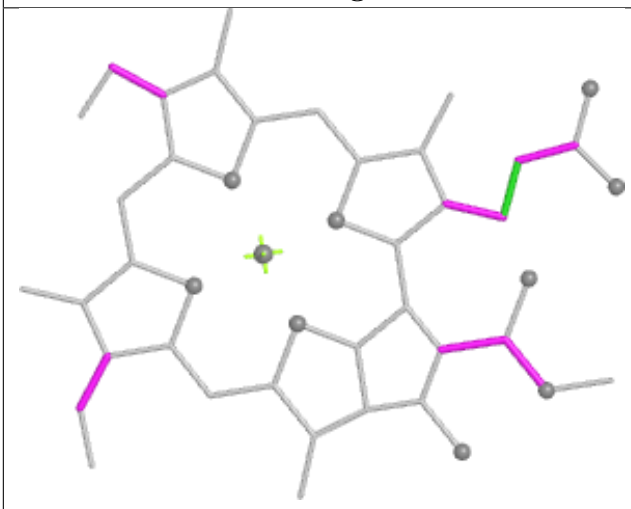

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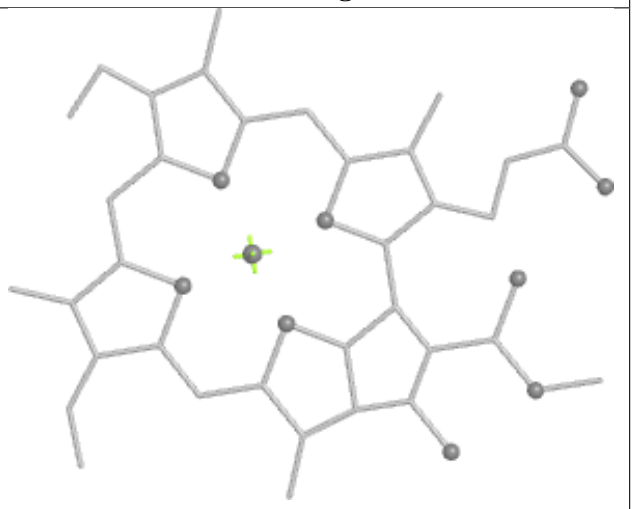
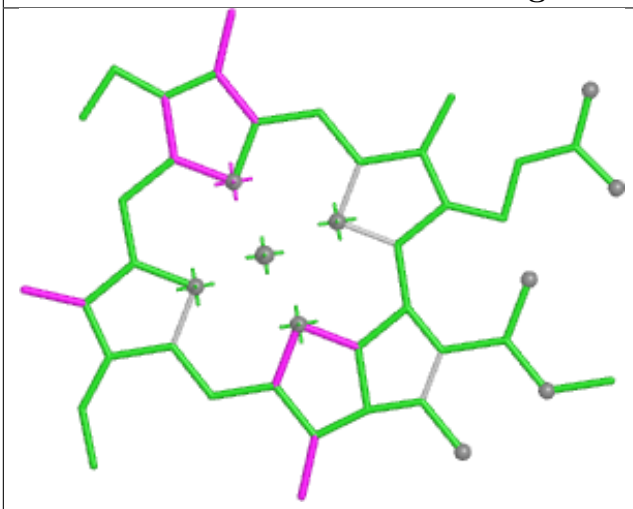


Rings

Ligand CLA 5 508



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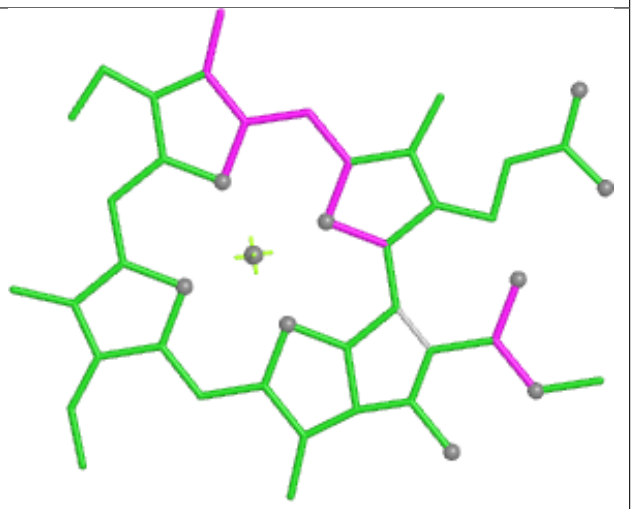

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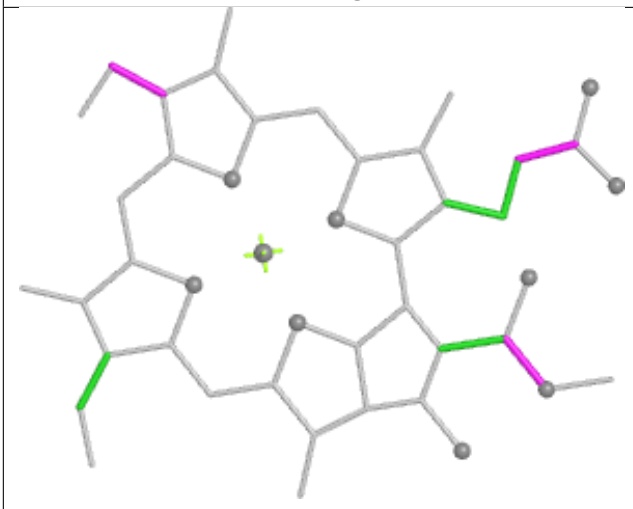
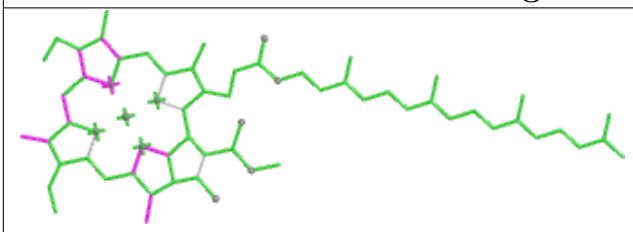


Torsions

Rings

Ligand CLA f 1231



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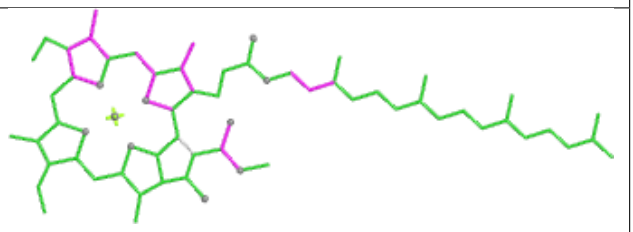

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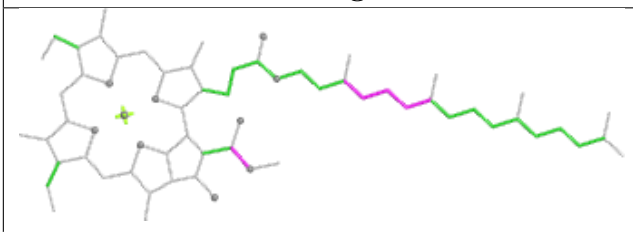

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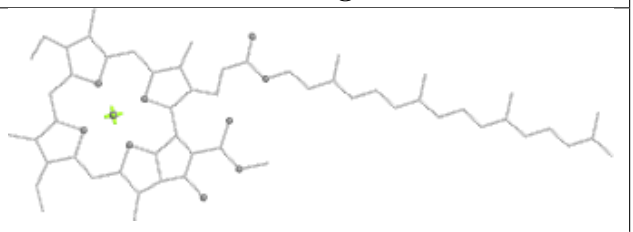
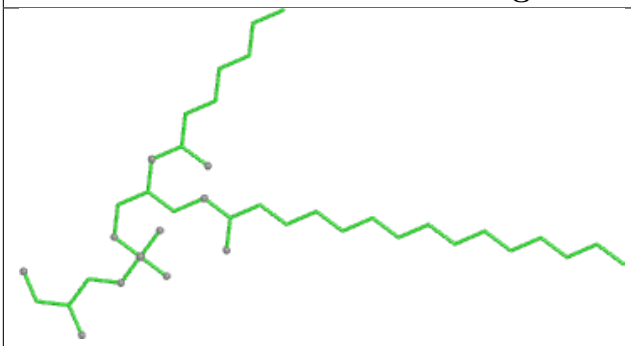


Rings

Ligand LHG H 1842



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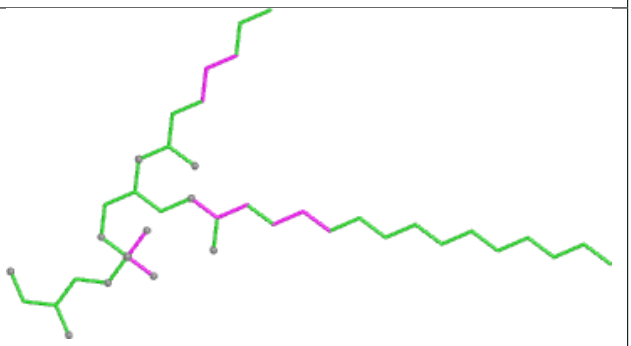

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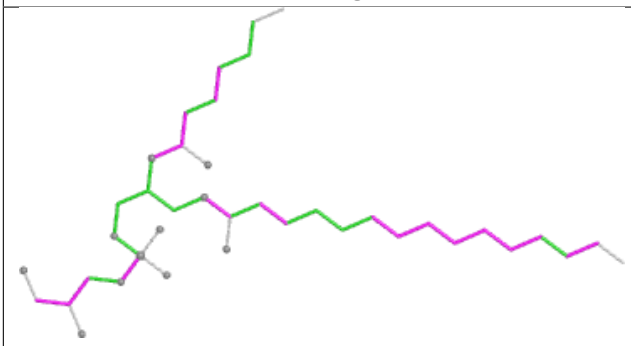

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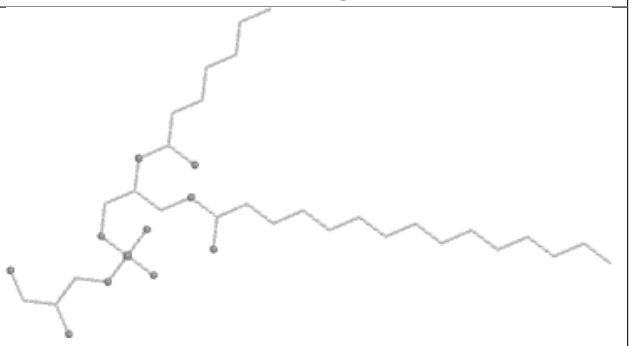
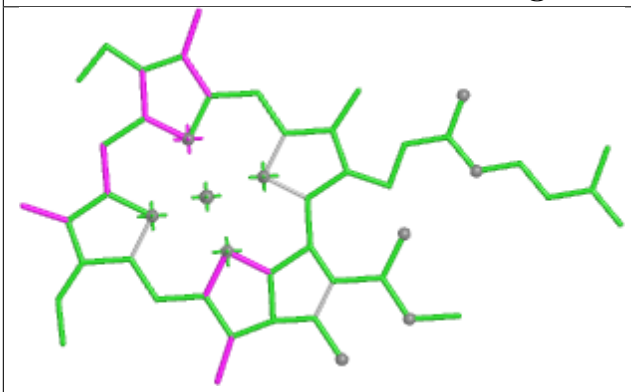


Rings

Ligand CLA 5 502



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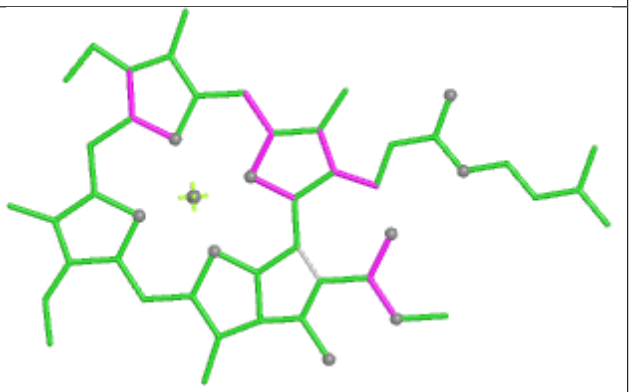
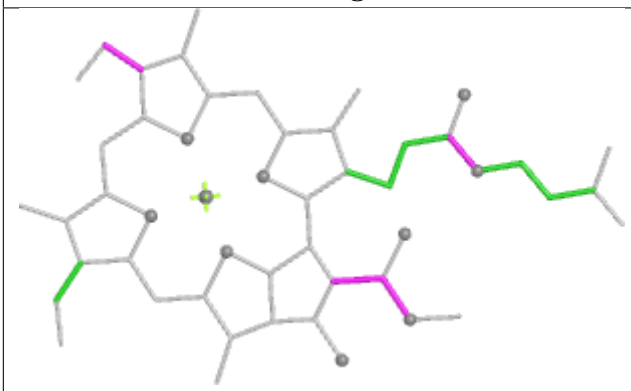


Bond angles



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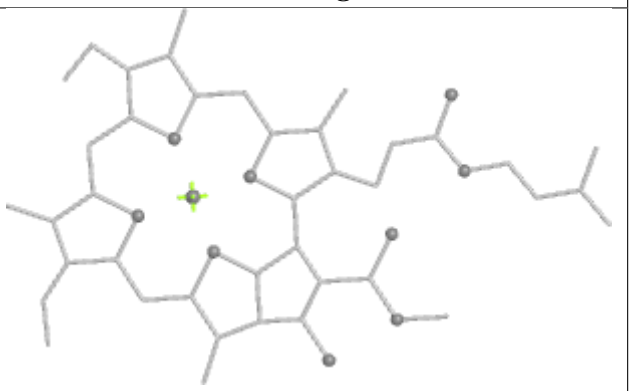
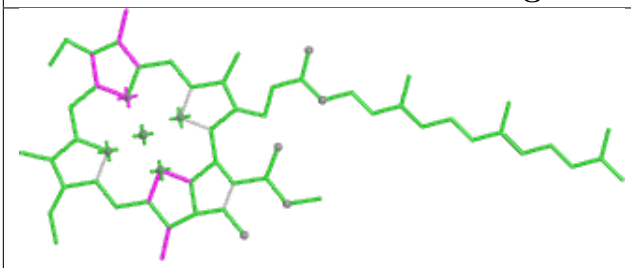
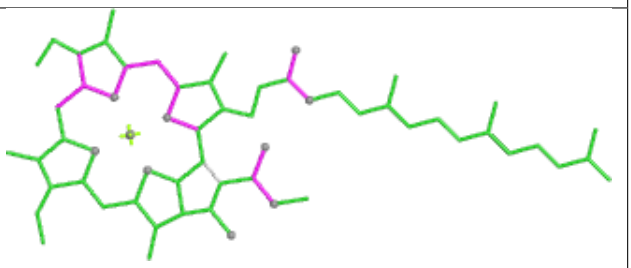
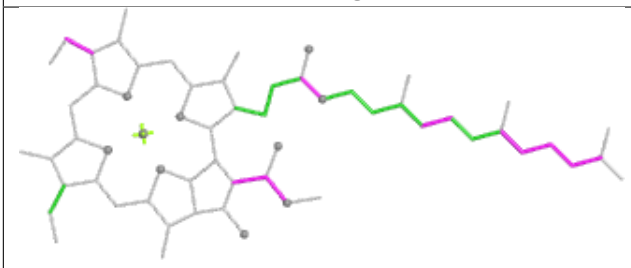
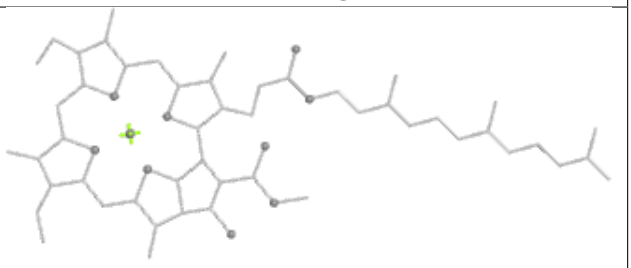


Rings

Ligand CLA Y 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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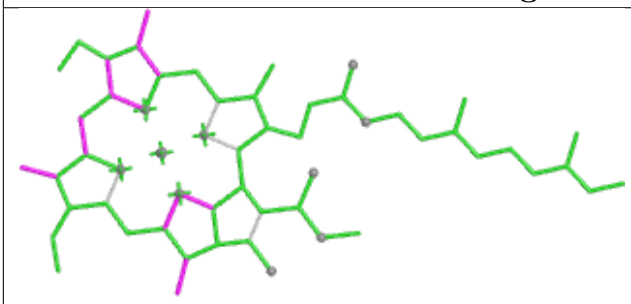
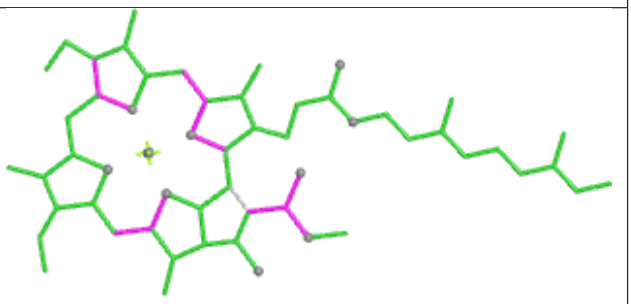
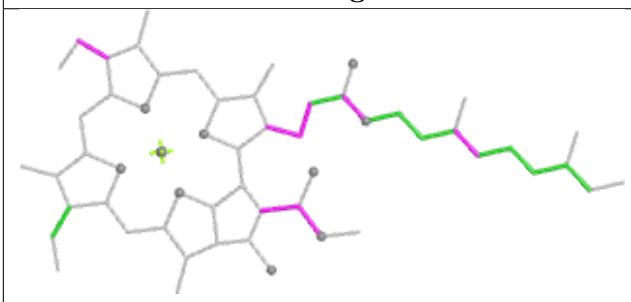
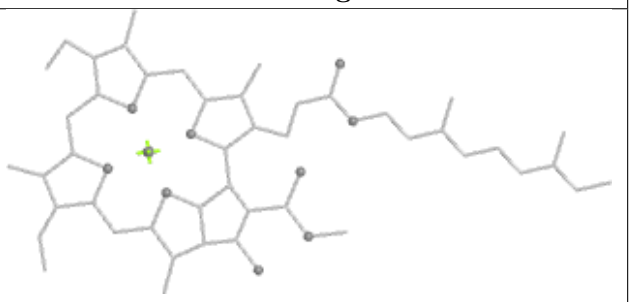
 Bond lengths	 Bond angles
 Torsions	 Rings

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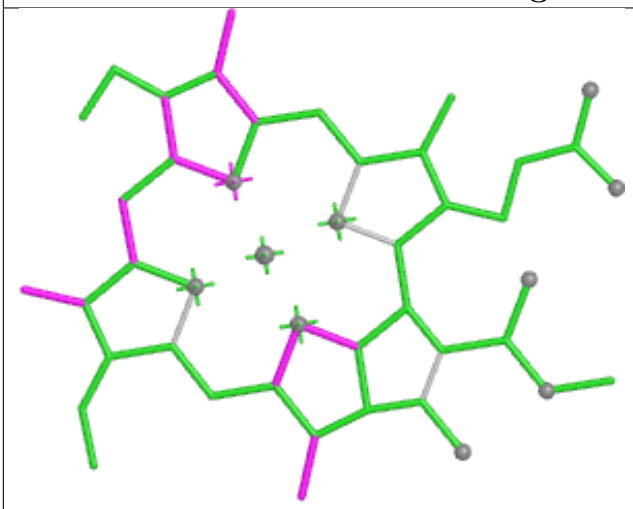
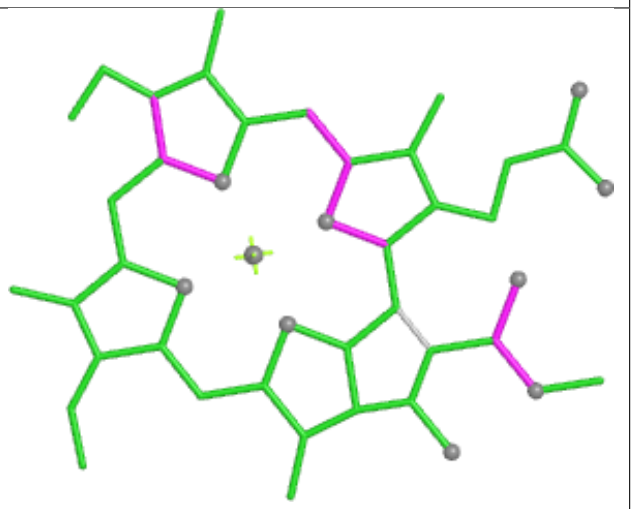
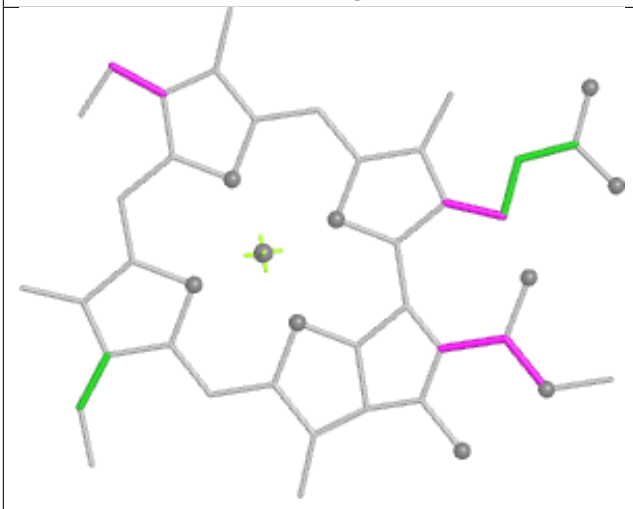


Bond lengths



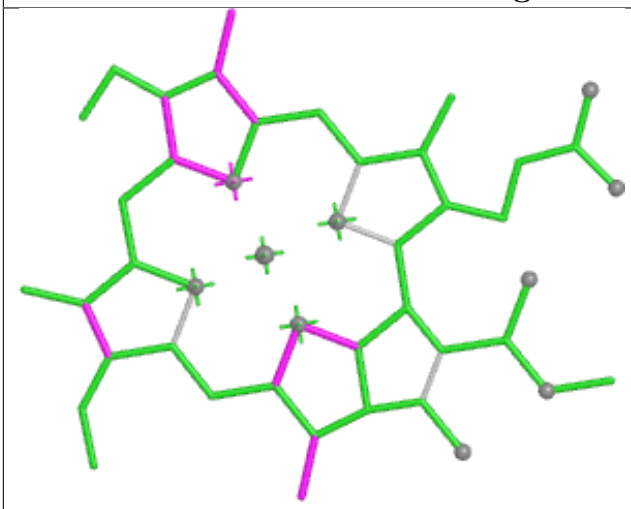
Bond angles



Torsions

Rings

Ligand CLA m 1105



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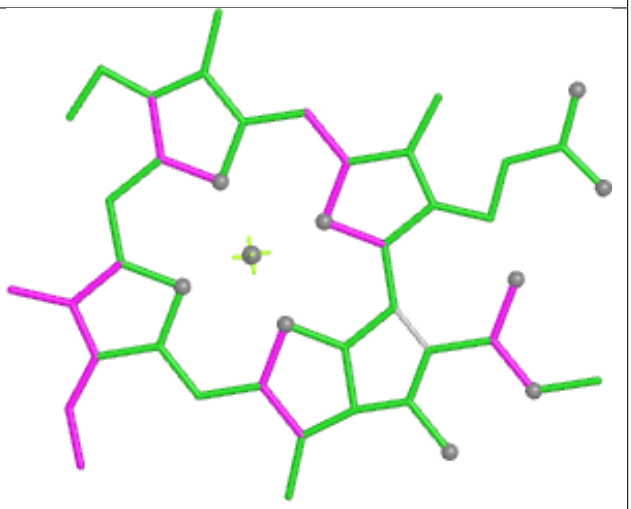

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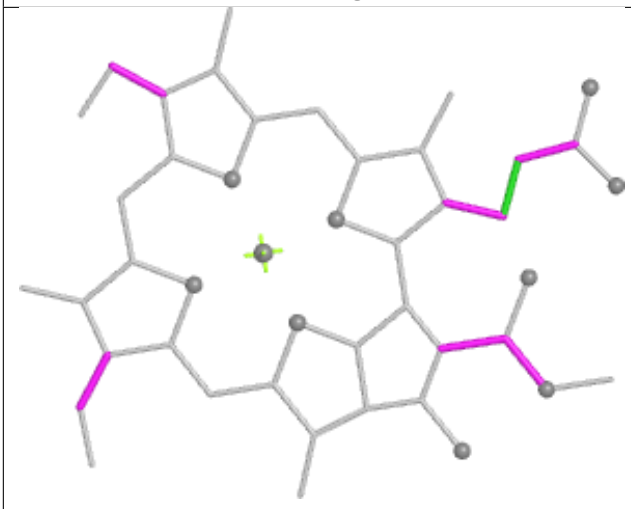
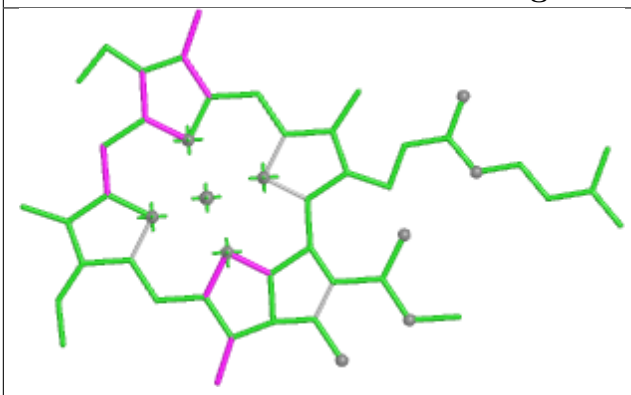


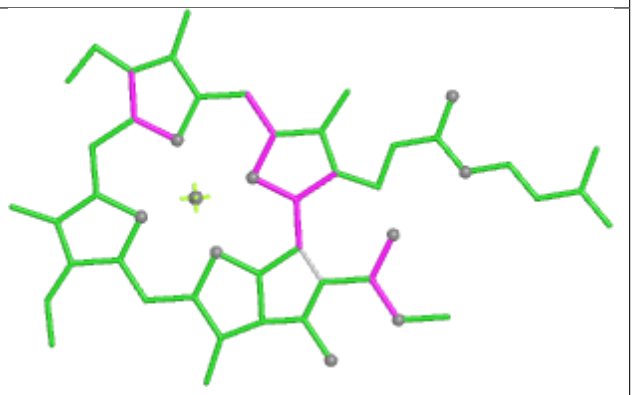
Torsions

Rings

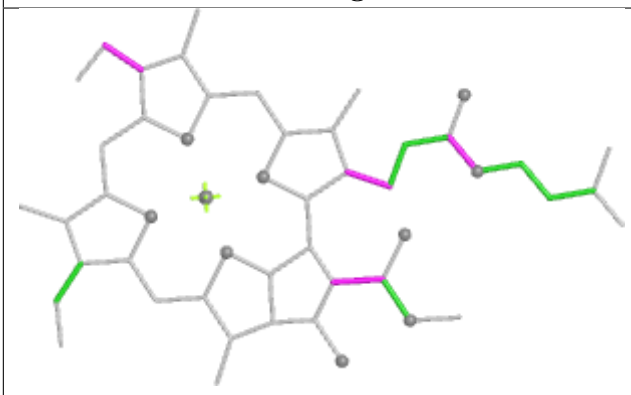
Ligand CLA t 502



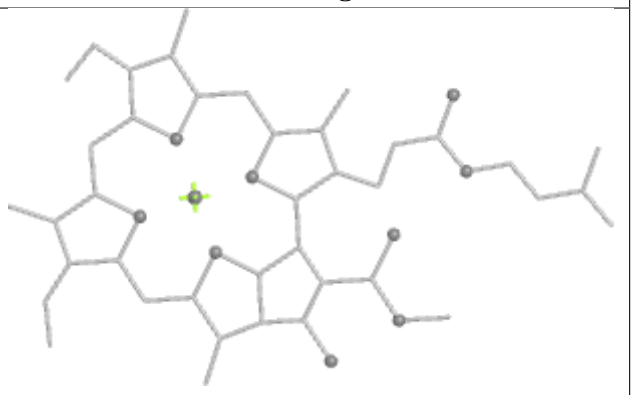
Bond lengths



Bond angles

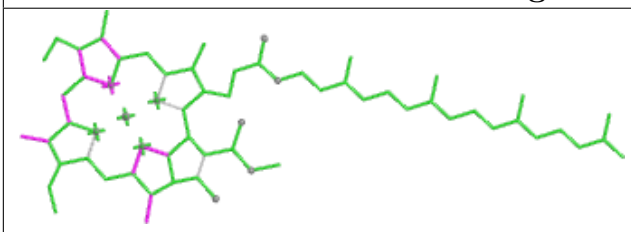


Torsions



Rings

Ligand CLA 3 501



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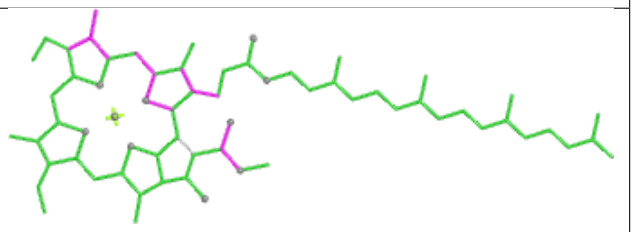
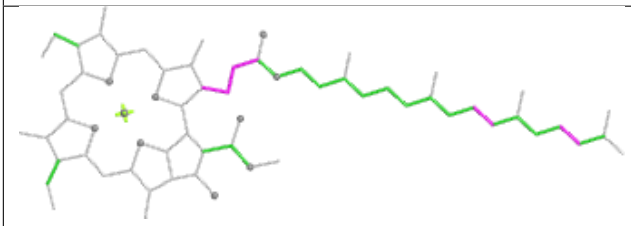


Bond angles



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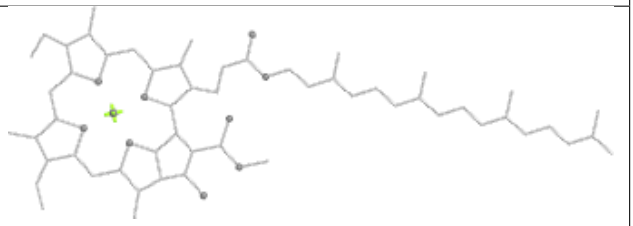
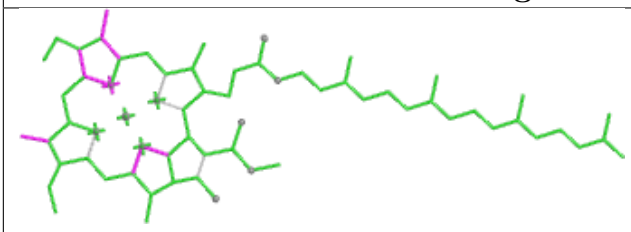


Rings

Ligand CLA G 1137



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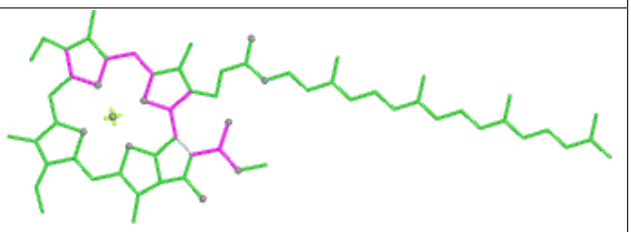
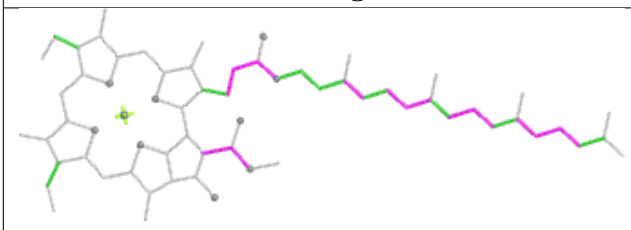
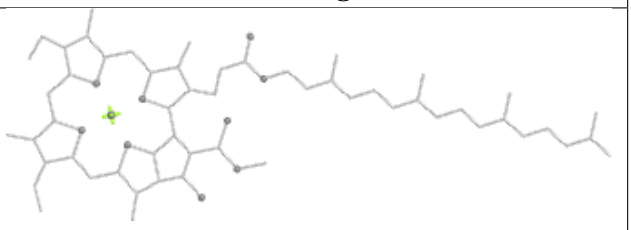


Bond angles

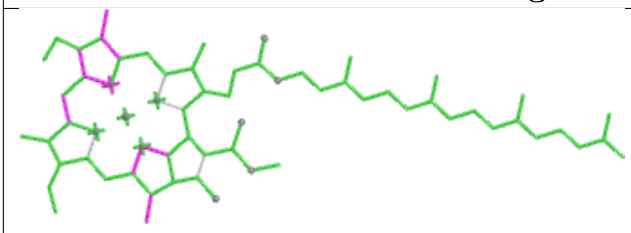


Torsions

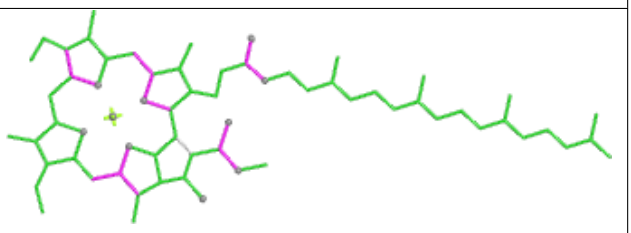


Rings

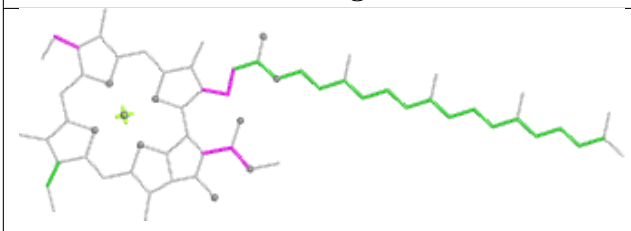
Ligand CLA a 503



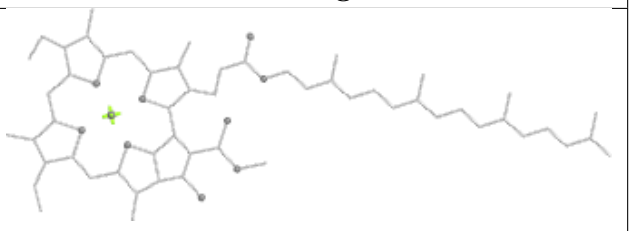
Bond lengths



Bond angles

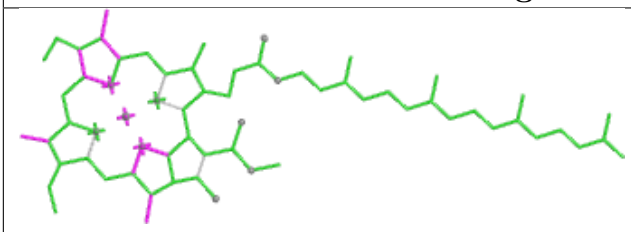


Torsions



Rings

Ligand CLA B 1021



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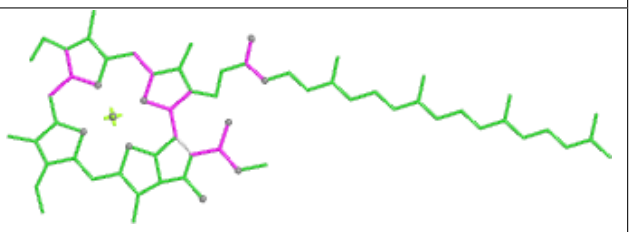
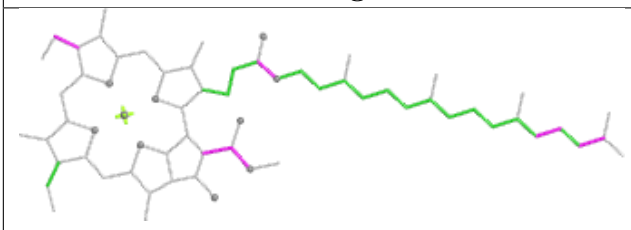
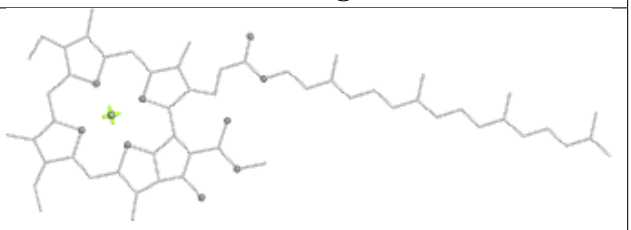


Bond angles

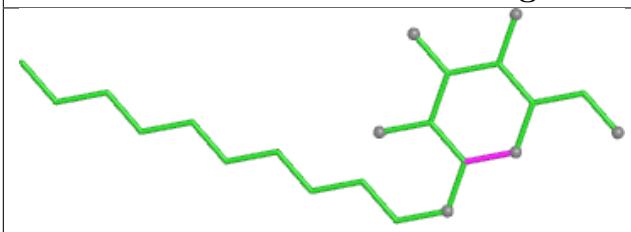


Torsions



Rings

Ligand LMU l 5105



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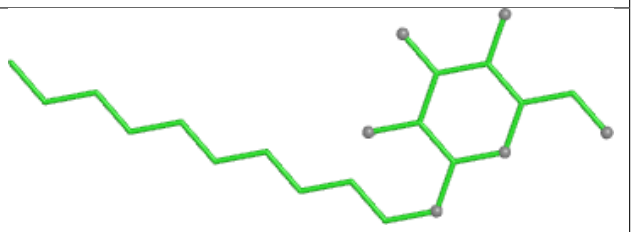
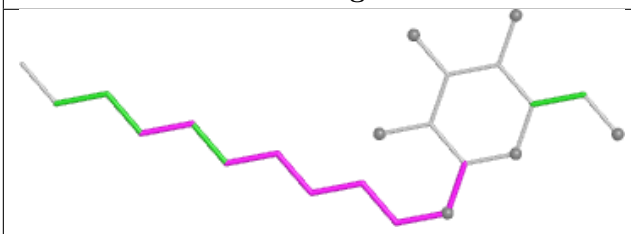
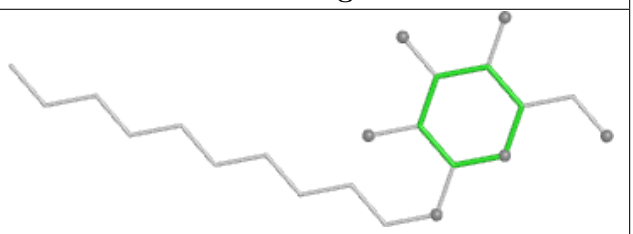


Bond angles

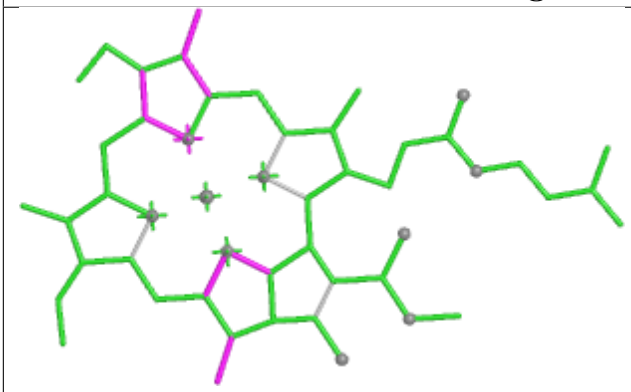


Torsions

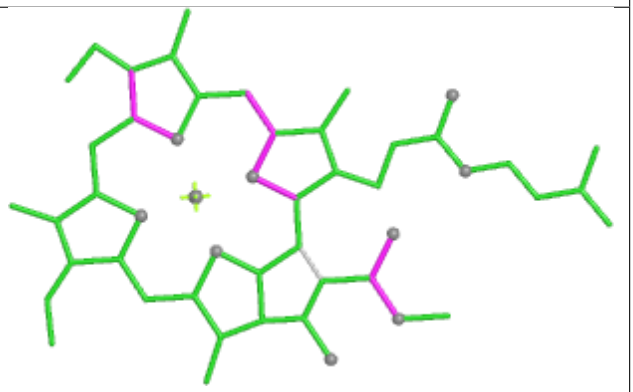


Rings

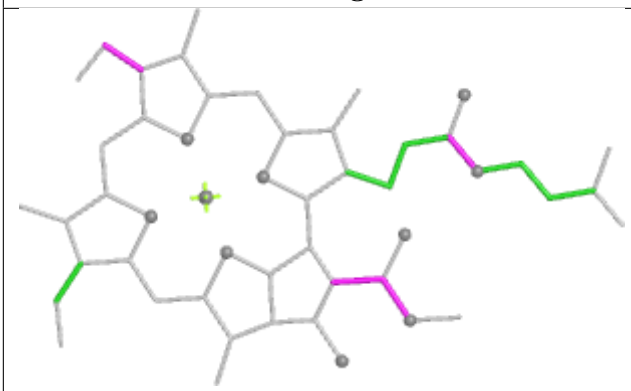
Ligand CLA v 502



Bond lengths



Bond angles



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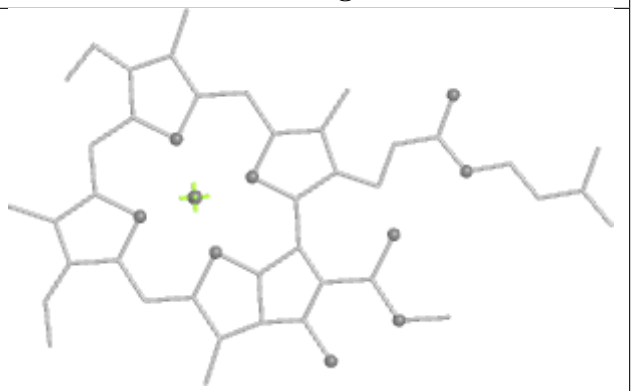
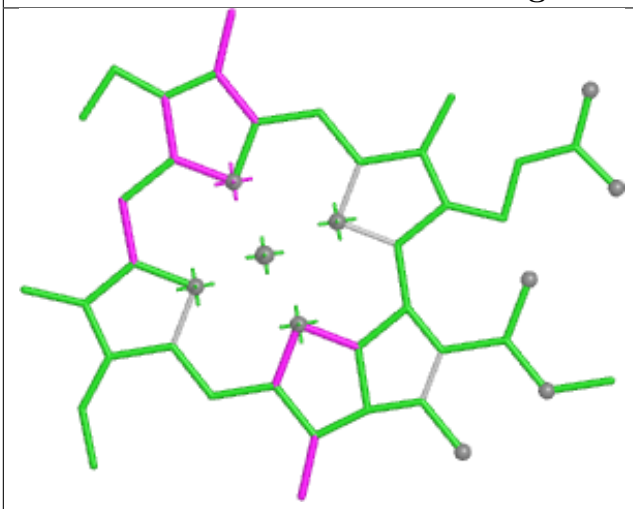
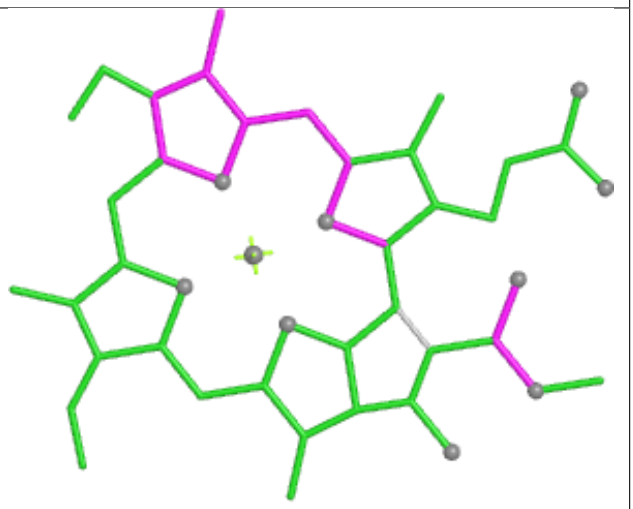


Rings

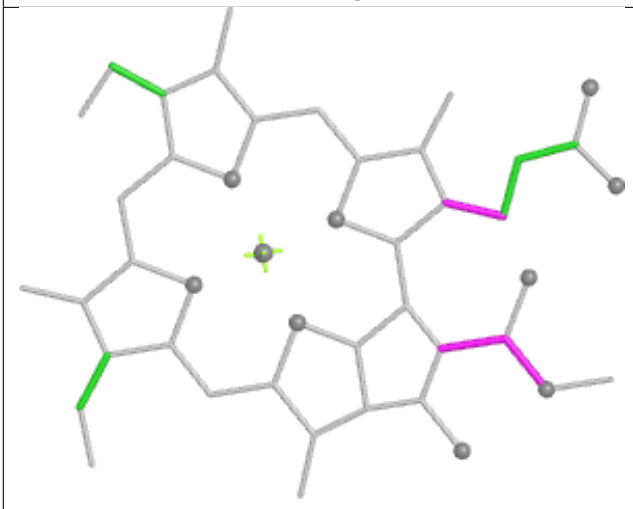
Ligand CLA 3 504



Bond lengths



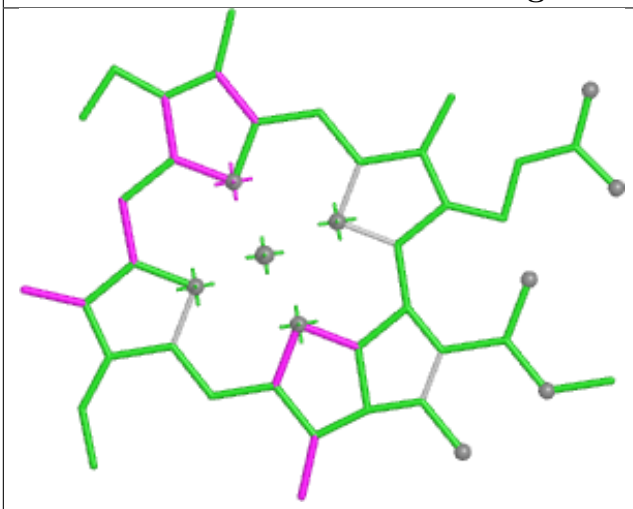
Bond angles



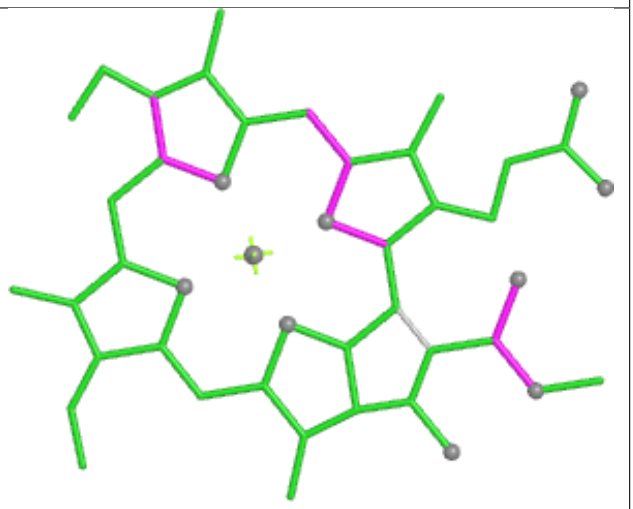
Torsions

Rings

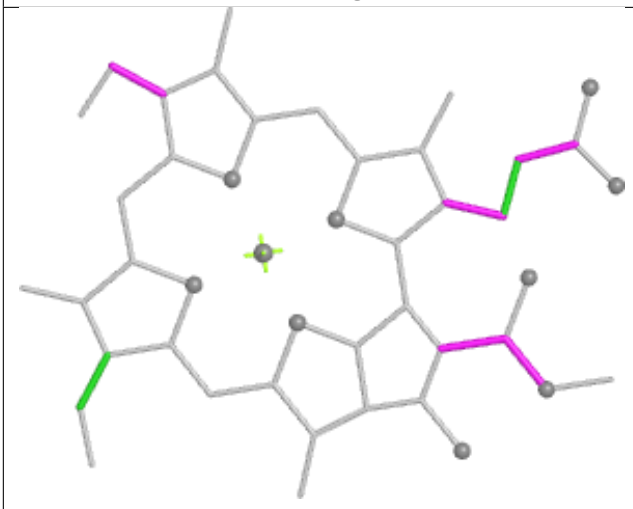
Ligand CLA d 517



Bond lengths



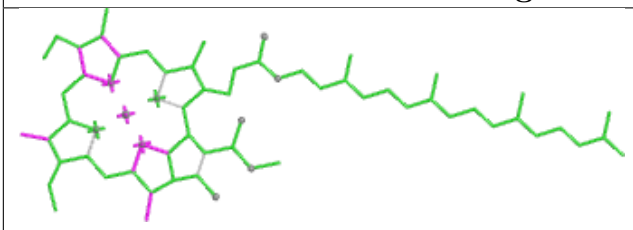
Bond angles



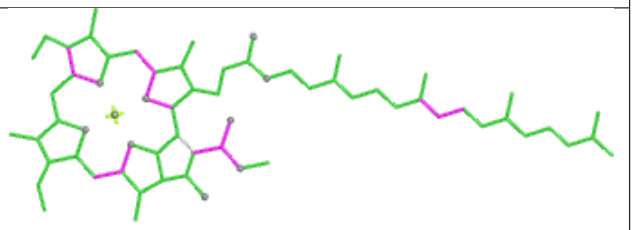
Torsions

Rings

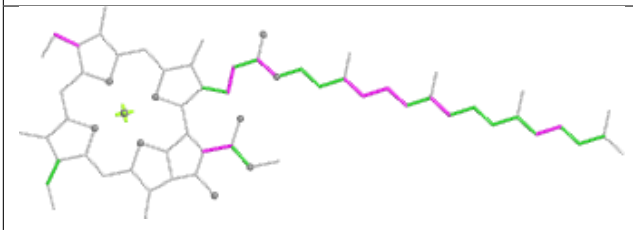
Ligand CLA B 1204



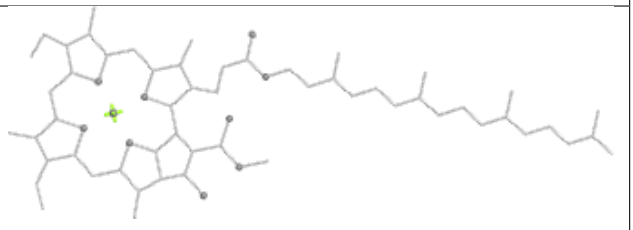
Bond lengths



Bond angles

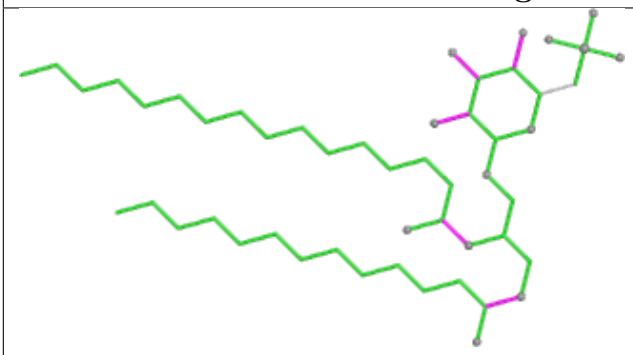


Torsions



Rings

Ligand SQD V 5216



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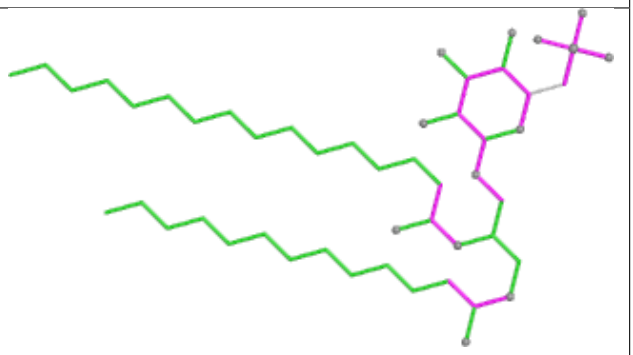
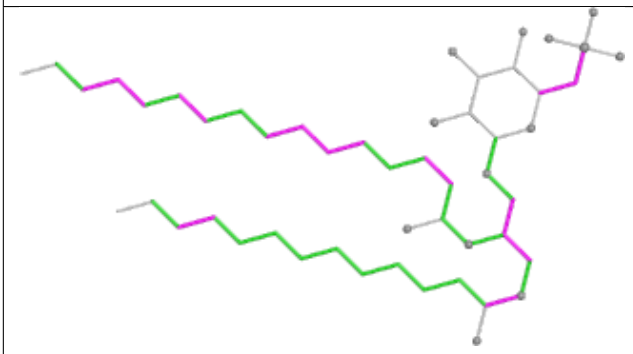
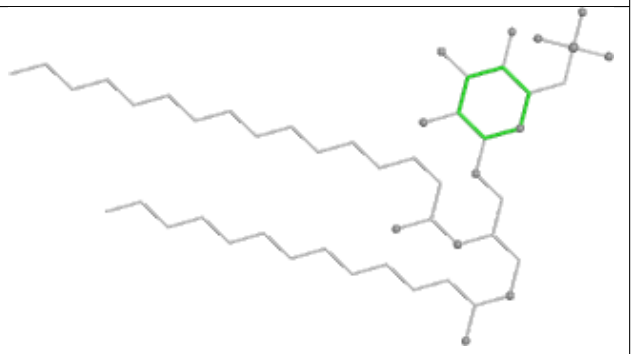


Bond angles



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

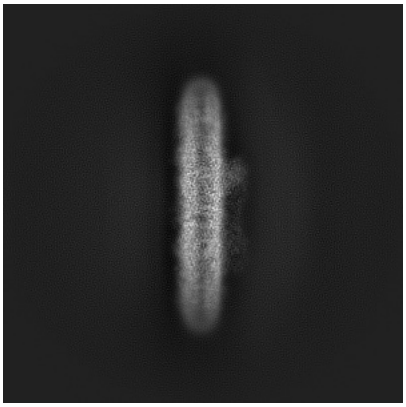
This section contains visualisations of the EMDB entry EMD-9995. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

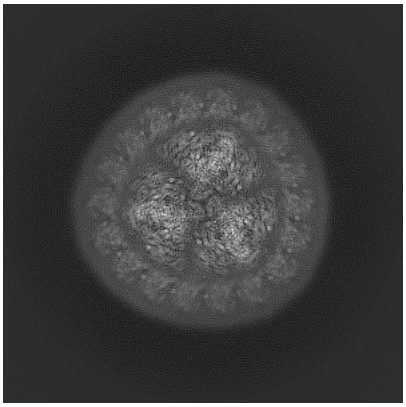
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

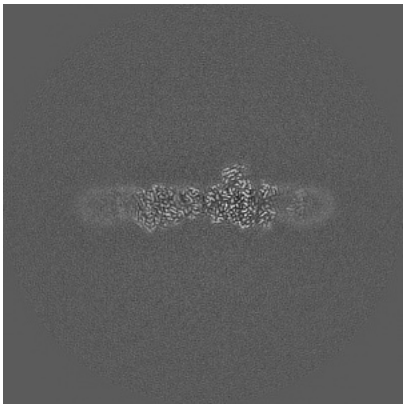


Z

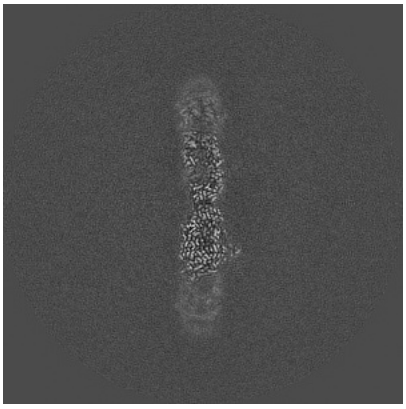
The images above show the map projected in three orthogonal directions.

6.2 Central slices

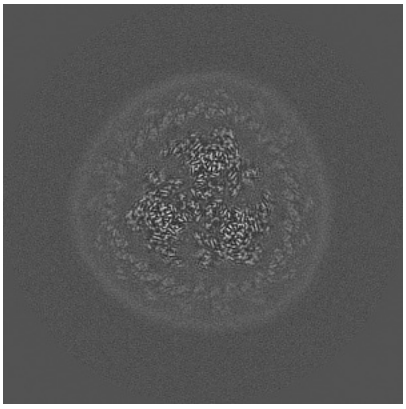
6.2.1 Primary map



X Index: 240



Y Index: 240

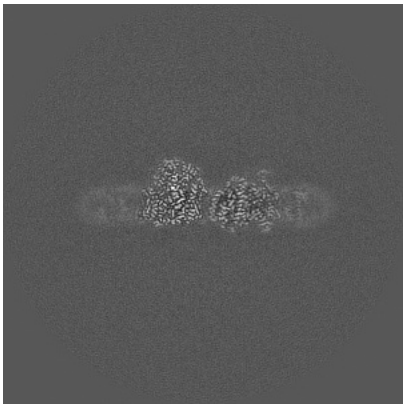


Z Index: 240

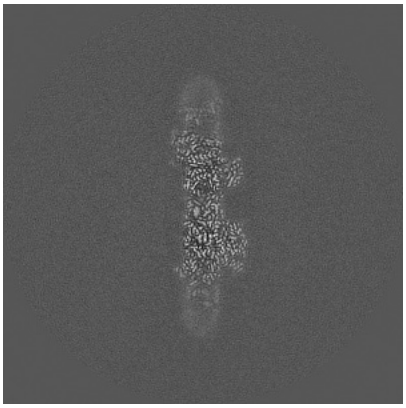
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

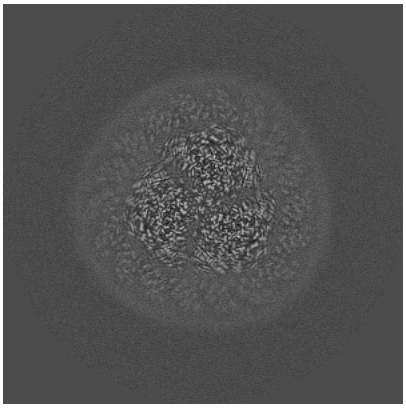
6.3.1 Primary map



X Index: 276



Y Index: 224

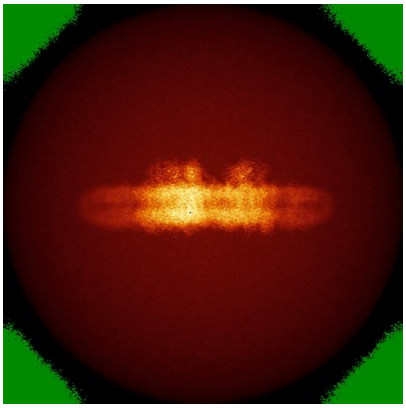


Z Index: 229

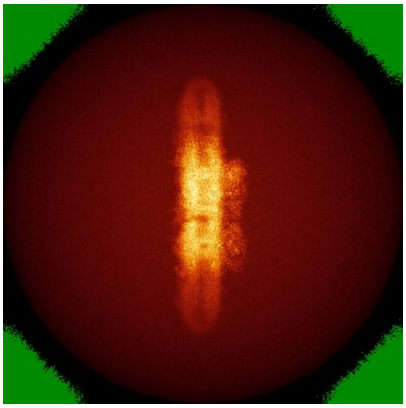
The images above show the largest variance slices of the map in three orthogonal directions.

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

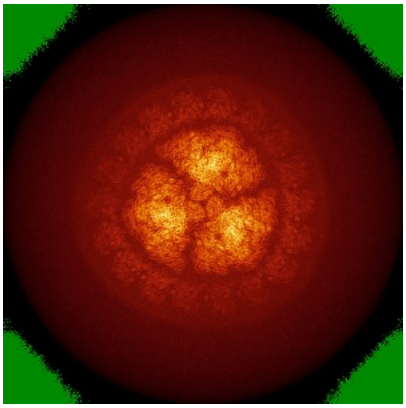
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

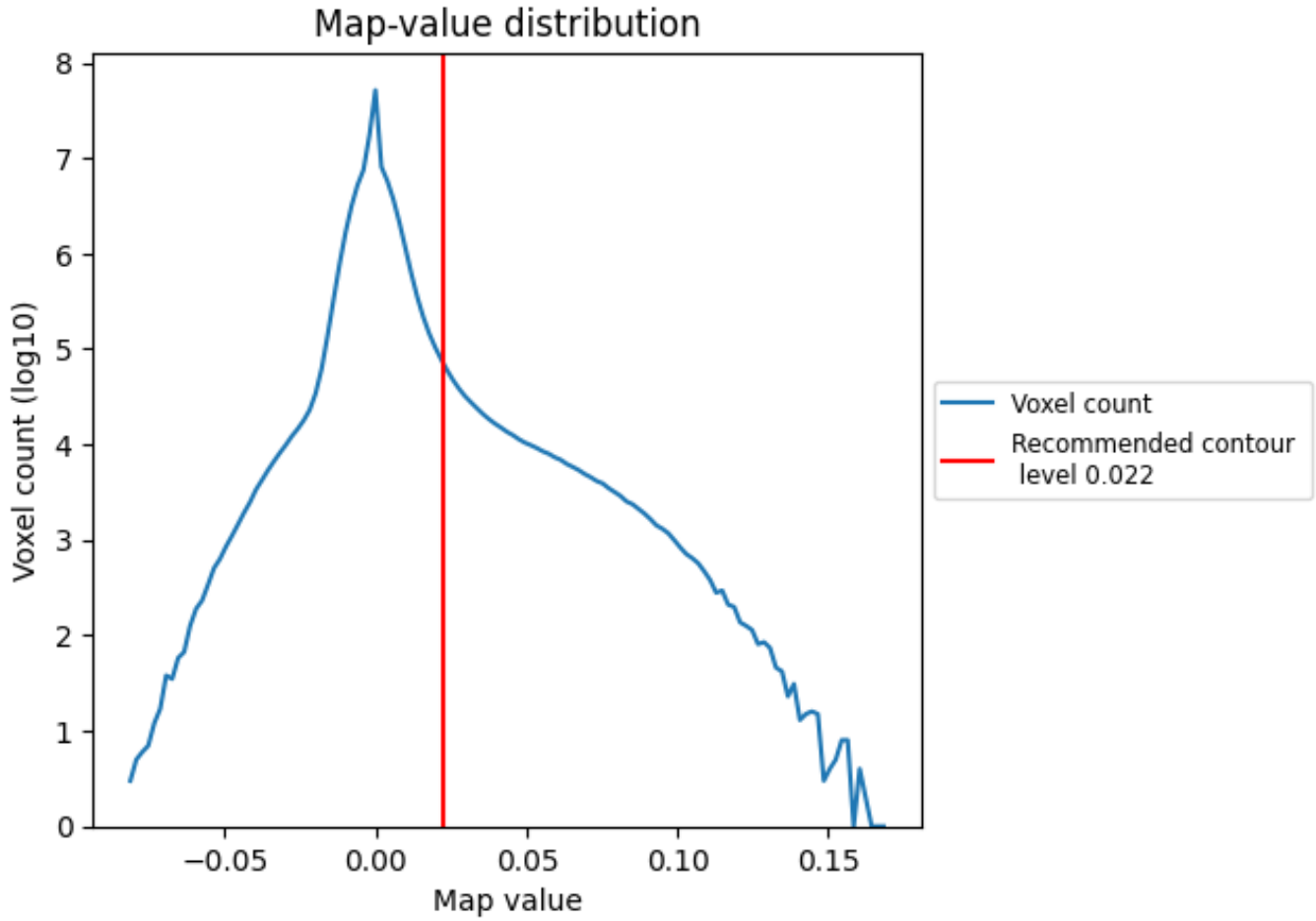
6.6 Mask visualisation (i)

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

7 Map analysis

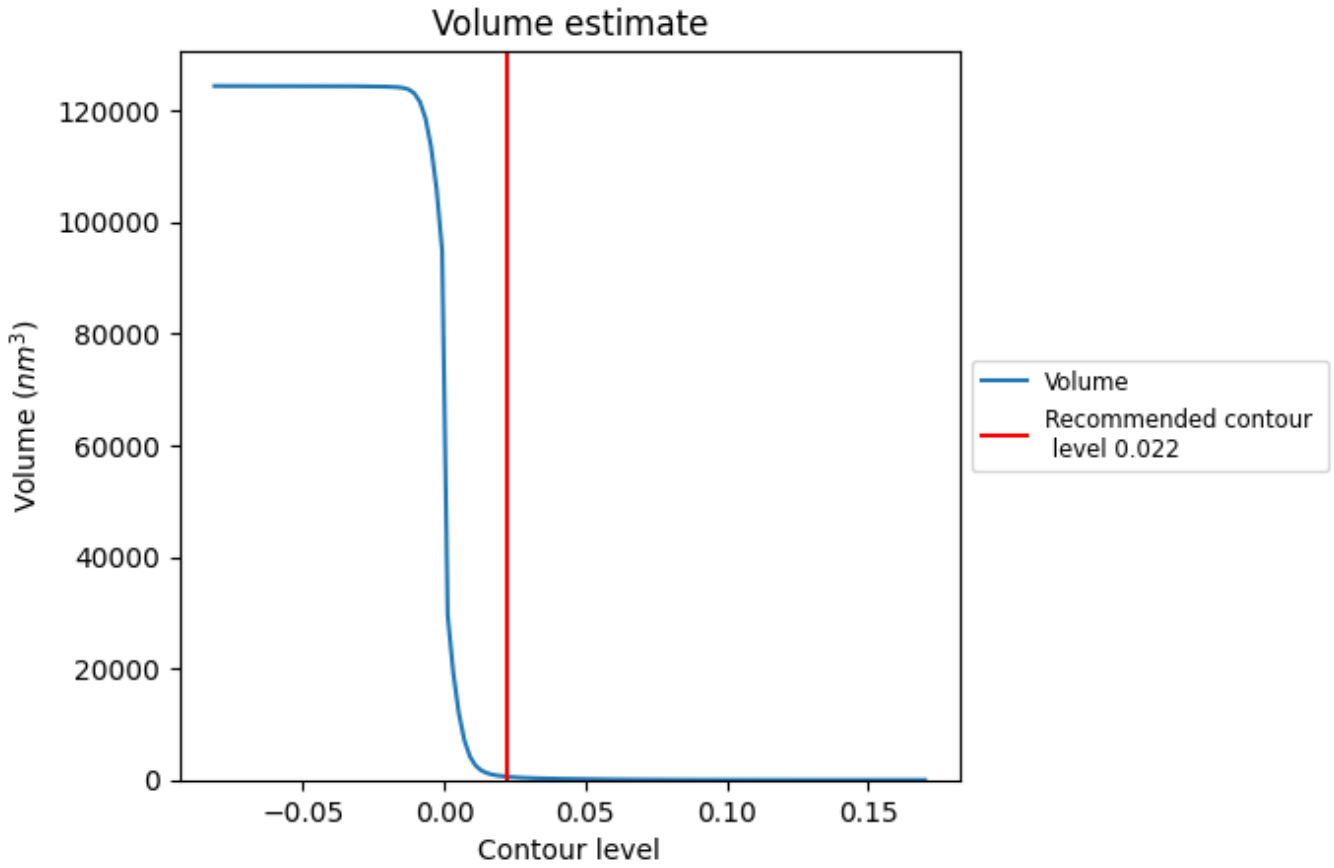
This section contains the results of statistical analysis of the map.

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.

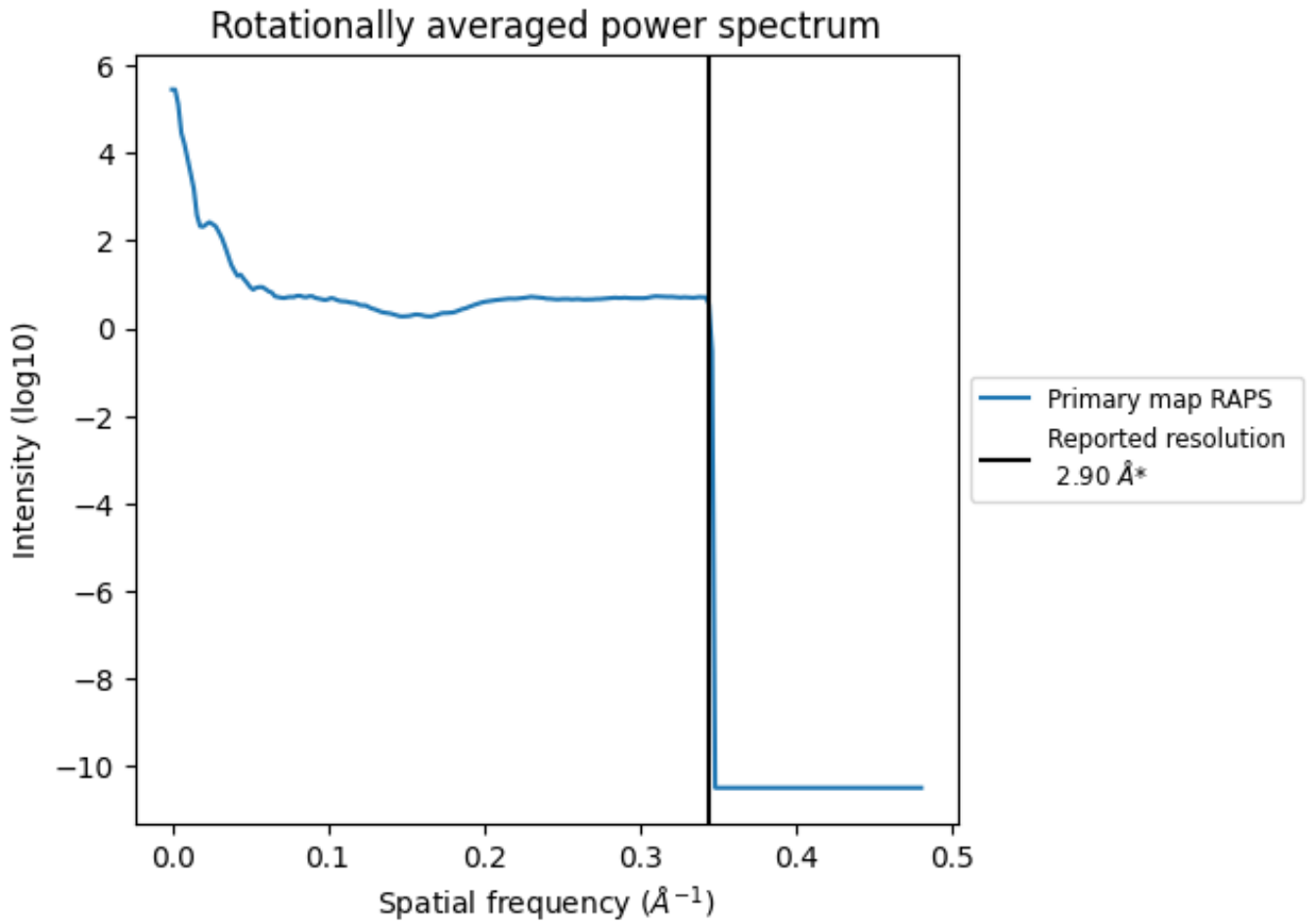
7.2 Volume estimate



The volume at the recommended contour level is 595 nm^3; this corresponds to an approximate mass of 538 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 0.345 Å^{-1}

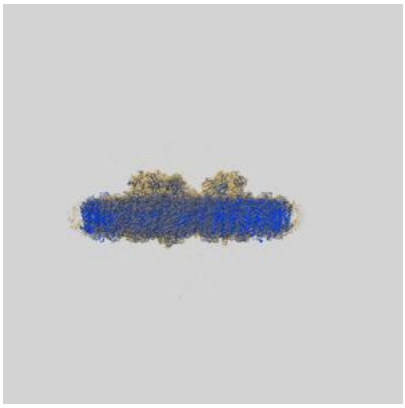
8 Fourier-Shell correlation

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

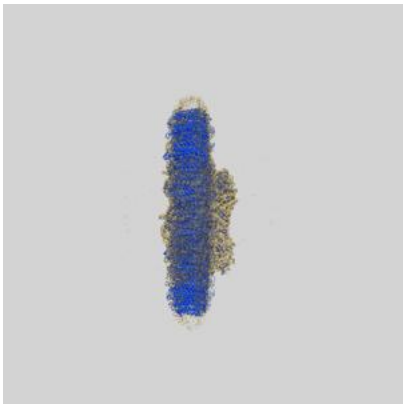
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9995 and PDB model 6KIG. Per-residue inclusion information can be found in section 3 on page 56.

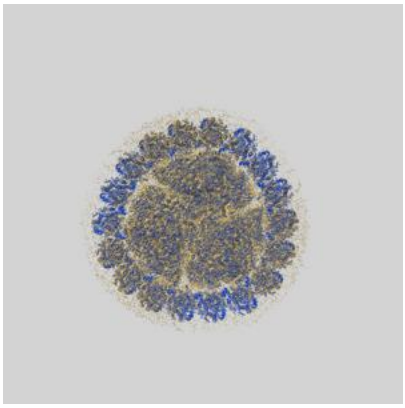
9.1 Map-model overlay



X



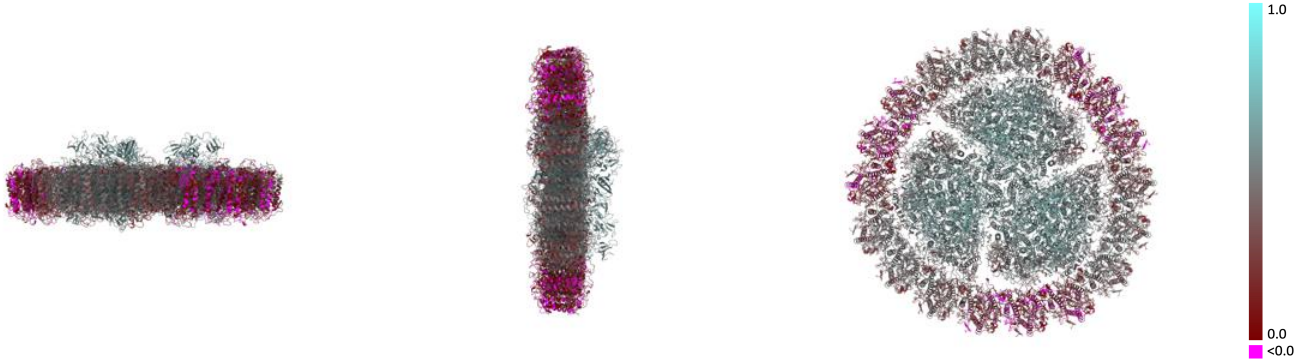
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

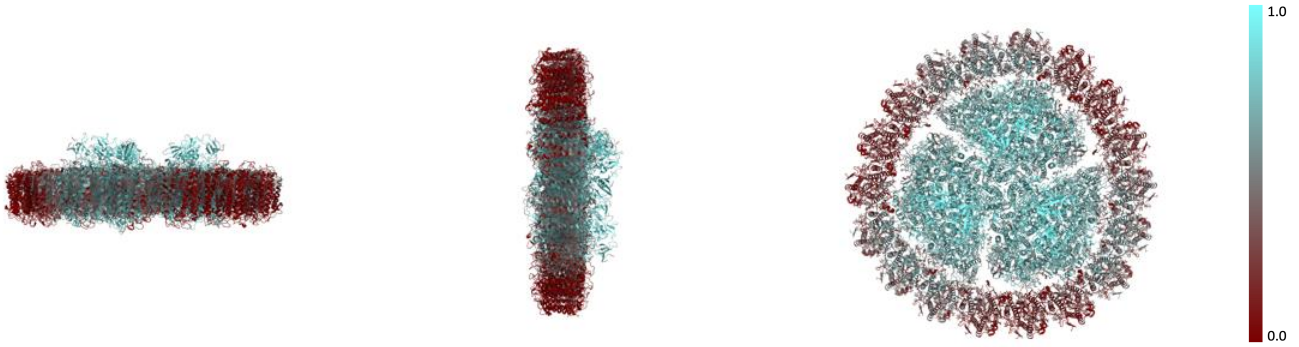
9.2 Q-score mapped to coordinate model



X Y Z

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

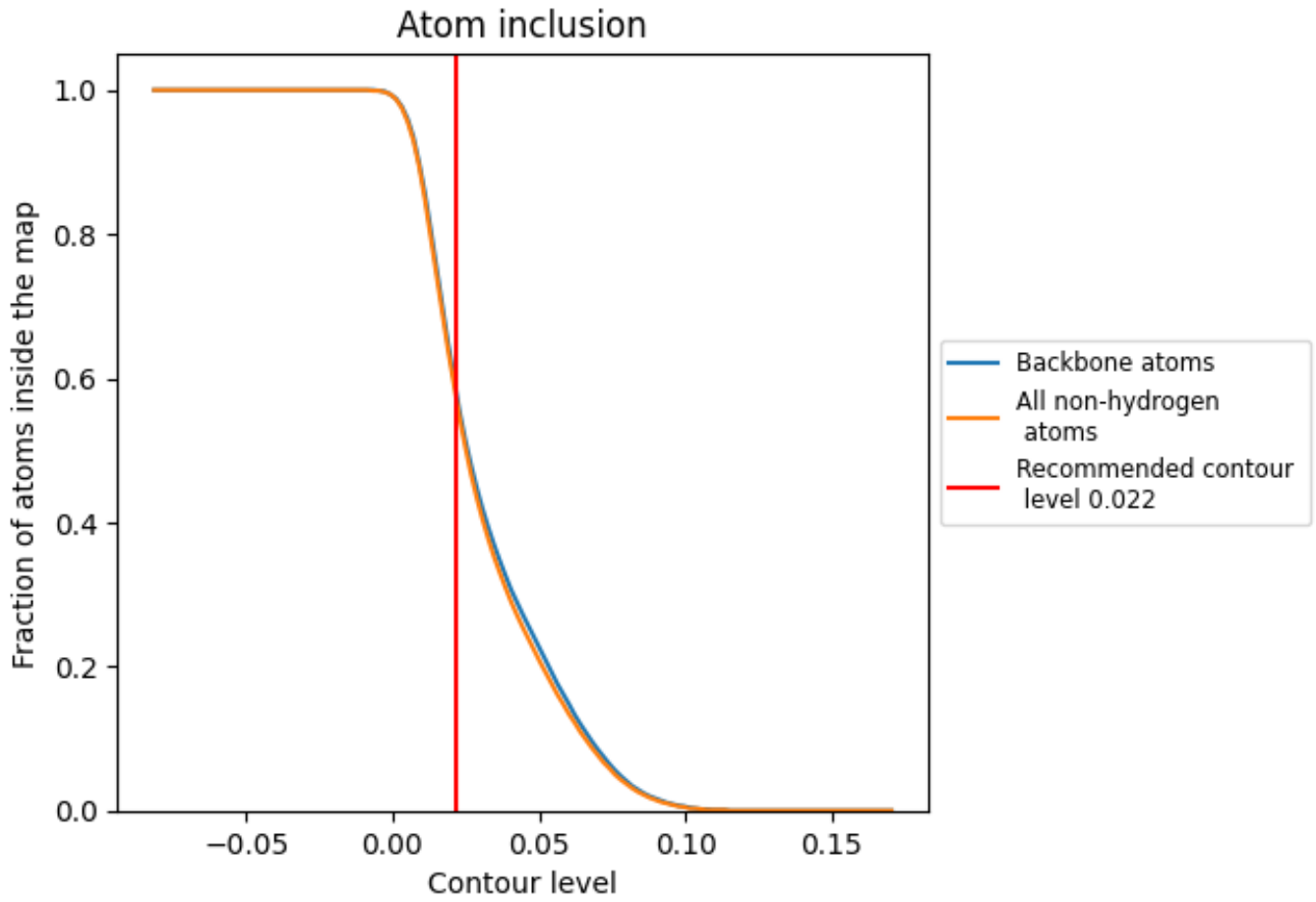
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5650	0.4190
1	0.4070	0.3640
2	0.4700	0.4180
3	0.3900	0.3830
4	0.1070	0.1410
5	0.0560	0.0860
6	0.1520	0.1850
A	0.8490	0.5780
B	0.8270	0.5450
C	0.9420	0.6070
D	0.8580	0.5770
E	0.7870	0.5410
F	0.7470	0.5290
G	0.8450	0.5770
H	0.8160	0.5370
I	0.8330	0.5720
J	0.7550	0.5460
K	0.5870	0.3890
L	0.8650	0.5930
M	0.7980	0.5290
N	0.9450	0.6070
O	0.8590	0.5780
Q	0.7810	0.5500
R	0.7440	0.5230
S	0.8250	0.5780
T	0.7360	0.5460
U	0.5810	0.3860
V	0.8690	0.5940
W	0.7790	0.5320
Y	0.4060	0.3660
Z	0.4670	0.4160
a	0.3870	0.3780
b	0.1040	0.1380
c	0.0530	0.0780
d	0.1450	0.1710

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Chain	Atom inclusion	Q-score
e	0.8420	0.5750
f	0.8210	0.5420
g	0.9420	0.6070
h	0.8690	0.5800
i	0.7950	0.5480
j	0.7500	0.5280
k	0.8410	0.5750
l	0.7470	0.5450
m	0.5790	0.3770
n	0.8670	0.5940
o	0.7820	0.5290
q	0.3920	0.3580
r	0.4580	0.4140
s	0.3910	0.3860
t	0.1100	0.1390
u	0.0560	0.0810
v	0.1540	0.1840