Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:15 AM JST

PDB ID	:	6KIF / pdb_00006kif
EMDB ID	:	EMD-9994
Title	:	Structure of cyanobacterial photosystem I-IsiA-flavodoxin 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	:	3.30 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:

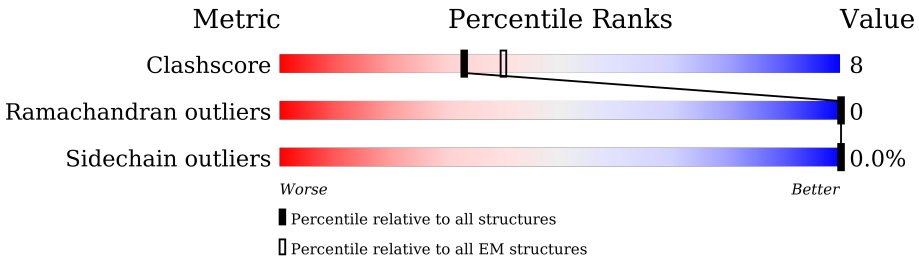
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

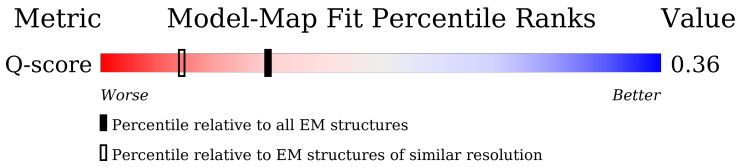
1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	83% 15%
1	G	763	83% 15%
1	e	763	85% 14%
2	B	734	82% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	734	82% 18%
2	f	734	82% 18%
3	C	81	80% 19%
3	N	81	79% 20%
3	g	81	81% 17%
4	D	141	79% 21%
4	O	141	81% 19%
4	h	141	79% 21%
5	E	75	11% 81% 13% 5%
5	Q	75	12% 84% 11% 5%
5	i	75	12% 85% 9% 5%
6	F	159	76% 9% 14%
6	R	159	75% 10% 14%
6	j	159	75% 10% 14%
7	I	38	8% 74% 26%
7	S	38	5% 79% 21%
7	k	38	8% 82% 18%
8	J	41	5% 80% 20%
8	T	41	5% 80% 20%
8	l	41	5% 80% 20%
9	K	84	19% 70% 23% 7%
9	U	84	23% 69% 24% 7%
9	m	84	15% 70% 23% 7%
10	L	166	76% 23%
10	V	166	76% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	n	166	76% 23%
11	M	29	83% 17%
11	W	29	86% 14%
11	o	29	86% 14%
12	P	172	58% 83% 15%
12	X	172	60% 83% 16%
12	p	172	58% 81% 17%
13	1	342	64% 89% 10%
13	2	342	65% 86% 13%
13	3	342	76% 87% 12%
13	4	342	97% 82% 17%
13	5	342	98% 89% 11%
13	6	342	94% 82% 17%
13	Y	342	65% 88% 11%
13	Z	342	65% 85% 14%
13	a	342	78% 88% 11%
13	b	342	97% 82% 18%
13	c	342	98% 89% 11%
13	d	342	93% 83% 16%
13	q	342	64% 89% 10%
13	r	342	65% 85% 14%
13	s	342	75% 87% 12%
13	t	342	96% 82% 18%
13	u	342	98% 89% 10%
13	v	342	93% 82% 17%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 144312 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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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 Flavodoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	169	Total	C	N	O	S	0	0
			1318	831	210	275	2		
12	X	169	Total	C	N	O	S	0	0
			1318	831	210	275	2		
12	p	169	Total	C	N	O	S	0	0
			1318	831	210	275	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-2	GLY	-	expression tag	UNP P10340
P	-1	SER	-	expression tag	UNP P10340
P	0	HIS	-	expression tag	UNP P10340
X	-2	GLY	-	expression tag	UNP P10340
X	-1	SER	-	expression tag	UNP P10340
X	0	HIS	-	expression tag	UNP P10340
p	-2	GLY	-	expression tag	UNP P10340
p	-1	SER	-	expression tag	UNP P10340
p	0	HIS	-	expression tag	UNP P10340

- Molecule 13 is a protein called Iron stress-induced chlorophyll-binding protein.

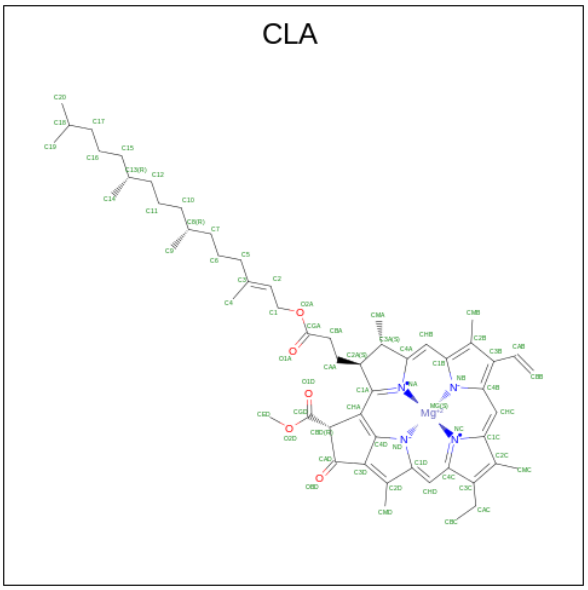
Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	4	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	5	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	6	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	Y	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	Z	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	a	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	b	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	c	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	d	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	q	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	r	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	t	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	u	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	v	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

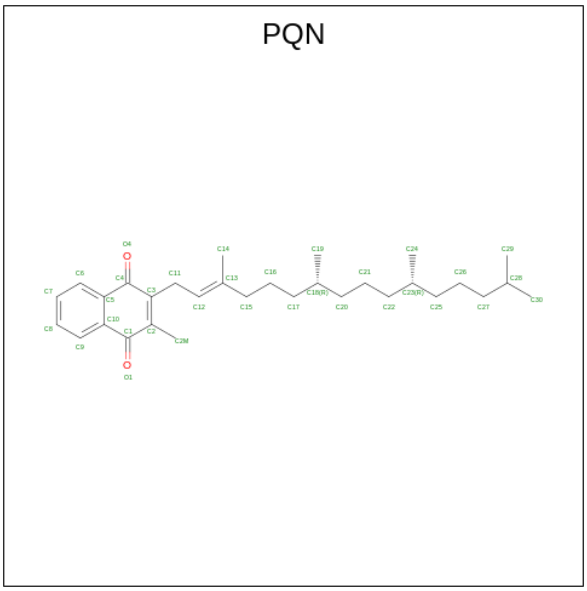
Mol	Chain	Residues	Atoms					AltConf
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

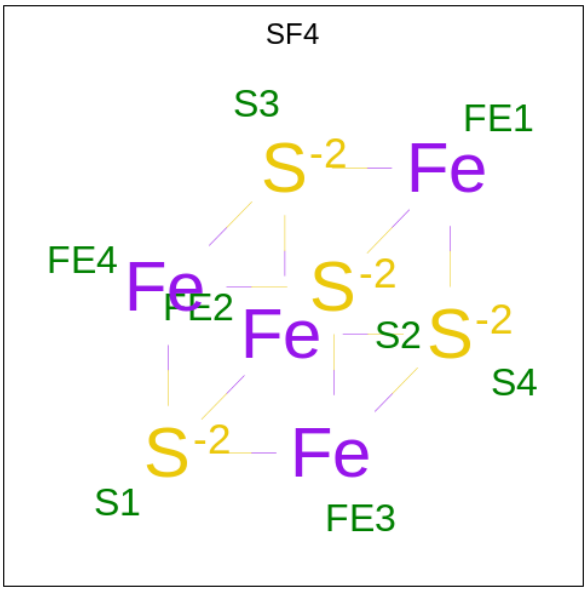
Mol	Chain	Residues	Atoms					AltConf
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



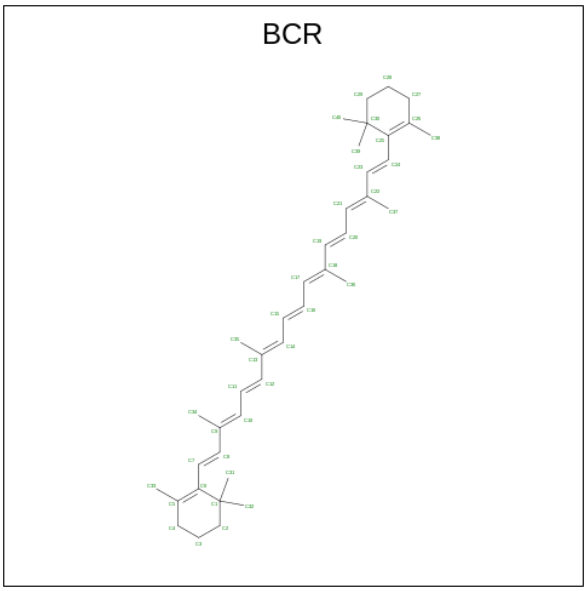
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C O 33 31 2	0
15	B	1	Total C O 33 31 2	0
15	G	1	Total C O 33 31 2	0
15	H	1	Total C O 33 31 2	0
15	e	1	Total C O 33 31 2	0
15	f	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	3	1	Total C 40 40	0
17	3	1	Total C 40 40	0
17	3	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
17	3	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

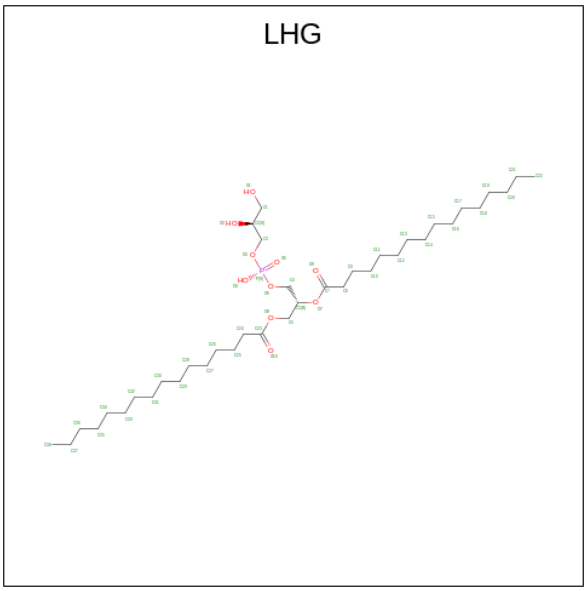
Mol	Chain	Residues	Atoms	AltConf
17	o	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	s	1	Total C 40 40	0
17	s	1	Total C 40 40	0
17	s	1	Total C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

Continued on next page...

Continued from previous page...

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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O P 43 32 10 1	0
18	A	1	Total C O P 35 24 10 1	0
18	A	1	Total C O P 43 32 10 1	0
18	A	1	Total C O P 40 29 10 1	0
18	A	1	Total C O P 47 36 10 1	0
18	A	1	Total C O P 35 24 10 1	0
18	A	1	Total C O P 42 31 10 1	0

Continued on next page...

Continued from previous page...

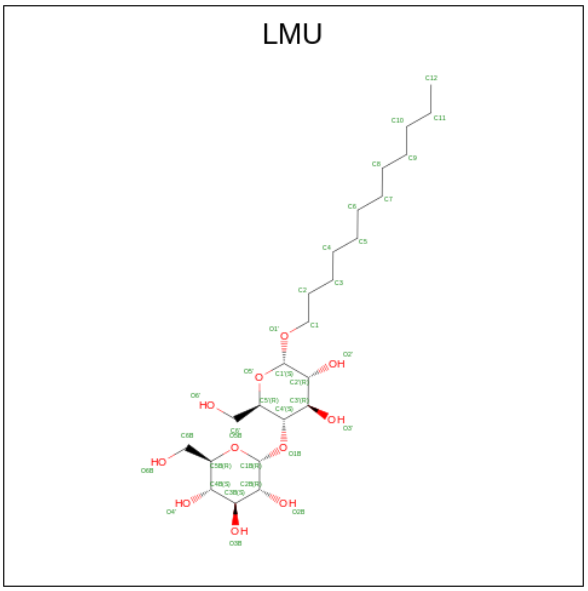
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	A	1	Total	C	O	P	0
			40	29	10	1	
18	B	1	Total	C	O	P	0
			37	26	10	1	
18	B	1	Total	C	O	P	0
			41	30	10	1	
18	I	1	Total	C	O	P	0
			48	37	10	1	
18	L	1	Total	C	O	P	0
			37	26	10	1	
18	L	1	Total	C	O	P	0
			41	30	10	1	
18	L	1	Total	C	O	P	0
			49	38	10	1	
18	G	1	Total	C	O	P	0
			43	32	10	1	
18	G	1	Total	C	O	P	0
			35	24	10	1	
18	G	1	Total	C	O	P	0
			43	32	10	1	
18	G	1	Total	C	O	P	0
			40	29	10	1	
18	G	1	Total	C	O	P	0
			47	36	10	1	
18	G	1	Total	C	O	P	0
			35	24	10	1	
18	G	1	Total	C	O	P	0
			42	31	10	1	
18	G	1	Total	C	O	P	0
			49	38	10	1	
18	G	1	Total	C	O	P	0
			40	29	10	1	
18	H	1	Total	C	O	P	0
			37	26	10	1	
18	H	1	Total	C	O	P	0
			41	30	10	1	
18	S	1	Total	C	O	P	0
			48	37	10	1	
18	V	1	Total	C	O	P	0
			37	26	10	1	

Continued on next page...

Continued from previous page...

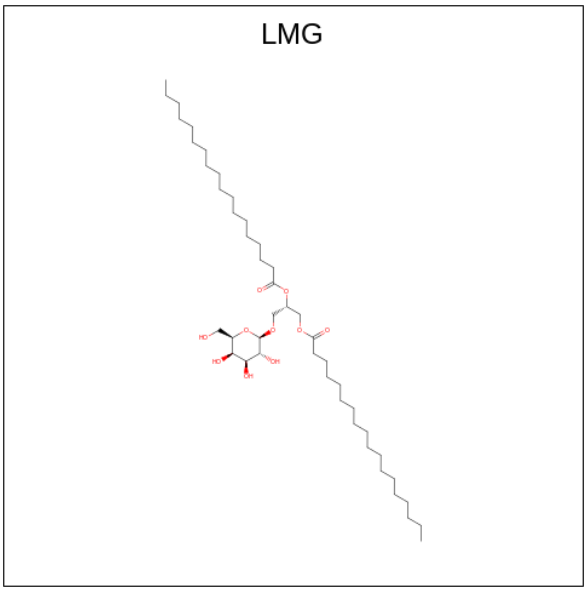
Mol	Chain	Residues	Atoms				AltConf
18	V	1	Total	C	O	P	0
			41	30	10	1	
18	V	1	Total	C	O	P	0
			49	38	10	1	
18	e	1	Total	C	O	P	0
			43	32	10	1	
18	e	1	Total	C	O	P	0
			35	24	10	1	
18	e	1	Total	C	O	P	0
			43	32	10	1	
18	e	1	Total	C	O	P	0
			40	29	10	1	
18	e	1	Total	C	O	P	0
			47	36	10	1	
18	e	1	Total	C	O	P	0
			35	24	10	1	
18	e	1	Total	C	O	P	0
			42	31	10	1	
18	e	1	Total	C	O	P	0
			49	38	10	1	
18	e	1	Total	C	O	P	0
			40	29	10	1	
18	f	1	Total	C	O	P	0
			37	26	10	1	
18	f	1	Total	C	O	P	0
			41	30	10	1	
18	k	1	Total	C	O	P	0
			48	37	10	1	
18	n	1	Total	C	O	P	0
			37	26	10	1	
18	n	1	Total	C	O	P	0
			41	30	10	1	
18	n	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 19 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



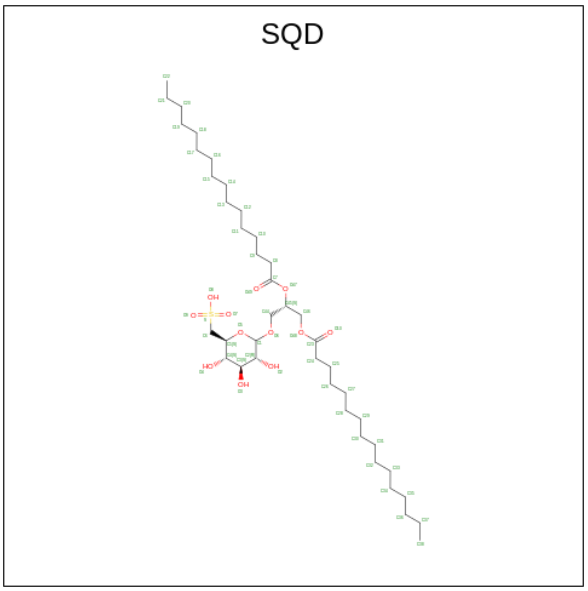
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total 35	C 24	O 11	0
19	A	1	Total 23	C 17	O 6	0
19	B	1	Total 35	C 24	O 11	0
19	J	1	Total 22	C 16	O 6	0
19	G	1	Total 35	C 24	O 11	0
19	G	1	Total 23	C 17	O 6	0
19	H	1	Total 35	C 24	O 11	0
19	T	1	Total 22	C 16	O 6	0
19	e	1	Total 35	C 24	O 11	0
19	e	1	Total 23	C 17	O 6	0
19	f	1	Total 35	C 24	O 11	0
19	l	1	Total 22	C 16	O 6	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			53	43	10	
20	J	1	Total	C	O	0
			32	22	10	
20	H	1	Total	C	O	0
			53	43	10	
20	T	1	Total	C	O	0
			32	22	10	
20	f	1	Total	C	O	0
			53	43	10	
20	l	1	Total	C	O	0
			32	22	10	

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



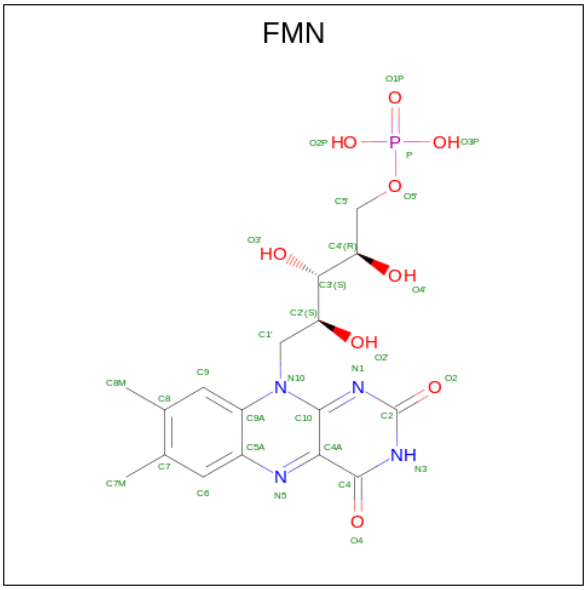
Mol	Chain	Residues	Atoms				AltConf
21	B	1	Total	C	O	S	0
			40	27	12	1	
21	L	1	Total	C	O	S	0
			46	33	12	1	
21	1	1	Total	C	O	S	0
			32	19	12	1	
21	2	1	Total	C	O	S	0
			28	15	12	1	
21	3	1	Total	C	O	S	0
			28	15	12	1	
21	4	1	Total	C	O	S	0
			26	13	12	1	
21	5	1	Total	C	O	S	0
			26	13	12	1	
21	6	1	Total	C	O	S	0
			26	13	12	1	
21	H	1	Total	C	O	S	0
			40	27	12	1	
21	V	1	Total	C	O	S	0
			46	33	12	1	
21	Y	1	Total	C	O	S	0
			32	19	12	1	
21	Z	1	Total	C	O	S	0
			28	15	12	1	
21	a	1	Total	C	O	S	0
			28	15	12	1	
21	b	1	Total	C	O	S	0
			26	13	12	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
21	c	1	Total	C	O	S	0
			26	13	12	1	
21	d	1	Total	C	O	S	0
			26	13	12	1	
21	f	1	Total	C	O	S	0
			40	27	12	1	
21	n	1	Total	C	O	S	0
			46	33	12	1	
21	q	1	Total	C	O	S	0
			32	19	12	1	
21	r	1	Total	C	O	S	0
			28	15	12	1	
21	s	1	Total	C	O	S	0
			28	15	12	1	
21	t	1	Total	C	O	S	0
			26	13	12	1	
21	u	1	Total	C	O	S	0
			26	13	12	1	
21	v	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 22 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total	C	N	O	P	0
			31	17	4	9	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			31	17	4	9	1	
22	p	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	9	Total	O	0
			9	9	
23	B	7	Total	O	0
			7	7	
23	F	1	Total	O	0
			1	1	
23	L	1	Total	O	0
			1	1	
23	G	9	Total	O	0
			9	9	
23	H	7	Total	O	0
			7	7	
23	R	1	Total	O	0
			1	1	
23	V	1	Total	O	0
			1	1	
23	e	9	Total	O	0
			9	9	
23	f	7	Total	O	0
			7	7	
23	j	1	Total	O	0
			1	1	
23	n	1	Total	O	0
			1	1	

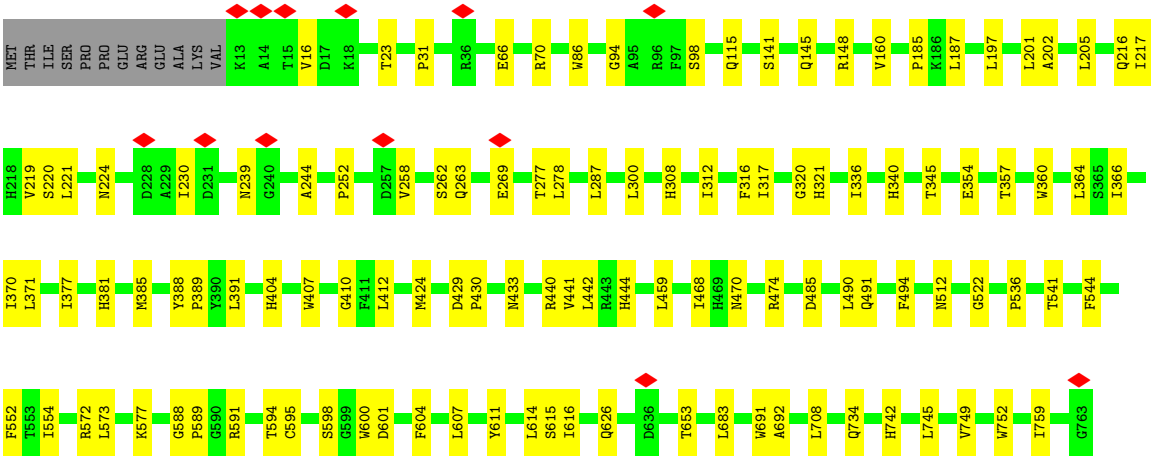
3 Residue-property plots (i)

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:

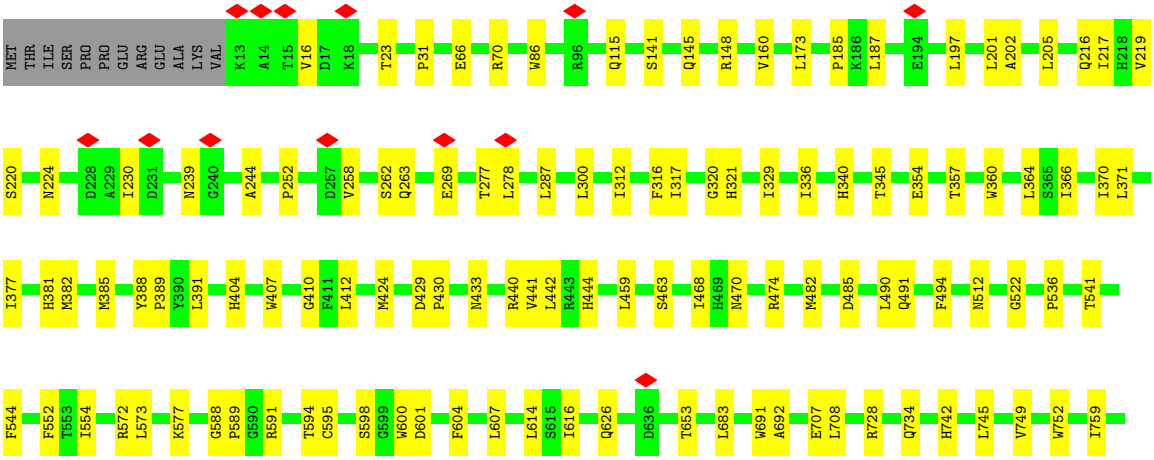




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain G:

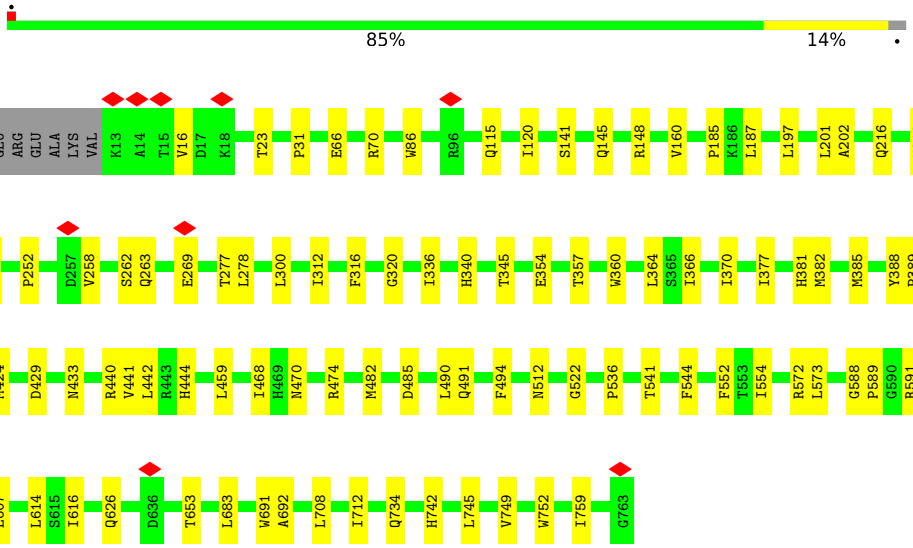






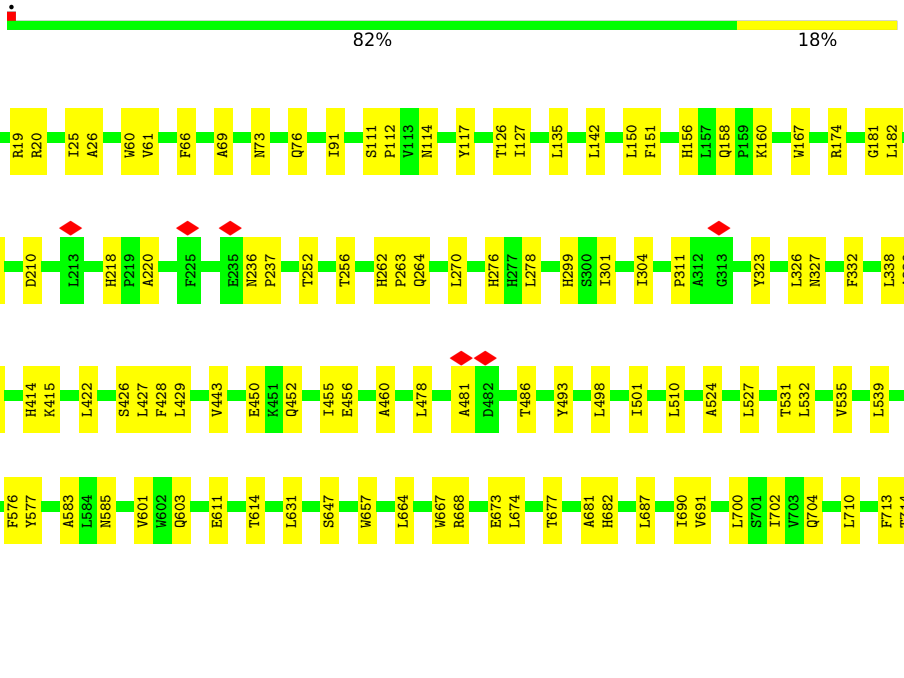
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e:



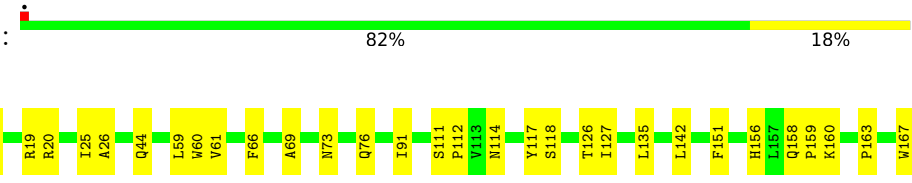
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

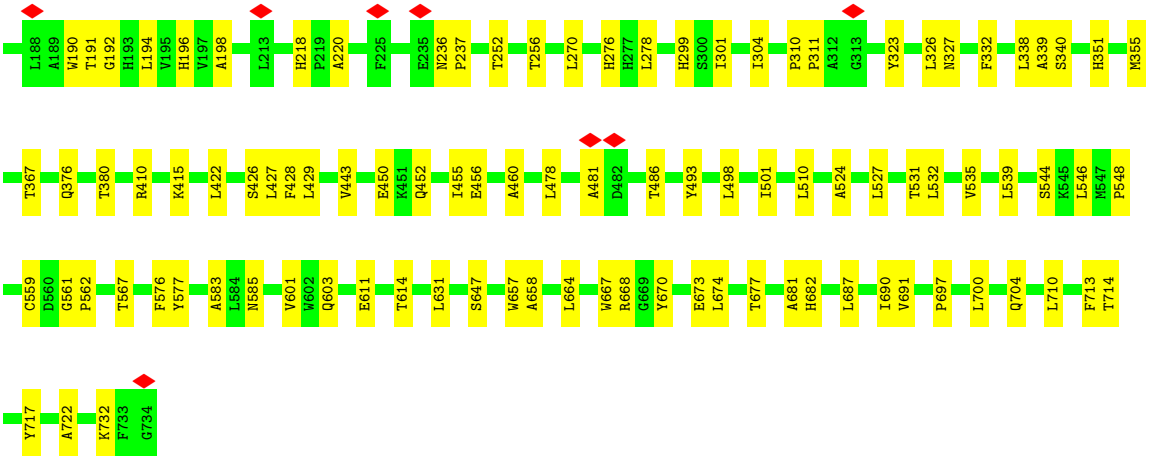
Chain B:



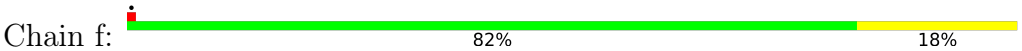
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

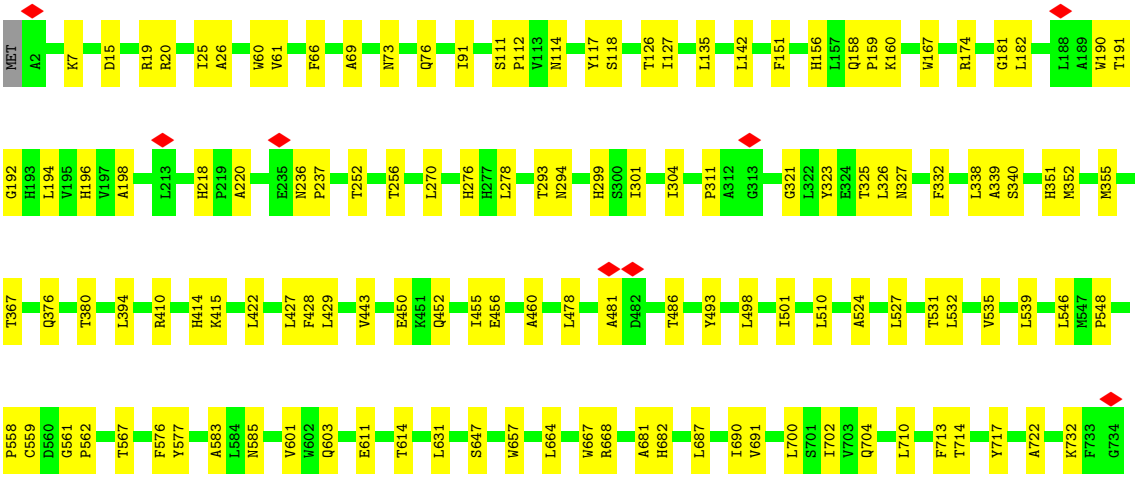
Chain H:



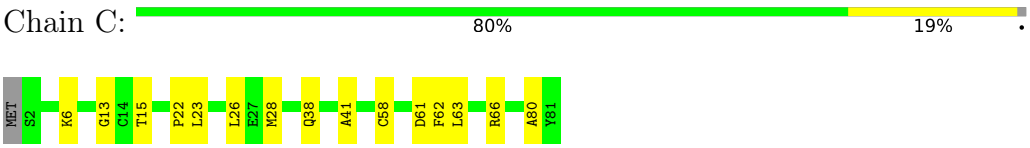


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

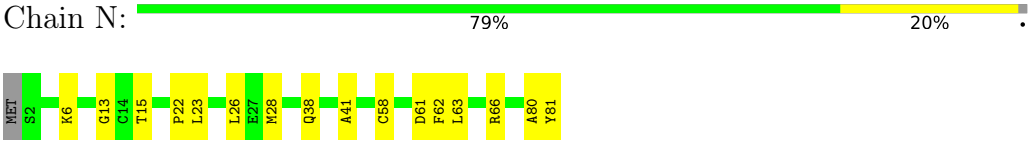




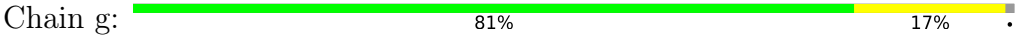
• Molecule 3: Photosystem I iron-sulfur center

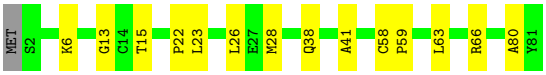


• Molecule 3: Photosystem I iron-sulfur center



• Molecule 3: Photosystem I iron-sulfur center





• 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:



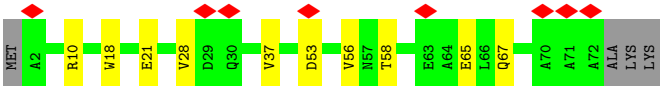




• Molecule 5: Photosystem I reaction center subunit IV

Chain E:

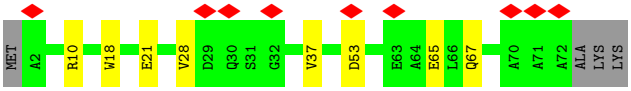




• Molecule 5: Photosystem I reaction center subunit IV

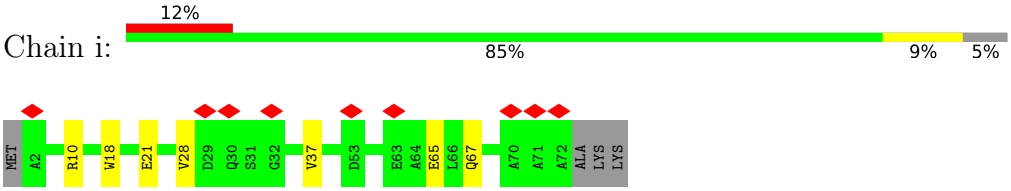
Chain Q:





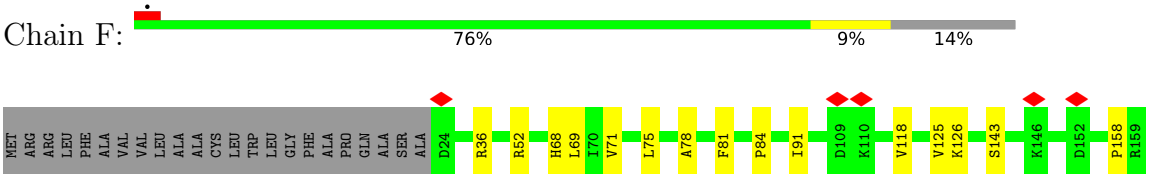
• Molecule 5: Photosystem I reaction center subunit IV

Chain i:



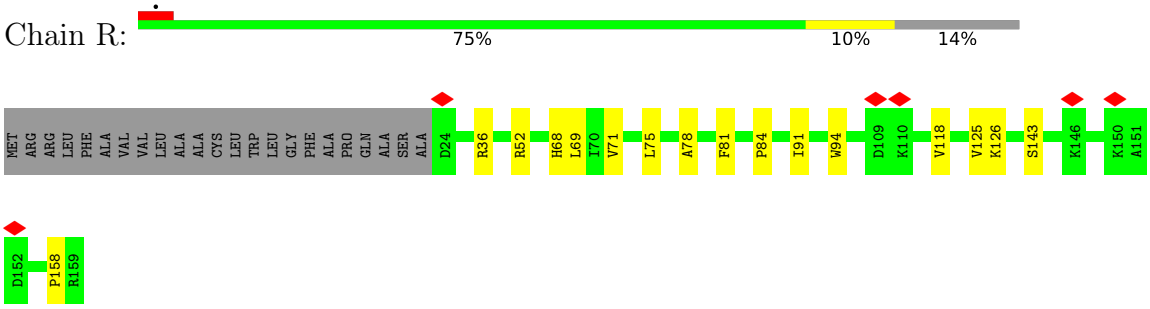
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



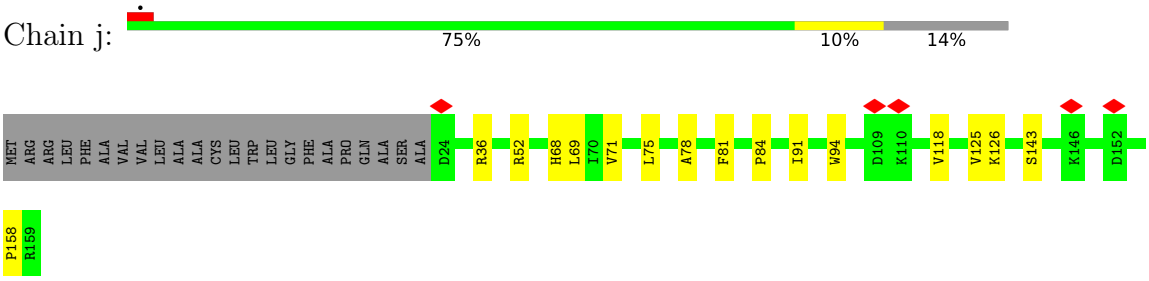
• Molecule 6: Photosystem I reaction center subunit III

Chain R:



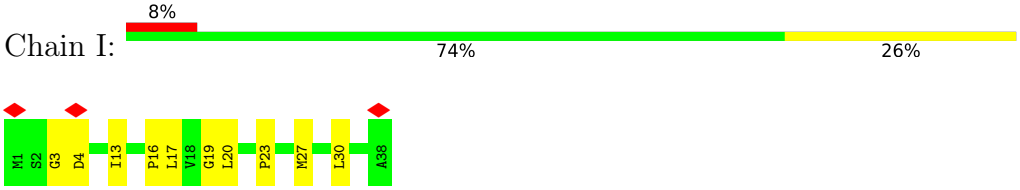
• Molecule 6: Photosystem I reaction center subunit III

Chain j:



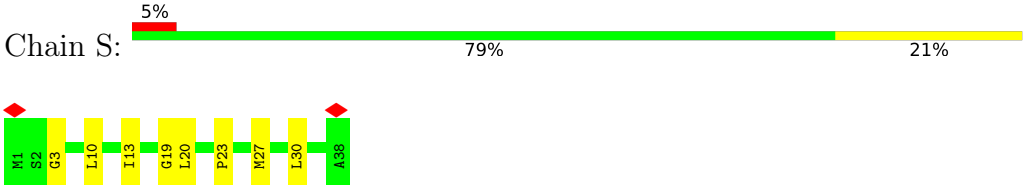
• Molecule 7: Photosystem I PsaI protein

Chain I:



• Molecule 7: Photosystem I PsaI protein

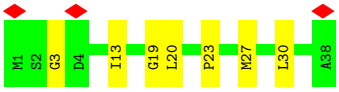
Chain S:



• Molecule 7: Photosystem I PsaI protein

Chain k:

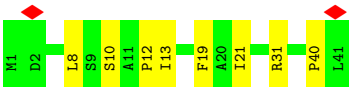




• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

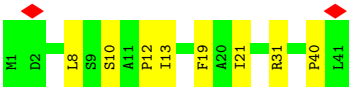




• Molecule 8: Photosystem I reaction center subunit IX

Chain T:

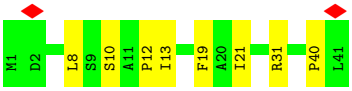




• Molecule 8: Photosystem I reaction center subunit IX

Chain l:

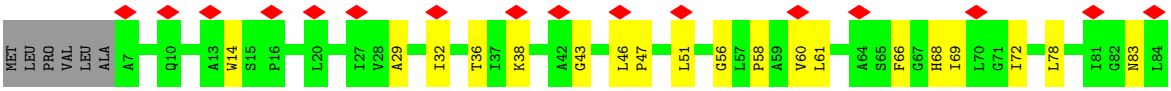




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:

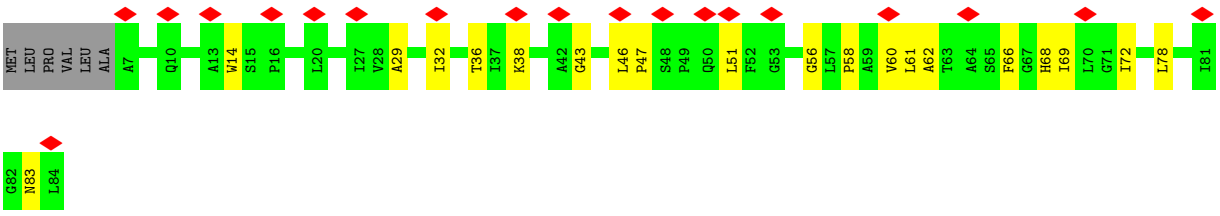




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain U:

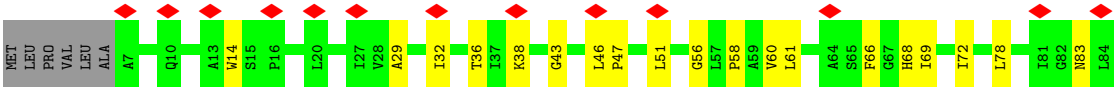




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain m:

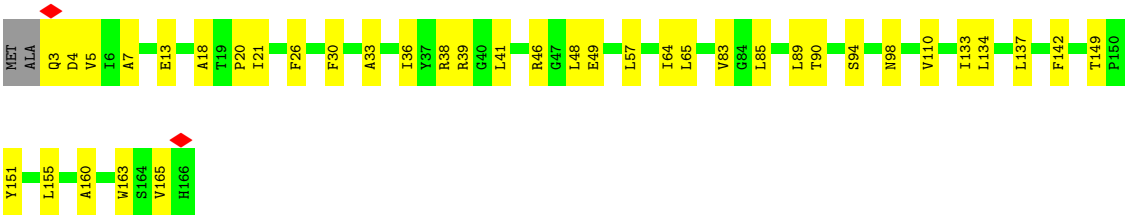




• Molecule 10: Photosystem I reaction center subunit XI

Chain L:





• Molecule 10: Photosystem I reaction center subunit XI

Chain V:

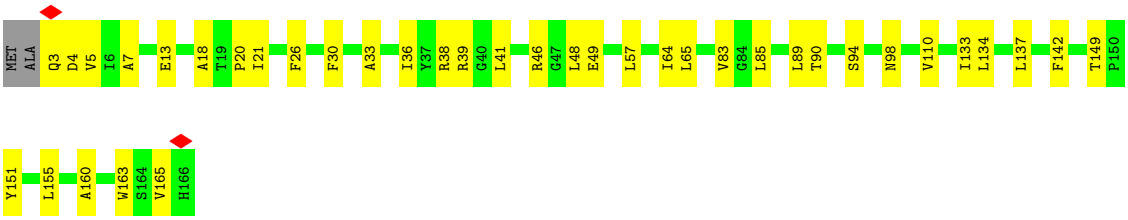




• Molecule 10: Photosystem I reaction center subunit XI

Chain n:

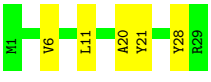




• Molecule 11: PsaM

Chain M:

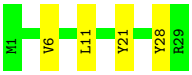




• Molecule 11: PsaM

Chain W:

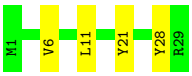




• Molecule 11: PsaM

Chain o:

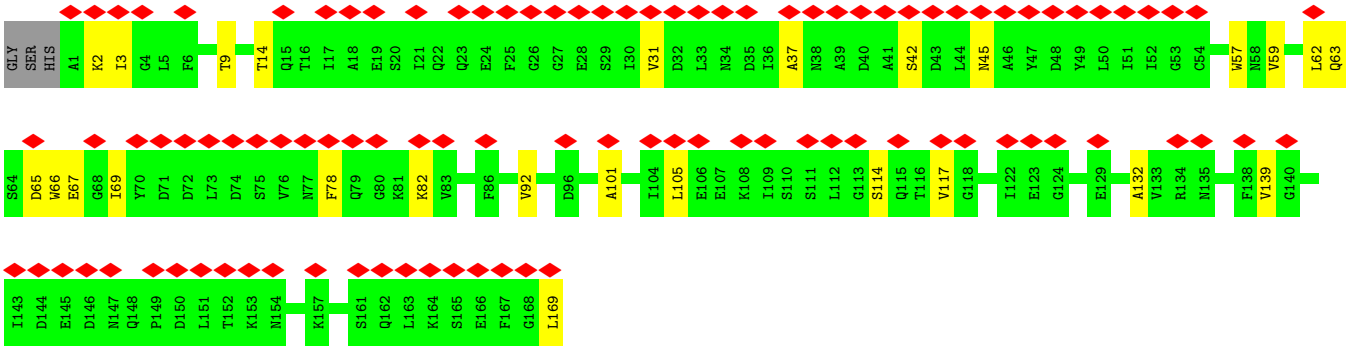




• Molecule 12: Flavodoxin

Chain P:

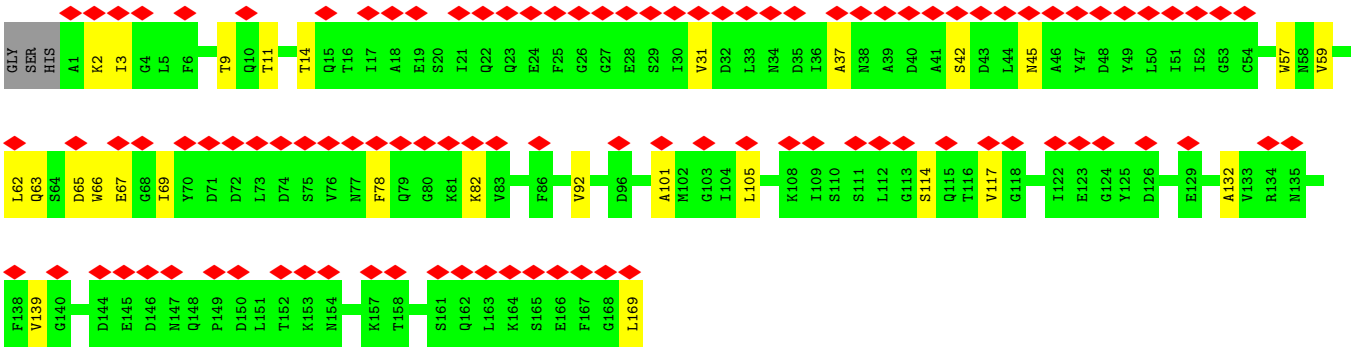




• Molecule 12: Flavodoxin

Chain X:

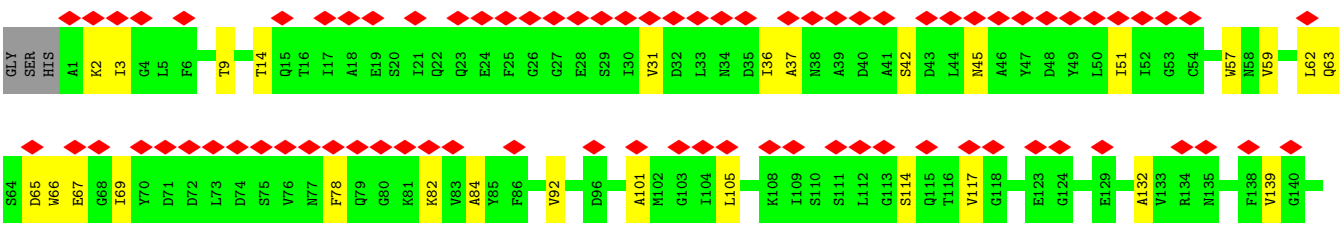


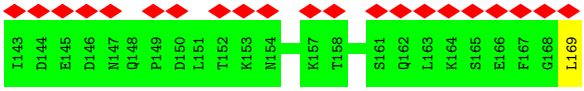


• Molecule 12: Flavodoxin

Chain p:



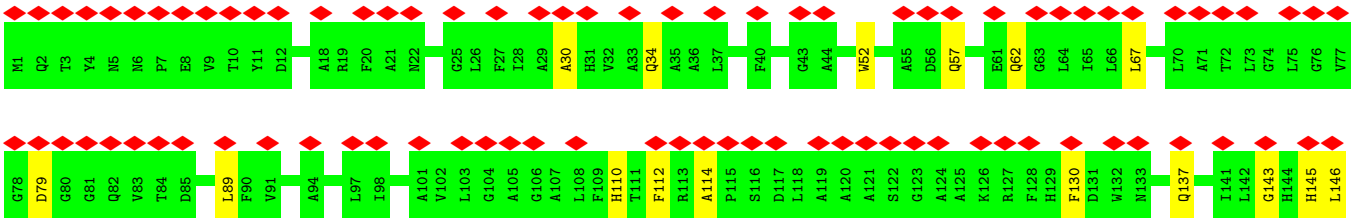




• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 1:

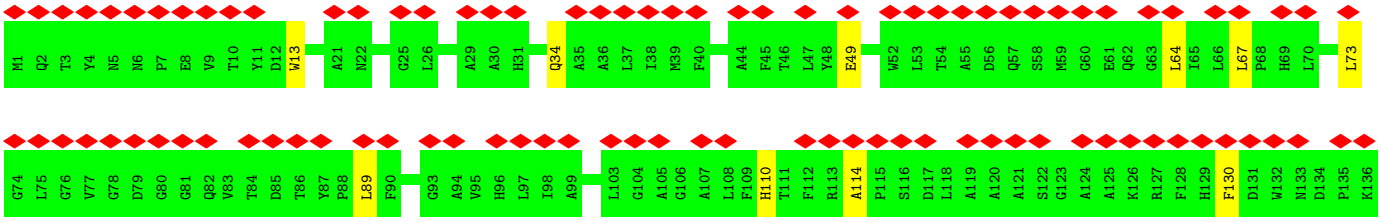




• Molecule 13: Iron stress-induced chlorophyll-binding protein

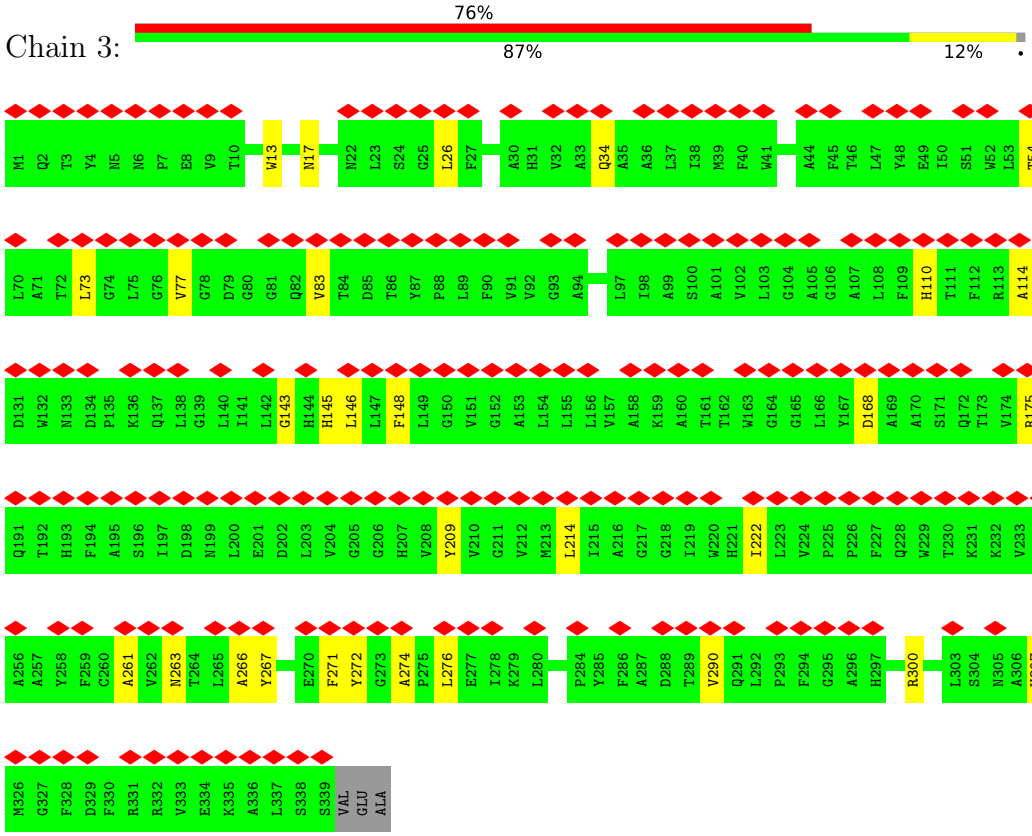
Chain 2:





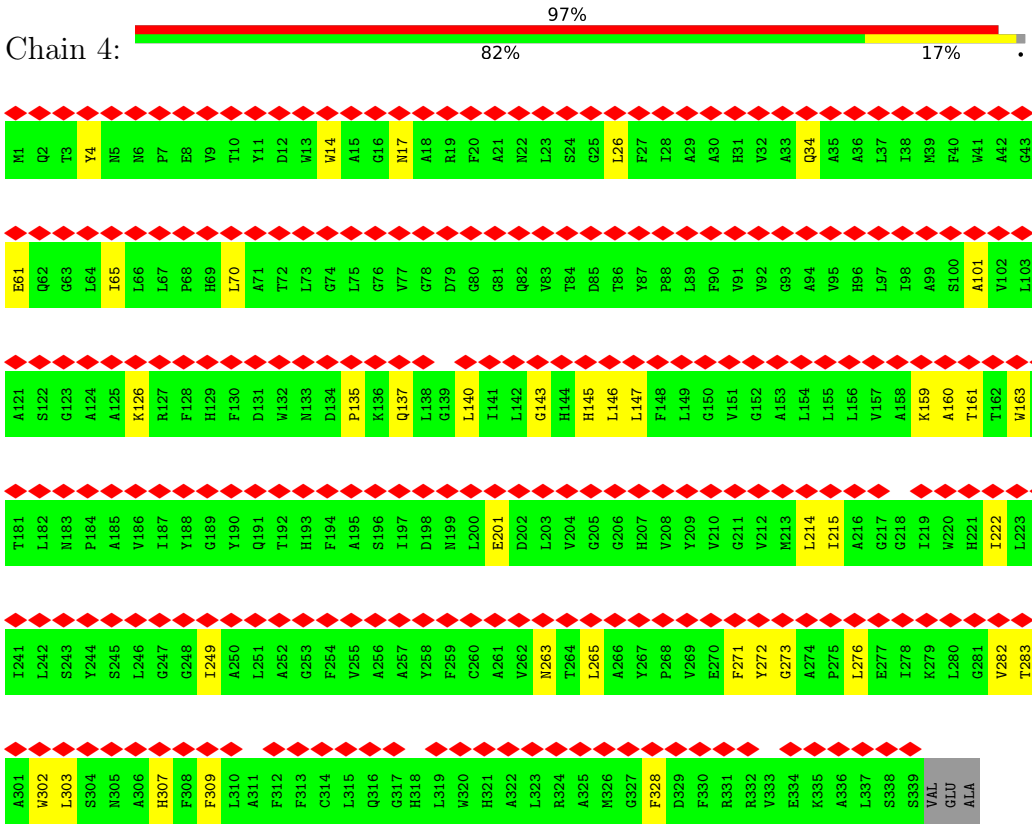
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 3:



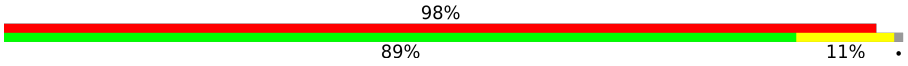
• Molecule 13: Iron stress-induced chlorophyll-binding protein

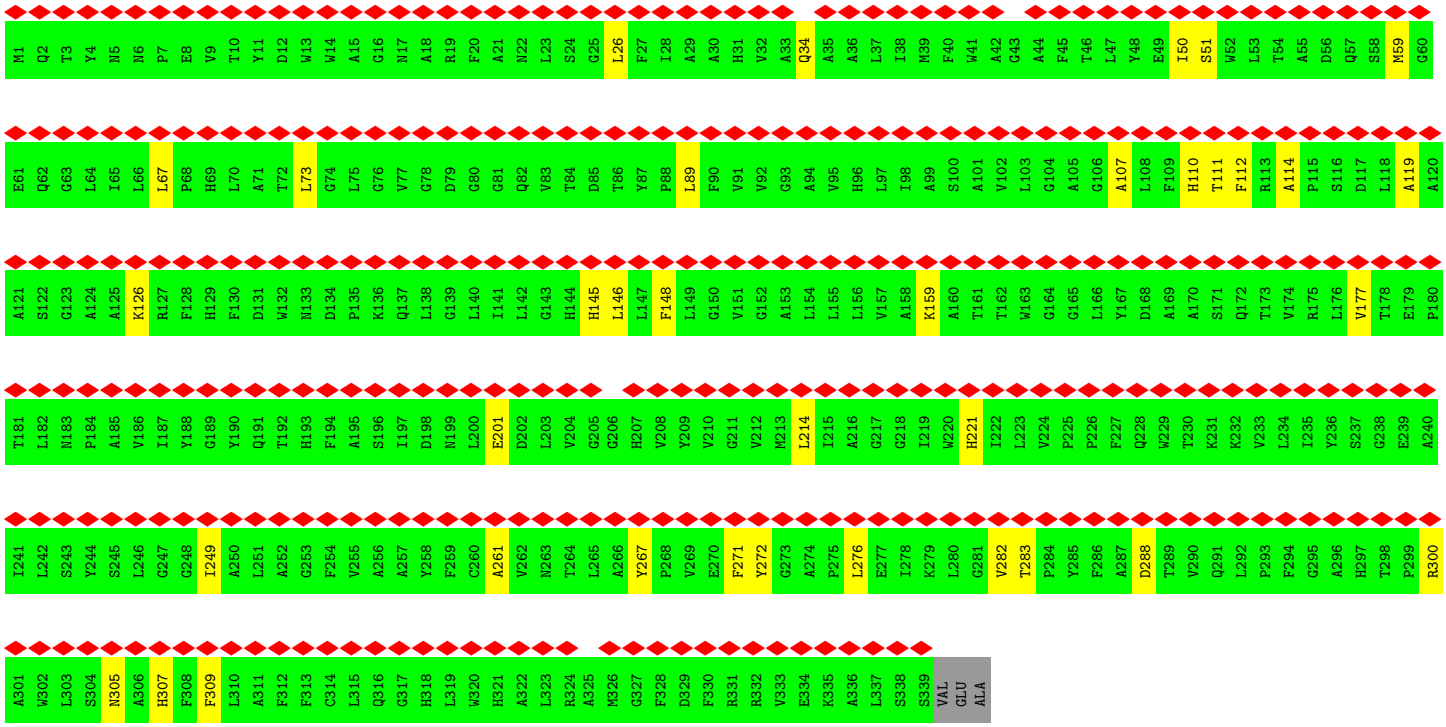
Chain 4:



• Molecule 13: Iron stress-induced chlorophyll-binding protein

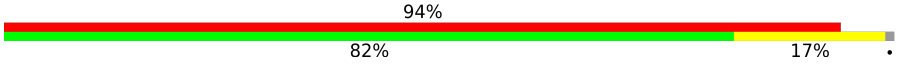
Chain 5:

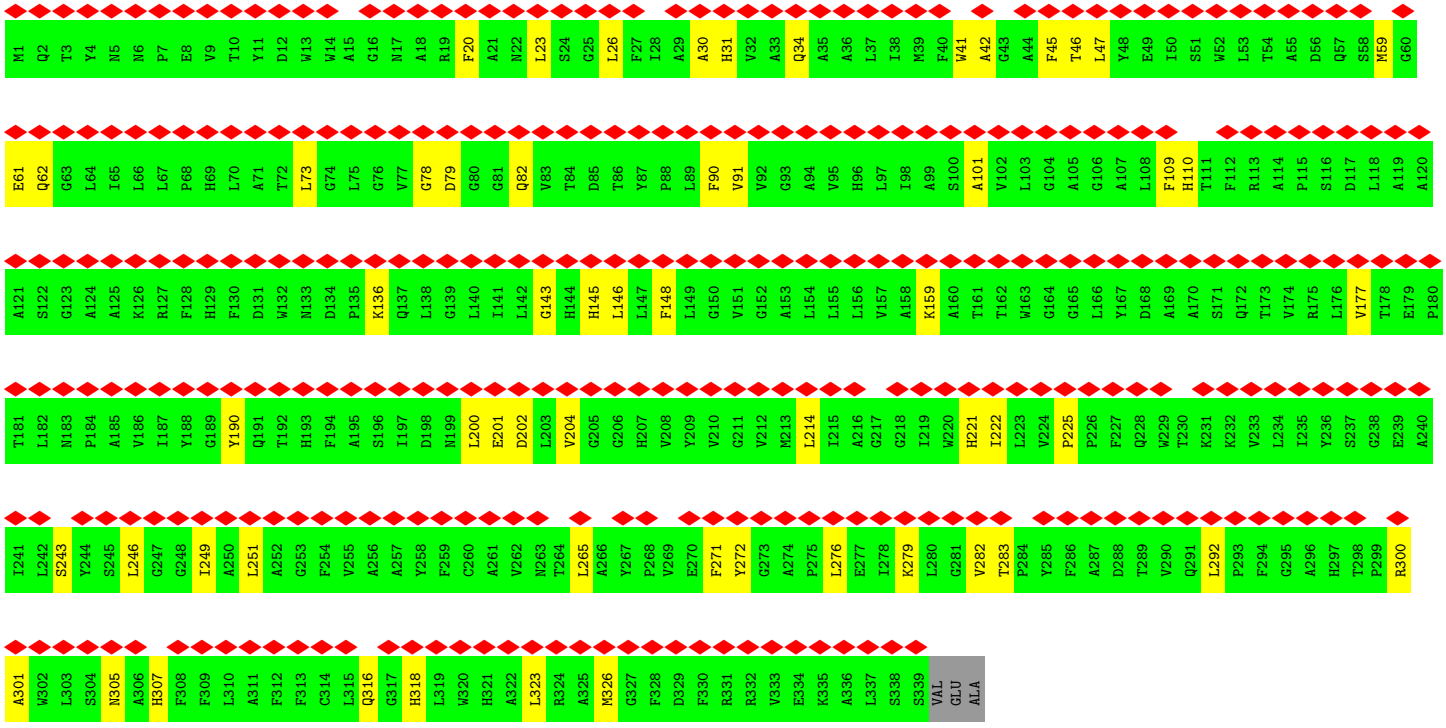




• Molecule 13: Iron stress-induced chlorophyll-binding protein

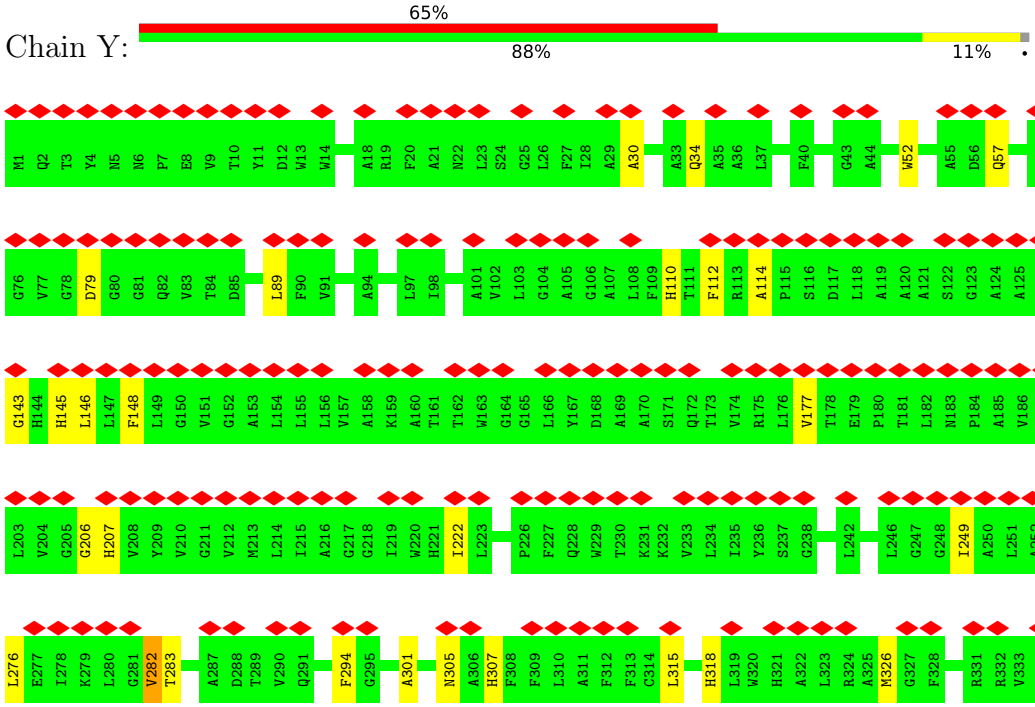
Chain 6:





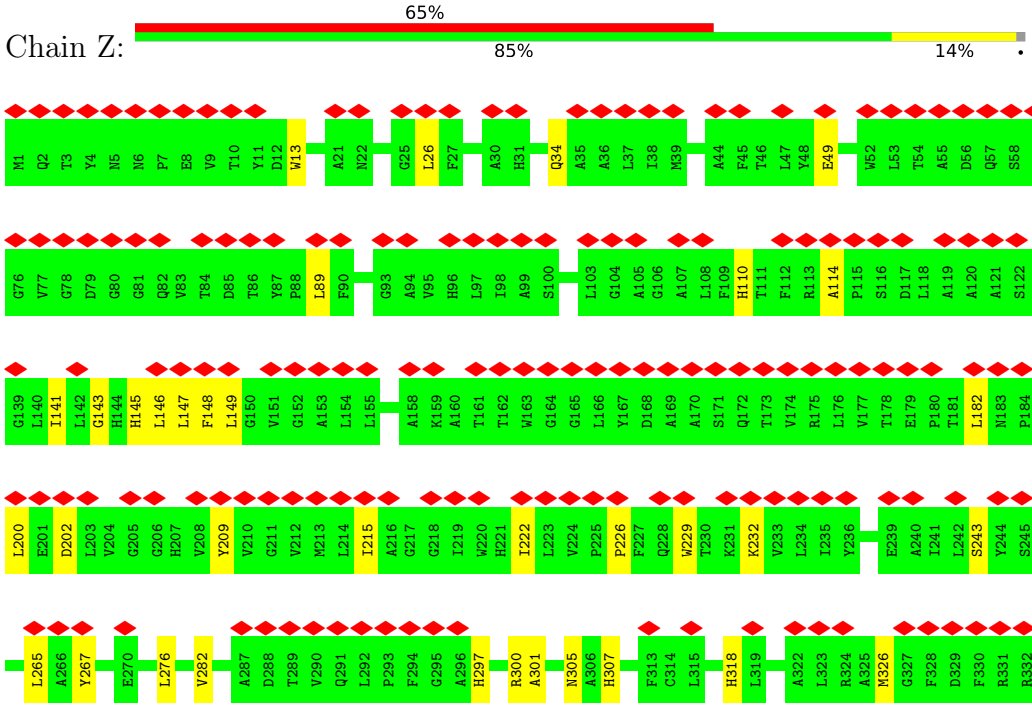
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain Y:



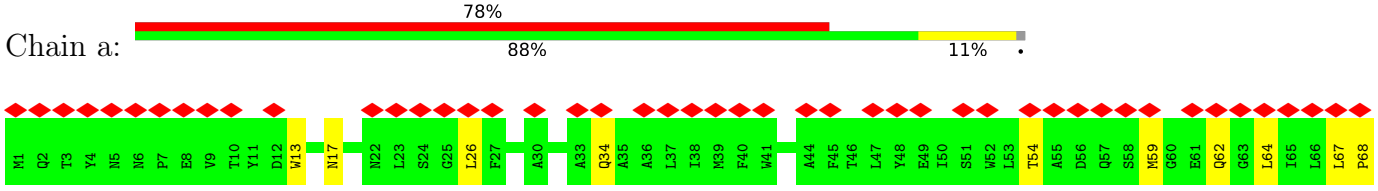
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain Z:



• Molecule 13: Iron stress-induced chlorophyll-binding protein

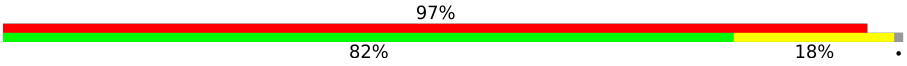
Chain a:

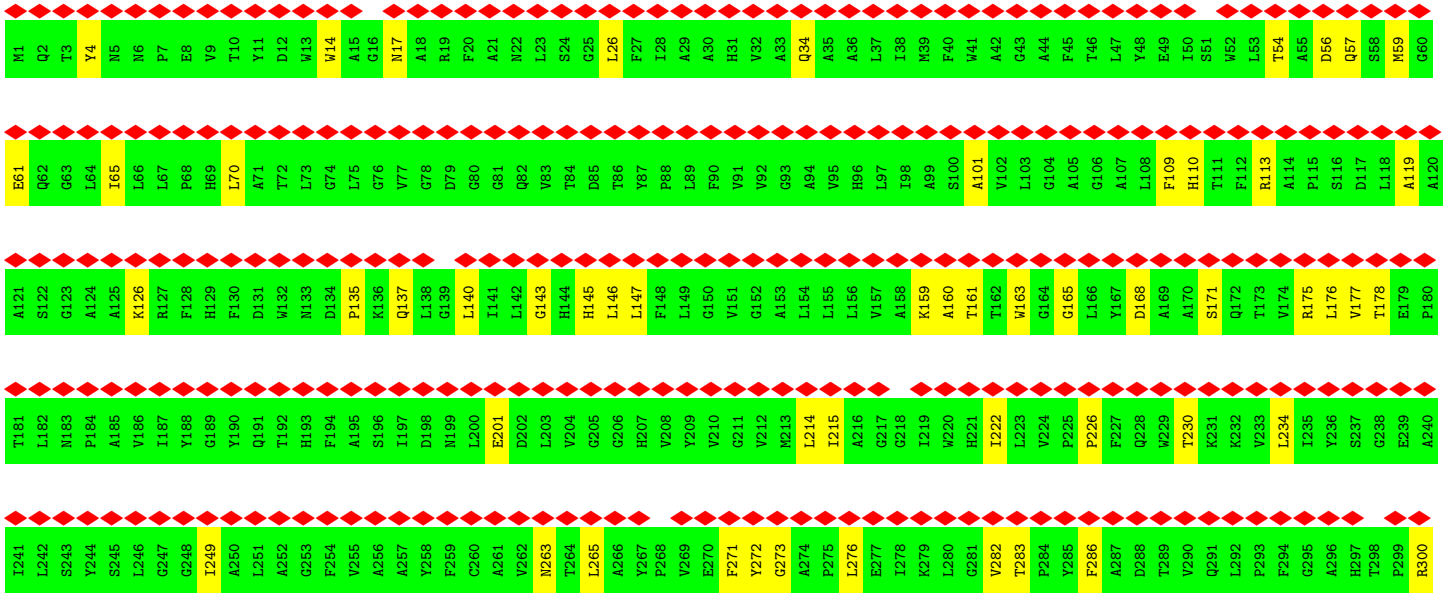




• Molecule 13: Iron stress-induced chlorophyll-binding protein

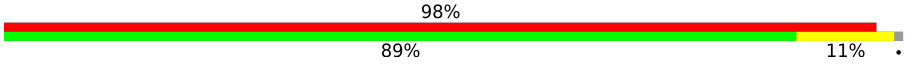
Chain b:

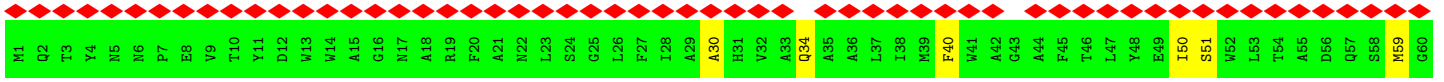


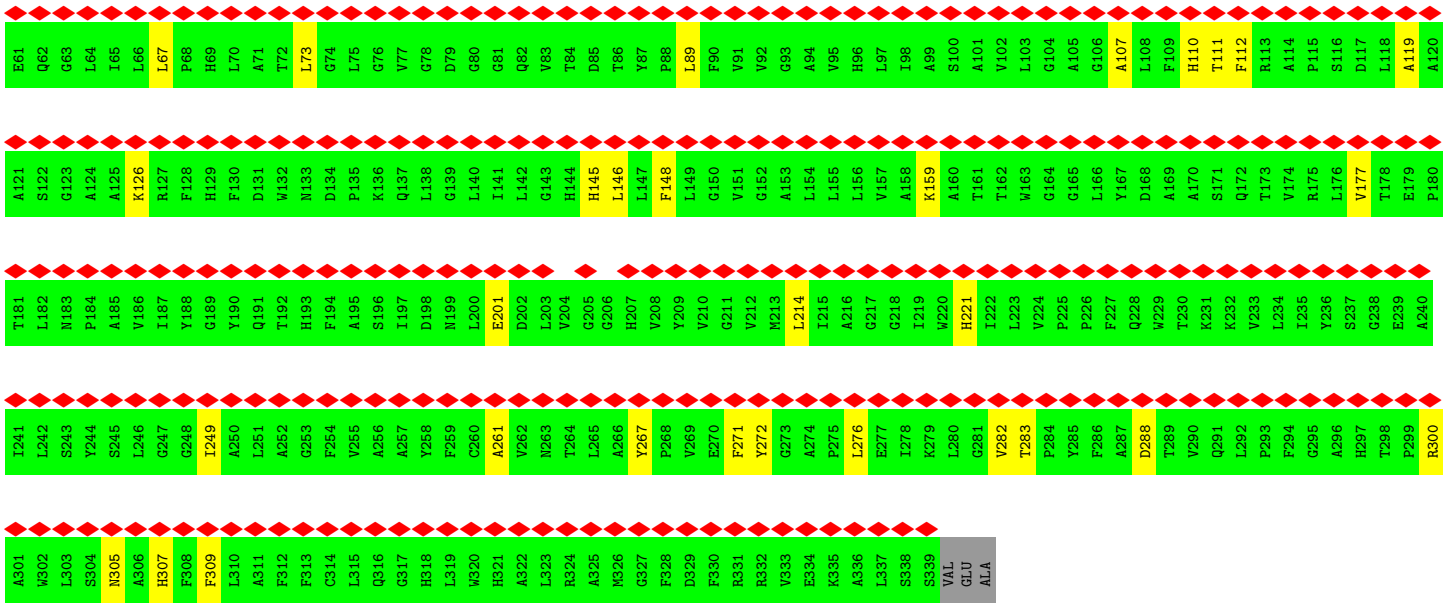


• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c:

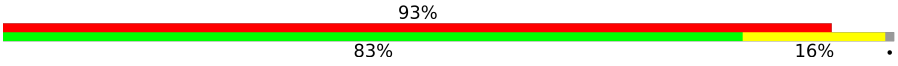


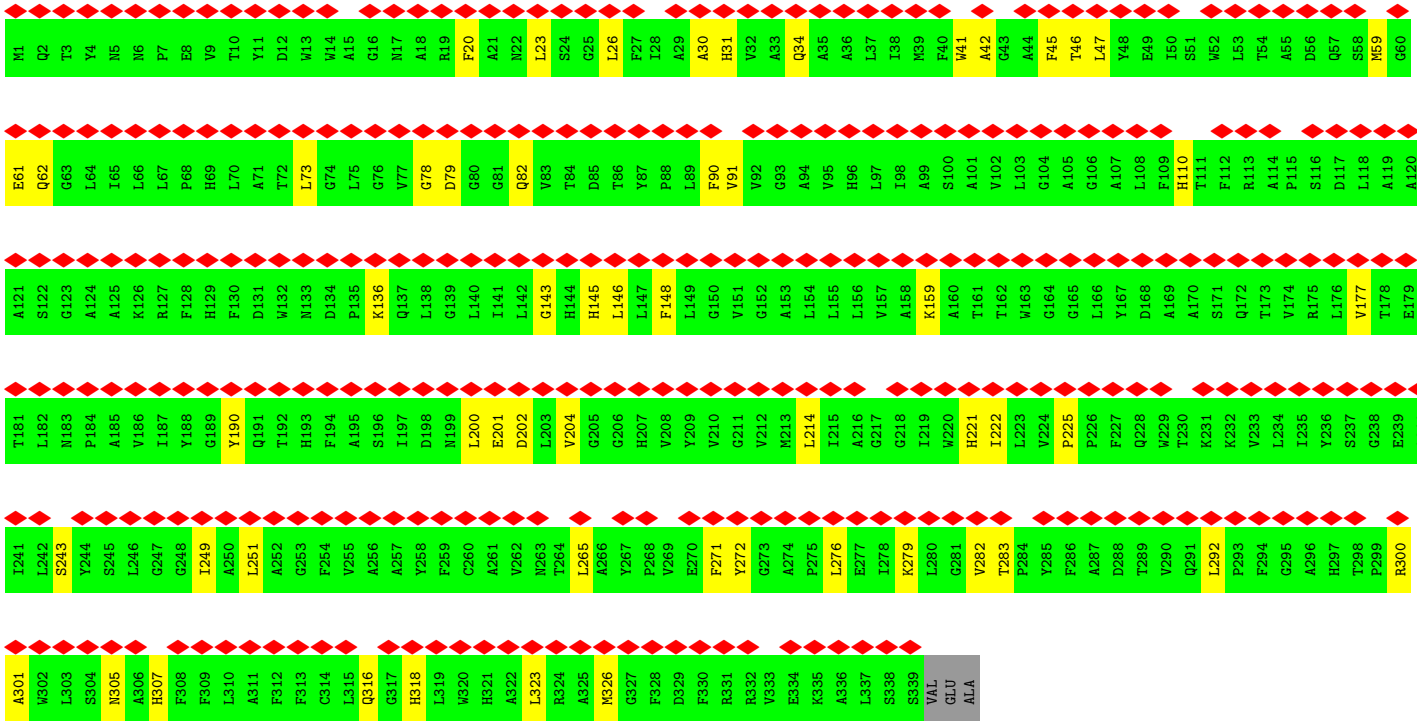




• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain d:

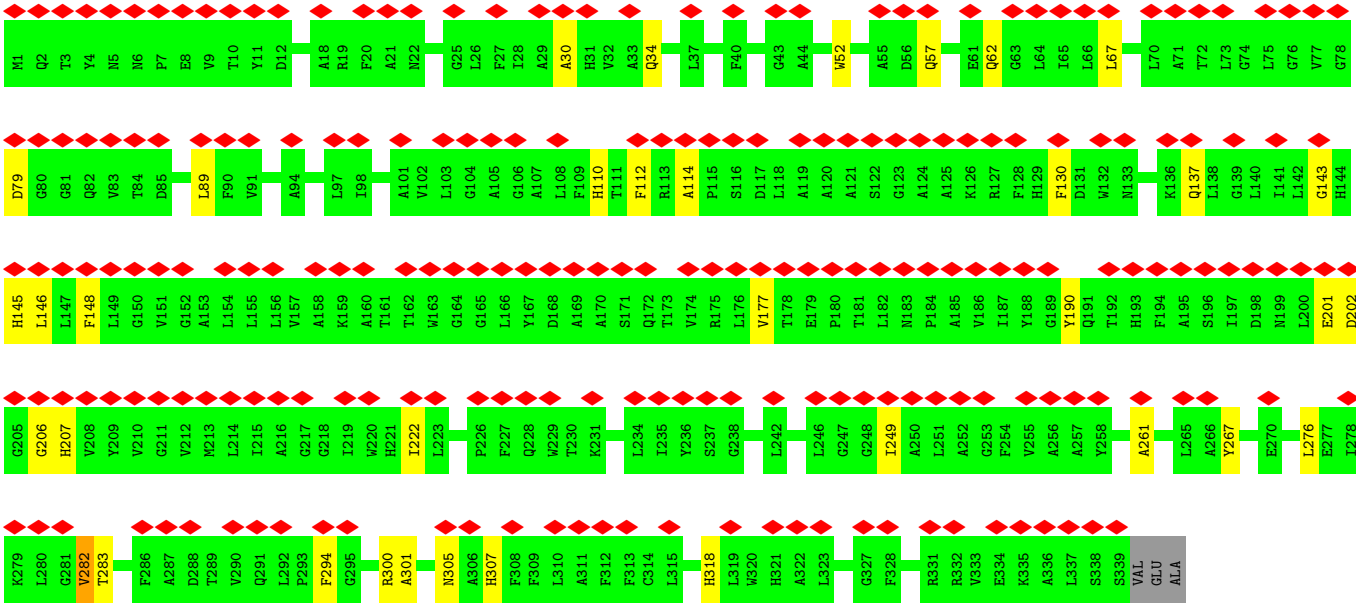




• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain q:

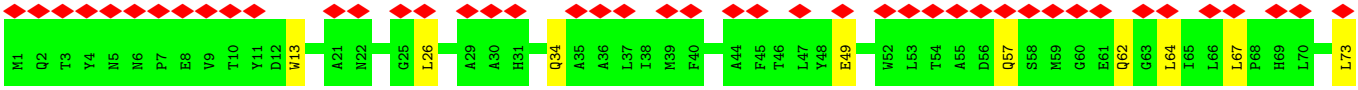


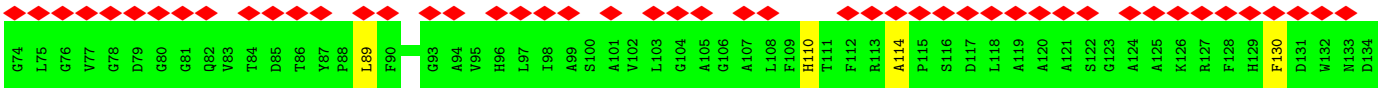


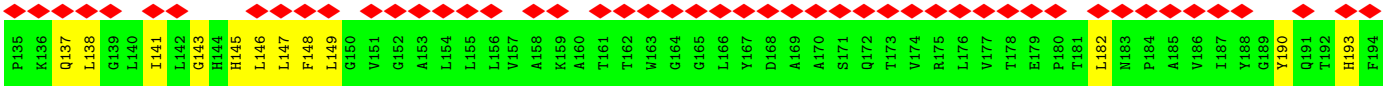
• Molecule 13: Iron stress-induced chlorophyll-binding protein

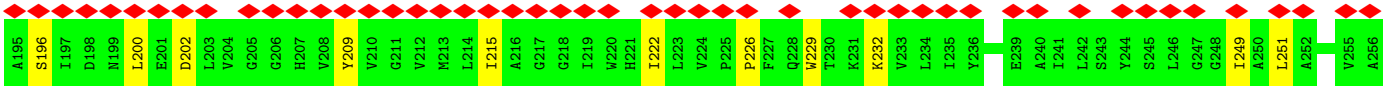
Chain r:









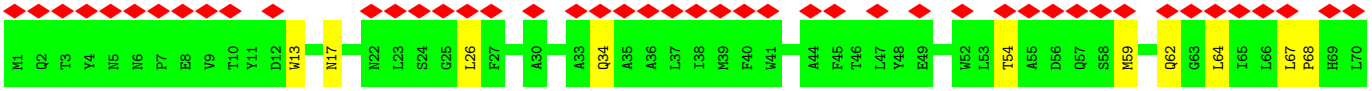


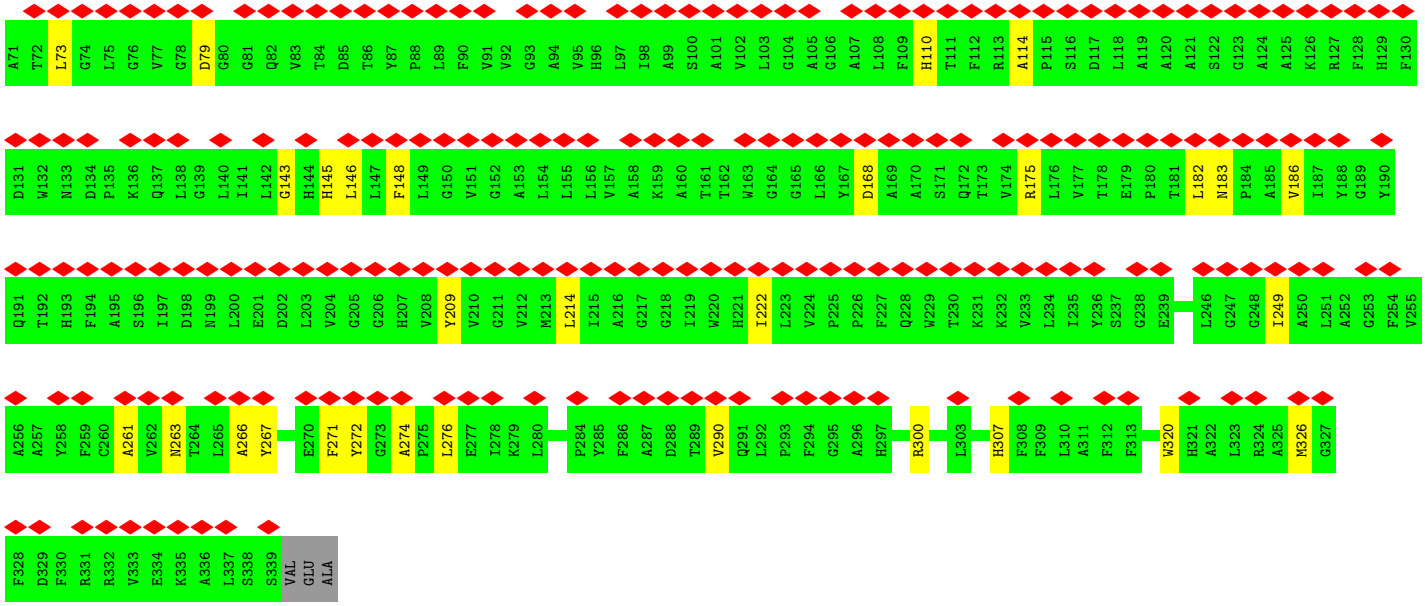


• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain s:

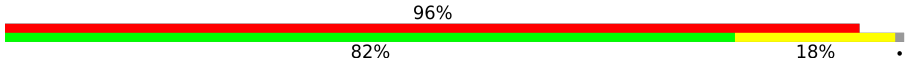


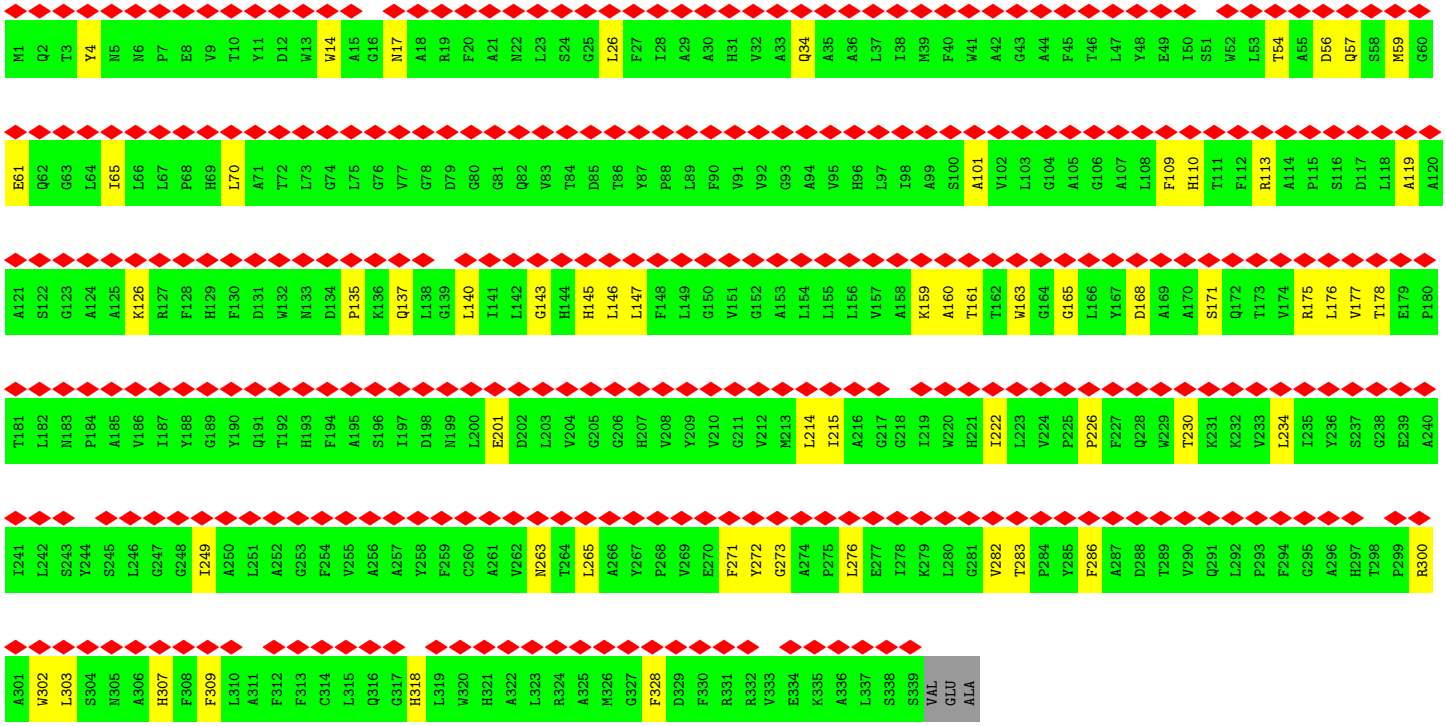




• Molecule 13: Iron stress-induced chlorophyll-binding protein

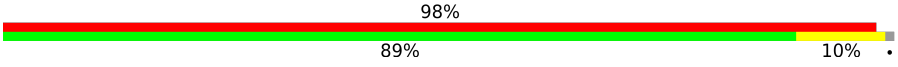
Chain t:

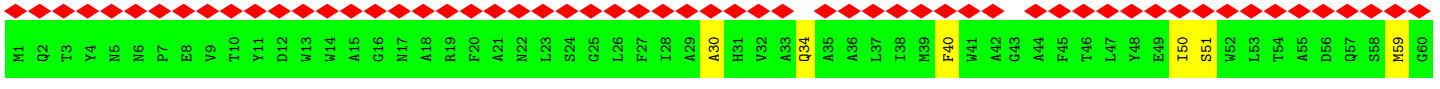


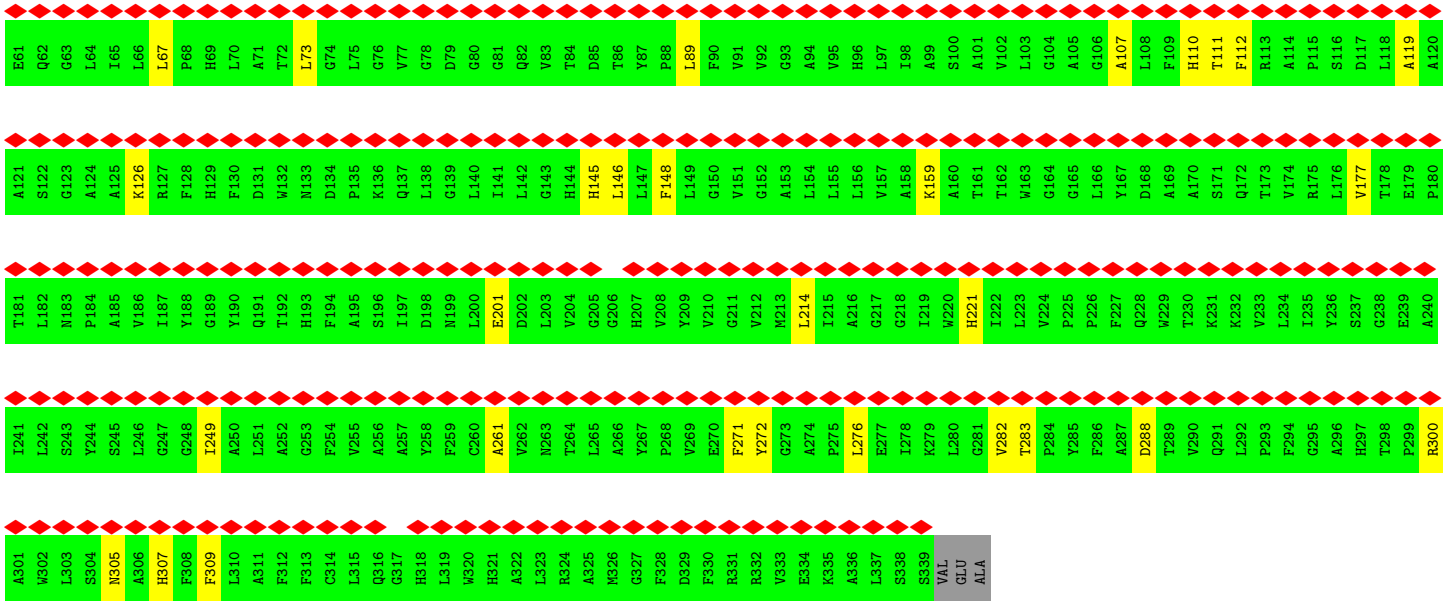


• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain u:

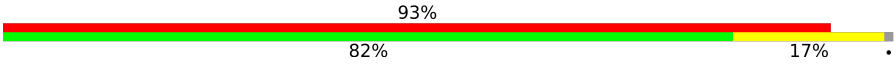


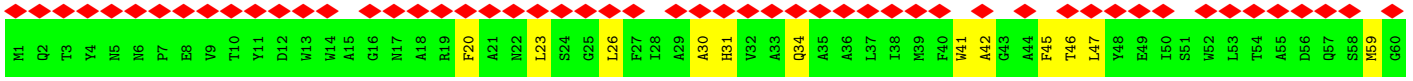


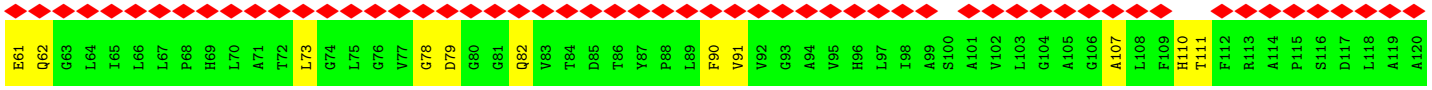


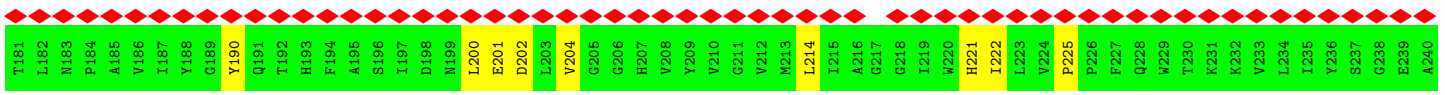
• Molecule 13: Iron stress-induced chlorophyll-binding protein

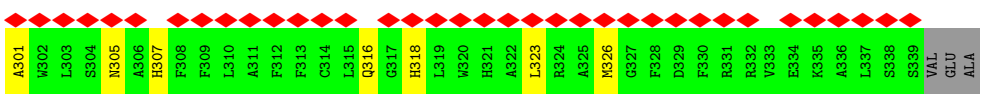
Chain v:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	29295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.50	0/6064	0.54	0/8274
1	G	0.50	0/6064	0.54	0/8274
1	e	0.50	0/6064	0.54	0/8274
2	B	0.42	0/5999	0.54	1/8199 (0.0%)
2	H	0.42	0/5999	0.54	1/8199 (0.0%)
2	f	0.42	0/5999	0.54	1/8199 (0.0%)
3	C	0.43	0/608	0.61	0/823
3	N	0.43	0/608	0.61	0/823
3	g	0.43	0/608	0.61	0/823
4	D	0.43	0/1124	0.56	0/1516
4	O	0.43	0/1124	0.56	0/1516
4	h	0.43	0/1124	0.56	0/1516
5	E	0.36	0/553	0.54	0/750
5	Q	0.36	0/553	0.54	0/750
5	i	0.36	0/553	0.54	0/750
6	F	0.39	0/1062	0.56	0/1442
6	R	0.39	0/1062	0.56	0/1442
6	j	0.39	0/1062	0.56	0/1442
7	I	0.45	0/289	0.66	0/393
7	S	0.45	0/289	0.66	0/393
7	k	0.45	0/289	0.66	0/393
8	J	0.35	0/346	0.50	0/469
8	T	0.35	0/346	0.50	0/469
8	l	0.35	0/346	0.50	0/469
9	K	0.30	0/560	0.57	0/765
9	U	0.31	0/560	0.57	0/765
9	m	0.31	0/560	0.57	0/765
10	L	0.36	0/1242	0.58	1/1696 (0.1%)
10	V	0.36	0/1242	0.58	1/1696 (0.1%)
10	n	0.36	0/1242	0.58	1/1696 (0.1%)
11	M	0.42	0/231	0.61	0/314
11	W	0.42	0/231	0.61	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	o	0.42	0/231	0.61	0/314
12	P	0.24	0/1344	0.45	0/1822
12	X	0.24	0/1344	0.45	0/1822
12	p	0.24	0/1344	0.45	0/1822
13	1	0.22	0/2689	0.45	1/3678 (0.0%)
13	2	0.21	0/2689	0.44	0/3678
13	3	0.19	0/2689	0.42	0/3678
13	4	0.19	0/2689	0.44	0/3678
13	5	0.19	0/2689	0.44	2/3678 (0.1%)
13	6	0.19	0/2689	0.43	0/3678
13	Y	0.22	0/2689	0.45	1/3678 (0.0%)
13	Z	0.22	0/2689	0.44	0/3678
13	a	0.19	0/2689	0.42	0/3678
13	b	0.19	0/2689	0.44	0/3678
13	c	0.19	0/2689	0.44	2/3678 (0.1%)
13	d	0.19	0/2689	0.43	0/3678
13	q	0.22	0/2689	0.45	1/3678 (0.0%)
13	r	0.22	0/2689	0.44	0/3678
13	s	0.19	0/2689	0.42	0/3678
13	t	0.19	0/2689	0.44	0/3678
13	u	0.19	0/2689	0.44	2/3678 (0.1%)
13	v	0.19	0/2689	0.43	0/3678
All	All	0.34	0/106668	0.50	15/145593 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	5	VAL	N-CA-C	7.05	117.84	110.72
10	V	5	VAL	N-CA-C	7.05	117.84	110.72
10	n	5	VAL	N-CA-C	7.05	117.84	110.72
13	1	282	VAL	N-CA-C	-5.65	107.37	112.12
13	Y	282	VAL	N-CA-C	-5.63	107.39	112.12
13	q	282	VAL	N-CA-C	-5.62	107.40	112.12
2	f	668	ARG	N-CA-C	5.57	117.35	111.28
2	B	668	ARG	N-CA-C	5.56	117.34	111.28
2	H	668	ARG	N-CA-C	5.55	117.33	111.28
13	5	288	ASP	CA-C-N	5.10	131.28	121.54
13	5	288	ASP	C-N-CA	5.10	131.28	121.54
13	c	288	ASP	CA-C-N	5.10	131.28	121.54
13	c	288	ASP	C-N-CA	5.10	131.28	121.54
13	u	288	ASP	CA-C-N	5.10	131.27	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	u	288	ASP	C-N-CA	5.10	131.27	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	94	0
1	G	5865	0	5744	98	0
1	e	5865	0	5744	85	0
2	B	5789	0	5575	106	0
2	H	5789	0	5575	110	0
2	f	5789	0	5575	104	0
3	C	598	0	579	9	0
3	N	598	0	579	10	0
3	g	598	0	579	9	0
4	D	1098	0	1099	21	0
4	O	1098	0	1099	20	0
4	h	1098	0	1099	20	0
5	E	543	0	525	7	0
5	Q	543	0	525	6	0
5	i	543	0	525	5	0
6	F	1036	0	1031	15	0
6	R	1036	0	1031	16	0
6	j	1036	0	1031	16	0
7	I	282	0	291	9	0
7	S	282	0	291	9	0
7	k	282	0	291	7	0
8	J	335	0	344	8	0
8	T	335	0	344	8	0
8	l	335	0	344	7	0
9	K	549	0	597	15	0
9	U	549	0	597	16	0
9	m	549	0	597	16	0
10	L	1210	0	1206	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	V	1210	0	1206	40	0
10	n	1210	0	1206	43	0
11	M	228	0	246	5	0
11	W	228	0	246	4	0
11	o	228	0	246	4	0
12	P	1318	0	1233	17	0
12	X	1318	0	1233	18	0
12	p	1318	0	1233	19	0
13	1	2605	0	2564	35	0
13	2	2605	0	2564	38	0
13	3	2605	0	2564	33	0
13	4	2605	0	2564	41	0
13	5	2605	0	2564	30	0
13	6	2605	0	2564	44	0
13	Y	2605	0	2564	38	0
13	Z	2605	0	2564	41	0
13	a	2605	0	2564	32	0
13	b	2605	0	2564	41	0
13	c	2605	0	2564	30	0
13	d	2605	0	2564	41	0
13	q	2605	0	2564	35	0
13	r	2605	0	2564	40	0
13	s	2605	0	2564	33	0
13	t	2605	0	2564	41	0
13	u	2605	0	2564	29	0
13	v	2605	0	2564	44	0
14	1	765	0	561	22	0
14	2	850	0	720	27	0
14	3	785	0	593	16	0
14	4	765	0	561	19	0
14	5	785	0	600	17	0
14	6	785	0	600	21	0
14	A	2712	0	2766	112	0
14	B	2515	0	2595	113	0
14	F	90	0	66	4	0
14	G	2712	0	2766	117	0
14	H	2515	0	2595	113	0
14	J	100	0	82	1	0
14	K	148	0	118	2	0
14	L	185	0	190	10	0
14	R	90	0	66	4	0
14	T	100	0	82	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	148	0	118	2	0
14	V	185	0	190	12	0
14	Y	765	0	561	24	0
14	Z	850	0	720	29	0
14	a	785	0	593	15	0
14	b	765	0	561	19	0
14	c	785	0	600	16	0
14	d	785	0	600	21	0
14	e	2712	0	2766	114	0
14	f	2515	0	2595	107	0
14	j	90	0	66	4	0
14	l	100	0	82	1	0
14	m	148	0	118	2	0
14	n	185	0	190	12	0
14	q	765	0	561	22	0
14	r	850	0	720	26	0
14	s	785	0	593	13	0
14	t	765	0	561	20	0
14	u	785	0	600	17	0
14	v	785	0	600	21	0
15	A	33	0	46	3	0
15	B	33	0	46	4	0
15	G	33	0	46	2	0
15	H	33	0	46	4	0
15	e	33	0	46	2	0
15	f	33	0	46	5	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	G	8	0	0	0	0
16	N	16	0	0	0	0
16	e	8	0	0	0	0
16	g	16	0	0	0	0
17	1	160	0	224	15	0
17	2	160	0	224	17	0
17	3	160	0	224	5	0
17	4	160	0	224	8	0
17	5	160	0	224	7	0
17	6	160	0	224	11	0
17	A	240	0	336	20	0
17	B	280	0	392	29	0
17	F	40	0	56	6	0
17	G	240	0	336	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	280	0	392	27	0
17	I	40	0	56	4	0
17	J	120	0	168	13	0
17	K	40	0	56	3	0
17	L	160	0	224	20	0
17	M	40	0	56	2	0
17	R	40	0	56	6	0
17	S	40	0	56	3	0
17	T	120	0	168	12	0
17	U	40	0	56	3	0
17	V	160	0	224	21	0
17	W	40	0	56	3	0
17	Y	160	0	224	12	0
17	Z	160	0	224	17	0
17	a	160	0	224	4	0
17	b	160	0	224	5	0
17	c	160	0	224	7	0
17	d	160	0	224	12	0
17	e	240	0	336	17	0
17	f	280	0	392	27	0
17	j	40	0	56	6	0
17	k	40	0	56	5	0
17	l	120	0	168	13	0
17	m	40	0	56	3	0
17	n	160	0	224	25	0
17	o	40	0	56	1	0
17	q	160	0	224	12	0
17	r	160	0	224	15	0
17	s	160	0	224	5	0
17	t	160	0	224	7	0
17	u	160	0	224	11	0
17	v	160	0	224	10	0
18	A	374	0	493	30	0
18	B	78	0	96	5	0
18	G	374	0	493	30	0
18	H	78	0	96	5	0
18	I	48	0	69	2	0
18	L	127	0	170	12	0
18	S	48	0	69	2	0
18	V	127	0	170	14	0
18	e	374	0	493	30	0
18	f	78	0	96	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	k	48	0	69	2	0
18	n	127	0	170	12	0
19	A	58	0	76	3	0
19	B	35	0	46	1	0
19	G	58	0	76	3	0
19	H	35	0	46	1	0
19	J	22	0	28	0	0
19	T	22	0	28	0	0
19	e	58	0	76	3	0
19	f	35	0	46	1	0
19	l	22	0	28	0	0
20	B	53	0	76	5	0
20	H	53	0	76	6	0
20	J	32	0	34	0	0
20	T	32	0	34	1	0
20	f	53	0	76	6	0
20	l	32	0	34	0	0
21	1	32	0	28	1	0
21	2	28	0	20	0	0
21	3	28	0	20	2	0
21	4	26	0	16	0	0
21	5	26	0	16	0	0
21	6	26	0	16	0	0
21	B	40	0	42	8	0
21	H	40	0	42	9	0
21	L	46	0	58	6	0
21	V	46	0	58	6	0
21	Y	32	0	28	1	0
21	Z	28	0	20	0	0
21	a	28	0	20	2	0
21	b	26	0	16	0	0
21	c	26	0	16	0	0
21	d	26	0	16	0	0
21	f	40	0	42	9	0
21	n	46	0	58	6	0
21	q	32	0	28	1	0
21	r	28	0	20	0	0
21	s	28	0	20	2	0
21	t	26	0	16	0	0
21	u	26	0	16	0	0
21	v	26	0	16	0	0
22	P	31	0	19	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	X	31	0	19	2	0
22	p	31	0	19	1	0
23	A	9	0	0	1	0
23	B	7	0	0	0	0
23	F	1	0	0	0	0
23	G	9	0	0	1	0
23	H	7	0	0	0	0
23	L	1	0	0	0	0
23	R	1	0	0	0	0
23	V	1	0	0	0	0
23	e	9	0	0	1	0
23	f	7	0	0	0	0
23	j	1	0	0	0	0
23	n	1	0	0	0	0
All	All	144312	0	142227	2417	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 (2417) 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)
10:n:3:GLN:HG2	10:n:4:ASP:H	0.93	1.09
10:L:3:GLN:HG2	10:L:4:ASP:H	0.93	1.06
10:V:3:GLN:HG2	10:V:4:ASP:H	0.93	1.05
10:L:3:GLN:HG2	10:L:4:ASP:N	1.75	1.00
10:V:3:GLN:HG2	10:V:4:ASP:N	1.75	0.98
10:n:3:GLN:HG2	10:n:4:ASP:N	1.75	0.97
10:n:3:GLN:CG	10:n:4:ASP:H	1.82	0.87
10:V:3:GLN:CG	10:V:4:ASP:H	1.82	0.87
17:L:4022:BCR:C24	10:n:137:LEU:HD13	2.04	0.87
18:A:5009:LHG:H131	17:1:521:BCR:H322	1.57	0.86
10:L:137:LEU:HD13	17:V:4022:BCR:C24	2.06	0.85
10:L:3:GLN:CG	10:L:4:ASP:H	1.82	0.85
18:G:5009:LHG:H131	17:Y:521:BCR:H322	1.57	0.85
18:e:5009:LHG:H131	17:q:521:BCR:H322	1.57	0.83
14:B:1207:CLA:H42	18:V:5221:LHG:H252	1.59	0.82
10:V:137:LEU:HD13	17:n:4022:BCR:C24	2.11	0.80
18:L:5221:LHG:H252	14:f:1207:CLA:H42	1.65	0.78
14:H:1207:CLA:H42	18:n:5221:LHG:H252	1.65	0.78
13:t:145:HIS:NE2	14:t:512:CLA:NA	2.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:145:HIS:NE2	14:b:512:CLA:NA	2.32	0.77
14:G:1013:CLA:H111	17:G:4011:BCR:H23C	1.67	0.76
13:4:145:HIS:NE2	14:4:512:CLA:NA	2.32	0.76
14:e:1130:CLA:H2	14:n:1502:CLA:H43	1.68	0.76
17:L:4022:BCR:H24C	10:n:137:LEU:HD13	1.67	0.75
14:e:1013:CLA:H111	17:e:4011:BCR:H23C	1.67	0.75
4:O:41:GLU:H	4:O:71:GLN:HE22	1.35	0.75
14:A:1013:CLA:H111	17:A:4011:BCR:H23C	1.67	0.74
13:Y:148:PHE:CZ	14:Y:516:CLA:HBC2	2.22	0.74
4:h:41:GLU:H	4:h:71:GLN:HE22	1.35	0.74
13:1:148:PHE:CZ	14:1:516:CLA:HBC2	2.22	0.74
14:A:1130:CLA:H2	14:L:1502:CLA:H43	1.68	0.74
14:G:1130:CLA:H2	14:V:1502:CLA:H43	1.68	0.74
13:q:148:PHE:CZ	14:q:516:CLA:HBC2	2.22	0.73
4:D:41:GLU:H	4:D:71:GLN:HE22	1.35	0.73
13:q:148:PHE:HZ	14:q:516:CLA:HBC2	1.54	0.73
9:K:60:VAL:HG22	14:K:1105:CLA:HAC2	1.71	0.72
14:d:505:CLA:H43	17:d:524:BCR:HC7	1.73	0.71
10:L:137:LEU:HD13	17:V:4022:BCR:H24C	1.71	0.71
13:1:52:TRP:CE3	14:1:504:CLA:HED3	2.25	0.71
13:q:52:TRP:CE3	14:q:504:CLA:HED3	2.25	0.71
1:G:410:GLY:HA3	1:G:614:LEU:HD11	1.73	0.71
1:A:410:GLY:HA3	1:A:614:LEU:HD11	1.73	0.71
9:U:60:VAL:HG22	14:U:1105:CLA:HAC2	1.71	0.71
13:Y:148:PHE:HZ	14:Y:516:CLA:HBC2	1.54	0.71
9:m:60:VAL:HG22	14:m:1105:CLA:HAC2	1.71	0.71
14:6:505:CLA:H43	17:6:524:BCR:HC7	1.72	0.71
13:Y:52:TRP:CE3	14:Y:504:CLA:HED3	2.25	0.71
14:B:1216:CLA:H2	14:B:1221:CLA:H102	1.71	0.71
14:H:1216:CLA:H2	14:H:1221:CLA:H102	1.71	0.71
14:v:505:CLA:H43	17:v:524:BCR:HC7	1.73	0.70
1:e:410:GLY:HA3	1:e:614:LEU:HD11	1.73	0.70
14:f:1216:CLA:H2	14:f:1221:CLA:H102	1.71	0.70
14:H:1222:CLA:HMA1	17:H:4010:BCR:H14C	1.74	0.70
14:e:1104:CLA:H42	14:e:1128:CLA:H2	1.74	0.70
13:1:148:PHE:HZ	14:1:516:CLA:HBC2	1.54	0.70
14:A:1104:CLA:H42	14:A:1128:CLA:H2	1.74	0.69
11:M:21:TYR:OH	10:V:26:PHE:HB2	1.92	0.69
13:c:146:LEU:HD21	14:c:506:CLA:HAB	1.75	0.69
13:5:146:LEU:HD21	14:5:506:CLA:HAB	1.75	0.69
13:s:110:HIS:NE2	14:s:513:CLA:NB	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:110:HIS:NE2	14:3:513:CLA:NB	2.40	0.69
13:a:110:HIS:NE2	14:a:513:CLA:NB	2.40	0.69
14:H:1234:CLA:H71	14:H:1235:CLA:H12	1.75	0.69
13:Y:222:ILE:HG23	14:Y:516:CLA:HMA1	1.75	0.69
14:B:1234:CLA:H71	14:B:1235:CLA:H12	1.75	0.69
14:G:1104:CLA:H42	14:G:1128:CLA:H2	1.74	0.69
13:q:222:ILE:HG23	14:q:516:CLA:HMA1	1.75	0.68
13:u:146:LEU:HD21	14:u:506:CLA:HAB	1.74	0.68
13:r:146:LEU:HD21	14:r:506:CLA:HAB	1.75	0.68
13:Y:318:HIS:NE2	14:Y:505:CLA:NB	2.42	0.68
14:f:1222:CLA:HMA1	17:f:4010:BCR:H14C	1.74	0.67
14:B:1222:CLA:HMA1	17:B:4010:BCR:H14C	1.74	0.67
13:1:222:ILE:HG23	14:1:516:CLA:HMA1	1.75	0.67
13:2:146:LEU:HD21	14:2:506:CLA:HAB	1.75	0.67
14:f:1234:CLA:H71	14:f:1235:CLA:H12	1.75	0.67
13:Z:146:LEU:HD21	14:Z:506:CLA:HAB	1.75	0.67
18:H:1855:LHG:HC82	18:H:1855:LHG:H252	1.77	0.67
10:V:137:LEU:HD13	17:n:4022:BCR:H24C	1.76	0.67
10:V:134:LEU:HD13	10:n:134:LEU:HD13	1.77	0.66
18:B:1855:LHG:HC82	18:B:1855:LHG:H252	1.77	0.66
5:E:10:ARG:HB3	5:E:67:GLN:HG2	1.78	0.66
5:Q:10:ARG:HB3	5:Q:67:GLN:HG2	1.77	0.66
14:f:1203:CLA:H152	14:f:1225:CLA:HBB2	1.79	0.65
13:1:318:HIS:NE2	14:1:505:CLA:NB	2.42	0.65
6:R:91:ILE:HG23	14:R:1301:CLA:HAA1	1.78	0.65
13:q:318:HIS:NE2	14:q:505:CLA:NB	2.42	0.65
10:L:134:LEU:HD13	10:V:134:LEU:HD13	1.78	0.65
18:f:1855:LHG:HC82	18:f:1855:LHG:H252	1.77	0.65
13:6:30:ALA:HB2	14:6:511:CLA:HMA1	1.79	0.65
10:V:133:ILE:CG2	10:n:48:LEU:HD21	2.27	0.65
5:i:10:ARG:HB3	5:i:67:GLN:HG2	1.77	0.65
13:v:30:ALA:HB2	14:v:511:CLA:HMA1	1.79	0.65
10:L:133:ILE:CG2	10:V:48:LEU:HD21	2.26	0.64
13:d:30:ALA:HB2	14:d:511:CLA:HMA1	1.79	0.64
6:j:91:ILE:HG23	14:j:1301:CLA:HAA1	1.78	0.64
13:3:272:TYR:HB3	13:3:300:ARG:HB2	1.80	0.64
13:a:272:TYR:HB3	13:a:300:ARG:HB2	1.80	0.64
14:A:1126:CLA:H201	17:J:4012:BCR:H12C	1.80	0.64
14:B:1207:CLA:H42	18:V:5221:LHG:C25	2.27	0.64
6:F:91:ILE:HG23	14:F:1301:CLA:HAA1	1.78	0.64
14:H:1239:CLA:HBA2	15:H:2002:PQN:H251	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:1203:CLA:H152	14:H:1225:CLA:HBB2	1.79	0.64
14:f:1214:CLA:HBA2	14:f:1223:CLA:HBB2	1.80	0.63
14:G:1136:CLA:HBC1	18:V:5220:LHG:H282	1.80	0.63
14:f:1239:CLA:HBA2	15:f:2002:PQN:H251	1.80	0.63
18:A:5005:LHG:HC61	17:2:521:BCR:HC22	1.81	0.63
14:B:1203:CLA:H152	14:B:1225:CLA:HBB2	1.79	0.63
17:A:4011:BCR:H362	14:B:1012:CLA:H2	1.80	0.63
13:s:272:TYR:HB3	13:s:300:ARG:HB2	1.80	0.63
11:W:21:TYR:OH	10:n:26:PHE:HB2	1.98	0.63
17:J:4013:BCR:H362	17:J:4012:BCR:H17C	1.81	0.63
14:e:1126:CLA:H201	17:l:4012:BCR:H12C	1.80	0.63
18:G:5005:LHG:HC61	17:Z:521:BCR:HC22	1.81	0.63
14:B:1214:CLA:HBA2	14:B:1223:CLA:HBB2	1.80	0.63
14:B:1239:CLA:HBA2	15:B:2002:PQN:H251	1.80	0.63
6:R:143:SER:HB2	13:b:14:TRP:CZ3	2.34	0.63
17:V:4022:BCR:H333	21:V:5216:SQD:C14	2.29	0.63
14:e:1136:CLA:HBC1	18:n:5220:LHG:H282	1.80	0.63
17:L:4022:BCR:H333	21:L:5216:SQD:C14	2.29	0.62
17:T:4013:BCR:H362	17:T:4012:BCR:H17C	1.81	0.62
14:G:1013:CLA:HBA2	2:H:427:LEU:HD12	1.82	0.62
14:H:1214:CLA:HBA2	14:H:1223:CLA:HBB2	1.80	0.62
4:O:73:ARG:NH1	4:O:106:GLU:OE2	2.31	0.62
18:e:5005:LHG:HC61	17:r:521:BCR:HC22	1.81	0.62
17:n:4022:BCR:H333	21:n:5216:SQD:C14	2.29	0.62
4:D:73:ARG:NH1	4:D:106:GLU:OE2	2.31	0.62
13:a:249:ILE:HG12	14:a:502:CLA:HAC1	1.81	0.62
13:s:249:ILE:HG12	14:s:502:CLA:HAC1	1.81	0.62
6:F:143:SER:HB2	13:4:14:TRP:CZ3	2.34	0.62
13:6:249:ILE:HG12	14:6:502:CLA:HAC1	1.82	0.62
14:G:1126:CLA:H201	17:T:4012:BCR:H12C	1.80	0.62
13:d:249:ILE:HG12	14:d:502:CLA:HAC1	1.82	0.62
1:e:752:TRP:NE1	14:e:1126:CLA:O1A	2.29	0.62
6:j:143:SER:HB2	13:t:14:TRP:CZ3	2.34	0.62
14:G:1101:CLA:H112	17:T:4013:BCR:H19C	1.82	0.62
17:e:4011:BCR:H362	14:f:1012:CLA:H2	1.80	0.62
14:A:1136:CLA:HBC1	18:L:5220:LHG:H282	1.80	0.62
13:d:272:TYR:HB3	13:d:300:ARG:HB2	1.81	0.62
10:L:26:PHE:HB2	11:o:21:TYR:OH	1.98	0.62
14:f:1217:CLA:HBB1	17:f:4004:BCR:H14C	1.82	0.62
10:L:94:SER:HB2	14:V:1501:CLA:HMD3	1.81	0.62
10:L:134:LEU:HD13	10:n:134:LEU:HD13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:272:TYR:HB3	13:6:300:ARG:HB2	1.81	0.62
4:h:73:ARG:NH1	4:h:106:GLU:OE2	2.31	0.62
14:A:1101:CLA:H112	17:J:4013:BCR:H19C	1.82	0.62
13:d:61:GLU:HG3	13:d:292:LEU:HD13	1.82	0.62
17:l:4013:BCR:H362	17:l:4012:BCR:H17C	1.81	0.62
13:v:61:GLU:HG3	13:v:292:LEU:HD13	1.82	0.62
13:v:249:ILE:HG12	14:v:502:CLA:HAC1	1.82	0.62
17:G:4011:BCR:H362	14:H:1012:CLA:H2	1.80	0.61
13:d:251:LEU:HD13	14:d:505:CLA:H122	1.82	0.61
14:B:1209:CLA:H71	14:B:1209:CLA:HBB1	1.83	0.61
13:2:34:GLN:OE1	14:2:510:CLA:NC	2.34	0.61
14:B:1217:CLA:HBB1	17:B:4004:BCR:H14C	1.82	0.61
14:B:1226:CLA:H42	20:B:5002:LMG:H302	1.82	0.61
14:e:1013:CLA:HBA2	2:f:427:LEU:HD12	1.82	0.61
13:3:249:ILE:HG12	14:3:502:CLA:HAC1	1.81	0.61
14:H:1217:CLA:HBB1	17:H:4004:BCR:H14C	1.82	0.61
14:f:1226:CLA:H42	20:f:5002:LMG:H302	1.82	0.61
13:v:272:TYR:HB3	13:v:300:ARG:HB2	1.81	0.61
1:A:752:TRP:NE1	14:A:1126:CLA:O1A	2.29	0.61
13:Z:34:GLN:OE1	14:Z:510:CLA:NC	2.34	0.61
13:r:34:GLN:OE1	14:r:510:CLA:NC	2.34	0.61
14:L:1501:CLA:HMD3	10:n:94:SER:HB2	1.82	0.61
14:f:1202:CLA:H8	14:f:1221:CLA:HBA2	1.83	0.61
4:h:32:TRP:NE1	4:h:50:MET:SD	2.72	0.61
14:A:1013:CLA:HBA2	2:B:427:LEU:HD12	1.82	0.61
14:H:1202:CLA:H8	14:H:1221:CLA:HBA2	1.83	0.61
1:A:86:TRP:HA	14:A:1105:CLA:HBB2	1.83	0.60
13:6:251:LEU:HD13	14:6:505:CLA:H122	1.82	0.60
1:G:86:TRP:HA	14:G:1105:CLA:HBB2	1.83	0.60
13:d:34:GLN:OE1	14:d:510:CLA:NC	2.34	0.60
14:e:1101:CLA:H112	17:l:4013:BCR:H19C	1.82	0.60
14:f:1209:CLA:H71	14:f:1209:CLA:HBB1	1.83	0.60
18:L:5221:LHG:C24	14:f:1207:CLA:H42	2.31	0.60
13:6:61:GLU:HG3	13:6:292:LEU:HD13	1.82	0.60
14:H:1226:CLA:H42	20:H:5002:LMG:H302	1.82	0.60
13:v:34:GLN:OE1	14:v:510:CLA:NC	2.34	0.60
14:B:1202:CLA:H8	14:B:1221:CLA:HBA2	1.83	0.60
13:v:251:LEU:HD13	14:v:505:CLA:H122	1.82	0.60
1:G:494:PHE:HB3	14:G:1135:CLA:H11	1.84	0.60
2:f:15:ASP:HB3	2:f:20:ARG:HB2	1.84	0.60
10:L:48:LEU:HD21	10:n:133:ILE:CG2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:494:PHE:HB3	14:e:1135:CLA:H11	1.84	0.60
4:D:32:TRP:NE1	4:D:50:MET:SD	2.72	0.60
13:u:34:GLN:OE1	14:u:510:CLA:NC	2.35	0.60
2:B:151:PHE:HE2	21:B:1852:SQD:H102	1.66	0.60
2:H:15:ASP:HB3	2:H:20:ARG:HB2	1.84	0.60
13:d:316:GLN:NE2	14:d:518:CLA:O1A	2.34	0.60
1:A:490:LEU:HD22	17:L:4219:BCR:H331	1.84	0.60
14:B:1225:CLA:H12	17:B:4005:BCR:H393	1.84	0.60
13:6:34:GLN:OE1	14:6:510:CLA:NC	2.34	0.59
2:H:151:PHE:HE2	21:H:1852:SQD:H102	1.66	0.59
14:f:1223:CLA:H122	17:f:4010:BCR:H17C	1.84	0.59
1:A:494:PHE:HB3	14:A:1135:CLA:H11	1.84	0.59
13:5:34:GLN:OE1	14:5:510:CLA:NC	2.35	0.59
1:G:490:LEU:HD22	17:V:4219:BCR:H331	1.84	0.59
14:A:1237:CLA:H141	10:L:85:LEU:HD11	1.85	0.59
13:6:316:GLN:NE2	14:6:518:CLA:O1A	2.34	0.59
13:c:34:GLN:OE1	14:c:510:CLA:NC	2.35	0.59
2:H:456:GLU:OE1	6:R:68:HIS:ND1	2.35	0.59
1:e:86:TRP:HA	14:e:1105:CLA:HBB2	1.83	0.59
14:B:1207:CLA:H42	18:V:5221:LHG:C24	2.32	0.59
1:G:607:LEU:HD21	14:G:1128:CLA:HBC1	1.83	0.59
14:G:1237:CLA:H141	10:V:85:LEU:HD11	1.85	0.59
1:e:490:LEU:HD22	17:n:4219:BCR:H331	1.84	0.59
2:f:151:PHE:HE2	21:f:1852:SQD:H102	1.66	0.59
14:f:1229:CLA:H192	17:j:4016:BCR:H17C	1.85	0.59
14:B:1223:CLA:H122	17:B:4010:BCR:H17C	1.85	0.59
13:Z:267:TYR:O	13:Z:300:ARG:NH2	2.36	0.59
13:r:267:TYR:O	13:r:300:ARG:NH2	2.36	0.59
1:A:607:LEU:HD21	14:A:1128:CLA:HBC1	1.83	0.59
1:G:370:ILE:HD11	14:G:1119:CLA:H71	1.85	0.59
14:H:1225:CLA:H12	17:H:4005:BCR:H393	1.84	0.59
14:f:1204:CLA:H111	17:k:4018:BCR:HC21	1.85	0.59
14:A:1103:CLA:H142	17:A:4003:BCR:H372	1.85	0.59
18:L:5221:LHG:C25	14:f:1207:CLA:H42	2.31	0.59
14:H:1209:CLA:H71	14:H:1209:CLA:HBB1	1.83	0.59
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.84	0.59
14:V:1501:CLA:H121	17:V:4022:BCR:HC8	1.85	0.59
1:e:607:LEU:HD21	14:e:1128:CLA:HBC1	1.83	0.59
14:B:1229:CLA:H192	17:F:4016:BCR:H17C	1.85	0.59
14:H:1229:CLA:H192	17:R:4016:BCR:H17C	1.85	0.59
14:n:1501:CLA:H121	17:n:4022:BCR:HC8	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:u:272:TYR:HB3	13:u:300:ARG:HB2	1.85	0.59
13:q:249:ILE:HG12	14:q:502:CLA:HAC1	1.85	0.58
15:G:2001:PQN:H162	17:H:4014:BCR:H382	1.85	0.58
14:e:1237:CLA:H141	10:n:85:LEU:HD11	1.85	0.58
14:f:1225:CLA:H12	17:f:4005:BCR:H393	1.84	0.58
14:f:1235:CLA:H172	17:j:4016:BCR:H272	1.85	0.58
15:A:2001:PQN:H162	17:B:4014:BCR:H382	1.85	0.58
10:L:160:ALA:HB1	10:L:165:VAL:HB	1.86	0.58
13:2:267:TYR:O	13:2:300:ARG:NH2	2.36	0.58
13:Y:145:HIS:NE2	14:Y:512:CLA:NA	2.51	0.58
15:e:2001:PQN:H162	17:f:4014:BCR:H382	1.85	0.58
13:v:316:GLN:NE2	14:v:518:CLA:O1A	2.34	0.58
10:L:155:LEU:HD22	7:k:13:ILE:HD11	1.85	0.58
18:L:5221:LHG:H241	14:f:1207:CLA:H42	1.86	0.58
9:U:51:LEU:O	14:U:1105:CLA:ND	2.37	0.58
13:s:34:GLN:OE1	14:s:510:CLA:NC	2.37	0.58
13:3:34:GLN:OE1	14:3:510:CLA:NC	2.37	0.58
14:H:1225:CLA:H203	17:H:4006:BCR:H15C	1.86	0.58
1:e:370:ILE:HD11	14:e:1119:CLA:H71	1.85	0.58
10:n:160:ALA:HB1	10:n:165:VAL:HB	1.86	0.58
14:L:1501:CLA:H121	17:L:4022:BCR:HC8	1.85	0.58
13:6:307:HIS:NE2	14:6:502:CLA:ND	2.52	0.58
14:H:1223:CLA:H122	17:H:4010:BCR:H17C	1.85	0.58
9:m:51:LEU:O	14:m:1105:CLA:ND	2.37	0.58
13:1:145:HIS:NE2	14:1:512:CLA:NA	2.51	0.58
13:Y:30:ALA:HB2	14:Y:511:CLA:HMA1	1.85	0.58
13:a:34:GLN:OE1	14:a:510:CLA:NC	2.37	0.58
2:f:456:GLU:OE1	6:j:68:HIS:ND1	2.35	0.58
13:q:30:ALA:HB2	14:q:511:CLA:HMA1	1.85	0.58
13:q:145:HIS:NE2	14:q:512:CLA:NA	2.51	0.58
12:X:2:LYS:HE2	12:X:169:LEU:HD12	1.86	0.58
13:Y:249:ILE:HG12	14:Y:502:CLA:HAC1	1.85	0.58
13:d:307:HIS:NE2	14:d:502:CLA:ND	2.52	0.58
9:K:51:LEU:O	14:K:1105:CLA:ND	2.37	0.58
13:5:272:TYR:HB3	13:5:300:ARG:HB2	1.85	0.58
13:v:307:HIS:NE2	14:v:502:CLA:ND	2.52	0.58
13:1:30:ALA:HB2	14:1:511:CLA:HMA1	1.85	0.57
14:H:1235:CLA:H172	17:R:4016:BCR:H272	1.85	0.57
13:b:175:ARG:NH2	13:b:176:LEU:O	2.37	0.57
14:B:1204:CLA:H111	17:I:4018:BCR:HC21	1.85	0.57
14:G:1103:CLA:H142	17:G:4003:BCR:H372	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:32:TRP:NE1	4:O:50:MET:SD	2.72	0.57
13:b:34:GLN:OE1	14:b:510:CLA:NC	2.38	0.57
13:t:175:ARG:NH2	13:t:176:LEU:O	2.37	0.57
12:P:2:LYS:HE2	12:P:169:LEU:HD12	1.86	0.57
1:G:277:THR:HB	9:U:14:TRP:HB2	1.86	0.57
13:c:272:TYR:HB3	13:c:300:ARG:HB2	1.85	0.57
14:e:1103:CLA:H142	17:e:4003:BCR:H372	1.85	0.57
13:4:175:ARG:NH2	13:4:176:LEU:O	2.37	0.57
1:G:412:LEU:HD21	14:G:1104:CLA:H142	1.87	0.57
14:H:1204:CLA:H111	17:S:4018:BCR:HC21	1.85	0.57
1:e:277:THR:HB	9:m:14:TRP:HB2	1.86	0.57
14:f:1225:CLA:H203	17:f:4006:BCR:H15C	1.86	0.57
14:H:1229:CLA:HBB2	17:H:4014:BCR:HC41	1.86	0.57
1:A:370:ILE:HD11	14:A:1119:CLA:H71	1.85	0.57
14:B:1235:CLA:H172	17:F:4016:BCR:H272	1.85	0.57
18:G:5007:LHG:HC82	13:Z:297:HIS:NE2	2.19	0.57
14:B:1225:CLA:H203	17:B:4006:BCR:H15C	1.86	0.57
12:p:2:LYS:HE2	12:p:169:LEU:HD12	1.86	0.57
13:t:34:GLN:OE1	14:t:510:CLA:NC	2.38	0.57
14:B:1210:CLA:H112	14:B:1210:CLA:H51	1.87	0.57
13:2:249:ILE:HG12	14:2:502:CLA:HAC1	1.87	0.57
1:e:278:LEU:HD21	9:m:72:ILE:HD12	1.87	0.57
1:A:278:LEU:HD21	9:K:72:ILE:HD12	1.87	0.57
14:B:1229:CLA:HBB2	17:B:4014:BCR:HC41	1.86	0.57
7:I:13:ILE:HD11	10:V:155:LEU:HD22	1.87	0.57
13:1:249:ILE:HG12	14:1:502:CLA:HAC1	1.85	0.57
2:H:603:GLN:HE21	2:H:732:LYS:HD3	1.70	0.57
1:A:160:VAL:HG22	18:A:5007:LHG:H281	1.87	0.56
13:4:34:GLN:OE1	14:4:510:CLA:NC	2.38	0.56
1:G:752:TRP:NE1	14:G:1126:CLA:O1A	2.29	0.56
2:f:603:GLN:HE21	2:f:732:LYS:HD3	1.70	0.56
13:s:320:TRP:HH2	21:s:822:SQD:H462	1.69	0.56
14:A:1103:CLA:H121	17:A:4002:BCR:HC41	1.87	0.56
13:6:148:PHE:HD2	14:6:512:CLA:H3A	1.71	0.56
1:G:269:GLU:HG3	13:Y:294:PHE:HD1	1.71	0.56
13:a:320:TRP:HH2	21:a:822:SQD:H462	1.69	0.56
1:e:216:GLN:HA	1:e:220:SER:HB2	1.87	0.56
3:g:63:LEU:HD12	3:g:66:ARG:HH21	1.70	0.56
13:v:148:PHE:HD2	14:v:512:CLA:H3A	1.70	0.56
1:A:216:GLN:HA	1:A:220:SER:HB2	1.87	0.56
1:A:277:THR:HB	9:K:14:TRP:HB2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:5007:LHG:HC82	13:2:297:HIS:NE2	2.19	0.56
10:V:160:ALA:HB1	10:V:165:VAL:HB	1.86	0.56
1:e:160:VAL:HG22	18:e:5007:LHG:H281	1.87	0.56
1:e:412:LEU:HD21	14:e:1104:CLA:H142	1.87	0.56
14:e:1103:CLA:H121	17:e:4002:BCR:HC41	1.88	0.56
14:f:1229:CLA:HBB2	17:f:4014:BCR:HC41	1.86	0.56
14:2:517:CLA:HBB1	17:2:524:BCR:H352	1.88	0.56
14:5:507:CLA:HED2	14:5:507:CLA:H2A	1.88	0.56
1:A:412:LEU:HD21	14:A:1104:CLA:H142	1.87	0.56
14:G:1122:CLA:HBB2	18:G:5003:LHG:HC82	1.88	0.56
4:O:9:PRO:HD2	4:O:57:LEU:HD13	1.88	0.56
1:e:269:GLU:HG3	13:q:294:PHE:HD1	1.70	0.56
14:r:517:CLA:HBB1	17:r:524:BCR:H352	1.88	0.56
2:B:26:ALA:HA	14:B:1226:CLA:H43	1.88	0.56
4:D:9:PRO:HD2	4:D:57:LEU:HD13	1.88	0.56
17:V:4219:BCR:H382	18:V:5221:LHG:H332	1.88	0.56
13:u:30:ALA:HB2	14:u:511:CLA:HMA1	1.86	0.56
1:A:23:THR:HG21	18:A:5008:LHG:HC91	1.87	0.56
2:B:603:GLN:HE21	2:B:732:LYS:HD3	1.70	0.56
13:3:320:TRP:HH2	21:3:822:SQD:H462	1.69	0.56
14:G:1103:CLA:H121	17:G:4002:BCR:HC41	1.87	0.56
13:d:148:PHE:HD2	14:d:512:CLA:H3A	1.71	0.56
17:n:4219:BCR:H382	18:n:5221:LHG:H332	1.88	0.56
3:N:63:LEU:HD12	3:N:66:ARG:HH21	1.70	0.56
13:c:30:ALA:HB2	14:c:511:CLA:HMA1	1.86	0.56
14:e:1105:CLA:HMB3	14:e:1106:CLA:HHB	1.88	0.56
1:G:23:THR:HG21	18:G:5008:LHG:HC91	1.87	0.56
1:G:216:GLN:HA	1:G:220:SER:HB2	1.87	0.56
14:H:1210:CLA:H112	14:H:1210:CLA:H51	1.87	0.56
14:H:1207:CLA:H42	18:n:5221:LHG:C25	2.35	0.56
14:e:1122:CLA:HBB2	18:e:5003:LHG:HC82	1.88	0.56
18:e:5007:LHG:HC82	13:r:297:HIS:NE2	2.19	0.56
2:B:548:PRO:HB3	6:F:158:PRO:HG2	1.88	0.56
10:L:38:ARG:O	10:L:46:ARG:NH2	2.39	0.56
17:L:4219:BCR:H382	18:L:5221:LHG:H332	1.88	0.56
4:h:61:ARG:NH1	4:h:63:GLU:OE1	2.39	0.56
14:u:507:CLA:HED2	14:u:507:CLA:H2A	1.88	0.56
1:G:160:VAL:HG22	18:G:5007:LHG:H281	1.87	0.55
10:V:38:ARG:O	10:V:46:ARG:NH2	2.39	0.55
1:A:589:PRO:HD3	2:B:561:GLY:HA2	1.89	0.55
13:1:34:GLN:OE1	14:1:510:CLA:NC	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:ARG:NH1	4:O:63:GLU:OE1	2.39	0.55
2:f:61:VAL:HG21	14:f:1225:CLA:H42	1.88	0.55
2:f:548:PRO:HB3	6:j:158:PRO:HG2	1.88	0.55
3:C:63:LEU:HD12	3:C:66:ARG:HH21	1.70	0.55
4:D:85:ILE:HB	4:D:98:HIS:HB3	1.88	0.55
4:O:85:ILE:HB	4:O:98:HIS:HB3	1.88	0.55
13:Z:249:ILE:HG12	14:Z:502:CLA:HAC1	1.87	0.55
1:e:23:THR:HG21	18:e:5008:LHG:HC91	1.87	0.55
4:h:31:THR:HA	4:h:55:ASN:O	2.06	0.55
2:B:61:VAL:HG21	14:B:1225:CLA:H42	1.88	0.55
14:B:1207:CLA:H42	18:V:5221:LHG:H241	1.89	0.55
4:D:31:THR:HA	4:D:55:ASN:O	2.06	0.55
14:4:508:CLA:HBB2	14:4:509:CLA:HED1	1.89	0.55
14:c:507:CLA:HED2	14:c:507:CLA:H2A	1.87	0.55
4:h:58:TYR:H	10:n:13:GLU:HG2	1.72	0.55
2:B:456:GLU:OE1	6:F:68:HIS:ND1	2.35	0.55
2:H:160:LYS:HB3	21:H:1852:SQD:S	2.47	0.55
14:H:1023:CLA:H122	17:S:4018:BCR:H281	1.89	0.55
4:O:31:THR:HA	4:O:55:ASN:O	2.06	0.55
14:Z:517:CLA:HBB1	17:Z:524:BCR:H352	1.87	0.55
4:h:9:PRO:HD2	4:h:57:LEU:HD13	1.88	0.55
14:L:1501:CLA:H102	14:L:1503:CLA:H122	1.89	0.55
12:P:42:SER:O	12:P:45:ASN:ND2	2.38	0.55
13:1:301:ALA:O	13:1:305:ASN:ND2	2.39	0.55
1:G:459:LEU:HB3	1:G:552:PHE:HB2	1.89	0.55
13:Y:301:ALA:O	13:Y:305:ASN:ND2	2.39	0.55
4:h:85:ILE:HB	4:h:98:HIS:HB3	1.89	0.55
13:q:34:GLN:OE1	14:q:510:CLA:NC	2.39	0.55
13:r:249:ILE:HG12	14:r:502:CLA:HAC1	1.87	0.55
14:B:1239:CLA:HBB1	17:B:4017:BCR:H363	1.89	0.55
10:L:83:VAL:HG11	10:V:142:PHE:CE1	2.42	0.55
2:H:351:HIS:ND1	14:H:1214:CLA:OBD	2.40	0.55
2:H:548:PRO:HB3	6:R:158:PRO:HG2	1.88	0.55
1:e:459:LEU:HB3	1:e:552:PHE:HB2	1.89	0.55
14:f:1231:CLA:H71	17:f:4010:BCR:H313	1.89	0.55
1:A:269:GLU:HG3	13:1:294:PHE:HD1	1.70	0.55
14:B:1207:CLA:H193	18:V:5221:LHG:H222	1.88	0.55
3:C:15:THR:HG22	3:C:28:MET:HG3	1.89	0.55
4:D:117:LYS:NZ	4:D:119:ASP:OD1	2.40	0.55
13:b:109:PHE:HE1	13:b:113:ARG:HH21	1.55	0.55
10:n:38:ARG:O	10:n:46:ARG:NH2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LYS:HB3	21:B:1852:SQD:S	2.47	0.55
13:6:110:HIS:NE2	14:6:513:CLA:NB	2.55	0.55
3:N:15:THR:HG22	3:N:28:MET:HG3	1.89	0.55
14:V:1501:CLA:H102	14:V:1503:CLA:H122	1.89	0.55
1:e:589:PRO:HD3	2:f:561:GLY:HA2	1.89	0.55
3:g:15:THR:HG22	3:g:28:MET:HG3	1.89	0.55
14:A:1122:CLA:HBB2	18:A:5003:LHG:HC82	1.88	0.55
14:B:1231:CLA:H71	17:B:4010:BCR:H313	1.89	0.55
1:G:278:LEU:HD21	9:U:72:ILE:HD12	1.87	0.55
2:H:26:ALA:HA	14:H:1226:CLA:H43	1.88	0.55
13:Y:34:GLN:OE1	14:Y:510:CLA:NC	2.39	0.55
13:d:110:HIS:NE2	14:d:513:CLA:NB	2.55	0.55
1:A:459:LEU:HB3	1:A:552:PHE:HB2	1.89	0.54
2:B:351:HIS:ND1	14:B:1214:CLA:OBD	2.40	0.54
4:D:61:ARG:NH1	4:D:63:GLU:OE1	2.39	0.54
21:L:5216:SQD:H242	18:k:5001:LHG:HC62	1.88	0.54
1:G:683:LEU:HD21	14:G:1126:CLA:H142	1.88	0.54
18:G:5004:LHG:H102	13:Z:282:VAL:HG13	1.89	0.54
10:V:33:ALA:HB1	14:V:1501:CLA:HAC1	1.89	0.54
1:e:683:LEU:HD21	14:e:1126:CLA:H142	1.88	0.54
2:f:26:ALA:HA	14:f:1226:CLA:H43	1.88	0.54
14:f:1210:CLA:H112	14:f:1210:CLA:H51	1.87	0.54
2:B:66:PHE:HZ	11:M:6:VAL:HG13	1.72	0.54
10:L:33:ALA:HB1	14:L:1501:CLA:HAC1	1.89	0.54
13:4:109:PHE:HE1	13:4:113:ARG:HH21	1.55	0.54
4:O:117:LYS:NZ	4:O:119:ASP:OD1	2.40	0.54
13:t:140:LEU:HA	13:t:222:ILE:HG22	1.90	0.54
13:5:148:PHE:HD2	14:5:512:CLA:H3A	1.73	0.54
14:G:1105:CLA:HMB3	14:G:1106:CLA:HHB	1.88	0.54
2:H:61:VAL:HG21	14:H:1225:CLA:H42	1.88	0.54
4:O:58:TYR:H	10:V:13:GLU:HG2	1.72	0.54
18:e:5004:LHG:H102	13:r:282:VAL:HG13	1.89	0.54
14:f:1023:CLA:H122	17:k:4018:BCR:H281	1.89	0.54
13:v:276:LEU:HD11	13:v:300:ARG:HG2	1.89	0.54
14:A:1105:CLA:HMB3	14:A:1106:CLA:HHB	1.88	0.54
13:6:200:LEU:HG	13:6:265:LEU:HD11	1.90	0.54
13:d:276:LEU:HD11	13:d:300:ARG:HG2	1.89	0.54
12:p:42:SER:O	12:p:45:ASN:ND2	2.38	0.54
13:v:110:HIS:NE2	14:v:513:CLA:NB	2.55	0.54
4:D:58:TYR:H	10:L:13:GLU:HG2	1.72	0.54
13:2:307:HIS:NE2	14:2:502:CLA:NA	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:589:PRO:HD3	2:H:561:GLY:HA2	1.88	0.54
14:G:1120:CLA:HMD2	17:G:4001:BCR:H24C	1.89	0.54
13:Y:110:HIS:NE2	14:Y:513:CLA:NB	2.56	0.54
1:A:683:LEU:HD21	14:A:1126:CLA:H142	1.88	0.54
14:B:1023:CLA:H122	17:I:4018:BCR:H281	1.89	0.54
13:1:110:HIS:NE2	14:1:513:CLA:NB	2.56	0.54
13:4:140:LEU:HA	13:4:222:ILE:HG22	1.90	0.54
13:6:145:HIS:NE2	14:6:512:CLA:NA	2.56	0.54
2:H:524:ALA:HB2	14:H:1235:CLA:HMA1	1.90	0.54
13:Z:307:HIS:NE2	14:Z:502:CLA:NA	2.56	0.54
2:f:351:HIS:ND1	14:f:1214:CLA:OBD	2.40	0.54
13:q:110:HIS:NE2	14:q:513:CLA:NB	2.56	0.54
4:O:39:VAL:HG22	4:O:49:VAL:HG22	1.90	0.54
14:d:505:CLA:H12	17:d:524:BCR:H312	1.90	0.54
2:f:160:LYS:HB3	21:f:1852:SQD:S	2.47	0.54
13:r:307:HIS:NE2	14:r:502:CLA:NA	2.56	0.54
2:B:524:ALA:HB2	14:B:1235:CLA:HMA1	1.90	0.54
13:3:145:HIS:NE2	14:3:512:CLA:NA	2.55	0.54
13:a:145:HIS:NE2	14:a:512:CLA:NA	2.55	0.54
13:d:200:LEU:HG	13:d:265:LEU:HD11	1.90	0.54
2:f:117:TYR:HA	2:f:367:THR:HG22	1.89	0.54
14:n:1501:CLA:H102	14:n:1503:CLA:H122	1.89	0.54
12:p:9:THR:HB	12:p:14:THR:HB	1.89	0.54
12:P:62:LEU:HD21	12:P:105:LEU:HG	1.90	0.54
18:V:5220:LHG:H311	18:V:5220:LHG:H171	1.90	0.54
10:n:33:ALA:HB1	14:n:1501:CLA:HAC1	1.89	0.54
14:t:508:CLA:HBB2	14:t:509:CLA:HED1	1.89	0.54
2:B:117:TYR:HA	2:B:367:THR:HG22	1.89	0.54
13:5:177:VAL:HG13	13:5:201:GLU:HG2	1.90	0.54
14:6:505:CLA:H12	17:6:524:BCR:H312	1.89	0.54
2:H:117:TYR:HA	2:H:367:THR:HG22	1.89	0.54
12:X:9:THR:HB	12:X:14:THR:HB	1.89	0.54
13:c:119:ALA:O	13:c:126:LYS:NZ	2.41	0.54
12:X:42:SER:O	12:X:45:ASN:ND2	2.38	0.53
13:Z:200:LEU:HG	13:Z:265:LEU:HD11	1.90	0.53
13:c:148:PHE:HD2	14:c:512:CLA:H3A	1.73	0.53
1:e:598:SER:OG	1:e:601:ASP:OD2	2.26	0.53
2:f:524:ALA:HB2	14:f:1235:CLA:HMA1	1.90	0.53
4:h:39:VAL:HG22	4:h:49:VAL:HG22	1.90	0.53
13:r:148:PHE:HD2	14:r:512:CLA:H3A	1.74	0.53
14:B:1220:CLA:HAA1	17:B:4009:BCR:H16C	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:200:LEU:HG	13:2:265:LEU:HD11	1.90	0.53
13:2:226:PRO:HA	14:2:506:CLA:HED3	1.91	0.53
13:5:119:ALA:O	13:5:126:LYS:NZ	2.41	0.53
14:H:1220:CLA:HAA1	17:H:4009:BCR:H16C	1.91	0.53
14:H:1231:CLA:H71	17:H:4010:BCR:H313	1.89	0.53
13:Z:148:PHE:HD2	14:Z:512:CLA:H3A	1.74	0.53
14:b:508:CLA:HBB2	14:b:509:CLA:HED1	1.89	0.53
14:f:1239:CLA:HBB1	17:f:4017:BCR:H363	1.89	0.53
4:h:79:LYS:HZ3	12:p:92:VAL:HG13	1.71	0.53
13:s:145:HIS:NE2	14:s:512:CLA:NA	2.55	0.53
8:J:12:PRO:HB2	17:J:4013:BCR:H381	1.90	0.53
18:L:5221:LHG:H222	14:f:1207:CLA:H193	1.88	0.53
14:G:1119:CLA:H61	17:G:4007:BCR:H352	1.90	0.53
14:H:1229:CLA:HAB	17:H:4014:BCR:H323	1.91	0.53
12:X:62:LEU:HD21	12:X:105:LEU:HG	1.90	0.53
13:r:200:LEU:HG	13:r:265:LEU:HD11	1.90	0.53
18:A:5004:LHG:H102	13:2:282:VAL:HG13	1.89	0.53
13:6:276:LEU:HD11	13:6:300:ARG:HG2	1.89	0.53
2:H:66:PHE:HZ	11:W:6:VAL:HG13	1.72	0.53
10:V:94:SER:HB2	14:n:1501:CLA:HMD3	1.89	0.53
1:A:16:VAL:HA	1:A:185:PRO:HA	1.91	0.53
14:H:1239:CLA:HBB1	17:H:4017:BCR:H363	1.89	0.53
13:d:73:LEU:O	13:d:159:LYS:NZ	2.42	0.53
13:t:109:PHE:HE1	13:t:113:ARG:HH21	1.55	0.53
13:u:119:ALA:O	13:u:126:LYS:NZ	2.41	0.53
13:v:73:LEU:O	13:v:159:LYS:NZ	2.42	0.53
14:A:1120:CLA:HMD2	17:A:4001:BCR:H24C	1.90	0.53
12:P:9:THR:HB	12:P:14:THR:HB	1.89	0.53
14:4:517:CLA:H2A	14:4:517:CLA:HED2	1.91	0.53
13:6:73:LEU:O	13:6:159:LYS:NZ	2.42	0.53
14:Z:513:CLA:HBB1	17:Z:523:BCR:H24C	1.90	0.53
13:d:145:HIS:NE2	14:d:512:CLA:NA	2.56	0.53
2:f:66:PHE:HZ	11:o:6:VAL:HG13	1.72	0.53
1:G:16:VAL:HA	1:G:185:PRO:HA	1.91	0.53
14:e:1120:CLA:HMD2	17:e:4001:BCR:H24C	1.90	0.53
13:v:145:HIS:NE2	14:v:512:CLA:NA	2.56	0.53
13:v:177:VAL:HG13	13:v:201:GLU:HG2	1.90	0.53
14:B:1234:CLA:H52	14:F:1302:CLA:HBB2	1.91	0.53
8:T:12:PRO:HB2	17:T:4013:BCR:H381	1.90	0.53
2:f:191:THR:HG21	2:f:278:LEU:HB2	1.91	0.53
14:f:1234:CLA:H52	14:j:1302:CLA:HBB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:12:PRO:HB2	17:l:4013:BCR:H381	1.90	0.53
12:p:62:LEU:HD21	12:p:105:LEU:HG	1.90	0.53
13:r:226:PRO:HA	14:r:506:CLA:HED3	1.91	0.53
13:s:168:ASP:OD2	13:s:175:ARG:NH2	2.42	0.53
13:u:177:VAL:HG13	13:u:201:GLU:HG2	1.90	0.53
4:D:39:VAL:HG22	4:D:49:VAL:HG22	1.90	0.53
13:2:148:PHE:HD2	14:2:512:CLA:H3A	1.74	0.53
7:S:13:ILE:HD11	10:n:155:LEU:HD22	1.91	0.53
9:U:47:PRO:HG2	21:Y:822:SQD:H262	1.91	0.53
13:a:168:ASP:OD2	13:a:175:ARG:NH2	2.42	0.53
13:b:26:LEU:HB3	14:b:511:CLA:HMA1	1.91	0.53
13:c:177:VAL:HG13	13:c:201:GLU:HG2	1.90	0.53
18:n:5220:LHG:H311	18:n:5220:LHG:H171	1.90	0.53
13:6:177:VAL:HG13	13:6:201:GLU:HG2	1.91	0.53
13:b:140:LEU:HA	13:b:222:ILE:HG22	1.90	0.53
14:f:1229:CLA:HAB	17:f:4014:BCR:H323	1.91	0.53
14:v:505:CLA:H12	17:v:524:BCR:H312	1.89	0.53
14:2:513:CLA:HBB1	17:2:523:BCR:H24C	1.90	0.52
13:4:146:LEU:HD22	13:4:214:LEU:HD22	1.91	0.52
1:G:598:SER:OG	1:G:601:ASP:OD2	2.26	0.52
13:Z:226:PRO:HA	14:Z:506:CLA:HED3	1.91	0.52
14:e:1118:CLA:H3A	9:m:61:LEU:HD23	1.91	0.52
2:f:158:GLN:HB3	21:f:1852:SQD:H5	1.92	0.52
14:f:1220:CLA:HAA1	17:f:4009:BCR:H16C	1.91	0.52
13:v:200:LEU:HG	13:v:265:LEU:HD11	1.90	0.52
2:H:191:THR:HG21	2:H:278:LEU:HB2	1.91	0.52
9:m:47:PRO:HG2	21:q:822:SQD:H262	1.91	0.52
14:r:513:CLA:HBB1	17:r:523:BCR:H24C	1.90	0.52
13:u:148:PHE:HD2	14:u:512:CLA:H3A	1.73	0.52
1:A:598:SER:OG	1:A:601:ASP:OD2	2.26	0.52
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.91	0.52
14:G:1237:CLA:H152	17:V:4020:BCR:H16C	1.91	0.52
2:H:158:GLN:HB3	21:H:1852:SQD:H5	1.92	0.52
2:H:181:GLY:HA3	14:H:1210:CLA:HBB1	1.91	0.52
13:Z:193:HIS:HB2	13:Z:196:SER:HB3	1.91	0.52
13:d:177:VAL:HG13	13:d:201:GLU:HG2	1.90	0.52
1:e:16:VAL:HA	1:e:185:PRO:HA	1.91	0.52
14:A:1124:CLA:HAB	17:A:4008:BCR:H311	1.92	0.52
10:L:142:PHE:CE1	10:n:83:VAL:HG11	2.43	0.52
13:2:193:HIS:HB2	13:2:196:SER:HB3	1.91	0.52
12:X:66:TRP:HA	12:X:69:ILE:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:s:513:CLA:HBB1	17:s:523:BCR:H402	1.92	0.52
1:A:708:LEU:HD21	14:A:1013:CLA:HED2	1.92	0.52
14:H:1204:CLA:HHB	14:H:1205:CLA:HHB	1.92	0.52
14:e:1119:CLA:H61	17:e:4007:BCR:H352	1.90	0.52
13:r:193:HIS:HB2	13:r:196:SER:HB3	1.91	0.52
13:t:146:LEU:HD22	13:t:214:LEU:HD22	1.91	0.52
13:t:273:GLY:O	13:t:300:ARG:NH2	2.39	0.52
12:P:66:TRP:HA	12:P:69:ILE:HG22	1.91	0.52
2:H:69:ALA:HB2	2:H:135:LEU:HB2	1.92	0.52
13:q:301:ALA:O	13:q:305:ASN:ND2	2.39	0.52
13:t:26:LEU:HB3	14:t:511:CLA:HMA1	1.91	0.52
13:t:272:TYR:HB3	13:t:300:ARG:HB2	1.92	0.52
14:A:1118:CLA:H3A	9:K:61:LEU:HD23	1.91	0.52
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.92	0.52
9:K:47:PRO:HG2	21:1:822:SQD:H262	1.91	0.52
13:b:230:THR:HG23	13:b:234:LEU:HD12	1.92	0.52
13:d:146:LEU:HD21	14:d:506:CLA:HAB	1.92	0.52
14:e:1237:CLA:H152	17:n:4020:BCR:H16C	1.91	0.52
17:n:4022:BCR:H333	21:n:5216:SQD:H142	1.92	0.52
14:t:517:CLA:HED2	14:t:517:CLA:H2A	1.90	0.52
18:L:5220:LHG:H311	18:L:5220:LHG:H171	1.90	0.52
13:1:148:PHE:HZ	14:1:516:CLA:CBC	2.22	0.52
14:G:1124:CLA:HAB	17:G:4008:BCR:H311	1.92	0.52
2:H:151:PHE:CE2	21:H:1852:SQD:H102	2.45	0.52
2:H:422:LEU:HD13	2:H:532:LEU:HA	1.92	0.52
14:H:1238:CLA:H2	14:H:1239:CLA:H122	1.92	0.52
15:H:2002:PQN:H242	17:H:4017:BCR:H17C	1.92	0.52
10:V:133:ILE:HG21	10:n:48:LEU:HD21	1.92	0.52
13:b:146:LEU:HD22	13:b:214:LEU:HD22	1.91	0.52
14:e:1124:CLA:HAB	17:e:4008:BCR:H311	1.92	0.52
14:f:1203:CLA:H191	20:f:5002:LMG:H252	1.92	0.52
13:v:177:VAL:HG21	13:v:204:VAL:HG21	1.91	0.52
2:B:338:LEU:HD21	14:B:1226:CLA:HAB	1.92	0.52
14:B:1203:CLA:H191	20:B:5002:LMG:H252	1.92	0.52
10:L:98:ASN:ND2	10:V:39:ARG:O	2.43	0.52
17:L:4022:BCR:H333	21:L:5216:SQD:H142	1.92	0.52
14:3:513:CLA:HBB1	17:3:523:BCR:H402	1.92	0.52
13:6:301:ALA:O	13:6:305:ASN:ND2	2.41	0.52
14:b:517:CLA:HED2	14:b:517:CLA:H2A	1.90	0.52
13:d:146:LEU:HD22	13:d:214:LEU:HD22	1.91	0.52
18:e:5004:LHG:H302	18:e:5006:LHG:H331	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:1012:CLA:H201	17:l:4012:BCR:H362	1.91	0.52
1:A:230:ILE:HG12	1:A:244:ALA:HA	1.92	0.52
14:B:1229:CLA:HAB	17:B:4014:BCR:H323	1.91	0.52
13:4:272:TYR:HB3	13:4:300:ARG:HB2	1.91	0.52
13:5:249:ILE:HG12	14:5:502:CLA:HAC1	1.92	0.52
14:H:1012:CLA:H201	17:T:4012:BCR:H362	1.91	0.52
14:H:1207:CLA:H42	18:n:5221:LHG:C24	2.39	0.52
4:O:79:LYS:HZ3	12:X:92:VAL:HG13	1.75	0.52
2:f:338:LEU:HD21	14:f:1226:CLA:HAB	1.92	0.52
14:f:1204:CLA:HHB	14:f:1205:CLA:HHB	1.92	0.52
13:v:146:LEU:HD22	13:v:214:LEU:HD22	1.91	0.52
14:B:1204:CLA:HHB	14:B:1205:CLA:HHB	1.92	0.51
14:B:1238:CLA:H2	14:B:1239:CLA:H122	1.92	0.51
4:D:79:LYS:HZ3	12:P:92:VAL:HG13	1.74	0.51
9:K:29:ALA:HA	9:K:32:ILE:HG22	1.92	0.51
12:P:62:LEU:HD23	12:P:101:ALA:HB1	1.92	0.51
4:h:117:LYS:NZ	4:h:119:ASP:OD1	2.39	0.51
13:u:249:ILE:HG12	14:u:502:CLA:HAC1	1.93	0.51
13:4:26:LEU:HB3	14:4:511:CLA:HMA1	1.91	0.51
12:X:62:LEU:HD23	12:X:101:ALA:HB1	1.92	0.51
13:Y:34:GLN:HG2	14:Y:509:CLA:HHB	1.93	0.51
1:e:708:LEU:HD21	14:e:1013:CLA:HED2	1.92	0.51
1:e:742:HIS:CE1	14:e:1140:CLA:NA	2.79	0.51
2:f:69:ALA:HB2	2:f:135:LEU:HB2	1.92	0.51
12:p:3:ILE:HB	12:p:31:VAL:HG22	1.93	0.51
12:p:66:TRP:HA	12:p:69:ILE:HG22	1.91	0.51
14:H:1203:CLA:H191	20:H:5002:LMG:H252	1.92	0.51
3:N:22:PRO:HG2	3:N:23:LEU:HD12	1.92	0.51
14:A:1119:CLA:H61	17:A:4007:BCR:H352	1.90	0.51
14:A:1237:CLA:H152	17:L:4020:BCR:H16C	1.91	0.51
12:P:37:ALA:HB2	12:P:65:ASP:OD2	2.11	0.51
13:d:177:VAL:HG21	13:d:204:VAL:HG21	1.91	0.51
13:t:230:THR:HG23	13:t:234:LEU:HD12	1.92	0.51
1:A:573:LEU:O	4:D:61:ARG:NH2	2.42	0.51
14:B:1229:CLA:H61	17:F:4016:BCR:HC32	1.93	0.51
12:P:3:ILE:HB	12:P:31:VAL:HG22	1.93	0.51
13:3:168:ASP:OD2	13:3:175:ARG:NH2	2.42	0.51
13:5:26:LEU:HB3	14:5:511:CLA:HMA1	1.90	0.51
13:Y:148:PHE:HZ	14:Y:516:CLA:CBC	2.22	0.51
2:f:60:TRP:NE1	14:f:1224:CLA:OBD	2.44	0.51
14:f:1206:CLA:H2A	14:f:1206:CLA:HED3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:22:PRO:HG2	3:g:23:LEU:HD12	1.92	0.51
13:v:190:TYR:HD2	17:v:524:BCR:H401	1.76	0.51
1:G:381:HIS:ND1	14:G:1116:CLA:OBD	2.44	0.51
14:G:1118:CLA:H3A	9:U:61:LEU:HD23	1.91	0.51
18:G:5004:LHG:H302	18:G:5006:LHG:H331	1.92	0.51
13:b:272:TYR:HB3	13:b:300:ARG:HB2	1.91	0.51
1:e:381:HIS:ND1	14:e:1116:CLA:OBD	2.44	0.51
9:m:29:ALA:HA	9:m:32:ILE:HG22	1.92	0.51
1:A:86:TRP:NE1	14:A:1126:CLA:OBD	2.43	0.51
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.92	0.51
10:L:64:ILE:HD12	10:L:160:ALA:HB2	1.93	0.51
13:1:34:GLN:HG2	14:1:509:CLA:HHB	1.93	0.51
14:A:1117:CLA:H203	14:A:1125:CLA:HAA1	1.93	0.51
2:B:181:GLY:HA3	14:B:1210:CLA:HBB1	1.91	0.51
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.92	0.51
18:S:5001:LHG:HC62	21:n:5216:SQD:H242	1.92	0.51
13:c:249:ILE:HG12	14:c:502:CLA:HAC1	1.92	0.51
14:f:1229:CLA:H61	17:j:4016:BCR:HC32	1.93	0.51
13:q:34:GLN:HG2	14:q:509:CLA:HHB	1.93	0.51
13:q:148:PHE:HZ	14:q:516:CLA:CBC	2.22	0.51
13:v:146:LEU:HD21	14:v:506:CLA:HAB	1.92	0.51
1:G:742:HIS:CE1	14:G:1140:CLA:NA	2.79	0.51
10:V:64:ILE:HD12	10:V:160:ALA:HB2	1.93	0.51
1:e:86:TRP:NE1	14:e:1126:CLA:OBD	2.43	0.51
14:f:1219:CLA:HBA2	14:f:1219:CLA:H43	1.93	0.51
1:A:381:HIS:ND1	14:A:1116:CLA:OBD	2.44	0.51
14:B:1012:CLA:H201	17:J:4012:BCR:H362	1.91	0.51
13:5:145:HIS:NE2	14:5:512:CLA:NA	2.59	0.51
17:6:522:BCR:HC41	13:Y:258:TYR:HB2	1.93	0.51
1:G:230:ILE:HG12	1:G:244:ALA:HA	1.92	0.51
2:H:60:TRP:NE1	14:H:1224:CLA:OBD	2.44	0.51
2:H:611:GLU:OE2	6:R:36:ARG:NH1	2.43	0.51
2:H:687:LEU:HB2	17:V:4020:BCR:H282	1.92	0.51
13:d:136:LYS:HG3	13:d:225:PRO:HB3	1.92	0.51
2:f:181:GLY:HA3	14:f:1210:CLA:HBB1	1.92	0.51
2:B:60:TRP:NE1	14:B:1224:CLA:OBD	2.44	0.50
13:3:148:PHE:HD2	14:3:512:CLA:H3A	1.76	0.50
13:6:177:VAL:HG21	13:6:204:VAL:HG21	1.91	0.50
13:6:190:TYR:HD2	17:6:524:BCR:H401	1.76	0.50
1:G:708:LEU:HD21	14:G:1013:CLA:HED2	1.92	0.50
18:G:5008:LHG:C7	13:Z:13:TRP:HE1	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:59:MET:HB2	13:d:271:PHE:HA	1.94	0.50
13:t:276:LEU:HG	13:t:300:ARG:HD2	1.93	0.50
1:A:742:HIS:CE1	14:A:1140:CLA:NA	2.79	0.50
14:A:1118:CLA:HBB1	17:K:4104:BCR:H342	1.94	0.50
13:6:146:LEU:HD21	14:6:506:CLA:HAB	1.92	0.50
1:G:345:THR:HG21	18:G:5003:LHG:HC11	1.94	0.50
14:H:1234:CLA:H52	14:R:1302:CLA:HBB2	1.91	0.50
4:O:121:ARG:NH1	5:Q:65:GLU:OE2	2.44	0.50
14:a:513:CLA:HBB1	17:a:523:BCR:H402	1.92	0.50
14:f:1238:CLA:H2	14:f:1239:CLA:H122	1.92	0.50
4:h:121:ARG:NH1	5:i:65:GLU:OE2	2.44	0.50
13:v:136:LYS:HG3	13:v:225:PRO:HB3	1.92	0.50
14:B:1219:CLA:HBA2	14:B:1219:CLA:H43	1.93	0.50
13:2:34:GLN:HG2	14:2:509:CLA:HHB	1.93	0.50
13:4:70:LEU:HD21	14:4:503:CLA:HED2	1.93	0.50
13:4:135:PRO:HB2	13:4:226:PRO:HD2	1.94	0.50
2:f:611:GLU:OE2	6:j:36:ARG:NH1	2.43	0.50
14:f:1202:CLA:H122	14:f:1202:CLA:HBD	1.93	0.50
15:f:2002:PQN:H242	17:f:4017:BCR:H17C	1.92	0.50
12:p:37:ALA:HB2	12:p:65:ASP:OD2	2.11	0.50
12:p:62:LEU:HD23	12:p:101:ALA:HB1	1.92	0.50
13:t:161:THR:HA	13:t:177:VAL:HB	1.93	0.50
18:A:5004:LHG:H302	18:A:5006:LHG:H331	1.92	0.50
2:B:158:GLN:HB3	21:B:1852:SQD:H5	1.92	0.50
15:B:2002:PQN:H242	17:B:4017:BCR:H17C	1.92	0.50
4:D:31:THR:O	4:D:83:TYR:HA	2.12	0.50
4:D:121:ARG:NH1	5:E:65:GLU:OE2	2.44	0.50
10:L:41:LEU:O	10:L:46:ARG:NH1	2.45	0.50
13:4:161:THR:HA	13:4:177:VAL:HB	1.93	0.50
13:6:136:LYS:HG3	13:6:225:PRO:HB3	1.92	0.50
18:G:5009:LHG:H131	17:Y:521:BCR:H313	1.94	0.50
19:G:1848:LMU:H5B	17:T:4013:BCR:HC21	1.94	0.50
17:V:4022:BCR:H333	21:V:5216:SQD:H142	1.92	0.50
12:X:3:ILE:HB	12:X:31:VAL:HG22	1.93	0.50
12:X:37:ALA:HB2	12:X:65:ASP:OD2	2.11	0.50
13:r:34:GLN:HG2	14:r:509:CLA:HHB	1.93	0.50
13:s:148:PHE:HD2	14:s:512:CLA:H3A	1.76	0.50
1:A:441:VAL:HG11	14:A:1119:CLA:H192	1.94	0.50
19:A:1848:LMU:O6B	8:J:31:ARG:NH1	2.44	0.50
9:U:29:ALA:HA	9:U:32:ILE:HG22	1.92	0.50
13:b:273:GLY:O	13:b:300:ARG:NH2	2.39	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:e:5008:LHG:C7	13:r:13:TRP:HE1	2.24	0.50
2:f:151:PHE:CE2	21:f:1852:SQD:H102	2.45	0.50
2:f:422:LEU:HD13	2:f:532:LEU:HA	1.92	0.50
13:t:263:ASN:HD21	13:t:265:LEU:HB3	1.77	0.50
18:A:5009:LHG:H131	17:1:521:BCR:H313	1.94	0.50
17:L:4022:BCR:H333	21:L:5216:SQD:H141	1.93	0.50
13:4:230:THR:HG23	13:4:234:LEU:HD12	1.92	0.50
13:6:146:LEU:HD22	13:6:214:LEU:HD22	1.91	0.50
1:G:692:ALA:HB3	14:G:1013:CLA:HBB2	1.94	0.50
2:H:338:LEU:HD21	14:H:1226:CLA:HAB	1.92	0.50
2:H:631:LEU:O	2:H:647:SER:OG	2.29	0.50
1:e:345:THR:HG21	18:e:5003:LHG:HC11	1.94	0.50
2:f:687:LEU:HB2	17:n:4020:BCR:H282	1.93	0.50
13:r:110:HIS:NE2	14:r:513:CLA:NB	2.60	0.50
13:r:261:ALA:HA	13:r:276:LEU:HD12	1.94	0.50
2:B:127:ILE:HG12	2:B:190:TRP:HH2	1.77	0.50
2:B:710:LEU:HD23	20:B:5002:LMG:H362	1.94	0.50
13:2:110:HIS:NE2	14:2:513:CLA:NB	2.60	0.50
2:H:452:GLN:NE2	2:H:614:THR:OG1	2.45	0.50
2:f:158:GLN:HG3	21:f:1852:SQD:H1	1.94	0.50
9:m:43:GLY:HA3	9:m:58:PRO:HG2	1.94	0.50
13:t:135:PRO:HB2	13:t:226:PRO:HD2	1.94	0.50
2:B:311:PRO:HD2	18:B:1842:LHG:HC31	1.94	0.50
2:B:452:GLN:NE2	2:B:614:THR:OG1	2.45	0.50
14:B:1206:CLA:H2A	14:B:1206:CLA:HED3	1.93	0.50
13:4:263:ASN:HD21	13:4:265:LEU:HB3	1.77	0.50
14:H:1219:CLA:HBA2	14:H:1219:CLA:H43	1.93	0.50
14:H:1229:CLA:H61	17:R:4016:BCR:HC32	1.93	0.50
13:c:145:HIS:NE2	14:c:512:CLA:NA	2.59	0.50
14:e:1118:CLA:HBB1	17:m:4104:BCR:H342	1.94	0.50
18:e:5009:LHG:H131	17:q:521:BCR:H313	1.94	0.50
2:f:311:PRO:HD2	18:f:1842:LHG:HC31	1.94	0.50
14:A:1119:CLA:H101	17:A:4008:BCR:H10C	1.94	0.50
18:A:5008:LHG:C7	13:2:13:TRP:HE1	2.24	0.50
13:2:261:ALA:HA	13:2:276:LEU:HD12	1.94	0.50
14:G:1117:CLA:H203	14:G:1125:CLA:HAA1	1.93	0.50
19:G:1848:LMU:O6B	8:T:31:ARG:NH1	2.44	0.50
17:V:4022:BCR:H333	21:V:5216:SQD:H141	1.94	0.50
13:b:263:ASN:HD21	13:b:265:LEU:HB3	1.77	0.50
19:e:1848:LMU:H5B	17:l:4013:BCR:HC21	1.94	0.50
2:H:311:PRO:HD2	18:H:1842:LHG:HC31	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:714:THR:HG21	20:H:5002:LMG:H402	1.94	0.49
18:H:1855:LHG:H192	14:R:1302:CLA:HBB1	1.94	0.49
13:Y:148:PHE:CE2	14:Y:512:CLA:HHB	2.47	0.49
13:Z:261:ALA:HA	13:Z:276:LEU:HD12	1.94	0.49
1:e:230:ILE:HG12	1:e:244:ALA:HA	1.92	0.49
10:n:64:ILE:HD12	10:n:160:ALA:HB2	1.93	0.49
13:q:148:PHE:CE2	14:q:512:CLA:HHB	2.47	0.49
1:A:626:GLN:HE21	1:A:759:ILE:HD13	1.78	0.49
14:A:1237:CLA:HAB	2:B:691:VAL:HG11	1.94	0.49
19:A:1848:LMU:H5B	17:J:4013:BCR:HC21	1.94	0.49
13:6:59:MET:HB2	13:6:271:PHE:HA	1.93	0.49
13:a:148:PHE:HD2	14:a:512:CLA:H3A	1.76	0.49
14:e:1117:CLA:H203	14:e:1125:CLA:HAA1	1.93	0.49
14:e:1119:CLA:H101	17:e:4008:BCR:H10C	1.94	0.49
13:q:143:GLY:HA3	13:q:222:ILE:HG13	1.94	0.49
13:v:59:MET:HB2	13:v:271:PHE:HA	1.94	0.49
2:B:151:PHE:CE2	21:B:1852:SQD:H102	2.45	0.49
18:B:1855:LHG:H192	14:F:1302:CLA:HBB1	1.94	0.49
13:1:148:PHE:CE2	14:1:512:CLA:HHB	2.47	0.49
14:4:513:CLA:HBB1	17:4:523:BCR:H402	1.94	0.49
14:G:1119:CLA:H101	17:G:4008:BCR:H10C	1.94	0.49
13:b:161:THR:HA	13:b:177:VAL:HB	1.93	0.49
2:f:498:LEU:HA	2:f:501:ILE:HG22	1.95	0.49
17:n:4022:BCR:H333	21:n:5216:SQD:H141	1.93	0.49
12:P:78:PHE:HB3	12:P:114:SER:HB3	1.95	0.49
14:H:1206:CLA:H2A	14:H:1206:CLA:HED3	1.93	0.49
14:H:1228:CLA:HBC1	14:H:1234:CLA:H18	1.94	0.49
4:O:31:THR:O	4:O:83:TYR:HA	2.12	0.49
10:V:41:LEU:O	10:V:46:ARG:NH1	2.45	0.49
13:Z:110:HIS:NE2	14:Z:513:CLA:NB	2.60	0.49
13:d:190:TYR:HD2	17:d:524:BCR:H401	1.76	0.49
13:d:282:VAL:HG23	13:d:283:THR:HG23	1.94	0.49
2:f:127:ILE:HG12	2:f:190:TRP:HH2	1.77	0.49
2:f:714:THR:HG21	20:f:5002:LMG:H402	1.94	0.49
13:t:70:LEU:HD21	14:t:503:CLA:HED2	1.93	0.49
14:t:513:CLA:HBB1	17:t:523:BCR:H402	1.94	0.49
13:u:145:HIS:NE2	14:u:512:CLA:NA	2.59	0.49
13:v:42:ALA:O	13:v:46:THR:OG1	2.30	0.49
14:B:1202:CLA:HBD	14:B:1202:CLA:H122	1.93	0.49
1:G:360:TRP:HB3	14:G:1103:CLA:HAC1	1.94	0.49
2:H:710:LEU:HD23	20:H:5002:LMG:H362	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:135:PRO:HB2	13:b:226:PRO:HD2	1.94	0.49
14:b:513:CLA:HBB1	17:b:523:BCR:H402	1.94	0.49
1:e:429:ASP:O	1:e:433:ASN:ND2	2.46	0.49
2:f:429:LEU:HD11	14:f:1235:CLA:HMB2	1.94	0.49
2:f:452:GLN:NE2	2:f:614:THR:OG1	2.45	0.49
13:r:301:ALA:O	13:r:305:ASN:ND2	2.42	0.49
13:v:301:ALA:O	13:v:305:ASN:ND2	2.41	0.49
14:A:1117:CLA:H8	14:A:1117:CLA:HAB	1.95	0.49
2:B:158:GLN:HG3	21:B:1852:SQD:H1	1.94	0.49
14:B:1228:CLA:HBC1	14:B:1234:CLA:H18	1.94	0.49
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.95	0.49
6:F:126:LYS:HB2	13:3:13:TRP:CE2	2.48	0.49
13:6:282:VAL:HG23	13:6:283:THR:HG23	1.94	0.49
1:G:86:TRP:NE1	14:G:1126:CLA:OBD	2.43	0.49
1:G:441:VAL:HG11	14:G:1119:CLA:H192	1.94	0.49
14:G:1118:CLA:HBB1	17:U:4104:BCR:H342	1.94	0.49
2:H:127:ILE:HG12	2:H:190:TRP:HH2	1.77	0.49
13:Z:34:GLN:HG2	14:Z:509:CLA:HHB	1.93	0.49
13:b:276:LEU:HG	13:b:300:ARG:HD2	1.93	0.49
14:e:1117:CLA:H8	14:e:1117:CLA:HAB	1.95	0.49
14:e:1237:CLA:HAB	2:f:691:VAL:HG11	1.94	0.49
4:h:31:THR:O	4:h:83:TYR:HA	2.12	0.49
10:n:41:LEU:O	10:n:46:ARG:NH1	2.45	0.49
14:r:512:CLA:H3A	14:r:512:CLA:HBA1	1.54	0.49
1:A:377:ILE:HG21	14:A:1117:CLA:H201	1.95	0.49
14:H:1207:CLA:H42	18:n:5221:LHG:H241	1.93	0.49
6:R:126:LYS:HB2	13:a:13:TRP:CE2	2.48	0.49
13:c:67:LEU:HD22	13:c:89:LEU:HD13	1.95	0.49
3:g:58:CYS:HB3	3:g:63:LEU:HD22	1.95	0.49
12:p:78:PHE:HB3	12:p:114:SER:HB3	1.95	0.49
1:A:345:THR:HG21	18:A:5003:LHG:HC11	1.94	0.49
1:A:589:PRO:HB3	2:B:559:CYS:SG	2.53	0.49
2:B:687:LEU:HB2	17:L:4020:BCR:H282	1.93	0.49
1:G:377:ILE:HG21	14:G:1117:CLA:H201	1.95	0.49
2:H:429:LEU:HD11	14:H:1235:CLA:HMB2	1.94	0.49
9:U:32:ILE:O	9:U:36:THR:OG1	2.29	0.49
13:Y:143:GLY:HA3	13:Y:222:ILE:HG13	1.94	0.49
13:d:20:PHE:HA	13:d:23:LEU:HD12	1.94	0.49
18:f:1855:LHG:H192	14:j:1302:CLA:HBB1	1.94	0.49
6:j:126:LYS:HB2	13:s:13:TRP:CE2	2.48	0.49
13:5:221:HIS:CE1	14:5:506:CLA:NA	2.81	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:5008:LHG:HC5	13:Z:13:TRP:NE1	2.28	0.49
2:H:158:GLN:HG3	21:H:1852:SQD:H1	1.94	0.49
14:H:1202:CLA:HBD	14:H:1202:CLA:H122	1.93	0.49
1:e:692:ALA:HB3	14:e:1013:CLA:HBB2	1.94	0.49
2:f:722:ALA:HB2	14:f:1224:CLA:HBB1	1.95	0.49
13:u:221:HIS:CE1	14:u:506:CLA:NA	2.81	0.49
6:F:143:SER:HB2	13:4:14:TRP:CH2	2.48	0.49
13:4:276:LEU:HG	13:4:300:ARG:HD2	1.93	0.49
3:N:58:CYS:HB3	3:N:63:LEU:HD22	1.95	0.49
13:b:70:LEU:HD21	14:b:503:CLA:HED2	1.93	0.49
13:c:221:HIS:CE1	14:c:506:CLA:NA	2.81	0.49
1:e:626:GLN:HE21	1:e:759:ILE:HD13	1.77	0.49
18:e:5008:LHG:HC5	13:r:13:TRP:NE1	2.28	0.49
6:j:143:SER:HB2	13:t:14:TRP:CH2	2.48	0.49
1:A:300:LEU:HD21	1:A:385:MET:HB3	1.95	0.48
13:1:143:GLY:HA3	13:1:222:ILE:HG13	1.94	0.48
1:G:429:ASP:O	1:G:433:ASN:ND2	2.46	0.48
1:G:589:PRO:HB3	2:H:559:CYS:SG	2.53	0.48
14:A:1137:CLA:H41	14:A:1137:CLA:H62	1.64	0.48
18:I:5001:LHG:HC62	21:V:5216:SQD:H242	1.95	0.48
9:K:43:GLY:HA3	9:K:58:PRO:HG2	1.94	0.48
13:2:148:PHE:CE2	14:2:512:CLA:HHB	2.48	0.48
13:4:273:GLY:O	13:4:300:ARG:NH2	2.39	0.48
13:5:67:LEU:HD22	13:5:89:LEU:HD13	1.95	0.48
19:e:1848:LMU:O6B	8:l:31:ARG:NH1	2.44	0.48
2:f:710:LEU:HD23	20:f:5002:LMG:H362	1.94	0.48
2:B:429:LEU:HD11	14:B:1235:CLA:HMB2	1.94	0.48
17:L:4219:BCR:H14C	18:L:5220:LHG:H331	1.95	0.48
14:G:1129:CLA:HMC1	14:G:1137:CLA:HAB	1.95	0.48
14:f:1215:CLA:HBA2	14:f:1215:CLA:H3A	1.63	0.48
13:r:148:PHE:CE2	14:r:512:CLA:HHB	2.48	0.48
13:u:305:ASN:HB3	17:u:521:BCR:HC8	1.95	0.48
13:v:20:PHE:HA	13:v:23:LEU:HD12	1.94	0.48
1:A:692:ALA:HB3	14:A:1013:CLA:HBB2	1.94	0.48
18:A:5008:LHG:HC5	13:2:13:TRP:NE1	2.28	0.48
2:H:15:ASP:OD2	2:H:19:ARG:NH2	2.47	0.48
12:X:78:PHE:HB3	12:X:114:SER:HB3	1.95	0.48
1:e:377:ILE:HG21	14:e:1117:CLA:H201	1.95	0.48
14:e:1129:CLA:HMC1	14:e:1137:CLA:HAB	1.95	0.48
13:r:49:GLU:HB3	13:r:64:LEU:HD22	1.96	0.48
2:B:151:PHE:CZ	21:B:1852:SQD:H252	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:GLU:OE2	6:F:36:ARG:NH1	2.43	0.48
10:L:133:ILE:HG21	10:V:48:LEU:HD21	1.93	0.48
1:G:626:GLN:HE21	1:G:759:ILE:HD13	1.78	0.48
13:a:320:TRP:CH2	21:a:822:SQD:H462	2.48	0.48
13:c:282:VAL:HG23	13:c:283:THR:HG23	1.95	0.48
2:f:376:GLN:O	2:f:380:THR:OG1	2.30	0.48
14:f:1228:CLA:HBC1	14:f:1234:CLA:H18	1.94	0.48
6:j:118:VAL:HA	8:l:10:SER:HA	1.96	0.48
13:u:67:LEU:HD22	13:u:89:LEU:HD13	1.95	0.48
14:A:1138:CLA:HAA2	14:B:1228:CLA:HMB2	1.96	0.48
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.95	0.48
2:B:714:THR:HG21	20:B:5002:LMG:H402	1.94	0.48
13:2:49:GLU:HB3	13:2:64:LEU:HD22	1.96	0.48
13:4:59:MET:HB2	13:4:271:PHE:HA	1.96	0.48
13:5:148:PHE:CE2	14:5:512:CLA:HHB	2.49	0.48
14:G:1129:CLA:HAB	14:G:1137:CLA:HBB2	1.96	0.48
14:G:1101:CLA:HHC	14:G:1101:CLA:HBB1	1.96	0.48
9:U:43:GLY:HA3	9:U:58:PRO:HG2	1.94	0.48
13:Z:49:GLU:HB3	13:Z:64:LEU:HD22	1.96	0.48
1:e:360:TRP:HB3	14:e:1103:CLA:HAC1	1.94	0.48
1:e:441:VAL:HG11	14:e:1119:CLA:H192	1.94	0.48
1:e:616:ILE:HD12	14:e:1011:CLA:H122	1.96	0.48
14:v:519:CLA:HED2	14:v:519:CLA:H2A	1.96	0.48
1:A:360:TRP:HB3	14:A:1103:CLA:HAC1	1.94	0.48
1:A:429:ASP:O	1:A:433:ASN:ND2	2.46	0.48
10:L:21:ILE:HD13	18:L:5218:LHG:H302	1.96	0.48
13:6:20:PHE:HA	13:6:23:LEU:HD12	1.94	0.48
14:6:519:CLA:HED2	14:6:519:CLA:H2A	1.96	0.48
14:G:1121:CLA:HAB	14:G:1801:CLA:HAB	1.96	0.48
1:e:589:PRO:HB3	2:f:559:CYS:SG	2.53	0.48
14:e:1138:CLA:HAA2	14:f:1228:CLA:HMB2	1.96	0.48
2:f:15:ASP:OD2	2:f:19:ARG:NH2	2.47	0.48
10:n:21:ILE:HD13	18:n:5218:LHG:H302	1.96	0.48
14:A:1104:CLA:H62	14:A:1104:CLA:H41	1.61	0.48
14:A:1121:CLA:HAB	14:A:1801:CLA:HAB	1.96	0.48
13:6:78:GLY:N	13:6:82:GLN:O	2.47	0.48
1:G:573:LEU:O	4:O:61:ARG:NH2	2.42	0.48
14:G:1115:CLA:H62	14:G:1115:CLA:H41	1.65	0.48
14:G:1237:CLA:HAB	2:H:691:VAL:HG11	1.94	0.48
2:H:722:ALA:HB2	14:H:1224:CLA:HBB1	1.95	0.48
4:O:79:LYS:NZ	12:X:92:VAL:HG13	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:67:LEU:HD22	13:Z:89:LEU:HD13	1.95	0.48
1:e:300:LEU:HD21	1:e:385:MET:HB3	1.95	0.48
14:e:1121:CLA:HAB	14:e:1801:CLA:HAB	1.96	0.48
14:f:1209:CLA:H3A	14:f:1209:CLA:HBA2	1.48	0.48
13:u:148:PHE:CE2	14:u:512:CLA:HHB	2.49	0.48
13:u:282:VAL:HG23	13:u:283:THR:HG23	1.95	0.48
13:v:78:GLY:N	13:v:82:GLN:O	2.47	0.48
2:B:493:TYR:HE1	14:B:1231:CLA:HED1	1.79	0.48
4:O:101:ASP:OD1	4:O:101:ASP:N	2.47	0.48
13:Z:148:PHE:CE2	14:Z:512:CLA:HHB	2.48	0.48
13:b:59:MET:HB2	13:b:271:PHE:HA	1.96	0.48
13:d:78:GLY:N	13:d:82:GLN:O	2.47	0.48
2:f:151:PHE:CZ	21:f:1852:SQD:H252	2.49	0.48
5:i:28:VAL:HG22	5:i:37:VAL:HG13	1.96	0.48
6:F:118:VAL:HA	8:J:10:SER:HA	1.96	0.48
13:2:67:LEU:HD22	13:2:89:LEU:HD13	1.95	0.48
13:3:320:TRP:CH2	21:3:822:SQD:H462	2.49	0.48
13:4:276:LEU:HB3	13:4:286:PHE:HB3	1.96	0.48
13:5:282:VAL:HG23	13:5:283:THR:HG23	1.95	0.48
14:G:1117:CLA:H8	14:G:1117:CLA:HAB	1.95	0.48
10:V:90:THR:HG21	10:V:133:ILE:HD12	1.96	0.48
17:V:4219:BCR:H14C	18:V:5220:LHG:H331	1.95	0.48
13:b:119:ALA:O	13:b:126:LYS:NZ	2.43	0.48
13:c:148:PHE:CE2	14:c:512:CLA:HHB	2.49	0.48
2:f:142:LEU:HG	17:f:4006:BCR:H382	1.96	0.48
10:n:90:THR:HG21	10:n:133:ILE:HD12	1.96	0.48
13:s:267:TYR:O	13:s:300:ARG:NH2	2.39	0.48
14:A:1114:CLA:HBB1	18:A:5005:LHG:H301	1.95	0.47
4:D:79:LYS:NZ	12:P:92:VAL:HG13	2.29	0.47
13:4:147:LEU:HD12	13:4:215:ILE:HG12	1.96	0.47
1:G:219:VAL:HG13	1:G:252:PRO:HB3	1.96	0.47
1:G:616:ILE:HD12	14:G:1011:CLA:H122	1.96	0.47
14:G:1114:CLA:HBB1	18:G:5005:LHG:H301	1.95	0.47
10:V:98:ASN:ND2	10:n:39:ARG:O	2.45	0.47
13:c:305:ASN:HB3	17:c:521:BCR:HC8	1.95	0.47
14:e:1109:CLA:H72	14:e:1101:CLA:HBB2	1.96	0.47
17:n:4219:BCR:H15C	17:n:4219:BCR:H351	1.75	0.47
13:s:320:TRP:CH2	21:s:822:SQD:H462	2.49	0.47
13:t:147:LEU:HD12	13:t:215:ILE:HG12	1.96	0.47
1:A:577:LYS:NZ	2:B:673:GLU:OE2	2.43	0.47
14:A:1109:CLA:H72	14:A:1101:CLA:HBB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1115:CLA:HBC1	14:A:1116:CLA:H121	1.96	0.47
14:A:1129:CLA:HMC1	14:A:1137:CLA:HAB	1.95	0.47
2:B:15:ASP:OD2	2:B:19:ARG:NH2	2.47	0.47
2:B:722:ALA:HB2	14:B:1224:CLA:HBB1	1.95	0.47
4:D:37:GLU:HA	4:D:50:MET:O	2.14	0.47
13:d:42:ALA:O	13:d:46:THR:OG1	2.30	0.47
4:h:37:GLU:HA	4:h:50:MET:O	2.14	0.47
13:v:282:VAL:HG23	13:v:283:THR:HG23	1.94	0.47
1:A:424:MET:HE1	1:A:442:LEU:HD11	1.97	0.47
10:L:90:THR:HG21	10:L:133:ILE:HD12	1.96	0.47
13:3:267:TYR:O	13:3:300:ARG:NH2	2.39	0.47
14:G:1103:CLA:H3A	14:G:1103:CLA:HBA1	1.57	0.47
2:H:151:PHE:CZ	21:H:1852:SQD:H252	2.49	0.47
5:Q:28:VAL:HG22	5:Q:37:VAL:HG13	1.96	0.47
6:R:143:SER:HB2	13:b:14:TRP:CH2	2.48	0.47
13:a:267:TYR:O	13:a:300:ARG:NH2	2.39	0.47
14:v:517:CLA:H3A	14:v:517:CLA:HBA1	1.55	0.47
1:A:485:ASP:OD1	1:A:491:GLN:NE2	2.45	0.47
2:B:114:ASN:ND2	14:B:1206:CLA:OBD	2.47	0.47
2:H:493:TYR:HE1	14:H:1231:CLA:HED1	1.79	0.47
14:H:1227:CLA:HAB	14:H:1236:CLA:HBB2	1.97	0.47
10:V:83:VAL:HG11	10:n:142:PHE:CE1	2.49	0.47
13:a:143:GLY:HA3	13:a:222:ILE:HG13	1.96	0.47
1:e:219:VAL:HG13	1:e:252:PRO:HB3	1.97	0.47
2:f:301:ILE:HG23	14:f:1216:CLA:HED2	1.97	0.47
2:f:355:MET:HE3	2:f:355:MET:HB2	1.74	0.47
1:A:258:VAL:O	1:A:262:SER:HB2	2.15	0.47
17:6:522:BCR:H352	13:Y:315:LEU:HD21	1.95	0.47
14:G:1138:CLA:HAA2	14:H:1228:CLA:HMB2	1.96	0.47
14:G:1130:CLA:H61	14:G:1130:CLA:H41	1.70	0.47
2:H:301:ILE:HG23	14:H:1216:CLA:HED2	1.97	0.47
2:H:376:GLN:O	2:H:380:THR:OG1	2.30	0.47
2:H:498:LEU:HA	2:H:501:ILE:HG22	1.94	0.47
6:R:118:VAL:HA	8:T:10:SER:HA	1.96	0.47
14:Y:518:CLA:HED2	14:Y:518:CLA:H2A	1.96	0.47
13:Z:145:HIS:NE2	14:Z:512:CLA:NA	2.62	0.47
14:Z:501:CLA:C4D	14:Z:503:CLA:H2	2.44	0.47
14:e:1115:CLA:HBC1	14:e:1116:CLA:H121	1.96	0.47
14:e:1129:CLA:HAB	14:e:1137:CLA:HBB2	1.96	0.47
13:t:59:MET:HB2	13:t:271:PHE:HA	1.96	0.47
13:t:276:LEU:HB3	13:t:286:PHE:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HG	17:B:4006:BCR:H382	1.96	0.47
13:1:261:ALA:HA	13:1:276:LEU:HD12	1.96	0.47
14:2:501:CLA:C4D	14:2:503:CLA:H2	2.44	0.47
13:4:249:ILE:HG12	14:4:502:CLA:HAC1	1.96	0.47
1:G:300:LEU:HD21	1:G:385:MET:HB3	1.95	0.47
1:G:440:ARG:O	1:G:444:HIS:ND1	2.43	0.47
14:G:1130:CLA:H52	14:V:1502:CLA:H12	1.96	0.47
14:d:519:CLA:HED2	14:d:519:CLA:H2A	1.96	0.47
1:e:522:GLY:HA2	1:e:536:PRO:HB3	1.97	0.47
1:e:573:LEU:O	4:h:61:ARG:NH2	2.42	0.47
13:r:145:HIS:NE2	14:r:512:CLA:NA	2.62	0.47
1:A:219:VAL:HG13	1:A:252:PRO:HB3	1.96	0.47
14:A:1119:CLA:H11	14:A:1125:CLA:H93	1.97	0.47
14:A:1130:CLA:H52	14:L:1502:CLA:H12	1.96	0.47
2:B:210:ASP:OD1	2:B:210:ASP:N	2.48	0.47
2:B:301:ILE:HG21	14:B:1221:CLA:HAC1	1.97	0.47
14:B:1216:CLA:H43	14:B:1223:CLA:H111	1.96	0.47
9:K:32:ILE:O	9:K:36:THR:OG1	2.29	0.47
13:3:148:PHE:CE2	14:3:512:CLA:HHB	2.50	0.47
13:5:305:ASN:HB3	17:5:521:BCR:HC8	1.95	0.47
1:G:66:GLU:HG3	1:G:187:LEU:HB2	1.97	0.47
1:G:66:GLU:OE2	1:G:70:ARG:NH2	2.48	0.47
1:G:490:LEU:HB2	1:G:541:THR:HG23	1.96	0.47
14:G:1115:CLA:HBC1	14:G:1116:CLA:H121	1.96	0.47
2:H:156:HIS:CE1	14:H:1208:CLA:NA	2.83	0.47
2:H:301:ILE:HG21	14:H:1221:CLA:HAC1	1.97	0.47
4:O:37:GLU:HA	4:O:50:MET:O	2.14	0.47
10:V:21:ILE:HD13	18:V:5218:LHG:H302	1.96	0.47
13:Y:112:PHE:HB2	13:Z:326:MET:HE3	1.97	0.47
13:b:276:LEU:HB3	13:b:286:PHE:HB3	1.96	0.47
1:e:258:VAL:O	1:e:262:SER:HB2	2.15	0.47
14:e:1101:CLA:HHC	14:e:1101:CLA:HBB1	1.96	0.47
2:f:156:HIS:CE1	14:f:1208:CLA:NA	2.83	0.47
12:p:57:TRP:NE1	22:p:170:FMN:O2P	2.45	0.47
13:r:67:LEU:HD22	13:r:89:LEU:HD13	1.95	0.47
14:r:505:CLA:H43	17:r:524:BCR:HC7	1.96	0.47
13:s:148:PHE:CE2	14:s:512:CLA:HHB	2.50	0.47
14:A:1139:CLA:H143	14:A:1139:CLA:H111	1.75	0.47
10:L:94:SER:HB2	14:V:1501:CLA:CMD	2.44	0.47
13:6:42:ALA:O	13:6:46:THR:OG1	2.30	0.47
14:G:1109:CLA:H72	14:G:1101:CLA:HBB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:LEU:HG	17:H:4006:BCR:H382	1.96	0.47
2:H:326:LEU:HD13	2:H:332:PHE:CD2	2.50	0.47
14:Z:505:CLA:H43	17:Z:524:BCR:HC7	1.96	0.47
13:a:146:LEU:HD22	13:a:214:LEU:HD22	1.97	0.47
1:e:424:MET:HE1	1:e:442:LEU:HD11	1.97	0.47
14:e:1114:CLA:HBB1	18:e:5005:LHG:H301	1.96	0.47
14:e:1137:CLA:H41	14:e:1137:CLA:H62	1.64	0.47
17:n:4219:BCR:H14C	18:n:5220:LHG:H331	1.96	0.47
13:q:261:ALA:HA	13:q:276:LEU:HD12	1.96	0.47
14:A:1129:CLA:HAB	14:A:1137:CLA:HBB2	1.96	0.47
2:B:326:LEU:HD13	2:B:332:PHE:CD2	2.50	0.47
1:G:512:ASN:HB2	14:G:1134:CLA:HED2	1.97	0.47
7:S:13:ILE:HG23	17:n:4219:BCR:C40	2.45	0.47
13:Y:146:LEU:HG	14:Y:507:CLA:HED1	1.97	0.47
13:Z:251:LEU:HD13	14:Z:505:CLA:H122	1.97	0.47
1:e:66:GLU:OE2	1:e:70:ARG:NH2	2.48	0.47
14:e:1128:CLA:H121	18:e:5001:LHG:H352	1.97	0.47
14:e:1130:CLA:H41	14:e:1130:CLA:H61	1.70	0.47
2:f:301:ILE:HG21	14:f:1221:CLA:HAC1	1.97	0.47
3:g:13:GLY:O	3:g:38:GLN:NE2	2.46	0.47
1:A:336:ILE:O	1:A:340:HIS:ND1	2.38	0.47
1:A:522:GLY:HA2	1:A:536:PRO:HB3	1.97	0.47
2:B:301:ILE:HG23	14:B:1216:CLA:HED2	1.97	0.47
13:1:112:PHE:HB2	13:2:326:MET:HE3	1.97	0.47
14:1:518:CLA:HED2	14:1:518:CLA:H2A	1.96	0.47
13:6:79:ASP:OD1	13:6:79:ASP:N	2.48	0.47
13:Y:261:ALA:HA	13:Y:276:LEU:HD12	1.96	0.47
14:Z:518:CLA:H3A	14:Z:518:CLA:C2	2.45	0.47
13:b:249:ILE:HG12	14:b:502:CLA:HAC1	1.96	0.47
10:n:7:ALA:HB3	10:n:18:ALA:HB3	1.97	0.47
13:s:68:PRO:HB3	13:s:271:PHE:HB3	1.97	0.47
13:t:119:ALA:O	13:t:126:LYS:NZ	2.43	0.47
1:A:66:GLU:OE2	1:A:70:ARG:NH2	2.48	0.46
14:A:1116:CLA:HBA2	14:A:1116:CLA:H3A	1.57	0.46
2:H:546:LEU:HD13	2:H:567:THR:HG22	1.97	0.46
14:H:1207:CLA:H193	18:n:5221:LHG:H222	1.96	0.46
6:R:125:VAL:HG12	13:a:13:TRP:HH2	1.80	0.46
8:l:21:ILE:HA	14:l:1302:CLA:HBB2	1.97	0.46
13:q:110:HIS:HA	13:q:114:ALA:HB3	1.98	0.46
14:r:518:CLA:C2	14:r:518:CLA:H3A	2.45	0.46
1:A:66:GLU:HG3	1:A:187:LEU:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1128:CLA:H121	18:A:5001:LHG:H352	1.97	0.46
13:2:182:LEU:O	13:2:209:TYR:OH	2.33	0.46
13:3:146:LEU:HD22	13:3:214:LEU:HD22	1.97	0.46
14:H:1216:CLA:H43	14:H:1223:CLA:H111	1.97	0.46
13:a:148:PHE:CE2	14:a:512:CLA:HHB	2.50	0.46
13:b:147:LEU:HD12	13:b:215:ILE:HG12	1.96	0.46
2:f:326:LEU:HD13	2:f:332:PHE:CD2	2.50	0.46
2:f:450:GLU:OE2	6:j:52:ARG:NE	2.43	0.46
2:f:493:TYR:HE1	14:f:1231:CLA:HED1	1.79	0.46
13:q:130:PHE:HA	13:q:137:GLN:HG2	1.97	0.46
1:A:616:ILE:HD12	14:A:1011:CLA:H122	1.96	0.46
14:A:1122:CLA:H62	14:A:1122:CLA:H41	1.67	0.46
2:B:182:LEU:HD13	14:B:1210:CLA:HHB	1.97	0.46
13:1:146:LEU:HG	14:1:507:CLA:HED1	1.97	0.46
17:1:522:BCR:H351	17:1:522:BCR:H15C	1.78	0.46
14:2:505:CLA:H43	17:2:524:BCR:HC7	1.96	0.46
13:3:143:GLY:HA3	13:3:222:ILE:HG13	1.96	0.46
1:e:512:ASN:HB2	14:e:1134:CLA:HED2	1.96	0.46
17:e:4003:BCR:H20C	17:e:4003:BCR:H361	1.82	0.46
14:f:1227:CLA:HAB	14:f:1236:CLA:HBB2	1.97	0.46
13:q:112:PHE:HB2	13:r:326:MET:HE3	1.97	0.46
13:q:146:LEU:HG	14:q:507:CLA:HED1	1.97	0.46
14:q:518:CLA:HED2	14:q:518:CLA:H2A	1.96	0.46
14:r:501:CLA:C4D	14:r:503:CLA:H2	2.44	0.46
14:t:501:CLA:HMB1	17:t:524:BCR:H23C	1.98	0.46
13:v:41:TRP:O	13:v:45:PHE:HB2	2.16	0.46
1:A:239:ASN:HD22	1:A:263:GLN:HE22	1.63	0.46
1:A:512:ASN:HB2	14:A:1134:CLA:HED2	1.97	0.46
14:A:1101:CLA:HBB1	14:A:1101:CLA:HHC	1.96	0.46
5:E:28:VAL:HG22	5:E:37:VAL:HG13	1.96	0.46
12:P:2:LYS:HG3	12:P:3:ILE:HG13	1.98	0.46
13:4:307:HIS:NE2	14:4:502:CLA:ND	2.63	0.46
1:G:145:GLN:HB3	1:G:388:TYR:HB3	1.98	0.46
2:H:174:ARG:HB2	14:H:1210:CLA:HBC2	1.97	0.46
2:H:237:PRO:HB3	2:H:256:THR:HG21	1.98	0.46
13:Y:110:HIS:HA	13:Y:114:ALA:HB3	1.97	0.46
14:Z:501:CLA:HMB2	17:Z:524:BCR:H23C	1.97	0.46
13:b:307:HIS:NE2	14:b:502:CLA:ND	2.63	0.46
1:e:595:CYS:HB2	2:f:667:TRP:HB3	1.98	0.46
17:e:4003:BCR:H15C	17:e:4003:BCR:H351	1.81	0.46
14:f:1218:CLA:H2	14:f:1218:CLA:H61	1.75	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:79:LYS:NZ	12:p:92:VAL:HG13	2.29	0.46
7:k:23:PRO:O	7:k:27:MET:HB2	2.16	0.46
13:s:143:GLY:HA3	13:s:222:ILE:HG13	1.96	0.46
13:t:249:ILE:HG12	14:t:502:CLA:HAC1	1.96	0.46
13:v:148:PHE:CD2	14:v:512:CLA:H3A	2.51	0.46
1:A:316:PHE:HZ	14:A:1117:CLA:H112	1.81	0.46
14:A:1106:CLA:H161	14:A:1106:CLA:H122	1.60	0.46
2:B:510:LEU:HD22	2:B:601:VAL:HG21	1.98	0.46
7:I:4:ASP:OD1	7:I:4:ASP:N	2.42	0.46
13:2:145:HIS:NE2	14:2:512:CLA:NA	2.62	0.46
14:2:501:CLA:HMB2	17:2:524:BCR:H23C	1.98	0.46
14:3:512:CLA:H3A	14:3:512:CLA:HBA1	1.62	0.46
13:5:261:ALA:HA	13:5:276:LEU:HD12	1.97	0.46
1:G:424:MET:HE1	1:G:442:LEU:HD11	1.97	0.46
14:H:1202:CLA:H3A	14:H:1202:CLA:HBA1	1.62	0.46
13:Z:148:PHE:CD2	14:Z:512:CLA:H3A	2.50	0.46
14:a:512:CLA:H3A	14:a:512:CLA:HBA1	1.63	0.46
13:d:301:ALA:O	13:d:305:ASN:ND2	2.41	0.46
1:e:66:GLU:HG3	1:e:187:LEU:HB2	1.97	0.46
1:e:490:LEU:HB2	1:e:541:THR:HG23	1.96	0.46
18:e:5008:LHG:HC5	13:r:13:TRP:CD1	2.51	0.46
2:f:510:LEU:HD22	2:f:601:VAL:HG21	1.98	0.46
2:f:577:TYR:OH	2:f:664:LEU:HD22	2.15	0.46
13:t:307:HIS:NE2	14:t:502:CLA:ND	2.63	0.46
14:A:1106:CLA:HBA2	14:A:1106:CLA:H3A	1.64	0.46
18:A:5008:LHG:HC5	13:2:13:TRP:CD1	2.51	0.46
18:A:5009:LHG:C13	17:1:521:BCR:H313	2.46	0.46
2:B:156:HIS:CE1	14:B:1208:CLA:NA	2.83	0.46
12:P:57:TRP:NE1	22:P:170:FMN:O2P	2.45	0.46
1:G:522:GLY:HA2	1:G:536:PRO:HB3	1.97	0.46
8:T:21:ILE:HA	14:T:1302:CLA:HBB2	1.97	0.46
14:e:1104:CLA:H62	14:e:1104:CLA:H41	1.61	0.46
4:h:101:ASP:OD1	4:h:101:ASP:N	2.47	0.46
6:j:84:PRO:HB3	17:l:4015:BCR:H362	1.98	0.46
6:j:125:VAL:HG12	13:s:13:TRP:HH2	1.80	0.46
10:n:3:GLN:CG	10:n:4:ASP:N	2.53	0.46
13:u:261:ALA:HA	13:u:276:LEU:HD12	1.97	0.46
2:B:237:PRO:HB3	2:B:256:THR:HG21	1.98	0.46
2:B:355:MET:HB2	2:B:355:MET:HE3	1.74	0.46
2:B:546:LEU:HD13	2:B:567:THR:HG22	1.97	0.46
14:F:1302:CLA:HMB1	17:F:4016:BCR:H24C	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:518:CLA:H3A	14:2:518:CLA:C2	2.45	0.46
14:3:517:CLA:HBA1	14:3:517:CLA:H3A	1.60	0.46
13:6:41:TRP:O	13:6:45:PHE:HB2	2.16	0.46
1:G:258:VAL:O	1:G:262:SER:HB2	2.15	0.46
2:H:450:GLU:OE2	6:R:52:ARG:NE	2.43	0.46
2:H:577:TYR:OH	2:H:664:LEU:HD22	2.15	0.46
14:H:1239:CLA:H91	14:H:1239:CLA:H112	1.81	0.46
18:H:1842:LHG:HC81	18:H:1842:LHG:H112	1.80	0.46
14:e:1119:CLA:H11	14:e:1125:CLA:H93	1.97	0.46
14:e:1130:CLA:H52	14:n:1502:CLA:H12	1.96	0.46
14:f:1216:CLA:H43	14:f:1223:CLA:H111	1.97	0.46
13:s:17:ASN:ND2	14:s:510:CLA:O1A	2.47	0.46
13:v:79:ASP:OD1	13:v:79:ASP:N	2.48	0.46
1:A:441:VAL:HA	1:A:444:HIS:CE1	2.51	0.46
2:B:577:TYR:OH	2:B:664:LEU:HD22	2.15	0.46
13:2:251:LEU:HD13	14:2:505:CLA:H122	1.97	0.46
1:G:316:PHE:HZ	14:G:1117:CLA:H112	1.81	0.46
14:G:1128:CLA:H121	18:G:5001:LHG:H352	1.97	0.46
14:H:1207:CLA:HAB	7:S:19:GLY:HA3	1.98	0.46
7:S:23:PRO:O	7:S:27:MET:HB2	2.16	0.46
13:Z:182:LEU:O	13:Z:209:TYR:OH	2.33	0.46
13:b:159:LYS:HA	13:b:163:TRP:HB2	1.98	0.46
14:d:517:CLA:H3A	14:d:517:CLA:HBA1	1.55	0.46
2:f:114:ASN:ND2	14:f:1206:CLA:OBD	2.46	0.46
2:f:546:LEU:HD13	2:f:567:THR:HG22	1.97	0.46
7:k:30:LEU:HD13	17:n:4019:BCR:HC8	1.98	0.46
10:n:163:TRP:CH2	17:n:4219:BCR:HC7	2.51	0.46
13:u:73:LEU:O	13:u:159:LYS:NZ	2.49	0.46
14:B:1227:CLA:HAB	14:B:1236:CLA:HBB2	1.97	0.46
13:1:130:PHE:HA	13:1:137:GLN:HG2	1.97	0.46
14:1:516:CLA:H3A	14:1:516:CLA:HBA1	1.44	0.46
13:5:73:LEU:O	13:5:159:LYS:NZ	2.49	0.46
2:H:182:LEU:HD13	14:H:1210:CLA:HHB	1.97	0.46
7:S:30:LEU:HD13	17:V:4019:BCR:HC8	1.98	0.46
10:V:49:GLU:OE2	14:V:1501:CLA:ND	2.49	0.46
13:Y:67:LEU:HD22	13:Y:89:LEU:HD13	1.98	0.46
13:Z:143:GLY:HA3	13:Z:222:ILE:HG13	1.98	0.46
13:c:261:ALA:HA	13:c:276:LEU:HD12	1.97	0.46
18:e:5009:LHG:C13	17:q:521:BCR:H313	2.46	0.46
12:p:2:LYS:HG3	12:p:3:ILE:HG13	1.98	0.46
13:q:67:LEU:HD22	13:q:89:LEU:HD13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:178:THR:OG1	13:t:201:GLU:OE2	2.34	0.46
2:B:73:ASN:HB2	2:B:76:GLN:HB2	1.97	0.46
14:B:1217:CLA:H3A	14:B:1217:CLA:HBA2	1.49	0.46
14:B:1207:CLA:HAB	7:I:19:GLY:HA3	1.98	0.46
6:F:75:LEU:HA	6:F:78:ALA:HB2	1.98	0.46
13:1:67:LEU:HD22	13:1:89:LEU:HD13	1.98	0.46
18:G:5008:LHG:HC5	13:Z:13:TRP:CD1	2.51	0.46
2:H:114:ASN:ND2	14:H:1206:CLA:OBD	2.47	0.46
2:H:410:ARG:NH2	14:H:1227:CLA:OBD	2.49	0.46
2:H:510:LEU:HD22	2:H:601:VAL:HG21	1.98	0.46
13:b:101:ALA:HB1	14:c:505:CLA:HAB	1.98	0.46
14:c:509:CLA:H92	14:c:509:CLA:H62	1.81	0.46
1:e:220:SER:O	1:e:224:ASN:HB2	2.16	0.46
2:f:174:ARG:HB2	14:f:1210:CLA:HBC2	1.97	0.46
2:f:237:PRO:HB3	2:f:256:THR:HG21	1.98	0.46
13:t:101:ALA:HB1	14:u:505:CLA:HAB	1.98	0.46
14:A:1139:CLA:H61	14:A:1139:CLA:H41	1.64	0.45
17:A:4002:BCR:H361	17:A:4002:BCR:H20C	1.76	0.45
2:B:25:ILE:HA	14:B:1201:CLA:HMD2	1.98	0.45
2:B:174:ARG:HB2	14:B:1210:CLA:HBC2	1.97	0.45
2:B:340:SER:HB3	14:B:1221:CLA:H2	1.97	0.45
14:B:1210:CLA:H42	17:B:4005:BCR:H21C	1.98	0.45
7:I:30:LEU:HD13	17:L:4019:BCR:HC8	1.98	0.45
10:L:163:TRP:CH2	17:L:4219:BCR:HC7	2.51	0.45
13:2:147:LEU:HD12	13:2:215:ILE:HG12	1.98	0.45
13:4:159:LYS:HA	13:4:163:TRP:HB2	1.98	0.45
2:H:25:ILE:HA	14:H:1201:CLA:HMD2	1.98	0.45
2:H:73:ASN:HB2	2:H:76:GLN:HB2	1.97	0.45
14:H:1210:CLA:H2	14:H:1210:CLA:H62	1.60	0.45
17:H:4006:BCR:H15C	17:H:4006:BCR:H351	1.81	0.45
6:R:84:PRO:HB3	17:T:4015:BCR:H362	1.98	0.45
13:Z:301:ALA:O	13:Z:305:ASN:ND2	2.42	0.45
14:b:501:CLA:HMB1	17:b:524:BCR:H23C	1.98	0.45
14:e:1119:CLA:H111	14:e:1119:CLA:H152	1.80	0.45
14:f:1210:CLA:H2	14:f:1210:CLA:H62	1.60	0.45
17:q:521:BCR:H24C	17:q:521:BCR:H371	1.78	0.45
13:t:159:LYS:HA	13:t:163:TRP:HB2	1.98	0.45
1:A:490:LEU:HB2	1:A:541:THR:HG23	1.96	0.45
14:A:1120:CLA:HED2	9:K:38:LYS:HD2	1.98	0.45
10:L:149:THR:HG22	10:L:151:TYR:H	1.81	0.45
13:1:110:HIS:HA	13:1:114:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:1104:CLA:H193	14:G:1104:CLA:H161	1.79	0.45
14:H:1210:CLA:H42	17:H:4005:BCR:H21C	1.98	0.45
14:R:1302:CLA:HMB1	17:R:4016:BCR:H24C	1.98	0.45
12:X:2:LYS:HG3	12:X:3:ILE:HG13	1.98	0.45
13:Z:147:LEU:HD12	13:Z:215:ILE:HG12	1.98	0.45
13:Z:149:LEU:HD21	14:Z:509:CLA:H61	1.97	0.45
13:c:73:LEU:O	13:c:159:LYS:NZ	2.49	0.45
13:d:41:TRP:O	13:d:45:PHE:HB2	2.16	0.45
13:r:148:PHE:CD2	14:r:512:CLA:H3A	2.50	0.45
17:u:522:BCR:H15C	17:u:522:BCR:H351	1.77	0.45
1:A:595:CYS:HB2	2:B:667:TRP:HB3	1.98	0.45
7:I:23:PRO:O	7:I:27:MET:HB2	2.16	0.45
10:L:48:LEU:HD21	10:n:133:ILE:HG21	1.98	0.45
13:2:148:PHE:CD2	14:2:512:CLA:H3A	2.50	0.45
13:4:178:THR:OG1	13:4:201:GLU:OE2	2.34	0.45
14:G:1119:CLA:H11	14:G:1125:CLA:H93	1.97	0.45
14:H:1216:CLA:HBA1	14:H:1216:CLA:H12	1.83	0.45
14:Y:512:CLA:H3A	14:Y:512:CLA:HBA1	1.68	0.45
13:a:68:PRO:HB3	13:a:271:PHE:HB3	1.97	0.45
17:b:524:BCR:H15C	17:b:524:BCR:H351	1.82	0.45
1:e:316:PHE:HZ	14:e:1117:CLA:H112	1.81	0.45
14:n:1501:CLA:HAA2	17:n:4022:BCR:H363	1.98	0.45
13:v:243:SER:O	13:v:318:HIS:ND1	2.50	0.45
1:A:115:GLN:NE2	14:A:1107:CLA:OBD	2.43	0.45
1:A:440:ARG:O	1:A:444:HIS:ND1	2.43	0.45
6:F:71:VAL:HG12	6:F:81:PHE:HB2	1.98	0.45
10:L:7:ALA:HB3	10:L:18:ALA:HB3	1.97	0.45
13:2:229:TRP:HA	13:2:232:LYS:HB2	1.98	0.45
13:3:68:PRO:HB3	13:3:271:PHE:HB3	1.97	0.45
13:5:267:TYR:O	13:5:300:ARG:NH2	2.45	0.45
14:G:1120:CLA:HED2	9:U:38:LYS:HD2	1.98	0.45
2:H:160:LYS:HB3	21:H:1852:SQD:O8	2.16	0.45
6:R:75:LEU:HA	6:R:78:ALA:HB2	1.98	0.45
1:e:239:ASN:HD22	1:e:263:GLN:HE22	1.63	0.45
2:f:25:ILE:HA	14:f:1201:CLA:HMD2	1.98	0.45
13:r:149:LEU:HD21	14:r:509:CLA:H61	1.97	0.45
13:s:146:LEU:HD22	13:s:214:LEU:HD22	1.97	0.45
14:B:1210:CLA:H62	14:B:1210:CLA:H2	1.60	0.45
13:4:119:ALA:O	13:4:126:LYS:NZ	2.43	0.45
2:H:340:SER:HB3	14:H:1221:CLA:H2	1.97	0.45
14:H:1209:CLA:H3A	14:H:1209:CLA:HBA2	1.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:178:THR:OG1	13:b:201:GLU:OE2	2.34	0.45
1:e:440:ARG:NH1	14:e:1129:CLA:O1D	2.50	0.45
17:e:4001:BCR:H23C	9:m:66:PHE:HB2	1.99	0.45
2:f:340:SER:HB3	14:f:1221:CLA:H2	1.97	0.45
14:f:1210:CLA:H42	17:f:4005:BCR:H21C	1.98	0.45
5:i:18:TRP:HB3	5:i:21:GLU:HB2	1.99	0.45
13:r:251:LEU:HD13	14:r:505:CLA:H122	1.97	0.45
14:r:501:CLA:HMB2	17:r:524:BCR:H23C	1.97	0.45
13:v:143:GLY:HA3	13:v:222:ILE:HG13	1.98	0.45
1:A:220:SER:O	1:A:224:ASN:HB2	2.16	0.45
17:A:4002:BCR:H15C	17:A:4002:BCR:H351	1.86	0.45
13:2:149:LEU:HD21	14:2:509:CLA:H61	1.97	0.45
1:G:220:SER:O	1:G:224:ASN:HB2	2.16	0.45
1:G:591:ARG:HH21	1:G:594:THR:HG21	1.81	0.45
14:H:1208:CLA:HMD3	21:H:1852:SQD:H101	1.99	0.45
14:H:1228:CLA:HBC2	14:H:1236:CLA:HMC2	1.99	0.45
10:V:163:TRP:CH2	17:V:4219:BCR:HC7	2.51	0.45
14:V:1503:CLA:H93	14:V:1503:CLA:H61	1.88	0.45
1:e:441:VAL:HA	1:e:444:HIS:CE1	2.51	0.45
18:e:5005:LHG:HC82	17:r:521:BCR:HC22	1.98	0.45
2:f:182:LEU:HD13	14:f:1210:CLA:HHB	1.97	0.45
14:j:1302:CLA:HMB1	17:j:4016:BCR:H24C	1.98	0.45
9:m:32:ILE:O	9:m:36:THR:OG1	2.29	0.45
10:n:149:THR:HG22	10:n:151:TYR:H	1.81	0.45
14:A:1110:CLA:H2	14:A:1110:CLA:H62	1.83	0.45
17:L:4019:BCR:H11C	17:L:4019:BCR:H341	1.81	0.45
14:2:519:CLA:HED2	14:2:519:CLA:H2A	1.99	0.45
13:5:112:PHE:HB2	13:6:326:MET:HE3	1.99	0.45
14:G:1126:CLA:HBA2	14:G:1126:CLA:H3A	1.63	0.45
18:G:5009:LHG:C13	17:Y:521:BCR:H313	2.46	0.45
10:V:7:ALA:HB3	10:V:18:ALA:HB3	1.97	0.45
13:c:110:HIS:NE2	14:c:513:CLA:NB	2.65	0.45
2:f:73:ASN:HB2	2:f:76:GLN:HB2	1.97	0.45
14:f:1228:CLA:HBC2	14:f:1236:CLA:HMC2	1.99	0.45
13:r:143:GLY:HA3	13:r:222:ILE:HG13	1.98	0.45
1:A:145:GLN:HB3	1:A:388:TYR:HB3	1.98	0.45
14:B:1228:CLA:HBC2	14:B:1236:CLA:HMC2	1.99	0.45
8:J:21:ILE:HA	14:J:1302:CLA:HBB2	1.97	0.45
14:2:501:CLA:H62	14:2:501:CLA:H41	1.70	0.45
17:2:522:BCR:H15C	17:2:522:BCR:H351	1.77	0.45
14:4:501:CLA:HMB1	17:4:524:BCR:H23C	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:441:VAL:HA	1:G:444:HIS:CE1	2.51	0.45
1:G:595:CYS:HB2	2:H:667:TRP:HB3	1.98	0.45
18:G:5005:LHG:HC82	17:Z:521:BCR:HC22	1.98	0.45
14:V:1501:CLA:HAA2	17:V:4022:BCR:H363	1.98	0.45
12:X:57:TRP:NE1	22:X:170:FMN:O2P	2.45	0.45
13:d:323:LEU:HA	13:d:326:MET:HE2	1.99	0.45
14:f:1207:CLA:HAB	7:k:19:GLY:HA3	1.98	0.45
17:r:521:BCR:H24C	17:r:521:BCR:H371	1.77	0.45
17:v:521:BCR:H15C	17:v:521:BCR:H351	1.84	0.45
2:B:576:PHE:HE1	14:B:1226:CLA:HAC2	1.82	0.45
14:B:1215:CLA:HBA2	14:B:1215:CLA:H3A	1.63	0.45
5:E:18:TRP:HB3	5:E:21:GLU:HB2	1.99	0.45
17:1:522:BCR:H371	17:1:522:BCR:H24C	1.86	0.45
13:2:130:PHE:HA	13:2:137:GLN:HG2	1.99	0.45
13:2:143:GLY:HA3	13:2:222:ILE:HG13	1.98	0.45
17:H:4009:BCR:H11C	17:H:4009:BCR:H341	1.81	0.45
3:N:6:LYS:HG3	4:O:139:TYR:HB2	1.99	0.45
3:N:26:LEU:HA	3:N:41:ALA:O	2.17	0.45
13:Y:130:PHE:HA	13:Y:137:GLN:HG2	1.97	0.45
2:f:160:LYS:HB3	21:f:1852:SQD:O8	2.16	0.45
2:f:576:PHE:HE1	14:f:1226:CLA:HAC2	1.82	0.45
17:A:4001:BCR:H23C	9:K:66:PHE:HB2	1.99	0.45
18:A:5008:LHG:HC82	13:2:13:TRP:HZ2	1.82	0.45
17:B:4004:BCR:H11C	17:B:4004:BCR:H341	1.83	0.45
10:L:49:GLU:OE2	14:L:1501:CLA:ND	2.49	0.45
14:2:505:CLA:HBA2	14:2:505:CLA:H11	1.80	0.45
13:3:307:HIS:NE2	14:3:502:CLA:ND	2.65	0.45
13:5:59:MET:HB2	13:5:271:PHE:HA	1.99	0.45
5:Q:18:TRP:HB3	5:Q:21:GLU:HB2	1.99	0.45
13:c:267:TYR:O	13:c:300:ARG:NH2	2.45	0.45
13:c:307:HIS:NE2	14:c:502:CLA:NA	2.65	0.45
13:d:243:SER:O	13:d:318:HIS:ND1	2.50	0.45
1:e:591:ARG:HH21	1:e:594:THR:HG21	1.81	0.45
14:f:1205:CLA:H143	14:f:1205:CLA:H161	1.88	0.45
14:r:518:CLA:H41	14:r:518:CLA:H61	1.70	0.45
14:B:1221:CLA:H151	14:B:1221:CLA:H112	1.81	0.44
6:F:125:VAL:HG12	13:3:13:TRP:HH2	1.80	0.44
10:L:30:PHE:CD1	21:L:5216:SQD:H122	2.53	0.44
10:L:163:TRP:HH2	17:L:4219:BCR:H311	1.83	0.44
14:G:1013:CLA:H143	14:G:1013:CLA:H161	1.85	0.44
14:G:1116:CLA:HBA2	14:G:1116:CLA:H3A	1.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:1121:CLA:HAB	14:G:1801:CLA:CAB	2.47	0.44
14:G:1122:CLA:H41	14:G:1122:CLA:H62	1.67	0.44
2:H:422:LEU:O	2:H:426:SER:OG	2.34	0.44
14:H:1206:CLA:H122	14:H:1206:CLA:H162	1.84	0.44
17:H:4010:BCR:H351	17:H:4010:BCR:H15C	1.72	0.44
13:Z:110:HIS:HA	13:Z:114:ALA:HB3	2.00	0.44
13:d:148:PHE:CD2	14:d:512:CLA:H3A	2.51	0.44
1:e:145:GLN:HB3	1:e:388:TYR:HB3	1.98	0.44
1:e:440:ARG:HD2	14:e:1129:CLA:HED3	1.99	0.44
3:g:6:LYS:HG3	4:h:139:TYR:HB2	1.99	0.44
13:r:182:LEU:O	13:r:209:TYR:OH	2.33	0.44
14:u:513:CLA:HBB1	17:u:523:BCR:H24C	1.99	0.44
1:A:148:ARG:HD3	1:A:389:PRO:HB2	1.99	0.44
1:A:440:ARG:NH1	14:A:1129:CLA:O1D	2.50	0.44
14:A:1124:CLA:H2	14:A:1124:CLA:H61	1.76	0.44
2:B:674:LEU:O	2:B:677:THR:OG1	2.34	0.44
13:3:17:ASN:ND2	14:3:510:CLA:O1A	2.47	0.44
17:3:523:BCR:H11C	17:3:523:BCR:H341	1.84	0.44
13:6:143:GLY:HA3	13:6:222:ILE:HG13	1.98	0.44
1:G:588:GLY:HA2	2:H:562:PRO:HD3	1.99	0.44
18:G:5008:LHG:HC82	13:Z:13:TRP:HZ2	1.82	0.44
2:H:670:TYR:OH	14:H:1023:CLA:OBD	2.26	0.44
2:H:674:LEU:O	2:H:677:THR:OG1	2.34	0.44
10:V:149:THR:HG22	10:V:151:TYR:H	1.81	0.44
14:e:1013:CLA:H93	14:e:1013:CLA:H61	1.83	0.44
14:e:1106:CLA:H122	14:e:1106:CLA:H161	1.60	0.44
14:e:1116:CLA:HBA2	14:e:1116:CLA:H3A	1.57	0.44
14:e:1137:CLA:H112	14:e:1137:CLA:H143	1.83	0.44
14:f:1202:CLA:HBA1	14:f:1202:CLA:H3A	1.62	0.44
3:g:26:LEU:HA	3:g:41:ALA:O	2.17	0.44
10:n:49:GLU:OE2	14:n:1501:CLA:ND	2.49	0.44
13:r:147:LEU:HD12	13:r:215:ILE:HG12	1.98	0.44
13:u:110:HIS:NE2	14:u:513:CLA:NB	2.65	0.44
13:v:323:LEU:HA	13:v:326:MET:HE2	1.99	0.44
1:A:308:HIS:HE2	14:A:1117:CLA:C2B	2.31	0.44
14:B:1023:CLA:H142	17:I:4018:BCR:H271	1.99	0.44
14:L:1501:CLA:HAA2	17:L:4022:BCR:H363	1.97	0.44
13:5:307:HIS:NE2	14:5:502:CLA:NA	2.65	0.44
1:G:239:ASN:HD22	1:G:263:GLN:HE22	1.63	0.44
17:R:4016:BCR:H24C	17:R:4016:BCR:H371	1.83	0.44
12:X:63:GLN:O	12:X:67:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:190:TYR:HE2	13:Y:202:ASP:HB3	1.83	0.44
17:Z:523:BCR:H15C	17:Z:523:BCR:H351	1.82	0.44
13:a:73:LEU:HD11	14:a:503:CLA:HAA2	1.99	0.44
14:a:517:CLA:HBA1	14:a:517:CLA:H3A	1.60	0.44
1:e:588:GLY:HA2	2:f:562:PRO:HD3	1.99	0.44
2:f:631:LEU:O	2:f:647:SER:OG	2.29	0.44
3:g:58:CYS:HA	3:g:59:PRO:HD3	1.86	0.44
10:n:30:PHE:CD1	21:n:5216:SQD:H122	2.53	0.44
13:u:107:ALA:O	13:u:111:THR:OG1	2.29	0.44
14:A:1121:CLA:HAB	14:A:1801:CLA:CAB	2.47	0.44
14:A:1137:CLA:H143	14:A:1137:CLA:H112	1.83	0.44
18:A:5001:LHG:H341	18:A:5001:LHG:H372	1.84	0.44
14:B:1226:CLA:H91	20:B:5002:LMG:H372	2.00	0.44
13:1:307:HIS:NE2	14:1:502:CLA:ND	2.66	0.44
17:2:521:BCR:H15C	17:2:521:BCR:H351	1.83	0.44
14:G:1104:CLA:H191	18:G:5001:LHG:H211	1.99	0.44
2:H:44:GLN:NE2	2:H:163:PRO:O	2.38	0.44
2:H:91:ILE:HB	2:H:112:PRO:HB2	2.00	0.44
14:H:1023:CLA:H142	17:S:4018:BCR:H271	1.99	0.44
14:H:1215:CLA:H13	14:H:1221:CLA:H162	2.00	0.44
5:Q:53:ASP:OD1	5:Q:53:ASP:N	2.43	0.44
10:V:20:PRO:HB3	18:V:5218:LHG:HC82	1.99	0.44
14:Z:505:CLA:HBC2	17:Z:524:BCR:H341	2.00	0.44
14:c:513:CLA:HBB1	17:c:523:BCR:H24C	1.99	0.44
1:e:745:LEU:HD22	14:e:1140:CLA:HMA1	2.00	0.44
6:j:71:VAL:HG12	6:j:81:PHE:HB2	1.98	0.44
14:r:519:CLA:HED2	14:r:519:CLA:H2A	1.99	0.44
13:u:307:HIS:NE2	14:u:502:CLA:NA	2.65	0.44
1:A:312:ILE:HD13	1:A:312:ILE:HA	1.85	0.44
14:A:1110:CLA:HBA2	14:A:1110:CLA:H3A	1.63	0.44
18:A:5005:LHG:HC82	17:2:521:BCR:HC22	1.98	0.44
2:B:160:LYS:HB3	21:B:1852:SQD:O8	2.16	0.44
14:2:505:CLA:HBC2	17:2:524:BCR:H341	2.00	0.44
13:5:107:ALA:O	13:5:111:THR:OG1	2.29	0.44
13:6:243:SER:O	13:6:318:HIS:ND1	2.50	0.44
1:G:440:ARG:NH1	14:G:1129:CLA:O1D	2.50	0.44
18:G:5005:LHG:C6	17:Z:521:BCR:HC22	2.48	0.44
13:Z:229:TRP:HA	13:Z:232:LYS:HB2	1.98	0.44
13:b:282:VAL:HG23	13:b:283:THR:HG23	2.00	0.44
1:e:404:HIS:CE1	14:e:1126:CLA:ND	2.86	0.44
1:e:474:ARG:HD2	1:e:653:THR:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:1103:CLA:H3A	14:e:1103:CLA:HBA1	1.57	0.44
14:e:1104:CLA:H191	18:e:5001:LHG:H211	1.99	0.44
14:e:1022:CLA:H13	17:f:4017:BCR:H10C	2.00	0.44
2:f:91:ILE:HB	2:f:112:PRO:HB2	2.00	0.44
2:f:352:MET:HE2	2:f:352:MET:HB3	1.79	0.44
14:f:1021:CLA:H62	14:f:1021:CLA:H102	1.82	0.44
17:f:4006:BCR:H371	17:f:4006:BCR:H24C	1.79	0.44
4:h:127:ASN:O	4:h:130:THR:OG1	2.34	0.44
13:s:26:LEU:HB3	14:s:511:CLA:HMA1	2.00	0.44
17:s:521:BCR:H351	17:s:521:BCR:H15C	1.77	0.44
13:v:246:LEU:HD23	13:v:246:LEU:HA	1.87	0.44
1:A:404:HIS:CE1	14:A:1126:CLA:ND	2.86	0.44
1:A:440:ARG:HD2	14:A:1129:CLA:HED3	1.99	0.44
14:A:1108:CLA:HBA2	14:A:1108:CLA:H3A	1.75	0.44
14:A:1022:CLA:H13	17:B:4017:BCR:H10C	2.00	0.44
2:B:380:THR:HG22	2:B:583:ALA:HB1	2.00	0.44
6:F:125:VAL:HG12	13:3:13:TRP:CH2	2.53	0.44
17:1:521:BCR:H15C	17:1:521:BCR:H351	1.82	0.44
13:3:73:LEU:HD11	14:3:503:CLA:HAA2	1.99	0.44
13:4:101:ALA:HB1	14:5:505:CLA:HAB	1.98	0.44
13:5:51:SER:HB2	13:6:279:LYS:HG3	2.00	0.44
13:5:110:HIS:NE2	14:5:513:CLA:NB	2.65	0.44
13:5:309:PHE:HD2	17:5:521:BCR:H10C	1.83	0.44
13:6:31:HIS:NE2	14:6:509:CLA:ND	2.65	0.44
13:6:101:ALA:HB1	14:Y:505:CLA:HAB	1.99	0.44
1:G:364:LEU:HD11	14:G:1128:CLA:HBB1	2.00	0.44
2:H:310:PRO:HA	2:H:311:PRO:HD3	1.88	0.44
2:H:355:MET:HE3	2:H:355:MET:HB2	1.74	0.44
2:H:380:THR:HG22	2:H:583:ALA:HB1	2.00	0.44
14:H:1221:CLA:H151	14:H:1221:CLA:H112	1.81	0.44
3:N:13:GLY:O	3:N:38:GLN:NE2	2.47	0.44
14:Z:519:CLA:H2A	14:Z:519:CLA:HED2	1.99	0.44
13:c:112:PHE:HB2	13:d:326:MET:HE3	1.99	0.44
17:d:521:BCR:H15C	17:d:521:BCR:H351	1.84	0.44
14:e:1108:CLA:H3A	14:e:1108:CLA:HBA2	1.75	0.44
14:e:1120:CLA:HED2	9:m:38:LYS:HD2	1.98	0.44
17:e:4001:BCR:H19C	9:m:69:ILE:HD11	2.00	0.44
14:f:1217:CLA:HBA2	14:f:1217:CLA:H3A	1.49	0.44
18:f:1855:LHG:H261	18:f:1855:LHG:H131	2.00	0.44
6:j:125:VAL:HG12	13:s:13:TRP:CH2	2.53	0.44
14:A:1126:CLA:H3A	14:A:1126:CLA:HBA2	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ASN:OD1	2:B:252:THR:OG1	2.36	0.44
2:B:415:LYS:HD2	2:B:539:LEU:HB3	2.00	0.44
3:C:13:GLY:O	3:C:38:GLN:NE2	2.46	0.44
13:3:274:ALA:HB3	13:3:290:VAL:HG22	2.00	0.44
13:4:110:HIS:NE2	14:4:513:CLA:NB	2.66	0.44
14:6:517:CLA:HBA1	14:6:517:CLA:H3A	1.55	0.44
1:G:440:ARG:HD2	14:G:1129:CLA:HED3	1.99	0.44
2:H:690:ILE:HG13	10:V:36:ILE:HG12	1.99	0.44
6:R:71:VAL:HG12	6:R:81:PHE:HB2	1.98	0.44
10:V:163:TRP:HH2	17:V:4219:BCR:H311	1.83	0.44
14:V:1501:CLA:H11	14:V:1501:CLA:H52	1.84	0.44
13:Y:307:HIS:NE2	14:Y:502:CLA:ND	2.66	0.44
13:a:182:LEU:O	13:a:209:TYR:OH	2.35	0.44
14:d:513:CLA:HBB1	17:d:523:BCR:H371	2.00	0.44
14:e:1110:CLA:H3A	14:e:1110:CLA:HBA2	1.63	0.44
2:f:713:PHE:O	2:f:717:TYR:HB2	2.18	0.44
6:j:75:LEU:HA	6:j:78:ALA:HB2	1.98	0.44
14:q:512:CLA:H3A	14:q:512:CLA:HBA1	1.68	0.44
14:q:516:CLA:HBA1	14:q:516:CLA:H3A	1.45	0.44
13:t:282:VAL:HG23	13:t:283:THR:HG23	2.00	0.44
13:u:309:PHE:HD2	17:u:521:BCR:H10C	1.83	0.44
13:v:31:HIS:NE2	14:v:509:CLA:ND	2.65	0.44
1:A:591:ARG:HH21	1:A:594:THR:HG21	1.81	0.44
14:A:1013:CLA:H93	14:A:1013:CLA:H61	1.83	0.44
14:A:1124:CLA:H12	14:A:1135:CLA:HMA3	2.00	0.44
14:A:1128:CLA:H91	14:A:1128:CLA:H112	1.82	0.44
2:B:410:ARG:O	2:B:414:HIS:ND1	2.44	0.44
2:B:690:ILE:HG13	10:L:36:ILE:HG12	1.99	0.44
3:C:26:LEU:HA	3:C:41:ALA:O	2.17	0.44
1:G:404:HIS:CE1	14:G:1126:CLA:ND	2.86	0.44
14:G:1022:CLA:H13	17:H:4017:BCR:H10C	2.00	0.44
17:G:4001:BCR:H23C	9:U:66:PHE:HB2	1.99	0.44
14:H:1215:CLA:HBA2	14:H:1215:CLA:H3A	1.63	0.44
2:f:194:LEU:HA	2:f:198:ALA:HB3	2.00	0.44
10:n:163:TRP:HH2	17:n:4219:BCR:H311	1.83	0.44
14:s:512:CLA:H3A	14:s:512:CLA:HBA1	1.63	0.44
13:t:57:GLN:HB3	13:t:61:GLU:HB2	2.00	0.44
13:u:309:PHE:CD2	17:u:521:BCR:H10C	2.53	0.44
1:A:31:PRO:HB3	14:A:1101:CLA:HAC1	2.00	0.44
1:A:370:ILE:HG21	14:A:1123:CLA:HMA3	2.00	0.44
1:A:474:ARG:HD2	1:A:653:THR:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1013:CLA:H143	14:A:1013:CLA:H161	1.85	0.44
2:B:196:HIS:NE2	14:B:1212:CLA:ND	2.66	0.44
14:B:1206:CLA:H3A	14:B:1207:CLA:CBB	2.48	0.44
3:C:6:LYS:HG3	4:D:139:TYR:HB2	1.99	0.44
6:F:84:PRO:HB3	17:J:4015:BCR:H362	1.98	0.44
13:1:190:TYR:HD2	17:1:524:BCR:H401	1.83	0.44
17:2:521:BCR:H24C	17:2:521:BCR:H371	1.77	0.44
14:3:505:CLA:H62	14:3:505:CLA:H41	1.75	0.44
13:4:282:VAL:HG23	13:4:283:THR:HG23	2.00	0.44
14:5:513:CLA:HBB1	17:5:523:BCR:H24C	1.99	0.44
14:6:513:CLA:HBB1	17:6:523:BCR:H371	2.00	0.44
1:G:115:GLN:NE2	14:G:1107:CLA:OBD	2.43	0.44
1:G:312:ILE:HD13	1:G:312:ILE:HA	1.85	0.44
14:G:1116:CLA:H93	14:G:1116:CLA:H61	1.89	0.44
2:H:478:LEU:HD21	14:H:1231:CLA:HED2	2.00	0.44
2:H:713:PHE:O	2:H:717:TYR:HB2	2.18	0.44
18:H:1855:LHG:H261	18:H:1855:LHG:H131	2.00	0.44
13:b:137:GLN:HE22	14:b:516:CLA:HED1	1.83	0.44
1:e:364:LEU:HD11	14:e:1128:CLA:HBB1	2.00	0.44
14:e:1121:CLA:HAB	14:e:1801:CLA:CAB	2.47	0.44
18:e:5008:LHG:HC82	13:r:13:TRP:HZ2	1.82	0.44
2:f:196:HIS:NE2	14:f:1212:CLA:ND	2.66	0.44
14:f:1208:CLA:HMD3	21:f:1852:SQD:H101	1.99	0.44
18:f:1842:LHG:HC81	18:f:1842:LHG:H112	1.80	0.44
10:n:20:PRO:HB3	18:n:5218:LHG:HC82	1.99	0.44
14:n:1503:CLA:H93	14:n:1503:CLA:H61	1.88	0.44
13:s:73:LEU:HD11	14:s:503:CLA:HAA2	1.99	0.44
13:s:307:HIS:NE2	14:s:502:CLA:ND	2.65	0.44
17:t:524:BCR:H11C	17:t:524:BCR:H341	1.79	0.44
14:v:513:CLA:HBB1	17:v:523:BCR:H371	2.00	0.44
18:A:5005:LHG:HC41	17:2:521:BCR:HC31	2.00	0.43
14:B:1208:CLA:HMD3	21:B:1852:SQD:H101	1.99	0.43
13:4:137:GLN:HE22	14:4:516:CLA:HED1	1.83	0.43
1:G:202:ALA:HB2	1:G:320:GLY:HA3	2.00	0.43
14:G:1124:CLA:H2	14:G:1124:CLA:H61	1.76	0.43
14:H:1218:CLA:HMD2	17:H:4004:BCR:H23C	2.00	0.43
17:U:4104:BCR:H15C	17:U:4104:BCR:H351	1.90	0.43
13:Z:130:PHE:HA	13:Z:137:GLN:HG2	1.99	0.43
13:c:51:SER:HB2	13:d:279:LYS:HG3	2.00	0.43
13:c:59:MET:HB2	13:c:271:PHE:HA	2.00	0.43
13:d:143:GLY:HA3	13:d:222:ILE:HG13	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:202:ALA:HB2	1:e:320:GLY:HA3	2.00	0.43
14:e:1110:CLA:H2	14:e:1110:CLA:H62	1.83	0.43
2:f:478:LEU:HD21	14:f:1231:CLA:HED2	2.00	0.43
14:f:1206:CLA:H3A	14:f:1207:CLA:CBB	2.48	0.43
14:f:1215:CLA:H13	14:f:1221:CLA:H162	2.00	0.43
13:q:190:TYR:HD2	17:q:524:BCR:H401	1.83	0.43
17:q:521:BCR:H15C	17:q:521:BCR:H351	1.82	0.43
13:t:168:ASP:HB3	13:t:171:SER:HB2	2.00	0.43
13:u:146:LEU:HD22	13:u:214:LEU:HD22	2.00	0.43
13:v:107:ALA:O	13:v:111:THR:OG1	2.29	0.43
2:B:478:LEU:HD21	14:B:1231:CLA:HED2	2.00	0.43
10:L:39:ARG:O	10:n:98:ASN:ND2	2.50	0.43
13:3:182:LEU:O	13:3:209:TYR:OH	2.35	0.43
13:4:4:TYR:OH	13:4:328:PHE:O	2.31	0.43
13:5:146:LEU:HD22	13:5:214:LEU:HD22	2.00	0.43
13:6:148:PHE:CD2	14:6:512:CLA:H3A	2.51	0.43
1:G:148:ARG:HD3	1:G:389:PRO:HB2	1.99	0.43
14:G:1104:CLA:H62	14:G:1104:CLA:H41	1.61	0.43
2:H:455:ILE:HD13	6:R:69:LEU:HB2	2.00	0.43
2:H:576:PHE:HE1	14:H:1226:CLA:HAC2	1.82	0.43
14:H:1206:CLA:H3A	14:H:1207:CLA:CBB	2.48	0.43
10:V:30:PHE:CD1	21:V:5216:SQD:H122	2.53	0.43
17:V:4219:BCR:H15C	17:V:4219:BCR:H351	1.75	0.43
14:Z:501:CLA:H41	14:Z:501:CLA:H62	1.70	0.43
13:a:307:HIS:NE2	14:a:502:CLA:ND	2.65	0.43
13:b:4:TYR:OH	13:b:328:PHE:O	2.31	0.43
13:c:309:PHE:CD2	17:c:521:BCR:H10C	2.53	0.43
13:d:190:TYR:HE2	13:d:202:ASP:HB3	1.83	0.43
14:e:1106:CLA:H61	14:e:1106:CLA:H92	1.78	0.43
2:f:236:ASN:OD1	2:f:236:ASN:N	2.51	0.43
17:f:4009:BCR:H351	17:f:4009:BCR:H15C	1.83	0.43
10:n:18:ALA:HB2	10:n:110:VAL:HG21	2.00	0.43
1:A:202:ALA:HB2	1:A:320:GLY:HA3	2.00	0.43
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.84	0.43
14:A:1134:CLA:H61	14:A:1134:CLA:H41	1.87	0.43
2:B:91:ILE:HB	2:B:112:PRO:HB2	2.00	0.43
14:B:1218:CLA:H61	14:B:1218:CLA:H2	1.75	0.43
17:K:4104:BCR:H15C	17:K:4104:BCR:H351	1.90	0.43
13:2:110:HIS:HA	13:2:114:ALA:HB3	2.00	0.43
17:2:524:BCR:H15C	17:2:524:BCR:H351	1.78	0.43
13:3:62:GLN:HB2	13:3:64:LEU:HG	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:261:ALA:HA	13:3:276:LEU:HD12	2.00	0.43
13:5:309:PHE:CD2	17:5:521:BCR:H10C	2.53	0.43
13:6:323:LEU:HA	13:6:326:MET:HE2	1.99	0.43
1:G:31:PRO:HB3	14:G:1101:CLA:HAC1	2.00	0.43
2:H:196:HIS:NE2	14:H:1212:CLA:ND	2.66	0.43
14:H:1226:CLA:H91	20:H:5002:LMG:H372	2.00	0.43
9:U:46:LEU:H	9:U:56:GLY:HA2	1.84	0.43
13:a:148:PHE:CD2	14:a:512:CLA:H3A	2.53	0.43
13:d:31:HIS:NE2	14:d:509:CLA:ND	2.65	0.43
1:e:148:ARG:HD3	1:e:389:PRO:HB2	1.99	0.43
2:f:481:ALA:HA	2:f:486:THR:HG21	2.00	0.43
2:f:585:ASN:HB2	14:f:1012:CLA:HBC2	2.00	0.43
14:f:1023:CLA:H142	17:k:4018:BCR:H271	1.99	0.43
14:f:1201:CLA:H91	14:f:1201:CLA:H112	1.77	0.43
14:f:1218:CLA:HMD2	17:f:4004:BCR:H23C	2.00	0.43
13:q:307:HIS:NE2	14:q:502:CLA:ND	2.66	0.43
13:r:229:TRP:HA	13:r:232:LYS:HB2	1.98	0.43
14:r:505:CLA:HBC2	17:r:524:BCR:H341	2.00	0.43
13:s:62:GLN:HB2	13:s:64:LEU:HG	2.01	0.43
13:t:110:HIS:NE2	14:t:513:CLA:NB	2.66	0.43
13:t:137:GLN:HE22	14:t:516:CLA:HED1	1.83	0.43
1:A:364:LEU:HD11	14:A:1128:CLA:HBB1	2.00	0.43
1:A:588:GLY:HA2	2:B:562:PRO:HD3	1.99	0.43
14:A:1121:CLA:HHB	14:A:1801:CLA:HBC3	2.01	0.43
2:B:713:PHE:O	2:B:717:TYR:HB2	2.18	0.43
14:B:1240:CLA:H62	14:B:1240:CLA:H41	1.87	0.43
17:B:4005:BCR:H15C	17:B:4005:BCR:H351	1.84	0.43
10:L:20:PRO:HB3	18:L:5218:LHG:HC82	1.99	0.43
17:L:4022:BCR:H11C	17:L:4022:BCR:H341	1.81	0.43
11:M:11:LEU:HD21	17:M:4021:BCR:H272	2.01	0.43
14:2:512:CLA:H3A	14:2:512:CLA:HBA1	1.54	0.43
1:G:482:MET:HE2	1:G:482:MET:HB3	1.85	0.43
2:H:481:ALA:HA	2:H:486:THR:HG21	2.00	0.43
13:Y:190:TYR:HD2	17:Y:524:BCR:H401	1.83	0.43
13:b:110:HIS:NE2	14:b:513:CLA:NB	2.66	0.43
13:b:307:HIS:NE2	14:b:502:CLA:NA	2.67	0.43
1:e:440:ARG:O	1:e:444:HIS:ND1	2.43	0.43
1:e:749:VAL:HG21	17:e:4011:BCR:HC8	2.01	0.43
2:f:410:ARG:NH2	14:f:1227:CLA:OBD	2.49	0.43
2:f:690:ILE:HG13	10:n:36:ILE:HG12	1.99	0.43
17:f:4009:BCR:H11C	17:f:4009:BCR:H341	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:o:11:LEU:HD21	17:o:4021:BCR:H272	2.01	0.43
13:r:110:HIS:HA	13:r:114:ALA:HB3	2.00	0.43
13:r:190:TYR:HE2	13:r:202:ASP:HB3	1.83	0.43
13:u:112:PHE:HB2	13:v:326:MET:HE3	1.99	0.43
17:v:522:BCR:H24C	17:v:522:BCR:H371	1.85	0.43
14:A:1133:CLA:H111	14:A:1133:CLA:H91	1.81	0.43
17:A:4001:BCR:H19C	9:K:69:ILE:HD11	2.00	0.43
14:B:1215:CLA:H13	14:B:1221:CLA:H162	2.00	0.43
14:B:1218:CLA:HMD2	17:B:4004:BCR:H23C	2.00	0.43
14:B:1221:CLA:H141	14:B:1221:CLA:H161	1.78	0.43
18:B:1842:LHG:H112	18:B:1842:LHG:HC81	1.80	0.43
8:J:40:PRO:HD2	17:J:4015:BCR:H382	2.01	0.43
14:H:1208:CLA:HAB	19:H:1843:LMU:H111	2.00	0.43
6:R:125:VAL:HG12	13:a:13:TRP:CH2	2.53	0.43
18:S:5001:LHG:H242	21:n:5216:SQD:H242	2.00	0.43
13:c:146:LEU:HD22	13:c:214:LEU:HD22	2.00	0.43
13:d:79:ASP:OD1	13:d:79:ASP:N	2.48	0.43
14:e:1128:CLA:H91	14:e:1128:CLA:H112	1.82	0.43
18:e:5005:LHG:HC41	17:r:521:BCR:HC31	2.01	0.43
2:f:299:HIS:HB3	2:f:304:ILE:HD11	2.01	0.43
14:f:1226:CLA:H91	20:f:5002:LMG:H372	2.00	0.43
13:q:177:VAL:HG13	13:q:201:GLU:HG2	2.01	0.43
13:s:148:PHE:CD2	14:s:512:CLA:H3A	2.53	0.43
13:u:59:MET:HB2	13:u:271:PHE:HA	2.00	0.43
14:A:1131:CLA:HBB2	10:L:65:LEU:HD13	2.00	0.43
2:B:410:ARG:NH2	14:B:1227:CLA:OBD	2.49	0.43
18:B:1855:LHG:H261	18:B:1855:LHG:H131	2.00	0.43
17:F:4016:BCR:H341	17:F:4016:BCR:H11C	1.75	0.43
14:L:1501:CLA:CMD	10:n:94:SER:HB2	2.47	0.43
13:1:148:PHE:CE1	14:1:516:CLA:HBC2	2.54	0.43
13:3:26:LEU:HB3	14:3:511:CLA:HMA1	2.00	0.43
17:6:522:BCR:H24C	17:6:522:BCR:H371	1.84	0.43
1:G:485:ASP:OD1	1:G:491:GLN:NE2	2.45	0.43
14:G:1137:CLA:H62	14:G:1137:CLA:H41	1.63	0.43
13:b:309:PHE:CD1	17:b:521:BCR:H12C	2.54	0.43
17:d:521:BCR:H371	17:d:521:BCR:H24C	1.84	0.43
14:e:1106:CLA:H91	14:e:1106:CLA:H112	1.85	0.43
14:e:1129:CLA:H11	14:e:1129:CLA:H51	1.84	0.43
2:f:236:ASN:OD1	2:f:252:THR:OG1	2.36	0.43
17:j:4016:BCR:H11C	17:j:4016:BCR:H341	1.75	0.43
13:q:190:TYR:HE2	13:q:202:ASP:HB3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:r:130:PHE:HA	13:r:137:GLN:HG2	1.99	0.43
17:s:522:BCR:H15C	17:s:522:BCR:H351	1.80	0.43
13:t:4:TYR:OH	13:t:328:PHE:O	2.31	0.43
17:t:524:BCR:H24C	17:t:524:BCR:H371	1.87	0.43
13:u:51:SER:HB2	13:v:279:LYS:HG3	2.00	0.43
1:A:317:ILE:O	1:A:321:HIS:ND1	2.46	0.43
12:P:82:LYS:HB3	12:P:117:VAL:HG21	2.01	0.43
14:1:513:CLA:HBB1	17:1:523:BCR:H402	2.01	0.43
13:3:59:MET:HE2	13:3:67:LEU:HB3	2.01	0.43
13:4:307:HIS:NE2	14:4:502:CLA:NA	2.67	0.43
13:6:190:TYR:HE2	13:6:202:ASP:HB3	1.83	0.43
1:G:370:ILE:HG21	14:G:1123:CLA:HMA3	2.00	0.43
1:G:745:LEU:HD22	14:G:1140:CLA:HMA1	2.00	0.43
18:G:5005:LHG:HC41	17:Z:521:BCR:HC31	2.00	0.43
2:H:236:ASN:OD1	2:H:236:ASN:N	2.51	0.43
17:V:4019:BCR:H15C	17:V:4019:BCR:H351	1.86	0.43
14:Y:505:CLA:HBC2	17:Y:524:BCR:H341	2.01	0.43
13:Z:190:TYR:HE2	13:Z:202:ASP:HB3	1.83	0.43
13:a:17:ASN:ND2	14:a:510:CLA:O1A	2.47	0.43
14:b:512:CLA:HAB	14:b:516:CLA:HMD2	2.01	0.43
2:f:7:LYS:HD2	11:o:28:TYR:CZ	2.54	0.43
2:f:455:ILE:HD13	6:j:69:LEU:HB2	2.00	0.43
17:l:4015:BCR:H15C	17:l:4015:BCR:H351	1.81	0.43
1:A:572:ARG:HD3	3:C:80:ALA:HB3	2.01	0.43
1:A:611:TYR:O	1:A:615:SER:OG	2.37	0.43
14:A:1104:CLA:H191	18:A:5001:LHG:H211	1.99	0.43
2:B:455:ILE:HD13	6:F:69:LEU:HB2	2.00	0.43
14:1:505:CLA:HBC2	17:1:524:BCR:H341	2.01	0.43
13:2:190:TYR:HE2	13:2:202:ASP:HB3	1.83	0.43
13:6:91:VAL:HG22	17:6:523:BCR:HC22	2.01	0.43
13:6:109:PHE:HB2	14:Y:505:CLA:HAA2	2.01	0.43
1:G:388:TYR:HB2	1:G:391:LEU:HB2	2.01	0.43
18:G:5005:LHG:O7	17:Z:521:BCR:HC22	2.19	0.43
2:H:585:ASN:HB2	14:H:1012:CLA:HBC2	2.00	0.43
17:R:4016:BCR:H341	17:R:4016:BCR:H11C	1.75	0.43
8:T:8:LEU:HA	8:T:13:ILE:HG21	2.01	0.43
14:Z:518:CLA:H61	14:Z:518:CLA:H41	1.70	0.43
13:a:261:ALA:HA	13:a:276:LEU:HD12	2.00	0.43
1:e:115:GLN:NE2	14:e:1107:CLA:OBD	2.43	0.43
1:e:485:ASP:OD1	1:e:491:GLN:NE2	2.44	0.43
14:e:1104:CLA:H201	18:e:5001:LHG:H221	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:1126:CLA:H143	14:e:1126:CLA:H112	1.81	0.43
14:e:1131:CLA:H111	15:f:2002:PQN:H201	2.01	0.43
17:q:522:BCR:H351	17:q:522:BCR:H15C	1.78	0.43
13:s:261:ALA:HA	13:s:276:LEU:HD12	2.00	0.43
13:u:50:ILE:HD11	13:u:89:LEU:HB2	2.00	0.43
1:A:752:TRP:HD1	14:A:1126:CLA:HMB2	1.84	0.43
17:I:4018:BCR:H20C	17:I:4018:BCR:H361	1.89	0.43
18:I:5001:LHG:H242	21:V:5216:SQD:H242	2.01	0.43
17:J:4015:BCR:H20C	17:J:4015:BCR:H361	1.88	0.43
13:1:190:TYR:HE2	13:1:202:ASP:HB3	1.83	0.43
1:G:371:LEU:HD12	1:G:371:LEU:HA	1.88	0.43
1:G:600:TRP:CD1	14:G:1128:CLA:HMD1	2.54	0.43
14:G:1121:CLA:HHB	14:G:1801:CLA:HBC3	2.01	0.43
14:G:1131:CLA:HBB2	10:V:65:LEU:HD13	2.00	0.43
14:G:1133:CLA:H192	14:G:1133:CLA:H162	1.88	0.43
2:H:299:HIS:HB3	2:H:304:ILE:HD11	2.01	0.43
14:Z:512:CLA:H3A	14:Z:512:CLA:HBA1	1.54	0.43
13:b:57:GLN:HB3	13:b:61:GLU:HB2	2.00	0.43
13:b:168:ASP:HB3	13:b:171:SER:HB2	2.00	0.43
1:e:31:PRO:HB3	14:e:1101:CLA:HAC1	2.00	0.43
1:e:370:ILE:HG21	14:e:1123:CLA:HMA3	2.00	0.43
14:e:1121:CLA:HHB	14:e:1801:CLA:HBC3	2.01	0.43
14:e:1124:CLA:H12	14:e:1135:CLA:HMA3	2.00	0.43
18:e:5005:LHG:O7	17:r:521:BCR:HC22	2.19	0.43
2:f:270:LEU:HD23	2:f:270:LEU:HA	1.89	0.43
17:f:4005:BCR:H15C	17:f:4005:BCR:H351	1.84	0.43
1:A:745:LEU:HD22	14:A:1140:CLA:HMA1	2.00	0.43
14:A:1102:CLA:HBA2	14:A:1102:CLA:H3A	1.81	0.43
14:A:1104:CLA:H161	14:A:1104:CLA:H193	1.79	0.43
18:A:5005:LHG:C6	17:2:521:BCR:HC22	2.48	0.43
14:B:1229:CLA:H2	14:B:1229:CLA:H62	1.81	0.43
4:D:101:ASP:OD1	4:D:101:ASP:N	2.47	0.43
17:J:4015:BCR:H11C	17:J:4015:BCR:H341	1.83	0.43
17:M:4021:BCR:H24C	17:M:4021:BCR:H371	1.83	0.43
13:1:177:VAL:HG13	13:1:201:GLU:HG2	2.01	0.43
13:4:160:ALA:HA	13:4:165:GLY:HA2	2.01	0.43
1:G:474:ARG:HD2	1:G:653:THR:HG21	2.00	0.43
1:G:572:ARG:HD3	3:N:80:ALA:HB3	2.00	0.43
1:G:734:GLN:HG3	18:G:5001:LHG:C7	2.49	0.43
1:G:752:TRP:HD1	14:G:1126:CLA:HMB2	1.84	0.43
14:G:1104:CLA:H201	18:G:5001:LHG:H221	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:1116:CLA:C4D	14:G:1125:CLA:HBB1	2.48	0.43
14:G:1123:CLA:H141	14:G:1123:CLA:H161	1.82	0.43
14:G:1128:CLA:H91	14:G:1128:CLA:H112	1.82	0.43
14:G:1133:CLA:H91	14:G:1133:CLA:H111	1.81	0.43
2:H:270:LEU:HD23	2:H:270:LEU:HA	1.89	0.43
2:H:415:LYS:HD2	2:H:539:LEU:HB3	2.00	0.43
14:H:1221:CLA:H112	14:H:1221:CLA:H72	1.73	0.43
10:V:18:ALA:HB2	10:V:110:VAL:HG21	2.00	0.43
13:a:59:MET:HE2	13:a:67:LEU:HB3	2.01	0.43
13:a:62:GLN:HB2	13:a:64:LEU:HG	2.01	0.43
13:c:148:PHE:CD2	14:c:512:CLA:H3A	2.53	0.43
2:f:380:THR:HG22	2:f:583:ALA:HB1	2.00	0.43
14:f:1208:CLA:HAB	19:f:1843:LMU:H111	2.00	0.43
14:n:1503:CLA:H111	14:n:1503:CLA:H91	1.84	0.43
17:n:4022:BCR:H15C	17:n:4022:BCR:H351	1.90	0.43
12:p:63:GLN:O	12:p:67:GLU:N	2.50	0.43
17:t:521:BCR:H24C	17:t:521:BCR:H371	1.87	0.43
17:u:524:BCR:H11C	17:u:524:BCR:H341	1.87	0.43
1:A:600:TRP:CD1	14:A:1128:CLA:HMD1	2.54	0.42
14:A:1137:CLA:HMC2	14:A:1130:CLA:HBC2	2.01	0.42
2:B:194:LEU:HA	2:B:198:ALA:HB3	2.00	0.42
2:B:236:ASN:OD1	2:B:236:ASN:N	2.51	0.42
17:B:4009:BCR:H15C	17:B:4009:BCR:H351	1.83	0.42
13:4:57:GLN:HB3	13:4:61:GLU:HB2	2.00	0.42
1:G:336:ILE:O	1:G:340:HIS:ND1	2.38	0.42
14:G:1137:CLA:HMC2	14:G:1130:CLA:HBC2	2.01	0.42
17:G:4002:BCR:H11C	17:G:4002:BCR:H341	1.83	0.42
2:H:7:LYS:HD2	11:W:28:TYR:CZ	2.54	0.42
13:a:26:LEU:HB3	14:a:511:CLA:HMA1	2.00	0.42
13:b:160:ALA:HA	13:b:165:GLY:HA2	2.01	0.42
13:c:309:PHE:HD2	17:c:521:BCR:H10C	1.83	0.42
2:f:410:ARG:O	2:f:414:HIS:ND1	2.44	0.42
14:f:1229:CLA:H62	14:f:1229:CLA:H2	1.81	0.42
14:q:513:CLA:HBB1	17:q:523:BCR:H402	2.01	0.42
13:s:263:ASN:HD21	13:s:266:ALA:H	1.67	0.42
13:t:307:HIS:NE2	14:t:502:CLA:NA	2.67	0.42
13:t:309:PHE:CD1	17:t:521:BCR:H12C	2.54	0.42
1:A:94:GLY:O	1:A:98:SER:OG	2.33	0.42
1:A:388:TYR:HB2	1:A:391:LEU:HB2	2.01	0.42
14:A:1116:CLA:C4D	14:A:1125:CLA:HBB1	2.48	0.42
17:A:4008:BCR:H11C	17:A:4008:BCR:H341	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:1220:CLA:HED3	14:B:1220:CLA:H2A	2.01	0.42
10:L:18:ALA:HB2	10:L:110:VAL:HG21	2.00	0.42
13:1:207:HIS:CE1	17:1:524:BCR:H381	2.54	0.42
14:2:502:CLA:HBD	14:2:503:CLA:H43	2.01	0.42
14:2:518:CLA:H61	14:2:518:CLA:H41	1.70	0.42
13:4:17:ASN:OD1	14:4:511:CLA:NC	2.52	0.42
14:G:1131:CLA:H111	15:H:2002:PQN:H201	2.01	0.42
2:H:428:PHE:CZ	17:T:4015:BCR:HC41	2.55	0.42
8:T:40:PRO:HD2	17:T:4015:BCR:H382	2.01	0.42
13:Y:177:VAL:HG13	13:Y:201:GLU:HG2	2.01	0.42
14:Y:513:CLA:HBB1	17:Y:523:BCR:H402	2.01	0.42
13:a:267:TYR:OH	14:a:502:CLA:O1D	2.36	0.42
13:a:274:ALA:HB3	13:a:290:VAL:HG22	2.00	0.42
13:c:50:ILE:HD11	13:c:89:LEU:HB2	2.00	0.42
17:d:523:BCR:H15C	17:d:523:BCR:H351	1.83	0.42
17:j:4016:BCR:H12C	17:j:4016:BCR:H15C	1.81	0.42
8:l:8:LEU:HA	8:l:13:ILE:HG21	2.01	0.42
8:l:40:PRO:HD2	17:l:4015:BCR:H382	2.01	0.42
13:r:138:LEU:HA	13:r:141:ILE:HD12	2.01	0.42
13:s:59:MET:HE2	13:s:67:LEU:HB3	2.01	0.42
17:A:4002:BCR:H24C	17:A:4002:BCR:H371	1.85	0.42
2:B:450:GLU:OE2	6:F:52:ARG:NE	2.43	0.42
2:B:585:ASN:HB2	14:B:1012:CLA:HBC2	2.00	0.42
14:B:1239:CLA:H112	14:B:1239:CLA:H91	1.81	0.42
14:B:1207:CLA:H91	14:B:1207:CLA:H112	1.87	0.42
9:K:46:LEU:H	9:K:56:GLY:HA2	1.84	0.42
17:K:4104:BCR:H11C	17:K:4104:BCR:H341	1.94	0.42
13:5:50:ILE:HD11	13:5:89:LEU:HB2	2.00	0.42
14:5:509:CLA:HBA1	14:5:509:CLA:H3A	1.81	0.42
14:G:1106:CLA:H91	14:G:1106:CLA:H112	1.85	0.42
14:G:1124:CLA:H12	14:G:1135:CLA:HMA3	2.00	0.42
17:G:4001:BCR:H19C	9:U:69:ILE:HD11	2.00	0.42
2:H:236:ASN:OD1	2:H:252:THR:OG1	2.36	0.42
2:H:527:LEU:HD12	14:H:1236:CLA:HED3	2.02	0.42
14:H:1220:CLA:HED3	14:H:1220:CLA:H2A	2.01	0.42
12:X:82:LYS:HB3	12:X:117:VAL:HG21	2.01	0.42
14:Z:502:CLA:HBD	14:Z:503:CLA:H43	2.01	0.42
13:b:302:TRP:HB3	14:b:504:CLA:HMB1	2.02	0.42
1:e:336:ILE:O	1:e:340:HIS:ND1	2.38	0.42
14:e:1116:CLA:C4D	14:e:1125:CLA:HBB1	2.48	0.42
14:e:1125:CLA:H161	14:e:1125:CLA:H122	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:1137:CLA:HMC2	14:e:1130:CLA:HBC2	2.01	0.42
15:e:2001:PQN:H142	15:e:2001:PQN:H112	1.82	0.42
18:e:5005:LHG:C6	17:r:521:BCR:HC22	2.48	0.42
2:f:167:TRP:CZ2	14:f:1208:CLA:HHB	2.54	0.42
2:f:276:HIS:HE2	14:f:1215:CLA:C2B	2.32	0.42
2:f:527:LEU:HD12	14:f:1236:CLA:HED3	2.02	0.42
14:f:1206:CLA:H3A	14:f:1206:CLA:HBA1	1.63	0.42
17:l:4015:BCR:H11C	17:l:4015:BCR:H341	1.83	0.42
13:q:79:ASP:OD1	13:q:79:ASP:N	2.52	0.42
13:q:148:PHE:CE1	14:q:516:CLA:HBC2	2.54	0.42
17:r:521:BCR:H15C	17:r:521:BCR:H351	1.83	0.42
17:u:524:BCR:H15C	17:u:524:BCR:H351	1.79	0.42
17:v:521:BCR:H371	17:v:521:BCR:H24C	1.84	0.42
14:A:1131:CLA:H111	15:B:2002:PQN:H201	2.01	0.42
17:3:524:BCR:H15C	17:3:524:BCR:H351	1.79	0.42
13:4:168:ASP:HB3	13:4:171:SER:HB2	2.00	0.42
1:G:749:VAL:HG21	17:G:4011:BCR:HC8	2.01	0.42
14:H:1229:CLA:H2	14:H:1229:CLA:H62	1.81	0.42
13:Y:148:PHE:CE1	14:Y:516:CLA:HBC2	2.54	0.42
14:e:1237:CLA:H13	10:n:89:LEU:HD21	2.02	0.42
2:f:126:THR:HG22	2:f:270:LEU:HD21	2.02	0.42
17:A:4002:BCR:H11C	17:A:4002:BCR:H341	1.83	0.42
2:B:276:HIS:HE2	14:B:1215:CLA:C2B	2.32	0.42
2:B:657:TRP:CZ3	14:B:1021:CLA:HHB	2.55	0.42
14:B:1012:CLA:H122	14:B:1012:CLA:H8	1.86	0.42
14:B:1209:CLA:H3A	14:B:1209:CLA:HBA2	1.47	0.42
14:B:1234:CLA:H143	14:B:1234:CLA:H111	1.81	0.42
17:1:523:BCR:H15C	17:1:523:BCR:H351	1.86	0.42
13:4:309:PHE:CD1	17:4:521:BCR:H12C	2.54	0.42
14:4:512:CLA:HAB	14:4:516:CLA:HMD2	2.01	0.42
1:G:407:TRP:HB3	14:G:1126:CLA:HMC3	2.02	0.42
14:G:1237:CLA:H202	17:V:4019:BCR:H391	2.02	0.42
2:H:167:TRP:CZ2	14:H:1208:CLA:HHB	2.54	0.42
14:H:1021:CLA:H62	14:H:1021:CLA:H102	1.83	0.42
17:H:4004:BCR:H361	17:H:4004:BCR:H20C	1.79	0.42
7:S:13:ILE:HG23	17:n:4219:BCR:H402	2.02	0.42
13:Y:148:PHE:HD2	14:Y:512:CLA:H3A	1.85	0.42
17:Z:524:BCR:H15C	17:Z:524:BCR:H351	1.78	0.42
17:a:524:BCR:H15C	17:a:524:BCR:H351	1.79	0.42
1:e:141:SER:HB3	14:e:1126:CLA:HAA2	2.02	0.42
1:e:544:PHE:CZ	17:n:4219:BCR:H332	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:1123:CLA:H141	14:e:1123:CLA:H161	1.82	0.42
14:e:1138:CLA:H202	14:e:1138:CLA:H162	1.84	0.42
2:f:111:SER:HB3	7:k:3:GLY:HA2	2.01	0.42
14:f:1201:CLA:H143	14:f:1201:CLA:H111	1.90	0.42
15:f:2002:PQN:H222	15:f:2002:PQN:H261	1.78	0.42
9:m:78:LEU:HD22	9:m:83:ASN:HB2	2.01	0.42
13:q:148:PHE:HD2	14:q:512:CLA:H3A	1.85	0.42
17:r:522:BCR:H351	17:r:522:BCR:H15C	1.77	0.42
13:s:274:ALA:HB3	13:s:290:VAL:HG22	2.00	0.42
1:A:544:PHE:CZ	17:L:4219:BCR:H332	2.55	0.42
1:A:734:GLN:HG3	18:A:5001:LHG:C7	2.49	0.42
18:A:5005:LHG:O7	17:2:521:BCR:HC22	2.19	0.42
2:B:7:LYS:HD2	11:M:28:TYR:CZ	2.54	0.42
2:B:299:HIS:HB3	2:B:304:ILE:HD11	2.01	0.42
2:B:428:PHE:CZ	17:J:4015:BCR:HC41	2.54	0.42
17:4:521:BCR:H11C	17:4:521:BCR:H341	1.88	0.42
1:G:459:LEU:O	1:G:463:SER:OG	2.28	0.42
14:G:1136:CLA:H92	14:G:1136:CLA:H62	1.81	0.42
14:G:1101:CLA:H51	8:T:19:PHE:HE2	1.85	0.42
17:H:4004:BCR:H11C	17:H:4004:BCR:H341	1.83	0.42
9:U:78:LEU:HD22	9:U:83:ASN:HB2	2.01	0.42
17:e:4008:BCR:H11C	17:e:4008:BCR:H341	1.90	0.42
14:f:1221:CLA:H161	14:f:1221:CLA:H141	1.78	0.42
17:k:4018:BCR:H24C	17:k:4018:BCR:H371	1.83	0.42
13:s:79:ASP:OD1	13:s:79:ASP:N	2.53	0.42
14:t:512:CLA:HAB	14:t:516:CLA:HMD2	2.01	0.42
13:v:91:VAL:HG22	17:v:523:BCR:HC22	2.01	0.42
1:A:691:TRP:CE2	14:A:1011:CLA:HBA2	2.54	0.42
14:A:1237:CLA:H202	17:L:4019:BCR:H391	2.02	0.42
18:A:5008:LHG:C8	13:2:13:TRP:CZ2	3.03	0.42
2:B:218:HIS:HD2	2:B:220:ALA:H	1.67	0.42
14:B:1221:CLA:H112	14:B:1221:CLA:H72	1.72	0.42
14:B:1229:CLA:H112	14:B:1229:CLA:H152	1.81	0.42
14:B:1207:CLA:HMA2	18:V:5221:LHG:H112	2.01	0.42
21:L:5216:SQD:H242	18:k:5001:LHG:H242	2.02	0.42
13:1:148:PHE:HD2	14:1:512:CLA:H3A	1.85	0.42
17:3:522:BCR:H24C	17:3:522:BCR:H371	1.87	0.42
13:6:59:MET:HA	13:6:62:GLN:HB2	2.02	0.42
14:6:505:CLA:H111	14:6:517:CLA:HBB2	2.02	0.42
14:G:1013:CLA:H141	14:H:1012:CLA:H151	2.02	0.42
14:G:1108:CLA:HBA2	14:G:1108:CLA:H3A	1.75	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:1237:CLA:H13	10:V:89:LEU:HD21	2.02	0.42
2:H:111:SER:HB3	7:S:3:GLY:HA2	2.01	0.42
2:H:657:TRP:CZ3	14:H:1021:CLA:HHB	2.55	0.42
14:H:1221:CLA:H141	14:H:1221:CLA:H161	1.78	0.42
13:Y:207:HIS:CE1	17:Y:524:BCR:H381	2.54	0.42
13:Z:138:LEU:HA	13:Z:141:ILE:HD12	2.01	0.42
13:c:221:HIS:HE1	14:c:506:CLA:NA	2.18	0.42
1:e:734:GLN:HG3	18:e:5001:LHG:C7	2.49	0.42
14:e:1106:CLA:HBA2	14:e:1106:CLA:H3A	1.64	0.42
14:e:1122:CLA:H91	14:e:1122:CLA:H111	1.89	0.42
14:f:1220:CLA:H2A	14:f:1220:CLA:HED3	2.01	0.42
17:f:4017:BCR:H20C	17:f:4017:BCR:H361	1.89	0.42
13:v:190:TYR:HE2	13:v:202:ASP:HB3	1.83	0.42
14:v:505:CLA:H111	14:v:517:CLA:HBB2	2.02	0.42
1:A:430:PRO:HG2	4:D:41:GLU:HB2	2.02	0.42
2:B:352:MET:HE2	2:B:352:MET:HB3	1.79	0.42
2:B:460:ALA:HB1	14:B:1234:CLA:HBD	2.02	0.42
2:B:481:ALA:HA	2:B:486:THR:HG21	2.00	0.42
5:E:10:ARG:HD3	5:E:21:GLU:O	2.20	0.42
1:G:382:MET:HE2	1:G:382:MET:HB3	1.93	0.42
15:G:2001:PQN:H142	15:G:2001:PQN:H112	1.82	0.42
18:G:5001:LHG:H341	18:G:5001:LHG:H372	1.84	0.42
4:O:127:ASN:O	4:O:130:THR:OG1	2.34	0.42
17:V:4022:BCR:H341	17:V:4022:BCR:H11C	1.82	0.42
1:e:407:TRP:HB3	14:e:1126:CLA:HMC3	2.02	0.42
1:e:572:ARG:HD3	3:g:80:ALA:HB3	2.01	0.42
14:e:1115:CLA:H41	14:e:1115:CLA:H62	1.65	0.42
14:e:1139:CLA:H143	14:e:1139:CLA:H111	1.74	0.42
9:m:46:LEU:H	9:m:56:GLY:HA2	1.84	0.42
13:q:207:HIS:CE1	17:q:524:BCR:H381	2.54	0.42
14:q:505:CLA:HBC2	17:q:524:BCR:H341	2.01	0.42
13:t:17:ASN:OD1	14:t:511:CLA:NC	2.52	0.42
17:u:523:BCR:H15C	17:u:523:BCR:H351	1.82	0.42
1:A:407:TRP:HB3	14:A:1126:CLA:HMC3	2.02	0.42
2:B:167:TRP:CZ2	14:B:1208:CLA:HHB	2.54	0.42
14:B:1206:CLA:H3A	14:B:1206:CLA:HBA1	1.63	0.42
14:B:1208:CLA:HAB	19:B:1843:LMU:H111	2.00	0.42
14:B:1224:CLA:HBA2	14:B:1224:CLA:H3A	1.67	0.42
18:L:5220:LHG:H151	18:L:5220:LHG:H292	2.02	0.42
13:5:221:HIS:HE1	14:5:506:CLA:NA	2.18	0.42
1:G:544:PHE:CZ	17:V:4219:BCR:H332	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:LEU:HA	2:H:198:ALA:HB3	2.00	0.42
17:H:4006:BCR:H24C	17:H:4006:BCR:H371	1.79	0.42
17:a:521:BCR:H15C	17:a:521:BCR:H351	1.77	0.42
1:e:554:ILE:HD11	14:e:1135:CLA:HBB1	2.02	0.42
2:f:415:LYS:HD2	2:f:539:LEU:HB3	2.00	0.42
14:f:1239:CLA:H91	14:f:1239:CLA:H112	1.81	0.42
17:l:4013:BCR:H15C	17:l:4013:BCR:H351	1.87	0.42
18:n:5220:LHG:H151	18:n:5220:LHG:H292	2.02	0.42
12:p:82:LYS:HB3	12:p:117:VAL:HG21	2.01	0.42
13:s:182:LEU:O	13:s:209:TYR:OH	2.35	0.42
13:v:59:MET:HA	13:v:62:GLN:HB2	2.02	0.42
14:A:1104:CLA:H201	18:A:5001:LHG:H221	2.01	0.42
14:A:1128:CLA:H142	14:A:1128:CLA:H111	1.83	0.42
17:A:4001:BCR:H11C	17:A:4001:BCR:H341	1.88	0.42
17:A:4008:BCR:H20C	17:A:4008:BCR:H361	1.83	0.42
2:B:192:GLY:O	2:B:196:HIS:HB2	2.20	0.42
2:B:262:HIS:HD1	2:B:264:GLN:H	1.67	0.42
2:B:422:LEU:O	2:B:426:SER:OG	2.34	0.42
14:B:1208:CLA:H61	14:B:1208:CLA:H2	1.84	0.42
10:L:57:LEU:HD13	14:L:1502:CLA:HMB2	2.02	0.42
12:P:63:GLN:O	12:P:67:GLU:N	2.50	0.42
13:2:301:ALA:O	13:2:305:ASN:ND2	2.42	0.42
13:3:54:THR:H	13:3:62:GLN:HE22	1.68	0.42
13:4:65:ILE:HB	13:4:303:LEU:HD21	2.02	0.42
14:G:1011:CLA:H62	14:G:1011:CLA:H102	1.82	0.42
14:G:1119:CLA:H111	14:G:1119:CLA:H152	1.81	0.42
17:G:4007:BCR:H11C	17:G:4007:BCR:H341	1.90	0.42
18:G:5008:LHG:C8	13:Z:13:TRP:CZ2	3.03	0.42
2:H:59:LEU:HD23	2:H:59:LEU:HA	1.92	0.42
2:H:276:HIS:HE2	14:H:1215:CLA:C2B	2.32	0.42
14:e:1112:CLA:HBC3	18:e:5006:LHG:H352	2.02	0.42
17:f:4010:BCR:H20C	17:f:4010:BCR:H361	1.86	0.42
17:n:4019:BCR:H20C	17:n:4019:BCR:H361	1.92	0.42
12:p:36:ILE:HD12	12:p:36:ILE:HA	1.96	0.42
17:q:522:BCR:H371	17:q:522:BCR:H24C	1.86	0.42
13:s:54:THR:H	13:s:62:GLN:HE22	1.68	0.42
13:t:160:ALA:HA	13:t:165:GLY:HA2	2.01	0.42
17:t:522:BCR:H20C	17:t:522:BCR:H361	1.95	0.42
18:A:5006:LHG:H241	13:1:52:TRP:CH2	2.55	0.41
17:B:4006:BCR:H15C	17:B:4006:BCR:H351	1.81	0.41
3:C:61:ASP:HA	3:C:62:PHE:HA	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:4016:BCR:H24C	17:F:4016:BCR:H371	1.83	0.41
8:J:8:LEU:HA	8:J:13:ILE:HG21	2.01	0.41
9:K:68:HIS:O	9:K:72:ILE:HG12	2.20	0.41
17:6:523:BCR:H11C	17:6:523:BCR:H341	1.91	0.41
1:G:430:PRO:HG2	4:O:41:GLU:HB2	2.02	0.41
1:G:691:TRP:CE2	14:G:1011:CLA:HBA2	2.54	0.41
14:G:1112:CLA:HBC3	18:G:5006:LHG:H352	2.02	0.41
3:N:61:ASP:HA	3:N:62:PHE:HA	1.81	0.41
20:T:5104:LMG:H292	20:T:5104:LMG:H321	1.89	0.41
17:U:4104:BCR:H11C	17:U:4104:BCR:H341	1.94	0.41
10:V:57:LEU:HD13	14:V:1502:CLA:HMB2	2.02	0.41
12:X:59:VAL:O	12:X:59:VAL:HG12	2.20	0.41
13:Y:79:ASP:OD1	13:Y:79:ASP:N	2.52	0.41
17:Y:521:BCR:H371	17:Y:521:BCR:H24C	1.78	0.41
13:b:17:ASN:OD1	14:b:511:CLA:NC	2.52	0.41
14:d:505:CLA:H111	14:d:517:CLA:HBB2	2.02	0.41
1:e:691:TRP:CE2	14:e:1011:CLA:HBA2	2.54	0.41
1:e:712:ILE:HD13	14:e:1138:CLA:HMD2	2.02	0.41
14:e:1131:CLA:HBB2	10:n:65:LEU:HD13	2.00	0.41
14:e:1101:CLA:H51	8:l:19:PHE:HE2	1.85	0.41
17:e:4008:BCR:H15C	17:e:4008:BCR:H351	1.77	0.41
2:f:218:HIS:HD2	2:f:220:ALA:H	1.67	0.41
2:f:326:LEU:HD12	2:f:326:LEU:O	2.20	0.41
14:f:1228:CLA:H52	14:f:1228:CLA:H12	1.77	0.41
14:n:1501:CLA:H11	14:n:1501:CLA:H52	1.84	0.41
17:r:521:BCR:H11C	17:r:521:BCR:H341	1.85	0.41
13:s:110:HIS:HA	13:s:114:ALA:HB3	2.02	0.41
17:u:521:BCR:H11C	17:u:521:BCR:H341	1.92	0.41
1:A:749:VAL:HG21	17:A:4011:BCR:HC8	2.01	0.41
15:A:2001:PQN:H162	15:A:2001:PQN:H193	1.89	0.41
17:A:4008:BCR:H15C	17:A:4008:BCR:H351	1.77	0.41
2:B:126:THR:HG22	2:B:270:LEU:HD21	2.02	0.41
13:3:267:TYR:OH	14:3:502:CLA:O1D	2.36	0.41
14:5:509:CLA:H92	14:5:509:CLA:H62	1.81	0.41
1:G:205:LEU:HD11	14:G:1127:CLA:H192	2.03	0.41
1:G:554:ILE:HD11	14:G:1135:CLA:HBB1	2.02	0.41
1:G:707:GLU:OE2	2:H:544:SER:OG	2.38	0.41
14:G:1116:CLA:H91	14:G:1116:CLA:H111	1.82	0.41
14:G:1137:CLA:H143	14:G:1137:CLA:H112	1.83	0.41
17:G:4011:BCR:H20C	17:G:4011:BCR:H361	1.87	0.41
2:H:192:GLY:O	2:H:196:HIS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:11:LEU:HD21	17:W:4021:BCR:H272	2.01	0.41
17:W:4021:BCR:H15C	17:W:4021:BCR:H351	1.81	0.41
17:Y:521:BCR:H11C	17:Y:521:BCR:H341	1.86	0.41
1:e:388:TYR:HB2	1:e:391:LEU:HB2	2.01	0.41
18:e:5006:LHG:H241	13:q:52:TRP:CH2	2.55	0.41
18:e:5008:LHG:C8	13:r:13:TRP:CZ2	3.03	0.41
2:f:159:PRO:HD2	21:f:1852:SQD:H5	2.02	0.41
2:f:192:GLY:O	2:f:196:HIS:HB2	2.20	0.41
9:m:68:HIS:O	9:m:72:ILE:HG12	2.20	0.41
13:q:206:GLY:HA3	17:q:524:BCR:H402	2.02	0.41
13:u:148:PHE:CD2	14:u:512:CLA:H3A	2.53	0.41
14:u:509:CLA:H92	14:u:509:CLA:H62	1.81	0.41
14:A:1112:CLA:HBC3	18:A:5006:LHG:H352	2.02	0.41
2:B:527:LEU:HD12	14:B:1236:CLA:HED3	2.02	0.41
14:B:1228:CLA:H12	14:B:1228:CLA:H52	1.77	0.41
17:B:4014:BCR:H24C	17:B:4014:BCR:H371	1.84	0.41
4:D:127:ASN:O	4:D:130:THR:OG1	2.34	0.41
17:L:4219:BCR:C40	7:k:13:ILE:HG23	2.50	0.41
13:1:258:TYR:HB2	17:v:522:BCR:HC41	2.02	0.41
13:3:263:ASN:HD21	13:3:266:ALA:H	1.67	0.41
17:4:523:BCR:H351	17:4:523:BCR:H15C	1.79	0.41
17:6:522:BCR:H15C	17:6:522:BCR:H351	1.79	0.41
17:6:524:BCR:H351	17:6:524:BCR:H15C	1.80	0.41
14:G:1128:CLA:H142	14:G:1128:CLA:H111	1.83	0.41
14:H:1210:CLA:H111	17:H:4005:BCR:H381	2.03	0.41
14:H:1234:CLA:H143	14:H:1234:CLA:H111	1.81	0.41
5:Q:10:ARG:HD3	5:Q:21:GLU:O	2.20	0.41
13:c:107:ALA:O	13:c:111:THR:OG1	2.29	0.41
13:d:91:VAL:HG22	17:d:523:BCR:HC22	2.01	0.41
17:d:524:BCR:H351	17:d:524:BCR:H15C	1.81	0.41
5:i:10:ARG:HD3	5:i:21:GLU:O	2.20	0.41
17:n:4022:BCR:H341	17:n:4022:BCR:H11C	1.81	0.41
12:p:132:ALA:HB1	12:p:139:VAL:HG22	2.03	0.41
13:q:57:GLN:HB2	13:q:62:GLN:HE21	1.85	0.41
17:s:522:BCR:H24C	17:s:522:BCR:H371	1.87	0.41
1:A:205:LEU:HD11	14:A:1127:CLA:H192	2.03	0.41
15:A:2001:PQN:H112	15:A:2001:PQN:H142	1.82	0.41
18:A:5008:LHG:C8	13:2:13:TRP:HZ2	2.34	0.41
2:B:326:LEU:O	2:B:326:LEU:HD12	2.20	0.41
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.35	0.41
14:B:1229:CLA:H193	14:B:1229:CLA:H162	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:4014:BCR:H15C	17:B:4014:BCR:H351	1.95	0.41
9:K:78:LEU:HD22	9:K:83:ASN:HB2	2.01	0.41
13:2:73:LEU:HD11	14:2:503:CLA:HAA2	2.03	0.41
13:2:138:LEU:HA	13:2:141:ILE:HD12	2.01	0.41
14:G:1115:CLA:H142	14:G:1115:CLA:H112	1.92	0.41
14:G:1126:CLA:H72	14:G:1126:CLA:H111	1.88	0.41
2:H:159:PRO:HD2	21:H:1852:SQD:H5	2.02	0.41
2:H:326:LEU:HD12	2:H:326:LEU:O	2.20	0.41
14:H:1206:CLA:H3A	14:H:1206:CLA:HBA1	1.63	0.41
14:H:1218:CLA:H61	14:H:1218:CLA:H2	1.75	0.41
13:b:54:THR:HG22	13:b:56:ASP:H	1.86	0.41
17:b:524:BCR:H11C	17:b:524:BCR:H341	1.79	0.41
14:e:1013:CLA:H122	14:e:1140:CLA:H101	2.03	0.41
14:e:1237:CLA:H202	17:n:4019:BCR:H391	2.02	0.41
2:f:118:SER:HA	14:f:1224:CLA:HMA2	2.03	0.41
2:f:700:LEU:HD22	2:f:704:GLN:NE2	2.35	0.41
17:f:4017:BCR:H371	17:f:4017:BCR:H24C	1.81	0.41
13:r:73:LEU:HD11	14:r:503:CLA:HAA2	2.03	0.41
1:A:141:SER:HB3	14:A:1126:CLA:HAA2	2.02	0.41
1:A:601:ASP:HA	1:A:604:PHE:HB3	2.03	0.41
14:A:1106:CLA:H61	14:A:1106:CLA:H92	1.78	0.41
2:B:339:ALA:HB2	17:B:4010:BCR:H372	2.03	0.41
15:B:2002:PQN:H261	15:B:2002:PQN:H222	1.78	0.41
7:I:17:LEU:HD23	7:I:17:LEU:HA	1.84	0.41
10:L:85:LEU:HD12	10:L:85:LEU:HA	1.89	0.41
17:1:524:BCR:H15C	17:1:524:BCR:H351	1.79	0.41
17:3:521:BCR:H351	17:3:521:BCR:H15C	1.77	0.41
13:4:54:THR:HG22	13:4:56:ASP:H	1.86	0.41
13:4:302:TRP:HB3	14:4:504:CLA:HMB1	2.02	0.41
1:G:197:LEU:O	1:G:201:LEU:HB2	2.21	0.41
14:G:1129:CLA:H51	14:G:1129:CLA:H11	1.84	0.41
18:G:5008:LHG:C8	13:Z:13:TRP:HZ2	2.33	0.41
14:H:1223:CLA:H13	17:H:4010:BCR:H15C	2.02	0.41
17:H:4004:BCR:H15C	17:H:4004:BCR:H351	1.83	0.41
13:a:54:THR:H	13:a:62:GLN:HE22	1.68	0.41
13:a:263:ASN:HD21	13:a:266:ALA:H	1.67	0.41
14:b:507:CLA:H2A	14:b:507:CLA:HED2	2.03	0.41
1:e:601:ASP:HA	1:e:604:PHE:HB3	2.03	0.41
14:e:1137:CLA:H92	14:e:1137:CLA:H61	1.90	0.41
2:f:428:PHE:CZ	17:l:4015:BCR:HC41	2.55	0.41
2:f:531:THR:O	2:f:535:VAL:HB	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:r:502:CLA:HBD	14:r:503:CLA:H43	2.01	0.41
17:r:524:BCR:H351	17:r:524:BCR:H15C	1.78	0.41
1:A:354:GLU:HA	1:A:357:THR:HG22	2.03	0.41
14:A:1237:CLA:H13	10:L:89:LEU:HD21	2.02	0.41
2:B:174:ARG:HB3	14:B:1221:CLA:HMD1	2.03	0.41
2:B:323:TYR:O	2:B:327:ASN:HB2	2.20	0.41
14:B:1207:CLA:C4	18:V:5221:LHG:H252	2.42	0.41
13:1:57:GLN:HB2	13:1:62:GLN:HE21	1.85	0.41
2:H:218:HIS:HD2	2:H:220:ALA:H	1.67	0.41
17:T:4015:BCR:H15C	17:T:4015:BCR:H351	1.81	0.41
9:U:68:HIS:O	9:U:72:ILE:HG12	2.20	0.41
17:Z:521:BCR:H371	17:Z:521:BCR:H24C	1.77	0.41
17:Z:524:BCR:H20C	17:Z:524:BCR:H361	1.91	0.41
17:a:522:BCR:H351	17:a:522:BCR:H15C	1.80	0.41
13:b:65:ILE:HB	13:b:303:LEU:HD21	2.02	0.41
13:d:59:MET:HA	13:d:62:GLN:HB2	2.02	0.41
1:e:312:ILE:HD13	1:e:312:ILE:HA	1.85	0.41
1:e:366:ILE:HD11	17:e:4007:BCR:HC7	2.03	0.41
14:e:1134:CLA:H61	14:e:1134:CLA:H41	1.87	0.41
18:e:5008:LHG:C8	13:r:13:TRP:HZ2	2.34	0.41
2:f:657:TRP:CZ3	14:f:1021:CLA:HHB	2.55	0.41
14:f:1229:CLA:H112	14:f:1229:CLA:H152	1.81	0.41
17:f:4006:BCR:H15C	17:f:4006:BCR:H351	1.81	0.41
14:t:512:CLA:H3A	14:t:512:CLA:HBA1	1.86	0.41
17:u:521:BCR:H15C	17:u:521:BCR:H351	1.81	0.41
14:A:1013:CLA:H122	14:A:1140:CLA:H101	2.03	0.41
14:A:1133:CLA:H192	14:A:1133:CLA:H162	1.88	0.41
5:E:53:ASP:OD1	5:E:53:ASP:N	2.43	0.41
13:3:110:HIS:HA	13:3:114:ALA:HB3	2.02	0.41
13:3:183:ASN:HD22	13:3:186:VAL:HG23	1.86	0.41
14:4:507:CLA:HED2	14:4:507:CLA:H2A	2.03	0.41
1:G:23:THR:HG21	18:G:5008:LHG:C9	2.51	0.41
1:G:366:ILE:HD11	17:G:4007:BCR:HC7	2.03	0.41
14:G:1106:CLA:H92	14:G:1106:CLA:H61	1.78	0.41
14:G:1119:CLA:H122	14:G:1122:CLA:H101	2.03	0.41
14:H:1207:CLA:H91	14:H:1207:CLA:H112	1.87	0.41
15:H:2002:PQN:H261	15:H:2002:PQN:H222	1.78	0.41
12:X:132:ALA:HB1	12:X:139:VAL:HG22	2.03	0.41
13:Z:26:LEU:HB3	14:Z:511:CLA:HMA1	2.03	0.41
13:Z:73:LEU:HD11	14:Z:503:CLA:HAA2	2.03	0.41
14:Z:505:CLA:H11	14:Z:505:CLA:HBA2	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:354:GLU:HA	1:e:357:THR:HG22	2.03	0.41
1:e:470:ASN:HB3	1:e:653:THR:HG22	2.02	0.41
2:f:394:LEU:HD23	2:f:394:LEU:HA	1.88	0.41
7:k:20:LEU:C	7:k:23:PRO:HD2	2.46	0.41
13:q:267:TYR:O	13:q:300:ARG:NH2	2.51	0.41
13:s:183:ASN:HD22	13:s:186:VAL:HG23	1.86	0.41
14:u:509:CLA:H3A	14:u:509:CLA:HBA1	1.81	0.41
13:v:47:LEU:HD23	13:v:47:LEU:HA	1.92	0.41
19:A:1849:LMU:H62	19:A:1849:LMU:H91	1.81	0.41
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.88	0.41
2:B:150:LEU:HD22	11:M:20:ALA:HA	2.03	0.41
2:B:262:HIS:HA	2:B:263:PRO:HD3	1.96	0.41
2:B:631:LEU:O	2:B:647:SER:OG	2.29	0.41
14:B:1223:CLA:H13	17:B:4010:BCR:H15C	2.02	0.41
17:J:4013:BCR:H15C	17:J:4013:BCR:H351	1.87	0.41
13:1:206:GLY:HA3	17:1:524:BCR:H402	2.02	0.41
14:G:1123:CLA:H193	14:G:1123:CLA:H162	1.84	0.41
2:H:339:ALA:HB2	17:H:4010:BCR:H372	2.03	0.41
2:H:697:PRO:O	3:N:81:TYR:OH	2.30	0.41
14:H:1201:CLA:H2A	14:H:1201:CLA:HED2	2.03	0.41
17:W:4021:BCR:H24C	17:W:4021:BCR:H371	1.83	0.41
13:Y:326:MET:H	13:Y:326:MET:HG2	1.72	0.41
17:Z:522:BCR:H24C	17:Z:522:BCR:H371	1.84	0.41
1:e:382:MET:HE2	1:e:382:MET:HB3	1.93	0.41
10:n:134:LEU:HD23	10:n:134:LEU:HA	1.92	0.41
17:n:4019:BCR:H15C	17:n:4019:BCR:H351	1.86	0.41
13:t:302:TRP:HB3	14:t:504:CLA:HMB1	2.02	0.41
17:u:521:BCR:H24C	17:u:521:BCR:H371	1.85	0.41
1:A:366:ILE:HD11	17:A:4007:BCR:HC7	2.03	0.41
14:A:1129:CLA:H11	14:A:1129:CLA:H51	1.84	0.41
14:B:1205:CLA:H51	14:B:1205:CLA:H8	1.87	0.41
17:B:4006:BCR:H371	17:B:4006:BCR:H24C	1.79	0.41
8:J:13:ILE:HD11	17:J:4013:BCR:H281	2.02	0.41
13:1:79:ASP:OD1	13:1:79:ASP:N	2.52	0.41
14:6:512:CLA:H2A	14:6:512:CLA:HED2	2.03	0.41
1:G:217:ILE:HD11	1:G:287:LEU:HD21	2.02	0.41
1:G:468:ILE:HG23	14:G:1022:CLA:H61	2.03	0.41
17:G:4003:BCR:H361	17:G:4003:BCR:H20C	1.82	0.41
18:G:5006:LHG:H241	13:Y:52:TRP:CH2	2.55	0.41
23:G:909:HOH:O	2:H:682:HIS:HB2	2.21	0.41
2:H:126:THR:HG22	2:H:270:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:LEU:HD23	2:H:142:LEU:HA	1.88	0.41
2:H:174:ARG:HB3	14:H:1221:CLA:HMD1	2.03	0.41
2:H:531:THR:O	2:H:535:VAL:HB	2.21	0.41
2:H:700:LEU:HD22	2:H:704:GLN:NE2	2.35	0.41
14:H:1234:CLA:H161	14:H:1234:CLA:H193	1.86	0.41
7:S:20:LEU:C	7:S:23:PRO:HD2	2.46	0.41
13:Y:206:GLY:HA3	17:Y:524:BCR:H402	2.02	0.41
17:Z:522:BCR:H15C	17:Z:522:BCR:H351	1.77	0.41
13:b:318:HIS:NE2	14:b:505:CLA:NC	2.69	0.41
13:c:40:PHE:HE2	14:d:519:CLA:HBA1	1.86	0.41
17:d:522:BCR:H351	17:d:522:BCR:H15C	1.79	0.41
1:e:197:LEU:O	1:e:201:LEU:HB2	2.21	0.41
1:e:468:ILE:HG23	14:e:1022:CLA:H61	2.03	0.41
1:e:482:MET:HE2	1:e:482:MET:HB3	1.85	0.41
14:e:1109:CLA:H141	14:e:1109:CLA:H161	1.90	0.41
14:e:1125:CLA:H91	14:e:1125:CLA:H112	1.91	0.41
14:e:1237:CLA:HED3	2:f:681:ALA:HB1	2.03	0.41
19:e:1849:LMU:H91	19:e:1849:LMU:H62	1.81	0.41
23:e:909:HOH:O	2:f:682:HIS:HB2	2.21	0.41
2:f:339:ALA:HB2	17:f:4010:BCR:H372	2.03	0.41
2:f:460:ALA:HB1	14:f:1234:CLA:HBD	2.02	0.41
2:f:558:PRO:HB3	2:f:702:ILE:HB	2.03	0.41
14:f:1206:CLA:H122	14:f:1206:CLA:H162	1.84	0.41
14:f:1216:CLA:H12	14:f:1216:CLA:HBA1	1.83	0.41
14:f:1224:CLA:HBA2	14:f:1224:CLA:H3A	1.67	0.41
17:k:4018:BCR:H11C	17:k:4018:BCR:H341	1.91	0.41
10:n:3:GLN:OE1	10:n:3:GLN:N	2.54	0.41
10:n:57:LEU:HD13	14:n:1502:CLA:HMB2	2.02	0.41
13:r:26:LEU:HB3	14:r:511:CLA:HMA1	2.03	0.41
13:s:326:MET:H	13:s:326:MET:HG2	1.72	0.41
13:t:54:THR:HG22	13:t:56:ASP:H	1.86	0.41
14:u:509:CLA:H91	14:u:512:CLA:HAA2	2.03	0.41
1:A:470:ASN:HB3	1:A:653:THR:HG22	2.02	0.41
14:A:1013:CLA:H141	14:B:1012:CLA:H151	2.02	0.41
2:B:111:SER:HB3	7:I:3:GLY:HA2	2.02	0.41
14:B:1204:CLA:H142	14:B:1204:CLA:H112	1.93	0.41
17:B:4017:BCR:H371	17:B:4017:BCR:H24C	1.81	0.41
7:I:20:LEU:C	7:I:23:PRO:HD2	2.46	0.41
12:P:59:VAL:O	12:P:59:VAL:HG12	2.20	0.41
17:2:523:BCR:H20C	17:2:523:BCR:H361	1.94	0.41
13:4:34:GLN:HG2	14:4:509:CLA:HHB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:509:CLA:O1A	14:4:510:CLA:HBB1	2.21	0.41
13:6:47:LEU:HD21	13:6:90:PHE:HD1	1.86	0.41
1:G:470:ASN:HB3	1:G:653:THR:HG22	2.02	0.41
14:G:1106:CLA:H161	14:G:1106:CLA:H122	1.60	0.41
14:H:1216:CLA:H111	14:H:1216:CLA:H91	1.84	0.41
12:X:11:THR:OG1	22:X:170:FMN:O1P	2.31	0.41
17:Y:524:BCR:H351	17:Y:524:BCR:H15C	1.79	0.41
13:Z:243:SER:O	13:Z:318:HIS:ND1	2.44	0.41
13:d:26:LEU:HD22	14:d:511:CLA:HAA2	2.03	0.41
14:e:1119:CLA:H122	14:e:1122:CLA:H101	2.03	0.41
2:f:323:TYR:O	2:f:327:ASN:HB2	2.20	0.41
14:f:1201:CLA:HED2	14:f:1201:CLA:H2A	2.03	0.41
15:f:2002:PQN:H2M1	15:f:2002:PQN:H111	1.89	0.41
17:m:4104:BCR:H15C	17:m:4104:BCR:H351	1.90	0.41
13:v:221:HIS:CE1	14:v:506:CLA:NA	2.89	0.41
17:v:523:BCR:H15C	17:v:523:BCR:H351	1.83	0.41
1:A:217:ILE:HD11	1:A:287:LEU:HD21	2.03	0.40
14:A:1237:CLA:HED3	2:B:681:ALA:HB1	2.03	0.40
14:B:1211:CLA:H12	14:B:1211:CLA:H52	1.90	0.40
14:B:1219:CLA:HBC2	14:B:1220:CLA:HBA1	2.03	0.40
10:L:3:GLN:N	10:L:3:GLN:OE1	2.54	0.40
13:3:148:PHE:CD2	14:3:512:CLA:H3A	2.53	0.40
17:4:524:BCR:H11C	17:4:524:BCR:H341	1.79	0.40
17:5:523:BCR:H15C	17:5:523:BCR:H351	1.82	0.40
1:G:141:SER:HB3	14:G:1126:CLA:HAA2	2.02	0.40
1:G:173:LEU:HD12	1:G:173:LEU:HA	1.95	0.40
1:G:440:ARG:NH2	10:V:4:ASP:OD1	2.54	0.40
1:G:728:ARG:HH11	1:G:728:ARG:HD3	1.77	0.40
14:G:1237:CLA:HED3	2:H:681:ALA:HB1	2.03	0.40
2:H:118:SER:HA	14:H:1224:CLA:HMA2	2.03	0.40
2:H:323:TYR:O	2:H:327:ASN:HB2	2.20	0.40
2:H:704:GLN:HG3	20:H:5002:LMG:H131	2.03	0.40
14:H:1215:CLA:H142	14:H:1215:CLA:H112	1.90	0.40
6:R:91:ILE:O	6:R:94:TRP:HB3	2.21	0.40
14:Y:516:CLA:H3A	14:Y:516:CLA:HBA1	1.45	0.40
13:Z:148:PHE:HE2	14:Z:512:CLA:HHB	1.86	0.40
13:d:47:LEU:HD21	13:d:90:PHE:HD1	1.86	0.40
13:d:221:HIS:CE1	14:d:506:CLA:NA	2.89	0.40
1:e:120:ILE:HD12	1:e:120:ILE:HA	1.88	0.40
14:e:1139:CLA:H41	14:e:1139:CLA:H61	1.64	0.40
17:s:523:BCR:H15C	17:s:523:BCR:H351	1.76	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:318:HIS:NE2	14:t:505:CLA:NC	2.69	0.40
14:t:507:CLA:H2A	14:t:507:CLA:HED2	2.03	0.40
13:u:40:PHE:HE2	14:v:519:CLA:HBA1	1.86	0.40
2:B:558:PRO:HB3	2:B:702:ILE:HB	2.03	0.40
13:1:305:ASN:HB3	17:1:521:BCR:HC8	2.03	0.40
14:1:512:CLA:H3A	14:1:512:CLA:HBA1	1.68	0.40
17:1:521:BCR:H24C	17:1:521:BCR:H371	1.79	0.40
13:4:143:GLY:HA3	13:4:222:ILE:HG23	2.03	0.40
1:G:354:GLU:HA	1:G:357:THR:HG22	2.03	0.40
19:G:1849:LMU:H62	19:G:1849:LMU:H91	1.81	0.40
13:Y:57:GLN:HB2	13:Y:62:GLN:HE21	1.86	0.40
13:a:110:HIS:HA	13:a:114:ALA:HB3	2.02	0.40
13:a:183:ASN:HD22	13:a:186:VAL:HG23	1.86	0.40
14:b:509:CLA:O1A	14:b:510:CLA:HBB1	2.21	0.40
18:e:5009:LHG:H241	9:m:14:TRP:HB3	2.04	0.40
2:f:704:GLN:HG3	20:f:5002:LMG:H131	2.03	0.40
14:f:1221:CLA:H151	14:f:1221:CLA:H112	1.81	0.40
12:p:51:ILE:HG12	12:p:84:ALA:HB3	2.03	0.40
13:u:73:LEU:HD23	13:u:73:LEU:HA	1.91	0.40
13:v:26:LEU:HD22	14:v:511:CLA:HAA2	2.03	0.40
1:A:197:LEU:O	1:A:201:LEU:HB2	2.21	0.40
23:A:909:HOH:O	2:B:682:HIS:HB2	2.21	0.40
2:B:270:LEU:HD23	2:B:270:LEU:HA	1.89	0.40
14:B:1201:CLA:H143	14:B:1201:CLA:H111	1.90	0.40
17:B:4009:BCR:H24C	17:B:4009:BCR:H371	1.94	0.40
7:I:16:PRO:HB2	17:V:4219:BCR:H291	2.02	0.40
17:4:524:BCR:H15C	17:4:524:BCR:H351	1.82	0.40
17:5:522:BCR:H15C	17:5:522:BCR:H351	1.77	0.40
13:6:246:LEU:HD23	13:6:246:LEU:HA	1.87	0.40
1:G:601:ASP:HA	1:G:604:PHE:HB3	2.03	0.40
14:G:1110:CLA:H3A	14:G:1110:CLA:HBA2	1.63	0.40
17:G:4008:BCR:H20C	17:G:4008:BCR:H361	1.83	0.40
2:H:460:ALA:HB1	14:H:1234:CLA:HBD	2.02	0.40
14:H:1023:CLA:H92	14:H:1023:CLA:H62	1.92	0.40
17:H:4010:BCR:H20C	17:H:4010:BCR:H361	1.86	0.40
7:S:10:LEU:HD23	7:S:10:LEU:HA	1.89	0.40
8:T:13:ILE:HD11	17:T:4013:BCR:H281	2.03	0.40
17:T:4013:BCR:H15C	17:T:4013:BCR:H351	1.87	0.40
18:V:5220:LHG:H151	18:V:5220:LHG:H292	2.02	0.40
17:Z:521:BCR:H351	17:Z:521:BCR:H15C	1.83	0.40
17:c:521:BCR:H11C	17:c:521:BCR:H341	1.92	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:523:BCR:H11C	17:c:523:BCR:H341	2.00	0.40
17:d:522:BCR:H371	17:d:522:BCR:H24C	1.85	0.40
14:e:1116:CLA:H93	14:e:1116:CLA:H61	1.89	0.40
4:h:89:PHE:HB2	4:h:93:ASP:HB3	2.02	0.40
6:j:91:ILE:O	6:j:94:TRP:HB3	2.21	0.40
17:l:4015:BCR:H371	17:l:4015:BCR:H24C	1.88	0.40
17:m:4104:BCR:H20C	17:m:4104:BCR:H361	1.83	0.40
17:n:4219:BCR:H24C	17:n:4219:BCR:H371	1.92	0.40
13:q:282:VAL:HG23	13:q:283:THR:HG23	2.04	0.40
13:r:57:GLN:HB2	13:r:62:GLN:HE21	1.87	0.40
13:t:65:ILE:HB	13:t:303:LEU:HD21	2.02	0.40
13:t:143:GLY:HA3	13:t:222:ILE:HG23	2.03	0.40
13:v:47:LEU:HD21	13:v:90:PHE:HD1	1.86	0.40
1:A:336:ILE:HG21	1:A:336:ILE:HD13	1.89	0.40
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.88	0.40
1:A:554:ILE:HD11	14:A:1135:CLA:HBB1	2.02	0.40
14:A:1115:CLA:H41	14:A:1115:CLA:H62	1.65	0.40
14:A:1101:CLA:H51	8:J:19:PHE:HE2	1.85	0.40
2:B:531:THR:O	2:B:535:VAL:HB	2.21	0.40
4:D:89:PHE:HB2	4:D:93:ASP:HB3	2.02	0.40
17:2:524:BCR:H20C	17:2:524:BCR:H361	1.91	0.40
13:5:110:HIS:HA	13:5:114:ALA:HB3	2.04	0.40
13:5:148:PHE:CD2	14:5:512:CLA:H3A	2.53	0.40
17:5:522:BCR:H371	17:5:522:BCR:H24C	1.88	0.40
13:6:26:LEU:HD22	14:6:511:CLA:HAA2	2.03	0.40
1:G:317:ILE:O	1:G:321:HIS:ND1	2.46	0.40
1:G:577:LYS:NZ	2:H:673:GLU:OE2	2.43	0.40
2:H:658:ALA:HB3	14:H:1023:CLA:HBB2	2.04	0.40
14:H:1205:CLA:H8	14:H:1205:CLA:H51	1.87	0.40
14:H:1219:CLA:HBC2	14:H:1220:CLA:HBA1	2.03	0.40
14:H:1230:CLA:H102	14:H:1230:CLA:H61	1.83	0.40
13:Y:282:VAL:HG23	13:Y:283:THR:HG23	2.04	0.40
13:Y:305:ASN:HB3	17:Y:521:BCR:HC8	2.03	0.40
17:c:522:BCR:H24C	17:c:522:BCR:H371	1.88	0.40
17:d:523:BCR:H11C	17:d:523:BCR:H341	1.91	0.40
18:e:5002:LHG:H342	18:e:5002:LHG:H371	1.94	0.40
2:f:293:THR:OG1	2:f:294:ASN:N	2.54	0.40
14:f:1223:CLA:H13	17:f:4010:BCR:H15C	2.02	0.40
12:p:59:VAL:O	12:p:59:VAL:HG12	2.20	0.40
14:t:517:CLA:H3A	14:t:517:CLA:HBA1	1.77	0.40
1:A:468:ILE:HG23	14:A:1022:CLA:H61	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:5004:LHG:H271	18:A:5005:LHG:H291	2.04	0.40
14:B:1210:CLA:H111	17:B:4005:BCR:H381	2.03	0.40
14:B:1216:CLA:H91	14:B:1216:CLA:H111	1.84	0.40
17:B:4010:BCR:H15C	17:B:4010:BCR:H351	1.72	0.40
5:E:56:VAL:HG12	5:E:58:THR:H	1.87	0.40
12:P:132:ALA:HB1	12:P:139:VAL:HG22	2.03	0.40
17:2:522:BCR:H24C	17:2:522:BCR:H371	1.84	0.40
13:3:77:VAL:HG12	13:3:83:VAL:HA	2.03	0.40
17:4:522:BCR:H24C	17:4:522:BCR:H371	1.90	0.40
13:6:221:HIS:CE1	14:6:506:CLA:NA	2.89	0.40
1:G:329:ILE:HD13	9:U:62:ALA:HB2	2.03	0.40
14:G:1013:CLA:H122	14:G:1140:CLA:H101	2.03	0.40
17:G:4003:BCR:H15C	17:G:4003:BCR:H351	1.80	0.40
14:H:1222:CLA:HBA2	14:H:1222:CLA:H3A	1.90	0.40
13:b:143:GLY:HA3	13:b:222:ILE:HG23	2.03	0.40
14:e:1013:CLA:H141	14:f:1012:CLA:H151	2.02	0.40
17:e:4008:BCR:H361	17:e:4008:BCR:H20C	1.83	0.40
2:f:321:GLY:O	2:f:325:THR:OG1	2.34	0.40
14:f:1210:CLA:H111	17:f:4005:BCR:H381	2.02	0.40
14:f:1207:CLA:H2A	14:f:1207:CLA:H2	2.04	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%)	724 (97%)	25 (3%)	0	100	100
1	G	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
1	e	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
2	B	731/734 (100%)	710 (97%)	21 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	731/734 (100%)	710 (97%)	21 (3%)	0	100	100
2	f	731/734 (100%)	710 (97%)	21 (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%)	133 (96%)	6 (4%)	0	100	100
4	O	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
4	h	139/141 (99%)	133 (96%)	6 (4%)	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%)	35 (97%)	1 (3%)	0	100	100
7	S	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	k	36/38 (95%)	35 (97%)	1 (3%)	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
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%)	158 (98%)	4 (2%)	0	100	100
10	V	162/166 (98%)	158 (98%)	4 (2%)	0	100	100
10	n	162/166 (98%)	158 (98%)	4 (2%)	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	P	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
12	X	167/172 (97%)	159 (95%)	8 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	p	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
13	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	2	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	4	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	Z	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	b	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	r	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	t	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	13287/13605 (98%)	12906 (97%)	381 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	600/611 (98%)	600 (100%)	0	100	100
2	B	583/584 (100%)	582 (100%)	1 (0%)	87	88
2	H	583/584 (100%)	582 (100%)	1 (0%)	87	88
2	f	583/584 (100%)	582 (100%)	1 (0%)	87	88
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	P	140/142 (99%)	140 (100%)	0	100	100
12	X	140/142 (99%)	140 (100%)	0	100	100
12	p	140/142 (99%)	140 (100%)	0	100	100
13	1	257/259 (99%)	257 (100%)	0	100	100
13	2	257/259 (99%)	257 (100%)	0	100	100
13	3	257/259 (99%)	257 (100%)	0	100	100
13	4	257/259 (99%)	257 (100%)	0	100	100
13	5	257/259 (99%)	257 (100%)	0	100	100
13	6	257/259 (99%)	257 (100%)	0	100	100
13	Y	257/259 (99%)	257 (100%)	0	100	100
13	Z	257/259 (99%)	257 (100%)	0	100	100
13	a	257/259 (99%)	257 (100%)	0	100	100
13	b	257/259 (99%)	257 (100%)	0	100	100
13	c	257/259 (99%)	257 (100%)	0	100	100
13	d	257/259 (99%)	257 (100%)	0	100	100
13	q	257/259 (99%)	257 (100%)	0	100	100
13	r	257/259 (99%)	257 (100%)	0	100	100
13	s	257/259 (99%)	257 (100%)	0	100	100
13	t	257/259 (99%)	257 (100%)	0	100	100
13	u	257/259 (99%)	257 (100%)	0	100	100
13	v	257/259 (99%)	257 (100%)	0	100	100
All	All	10437/10593 (98%)	10434 (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 (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	GLN
1	A	135	HIS
1	A	179	HIS
1	A	181	HIS
1	A	192	ASN
1	A	253	HIS
1	A	263	GLN
1	A	612	ASN
2	B	98	GLN
2	B	156	HIS
2	B	218	HIS
2	B	452	GLN
2	B	603	GLN
2	B	689	ASN
2	B	704	GLN
4	D	71	GLN
4	D	127	ASN
4	D	137	GLN
6	F	77	HIS
8	J	39	HIS
9	K	26	ASN
9	K	80	ASN
10	L	44	ASN
12	P	38	ASN
12	P	79	GLN
13	1	57	GLN
13	1	221	HIS
13	2	129	HIS
13	2	263	ASN
13	2	316	GLN
13	3	221	HIS
13	3	263	ASN
13	4	62	GLN
13	4	129	HIS
13	4	137	GLN
13	4	263	ASN
13	6	133	ASN
13	6	263	ASN
1	G	19	ASN
1	G	115	GLN
1	G	135	HIS
1	G	179	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	181	HIS
1	G	192	ASN
1	G	253	HIS
1	G	263	GLN
2	H	98	GLN
2	H	156	HIS
2	H	218	HIS
2	H	452	GLN
2	H	603	GLN
2	H	689	ASN
2	H	704	GLN
4	O	71	GLN
4	O	127	ASN
4	O	137	GLN
6	R	55	ASN
6	R	77	HIS
8	T	39	HIS
9	U	26	ASN
10	V	44	ASN
12	X	38	ASN
12	X	79	GLN
13	Y	57	GLN
13	Y	221	HIS
13	Z	129	HIS
13	Z	263	ASN
13	Z	291	GLN
13	Z	316	GLN
13	a	221	HIS
13	a	263	ASN
13	b	62	GLN
13	b	129	HIS
13	b	137	GLN
13	b	263	ASN
13	d	133	ASN
13	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	253	HIS
1	e	263	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	612	ASN
2	f	34	HIS
2	f	98	GLN
2	f	122	HIS
2	f	132	ASN
2	f	218	HIS
2	f	350	GLN
2	f	452	GLN
2	f	603	GLN
2	f	689	ASN
2	f	704	GLN
4	h	71	GLN
4	h	127	ASN
4	h	137	GLN
5	i	67	GLN
6	j	77	HIS
8	l	39	HIS
9	m	26	ASN
10	n	44	ASN
12	p	38	ASN
12	p	79	GLN
13	q	57	GLN
13	q	221	HIS
13	r	129	HIS
13	r	263	ASN
13	r	291	GLN
13	r	316	GLN
13	s	221	HIS
13	s	263	ASN
13	t	62	GLN
13	t	129	HIS
13	t	137	GLN
13	t	263	ASN
13	v	133	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)

843 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	$\#\|Z\| > 2$
17	BCR	W	4021	-	41,41,41	0.77	0	56,56,56	1.91	15 (26%)
14	CLA	B	1212	2	55,59,73	1.37	9 (16%)	66,96,113	1.49	6 (9%)
14	CLA	V	1501	10	64,68,73	1.33	11 (17%)	77,107,113	1.42	9 (11%)
17	BCR	J	4012	-	41,41,41	0.72	0	56,56,56	1.75	12 (21%)
14	CLA	s	507	-	49,53,73	1.47	7 (14%)	59,89,113	1.51	6 (10%)
17	BCR	r	522	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	s	516	13	49,53,73	1.47	7 (14%)	59,89,113	1.71	9 (15%)
14	CLA	m	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.49	10 (14%)
14	CLA	f	1012	23	69,73,73	1.28	11 (15%)	83,113,113	1.42	10 (12%)
17	BCR	d	521	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
20	LMG	l	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	Z	509	13	69,73,73	1.26	10 (14%)	83,113,113	1.39	8 (9%)
18	LHG	G	5009	-	41,41,48	0.67	0	44,47,54	1.22	4 (9%)
17	BCR	n	4022	-	41,41,41	0.79	0	56,56,56	1.82	10 (17%)
17	BCR	V	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	G	1131	1	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
18	LHG	B	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
20	LMG	T	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	e	1114	23	49,53,73	1.51	9 (18%)	59,89,113	1.56	9 (15%)
18	LHG	e	5008	-	34,34,48	0.71	1 (2%)	37,40,54	1.25	4 (10%)
14	CLA	B	1228	2	59,63,73	1.31	10 (16%)	71,101,113	1.51	7 (9%)
14	CLA	A	1127	1	69,73,73	1.25	10 (14%)	83,113,113	1.40	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	H	4009	-	41,41,41	0.78	0	56,56,56	1.90	20 (35%)
14	CLA	q	503	13	49,53,73	1.48	8 (16%)	59,89,113	1.52	5 (8%)
19	LMU	G	1849	-	23,23,36	1.18	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	A	1137	1	64,68,73	1.31	8 (12%)	77,107,113	1.46	9 (11%)
14	CLA	5	511	13	49,53,73	1.49	7 (14%)	59,89,113	1.54	8 (13%)
14	CLA	4	512	13	49,53,73	1.47	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	6	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.46	8 (13%)
17	BCR	b	524	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
17	BCR	a	524	-	41,41,41	0.78	0	56,56,56	1.93	18 (32%)
14	CLA	U	1105	9	49,53,73	1.47	8 (16%)	59,89,113	1.68	8 (13%)
14	CLA	5	507	-	49,53,73	1.45	8 (16%)	59,89,113	1.55	7 (11%)
14	CLA	m	1105	9	49,53,73	1.48	8 (16%)	59,89,113	1.67	8 (13%)
14	CLA	H	1226	2	59,63,73	1.49	11 (18%)	71,101,113	1.83	18 (25%)
14	CLA	A	1115	1	64,68,73	1.29	11 (17%)	77,107,113	1.49	8 (10%)
14	CLA	f	1216	23	64,68,73	1.33	10 (15%)	77,107,113	1.51	10 (12%)
14	CLA	H	1238	23	69,73,73	1.24	10 (14%)	83,113,113	1.49	12 (14%)
14	CLA	Y	519	13	49,53,73	1.50	10 (20%)	59,89,113	1.42	6 (10%)
14	CLA	f	1236	2	54,58,73	1.40	9 (16%)	65,95,113	1.43	9 (13%)
14	CLA	f	1232	23	59,63,73	1.34	10 (16%)	71,101,113	1.50	8 (11%)
14	CLA	f	1205	2	69,73,73	1.25	11 (15%)	83,113,113	1.50	10 (12%)
14	CLA	G	1137	1	64,68,73	1.31	8 (12%)	77,107,113	1.46	9 (11%)
17	BCR	G	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
17	BCR	f	4017	-	41,41,41	0.97	3 (7%)	56,56,56	1.82	12 (21%)
14	CLA	A	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.69	14 (16%)
14	CLA	c	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.57	6 (10%)
14	CLA	H	1206	2	69,73,73	1.29	12 (17%)	83,113,113	1.48	11 (13%)
14	CLA	B	1208	2	69,73,73	1.23	9 (13%)	83,113,113	1.28	7 (8%)
14	CLA	A	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.54	12 (14%)
14	CLA	J	1302	8	59,63,73	1.31	9 (15%)	71,101,113	1.47	7 (9%)
14	CLA	1	503	13	49,53,73	1.48	8 (16%)	59,89,113	1.52	5 (8%)
14	CLA	A	1124	23	64,68,73	1.33	11 (17%)	77,107,113	1.46	10 (12%)
14	CLA	3	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
14	CLA	f	1207	2	69,73,73	1.25	9 (13%)	83,113,113	1.32	4 (4%)
14	CLA	d	518	13	49,53,73	1.46	8 (16%)	59,89,113	1.49	4 (6%)
14	CLA	f	1206	2	69,73,73	1.28	12 (17%)	83,113,113	1.49	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	e	1125	1	69,73,73	1.26	11 (15%)	83,113,113	1.47	9 (10%)
14	CLA	b	502	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	6 (10%)
14	CLA	G	1134	1	60,64,73	1.31	9 (15%)	72,102,113	1.51	9 (12%)
18	LHG	n	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
14	CLA	A	1138	1	69,73,73	1.23	9 (13%)	83,113,113	1.45	6 (7%)
14	CLA	e	1011	1	69,73,73	1.27	8 (11%)	83,113,113	1.66	14 (16%)
14	CLA	Z	507	-	49,53,73	1.46	9 (18%)	59,89,113	1.53	8 (13%)
17	BCR	A	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
14	CLA	t	512	13	49,53,73	1.47	8 (16%)	59,89,113	1.48	5 (8%)
17	BCR	t	522	-	41,41,41	0.74	0	56,56,56	1.91	19 (33%)
14	CLA	e	1237	23	69,73,73	1.27	13 (18%)	83,113,113	1.54	10 (12%)
14	CLA	H	1208	2	69,73,73	1.23	10 (14%)	83,113,113	1.28	7 (8%)
14	CLA	s	509	13	49,53,73	1.48	11 (22%)	59,89,113	1.57	8 (13%)
14	CLA	F	1302	6	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
14	CLA	A	1801	18	49,53,73	1.44	11 (22%)	59,89,113	1.51	7 (11%)
14	CLA	B	1235	2	69,73,73	1.27	11 (15%)	83,113,113	1.41	7 (8%)
14	CLA	G	1111	1	69,73,73	1.25	11 (15%)	83,113,113	1.40	7 (8%)
14	CLA	H	1225	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	11 (13%)
14	CLA	v	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	6 (10%)
17	BCR	A	4003	-	41,41,41	0.88	1 (2%)	56,56,56	1.78	14 (25%)
17	BCR	n	4219	-	41,41,41	1.09	5 (12%)	56,56,56	2.26	23 (41%)
18	LHG	e	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	A	1134	1	60,64,73	1.32	9 (15%)	72,102,113	1.50	9 (12%)
14	CLA	4	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	5 (8%)
14	CLA	q	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
14	CLA	Z	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.43	5 (8%)
14	CLA	u	502	13	49,53,73	1.50	8 (16%)	59,89,113	1.57	6 (10%)
14	CLA	4	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.58	7 (11%)
17	BCR	H	4017	-	41,41,41	0.97	4 (9%)	56,56,56	1.82	12 (21%)
17	BCR	a	522	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)
14	CLA	G	1113	1	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
14	CLA	R	1302	6	49,53,73	1.48	9 (18%)	59,89,113	1.49	7 (11%)
14	CLA	B	1221	23	66,70,73	1.32	11 (16%)	79,109,113	1.54	12 (15%)
14	CLA	a	513	13	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	1	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.46	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	f	1240	18	69,73,73	1.26	9 (13%)	83,113,113	1.35	8 (9%)
14	CLA	T	1303	8	49,53,73	1.47	10 (20%)	59,89,113	1.60	8 (13%)
14	CLA	G	1104	1	69,73,73	1.26	13 (18%)	83,113,113	1.47	13 (15%)
14	CLA	G	1138	1	69,73,73	1.23	9 (13%)	83,113,113	1.46	6 (7%)
14	CLA	r	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.46	6 (10%)
17	BCR	3	522	-	41,41,41	0.69	0	56,56,56	2.04	18 (32%)
14	CLA	e	1121	1	59,63,73	1.36	11 (18%)	71,101,113	1.55	10 (14%)
14	CLA	G	1139	23	69,73,73	1.27	11 (15%)	83,113,113	1.28	6 (7%)
14	CLA	F	1301	23	49,53,73	1.49	11 (22%)	59,89,113	1.47	5 (8%)
14	CLA	t	511	13	49,53,73	1.50	9 (18%)	59,89,113	1.51	9 (15%)
14	CLA	H	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.45	10 (12%)
14	CLA	2	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)
14	CLA	f	1229	2	69,73,73	1.23	10 (14%)	83,113,113	1.45	9 (10%)
20	LMG	B	5002	-	53,53,55	0.85	3 (5%)	61,61,63	1.51	12 (19%)
17	BCR	A	4011	-	41,41,41	0.82	0	56,56,56	1.79	12 (21%)
18	LHG	A	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
14	CLA	t	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.58	7 (11%)
14	CLA	Y	516	13	49,53,73	1.46	10 (20%)	59,89,113	1.48	6 (10%)
14	CLA	B	1205	2	69,73,73	1.26	11 (15%)	83,113,113	1.50	10 (12%)
17	BCR	6	524	-	41,41,41	0.78	0	56,56,56	1.85	15 (26%)
14	CLA	v	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
14	CLA	G	1118	1	64,68,73	1.28	11 (17%)	77,107,113	1.46	7 (9%)
15	PQN	B	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.31	6 (14%)
14	CLA	A	1132	1	69,73,73	1.25	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	H	1215	2	69,73,73	1.26	10 (14%)	83,113,113	1.55	11 (13%)
17	BCR	J	4013	-	41,41,41	0.77	0	56,56,56	1.93	16 (28%)
17	BCR	B	4006	-	41,41,41	0.78	0	56,56,56	2.09	18 (32%)
14	CLA	H	1204	2	69,73,73	1.22	10 (14%)	83,113,113	1.33	7 (8%)
17	BCR	s	524	-	41,41,41	0.77	0	56,56,56	1.93	18 (32%)
14	CLA	H	1228	2	59,63,73	1.30	10 (16%)	71,101,113	1.51	7 (9%)
14	CLA	f	1215	2	69,73,73	1.26	10 (14%)	83,113,113	1.56	11 (13%)
14	CLA	u	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.42	5 (8%)
17	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
14	CLA	v	510	13	49,53,73	1.49	10 (20%)	59,89,113	1.48	4 (6%)
14	CLA	s	505	13	59,63,73	1.33	8 (13%)	71,101,113	1.36	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	Y	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	e	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.69	14 (16%)
17	BCR	Z	523	-	41,41,41	0.72	0	56,56,56	1.76	17 (30%)
21	SQD	6	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	A	1118	1	64,68,73	1.28	11 (17%)	77,107,113	1.46	7 (9%)
18	LHG	L	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	A	1133	1	69,73,73	1.23	10 (14%)	83,113,113	1.39	7 (8%)
14	CLA	q	505	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
17	BCR	L	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	5	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.58	6 (10%)
14	CLA	G	1140	1	69,73,73	1.26	10 (14%)	83,113,113	1.46	9 (10%)
17	BCR	v	524	-	41,41,41	0.78	0	56,56,56	1.84	15 (26%)
14	CLA	d	511	13	49,53,73	1.49	8 (16%)	59,89,113	1.55	5 (8%)
14	CLA	f	1231	23	69,73,73	1.22	9 (13%)	83,113,113	1.36	9 (10%)
14	CLA	e	1132	1	69,73,73	1.25	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	a	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
14	CLA	c	518	13	49,53,73	1.47	9 (18%)	59,89,113	1.43	6 (10%)
18	LHG	G	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
18	LHG	e	5009	-	41,41,48	0.67	0	44,47,54	1.22	4 (9%)
17	BCR	B	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.30	21 (37%)
14	CLA	e	1131	1	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
14	CLA	A	1114	23	49,53,73	1.50	9 (18%)	59,89,113	1.57	9 (15%)
18	LHG	A	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.22	4 (8%)
17	BCR	2	522	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	6	503	13	49,53,73	1.48	8 (16%)	59,89,113	1.55	5 (8%)
14	CLA	6	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
14	CLA	v	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
14	CLA	B	1230	2	64,68,73	1.30	10 (15%)	77,107,113	1.40	7 (9%)
14	CLA	r	516	13	49,53,73	1.46	8 (16%)	59,89,113	1.50	6 (10%)
17	BCR	f	4014	-	41,41,41	0.83	1 (2%)	56,56,56	1.90	23 (41%)
14	CLA	B	1204	2	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)
14	CLA	b	519	13	49,53,73	1.49	10 (20%)	59,89,113	1.50	6 (10%)
14	CLA	s	518	13	59,63,73	1.35	10 (16%)	71,101,113	1.37	5 (7%)
14	CLA	B	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.37	9 (11%)
14	CLA	K	1103	9	52,56,73	1.43	9 (17%)	62,92,113	1.51	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	f	1214	2	69,73,73	1.26	9 (13%)	83,113,113	1.45	6 (7%)
17	BCR	b	523	-	41,41,41	0.73	0	56,56,56	1.77	14 (25%)
14	CLA	a	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.57	8 (13%)
14	CLA	e	1140	1	69,73,73	1.25	10 (14%)	83,113,113	1.46	9 (10%)
21	SQD	b	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
17	BCR	f	4005	-	41,41,41	0.77	0	56,56,56	1.72	12 (21%)
14	CLA	4	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	4 (6%)
14	CLA	G	1106	1	69,73,73	1.22	11 (15%)	83,113,113	1.42	9 (10%)
14	CLA	B	1234	2	69,73,73	1.29	11 (15%)	83,113,113	1.49	11 (13%)
14	CLA	u	503	13	49,53,73	1.48	9 (18%)	59,89,113	1.55	8 (13%)
18	LHG	A	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	e	1102	1	59,63,73	1.35	12 (20%)	71,101,113	1.45	8 (11%)
17	BCR	J	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
17	BCR	T	4012	-	41,41,41	0.72	0	56,56,56	1.76	13 (23%)
21	SQD	1	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
14	CLA	q	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.52	5 (8%)
14	CLA	d	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.46	7 (11%)
18	LHG	G	5007	-	46,46,48	0.60	0	49,52,54	1.20	4 (8%)
14	CLA	d	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	B	1238	23	69,73,73	1.23	10 (14%)	83,113,113	1.48	11 (13%)
18	LHG	e	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	v	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.46	8 (13%)
18	LHG	G	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
14	CLA	4	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	6 (10%)
14	CLA	A	1106	1	69,73,73	1.23	11 (15%)	83,113,113	1.41	9 (10%)
14	CLA	e	1101	1	69,73,73	1.28	10 (14%)	83,113,113	1.55	12 (14%)
14	CLA	G	1119	23	69,73,73	1.32	10 (14%)	83,113,113	1.53	14 (16%)
14	CLA	G	1105	1	59,63,73	1.31	9 (15%)	71,101,113	1.49	9 (12%)
14	CLA	H	1219	2	67,71,73	1.28	10 (14%)	80,110,113	1.34	10 (12%)
18	LHG	A	5007	-	46,46,48	0.60	0	49,52,54	1.20	4 (8%)
19	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
14	CLA	H	1203	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	b	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.49	4 (6%)
14	CLA	3	503	13	49,53,73	1.49	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	H	1221	23	66,70,73	1.32	11 (16%)	79,109,113	1.54	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	4	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
14	CLA	r	509	13	69,73,73	1.26	11 (15%)	83,113,113	1.38	8 (9%)
18	LHG	A	5008	-	34,34,48	0.70	1 (2%)	37,40,54	1.25	4 (10%)
14	CLA	d	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	6	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.47	6 (10%)
14	CLA	B	1012	23	69,73,73	1.28	11 (15%)	83,113,113	1.42	10 (12%)
14	CLA	Z	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.60	10 (16%)
14	CLA	f	1218	2	64,68,73	1.30	9 (14%)	77,107,113	1.35	5 (6%)
14	CLA	v	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.56	5 (8%)
19	LMU	e	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
21	SQD	Y	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
18	LHG	f	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.25	3 (7%)
14	CLA	u	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.65	6 (10%)
17	BCR	a	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
21	SQD	L	5216	-	45,46,54	1.01	5 (11%)	54,57,65	1.69	11 (20%)
14	CLA	A	1119	23	69,73,73	1.32	10 (14%)	83,113,113	1.54	14 (16%)
14	CLA	H	1214	2	69,73,73	1.26	9 (13%)	83,113,113	1.45	7 (8%)
14	CLA	c	503	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
14	CLA	s	519	13	49,53,73	1.47	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	1	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
17	BCR	d	523	-	41,41,41	0.72	0	56,56,56	1.72	14 (25%)
14	CLA	G	1116	1	64,68,73	1.30	11 (17%)	77,107,113	1.36	9 (11%)
14	CLA	f	1212	2	55,59,73	1.37	9 (16%)	66,96,113	1.49	6 (9%)
14	CLA	j	1301	23	49,53,73	1.49	11 (22%)	59,89,113	1.47	5 (8%)
14	CLA	r	501	13	64,68,73	1.28	9 (14%)	77,107,113	1.46	7 (9%)
14	CLA	t	502	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	5 (8%)
14	CLA	e	1109	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	8 (9%)
14	CLA	e	1133	1	69,73,73	1.23	10 (14%)	83,113,113	1.40	7 (8%)
16	SF4	C	3002	3	0,12,12	-	-	-		
17	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.75	12 (21%)
14	CLA	4	505	13	49,53,73	1.46	10 (20%)	59,89,113	1.43	4 (6%)
14	CLA	H	1213	2	65,69,73	1.26	11 (16%)	78,108,113	1.48	10 (12%)
14	CLA	e	1124	23	64,68,73	1.33	11 (17%)	77,107,113	1.46	11 (14%)
14	CLA	f	1210	2	69,73,73	1.27	12 (17%)	83,113,113	1.36	10 (12%)
14	CLA	b	503	13	49,53,73	1.50	9 (18%)	59,89,113	1.55	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	Z	522	-	41,41,41	0.75	0	56,56,56	1.86	17 (30%)
14	CLA	6	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	c	504	-	49,53,73	1.48	9 (18%)	59,89,113	1.54	5 (8%)
17	BCR	u	524	-	41,41,41	0.71	0	56,56,56	1.74	11 (19%)
14	CLA	s	504	-	49,53,73	1.48	9 (18%)	59,89,113	1.57	9 (15%)
14	CLA	G	1133	1	69,73,73	1.23	11 (15%)	83,113,113	1.40	7 (8%)
14	CLA	e	1104	1	69,73,73	1.27	13 (18%)	83,113,113	1.47	13 (15%)
14	CLA	e	1120	1	54,58,73	1.37	12 (22%)	65,95,113	1.57	10 (15%)
14	CLA	a	503	13	49,53,73	1.49	8 (16%)	59,89,113	1.51	7 (11%)
17	BCR	n	4020	-	41,41,41	0.98	2 (4%)	56,56,56	1.67	14 (25%)
16	SF4	g	3002	3	0,12,12	-	-	-		
14	CLA	A	1116	1	64,68,73	1.30	11 (17%)	77,107,113	1.35	9 (11%)
14	CLA	e	1137	1	64,68,73	1.31	8 (12%)	77,107,113	1.46	9 (11%)
14	CLA	e	1117	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	11 (13%)
17	BCR	A	4007	-	41,41,41	0.87	0	56,56,56	2.10	20 (35%)
17	BCR	e	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
14	CLA	G	1120	1	54,58,73	1.37	12 (22%)	65,95,113	1.57	10 (15%)
14	CLA	u	504	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	5 (8%)
22	FMN	P	170	-	33,33,33	1.13	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	K	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.49	10 (14%)
14	CLA	5	519	13	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	Y	512	13	49,53,73	1.47	10 (20%)	59,89,113	1.39	4 (6%)
14	CLA	2	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.46	5 (8%)
21	SQD	f	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	d	517	-	49,53,73	1.45	7 (14%)	59,89,113	1.47	6 (10%)
14	CLA	G	1022	23	69,73,73	1.32	10 (14%)	83,113,113	1.38	12 (14%)
14	CLA	L	1501	10	64,68,73	1.32	11 (17%)	77,107,113	1.41	9 (11%)
14	CLA	Y	502	13	49,53,73	1.47	9 (18%)	59,89,113	1.53	7 (11%)
14	CLA	1	519	13	49,53,73	1.49	10 (20%)	59,89,113	1.43	5 (8%)
14	CLA	H	1217	2	64,68,73	1.29	9 (14%)	77,107,113	1.33	5 (6%)
17	BCR	3	524	-	41,41,41	0.78	0	56,56,56	1.93	18 (32%)
14	CLA	B	1209	2	57,61,73	1.38	11 (19%)	68,98,113	1.54	8 (11%)
14	CLA	e	1110	1	57,61,73	1.37	10 (17%)	68,98,113	1.45	7 (10%)
14	CLA	f	1220	2	59,63,73	1.36	10 (16%)	71,101,113	1.53	8 (11%)
14	CLA	f	1226	2	59,63,73	1.48	11 (18%)	71,101,113	1.81	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	K	1105	9	49,53,73	1.48	8 (16%)	59,89,113	1.67	8 (13%)
17	BCR	b	521	-	41,41,41	0.68	0	56,56,56	1.78	11 (19%)
14	CLA	f	1217	2	64,68,73	1.28	9 (14%)	77,107,113	1.33	5 (6%)
19	LMU	e	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	s	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
14	CLA	H	1209	2	57,61,73	1.38	11 (19%)	68,98,113	1.53	8 (11%)
14	CLA	A	1120	1	54,58,73	1.37	12 (22%)	65,95,113	1.57	10 (15%)
17	BCR	G	4002	-	41,41,41	0.88	1 (2%)	56,56,56	1.94	16 (28%)
17	BCR	G	4011	-	41,41,41	0.81	0	56,56,56	1.78	12 (21%)
14	CLA	e	1130	1	60,64,73	1.33	11 (18%)	72,102,113	1.54	11 (15%)
14	CLA	A	1022	23	69,73,73	1.32	10 (14%)	83,113,113	1.38	12 (14%)
14	CLA	H	1222	23	54,58,73	1.40	11 (20%)	65,95,113	1.55	10 (15%)
14	CLA	e	1129	1	57,61,73	1.41	10 (17%)	68,98,113	1.51	11 (16%)
19	LMU	l	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
17	BCR	B	4014	-	41,41,41	0.83	1 (2%)	56,56,56	1.89	23 (41%)
14	CLA	f	1222	23	54,58,73	1.40	10 (18%)	65,95,113	1.54	10 (15%)
19	LMU	T	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
14	CLA	v	508	13	49,53,73	1.48	9 (18%)	59,89,113	1.60	11 (18%)
14	CLA	v	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.48	6 (10%)
14	CLA	q	510	13	49,53,73	1.49	10 (20%)	59,89,113	1.45	4 (6%)
17	BCR	G	4007	-	41,41,41	0.87	0	56,56,56	2.11	20 (35%)
17	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
14	CLA	5	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.45	4 (6%)
14	CLA	Z	501	13	64,68,73	1.28	10 (15%)	77,107,113	1.46	6 (7%)
14	CLA	a	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.60	8 (13%)
14	CLA	3	509	13	49,53,73	1.49	10 (20%)	59,89,113	1.57	8 (13%)
17	BCR	A	4002	-	41,41,41	0.88	1 (2%)	56,56,56	1.94	16 (28%)
14	CLA	a	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
14	CLA	3	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	8 (13%)
19	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	q	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	7 (11%)
14	CLA	2	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
17	BCR	n	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	H	1201	2	64,68,73	1.26	9 (14%)	77,107,113	1.50	10 (12%)
17	BCR	e	4011	-	41,41,41	0.83	0	56,56,56	1.78	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	v	503	13	49,53,73	1.47	8 (16%)	59,89,113	1.55	5 (8%)
17	BCR	S	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	16 (28%)
14	CLA	u	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.44	4 (6%)
14	CLA	B	1202	2	69,73,73	1.22	10 (14%)	83,113,113	1.42	8 (9%)
14	CLA	1	509	13	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
14	CLA	v	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.49	5 (8%)
17	BCR	T	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
14	CLA	4	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	Y	503	13	49,53,73	1.49	8 (16%)	59,89,113	1.53	5 (8%)
14	CLA	A	1108	1	58,62,73	1.34	10 (17%)	69,99,113	1.45	7 (10%)
14	CLA	r	507	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	8 (13%)
14	CLA	4	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	6	518	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
18	LHG	I	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
14	CLA	q	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	e	1111	1	69,73,73	1.24	11 (15%)	83,113,113	1.40	8 (9%)
14	CLA	f	1239	2	69,73,73	1.26	9 (13%)	83,113,113	1.65	13 (15%)
17	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.83	11 (19%)
14	CLA	v	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.54	6 (10%)
14	CLA	2	509	13	69,73,73	1.26	10 (14%)	83,113,113	1.38	8 (9%)
21	SQD	3	822	-	27,28,54	1.29	5 (18%)	36,39,65	1.80	11 (30%)
14	CLA	f	1227	2	64,68,73	1.29	10 (15%)	77,107,113	1.45	7 (9%)
14	CLA	Z	519	13	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
17	BCR	u	522	-	41,41,41	0.75	0	56,56,56	1.94	21 (37%)
16	SF4	A	3001	2,1	0,12,12	-	-	-		
14	CLA	Z	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.45	5 (8%)
14	CLA	2	507	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	8 (13%)
14	CLA	5	516	13	49,53,73	1.47	9 (18%)	59,89,113	1.42	4 (6%)
14	CLA	r	502	13	49,53,73	1.46	8 (16%)	59,89,113	1.58	8 (13%)
14	CLA	f	1211	2	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	G	1128	1	69,73,73	1.36	11 (15%)	83,113,113	1.60	12 (14%)
14	CLA	Y	511	13	49,53,73	1.49	8 (16%)	59,89,113	1.54	8 (13%)
19	LMU	H	1843	-	36,36,36	1.17	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	f	1203	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	1	516	13	49,53,73	1.46	10 (20%)	59,89,113	1.47	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	G	1130	1	60,64,73	1.33	11 (18%)	72,102,113	1.55	11 (15%)
14	CLA	t	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	6 (10%)
14	CLA	a	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.40	5 (8%)
14	CLA	b	510	13	49,53,73	1.46	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	e	1122	1	64,68,73	1.31	11 (17%)	77,107,113	1.44	8 (10%)
17	BCR	K	4104	-	41,41,41	0.78	0	56,56,56	1.88	16 (28%)
18	LHG	L	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
18	LHG	V	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
14	CLA	1	501	13	49,53,73	1.47	8 (16%)	59,89,113	1.53	4 (6%)
17	BCR	B	4017	-	41,41,41	0.97	3 (7%)	56,56,56	1.82	12 (21%)
14	CLA	B	1201	2	64,68,73	1.27	9 (14%)	77,107,113	1.50	10 (12%)
14	CLA	f	1223	2	69,73,73	1.26	10 (14%)	83,113,113	1.47	7 (8%)
14	CLA	u	506	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	5 (8%)
14	CLA	A	1128	1	69,73,73	1.36	11 (15%)	83,113,113	1.60	12 (14%)
14	CLA	G	1801	18	49,53,73	1.44	11 (22%)	59,89,113	1.52	6 (10%)
18	LHG	n	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
17	BCR	Y	523	-	41,41,41	0.74	0	56,56,56	1.69	14 (25%)
14	CLA	t	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.51	4 (6%)
17	BCR	1	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	V	1502	10	69,73,73	1.25	11 (15%)	83,113,113	1.42	9 (10%)
14	CLA	B	1231	23	69,73,73	1.22	9 (13%)	83,113,113	1.36	9 (10%)
14	CLA	H	1212	2	55,59,73	1.37	9 (16%)	66,96,113	1.50	6 (9%)
14	CLA	Y	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.71	8 (13%)
16	SF4	N	3003	3	0,12,12	-	-	-		
14	CLA	e	1118	1	64,68,73	1.28	11 (17%)	77,107,113	1.46	7 (9%)
14	CLA	t	501	13	49,53,73	1.48	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	A	1136	1	69,73,73	1.28	10 (14%)	83,113,113	1.47	9 (10%)
14	CLA	B	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.45	9 (10%)
14	CLA	e	1103	1	69,73,73	1.28	12 (17%)	83,113,113	1.58	10 (12%)
14	CLA	t	505	13	49,53,73	1.47	10 (20%)	59,89,113	1.43	4 (6%)
18	LHG	B	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.26	3 (7%)
14	CLA	3	505	13	59,63,73	1.33	9 (15%)	71,101,113	1.35	4 (5%)
17	BCR	2	523	-	41,41,41	0.72	0	56,56,56	1.75	17 (30%)
14	CLA	b	512	13	49,53,73	1.46	8 (16%)	59,89,113	1.47	5 (8%)
17	BCR	b	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LHG	A	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
14	CLA	s	506	13	49,53,73	1.49	9 (18%)	59,89,113	1.50	7 (11%)
22	FMN	p	170	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	H	1205	2	69,73,73	1.26	11 (15%)	83,113,113	1.50	10 (12%)
14	CLA	r	503	13	69,73,73	1.25	7 (10%)	83,113,113	1.35	7 (8%)
14	CLA	H	1211	2	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	Y	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
14	CLA	H	1223	2	69,73,73	1.25	9 (13%)	83,113,113	1.47	7 (8%)
20	LMG	J	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
17	BCR	f	4006	-	41,41,41	0.77	0	56,56,56	2.09	18 (32%)
14	CLA	V	1503	23	64,68,73	1.28	10 (15%)	77,107,113	1.42	5 (6%)
14	CLA	Z	516	13	49,53,73	1.47	8 (16%)	59,89,113	1.52	6 (10%)
14	CLA	Z	502	13	49,53,73	1.47	9 (18%)	59,89,113	1.59	8 (13%)
14	CLA	G	1115	1	64,68,73	1.29	11 (17%)	77,107,113	1.48	8 (10%)
17	BCR	6	523	-	41,41,41	0.72	0	56,56,56	1.72	14 (25%)
14	CLA	G	1136	1	69,73,73	1.27	9 (13%)	83,113,113	1.46	9 (10%)
14	CLA	r	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	a	519	13	49,53,73	1.47	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	d	513	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	2	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	A	1131	1	69,73,73	1.25	9 (13%)	83,113,113	1.37	8 (9%)
14	CLA	q	519	13	49,53,73	1.49	10 (20%)	59,89,113	1.44	6 (10%)
14	CLA	b	511	13	49,53,73	1.50	10 (20%)	59,89,113	1.51	9 (15%)
14	CLA	e	1105	1	59,63,73	1.32	10 (16%)	71,101,113	1.49	9 (12%)
14	CLA	e	1112	1	54,58,73	1.39	12 (22%)	65,95,113	1.54	7 (10%)
14	CLA	1	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.71	7 (11%)
16	SF4	C	3003	3	0,12,12	-	-	-		
17	BCR	B	4004	-	41,41,41	0.73	0	56,56,56	1.85	14 (25%)
14	CLA	b	517	-	49,53,73	1.48	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	f	1238	23	69,73,73	1.24	10 (14%)	83,113,113	1.48	11 (13%)
14	CLA	G	1108	1	58,62,73	1.34	10 (17%)	69,99,113	1.45	8 (11%)
14	CLA	t	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	f	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	10 (12%)
14	CLA	H	1232	23	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	T	1302	8	59,63,73	1.30	9 (15%)	71,101,113	1.46	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	SQD	v	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	a	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.53	8 (13%)
14	CLA	b	504	-	49,53,73	1.48	7 (14%)	59,89,113	1.48	5 (8%)
14	CLA	3	506	13	49,53,73	1.49	10 (20%)	59,89,113	1.51	7 (11%)
14	CLA	c	509	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
16	SF4	g	3003	3	0,12,12	-	-	-		
17	BCR	Y	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
18	LHG	L	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
14	CLA	e	1113	1	49,53,73	1.45	11 (22%)	59,89,113	1.59	8 (13%)
17	BCR	H	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.31	21 (37%)
14	CLA	q	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.72	8 (13%)
17	BCR	T	4013	-	41,41,41	0.78	0	56,56,56	1.93	16 (28%)
14	CLA	d	508	13	49,53,73	1.49	9 (18%)	59,89,113	1.59	11 (18%)
14	CLA	f	1202	2	69,73,73	1.23	11 (15%)	83,113,113	1.42	8 (9%)
14	CLA	a	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.52	6 (10%)
14	CLA	B	1222	23	54,58,73	1.40	10 (18%)	65,95,113	1.54	10 (15%)
14	CLA	Y	501	13	49,53,73	1.47	9 (18%)	59,89,113	1.53	4 (6%)
17	BCR	L	4219	-	41,41,41	1.09	5 (12%)	56,56,56	2.26	23 (41%)
17	BCR	f	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.30	21 (37%)
21	SQD	5	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
14	CLA	b	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.58	8 (13%)
14	CLA	A	1105	1	59,63,73	1.31	10 (16%)	71,101,113	1.49	9 (12%)
17	BCR	5	524	-	41,41,41	0.71	0	56,56,56	1.74	12 (21%)
14	CLA	u	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
14	CLA	H	1012	23	69,73,73	1.28	11 (15%)	83,113,113	1.42	10 (12%)
17	BCR	r	524	-	41,41,41	0.74	0	56,56,56	1.76	13 (23%)
14	CLA	5	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)
14	CLA	s	512	13	49,53,73	1.50	10 (20%)	59,89,113	1.39	5 (8%)
14	CLA	r	519	13	49,53,73	1.48	9 (18%)	59,89,113	1.50	7 (11%)
17	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.76	12 (21%)
18	LHG	e	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
17	BCR	q	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	4	513	13	49,53,73	1.49	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	2	502	13	49,53,73	1.47	9 (18%)	59,89,113	1.58	8 (13%)
14	CLA	f	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.49	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	s	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.60	8 (13%)
14	CLA	4	517	-	49,53,73	1.49	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	f	1209	2	57,61,73	1.38	11 (19%)	68,98,113	1.54	8 (11%)
14	CLA	f	1225	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	11 (13%)
17	BCR	f	4009	-	41,41,41	0.78	0	56,56,56	1.89	18 (32%)
14	CLA	b	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
14	CLA	u	519	13	49,53,73	1.47	8 (16%)	59,89,113	1.48	6 (10%)
14	CLA	3	510	13	49,53,73	1.47	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	6	511	13	49,53,73	1.50	8 (16%)	59,89,113	1.54	5 (8%)
14	CLA	2	501	13	64,68,73	1.28	9 (14%)	77,107,113	1.46	7 (9%)
14	CLA	B	1021	2	69,73,73	1.27	10 (14%)	83,113,113	1.39	8 (9%)
21	SQD	a	822	-	27,28,54	1.30	5 (18%)	36,39,65	1.79	10 (27%)
14	CLA	B	1207	2	69,73,73	1.25	9 (13%)	83,113,113	1.31	4 (4%)
21	SQD	V	5216	-	45,46,54	1.01	5 (11%)	54,57,65	1.69	11 (20%)
17	BCR	o	4021	-	41,41,41	0.77	0	56,56,56	1.91	15 (26%)
21	SQD	q	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
17	BCR	v	523	-	41,41,41	0.72	0	56,56,56	1.72	15 (26%)
14	CLA	B	1226	2	59,63,73	1.49	11 (18%)	71,101,113	1.81	17 (23%)
14	CLA	e	1119	23	69,73,73	1.32	10 (14%)	83,113,113	1.54	14 (16%)
14	CLA	q	516	13	49,53,73	1.46	10 (20%)	59,89,113	1.48	6 (10%)
14	CLA	d	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.56	5 (8%)
14	CLA	G	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.55	12 (14%)
14	CLA	B	1223	2	69,73,73	1.25	11 (15%)	83,113,113	1.47	7 (8%)
14	CLA	r	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	10 (16%)
14	CLA	B	1219	2	67,71,73	1.28	9 (13%)	80,110,113	1.35	10 (12%)
14	CLA	G	1135	1	59,63,73	1.36	8 (13%)	71,101,113	1.61	13 (18%)
14	CLA	6	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	7 (11%)
14	CLA	d	505	13	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
14	CLA	e	1135	1	59,63,73	1.37	9 (15%)	71,101,113	1.60	13 (18%)
21	SQD	n	5216	-	45,46,54	1.02	5 (11%)	54,57,65	1.68	11 (20%)
14	CLA	e	1116	1	64,68,73	1.31	11 (17%)	77,107,113	1.35	9 (11%)
14	CLA	1	512	13	49,53,73	1.47	11 (22%)	59,89,113	1.39	4 (6%)
14	CLA	J	1303	8	49,53,73	1.46	10 (20%)	59,89,113	1.60	8 (13%)
14	CLA	A	1237	23	69,73,73	1.27	13 (18%)	83,113,113	1.53	10 (12%)
17	BCR	1	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LHG	e	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
16	SF4	e	3001	2,1	0,12,12	-	-	-		
14	CLA	v	511	13	49,53,73	1.50	7 (14%)	59,89,113	1.54	5 (8%)
14	CLA	e	1107	1	69,73,73	1.31	10 (14%)	83,113,113	1.40	10 (12%)
14	CLA	5	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.49	5 (8%)
14	CLA	H	1207	2	69,73,73	1.25	9 (13%)	83,113,113	1.32	4 (4%)
17	BCR	H	4014	-	41,41,41	0.83	0	56,56,56	1.89	23 (41%)
14	CLA	B	1211	2	59,63,73	1.33	11 (18%)	71,101,113	1.49	8 (11%)
14	CLA	H	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.49	11 (13%)
17	BCR	e	4003	-	41,41,41	0.87	1 (2%)	56,56,56	1.78	14 (25%)
14	CLA	e	1127	1	69,73,73	1.26	11 (15%)	83,113,113	1.40	11 (13%)
14	CLA	H	1230	2	64,68,73	1.31	10 (15%)	77,107,113	1.39	6 (7%)
17	BCR	6	521	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
14	CLA	A	1135	1	59,63,73	1.36	9 (15%)	71,101,113	1.61	13 (18%)
17	BCR	L	4020	-	41,41,41	0.98	2 (4%)	56,56,56	1.67	15 (26%)
17	BCR	4	524	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
17	BCR	G	4003	-	41,41,41	0.87	1 (2%)	56,56,56	1.78	14 (25%)
14	CLA	a	518	13	59,63,73	1.35	9 (15%)	71,101,113	1.38	5 (7%)
14	CLA	B	1213	2	65,69,73	1.26	10 (15%)	78,108,113	1.48	10 (12%)
14	CLA	s	503	13	49,53,73	1.49	8 (16%)	59,89,113	1.50	7 (11%)
17	BCR	q	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	5	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	4 (6%)
17	BCR	v	521	-	41,41,41	0.68	0	56,56,56	1.79	12 (21%)
19	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
14	CLA	Y	505	13	49,53,73	1.46	8 (16%)	59,89,113	1.49	4 (6%)
14	CLA	3	519	13	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	f	1208	2	69,73,73	1.23	9 (13%)	83,113,113	1.28	7 (8%)
14	CLA	e	1022	23	69,73,73	1.32	10 (14%)	83,113,113	1.38	12 (14%)
14	CLA	f	1228	2	59,63,73	1.31	10 (16%)	71,101,113	1.51	7 (9%)
14	CLA	d	519	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	5 (8%)
14	CLA	B	1240	18	69,73,73	1.26	9 (13%)	83,113,113	1.35	8 (9%)
17	BCR	M	4021	-	41,41,41	0.76	0	56,56,56	1.91	15 (26%)
21	SQD	Z	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	A	1110	1	57,61,73	1.37	10 (17%)	68,98,113	1.45	7 (10%)
14	CLA	A	1102	1	59,63,73	1.35	12 (20%)	71,101,113	1.45	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	5	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.54	5 (8%)
14	CLA	r	505	13	69,73,73	1.23	8 (11%)	83,113,113	1.32	7 (8%)
14	CLA	a	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	G	1102	1	59,63,73	1.35	11 (18%)	71,101,113	1.45	8 (11%)
14	CLA	t	503	13	49,53,73	1.51	9 (18%)	59,89,113	1.55	6 (10%)
17	BCR	u	523	-	41,41,41	0.78	0	56,56,56	1.79	15 (26%)
21	SQD	u	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
14	CLA	A	1109	1	69,73,73	1.25	11 (15%)	83,113,113	1.47	8 (9%)
15	PQN	A	2001	-	34,34,34	2.81	11 (32%)	42,45,45	2.19	6 (14%)
14	CLA	1	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.64	7 (11%)
17	BCR	4	523	-	41,41,41	0.74	0	56,56,56	1.77	14 (25%)
21	SQD	t	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
15	PQN	f	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.30	6 (14%)
14	CLA	b	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.42	4 (6%)
14	CLA	c	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.55	6 (10%)
14	CLA	H	1235	2	69,73,73	1.27	11 (15%)	83,113,113	1.41	7 (8%)
14	CLA	c	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
14	CLA	1	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	2	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	10 (16%)
14	CLA	j	1302	6	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
14	CLA	q	511	13	49,53,73	1.49	9 (18%)	59,89,113	1.52	9 (15%)
14	CLA	m	1103	9	52,56,73	1.43	10 (19%)	62,92,113	1.50	6 (9%)
14	CLA	s	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
17	BCR	t	524	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
14	CLA	1	517	-	49,53,73	1.46	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	H	1240	18	69,73,73	1.26	9 (13%)	83,113,113	1.35	8 (9%)
14	CLA	Z	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.39	5 (8%)
17	BCR	c	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	c	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
17	BCR	e	4007	-	41,41,41	0.87	0	56,56,56	2.10	19 (33%)
14	CLA	H	1236	2	54,58,73	1.41	9 (16%)	65,95,113	1.43	9 (13%)
14	CLA	c	519	13	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	e	1128	1	69,73,73	1.36	11 (15%)	83,113,113	1.60	12 (14%)
14	CLA	R	1301	23	49,53,73	1.48	11 (22%)	59,89,113	1.47	5 (8%)
17	BCR	r	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	e	1108	1	58,62,73	1.34	8 (13%)	69,99,113	1.45	7 (10%)
14	CLA	a	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	8 (13%)
14	CLA	q	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.65	10 (16%)
14	CLA	u	509	13	69,73,73	1.24	10 (14%)	83,113,113	1.35	7 (8%)
17	BCR	1	523	-	41,41,41	0.75	0	56,56,56	1.69	13 (23%)
14	CLA	6	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	6 (10%)
14	CLA	2	503	13	69,73,73	1.25	8 (11%)	83,113,113	1.35	6 (7%)
17	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
14	CLA	v	505	13	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
18	LHG	G	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	c	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.43	5 (8%)
14	CLA	q	518	13	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	B	1214	2	69,73,73	1.26	9 (13%)	83,113,113	1.45	6 (7%)
14	CLA	G	1110	1	57,61,73	1.37	10 (17%)	68,98,113	1.45	7 (10%)
17	BCR	u	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	v	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	d	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
18	LHG	G	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
17	BCR	H	4005	-	41,41,41	0.76	0	56,56,56	1.73	12 (21%)
14	CLA	d	503	13	49,53,73	1.47	8 (16%)	59,89,113	1.54	5 (8%)
15	PQN	G	2001	-	34,34,34	2.82	11 (32%)	42,45,45	2.20	6 (14%)
14	CLA	G	1127	1	69,73,73	1.25	10 (14%)	83,113,113	1.39	11 (13%)
14	CLA	B	1210	2	69,73,73	1.26	12 (17%)	83,113,113	1.36	10 (12%)
14	CLA	r	506	13	49,53,73	1.46	9 (18%)	59,89,113	1.49	7 (11%)
14	CLA	c	511	13	49,53,73	1.49	7 (14%)	59,89,113	1.54	9 (15%)
14	CLA	1	511	13	49,53,73	1.49	8 (16%)	59,89,113	1.53	8 (13%)
21	SQD	s	822	-	27,28,54	1.29	5 (18%)	36,39,65	1.80	10 (27%)
14	CLA	B	1215	2	69,73,73	1.26	10 (14%)	83,113,113	1.55	11 (13%)
14	CLA	5	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.65	7 (11%)
14	CLA	2	516	13	49,53,73	1.46	8 (16%)	59,89,113	1.51	6 (10%)
14	CLA	f	1021	2	69,73,73	1.27	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	q	506	13	49,53,73	1.47	8 (16%)	59,89,113	1.45	6 (10%)
17	BCR	A	4001	-	41,41,41	0.79	0	56,56,56	1.69	11 (19%)
14	CLA	A	1113	1	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
14	CLA	f	1204	2	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	s	513	13	49,53,73	1.48	8 (16%)	59,89,113	1.47	5 (8%)
17	BCR	U	4104	-	41,41,41	0.78	0	56,56,56	1.88	16 (28%)
14	CLA	3	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.52	6 (10%)
14	CLA	f	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.37	9 (11%)
14	CLA	6	513	13	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	H	1216	23	64,68,73	1.34	11 (17%)	77,107,113	1.52	10 (12%)
14	CLA	B	1236	2	54,58,73	1.41	9 (16%)	65,95,113	1.43	9 (13%)
17	BCR	5	523	-	41,41,41	0.78	1 (2%)	56,56,56	1.78	15 (26%)
15	PQN	H	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.30	6 (14%)
14	CLA	G	1123	23	69,73,73	1.26	11 (15%)	83,113,113	1.38	9 (10%)
14	CLA	s	517	-	49,53,73	1.49	10 (20%)	59,89,113	1.45	4 (6%)
14	CLA	4	503	13	49,53,73	1.50	9 (18%)	59,89,113	1.55	6 (10%)
17	BCR	4	521	-	41,41,41	0.67	0	56,56,56	1.79	11 (19%)
14	CLA	G	1114	23	49,53,73	1.51	9 (18%)	59,89,113	1.57	9 (15%)
17	BCR	H	4004	-	41,41,41	0.73	0	56,56,56	1.85	14 (25%)
14	CLA	5	509	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	A	1125	1	69,73,73	1.26	11 (15%)	83,113,113	1.46	8 (9%)
14	CLA	Y	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.46	4 (6%)
17	BCR	l	4013	-	41,41,41	0.77	0	56,56,56	1.93	16 (28%)
18	LHG	V	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	3	516	13	49,53,73	1.48	7 (14%)	59,89,113	1.71	9 (15%)
18	LHG	V	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
14	CLA	H	1231	23	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
17	BCR	F	4016	-	41,41,41	0.82	0	56,56,56	1.91	11 (19%)
17	BCR	G	4001	-	41,41,41	0.79	0	56,56,56	1.68	11 (19%)
14	CLA	Z	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	t	513	13	49,53,73	1.49	8 (16%)	59,89,113	1.49	4 (6%)
14	CLA	3	502	13	49,53,73	1.48	8 (16%)	59,89,113	1.60	8 (13%)
17	BCR	B	4005	-	41,41,41	0.76	0	56,56,56	1.72	12 (21%)
14	CLA	3	513	13	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	c	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.64	8 (13%)
14	CLA	e	1134	1	60,64,73	1.32	9 (15%)	72,102,113	1.50	9 (12%)
14	CLA	Z	518	13	59,63,73	1.33	9 (15%)	71,101,113	1.41	5 (7%)
20	LMG	f	5002	-	53,53,55	0.85	2 (3%)	61,61,63	1.51	12 (19%)
14	CLA	A	1126	1	69,73,73	1.23	12 (17%)	83,113,113	1.38	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	V	4022	-	41,41,41	0.78	0	56,56,56	1.81	10 (17%)
14	CLA	4	501	13	49,53,73	1.47	8 (16%)	59,89,113	1.50	5 (8%)
14	CLA	u	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
14	CLA	A	1123	23	69,73,73	1.25	11 (15%)	83,113,113	1.38	9 (10%)
18	LHG	n	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	t	504	-	49,53,73	1.49	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	u	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
14	CLA	H	1227	2	64,68,73	1.30	11 (17%)	77,107,113	1.44	7 (9%)
14	CLA	f	1219	2	67,71,73	1.27	10 (14%)	80,110,113	1.35	10 (12%)
14	CLA	B	1239	2	69,73,73	1.26	9 (13%)	83,113,113	1.65	14 (16%)
21	SQD	c	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
17	BCR	c	523	-	41,41,41	0.78	1 (2%)	56,56,56	1.78	15 (26%)
14	CLA	e	1115	1	64,68,73	1.29	11 (17%)	77,107,113	1.48	8 (10%)
14	CLA	G	1117	1	69,73,73	1.27	10 (14%)	83,113,113	1.44	11 (13%)
14	CLA	e	1136	1	69,73,73	1.27	9 (13%)	83,113,113	1.46	9 (10%)
14	CLA	4	511	13	49,53,73	1.50	10 (20%)	59,89,113	1.51	9 (15%)
14	CLA	e	1801	18	49,53,73	1.44	11 (22%)	59,89,113	1.51	7 (11%)
17	BCR	Z	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
18	LHG	S	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
17	BCR	B	4009	-	41,41,41	0.77	0	56,56,56	1.90	18 (32%)
17	BCR	1	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	B	1227	2	64,68,73	1.30	11 (17%)	77,107,113	1.45	7 (9%)
14	CLA	B	1225	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	10 (12%)
14	CLA	G	1129	1	57,61,73	1.41	10 (17%)	68,98,113	1.52	11 (16%)
14	CLA	d	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.55	7 (11%)
18	LHG	e	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
14	CLA	n	1501	10	64,68,73	1.33	10 (15%)	77,107,113	1.41	9 (11%)
14	CLA	A	1130	1	60,64,73	1.33	11 (18%)	72,102,113	1.54	11 (15%)
14	CLA	U	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.49	10 (14%)
14	CLA	b	513	13	49,53,73	1.49	9 (18%)	59,89,113	1.49	4 (6%)
14	CLA	l	1303	8	49,53,73	1.47	10 (20%)	59,89,113	1.61	8 (13%)
14	CLA	n	1502	10	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
14	CLA	Z	503	13	69,73,73	1.26	8 (11%)	83,113,113	1.35	6 (7%)
14	CLA	G	1125	1	69,73,73	1.26	11 (15%)	83,113,113	1.46	8 (9%)
14	CLA	e	1126	1	69,73,73	1.23	12 (17%)	83,113,113	1.38	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	l	1302	8	59,63,73	1.30	9 (15%)	71,101,113	1.46	7 (9%)
14	CLA	A	1117	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	11 (13%)
14	CLA	B	1220	2	59,63,73	1.35	10 (16%)	71,101,113	1.54	8 (11%)
14	CLA	A	1139	23	69,73,73	1.27	11 (15%)	83,113,113	1.29	7 (8%)
14	CLA	e	1123	23	69,73,73	1.25	11 (15%)	83,113,113	1.38	9 (10%)
14	CLA	s	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	7 (11%)
14	CLA	3	518	13	59,63,73	1.35	9 (15%)	71,101,113	1.38	5 (7%)
14	CLA	B	1216	23	64,68,73	1.33	10 (15%)	77,107,113	1.51	10 (12%)
17	BCR	V	4219	-	41,41,41	1.08	5 (12%)	56,56,56	2.26	23 (41%)
17	BCR	d	524	-	41,41,41	0.79	0	56,56,56	1.84	15 (26%)
14	CLA	v	513	13	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	b	501	13	49,53,73	1.47	9 (18%)	59,89,113	1.49	5 (8%)
14	CLA	Y	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	Z	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.55	7 (11%)
18	LHG	f	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
14	CLA	6	505	13	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
14	CLA	6	517	-	49,53,73	1.46	8 (16%)	59,89,113	1.47	6 (10%)
14	CLA	n	1503	23	64,68,73	1.28	10 (15%)	77,107,113	1.42	5 (6%)
17	BCR	5	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	A	1111	1	69,73,73	1.25	11 (15%)	83,113,113	1.40	9 (10%)
14	CLA	B	1218	2	64,68,73	1.30	9 (14%)	77,107,113	1.34	5 (6%)
14	CLA	e	1139	23	69,73,73	1.27	11 (15%)	83,113,113	1.28	7 (8%)
14	CLA	A	1122	1	64,68,73	1.30	11 (17%)	77,107,113	1.44	8 (10%)
14	CLA	G	1237	23	69,73,73	1.27	13 (18%)	83,113,113	1.53	10 (12%)
18	LHG	G	5008	-	34,34,48	0.71	1 (2%)	37,40,54	1.25	3 (8%)
14	CLA	B	1206	2	69,73,73	1.29	12 (17%)	83,113,113	1.48	11 (13%)
14	CLA	Y	509	13	49,53,73	1.49	9 (18%)	59,89,113	1.52	8 (13%)
17	BCR	2	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
18	LHG	G	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	2	518	13	59,63,73	1.33	8 (13%)	71,101,113	1.41	5 (7%)
14	CLA	H	1220	2	59,63,73	1.35	10 (16%)	71,101,113	1.54	8 (11%)
18	LHG	H	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.26	3 (7%)
17	BCR	R	4016	-	41,41,41	0.81	0	56,56,56	1.91	12 (21%)
14	CLA	A	1011	1	69,73,73	1.27	8 (11%)	83,113,113	1.66	14 (16%)
16	SF4	N	3002	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	t	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.63	9 (15%)
14	CLA	5	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.56	6 (10%)
14	CLA	5	503	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
17	BCR	c	522	-	41,41,41	0.76	0	56,56,56	1.94	20 (35%)
14	CLA	5	506	13	49,53,73	1.47	10 (20%)	59,89,113	1.46	5 (8%)
14	CLA	a	504	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)
14	CLA	G	1103	1	69,73,73	1.28	12 (17%)	83,113,113	1.58	11 (13%)
14	CLA	v	518	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
17	BCR	t	523	-	41,41,41	0.73	0	56,56,56	1.77	14 (25%)
18	LHG	A	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	L	1502	10	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
17	BCR	V	4020	-	41,41,41	0.99	2 (4%)	56,56,56	1.67	15 (26%)
14	CLA	G	1121	1	59,63,73	1.36	11 (18%)	71,101,113	1.55	10 (14%)
19	LMU	J	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
14	CLA	2	505	13	69,73,73	1.23	9 (13%)	83,113,113	1.33	7 (8%)
18	LHG	H	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
14	CLA	f	1213	2	65,69,73	1.26	11 (16%)	78,108,113	1.48	9 (11%)
14	CLA	G	1011	1	69,73,73	1.27	8 (11%)	83,113,113	1.66	14 (16%)
14	CLA	f	1230	2	64,68,73	1.30	10 (15%)	77,107,113	1.39	6 (7%)
17	BCR	s	522	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)
14	CLA	c	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.46	4 (6%)
17	BCR	v	522	-	41,41,41	0.71	0	56,56,56	1.89	19 (33%)
17	BCR	H	4006	-	41,41,41	0.78	0	56,56,56	2.09	18 (32%)
14	CLA	A	1103	1	69,73,73	1.28	12 (17%)	83,113,113	1.58	11 (13%)
17	BCR	6	522	-	41,41,41	0.72	0	56,56,56	1.89	19 (33%)
14	CLA	5	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
14	CLA	4	509	13	49,53,73	1.48	11 (22%)	59,89,113	1.59	9 (15%)
14	CLA	1	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	7 (11%)
14	CLA	H	1021	2	69,73,73	1.26	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	a	506	13	49,53,73	1.48	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	f	1235	2	69,73,73	1.27	12 (17%)	83,113,113	1.42	7 (8%)
14	CLA	B	1232	23	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	A	1121	1	59,63,73	1.36	11 (18%)	71,101,113	1.55	10 (14%)
21	SQD	B	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	L	1503	23	64,68,73	1.28	10 (15%)	77,107,113	1.42	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	t	517	-	49,53,73	1.48	7 (14%)	59,89,113	1.53	6 (10%)
14	CLA	a	505	13	59,63,73	1.34	9 (15%)	71,101,113	1.35	5 (7%)
14	CLA	b	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.63	9 (15%)
16	SF4	G	3001	2,1	0,12,12	-	-	-		
21	SQD	H	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	B	1217	2	64,68,73	1.29	9 (14%)	77,107,113	1.33	5 (6%)
14	CLA	r	512	13	49,53,73	1.48	10 (20%)	59,89,113	1.40	5 (8%)
20	LMG	H	5002	-	53,53,55	0.86	3 (5%)	61,61,63	1.51	12 (19%)
15	PQN	e	2001	-	34,34,34	2.81	11 (32%)	42,45,45	2.19	6 (14%)
14	CLA	4	502	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	5 (8%)
14	CLA	H	1239	2	69,73,73	1.27	10 (14%)	83,113,113	1.65	13 (15%)
18	LHG	k	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
14	CLA	G	1124	23	64,68,73	1.33	11 (17%)	77,107,113	1.46	10 (12%)
14	CLA	6	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
14	CLA	A	1104	1	69,73,73	1.26	13 (18%)	83,113,113	1.47	13 (15%)
17	BCR	l	4012	-	41,41,41	0.73	0	56,56,56	1.75	12 (21%)
14	CLA	e	1106	1	69,73,73	1.23	11 (15%)	83,113,113	1.41	8 (9%)
14	CLA	t	509	13	49,53,73	1.48	11 (22%)	59,89,113	1.58	9 (15%)
14	CLA	v	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
14	CLA	4	506	13	49,53,73	1.48	9 (18%)	59,89,113	1.51	5 (8%)
14	CLA	b	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.58	7 (11%)
19	LMU	f	1843	-	36,36,36	1.16	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	2	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
14	CLA	G	1132	1	69,73,73	1.25	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	c	516	13	49,53,73	1.47	9 (18%)	59,89,113	1.41	4 (6%)
17	BCR	r	523	-	41,41,41	0.72	0	56,56,56	1.75	17 (30%)
17	BCR	t	521	-	41,41,41	0.67	0	56,56,56	1.79	10 (17%)
21	SQD	r	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	c	506	13	49,53,73	1.47	10 (20%)	59,89,113	1.46	5 (8%)
14	CLA	A	1129	1	57,61,73	1.41	10 (17%)	68,98,113	1.52	11 (16%)
14	CLA	1	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.46	7 (11%)
14	CLA	3	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.39	5 (8%)
17	BCR	q	523	-	41,41,41	0.75	0	56,56,56	1.68	13 (23%)
14	CLA	H	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.36	9 (11%)
17	BCR	c	524	-	41,41,41	0.72	0	56,56,56	1.74	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	f	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.74	12 (14%)
18	LHG	A	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	d	512	13	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
17	BCR	d	522	-	41,41,41	0.71	0	56,56,56	1.89	19 (33%)
17	BCR	k	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	16 (28%)
14	CLA	b	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	u	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.49	5 (8%)
17	BCR	I	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	17 (30%)
14	CLA	u	516	13	49,53,73	1.47	9 (18%)	59,89,113	1.41	4 (6%)
14	CLA	6	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.56	5 (8%)
14	CLA	Y	518	13	49,53,73	1.48	7 (14%)	59,89,113	1.52	6 (10%)
14	CLA	a	516	13	49,53,73	1.48	7 (14%)	59,89,113	1.71	9 (15%)
14	CLA	e	1138	1	69,73,73	1.23	9 (13%)	83,113,113	1.44	6 (7%)
21	SQD	2	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	G	1112	1	54,58,73	1.39	12 (22%)	65,95,113	1.53	7 (10%)
14	CLA	6	508	13	49,53,73	1.49	9 (18%)	59,89,113	1.60	11 (18%)
14	CLA	Z	505	13	69,73,73	1.23	7 (10%)	83,113,113	1.33	7 (8%)
14	CLA	G	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.69	14 (16%)
14	CLA	f	1221	23	66,70,73	1.32	11 (16%)	79,109,113	1.53	12 (15%)
14	CLA	r	517	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	c	510	13	49,53,73	1.47	10 (20%)	59,89,113	1.49	5 (8%)
14	CLA	u	511	13	49,53,73	1.49	7 (14%)	59,89,113	1.54	9 (15%)
14	CLA	5	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
17	BCR	5	522	-	41,41,41	0.76	0	56,56,56	1.94	20 (35%)
17	BCR	j	4016	-	41,41,41	0.82	0	56,56,56	1.91	11 (19%)
14	CLA	Y	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	7 (11%)
14	CLA	q	517	-	49,53,73	1.46	9 (18%)	59,89,113	1.45	5 (8%)
17	BCR	Y	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	H	1218	2	64,68,73	1.30	9 (14%)	77,107,113	1.36	5 (6%)
14	CLA	A	1140	1	69,73,73	1.26	10 (14%)	83,113,113	1.47	9 (10%)
14	CLA	B	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.74	12 (14%)
22	FMN	X	170	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	2	519	13	49,53,73	1.48	9 (18%)	59,89,113	1.50	7 (11%)
14	CLA	H	1210	2	69,73,73	1.27	11 (15%)	83,113,113	1.36	10 (12%)
14	CLA	q	512	13	49,53,73	1.47	10 (20%)	59,89,113	1.38	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	Y	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
14	CLA	A	1112	1	54,58,73	1.39	12 (22%)	65,95,113	1.54	7 (10%)
18	LHG	G	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	6	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	d	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
14	CLA	t	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	4 (6%)
14	CLA	r	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)
14	CLA	s	510	13	49,53,73	1.47	10 (20%)	59,89,113	1.49	5 (8%)
17	BCR	L	4022	-	41,41,41	0.79	0	56,56,56	1.82	10 (17%)
21	SQD	4	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
14	CLA	Y	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.64	8 (13%)
14	CLA	A	1107	1	69,73,73	1.31	10 (14%)	83,113,113	1.40	10 (12%)
17	BCR	l	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
14	CLA	3	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
14	CLA	q	509	13	49,53,73	1.49	10 (20%)	59,89,113	1.51	8 (13%)
18	LHG	e	5007	-	46,46,48	0.61	0	49,52,54	1.20	4 (8%)
14	CLA	3	504	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)
14	CLA	H	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.75	12 (14%)
14	CLA	r	511	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	8 (13%)
17	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	4	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.63	9 (15%)
18	LHG	A	5009	-	41,41,48	0.67	0	44,47,54	1.22	5 (11%)
14	CLA	2	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.55	7 (11%)
14	CLA	6	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.55	6 (10%)
21	SQD	d	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	1	505	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
17	BCR	m	4104	-	41,41,41	0.79	0	56,56,56	1.88	16 (28%)
14	CLA	c	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	4 (6%)
14	CLA	1	518	13	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
17	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
19	LMU	B	1843	-	36,36,36	1.16	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	Z	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
17	BCR	e	4001	-	41,41,41	0.79	0	56,56,56	1.69	11 (19%)
14	CLA	G	1122	1	64,68,73	1.31	11 (17%)	77,107,113	1.43	8 (10%)
14	CLA	u	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.56	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LHG	e	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	G	1126	1	69,73,73	1.24	12 (17%)	83,113,113	1.38	7 (8%)
14	CLA	G	1107	1	69,73,73	1.31	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	G	1109	1	69,73,73	1.25	11 (15%)	83,113,113	1.47	8 (9%)
14	CLA	B	1203	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	Z	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	t	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	r	518	13	59,63,73	1.33	9 (15%)	71,101,113	1.41	6 (8%)
14	CLA	2	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.39	5 (8%)
14	CLA	u	517	-	49,53,73	1.49	10 (20%)	59,89,113	1.42	4 (6%)
14	CLA	3	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
17	BCR	e	4002	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	16 (28%)
14	CLA	U	1103	9	52,56,73	1.44	10 (19%)	62,92,113	1.51	6 (9%)
14	CLA	d	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	6 (10%)
14	CLA	H	1202	2	69,73,73	1.22	11 (15%)	83,113,113	1.42	8 (9%)
17	BCR	f	4004	-	41,41,41	0.74	0	56,56,56	1.85	14 (25%)

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
17	BCR	W	4021	-	-	6/29/63/63	0/2/2/2
14	CLA	B	1212	2	-	8/23/99/115	-
14	CLA	V	1501	10	-	11/33/109/115	-
17	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	s	507	-	-	7/15/91/115	-
17	BCR	r	522	-	-	6/29/63/63	0/2/2/2
14	CLA	s	516	13	-	9/15/91/115	-
14	CLA	m	1401	-	-	10/27/103/115	-
14	CLA	f	1012	23	-	15/39/115/115	-
17	BCR	d	521	-	-	5/29/63/63	0/2/2/2
20	LMG	l	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	Z	509	13	-	3/39/115/115	-
18	LHG	G	5009	-	-	28/46/46/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	n	4022	-	-	3/29/63/63	0/2/2/2
17	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	G	1131	1	-	8/39/115/115	-
18	LHG	B	1855	-	-	24/45/45/53	-
20	LMG	T	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	e	1114	23	-	3/15/91/115	-
18	LHG	e	5008	-	-	18/39/39/53	-
14	CLA	B	1228	2	-	6/27/103/115	-
14	CLA	A	1127	1	-	12/39/115/115	-
17	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
14	CLA	q	503	13	-	9/15/91/115	-
19	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	A	1137	1	-	20/33/109/115	-
14	CLA	5	511	13	-	3/15/91/115	-
14	CLA	4	512	13	-	5/15/91/115	-
14	CLA	6	516	13	-	11/15/91/115	-
17	BCR	b	524	-	-	4/29/63/63	0/2/2/2
17	BCR	a	524	-	-	5/29/63/63	0/2/2/2
14	CLA	U	1105	9	-	10/15/91/115	-
14	CLA	5	507	-	-	9/15/91/115	-
14	CLA	m	1105	9	-	10/15/91/115	-
14	CLA	H	1226	2	-	7/27/103/115	-
14	CLA	A	1115	1	-	13/33/109/115	-
14	CLA	f	1216	23	-	13/33/109/115	-
14	CLA	H	1238	23	-	4/39/115/115	-
14	CLA	Y	519	13	-	8/15/91/115	-
14	CLA	f	1236	2	-	5/21/97/115	-
14	CLA	f	1232	23	-	6/27/103/115	-
14	CLA	f	1205	2	-	10/39/115/115	-
14	CLA	G	1137	1	-	20/33/109/115	-
17	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
17	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1013	-	-	13/39/115/115	-
14	CLA	c	502	13	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1206	2	-	15/39/115/115	-
14	CLA	B	1208	2	-	17/39/115/115	-
14	CLA	A	1101	1	-	18/39/115/115	-
14	CLA	J	1302	8	-	14/27/103/115	-
14	CLA	1	503	13	-	9/15/91/115	-
14	CLA	A	1124	23	-	13/33/109/115	-
14	CLA	3	501	13	-	6/15/91/115	-
14	CLA	f	1207	2	-	18/39/115/115	-
14	CLA	d	518	13	-	9/15/91/115	-
14	CLA	f	1206	2	-	15/39/115/115	-
14	CLA	e	1125	1	-	12/39/115/115	-
14	CLA	b	502	13	-	5/15/91/115	-
14	CLA	G	1134	1	-	11/29/105/115	-
18	LHG	n	5220	-	-	28/45/45/53	-
14	CLA	A	1138	1	-	14/39/115/115	-
14	CLA	e	1011	1	-	12/39/115/115	-
14	CLA	Z	507	-	-	10/15/91/115	-
17	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
14	CLA	t	512	13	-	5/15/91/115	-
17	BCR	t	522	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1237	23	-	25/39/115/115	-
14	CLA	H	1208	2	-	17/39/115/115	-
14	CLA	s	509	13	-	2/15/91/115	-
14	CLA	F	1302	6	-	9/15/91/115	-
14	CLA	A	1801	18	-	7/15/91/115	-
14	CLA	B	1235	2	-	9/39/115/115	-
14	CLA	G	1111	1	-	20/39/115/115	-
14	CLA	H	1225	2	-	7/39/115/115	-
14	CLA	v	509	13	-	4/15/91/115	-
17	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
17	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
18	LHG	e	5003	14	-	17/44/44/53	-
14	CLA	A	1134	1	-	11/29/105/115	-
14	CLA	4	504	-	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	q	513	13	-	6/15/91/115	-
14	CLA	Z	513	13	-	4/15/91/115	-
14	CLA	u	502	13	-	7/15/91/115	-
14	CLA	4	507	-	-	8/15/91/115	-
17	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
17	BCR	a	522	-	-	5/29/63/63	0/2/2/2
14	CLA	G	1113	1	-	6/15/91/115	-
14	CLA	R	1302	6	-	9/15/91/115	-
14	CLA	B	1221	23	-	14/36/112/115	-
14	CLA	a	513	13	-	5/15/91/115	-
14	CLA	1	510	13	-	6/15/91/115	-
14	CLA	f	1240	18	-	15/39/115/115	-
14	CLA	T	1303	8	-	6/15/91/115	-
14	CLA	G	1104	1	-	10/39/115/115	-
14	CLA	G	1138	1	-	14/39/115/115	-
14	CLA	r	510	13	-	7/15/91/115	-
17	BCR	3	522	-	-	5/29/63/63	0/2/2/2
14	CLA	e	1121	1	-	10/27/103/115	-
14	CLA	G	1139	23	-	20/39/115/115	-
14	CLA	F	1301	23	-	3/15/91/115	-
14	CLA	t	511	13	-	5/15/91/115	-
14	CLA	H	1229	2	-	12/39/115/115	-
14	CLA	2	513	13	-	4/15/91/115	-
14	CLA	f	1229	2	-	12/39/115/115	-
20	LMG	B	5002	-	-	24/48/68/70	0/1/1/1
17	BCR	A	4011	-	-	13/29/63/63	0/2/2/2
18	LHG	A	5006	-	-	26/44/44/53	-
14	CLA	t	507	-	-	8/15/91/115	-
14	CLA	Y	516	13	-	14/15/91/115	-
14	CLA	B	1205	2	-	10/39/115/115	-
17	BCR	6	524	-	-	5/29/63/63	0/2/2/2
14	CLA	v	512	13	-	9/15/91/115	-
14	CLA	G	1118	1	-	10/33/109/115	-
15	PQN	B	2002	-	-	6/23/43/43	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1132	1	-	18/39/115/115	-
14	CLA	H	1215	2	-	19/39/115/115	-
17	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
17	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1204	2	-	13/39/115/115	-
17	BCR	s	524	-	-	5/29/63/63	0/2/2/2
14	CLA	H	1228	2	-	6/27/103/115	-
14	CLA	f	1215	2	-	19/39/115/115	-
14	CLA	u	513	13	-	7/15/91/115	-
17	BCR	q	522	-	-	6/29/63/63	0/2/2/2
14	CLA	v	510	13	-	10/15/91/115	-
14	CLA	s	505	13	-	11/27/103/115	-
17	BCR	Y	521	-	-	7/29/63/63	0/2/2/2
14	CLA	e	1013	-	-	13/39/115/115	-
17	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
21	SQD	6	822	-	-	7/19/39/69	0/1/1/1
14	CLA	A	1118	1	-	10/33/109/115	-
18	LHG	L	5218	-	-	19/41/41/53	-
14	CLA	A	1133	1	-	17/39/115/115	-
14	CLA	q	505	13	-	6/15/91/115	-
17	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	5	502	13	-	7/15/91/115	-
14	CLA	G	1140	1	-	14/39/115/115	-
17	BCR	v	524	-	-	5/29/63/63	0/2/2/2
14	CLA	d	511	13	-	8/15/91/115	-
14	CLA	f	1231	23	-	8/39/115/115	-
14	CLA	e	1132	1	-	18/39/115/115	-
14	CLA	a	517	-	-	9/15/91/115	-
14	CLA	c	518	13	-	5/15/91/115	-
18	LHG	G	5004	-	-	18/39/39/53	-
18	LHG	e	5009	-	-	28/46/46/53	-
17	BCR	B	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	e	1131	1	-	8/39/115/115	-
14	CLA	A	1114	23	-	3/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	A	5002	-	-	22/47/47/53	-
17	BCR	2	522	-	-	6/29/63/63	0/2/2/2
14	CLA	6	503	13	-	8/15/91/115	-
14	CLA	6	512	13	-	9/15/91/115	-
14	CLA	v	504	-	-	6/15/91/115	-
14	CLA	B	1230	2	-	12/33/109/115	-
14	CLA	r	516	13	-	8/15/91/115	-
17	BCR	f	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1204	2	-	13/39/115/115	-
14	CLA	b	519	13	-	10/15/91/115	-
14	CLA	s	518	13	-	11/27/103/115	-
14	CLA	B	1224	2	-	7/33/109/115	-
14	CLA	K	1103	9	-	10/19/95/115	-
14	CLA	f	1214	2	-	14/39/115/115	-
17	BCR	b	523	-	-	5/29/63/63	0/2/2/2
14	CLA	a	509	13	-	2/15/91/115	-
14	CLA	e	1140	1	-	14/39/115/115	-
21	SQD	b	822	-	-	10/19/39/69	0/1/1/1
17	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	4	518	13	-	6/15/91/115	-
14	CLA	G	1106	1	-	23/39/115/115	-
14	CLA	B	1234	2	-	15/39/115/115	-
14	CLA	u	503	13	-	9/15/91/115	-
18	LHG	A	5005	-	-	28/47/47/53	-
14	CLA	e	1102	1	-	7/27/103/115	-
17	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
17	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
21	SQD	1	822	-	-	10/27/47/69	0/1/1/1
14	CLA	q	501	13	-	11/15/91/115	-
14	CLA	d	516	13	-	11/15/91/115	-
18	LHG	G	5007	-	-	23/51/51/53	-
14	CLA	d	506	13	-	8/15/91/115	-
14	CLA	B	1238	23	-	4/39/115/115	-
18	LHG	e	5001	-	-	23/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	v	516	13	-	11/15/91/115	-
18	LHG	G	5002	-	-	22/47/47/53	-
14	CLA	4	519	13	-	10/15/91/115	-
14	CLA	A	1106	1	-	23/39/115/115	-
14	CLA	e	1101	1	-	18/39/115/115	-
14	CLA	G	1119	23	-	14/39/115/115	-
14	CLA	G	1105	1	-	8/27/103/115	-
14	CLA	H	1219	2	-	20/37/113/115	-
18	LHG	A	5007	-	-	23/51/51/53	-
19	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
14	CLA	H	1203	2	-	16/39/115/115	-
14	CLA	b	518	13	-	6/15/91/115	-
14	CLA	3	503	13	-	9/15/91/115	-
14	CLA	H	1221	23	-	14/36/112/115	-
17	BCR	4	522	-	-	4/29/63/63	0/2/2/2
14	CLA	r	509	13	-	4/39/115/115	-
18	LHG	A	5008	-	-	18/39/39/53	-
14	CLA	d	507	-	-	7/15/91/115	-
14	CLA	6	519	13	-	8/15/91/115	-
14	CLA	B	1012	23	-	15/39/115/115	-
14	CLA	Z	508	13	-	4/15/91/115	-
14	CLA	f	1218	2	-	9/33/109/115	-
14	CLA	v	501	13	-	9/15/91/115	-
19	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
21	SQD	Y	822	-	-	10/27/47/69	0/1/1/1
18	LHG	f	1842	14	-	19/41/41/53	-
14	CLA	u	508	13	-	6/15/91/115	-
17	BCR	a	521	-	-	7/29/63/63	0/2/2/2
21	SQD	L	5216	-	-	17/41/61/69	0/1/1/1
14	CLA	A	1119	23	-	15/39/115/115	-
14	CLA	H	1214	2	-	14/39/115/115	-
14	CLA	c	503	13	-	9/15/91/115	-
14	CLA	s	519	13	-	7/15/91/115	-
14	CLA	1	513	13	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	d	523	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1116	1	-	9/33/109/115	-
14	CLA	f	1212	2	-	8/23/99/115	-
14	CLA	j	1301	23	-	3/15/91/115	-
14	CLA	r	501	13	-	13/33/109/115	-
14	CLA	t	502	13	-	5/15/91/115	-
14	CLA	e	1109	1	-	16/39/115/115	-
14	CLA	e	1133	1	-	17/39/115/115	-
17	BCR	Z	524	-	-	3/29/63/63	0/2/2/2
16	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	4	505	13	-	5/15/91/115	-
14	CLA	H	1213	2	-	11/35/111/115	-
14	CLA	e	1124	23	-	13/33/109/115	-
14	CLA	f	1210	2	-	22/39/115/115	-
14	CLA	b	503	13	-	4/15/91/115	-
17	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
14	CLA	6	506	13	-	8/15/91/115	-
14	CLA	c	504	-	-	5/15/91/115	-
17	BCR	u	524	-	-	2/29/63/63	0/2/2/2
14	CLA	s	504	-	-	7/15/91/115	-
14	CLA	G	1133	1	-	17/39/115/115	-
14	CLA	e	1104	1	-	10/39/115/115	-
14	CLA	e	1120	1	-	11/21/97/115	-
14	CLA	a	503	13	-	9/15/91/115	-
17	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
16	SF4	g	3002	3	-	-	0/6/5/5
14	CLA	A	1116	1	-	9/33/109/115	-
14	CLA	e	1137	1	-	20/33/109/115	-
14	CLA	e	1117	1	-	13/39/115/115	-
17	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
17	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1120	1	-	11/21/97/115	-
14	CLA	u	504	-	-	5/15/91/115	-
22	FMN	P	170	-	-	0/18/18/18	0/3/3/3
14	CLA	K	1401	-	-	10/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	5	519	13	-	8/15/91/115	-
14	CLA	Y	512	13	-	7/15/91/115	-
14	CLA	2	510	13	-	7/15/91/115	-
21	SQD	f	1852	-	-	18/35/55/69	0/1/1/1
14	CLA	d	517	-	-	12/15/91/115	-
14	CLA	G	1022	23	-	9/39/115/115	-
14	CLA	L	1501	10	-	11/33/109/115	-
14	CLA	Y	502	13	-	4/15/91/115	-
14	CLA	1	519	13	-	8/15/91/115	-
14	CLA	H	1217	2	-	14/33/109/115	-
17	BCR	3	524	-	-	5/29/63/63	0/2/2/2
14	CLA	B	1209	2	-	11/25/101/115	-
14	CLA	e	1110	1	-	12/25/101/115	-
14	CLA	f	1220	2	-	11/27/103/115	-
14	CLA	f	1226	2	-	7/27/103/115	-
14	CLA	K	1105	9	-	10/15/91/115	-
17	BCR	b	521	-	-	10/29/63/63	0/2/2/2
14	CLA	f	1217	2	-	14/33/109/115	-
19	LMU	e	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	s	508	13	-	4/15/91/115	-
14	CLA	H	1209	2	-	11/25/101/115	-
14	CLA	A	1120	1	-	11/21/97/115	-
17	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
17	BCR	G	4011	-	-	13/29/63/63	0/2/2/2
14	CLA	e	1130	1	-	7/29/105/115	-
14	CLA	A	1022	23	-	9/39/115/115	-
14	CLA	H	1222	23	-	2/21/97/115	-
14	CLA	e	1129	1	-	10/25/101/115	-
19	LMU	l	5105	-	-	9/13/33/61	0/1/1/2
17	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	f	1222	23	-	2/21/97/115	-
19	LMU	T	5105	-	-	9/13/33/61	0/1/1/2
14	CLA	v	508	13	-	6/15/91/115	-
14	CLA	v	519	13	-	8/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	q	510	13	-	6/15/91/115	-
17	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
17	BCR	a	523	-	-	4/29/63/63	0/2/2/2
14	CLA	5	505	13	-	5/15/91/115	-
14	CLA	Z	501	13	-	13/33/109/115	-
14	CLA	a	502	13	-	3/15/91/115	-
14	CLA	3	509	13	-	2/15/91/115	-
17	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
14	CLA	a	508	13	-	4/15/91/115	-
14	CLA	3	508	13	-	4/15/91/115	-
19	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	q	502	13	-	4/15/91/115	-
14	CLA	2	517	-	-	9/15/91/115	-
17	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1201	2	-	8/33/109/115	-
17	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
14	CLA	v	503	13	-	8/15/91/115	-
17	BCR	S	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	u	505	13	-	5/15/91/115	-
14	CLA	B	1202	2	-	12/39/115/115	-
14	CLA	1	509	13	-	5/15/91/115	-
14	CLA	v	506	13	-	8/15/91/115	-
17	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
14	CLA	4	510	13	-	7/15/91/115	-
14	CLA	Y	503	13	-	9/15/91/115	-
14	CLA	A	1108	1	-	16/26/102/115	-
14	CLA	r	507	-	-	10/15/91/115	-
14	CLA	4	516	13	-	9/15/91/115	-
14	CLA	6	518	13	-	9/15/91/115	-
18	LHG	I	5001	-	-	25/52/52/53	-
14	CLA	q	507	-	-	8/15/91/115	-
14	CLA	e	1111	1	-	20/39/115/115	-
14	CLA	f	1239	2	-	16/39/115/115	-
17	BCR	s	521	-	-	7/29/63/63	0/2/2/2
14	CLA	v	502	13	-	3/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	509	13	-	3/39/115/115	-
21	SQD	3	822	-	-	9/23/43/69	0/1/1/1
14	CLA	f	1227	2	-	13/33/109/115	-
14	CLA	Z	519	13	-	7/15/91/115	-
17	BCR	u	522	-	-	5/29/63/63	0/2/2/2
16	SF4	A	3001	2,1	-	-	0/6/5/5
14	CLA	Z	510	13	-	7/15/91/115	-
14	CLA	2	507	-	-	10/15/91/115	-
14	CLA	5	516	13	-	7/15/91/115	-
14	CLA	r	502	13	-	3/15/91/115	-
14	CLA	f	1211	2	-	8/27/103/115	-
14	CLA	G	1128	1	-	10/39/115/115	-
14	CLA	Y	511	13	-	4/15/91/115	-
19	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	f	1203	2	-	16/39/115/115	-
14	CLA	1	516	13	-	14/15/91/115	-
14	CLA	G	1130	1	-	7/29/105/115	-
14	CLA	t	519	13	-	10/15/91/115	-
14	CLA	a	512	13	-	3/15/91/115	-
14	CLA	b	510	13	-	7/15/91/115	-
14	CLA	e	1122	1	-	14/33/109/115	-
17	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
18	LHG	L	5220	-	-	28/45/45/53	-
18	LHG	V	5221	-	-	31/53/53/53	-
14	CLA	1	501	13	-	11/15/91/115	-
17	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	B	1201	2	-	8/33/109/115	-
14	CLA	f	1223	2	-	10/39/115/115	-
14	CLA	u	506	13	-	8/15/91/115	-
14	CLA	A	1128	1	-	10/39/115/115	-
14	CLA	G	1801	18	-	7/15/91/115	-
18	LHG	n	5221	-	-	31/53/53/53	-
17	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
14	CLA	t	510	13	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	1	521	-	-	7/29/63/63	0/2/2/2
14	CLA	V	1502	10	-	10/39/115/115	-
14	CLA	B	1231	23	-	8/39/115/115	-
14	CLA	H	1212	2	-	8/23/99/115	-
14	CLA	Y	508	13	-	5/15/91/115	-
16	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	e	1118	1	-	10/33/109/115	-
14	CLA	t	501	13	-	8/15/91/115	-
14	CLA	A	1136	1	-	10/39/115/115	-
14	CLA	B	1229	2	-	13/39/115/115	-
14	CLA	e	1103	1	-	21/39/115/115	-
14	CLA	t	505	13	-	5/15/91/115	-
18	LHG	B	1842	14	-	19/41/41/53	-
14	CLA	3	505	13	-	11/27/103/115	-
17	BCR	2	523	-	-	6/29/63/63	0/2/2/2
14	CLA	b	512	13	-	5/15/91/115	-
17	BCR	b	522	-	-	4/29/63/63	0/2/2/2
18	LHG	A	5004	-	-	18/39/39/53	-
14	CLA	s	506	13	-	8/15/91/115	-
22	FMN	p	170	-	-	0/18/18/18	0/3/3/3
14	CLA	H	1205	2	-	10/39/115/115	-
14	CLA	r	503	13	-	10/39/115/115	-
14	CLA	H	1211	2	-	8/27/103/115	-
14	CLA	Y	517	-	-	9/15/91/115	-
14	CLA	H	1223	2	-	9/39/115/115	-
20	LMG	J	5104	-	-	13/27/47/70	0/1/1/1
17	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	V	1503	23	-	10/33/109/115	-
14	CLA	Z	516	13	-	8/15/91/115	-
14	CLA	Z	502	13	-	3/15/91/115	-
14	CLA	G	1115	1	-	13/33/109/115	-
17	BCR	6	523	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1136	1	-	10/39/115/115	-
14	CLA	r	504	-	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	519	13	-	7/15/91/115	-
14	CLA	d	513	13	-	5/15/91/115	-
14	CLA	2	504	-	-	9/15/91/115	-
14	CLA	A	1131	1	-	8/39/115/115	-
14	CLA	q	519	13	-	8/15/91/115	-
14	CLA	b	511	13	-	5/15/91/115	-
14	CLA	e	1105	1	-	7/27/103/115	-
14	CLA	e	1112	1	-	4/21/97/115	-
14	CLA	1	508	13	-	5/15/91/115	-
17	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
16	SF4	C	3003	3	-	-	0/6/5/5
14	CLA	b	517	-	-	7/15/91/115	-
14	CLA	f	1238	23	-	4/39/115/115	-
14	CLA	G	1108	1	-	16/26/102/115	-
14	CLA	t	516	13	-	9/15/91/115	-
14	CLA	f	1201	2	-	8/33/109/115	-
14	CLA	H	1232	23	-	6/27/103/115	-
14	CLA	T	1302	8	-	14/27/103/115	-
21	SQD	v	822	-	-	7/19/39/69	0/1/1/1
14	CLA	a	511	13	-	2/15/91/115	-
14	CLA	b	504	-	-	6/15/91/115	-
14	CLA	3	506	13	-	8/15/91/115	-
14	CLA	c	509	13	-	13/39/115/115	-
16	SF4	g	3003	3	-	-	0/6/5/5
17	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
18	LHG	L	5221	-	-	31/53/53/53	-
14	CLA	e	1113	1	-	6/15/91/115	-
17	BCR	H	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	q	508	13	-	5/15/91/115	-
17	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
14	CLA	d	508	13	-	6/15/91/115	-
14	CLA	f	1202	2	-	12/39/115/115	-
14	CLA	a	507	-	-	7/15/91/115	-
14	CLA	B	1222	23	-	2/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	501	13	-	11/15/91/115	-
17	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
17	BCR	f	4010	-	-	7/29/63/63	0/2/2/2
21	SQD	5	822	-	-	3/19/39/69	0/1/1/1
14	CLA	b	509	13	-	6/15/91/115	-
14	CLA	A	1105	1	-	7/27/103/115	-
17	BCR	5	524	-	-	2/29/63/63	0/2/2/2
14	CLA	u	512	13	-	7/15/91/115	-
14	CLA	H	1012	23	-	15/39/115/115	-
17	BCR	r	524	-	-	3/29/63/63	0/2/2/2
14	CLA	5	513	13	-	7/15/91/115	-
14	CLA	s	512	13	-	3/15/91/115	-
14	CLA	r	519	13	-	7/15/91/115	-
17	BCR	2	524	-	-	3/29/63/63	0/2/2/2
18	LHG	e	5002	-	-	22/47/47/53	-
17	BCR	q	524	-	-	2/29/63/63	0/2/2/2
14	CLA	4	513	13	-	7/15/91/115	-
14	CLA	2	502	13	-	3/15/91/115	-
14	CLA	f	1234	2	-	15/39/115/115	-
14	CLA	s	502	13	-	3/15/91/115	-
14	CLA	4	517	-	-	7/15/91/115	-
14	CLA	f	1209	2	-	11/25/101/115	-
14	CLA	f	1225	2	-	7/39/115/115	-
17	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
14	CLA	b	506	13	-	6/15/91/115	-
14	CLA	u	519	13	-	8/15/91/115	-
14	CLA	3	510	13	-	8/15/91/115	-
14	CLA	6	511	13	-	7/15/91/115	-
14	CLA	2	501	13	-	13/33/109/115	-
14	CLA	B	1021	2	-	11/39/115/115	-
21	SQD	a	822	-	-	9/23/43/69	0/1/1/1
14	CLA	B	1207	2	-	18/39/115/115	-
21	SQD	V	5216	-	-	17/41/61/69	0/1/1/1
17	BCR	o	4021	-	-	6/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SQD	q	822	-	-	10/27/47/69	0/1/1/1
17	BCR	v	523	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1226	2	-	7/27/103/115	-
14	CLA	e	1119	23	-	15/39/115/115	-
14	CLA	q	516	13	-	14/15/91/115	-
14	CLA	d	501	13	-	9/15/91/115	-
14	CLA	G	1101	1	-	18/39/115/115	-
14	CLA	B	1223	2	-	9/39/115/115	-
14	CLA	r	508	13	-	4/15/91/115	-
14	CLA	B	1219	2	-	20/37/113/115	-
14	CLA	G	1135	1	-	10/27/103/115	-
14	CLA	6	504	-	-	6/15/91/115	-
14	CLA	d	505	13	-	15/39/115/115	-
14	CLA	e	1135	1	-	10/27/103/115	-
21	SQD	n	5216	-	-	17/41/61/69	0/1/1/1
14	CLA	e	1116	1	-	9/33/109/115	-
14	CLA	1	512	13	-	7/15/91/115	-
14	CLA	J	1303	8	-	6/15/91/115	-
14	CLA	A	1237	23	-	24/39/115/115	-
17	BCR	1	522	-	-	6/29/63/63	0/2/2/2
18	LHG	e	5006	-	-	26/44/44/53	-
16	SF4	e	3001	2,1	-	-	0/6/5/5
14	CLA	v	511	13	-	7/15/91/115	-
14	CLA	e	1107	1	-	16/39/115/115	-
14	CLA	5	510	13	-	9/15/91/115	-
14	CLA	H	1207	2	-	18/39/115/115	-
17	BCR	H	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1211	2	-	8/27/103/115	-
14	CLA	H	1234	2	-	15/39/115/115	-
17	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
14	CLA	e	1127	1	-	12/39/115/115	-
14	CLA	H	1230	2	-	12/33/109/115	-
17	BCR	6	521	-	-	5/29/63/63	0/2/2/2
14	CLA	A	1135	1	-	10/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
17	BCR	4	524	-	-	4/29/63/63	0/2/2/2
17	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
14	CLA	a	518	13	-	11/27/103/115	-
14	CLA	B	1213	2	-	11/35/111/115	-
14	CLA	s	503	13	-	9/15/91/115	-
17	BCR	q	521	-	-	7/29/63/63	0/2/2/2
14	CLA	5	517	-	-	12/15/91/115	-
17	BCR	v	521	-	-	5/29/63/63	0/2/2/2
19	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
14	CLA	Y	505	13	-	6/15/91/115	-
14	CLA	3	519	13	-	7/15/91/115	-
14	CLA	f	1208	2	-	17/39/115/115	-
14	CLA	e	1022	23	-	9/39/115/115	-
14	CLA	f	1228	2	-	6/27/103/115	-
14	CLA	d	519	13	-	8/15/91/115	-
14	CLA	B	1240	18	-	15/39/115/115	-
17	BCR	M	4021	-	-	6/29/63/63	0/2/2/2
21	SQD	Z	822	-	-	7/22/42/69	0/1/1/1
14	CLA	A	1110	1	-	12/25/101/115	-
14	CLA	A	1102	1	-	7/27/103/115	-
14	CLA	5	504	-	-	5/15/91/115	-
14	CLA	r	505	13	-	14/39/115/115	-
14	CLA	a	510	13	-	8/15/91/115	-
14	CLA	G	1102	1	-	7/27/103/115	-
14	CLA	t	503	13	-	4/15/91/115	-
17	BCR	u	523	-	-	4/29/63/63	0/2/2/2
21	SQD	u	822	-	-	3/19/39/69	0/1/1/1
14	CLA	A	1109	1	-	16/39/115/115	-
15	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	1	504	-	-	7/15/91/115	-
17	BCR	4	523	-	-	5/29/63/63	0/2/2/2
21	SQD	t	822	-	-	10/19/39/69	0/1/1/1
15	PQN	f	2002	-	-	6/23/43/43	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	505	13	-	5/15/91/115	-
14	CLA	c	501	13	-	8/15/91/115	-
14	CLA	H	1235	2	-	9/39/115/115	-
14	CLA	c	507	-	-	9/15/91/115	-
14	CLA	1	507	-	-	8/15/91/115	-
14	CLA	2	508	13	-	4/15/91/115	-
14	CLA	j	1302	6	-	9/15/91/115	-
14	CLA	q	511	13	-	4/15/91/115	-
14	CLA	m	1103	9	-	10/19/95/115	-
14	CLA	s	511	13	-	2/15/91/115	-
17	BCR	t	524	-	-	4/29/63/63	0/2/2/2
14	CLA	1	517	-	-	9/15/91/115	-
14	CLA	H	1240	18	-	15/39/115/115	-
14	CLA	Z	512	13	-	5/15/91/115	-
17	BCR	c	521	-	-	7/29/63/63	0/2/2/2
14	CLA	c	512	13	-	7/15/91/115	-
17	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
14	CLA	H	1236	2	-	5/21/97/115	-
14	CLA	c	519	13	-	8/15/91/115	-
14	CLA	e	1128	1	-	10/39/115/115	-
14	CLA	R	1301	23	-	3/15/91/115	-
17	BCR	r	521	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1108	1	-	16/26/102/115	-
14	CLA	a	501	13	-	6/15/91/115	-
14	CLA	q	504	-	-	7/15/91/115	-
14	CLA	u	509	13	-	13/39/115/115	-
17	BCR	1	523	-	-	6/29/63/63	0/2/2/2
14	CLA	6	509	13	-	4/15/91/115	-
14	CLA	2	503	13	-	10/39/115/115	-
17	BCR	s	523	-	-	4/29/63/63	0/2/2/2
14	CLA	v	505	13	-	15/39/115/115	-
18	LHG	G	5005	-	-	28/47/47/53	-
14	CLA	c	513	13	-	7/15/91/115	-
14	CLA	q	518	13	-	8/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1214	2	-	14/39/115/115	-
14	CLA	G	1110	1	-	12/25/101/115	-
17	BCR	u	521	-	-	7/29/63/63	0/2/2/2
14	CLA	v	507	-	-	7/15/91/115	-
14	CLA	d	510	13	-	10/15/91/115	-
18	LHG	G	5006	-	-	26/44/44/53	-
17	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	d	503	13	-	8/15/91/115	-
15	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	G	1127	1	-	12/39/115/115	-
14	CLA	B	1210	2	-	22/39/115/115	-
14	CLA	r	506	13	-	7/15/91/115	-
14	CLA	c	511	13	-	3/15/91/115	-
14	CLA	1	511	13	-	4/15/91/115	-
21	SQD	s	822	-	-	9/23/43/69	0/1/1/1
14	CLA	B	1215	2	-	19/39/115/115	-
14	CLA	5	508	13	-	6/15/91/115	-
14	CLA	2	516	13	-	8/15/91/115	-
14	CLA	f	1021	2	-	11/39/115/115	-
14	CLA	q	506	13	-	5/15/91/115	-
17	BCR	A	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	A	1113	1	-	6/15/91/115	-
14	CLA	f	1204	2	-	13/39/115/115	-
14	CLA	s	513	13	-	5/15/91/115	-
17	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
14	CLA	3	507	-	-	7/15/91/115	-
14	CLA	f	1224	2	-	7/33/109/115	-
14	CLA	6	513	13	-	5/15/91/115	-
14	CLA	H	1216	23	-	13/33/109/115	-
14	CLA	B	1236	2	-	5/21/97/115	-
17	BCR	5	523	-	-	4/29/63/63	0/2/2/2
15	PQN	H	2002	-	-	6/23/43/43	0/2/2/2
14	CLA	G	1123	23	-	11/39/115/115	-
14	CLA	s	517	-	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	4	503	13	-	4/15/91/115	-
17	BCR	4	521	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1114	23	-	3/15/91/115	-
17	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	5	509	13	-	13/39/115/115	-
14	CLA	A	1125	1	-	12/39/115/115	-
14	CLA	Y	510	13	-	6/15/91/115	-
17	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
18	LHG	V	5218	-	-	19/41/41/53	-
14	CLA	3	516	13	-	9/15/91/115	-
18	LHG	V	5220	-	-	28/45/45/53	-
14	CLA	H	1231	23	-	8/39/115/115	-
17	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
17	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	504	-	-	9/15/91/115	-
14	CLA	t	513	13	-	7/15/91/115	-
14	CLA	3	502	13	-	3/15/91/115	-
17	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	3	513	13	-	5/15/91/115	-
14	CLA	c	508	13	-	6/15/91/115	-
14	CLA	e	1134	1	-	11/29/105/115	-
14	CLA	Z	518	13	-	16/27/103/115	-
20	LMG	f	5002	-	-	24/48/68/70	0/1/1/1
14	CLA	A	1126	1	-	18/39/115/115	-
17	BCR	V	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	4	501	13	-	8/15/91/115	-
14	CLA	u	518	13	-	5/15/91/115	-
14	CLA	A	1123	23	-	11/39/115/115	-
18	LHG	n	5218	-	-	19/41/41/53	-
14	CLA	t	504	-	-	6/15/91/115	-
14	CLA	u	507	-	-	9/15/91/115	-
14	CLA	H	1227	2	-	13/33/109/115	-
14	CLA	f	1219	2	-	20/37/113/115	-
14	CLA	B	1239	2	-	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SQD	c	822	-	-	3/19/39/69	0/1/1/1
17	BCR	c	523	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1115	1	-	12/33/109/115	-
14	CLA	G	1117	1	-	13/39/115/115	-
14	CLA	e	1136	1	-	10/39/115/115	-
14	CLA	4	511	13	-	5/15/91/115	-
14	CLA	e	1801	18	-	7/15/91/115	-
17	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
18	LHG	S	5001	-	-	25/52/52/53	-
17	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
17	BCR	1	524	-	-	2/29/63/63	0/2/2/2
14	CLA	B	1227	2	-	13/33/109/115	-
14	CLA	B	1225	2	-	7/39/115/115	-
14	CLA	G	1129	1	-	10/25/101/115	-
14	CLA	d	502	13	-	3/15/91/115	-
18	LHG	e	5004	-	-	18/39/39/53	-
14	CLA	n	1501	10	-	11/33/109/115	-
14	CLA	A	1130	1	-	7/29/105/115	-
14	CLA	U	1401	-	-	10/27/103/115	-
14	CLA	b	513	13	-	7/15/91/115	-
14	CLA	l	1303	8	-	6/15/91/115	-
14	CLA	n	1502	10	-	10/39/115/115	-
14	CLA	Z	503	13	-	10/39/115/115	-
14	CLA	G	1125	1	-	12/39/115/115	-
14	CLA	e	1126	1	-	18/39/115/115	-
14	CLA	l	1302	8	-	14/27/103/115	-
14	CLA	A	1117	1	-	13/39/115/115	-
14	CLA	B	1220	2	-	11/27/103/115	-
14	CLA	A	1139	23	-	20/39/115/115	-
14	CLA	e	1123	23	-	11/39/115/115	-
14	CLA	s	501	13	-	6/15/91/115	-
14	CLA	3	518	13	-	11/27/103/115	-
14	CLA	B	1216	23	-	13/33/109/115	-
17	BCR	V	4219	-	-	2/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	d	524	-	-	5/29/63/63	0/2/2/2
14	CLA	v	513	13	-	5/15/91/115	-
14	CLA	b	501	13	-	8/15/91/115	-
14	CLA	Y	507	-	-	8/15/91/115	-
14	CLA	Z	511	13	-	5/15/91/115	-
18	LHG	f	1855	-	-	24/45/45/53	-
14	CLA	6	505	13	-	15/39/115/115	-
14	CLA	6	517	-	-	12/15/91/115	-
14	CLA	n	1503	23	-	10/33/109/115	-
17	BCR	5	521	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1111	1	-	20/39/115/115	-
14	CLA	B	1218	2	-	9/33/109/115	-
14	CLA	e	1139	23	-	20/39/115/115	-
14	CLA	A	1122	1	-	14/33/109/115	-
14	CLA	G	1237	23	-	25/39/115/115	-
18	LHG	G	5008	-	-	18/39/39/53	-
14	CLA	B	1206	2	-	15/39/115/115	-
14	CLA	Y	509	13	-	5/15/91/115	-
17	BCR	2	521	-	-	4/29/63/63	0/2/2/2
18	LHG	G	5003	14	-	17/44/44/53	-
14	CLA	2	518	13	-	16/27/103/115	-
14	CLA	H	1220	2	-	11/27/103/115	-
18	LHG	H	1842	14	-	19/41/41/53	-
17	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1011	1	-	12/39/115/115	-
16	SF4	N	3002	3	-	-	0/6/5/5
14	CLA	t	508	13	-	6/15/91/115	-
14	CLA	5	501	13	-	8/15/91/115	-
14	CLA	5	503	13	-	9/15/91/115	-
17	BCR	c	522	-	-	5/29/63/63	0/2/2/2
14	CLA	5	506	13	-	8/15/91/115	-
14	CLA	a	504	-	-	7/15/91/115	-
14	CLA	G	1103	1	-	21/39/115/115	-
14	CLA	v	518	13	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	t	523	-	-	5/29/63/63	0/2/2/2
18	LHG	A	5003	14	-	17/44/44/53	-
14	CLA	L	1502	10	-	10/39/115/115	-
17	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1121	1	-	10/27/103/115	-
19	LMU	J	5105	-	-	9/13/33/61	0/1/1/2
14	CLA	2	505	13	-	14/39/115/115	-
18	LHG	H	1855	-	-	24/45/45/53	-
14	CLA	f	1213	2	-	11/35/111/115	-
14	CLA	G	1011	1	-	12/39/115/115	-
14	CLA	f	1230	2	-	12/33/109/115	-
17	BCR	s	522	-	-	5/29/63/63	0/2/2/2
14	CLA	c	505	13	-	5/15/91/115	-
17	BCR	v	522	-	-	5/29/63/63	0/2/2/2
17	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	A	1103	1	-	21/39/115/115	-
17	BCR	6	522	-	-	5/29/63/63	0/2/2/2
14	CLA	5	518	13	-	5/15/91/115	-
14	CLA	4	509	13	-	6/15/91/115	-
14	CLA	1	502	13	-	4/15/91/115	-
14	CLA	H	1021	2	-	11/39/115/115	-
14	CLA	a	506	13	-	8/15/91/115	-
14	CLA	f	1235	2	-	9/39/115/115	-
14	CLA	B	1232	23	-	6/27/103/115	-
14	CLA	A	1121	1	-	10/27/103/115	-
21	SQD	B	1852	-	-	18/35/55/69	0/1/1/1
14	CLA	L	1503	23	-	10/33/109/115	-
14	CLA	t	517	-	-	7/15/91/115	-
14	CLA	a	505	13	-	11/27/103/115	-
14	CLA	b	508	13	-	6/15/91/115	-
21	SQD	H	1852	-	-	18/35/55/69	0/1/1/1
16	SF4	G	3001	2,1	-	-	0/6/5/5
14	CLA	B	1217	2	-	14/33/109/115	-
14	CLA	r	512	13	-	5/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	H	5002	-	-	24/48/68/70	0/1/1/1
15	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	4	502	13	-	5/15/91/115	-
14	CLA	H	1239	2	-	16/39/115/115	-
18	LHG	k	5001	-	-	25/52/52/53	-
14	CLA	G	1124	23	-	13/33/109/115	-
14	CLA	6	510	13	-	10/15/91/115	-
14	CLA	A	1104	1	-	10/39/115/115	-
17	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	e	1106	1	-	23/39/115/115	-
14	CLA	t	509	13	-	6/15/91/115	-
14	CLA	v	517	-	-	12/15/91/115	-
14	CLA	4	506	13	-	6/15/91/115	-
14	CLA	b	507	-	-	8/15/91/115	-
19	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	2	506	13	-	7/15/91/115	-
14	CLA	G	1132	1	-	18/39/115/115	-
14	CLA	c	516	13	-	7/15/91/115	-
17	BCR	r	523	-	-	6/29/63/63	0/2/2/2
17	BCR	t	521	-	-	10/29/63/63	0/2/2/2
21	SQD	r	822	-	-	7/22/42/69	0/1/1/1
14	CLA	c	506	13	-	8/15/91/115	-
14	CLA	A	1129	1	-	10/25/101/115	-
14	CLA	1	506	13	-	5/15/91/115	-
14	CLA	3	512	13	-	3/15/91/115	-
17	BCR	q	523	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1224	2	-	7/33/109/115	-
17	BCR	c	524	-	-	2/29/63/63	0/2/2/2
14	CLA	f	1023	-	-	10/39/115/115	-
18	LHG	A	5001	-	-	23/53/53/53	-
14	CLA	d	512	13	-	9/15/91/115	-
17	BCR	d	522	-	-	5/29/63/63	0/2/2/2
17	BCR	k	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	b	516	13	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	u	510	13	-	9/15/91/115	-
17	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	u	516	13	-	7/15/91/115	-
14	CLA	6	501	13	-	9/15/91/115	-
14	CLA	Y	518	13	-	8/15/91/115	-
14	CLA	a	516	13	-	9/15/91/115	-
14	CLA	e	1138	1	-	14/39/115/115	-
21	SQD	2	822	-	-	7/22/42/69	0/1/1/1
14	CLA	G	1112	1	-	4/21/97/115	-
14	CLA	6	508	13	-	6/15/91/115	-
14	CLA	Z	505	13	-	14/39/115/115	-
14	CLA	G	1013	-	-	14/39/115/115	-
14	CLA	f	1221	23	-	14/36/112/115	-
14	CLA	r	517	-	-	9/15/91/115	-
14	CLA	c	510	13	-	9/15/91/115	-
14	CLA	u	511	13	-	3/15/91/115	-
14	CLA	5	512	13	-	7/15/91/115	-
17	BCR	5	522	-	-	5/29/63/63	0/2/2/2
17	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	Y	506	13	-	5/15/91/115	-
14	CLA	q	517	-	-	9/15/91/115	-
17	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
14	CLA	H	1218	2	-	9/33/109/115	-
14	CLA	A	1140	1	-	14/39/115/115	-
14	CLA	B	1023	-	-	10/39/115/115	-
22	FMN	X	170	-	-	0/18/18/18	0/3/3/3
14	CLA	2	519	13	-	7/15/91/115	-
14	CLA	H	1210	2	-	22/39/115/115	-
14	CLA	q	512	13	-	7/15/91/115	-
14	CLA	Y	513	13	-	6/15/91/115	-
14	CLA	A	1112	1	-	4/21/97/115	-
18	LHG	G	5001	-	-	23/53/53/53	-
14	CLA	6	507	-	-	7/15/91/115	-
14	CLA	d	504	-	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	t	518	13	-	6/15/91/115	-
14	CLA	r	513	13	-	4/15/91/115	-
14	CLA	s	510	13	-	8/15/91/115	-
17	BCR	L	4022	-	-	3/29/63/63	0/2/2/2
21	SQD	4	822	-	-	10/19/39/69	0/1/1/1
14	CLA	Y	504	-	-	7/15/91/115	-
14	CLA	A	1107	1	-	16/39/115/115	-
17	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
14	CLA	3	517	-	-	9/15/91/115	-
14	CLA	q	509	13	-	5/15/91/115	-
18	LHG	e	5007	-	-	23/51/51/53	-
14	CLA	3	504	-	-	7/15/91/115	-
14	CLA	H	1023	-	-	10/39/115/115	-
14	CLA	r	511	13	-	4/15/91/115	-
17	BCR	3	521	-	-	7/29/63/63	0/2/2/2
14	CLA	4	508	13	-	6/15/91/115	-
18	LHG	A	5009	-	-	28/46/46/53	-
14	CLA	2	511	13	-	4/15/91/115	-
14	CLA	6	502	13	-	3/15/91/115	-
21	SQD	d	822	-	-	7/19/39/69	0/1/1/1
14	CLA	1	505	13	-	6/15/91/115	-
17	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
14	CLA	c	517	-	-	12/15/91/115	-
14	CLA	1	518	13	-	8/15/91/115	-
17	BCR	3	523	-	-	4/29/63/63	0/2/2/2
19	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	Z	506	13	-	7/15/91/115	-
17	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	G	1122	1	-	14/33/109/115	-
14	CLA	u	501	13	-	8/15/91/115	-
18	LHG	e	5005	-	-	28/47/47/53	-
14	CLA	G	1126	1	-	18/39/115/115	-
14	CLA	G	1107	1	-	16/39/115/115	-
14	CLA	G	1109	1	-	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1203	2	-	16/39/115/115	-
14	CLA	Z	517	-	-	9/15/91/115	-
14	CLA	t	506	13	-	6/15/91/115	-
14	CLA	r	518	13	-	16/27/103/115	-
14	CLA	2	512	13	-	5/15/91/115	-
14	CLA	u	517	-	-	12/15/91/115	-
14	CLA	3	511	13	-	2/15/91/115	-
17	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
14	CLA	U	1103	9	-	10/19/95/115	-
14	CLA	d	509	13	-	4/15/91/115	-
14	CLA	H	1202	2	-	12/39/115/115	-
17	BCR	f	4004	-	-	8/29/63/63	0/2/2/2

All (6040) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	2001	PQN	C12-C13	8.46	1.53	1.33
15	A	2001	PQN	C12-C13	8.44	1.53	1.33
15	e	2001	PQN	C12-C13	8.44	1.53	1.33
15	B	2002	PQN	C12-C13	8.38	1.53	1.33
15	H	2002	PQN	C12-C13	8.38	1.53	1.33
15	f	2002	PQN	C12-C13	8.37	1.53	1.33
15	f	2002	PQN	O1-C1	7.94	1.40	1.23
15	H	2002	PQN	O1-C1	7.93	1.40	1.23
15	B	2002	PQN	O1-C1	7.93	1.40	1.23
15	G	2001	PQN	O1-C1	7.55	1.39	1.23
15	A	2001	PQN	O1-C1	7.55	1.39	1.23
15	e	2001	PQN	O1-C1	7.53	1.39	1.23
15	A	2001	PQN	O4-C4	7.25	1.38	1.23
15	e	2001	PQN	O4-C4	7.24	1.38	1.23
15	G	2001	PQN	O4-C4	7.24	1.38	1.23
15	B	2002	PQN	O4-C4	6.95	1.37	1.23
15	H	2002	PQN	O4-C4	6.94	1.37	1.23
15	f	2002	PQN	O4-C4	6.93	1.37	1.23
15	B	2002	PQN	C2-C1	-5.02	1.37	1.48
15	f	2002	PQN	C2-C1	-5.00	1.37	1.48
15	H	2002	PQN	C2-C1	-5.00	1.37	1.48
15	G	2001	PQN	C2-C1	-4.83	1.37	1.48
15	e	2001	PQN	C2-C1	-4.82	1.37	1.48
15	A	2001	PQN	C2-C1	-4.82	1.37	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1128	CLA	CMB-C2B	-4.05	1.42	1.50
14	H	1229	CLA	C4D-ND	-4.03	1.32	1.37
14	e	1128	CLA	CMB-C2B	-4.03	1.42	1.50
14	B	1023	CLA	C4D-ND	-4.03	1.32	1.37
14	B	1229	CLA	C4D-ND	-4.02	1.32	1.37
14	G	1128	CLA	CMB-C2B	-4.02	1.42	1.50
14	H	1023	CLA	C4D-ND	-4.02	1.32	1.37
19	l	5105	LMU	O5'-C1'	4.01	1.52	1.41
14	f	1023	CLA	C4D-ND	-4.01	1.32	1.37
19	T	5105	LMU	O5'-C1'	4.01	1.52	1.41
19	J	5105	LMU	O5'-C1'	3.99	1.52	1.41
14	f	1229	CLA	C4D-ND	-3.98	1.32	1.37
14	B	1234	CLA	C4D-ND	-3.97	1.32	1.37
14	t	503	CLA	C1D-ND	3.97	1.42	1.37
14	f	1226	CLA	CMB-C2B	-3.96	1.42	1.50
14	f	1234	CLA	C4D-ND	-3.96	1.32	1.37
14	B	1226	CLA	CMB-C2B	-3.95	1.42	1.50
14	H	1226	CLA	CMD-C2D	-3.95	1.42	1.50
14	B	1226	CLA	CMD-C2D	-3.94	1.42	1.50
14	s	503	CLA	C1D-ND	3.94	1.42	1.37
14	3	503	CLA	C1D-ND	3.94	1.42	1.37
22	P	170	FMN	C4A-N5	3.93	1.38	1.30
22	X	170	FMN	C4A-N5	3.92	1.38	1.30
14	e	1109	CLA	C4D-ND	-3.92	1.32	1.37
14	H	1234	CLA	C4D-ND	-3.92	1.32	1.37
14	n	1502	CLA	C4D-ND	-3.92	1.32	1.37
14	f	1226	CLA	CMD-C2D	-3.92	1.42	1.50
14	H	1226	CLA	CMB-C2B	-3.92	1.42	1.50
14	V	1502	CLA	C4D-ND	-3.91	1.32	1.37
14	4	503	CLA	C1D-ND	3.91	1.42	1.37
14	G	1109	CLA	C4D-ND	-3.91	1.32	1.37
22	p	170	FMN	C4A-N5	3.91	1.38	1.30
14	A	1109	CLA	C4D-ND	-3.91	1.32	1.37
14	L	1502	CLA	C4D-ND	-3.90	1.32	1.37
14	a	503	CLA	C1D-ND	3.89	1.42	1.37
14	A	1022	CLA	C4D-ND	-3.89	1.32	1.37
14	G	1122	CLA	C4D-ND	-3.87	1.32	1.37
14	e	1022	CLA	C4D-ND	-3.87	1.32	1.37
14	G	1022	CLA	C4D-ND	-3.87	1.32	1.37
14	e	1135	CLA	C4D-ND	-3.87	1.32	1.37
14	A	1122	CLA	C4D-ND	-3.86	1.32	1.37
14	A	1132	CLA	C4D-ND	-3.86	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	503	CLA	C1D-ND	3.86	1.42	1.37
14	G	1135	CLA	C4D-ND	-3.85	1.32	1.37
14	e	1122	CLA	C4D-ND	-3.85	1.32	1.37
14	A	1135	CLA	C4D-ND	-3.84	1.32	1.37
14	e	1132	CLA	C4D-ND	-3.83	1.32	1.37
14	t	516	CLA	C1D-ND	3.83	1.42	1.37
14	t	507	CLA	C1D-ND	3.82	1.42	1.37
14	A	1128	CLA	C4D-ND	-3.82	1.32	1.37
14	m	1105	CLA	C1D-ND	3.82	1.42	1.37
14	G	1128	CLA	C4D-ND	-3.82	1.32	1.37
14	b	516	CLA	C1D-ND	3.82	1.42	1.37
14	f	1204	CLA	C4D-ND	-3.81	1.32	1.37
14	G	1132	CLA	C4D-ND	-3.81	1.32	1.37
14	u	511	CLA	C1D-ND	3.81	1.42	1.37
14	e	1125	CLA	C4D-ND	-3.80	1.32	1.37
14	K	1105	CLA	C1D-ND	3.80	1.42	1.37
14	e	1115	CLA	C4D-ND	-3.80	1.32	1.37
14	f	1203	CLA	C4D-ND	-3.79	1.32	1.37
14	v	503	CLA	C1D-ND	3.79	1.42	1.37
14	H	1204	CLA	C4D-ND	-3.79	1.32	1.37
14	B	1204	CLA	C4D-ND	-3.79	1.32	1.37
14	6	503	CLA	C1D-ND	3.78	1.42	1.37
14	4	516	CLA	C1D-ND	3.78	1.42	1.37
14	A	1115	CLA	C4D-ND	-3.78	1.32	1.37
14	e	1128	CLA	C4D-ND	-3.78	1.32	1.37
14	v	511	CLA	C1D-ND	3.78	1.42	1.37
14	G	1115	CLA	C4D-ND	-3.78	1.32	1.37
14	e	1129	CLA	C4D-ND	-3.78	1.32	1.37
14	G	1137	CLA	C4D-ND	-3.78	1.32	1.37
14	d	503	CLA	C1D-ND	3.77	1.42	1.37
14	4	507	CLA	C1D-ND	3.77	1.42	1.37
14	A	1129	CLA	C4D-ND	-3.77	1.32	1.37
14	3	513	CLA	C1D-ND	3.77	1.42	1.37
14	G	1140	CLA	C4D-ND	-3.77	1.32	1.37
14	6	511	CLA	C1D-ND	3.77	1.42	1.37
14	a	513	CLA	C1D-ND	3.77	1.42	1.37
14	A	1119	CLA	C4D-ND	-3.76	1.32	1.37
14	e	1119	CLA	C4D-ND	-3.76	1.32	1.37
14	5	511	CLA	C1D-ND	3.76	1.42	1.37
14	B	1203	CLA	C4D-ND	-3.76	1.32	1.37
14	Z	516	CLA	C1D-ND	3.76	1.42	1.37
14	r	516	CLA	C1D-ND	3.75	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1111	CLA	C4D-ND	-3.75	1.32	1.37
14	G	1129	CLA	C4D-ND	-3.75	1.32	1.37
14	s	513	CLA	C1D-ND	3.75	1.42	1.37
14	H	1203	CLA	C4D-ND	-3.75	1.32	1.37
14	Z	503	CLA	C1D-ND	3.75	1.42	1.37
14	t	502	CLA	C1D-ND	3.75	1.42	1.37
14	b	502	CLA	C1D-ND	3.75	1.42	1.37
14	A	1137	CLA	C4D-ND	-3.75	1.32	1.37
14	4	502	CLA	C1D-ND	3.74	1.42	1.37
14	U	1105	CLA	C1D-ND	3.74	1.42	1.37
14	f	1235	CLA	C4D-ND	-3.74	1.32	1.37
14	r	517	CLA	C1D-ND	3.74	1.42	1.37
14	v	506	CLA	C1D-ND	3.74	1.42	1.37
14	b	506	CLA	C1D-ND	3.74	1.42	1.37
14	u	517	CLA	C1D-ND	3.73	1.42	1.37
14	A	1125	CLA	C4D-ND	-3.73	1.32	1.37
14	6	506	CLA	C1D-ND	3.73	1.42	1.37
14	e	1124	CLA	C4D-ND	-3.73	1.32	1.37
14	s	507	CLA	C1D-ND	3.72	1.42	1.37
14	t	506	CLA	C1D-ND	3.72	1.42	1.37
14	b	507	CLA	C1D-ND	3.72	1.42	1.37
14	c	511	CLA	C1D-ND	3.72	1.42	1.37
14	t	517	CLA	C1D-ND	3.72	1.42	1.37
14	Z	517	CLA	C1D-ND	3.72	1.42	1.37
14	2	516	CLA	C1D-ND	3.72	1.42	1.37
14	s	506	CLA	C1D-ND	3.72	1.42	1.37
14	t	504	CLA	C1D-ND	3.72	1.42	1.37
14	e	1137	CLA	C4D-ND	-3.72	1.32	1.37
14	d	511	CLA	C1D-ND	3.72	1.42	1.37
14	G	1111	CLA	C4D-ND	-3.71	1.32	1.37
14	2	517	CLA	C1D-ND	3.71	1.42	1.37
14	G	1124	CLA	C4D-ND	-3.71	1.32	1.37
14	s	519	CLA	C1D-ND	3.71	1.42	1.37
14	G	1119	CLA	C4D-ND	-3.71	1.32	1.37
14	H	1012	CLA	C4D-ND	-3.71	1.32	1.37
14	A	1103	CLA	C4D-ND	-3.70	1.32	1.37
14	A	1140	CLA	C4D-ND	-3.70	1.32	1.37
14	3	519	CLA	C1D-ND	3.70	1.42	1.37
14	4	504	CLA	C1D-ND	3.70	1.42	1.37
14	a	518	CLA	C1D-ND	3.70	1.42	1.37
14	e	1136	CLA	C4D-ND	-3.70	1.32	1.37
14	f	1236	CLA	C4D-ND	-3.70	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	506	CLA	C1D-ND	3.70	1.42	1.37
14	B	1235	CLA	C4D-ND	-3.70	1.32	1.37
14	2	503	CLA	C1D-ND	3.70	1.42	1.37
14	u	508	CLA	C1D-ND	3.70	1.42	1.37
14	r	503	CLA	C1D-ND	3.70	1.42	1.37
14	G	1125	CLA	C4D-ND	-3.69	1.32	1.37
14	4	506	CLA	C1D-ND	3.69	1.42	1.37
14	Y	519	CLA	C1D-ND	3.69	1.42	1.37
14	H	1235	CLA	C4D-ND	-3.69	1.32	1.37
14	1	506	CLA	C1D-ND	3.69	1.42	1.37
14	a	506	CLA	C1D-ND	3.69	1.42	1.37
14	q	519	CLA	C1D-ND	3.69	1.42	1.37
14	A	1124	CLA	C4D-ND	-3.69	1.32	1.37
14	b	504	CLA	C1D-ND	3.69	1.42	1.37
14	u	503	CLA	C1D-ND	3.69	1.42	1.37
14	Y	506	CLA	C1D-ND	3.69	1.42	1.37
14	e	1111	CLA	C4D-ND	-3.69	1.32	1.37
14	1	519	CLA	C1D-ND	3.69	1.42	1.37
14	e	1140	CLA	C4D-ND	-3.69	1.32	1.37
14	G	1136	CLA	C4D-ND	-3.68	1.32	1.37
14	5	517	CLA	C1D-ND	3.68	1.42	1.37
14	A	1136	CLA	C4D-ND	-3.68	1.32	1.37
14	3	507	CLA	C1D-ND	3.68	1.42	1.37
15	H	2002	PQN	C3-C4	-3.68	1.37	1.47
14	3	506	CLA	C1D-ND	3.68	1.42	1.37
14	5	503	CLA	C1D-ND	3.68	1.42	1.37
14	3	518	CLA	C1D-ND	3.68	1.42	1.37
14	r	507	CLA	C1D-ND	3.68	1.42	1.37
14	v	519	CLA	C1D-ND	3.68	1.42	1.37
14	t	511	CLA	C1D-ND	3.68	1.42	1.37
14	e	1131	CLA	C4D-ND	-3.68	1.32	1.37
14	s	517	CLA	C1D-ND	3.68	1.42	1.37
14	G	1103	CLA	C4D-ND	-3.68	1.32	1.37
14	q	508	CLA	C1D-ND	3.67	1.42	1.37
14	e	1103	CLA	C4D-ND	-3.67	1.32	1.37
14	B	1236	CLA	C4D-ND	-3.67	1.32	1.37
14	q	511	CLA	C1D-ND	3.67	1.42	1.37
15	B	2002	PQN	C3-C4	-3.67	1.38	1.47
14	4	517	CLA	C1D-ND	3.67	1.42	1.37
14	6	519	CLA	C1D-ND	3.67	1.42	1.37
14	G	1117	CLA	C4D-ND	-3.67	1.32	1.37
14	B	1012	CLA	C4D-ND	-3.67	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1127	CLA	C4D-ND	-3.67	1.32	1.37
14	3	517	CLA	C1D-ND	3.67	1.42	1.37
14	v	507	CLA	C1D-ND	3.67	1.42	1.37
14	e	1139	CLA	C4D-ND	-3.66	1.32	1.37
14	c	519	CLA	C1D-ND	3.66	1.42	1.37
14	1	508	CLA	C1D-ND	3.66	1.42	1.37
14	c	508	CLA	C1D-ND	3.66	1.42	1.37
14	t	510	CLA	C1D-ND	3.66	1.42	1.37
14	G	1127	CLA	C4D-ND	-3.66	1.32	1.37
14	5	519	CLA	C1D-ND	3.66	1.42	1.37
14	b	511	CLA	C1D-ND	3.66	1.42	1.37
14	a	507	CLA	C1D-ND	3.66	1.42	1.37
14	e	1127	CLA	C4D-ND	-3.66	1.32	1.37
14	Y	511	CLA	C1D-ND	3.66	1.42	1.37
14	T	1303	CLA	C1D-ND	3.66	1.42	1.37
19	G	1849	LMU	O5'-C1'	3.66	1.51	1.41
14	4	513	CLA	C1D-ND	3.66	1.42	1.37
14	A	1131	CLA	C4D-ND	-3.65	1.32	1.37
14	b	517	CLA	C1D-ND	3.65	1.42	1.37
14	q	513	CLA	C1D-ND	3.65	1.42	1.37
14	q	506	CLA	C1D-ND	3.65	1.42	1.37
14	Y	513	CLA	C1D-ND	3.65	1.42	1.37
14	b	508	CLA	C1D-ND	3.65	1.42	1.37
14	1	513	CLA	C1D-ND	3.65	1.42	1.37
14	Y	503	CLA	C1D-ND	3.65	1.42	1.37
14	c	517	CLA	C1D-ND	3.65	1.42	1.37
14	e	1117	CLA	C4D-ND	-3.64	1.32	1.37
14	G	1131	CLA	C4D-ND	-3.64	1.32	1.37
14	2	507	CLA	C1D-ND	3.64	1.42	1.37
15	f	2002	PQN	C3-C4	-3.64	1.38	1.47
14	4	511	CLA	C1D-ND	3.64	1.42	1.37
14	Y	508	CLA	C1D-ND	3.64	1.42	1.37
14	H	1236	CLA	C4D-ND	-3.63	1.32	1.37
14	b	513	CLA	C1D-ND	3.63	1.42	1.37
14	t	513	CLA	C1D-ND	3.63	1.42	1.37
14	s	518	CLA	C1D-ND	3.63	1.42	1.37
14	r	511	CLA	C1D-ND	3.63	1.42	1.37
14	G	1139	CLA	C4D-ND	-3.63	1.32	1.37
14	c	503	CLA	C1D-ND	3.63	1.42	1.37
14	A	1139	CLA	C4D-ND	-3.63	1.32	1.37
14	1	511	CLA	C1D-ND	3.63	1.42	1.37
19	A	1849	LMU	O5'-C1'	3.63	1.51	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	u	507	CLA	C1D-ND	3.63	1.42	1.37
14	d	519	CLA	C1D-ND	3.62	1.42	1.37
14	b	518	CLA	C1D-ND	3.62	1.42	1.37
14	5	508	CLA	C1D-ND	3.62	1.42	1.37
14	Y	505	CLA	C1D-ND	3.62	1.42	1.37
14	1	518	CLA	C1D-ND	3.62	1.42	1.37
14	Z	507	CLA	C1D-ND	3.62	1.42	1.37
14	b	510	CLA	C1D-ND	3.62	1.42	1.37
14	u	502	CLA	C1D-ND	3.62	1.42	1.37
14	d	501	CLA	C1D-ND	3.62	1.42	1.37
14	q	509	CLA	C1D-ND	3.62	1.42	1.37
14	e	1105	CLA	C4D-ND	-3.62	1.32	1.37
14	4	510	CLA	C1D-ND	3.62	1.42	1.37
14	n	1503	CLA	C1D-ND	3.62	1.42	1.37
14	a	517	CLA	C1D-ND	3.62	1.42	1.37
14	J	1303	CLA	C1D-ND	3.62	1.42	1.37
14	4	508	CLA	C1D-ND	3.62	1.42	1.37
14	a	519	CLA	C1D-ND	3.62	1.42	1.37
14	u	519	CLA	C1D-ND	3.62	1.42	1.37
14	G	1011	CLA	C4D-ND	-3.62	1.32	1.37
14	f	1209	CLA	C1D-ND	3.61	1.42	1.37
14	v	501	CLA	C1D-ND	3.61	1.42	1.37
19	e	1849	LMU	O5'-C1'	3.61	1.51	1.41
14	A	1133	CLA	C4D-ND	-3.61	1.32	1.37
14	H	1225	CLA	C4D-ND	-3.61	1.32	1.37
14	a	501	CLA	C1D-ND	3.61	1.42	1.37
14	b	501	CLA	C1D-ND	3.61	1.42	1.37
14	Y	509	CLA	C1D-ND	3.61	1.42	1.37
14	6	507	CLA	C1D-ND	3.61	1.42	1.37
14	Y	517	CLA	C1D-ND	3.61	1.42	1.37
14	Z	504	CLA	C1D-ND	3.61	1.42	1.37
14	q	505	CLA	C1D-ND	3.61	1.42	1.37
14	q	503	CLA	C1D-ND	3.60	1.42	1.37
14	A	1117	CLA	C4D-ND	-3.60	1.32	1.37
14	u	501	CLA	C1D-ND	3.60	1.42	1.37
14	A	1011	CLA	C4D-ND	-3.60	1.32	1.37
14	B	1217	CLA	C1D-ND	3.60	1.42	1.37
14	5	501	CLA	C1D-ND	3.60	1.42	1.37
14	Y	518	CLA	C1D-ND	3.60	1.42	1.37
14	f	1012	CLA	C4D-ND	-3.60	1.32	1.37
14	Y	507	CLA	C1D-ND	3.60	1.42	1.37
14	e	1011	CLA	C4D-ND	-3.60	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	511	CLA	C1D-ND	3.60	1.42	1.37
14	d	507	CLA	C1D-ND	3.60	1.42	1.37
14	c	501	CLA	C1D-ND	3.60	1.42	1.37
14	q	518	CLA	C1D-ND	3.60	1.42	1.37
14	V	1503	CLA	C1D-ND	3.60	1.42	1.37
14	e	1133	CLA	C4D-ND	-3.60	1.32	1.37
14	1	507	CLA	C1D-ND	3.60	1.42	1.37
14	6	501	CLA	C1D-ND	3.60	1.42	1.37
14	G	1105	CLA	C4D-ND	-3.60	1.32	1.37
14	G	1237	CLA	C4D-ND	-3.60	1.32	1.37
14	A	1105	CLA	C4D-ND	-3.59	1.32	1.37
14	3	511	CLA	C1D-ND	3.59	1.42	1.37
14	q	517	CLA	C1D-ND	3.59	1.42	1.37
14	B	1209	CLA	C1D-ND	3.59	1.42	1.37
14	4	518	CLA	C1D-ND	3.59	1.42	1.37
14	H	1217	CLA	C1D-ND	3.59	1.42	1.37
14	t	501	CLA	C1D-ND	3.59	1.42	1.37
14	f	1217	CLA	C1D-ND	3.59	1.42	1.37
14	6	513	CLA	C1D-ND	3.58	1.42	1.37
14	e	1104	CLA	C4D-ND	-3.58	1.32	1.37
14	j	1301	CLA	C4D-ND	-3.58	1.32	1.37
14	r	509	CLA	C1D-ND	3.58	1.42	1.37
14	v	510	CLA	C1D-ND	3.58	1.42	1.37
14	G	1102	CLA	C4D-ND	-3.58	1.32	1.37
14	r	504	CLA	C1D-ND	3.58	1.42	1.37
14	t	519	CLA	C1D-ND	3.58	1.42	1.37
14	L	1503	CLA	C1D-ND	3.58	1.42	1.37
14	G	1133	CLA	C4D-ND	-3.58	1.32	1.37
14	4	501	CLA	C1D-ND	3.58	1.42	1.37
14	b	519	CLA	C1D-ND	3.58	1.42	1.37
14	A	1013	CLA	C4D-ND	-3.58	1.32	1.37
14	1	503	CLA	C1D-ND	3.57	1.42	1.37
14	f	1225	CLA	C4D-ND	-3.57	1.32	1.37
14	2	504	CLA	C1D-ND	3.57	1.42	1.37
14	d	513	CLA	C1D-ND	3.57	1.42	1.37
15	e	2001	PQN	C3-C4	-3.57	1.38	1.47
14	c	502	CLA	C1D-ND	3.57	1.42	1.37
14	1	509	CLA	C1D-ND	3.57	1.42	1.37
14	5	502	CLA	C1D-ND	3.57	1.42	1.37
14	c	507	CLA	C1D-ND	3.57	1.42	1.37
14	d	516	CLA	C1D-ND	3.57	1.42	1.37
14	e	1113	CLA	C4D-ND	-3.57	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5	507	CLA	C1D-ND	3.57	1.42	1.37
14	A	1237	CLA	C4D-ND	-3.57	1.32	1.37
14	q	507	CLA	C1D-ND	3.57	1.42	1.37
14	1	505	CLA	C1D-ND	3.57	1.42	1.37
14	Z	511	CLA	C1D-ND	3.56	1.42	1.37
14	d	504	CLA	C1D-ND	3.56	1.42	1.37
14	t	509	CLA	C1D-ND	3.56	1.42	1.37
14	5	518	CLA	C1D-ND	3.56	1.42	1.37
14	3	501	CLA	C1D-ND	3.56	1.42	1.37
14	u	518	CLA	C1D-ND	3.56	1.42	1.37
14	a	511	CLA	C1D-ND	3.56	1.42	1.37
14	l	1303	CLA	C1D-ND	3.56	1.42	1.37
14	B	1212	CLA	C1D-ND	3.56	1.42	1.37
14	s	511	CLA	C1D-ND	3.56	1.42	1.37
14	B	1225	CLA	C4D-ND	-3.55	1.32	1.37
14	1	517	CLA	C1D-ND	3.55	1.42	1.37
14	A	1104	CLA	C4D-ND	-3.55	1.32	1.37
14	Y	510	CLA	C1D-ND	3.55	1.42	1.37
14	r	513	CLA	C1D-ND	3.55	1.42	1.37
14	G	1013	CLA	C4D-ND	-3.55	1.32	1.37
14	6	504	CLA	C1D-ND	3.55	1.42	1.37
14	t	508	CLA	C1D-ND	3.55	1.42	1.37
14	d	509	CLA	C1D-ND	3.55	1.42	1.37
14	G	1104	CLA	C4D-ND	-3.55	1.32	1.37
14	G	1113	CLA	C4D-ND	-3.55	1.32	1.37
15	A	2001	PQN	C3-C4	-3.55	1.38	1.47
14	c	504	CLA	C1D-ND	3.54	1.42	1.37
14	f	1212	CLA	C1D-ND	3.54	1.42	1.37
14	6	510	CLA	C1D-ND	3.54	1.42	1.37
14	G	1130	CLA	C4D-ND	-3.54	1.32	1.37
14	H	1212	CLA	C1D-ND	3.54	1.42	1.37
14	e	1013	CLA	C4D-ND	-3.54	1.32	1.37
14	6	502	CLA	C1D-ND	3.54	1.42	1.37
14	A	1130	CLA	C4D-ND	-3.54	1.32	1.37
14	F	1301	CLA	C4D-ND	-3.54	1.32	1.37
14	t	518	CLA	C1D-ND	3.54	1.42	1.37
14	v	513	CLA	C1D-ND	3.54	1.42	1.37
14	6	516	CLA	C1D-ND	3.54	1.42	1.37
14	c	513	CLA	C1D-ND	3.54	1.42	1.37
14	5	513	CLA	C1D-ND	3.54	1.42	1.37
14	f	1224	CLA	C1D-ND	3.54	1.42	1.37
14	A	1113	CLA	C4D-ND	-3.53	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1223	CLA	C4D-ND	-3.53	1.32	1.37
14	f	1202	CLA	C4D-ND	-3.53	1.32	1.37
14	4	519	CLA	C1D-ND	3.53	1.42	1.37
15	G	2001	PQN	C3-C4	-3.53	1.38	1.47
14	G	1120	CLA	C4D-ND	-3.53	1.32	1.37
14	s	502	CLA	C1D-ND	3.53	1.42	1.37
14	v	509	CLA	C1D-ND	3.53	1.42	1.37
14	v	517	CLA	C1D-ND	3.53	1.42	1.37
14	a	508	CLA	C1D-ND	3.53	1.42	1.37
14	H	1223	CLA	C4D-ND	-3.53	1.32	1.37
14	c	518	CLA	C1D-ND	3.53	1.42	1.37
14	e	1237	CLA	C4D-ND	-3.53	1.32	1.37
14	A	1120	CLA	C4D-ND	-3.53	1.32	1.37
14	f	1223	CLA	C4D-ND	-3.53	1.32	1.37
14	6	508	CLA	C1D-ND	3.53	1.42	1.37
14	H	1210	CLA	C4D-ND	-3.53	1.32	1.37
14	v	516	CLA	C1D-ND	3.53	1.42	1.37
14	d	508	CLA	C1D-ND	3.53	1.42	1.37
14	H	1209	CLA	C1D-ND	3.53	1.42	1.37
14	b	509	CLA	C1D-ND	3.53	1.42	1.37
14	A	1102	CLA	C4D-ND	-3.52	1.32	1.37
14	f	1239	CLA	C1D-ND	3.52	1.42	1.37
14	6	509	CLA	C1D-ND	3.52	1.42	1.37
14	v	502	CLA	C1D-ND	3.52	1.42	1.37
14	2	513	CLA	C1D-ND	3.52	1.42	1.37
14	c	516	CLA	C1D-ND	3.52	1.42	1.37
14	2	509	CLA	C1D-ND	3.52	1.42	1.37
14	5	516	CLA	C1D-ND	3.52	1.42	1.37
14	H	1224	CLA	C1D-ND	3.52	1.42	1.37
14	v	518	CLA	C1D-ND	3.52	1.42	1.37
14	u	504	CLA	C1D-ND	3.52	1.42	1.37
14	4	509	CLA	C1D-ND	3.51	1.42	1.37
14	v	504	CLA	C1D-ND	3.51	1.42	1.37
14	q	510	CLA	C1D-ND	3.51	1.42	1.37
14	d	505	CLA	C1D-ND	3.51	1.42	1.37
14	e	1102	CLA	C4D-ND	-3.51	1.32	1.37
14	e	1120	CLA	C4D-ND	-3.51	1.32	1.37
14	f	1215	CLA	C4D-ND	-3.51	1.32	1.37
19	H	1843	LMU	O5'-C1'	3.51	1.50	1.41
14	G	1107	CLA	C4D-ND	-3.51	1.32	1.37
14	e	1130	CLA	C4D-ND	-3.51	1.32	1.37
14	Y	501	CLA	C1D-ND	3.51	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1107	CLA	C4D-ND	-3.51	1.32	1.37
14	6	518	CLA	C1D-ND	3.51	1.42	1.37
14	B	1210	CLA	C4D-ND	-3.51	1.32	1.37
14	f	1223	CLA	C1D-ND	3.51	1.42	1.37
14	u	509	CLA	C1D-ND	3.51	1.42	1.37
14	B	1224	CLA	C1D-ND	3.51	1.42	1.37
14	5	504	CLA	C1D-ND	3.51	1.42	1.37
14	a	502	CLA	C1D-ND	3.51	1.42	1.37
14	s	501	CLA	C1D-ND	3.50	1.42	1.37
14	u	513	CLA	C1D-ND	3.50	1.42	1.37
14	B	1202	CLA	C4D-ND	-3.50	1.32	1.37
14	2	501	CLA	C1D-ND	3.50	1.42	1.37
14	3	509	CLA	C1D-ND	3.50	1.42	1.37
14	G	1121	CLA	C4D-ND	-3.50	1.32	1.37
14	1	510	CLA	C1D-ND	3.50	1.42	1.37
14	2	506	CLA	C1D-ND	3.50	1.42	1.37
14	s	504	CLA	C1D-ND	3.50	1.42	1.37
14	u	516	CLA	C1D-ND	3.50	1.42	1.37
14	R	1301	CLA	C4D-ND	-3.50	1.32	1.37
14	Z	508	CLA	C1D-ND	3.50	1.42	1.37
14	Z	501	CLA	C1D-ND	3.50	1.42	1.37
14	6	505	CLA	C1D-ND	3.50	1.42	1.37
14	c	509	CLA	C1D-ND	3.50	1.42	1.37
14	d	510	CLA	C1D-ND	3.50	1.42	1.37
14	1	501	CLA	C1D-ND	3.49	1.42	1.37
14	H	1215	CLA	C4D-ND	-3.49	1.32	1.37
14	v	508	CLA	C1D-ND	3.49	1.42	1.37
14	3	508	CLA	C1D-ND	3.49	1.42	1.37
14	U	1103	CLA	C1D-ND	3.49	1.42	1.37
14	B	1215	CLA	C4D-ND	-3.49	1.32	1.37
14	3	504	CLA	C1D-ND	3.49	1.42	1.37
14	r	501	CLA	C1D-ND	3.49	1.42	1.37
14	5	509	CLA	C1D-ND	3.49	1.42	1.37
14	e	1116	CLA	C1D-ND	3.49	1.42	1.37
14	e	1121	CLA	C4D-ND	-3.49	1.32	1.37
14	t	512	CLA	C1D-ND	3.49	1.42	1.37
14	A	1106	CLA	C4D-ND	-3.48	1.32	1.37
14	B	1239	CLA	C1D-ND	3.48	1.42	1.37
14	a	510	CLA	C1D-ND	3.48	1.42	1.37
19	B	1843	LMU	O5'-C1'	3.48	1.50	1.41
14	A	1107	CLA	C4D-ND	-3.48	1.32	1.37
14	Z	506	CLA	C1D-ND	3.48	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1216	CLA	C4D-ND	-3.48	1.32	1.37
14	f	1214	CLA	C4D-ND	-3.48	1.32	1.37
14	s	508	CLA	C1D-ND	3.48	1.42	1.37
14	H	1207	CLA	C4D-ND	-3.48	1.32	1.37
14	f	1222	CLA	C4D-ND	-3.48	1.32	1.37
14	3	502	CLA	C1D-ND	3.48	1.42	1.37
14	q	501	CLA	C1D-ND	3.47	1.42	1.37
14	A	1116	CLA	C4D-ND	-3.47	1.32	1.37
14	H	1202	CLA	C4D-ND	-3.47	1.32	1.37
14	A	1101	CLA	C3B-C4B	3.47	1.50	1.42
14	B	1207	CLA	C4D-ND	-3.47	1.32	1.37
14	e	1101	CLA	C3B-C4B	3.47	1.50	1.42
14	c	510	CLA	C1D-ND	3.47	1.42	1.37
14	d	502	CLA	C1D-ND	3.47	1.42	1.37
14	f	1240	CLA	C1D-ND	3.47	1.42	1.37
14	e	1118	CLA	C4D-ND	-3.47	1.32	1.37
14	A	1116	CLA	C1D-ND	3.47	1.42	1.37
14	B	1223	CLA	C1D-ND	3.47	1.42	1.37
14	B	1240	CLA	C1D-ND	3.47	1.42	1.37
14	2	508	CLA	C1D-ND	3.47	1.42	1.37
14	u	510	CLA	C1D-ND	3.47	1.42	1.37
14	G	1106	CLA	C4D-ND	-3.47	1.32	1.37
14	H	1223	CLA	C1D-ND	3.47	1.42	1.37
14	B	1231	CLA	C4D-ND	-3.47	1.32	1.37
14	r	508	CLA	C1D-ND	3.47	1.42	1.37
14	Y	504	CLA	C1D-ND	3.47	1.42	1.37
14	f	1216	CLA	C4D-ND	-3.46	1.32	1.37
14	Z	513	CLA	C1D-ND	3.46	1.42	1.37
19	f	1843	LMU	O5'-C1'	3.46	1.50	1.41
14	G	1011	CLA	C1D-ND	3.46	1.42	1.37
14	f	1210	CLA	C4D-ND	-3.46	1.32	1.37
14	B	1214	CLA	C4D-ND	-3.46	1.32	1.37
14	H	1239	CLA	C1D-ND	3.46	1.42	1.37
15	f	2002	PQN	C10-C1	-3.46	1.41	1.48
14	H	1214	CLA	C1D-ND	3.46	1.42	1.37
14	e	1116	CLA	C4D-ND	-3.46	1.32	1.37
14	f	1207	CLA	C4D-ND	-3.46	1.32	1.37
14	3	510	CLA	C1D-ND	3.46	1.42	1.37
14	d	517	CLA	C1D-ND	3.46	1.42	1.37
14	d	518	CLA	C1D-ND	3.46	1.42	1.37
14	6	517	CLA	C1D-ND	3.45	1.42	1.37
14	Z	509	CLA	C1D-ND	3.45	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1231	CLA	C4D-ND	-3.45	1.32	1.37
14	v	505	CLA	C1D-ND	3.45	1.42	1.37
14	a	509	CLA	C1D-ND	3.45	1.42	1.37
14	G	1101	CLA	C3B-C4B	3.45	1.50	1.42
14	a	504	CLA	C1D-ND	3.45	1.42	1.37
14	Z	519	CLA	C1D-ND	3.45	1.42	1.37
14	f	1214	CLA	C1D-ND	3.45	1.42	1.37
14	G	1116	CLA	C1D-ND	3.45	1.42	1.37
14	f	1203	CLA	C1D-ND	3.45	1.42	1.37
14	5	510	CLA	C1D-ND	3.44	1.42	1.37
14	H	1222	CLA	C4D-ND	-3.44	1.33	1.37
14	B	1216	CLA	C4D-ND	-3.44	1.33	1.37
14	2	519	CLA	C1D-ND	3.44	1.42	1.37
14	4	512	CLA	C1D-ND	3.44	1.42	1.37
14	A	1121	CLA	C4D-ND	-3.44	1.33	1.37
14	e	1112	CLA	C4D-ND	-3.44	1.33	1.37
14	q	502	CLA	C1D-ND	3.44	1.42	1.37
14	u	506	CLA	C1D-ND	3.44	1.42	1.37
14	e	1106	CLA	C4D-ND	-3.44	1.33	1.37
14	5	506	CLA	C1D-ND	3.44	1.42	1.37
14	B	1214	CLA	C1D-ND	3.43	1.42	1.37
14	G	1116	CLA	C4D-ND	-3.43	1.33	1.37
14	f	1231	CLA	C4D-ND	-3.43	1.33	1.37
14	K	1401	CLA	C4D-ND	-3.43	1.33	1.37
14	H	1240	CLA	C1D-ND	3.43	1.42	1.37
14	r	506	CLA	C1D-ND	3.43	1.42	1.37
14	Y	516	CLA	C4D-ND	-3.43	1.33	1.37
14	q	516	CLA	C4D-ND	-3.43	1.33	1.37
14	m	1103	CLA	C1D-ND	3.43	1.42	1.37
14	n	1501	CLA	C4D-ND	-3.43	1.33	1.37
14	B	1222	CLA	C4D-ND	-3.43	1.33	1.37
14	K	1103	CLA	C1D-ND	3.43	1.42	1.37
14	a	505	CLA	C1D-ND	3.43	1.42	1.37
14	B	1238	CLA	C4D-ND	-3.43	1.33	1.37
14	1	516	CLA	C4D-ND	-3.43	1.33	1.37
14	r	519	CLA	C1D-ND	3.42	1.42	1.37
14	s	510	CLA	C1D-ND	3.42	1.42	1.37
15	B	2002	PQN	C10-C1	-3.42	1.41	1.48
14	b	512	CLA	C1D-ND	3.42	1.42	1.37
14	A	1122	CLA	C1D-ND	3.42	1.42	1.37
14	H	1203	CLA	C1D-ND	3.42	1.42	1.37
14	A	1118	CLA	C4D-ND	-3.42	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	U	1401	CLA	C4D-ND	-3.42	1.33	1.37
14	s	509	CLA	C1D-ND	3.42	1.42	1.37
14	e	1122	CLA	C1D-ND	3.42	1.42	1.37
14	r	518	CLA	C1D-ND	3.41	1.42	1.37
14	G	1118	CLA	C4D-ND	-3.41	1.33	1.37
14	B	1203	CLA	C1D-ND	3.41	1.42	1.37
14	c	506	CLA	C1D-ND	3.41	1.42	1.37
14	t	504	CLA	C4B-NB	3.41	1.42	1.37
14	L	1501	CLA	C4D-ND	-3.41	1.33	1.37
14	s	505	CLA	C1D-ND	3.41	1.42	1.37
14	H	1214	CLA	C4D-ND	-3.41	1.33	1.37
14	G	1122	CLA	C1D-ND	3.40	1.42	1.37
14	u	505	CLA	C1D-ND	3.40	1.42	1.37
14	f	1238	CLA	C4D-ND	-3.40	1.33	1.37
14	m	1401	CLA	C4D-ND	-3.40	1.33	1.37
14	f	1218	CLA	C4D-ND	-3.40	1.33	1.37
14	f	1220	CLA	C4D-ND	-3.40	1.33	1.37
15	H	2002	PQN	C10-C1	-3.40	1.41	1.48
14	H	1218	CLA	C4D-ND	-3.40	1.33	1.37
14	B	1218	CLA	C4D-ND	-3.39	1.33	1.37
14	B	1220	CLA	C4D-ND	-3.39	1.33	1.37
14	3	505	CLA	C1D-ND	3.39	1.42	1.37
14	H	1238	CLA	C4D-ND	-3.39	1.33	1.37
14	1	504	CLA	C1D-ND	3.39	1.42	1.37
14	c	505	CLA	C1D-ND	3.39	1.42	1.37
14	t	501	CLA	C4B-NB	3.39	1.42	1.37
14	5	505	CLA	C1D-ND	3.39	1.41	1.37
14	H	1212	CLA	C4D-ND	-3.39	1.33	1.37
14	f	1221	CLA	C4D-ND	-3.38	1.33	1.37
14	B	1206	CLA	C4D-ND	-3.38	1.33	1.37
14	2	518	CLA	C1D-ND	3.38	1.41	1.37
14	B	1221	CLA	C4D-ND	-3.38	1.33	1.37
14	G	1126	CLA	C4D-ND	-3.38	1.33	1.37
14	A	1112	CLA	C4D-ND	-3.38	1.33	1.37
14	1	502	CLA	C1D-ND	3.38	1.41	1.37
14	V	1501	CLA	C4D-ND	-3.38	1.33	1.37
14	v	513	CLA	C4B-NB	3.38	1.41	1.37
14	B	1212	CLA	C4D-ND	-3.38	1.33	1.37
14	H	1211	CLA	C4D-ND	-3.37	1.33	1.37
14	H	1226	CLA	C4D-ND	-3.37	1.33	1.37
19	e	1848	LMU	O5'-C1'	3.37	1.50	1.41
14	A	1011	CLA	C1D-ND	3.37	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	501	CLA	C4B-NB	3.37	1.41	1.37
14	A	1126	CLA	C4D-ND	-3.37	1.33	1.37
14	q	504	CLA	C1D-ND	3.37	1.41	1.37
14	B	1021	CLA	C4D-ND	-3.37	1.33	1.37
14	f	1226	CLA	C4D-ND	-3.37	1.33	1.37
19	G	1848	LMU	O5'-C1'	3.37	1.50	1.41
14	H	1220	CLA	C4D-ND	-3.37	1.33	1.37
14	2	502	CLA	C1D-ND	3.37	1.41	1.37
19	A	1848	LMU	O5'-C1'	3.36	1.50	1.41
14	m	1401	CLA	C1D-ND	3.36	1.41	1.37
14	a	517	CLA	C4B-NB	3.36	1.41	1.37
19	G	1848	LMU	O5B-C1B	3.36	1.50	1.41
14	H	1227	CLA	C4D-ND	-3.36	1.33	1.37
14	f	1206	CLA	C4D-ND	-3.36	1.33	1.37
14	e	1011	CLA	C1D-ND	3.36	1.41	1.37
14	f	1212	CLA	C4D-ND	-3.35	1.33	1.37
14	G	1114	CLA	C1D-ND	3.35	1.41	1.37
14	e	1126	CLA	C4D-ND	-3.35	1.33	1.37
14	H	1206	CLA	C4D-ND	-3.35	1.33	1.37
14	Z	502	CLA	C1D-ND	3.35	1.41	1.37
14	Z	518	CLA	C1D-ND	3.35	1.41	1.37
14	f	1021	CLA	C4D-ND	-3.35	1.33	1.37
14	G	1101	CLA	C4B-NB	3.35	1.41	1.37
14	B	1226	CLA	C4D-ND	-3.35	1.33	1.37
14	H	1221	CLA	C4D-ND	-3.35	1.33	1.37
14	4	504	CLA	C4B-NB	3.34	1.41	1.37
14	G	1112	CLA	C4D-ND	-3.34	1.33	1.37
14	4	501	CLA	C4B-NB	3.34	1.41	1.37
14	e	1101	CLA	C4B-NB	3.34	1.41	1.37
19	e	1848	LMU	O5B-C1B	3.34	1.50	1.41
14	A	1134	CLA	C4D-ND	-3.34	1.33	1.37
14	B	1232	CLA	C4D-ND	-3.33	1.33	1.37
14	U	1103	CLA	C4D-ND	-3.33	1.33	1.37
19	A	1848	LMU	O5B-C1B	3.33	1.50	1.41
14	H	1021	CLA	C4D-ND	-3.33	1.33	1.37
14	f	1235	CLA	C1D-ND	3.33	1.41	1.37
14	f	1211	CLA	C1D-ND	3.33	1.41	1.37
14	e	1134	CLA	C4D-ND	-3.33	1.33	1.37
19	H	1843	LMU	O5B-C1B	3.33	1.50	1.41
21	t	822	SQD	O47-C7	3.33	1.42	1.35
14	n	1503	CLA	C4D-ND	-3.33	1.33	1.37
14	R	1302	CLA	C1D-ND	3.33	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1211	CLA	C4D-ND	-3.33	1.33	1.37
14	f	1232	CLA	C4D-ND	-3.33	1.33	1.37
14	K	1401	CLA	C1D-ND	3.33	1.41	1.37
14	B	1211	CLA	C4D-ND	-3.33	1.33	1.37
14	B	1227	CLA	C4D-ND	-3.32	1.33	1.37
14	f	1224	CLA	C4D-ND	-3.32	1.33	1.37
14	e	1114	CLA	C1D-ND	3.32	1.41	1.37
14	r	502	CLA	C1D-ND	3.32	1.41	1.37
21	4	822	SQD	O47-C7	3.32	1.42	1.35
14	3	516	CLA	C1D-ND	3.32	1.41	1.37
21	b	822	SQD	O47-C7	3.32	1.42	1.35
19	B	1843	LMU	O5B-C1B	3.32	1.50	1.41
14	t	509	CLA	C4B-NB	3.32	1.41	1.37
14	L	1503	CLA	C4D-ND	-3.32	1.33	1.37
14	r	510	CLA	C1D-ND	3.32	1.41	1.37
14	V	1503	CLA	C4D-ND	-3.32	1.33	1.37
14	A	1114	CLA	C1D-ND	3.31	1.41	1.37
14	u	517	CLA	C4B-NB	3.31	1.41	1.37
14	f	1208	CLA	C4D-ND	-3.31	1.33	1.37
14	G	1134	CLA	C4D-ND	-3.31	1.33	1.37
14	e	1110	CLA	C4D-ND	-3.31	1.33	1.37
14	6	513	CLA	C4B-NB	3.31	1.41	1.37
14	A	1110	CLA	C4D-ND	-3.31	1.33	1.37
14	H	1230	CLA	C4D-ND	-3.31	1.33	1.37
14	s	501	CLA	C4D-ND	-3.31	1.33	1.37
14	A	1101	CLA	C4B-NB	3.31	1.41	1.37
14	Z	510	CLA	C1D-ND	3.30	1.41	1.37
14	b	513	CLA	C4B-NB	3.30	1.41	1.37
14	2	510	CLA	C1D-ND	3.30	1.41	1.37
14	H	1218	CLA	C1D-ND	3.30	1.41	1.37
14	B	1224	CLA	C4D-ND	-3.30	1.33	1.37
19	f	1843	LMU	O5B-C1B	3.30	1.50	1.41
14	B	1207	CLA	C1D-ND	3.30	1.41	1.37
14	U	1401	CLA	C1D-ND	3.30	1.41	1.37
14	e	1134	CLA	C1D-ND	3.30	1.41	1.37
14	J	1302	CLA	C1D-ND	3.30	1.41	1.37
14	s	516	CLA	C1D-ND	3.30	1.41	1.37
14	5	513	CLA	C4B-NB	3.30	1.41	1.37
14	H	1211	CLA	C1D-ND	3.30	1.41	1.37
14	e	1138	CLA	C4D-ND	-3.30	1.33	1.37
14	3	501	CLA	C4D-ND	-3.30	1.33	1.37
14	s	506	CLA	C4D-ND	-3.30	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Y	502	CLA	C1D-ND	3.30	1.41	1.37
14	d	513	CLA	C4B-NB	3.30	1.41	1.37
14	j	1302	CLA	C1D-ND	3.30	1.41	1.37
14	s	512	CLA	C4B-NB	3.30	1.41	1.37
14	B	1218	CLA	C1D-ND	3.29	1.41	1.37
14	H	1206	CLA	CMB-C2B	-3.29	1.43	1.50
14	2	506	CLA	C4D-ND	-3.29	1.33	1.37
14	a	501	CLA	C4D-ND	-3.29	1.33	1.37
14	F	1302	CLA	C1D-ND	3.29	1.41	1.37
14	Z	508	CLA	C4D-ND	-3.29	1.33	1.37
14	b	519	CLA	C4D-ND	-3.29	1.33	1.37
14	v	505	CLA	C4D-ND	-3.29	1.33	1.37
14	B	1222	CLA	C1D-ND	3.29	1.41	1.37
14	H	1207	CLA	C1D-ND	3.29	1.41	1.37
14	B	1230	CLA	C4D-ND	-3.29	1.33	1.37
14	v	510	CLA	C4D-ND	-3.29	1.33	1.37
14	Z	506	CLA	C4D-ND	-3.29	1.33	1.37
14	f	1222	CLA	C1D-ND	3.29	1.41	1.37
14	c	517	CLA	C4B-NB	3.29	1.41	1.37
14	s	506	CLA	C4B-NB	3.28	1.41	1.37
14	a	516	CLA	C1D-ND	3.28	1.41	1.37
14	s	517	CLA	C4B-NB	3.28	1.41	1.37
14	e	1801	CLA	C4D-ND	-3.28	1.33	1.37
14	d	512	CLA	C1D-ND	3.28	1.41	1.37
14	4	509	CLA	C4B-NB	3.28	1.41	1.37
14	2	508	CLA	C4D-ND	-3.28	1.33	1.37
14	f	1227	CLA	C4D-ND	-3.28	1.33	1.37
14	f	1208	CLA	C1D-ND	3.28	1.41	1.37
14	f	1218	CLA	C1D-ND	3.28	1.41	1.37
14	A	1801	CLA	C4D-ND	-3.28	1.33	1.37
14	c	501	CLA	C4D-ND	-3.28	1.33	1.37
14	b	504	CLA	C4B-NB	3.28	1.41	1.37
21	c	822	SQD	O47-C7	3.28	1.42	1.35
14	G	1138	CLA	C4D-ND	-3.28	1.33	1.37
14	B	1206	CLA	CMB-C2B	-3.28	1.43	1.50
14	r	508	CLA	C4D-ND	-3.28	1.33	1.37
14	n	1501	CLA	C1D-ND	3.28	1.41	1.37
14	A	1134	CLA	C1D-ND	3.28	1.41	1.37
14	f	1207	CLA	C1D-ND	3.28	1.41	1.37
14	l	1303	CLA	C4B-NB	3.28	1.41	1.37
14	b	509	CLA	C4B-NB	3.28	1.41	1.37
14	5	506	CLA	C4D-ND	-3.28	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	506	CLA	C4B-NB	3.28	1.41	1.37
14	H	1232	CLA	C4D-ND	-3.27	1.33	1.37
14	u	506	CLA	C4D-ND	-3.27	1.33	1.37
14	r	505	CLA	C1D-ND	3.27	1.41	1.37
14	K	1103	CLA	C4D-ND	-3.27	1.33	1.37
14	u	513	CLA	C4B-NB	3.27	1.41	1.37
14	m	1103	CLA	C4D-ND	-3.27	1.33	1.37
21	5	822	SQD	O47-C7	3.27	1.42	1.35
14	3	517	CLA	C4B-NB	3.27	1.41	1.37
14	l	1302	CLA	C1D-ND	3.27	1.41	1.37
14	r	519	CLA	C4D-ND	-3.27	1.33	1.37
14	B	1235	CLA	C1D-ND	3.27	1.41	1.37
14	b	502	CLA	C4B-NB	3.27	1.41	1.37
14	G	1801	CLA	C4D-ND	-3.27	1.33	1.37
14	B	1208	CLA	C4D-ND	-3.27	1.33	1.37
14	5	501	CLA	C4D-ND	-3.27	1.33	1.37
14	H	1208	CLA	C4D-ND	-3.27	1.33	1.37
14	H	1224	CLA	C4D-ND	-3.27	1.33	1.37
21	u	822	SQD	O47-C7	3.27	1.42	1.35
14	1	512	CLA	C1D-ND	3.27	1.41	1.37
14	Y	509	CLA	C4D-ND	-3.27	1.33	1.37
21	d	822	SQD	O47-C7	3.27	1.42	1.35
14	Y	512	CLA	C1D-ND	3.27	1.41	1.37
21	6	822	SQD	O47-C7	3.27	1.42	1.35
14	G	1134	CLA	C1D-ND	3.27	1.41	1.37
14	f	1210	CLA	C1D-ND	3.27	1.41	1.37
14	b	505	CLA	C1D-ND	3.27	1.41	1.37
14	c	513	CLA	C4B-NB	3.26	1.41	1.37
14	A	1138	CLA	C4D-ND	-3.26	1.33	1.37
14	T	1302	CLA	C1D-ND	3.26	1.41	1.37
14	c	506	CLA	C4D-ND	-3.26	1.33	1.37
14	6	512	CLA	C1D-ND	3.26	1.41	1.37
14	6	505	CLA	C4D-ND	-3.26	1.33	1.37
14	f	1206	CLA	CMB-C2B	-3.26	1.43	1.50
14	B	1211	CLA	C1D-ND	3.26	1.41	1.37
14	H	1228	CLA	C1D-ND	3.26	1.41	1.37
14	f	1230	CLA	C4D-ND	-3.26	1.33	1.37
14	m	1105	CLA	C4B-NB	3.26	1.41	1.37
14	q	501	CLA	C4D-ND	-3.26	1.33	1.37
14	4	502	CLA	C4B-NB	3.26	1.41	1.37
14	d	505	CLA	C4D-ND	-3.26	1.33	1.37
14	f	1240	CLA	C4D-ND	-3.26	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1239	CLA	C4D-ND	-3.26	1.33	1.37
14	B	1228	CLA	C1D-ND	3.26	1.41	1.37
14	r	506	CLA	C4D-ND	-3.26	1.33	1.37
14	L	1501	CLA	C1D-ND	3.26	1.41	1.37
14	2	505	CLA	C1D-ND	3.26	1.41	1.37
14	Y	501	CLA	C4D-ND	-3.25	1.33	1.37
21	v	822	SQD	O47-C7	3.25	1.42	1.35
14	2	509	CLA	C4D-ND	-3.25	1.33	1.37
14	b	506	CLA	C4B-NB	3.25	1.41	1.37
14	q	512	CLA	C1D-ND	3.25	1.41	1.37
14	6	501	CLA	C4D-ND	-3.25	1.33	1.37
14	G	1110	CLA	C4D-ND	-3.25	1.33	1.37
14	q	509	CLA	C4D-ND	-3.25	1.33	1.37
14	v	501	CLA	C4D-ND	-3.25	1.33	1.37
14	4	513	CLA	C4B-NB	3.25	1.41	1.37
14	1	502	CLA	C4D-ND	-3.25	1.33	1.37
14	u	501	CLA	C4D-ND	-3.25	1.33	1.37
14	B	1208	CLA	C1D-ND	3.25	1.41	1.37
14	1	509	CLA	C4D-ND	-3.25	1.33	1.37
14	Y	503	CLA	C4D-ND	-3.24	1.33	1.37
14	v	511	CLA	C4B-NB	3.24	1.41	1.37
14	a	513	CLA	C4B-NB	3.24	1.41	1.37
14	V	1501	CLA	C1D-ND	3.24	1.41	1.37
14	1	519	CLA	C4D-ND	-3.24	1.33	1.37
14	T	1303	CLA	C4B-NB	3.24	1.41	1.37
14	3	506	CLA	C4D-ND	-3.24	1.33	1.37
14	Z	503	CLA	C4D-ND	-3.24	1.33	1.37
14	6	508	CLA	C4D-ND	-3.24	1.33	1.37
14	3	512	CLA	C4B-NB	3.24	1.41	1.37
14	Z	505	CLA	C1D-ND	3.24	1.41	1.37
14	f	1228	CLA	C1D-ND	3.24	1.41	1.37
14	v	512	CLA	C1D-ND	3.24	1.41	1.37
14	1	501	CLA	C4D-ND	-3.24	1.33	1.37
14	f	1202	CLA	C1D-ND	3.24	1.41	1.37
14	H	1208	CLA	C1D-ND	3.23	1.41	1.37
14	d	501	CLA	C4D-ND	-3.23	1.33	1.37
14	r	509	CLA	C4D-ND	-3.23	1.33	1.37
14	A	1101	CLA	C4D-ND	-3.23	1.33	1.37
14	c	516	CLA	C4B-NB	3.23	1.41	1.37
14	q	506	CLA	C4B-NB	3.23	1.41	1.37
14	4	505	CLA	C1D-ND	3.23	1.41	1.37
14	5	517	CLA	C4B-NB	3.23	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	s	512	CLA	C1D-ND	3.23	1.41	1.37
14	t	505	CLA	C1D-ND	3.23	1.41	1.37
14	f	1238	CLA	C1D-ND	3.23	1.41	1.37
14	B	1213	CLA	C4D-ND	-3.23	1.33	1.37
14	3	512	CLA	C1D-ND	3.23	1.41	1.37
14	4	506	CLA	C4B-NB	3.23	1.41	1.37
14	6	512	CLA	C4B-NB	3.23	1.41	1.37
14	H	1222	CLA	C1D-ND	3.23	1.41	1.37
14	a	512	CLA	C4B-NB	3.23	1.41	1.37
14	6	510	CLA	C4D-ND	-3.23	1.33	1.37
14	G	1114	CLA	C4D-ND	-3.23	1.33	1.37
14	Y	519	CLA	C4D-ND	-3.23	1.33	1.37
14	d	508	CLA	C4D-ND	-3.23	1.33	1.37
14	4	519	CLA	C4D-ND	-3.23	1.33	1.37
14	3	518	CLA	C4D-ND	-3.23	1.33	1.37
14	u	508	CLA	C4D-ND	-3.23	1.33	1.37
14	A	1114	CLA	C4B-NB	3.23	1.41	1.37
14	t	513	CLA	C4B-NB	3.23	1.41	1.37
14	j	1301	CLA	C1D-ND	3.22	1.41	1.37
14	H	1239	CLA	C4D-ND	-3.22	1.33	1.37
14	a	508	CLA	C4D-ND	-3.22	1.33	1.37
14	f	1228	CLA	C4D-ND	-3.22	1.33	1.37
14	A	1114	CLA	C4D-ND	-3.22	1.33	1.37
14	2	519	CLA	C4D-ND	-3.22	1.33	1.37
14	s	513	CLA	C4B-NB	3.22	1.41	1.37
14	H	1213	CLA	C4D-ND	-3.22	1.33	1.37
14	q	502	CLA	C4D-ND	-3.22	1.33	1.37
14	H	1219	CLA	C1D-ND	3.22	1.41	1.37
14	a	512	CLA	C1D-ND	3.22	1.41	1.37
14	u	516	CLA	C4B-NB	3.22	1.41	1.37
14	G	1132	CLA	C1D-ND	3.22	1.41	1.37
14	B	1239	CLA	C4D-ND	-3.22	1.33	1.37
14	B	1240	CLA	C4D-ND	-3.22	1.33	1.37
14	s	518	CLA	C4D-ND	-3.22	1.33	1.37
14	G	1114	CLA	C4B-NB	3.22	1.41	1.37
14	q	503	CLA	C4D-ND	-3.22	1.33	1.37
14	e	1114	CLA	C4B-NB	3.22	1.41	1.37
14	K	1105	CLA	C4B-NB	3.22	1.41	1.37
14	t	502	CLA	C4B-NB	3.22	1.41	1.37
14	3	508	CLA	C4D-ND	-3.22	1.33	1.37
14	v	508	CLA	C4D-ND	-3.22	1.33	1.37
14	2	512	CLA	C4B-NB	3.22	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1113	CLA	C1D-ND	3.22	1.41	1.37
14	H	1235	CLA	C1D-ND	3.22	1.41	1.37
14	H	1238	CLA	C1D-ND	3.22	1.41	1.37
14	d	516	CLA	C4B-NB	3.22	1.41	1.37
14	s	504	CLA	C4B-NB	3.22	1.41	1.37
14	e	1108	CLA	C4D-ND	-3.22	1.33	1.37
14	c	512	CLA	C1D-ND	3.22	1.41	1.37
14	A	1108	CLA	C4D-ND	-3.22	1.33	1.37
14	e	1110	CLA	C1D-ND	3.22	1.41	1.37
14	a	506	CLA	C4D-ND	-3.21	1.33	1.37
14	r	518	CLA	C4D-ND	-3.21	1.33	1.37
14	Y	506	CLA	C4B-NB	3.21	1.41	1.37
14	f	1234	CLA	C1D-ND	3.21	1.41	1.37
14	e	1114	CLA	C4D-ND	-3.21	1.33	1.37
14	q	519	CLA	C4D-ND	-3.21	1.33	1.37
14	5	516	CLA	C4B-NB	3.21	1.41	1.37
14	v	516	CLA	C4B-NB	3.21	1.41	1.37
14	a	506	CLA	C4B-NB	3.21	1.41	1.37
14	u	503	CLA	C4B-NB	3.21	1.41	1.37
14	s	508	CLA	C4D-ND	-3.21	1.33	1.37
14	J	1303	CLA	C4B-NB	3.21	1.41	1.37
14	u	510	CLA	C4D-ND	-3.21	1.33	1.37
14	H	1219	CLA	C4B-NB	3.21	1.41	1.37
14	H	1228	CLA	C4D-ND	-3.21	1.33	1.37
14	B	1228	CLA	C4D-ND	-3.21	1.33	1.37
14	1	504	CLA	C4D-ND	-3.21	1.33	1.37
14	Z	509	CLA	C4D-ND	-3.21	1.33	1.37
14	f	1213	CLA	C4D-ND	-3.21	1.33	1.37
14	B	1201	CLA	C1D-ND	3.21	1.41	1.37
14	u	519	CLA	C4B-NB	3.21	1.41	1.37
14	e	1101	CLA	C4D-ND	-3.21	1.33	1.37
14	Z	519	CLA	C4D-ND	-3.21	1.33	1.37
14	Y	502	CLA	C4D-ND	-3.20	1.33	1.37
14	B	1219	CLA	C4B-NB	3.20	1.41	1.37
14	6	516	CLA	C4B-NB	3.20	1.41	1.37
14	Z	512	CLA	C4B-NB	3.20	1.41	1.37
14	3	519	CLA	C4D-ND	-3.20	1.33	1.37
14	q	504	CLA	C4D-ND	-3.20	1.33	1.37
14	A	1110	CLA	C1D-ND	3.20	1.41	1.37
14	5	512	CLA	C1D-ND	3.20	1.41	1.37
14	H	1210	CLA	C1D-ND	3.20	1.41	1.37
14	t	517	CLA	C4D-ND	-3.20	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	518	CLA	C4D-ND	-3.20	1.33	1.37
14	G	1110	CLA	C1D-ND	3.20	1.41	1.37
14	U	1105	CLA	C4B-NB	3.20	1.41	1.37
14	d	512	CLA	C4B-NB	3.20	1.41	1.37
14	2	503	CLA	C4D-ND	-3.20	1.33	1.37
14	H	1217	CLA	C4B-NB	3.20	1.41	1.37
14	t	506	CLA	C4B-NB	3.20	1.41	1.37
14	1	503	CLA	C4D-ND	-3.20	1.33	1.37
14	B	1238	CLA	C1D-ND	3.20	1.41	1.37
14	u	502	CLA	C4B-NB	3.20	1.41	1.37
14	d	510	CLA	C4D-ND	-3.20	1.33	1.37
14	B	1210	CLA	C1D-ND	3.20	1.41	1.37
14	1	506	CLA	C4B-NB	3.20	1.41	1.37
14	Y	504	CLA	C4B-NB	3.20	1.41	1.37
14	e	1135	CLA	MG-NB	-3.19	1.99	2.05
14	A	1136	CLA	C1D-ND	3.19	1.41	1.37
14	1	504	CLA	C4B-NB	3.19	1.41	1.37
14	2	504	CLA	C4B-NB	3.19	1.41	1.37
14	e	1107	CLA	CMD-C2D	-3.19	1.44	1.50
14	6	510	CLA	C4B-NB	3.19	1.41	1.37
14	H	1240	CLA	C4D-ND	-3.19	1.33	1.37
14	c	510	CLA	C4D-ND	-3.19	1.33	1.37
14	t	519	CLA	C4D-ND	-3.19	1.33	1.37
14	G	1107	CLA	CMD-C2D	-3.19	1.44	1.50
14	t	503	CLA	C4B-NB	3.19	1.41	1.37
14	5	517	CLA	C4D-ND	-3.19	1.33	1.37
14	G	1108	CLA	C4D-ND	-3.19	1.33	1.37
14	B	1219	CLA	C1D-ND	3.19	1.41	1.37
14	2	513	CLA	C4B-NB	3.19	1.41	1.37
14	b	511	CLA	C4B-NB	3.19	1.41	1.37
14	2	518	CLA	C4D-ND	-3.19	1.33	1.37
14	F	1301	CLA	C1D-ND	3.19	1.41	1.37
14	5	503	CLA	C4B-NB	3.19	1.41	1.37
14	5	510	CLA	C4D-ND	-3.19	1.33	1.37
14	Y	505	CLA	C4D-ND	-3.19	1.33	1.37
14	b	508	CLA	C4D-ND	-3.19	1.33	1.37
14	B	1217	CLA	C4B-NB	3.19	1.41	1.37
14	b	517	CLA	C4B-NB	3.19	1.41	1.37
14	e	1136	CLA	C1D-ND	3.19	1.41	1.37
14	v	512	CLA	C4B-NB	3.19	1.41	1.37
14	B	1202	CLA	C1D-ND	3.19	1.41	1.37
14	6	511	CLA	C4B-NB	3.19	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	505	CLA	C4D-ND	-3.19	1.33	1.37
14	R	1301	CLA	C1D-ND	3.19	1.41	1.37
14	3	509	CLA	C4D-ND	-3.19	1.33	1.37
14	q	504	CLA	C4B-NB	3.18	1.41	1.37
14	r	504	CLA	C4B-NB	3.18	1.41	1.37
14	1	518	CLA	C4D-ND	-3.18	1.33	1.37
14	A	1107	CLA	CMD-C2D	-3.18	1.44	1.50
14	f	1215	CLA	C1D-ND	3.18	1.41	1.37
14	r	512	CLA	C4B-NB	3.18	1.41	1.37
14	t	516	CLA	C4B-NB	3.18	1.41	1.37
14	G	1101	CLA	C4D-ND	-3.18	1.33	1.37
14	s	509	CLA	C4D-ND	-3.18	1.33	1.37
14	3	513	CLA	C4B-NB	3.18	1.41	1.37
14	f	1201	CLA	C1D-ND	3.18	1.41	1.37
14	v	509	CLA	C4B-NB	3.18	1.41	1.37
14	s	519	CLA	C4D-ND	-3.18	1.33	1.37
14	G	1135	CLA	MG-NB	-3.18	1.99	2.05
14	H	1236	CLA	C4B-NB	3.18	1.41	1.37
14	H	1232	CLA	C1D-ND	3.18	1.41	1.37
14	f	1232	CLA	C1D-ND	3.18	1.41	1.37
14	5	508	CLA	C4D-ND	-3.18	1.33	1.37
14	t	511	CLA	C4B-NB	3.18	1.41	1.37
14	4	508	CLA	C4D-ND	-3.18	1.33	1.37
14	d	509	CLA	C4D-ND	-3.18	1.33	1.37
14	A	1132	CLA	C1D-ND	3.18	1.41	1.37
14	B	1215	CLA	C1D-ND	3.18	1.41	1.37
14	6	509	CLA	C4B-NB	3.18	1.41	1.37
14	5	509	CLA	C4D-ND	-3.18	1.33	1.37
14	u	504	CLA	C4B-NB	3.18	1.41	1.37
14	B	1232	CLA	C1D-ND	3.18	1.41	1.37
14	u	517	CLA	C4D-ND	-3.18	1.33	1.37
14	f	1219	CLA	C4B-NB	3.18	1.41	1.37
14	H	1201	CLA	C4D-ND	-3.17	1.33	1.37
14	v	509	CLA	C4D-ND	-3.17	1.33	1.37
14	1	513	CLA	C4B-NB	3.17	1.41	1.37
14	Y	513	CLA	C4B-NB	3.17	1.41	1.37
14	F	1302	CLA	C4D-ND	-3.17	1.33	1.37
14	u	512	CLA	C1D-ND	3.17	1.41	1.37
14	Y	508	CLA	C4D-ND	-3.17	1.33	1.37
14	6	509	CLA	C4D-ND	-3.17	1.33	1.37
14	d	511	CLA	C4D-ND	-3.17	1.33	1.37
14	t	508	CLA	C4D-ND	-3.17	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	u	505	CLA	C4D-ND	-3.17	1.33	1.37
14	4	516	CLA	C4B-NB	3.17	1.41	1.37
14	c	503	CLA	C4B-NB	3.17	1.41	1.37
14	v	502	CLA	C4D-ND	-3.17	1.33	1.37
21	a	822	SQD	O48-C23	3.17	1.42	1.33
14	s	517	CLA	C4D-ND	-3.17	1.33	1.37
14	f	1217	CLA	C4B-NB	3.17	1.41	1.37
14	H	1201	CLA	C1D-ND	3.17	1.41	1.37
14	Z	506	CLA	C4B-NB	3.17	1.41	1.37
14	Z	513	CLA	C4B-NB	3.17	1.41	1.37
14	b	516	CLA	C4B-NB	3.17	1.41	1.37
14	1	506	CLA	C4D-ND	-3.17	1.33	1.37
14	c	508	CLA	C4D-ND	-3.17	1.33	1.37
14	B	1236	CLA	C4B-NB	3.17	1.41	1.37
14	f	1219	CLA	C1D-ND	3.17	1.41	1.37
14	c	509	CLA	C4D-ND	-3.17	1.33	1.37
14	1	508	CLA	C4D-ND	-3.16	1.33	1.37
14	R	1302	CLA	C4D-ND	-3.16	1.33	1.37
14	a	504	CLA	C4B-NB	3.16	1.41	1.37
14	q	510	CLA	C4B-NB	3.16	1.41	1.37
14	q	508	CLA	C4D-ND	-3.16	1.33	1.37
14	B	1234	CLA	C1D-ND	3.16	1.41	1.37
14	2	506	CLA	C4B-NB	3.16	1.41	1.37
14	6	516	CLA	C4D-ND	-3.16	1.33	1.37
14	3	504	CLA	C4B-NB	3.16	1.41	1.37
14	e	1125	CLA	C1D-ND	3.16	1.41	1.37
14	Z	518	CLA	C4D-ND	-3.16	1.33	1.37
14	A	1113	CLA	C1D-ND	3.16	1.41	1.37
14	Y	504	CLA	C4D-ND	-3.16	1.33	1.37
14	B	1201	CLA	C4D-ND	-3.16	1.33	1.37
14	q	518	CLA	C4D-ND	-3.16	1.33	1.37
14	t	505	CLA	C4D-ND	-3.16	1.33	1.37
14	d	516	CLA	C4D-ND	-3.16	1.33	1.37
14	G	1123	CLA	C1D-ND	3.16	1.41	1.37
14	G	1138	CLA	C1D-ND	3.16	1.41	1.37
14	r	517	CLA	C4B-NB	3.16	1.41	1.37
14	H	1205	CLA	C4D-ND	-3.16	1.33	1.37
14	G	1136	CLA	C1D-ND	3.16	1.41	1.37
14	H	1216	CLA	C1D-ND	3.16	1.41	1.37
14	e	1132	CLA	C1D-ND	3.16	1.41	1.37
14	v	510	CLA	C4B-NB	3.16	1.41	1.37
14	a	509	CLA	C4D-ND	-3.16	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	v	516	CLA	C4D-ND	-3.16	1.33	1.37
14	3	501	CLA	C4B-NB	3.16	1.41	1.37
14	b	517	CLA	C4D-ND	-3.16	1.33	1.37
14	v	511	CLA	C4D-ND	-3.16	1.33	1.37
14	d	509	CLA	C4B-NB	3.16	1.41	1.37
14	H	1215	CLA	C1D-ND	3.15	1.41	1.37
14	2	513	CLA	C4D-ND	-3.15	1.33	1.37
14	q	511	CLA	C4D-ND	-3.15	1.33	1.37
14	4	517	CLA	C4D-ND	-3.15	1.33	1.37
14	u	504	CLA	C4D-ND	-3.15	1.33	1.37
14	5	502	CLA	C4B-NB	3.15	1.41	1.37
14	G	1119	CLA	C1D-ND	3.15	1.41	1.37
14	3	516	CLA	C4D-ND	-3.15	1.33	1.37
14	6	502	CLA	C4D-ND	-3.15	1.33	1.37
14	a	516	CLA	C4D-ND	-3.15	1.33	1.37
14	5	519	CLA	C4B-NB	3.15	1.41	1.37
14	Y	518	CLA	C4B-NB	3.15	1.41	1.37
14	c	502	CLA	C4B-NB	3.15	1.41	1.37
14	r	513	CLA	C4B-NB	3.15	1.41	1.37
14	s	501	CLA	C4B-NB	3.15	1.41	1.37
14	Z	513	CLA	C4D-ND	-3.15	1.33	1.37
14	r	513	CLA	C4D-ND	-3.15	1.33	1.37
14	Z	504	CLA	C4B-NB	3.15	1.41	1.37
14	5	505	CLA	C4D-ND	-3.15	1.33	1.37
14	Y	510	CLA	C4D-ND	-3.15	1.33	1.37
14	s	516	CLA	C4D-ND	-3.15	1.33	1.37
21	3	822	SQD	O48-C23	3.15	1.42	1.33
14	r	501	CLA	C4D-ND	-3.15	1.33	1.37
14	r	503	CLA	C4D-ND	-3.15	1.33	1.37
14	G	1137	CLA	C1D-ND	3.15	1.41	1.37
14	Y	519	CLA	C4B-NB	3.15	1.41	1.37
14	e	1113	CLA	C1D-ND	3.15	1.41	1.37
14	A	1135	CLA	MG-NB	-3.15	1.99	2.05
21	Y	822	SQD	O48-C23	3.15	1.42	1.33
14	q	519	CLA	C4B-NB	3.15	1.41	1.37
14	6	511	CLA	C4D-ND	-3.15	1.33	1.37
14	Z	510	CLA	C4D-ND	-3.15	1.33	1.37
14	d	511	CLA	C4B-NB	3.15	1.41	1.37
14	c	505	CLA	C4D-ND	-3.15	1.33	1.37
14	c	517	CLA	C4D-ND	-3.15	1.33	1.37
14	s	503	CLA	C4D-ND	-3.15	1.33	1.37
21	1	822	SQD	O48-C23	3.15	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1225	CLA	CMD-C2D	-3.15	1.44	1.50
14	r	516	CLA	C4B-NB	3.14	1.41	1.37
14	2	516	CLA	C4B-NB	3.14	1.41	1.37
14	5	503	CLA	C4D-ND	-3.14	1.33	1.37
14	f	1201	CLA	C4D-ND	-3.14	1.33	1.37
21	q	822	SQD	O48-C23	3.14	1.42	1.33
14	H	1234	CLA	C1D-ND	3.14	1.41	1.37
14	e	1123	CLA	C1D-ND	3.14	1.41	1.37
14	2	505	CLA	C4D-ND	-3.14	1.33	1.37
14	H	1231	CLA	C1D-ND	3.14	1.41	1.37
14	2	510	CLA	C4D-ND	-3.14	1.33	1.37
14	1	505	CLA	C4D-ND	-3.14	1.33	1.37
14	Z	501	CLA	C4D-ND	-3.14	1.33	1.37
14	a	505	CLA	C4D-ND	-3.14	1.33	1.37
14	r	507	CLA	C4D-ND	-3.14	1.33	1.37
21	s	822	SQD	O48-C23	3.14	1.42	1.33
14	4	505	CLA	C4D-ND	-3.14	1.33	1.37
14	j	1302	CLA	C4D-ND	-3.14	1.33	1.37
14	r	505	CLA	C4D-ND	-3.14	1.33	1.37
14	v	517	CLA	C4D-ND	-3.14	1.33	1.37
14	6	508	CLA	C4B-NB	3.14	1.41	1.37
14	2	501	CLA	C4D-ND	-3.14	1.33	1.37
14	q	505	CLA	C4D-ND	-3.14	1.33	1.37
14	f	1225	CLA	CMD-C2D	-3.14	1.44	1.50
14	q	506	CLA	C4D-ND	-3.14	1.33	1.37
14	q	513	CLA	C4B-NB	3.14	1.41	1.37
14	Y	506	CLA	C4D-ND	-3.13	1.33	1.37
14	c	503	CLA	C4D-ND	-3.13	1.33	1.37
14	A	1119	CLA	C1D-ND	3.13	1.41	1.37
14	e	1138	CLA	C1D-ND	3.13	1.41	1.37
14	B	1236	CLA	C1D-ND	3.13	1.41	1.37
14	c	519	CLA	C4B-NB	3.13	1.41	1.37
14	4	517	CLA	C4B-NB	3.13	1.41	1.37
14	Z	516	CLA	C4B-NB	3.13	1.41	1.37
14	f	1216	CLA	CMB-C2B	-3.13	1.44	1.50
14	3	507	CLA	C4D-ND	-3.13	1.33	1.37
14	Z	517	CLA	C4D-ND	-3.13	1.33	1.37
14	a	507	CLA	C4D-ND	-3.13	1.33	1.37
14	A	1125	CLA	C1D-ND	3.13	1.41	1.37
14	5	504	CLA	C4B-NB	3.13	1.41	1.37
14	e	1119	CLA	C1D-ND	3.13	1.41	1.37
14	B	1219	CLA	C4D-ND	-3.13	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	c	519	CLA	C4D-ND	-3.13	1.33	1.37
14	A	1137	CLA	C1D-ND	3.13	1.41	1.37
14	B	1231	CLA	C1D-ND	3.13	1.41	1.37
14	4	503	CLA	C4B-NB	3.13	1.41	1.37
14	d	510	CLA	C4B-NB	3.13	1.41	1.37
14	c	504	CLA	C4D-ND	-3.13	1.33	1.37
14	B	1225	CLA	CMD-C2D	-3.13	1.44	1.50
14	Y	517	CLA	C4D-ND	-3.13	1.33	1.37
14	s	510	CLA	C4D-ND	-3.13	1.33	1.37
14	e	1137	CLA	C1D-ND	3.13	1.41	1.37
14	H	1216	CLA	CMB-C2B	-3.13	1.44	1.50
14	q	501	CLA	C4B-NB	3.13	1.41	1.37
14	d	502	CLA	C4D-ND	-3.13	1.33	1.37
14	2	517	CLA	C4D-ND	-3.12	1.33	1.37
14	1	519	CLA	C4B-NB	3.12	1.41	1.37
14	1	511	CLA	C4D-ND	-3.12	1.33	1.37
14	Y	511	CLA	C4D-ND	-3.12	1.33	1.37
14	d	503	CLA	C4D-ND	-3.12	1.33	1.37
14	4	511	CLA	C4B-NB	3.12	1.41	1.37
14	B	1205	CLA	C4D-ND	-3.12	1.33	1.37
14	a	519	CLA	C4D-ND	-3.12	1.33	1.37
14	b	505	CLA	C4D-ND	-3.12	1.33	1.37
14	A	1123	CLA	C1D-ND	3.12	1.41	1.37
14	G	1118	CLA	C1D-ND	3.12	1.41	1.37
14	G	1140	CLA	C1D-ND	3.12	1.41	1.37
14	q	507	CLA	C4B-NB	3.12	1.41	1.37
14	3	517	CLA	C4D-ND	-3.12	1.33	1.37
14	5	519	CLA	C4D-ND	-3.12	1.33	1.37
14	Y	518	CLA	C4D-ND	-3.12	1.33	1.37
14	e	1107	CLA	CMB-C2B	-3.12	1.44	1.50
14	6	517	CLA	C4D-ND	-3.12	1.33	1.37
14	s	512	CLA	C4D-ND	-3.12	1.33	1.37
14	6	501	CLA	C4B-NB	3.12	1.41	1.37
14	d	506	CLA	C4B-NB	3.12	1.41	1.37
14	a	503	CLA	C4D-ND	-3.12	1.33	1.37
14	e	1123	CLA	C4D-ND	-3.12	1.33	1.37
14	v	506	CLA	C4D-ND	-3.12	1.33	1.37
14	Z	512	CLA	C3B-C4B	3.12	1.50	1.42
14	6	506	CLA	C4B-NB	3.12	1.41	1.37
14	c	504	CLA	C4B-NB	3.12	1.41	1.37
14	t	512	CLA	C4B-NB	3.12	1.41	1.37
14	5	504	CLA	C4D-ND	-3.12	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	503	CLA	C4D-ND	-3.12	1.33	1.37
14	G	1123	CLA	C4D-ND	-3.12	1.33	1.37
14	v	503	CLA	C4D-ND	-3.12	1.33	1.37
14	2	507	CLA	C4D-ND	-3.12	1.33	1.37
14	Z	502	CLA	C4D-ND	-3.12	1.33	1.37
14	u	509	CLA	C4D-ND	-3.12	1.33	1.37
14	A	1118	CLA	C1D-ND	3.12	1.41	1.37
14	f	1205	CLA	C4D-ND	-3.12	1.33	1.37
14	Z	507	CLA	C4D-ND	-3.11	1.33	1.37
14	v	519	CLA	C4D-ND	-3.11	1.33	1.37
14	A	1138	CLA	C1D-ND	3.11	1.41	1.37
14	1	510	CLA	C4B-NB	3.11	1.41	1.37
14	1	518	CLA	C4B-NB	3.11	1.41	1.37
14	v	504	CLA	C4B-NB	3.11	1.41	1.37
14	A	1107	CLA	CMB-C2B	-3.11	1.44	1.50
14	t	518	CLA	C4D-ND	-3.11	1.33	1.37
14	e	1112	CLA	C1D-ND	3.11	1.41	1.37
14	e	1128	CLA	C1B-NB	-3.11	1.34	1.37
14	3	509	CLA	C4B-NB	3.11	1.41	1.37
14	A	1123	CLA	C4D-ND	-3.11	1.33	1.37
14	B	1216	CLA	CMB-C2B	-3.11	1.44	1.50
14	6	519	CLA	C4D-ND	-3.11	1.33	1.37
14	Z	516	CLA	C4D-ND	-3.11	1.33	1.37
14	B	1216	CLA	C1D-ND	3.11	1.41	1.37
14	1	517	CLA	C4D-ND	-3.11	1.33	1.37
14	3	503	CLA	C4D-ND	-3.11	1.33	1.37
14	a	510	CLA	C4D-ND	-3.11	1.33	1.37
14	r	510	CLA	C4D-ND	-3.11	1.33	1.37
14	G	1125	CLA	C1D-ND	3.11	1.41	1.37
14	a	517	CLA	C4D-ND	-3.11	1.33	1.37
14	r	511	CLA	C4D-ND	-3.11	1.33	1.37
14	2	512	CLA	C3B-C4B	3.11	1.50	1.42
14	a	512	CLA	C3B-C4B	3.11	1.50	1.42
14	f	1231	CLA	C1D-ND	3.11	1.41	1.37
21	B	1852	SQD	O48-C23	3.11	1.42	1.33
14	u	519	CLA	C4D-ND	-3.11	1.33	1.37
14	e	1136	CLA	C3B-C4B	3.11	1.50	1.42
14	a	509	CLA	C4B-NB	3.11	1.41	1.37
14	f	1236	CLA	C4B-NB	3.11	1.41	1.37
14	f	1236	CLA	C1D-ND	3.11	1.41	1.37
14	1	510	CLA	C4D-ND	-3.10	1.33	1.37
14	r	512	CLA	C3B-C4B	3.10	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	509	CLA	C4D-ND	-3.10	1.33	1.37
14	B	1227	CLA	C1D-ND	3.10	1.41	1.37
14	Z	504	CLA	C4D-ND	-3.10	1.33	1.37
14	Z	512	CLA	C1D-ND	3.10	1.41	1.37
14	a	502	CLA	C4B-NB	3.10	1.41	1.37
14	t	517	CLA	C4B-NB	3.10	1.41	1.37
14	b	518	CLA	C4D-ND	-3.10	1.33	1.37
14	s	511	CLA	C4B-NB	3.10	1.41	1.37
14	A	1129	CLA	MG-NB	-3.10	1.99	2.05
14	6	506	CLA	C4D-ND	-3.10	1.33	1.37
14	t	513	CLA	C4D-ND	-3.10	1.33	1.37
14	Y	517	CLA	C4B-NB	3.10	1.41	1.37
14	f	1216	CLA	C1D-ND	3.10	1.41	1.37
14	G	1129	CLA	MG-NB	-3.10	1.99	2.05
14	q	518	CLA	C4B-NB	3.10	1.41	1.37
14	2	516	CLA	C4D-ND	-3.10	1.33	1.37
14	a	502	CLA	C4D-ND	-3.10	1.33	1.37
14	u	502	CLA	C4D-ND	-3.10	1.33	1.37
14	b	512	CLA	C4B-NB	3.10	1.41	1.37
14	H	1202	CLA	C1D-ND	3.10	1.41	1.37
14	Y	501	CLA	C4B-NB	3.10	1.41	1.37
14	b	503	CLA	C4B-NB	3.10	1.41	1.37
14	v	506	CLA	C4B-NB	3.10	1.41	1.37
14	r	516	CLA	C4D-ND	-3.10	1.33	1.37
14	G	1128	CLA	C1B-NB	-3.10	1.34	1.37
14	r	506	CLA	C4B-NB	3.10	1.41	1.37
14	b	519	CLA	C4B-NB	3.10	1.41	1.37
14	v	501	CLA	C4B-NB	3.10	1.41	1.37
14	3	510	CLA	C4D-ND	-3.10	1.33	1.37
14	e	1801	CLA	C1D-ND	3.09	1.41	1.37
14	3	512	CLA	C3B-C4B	3.09	1.50	1.42
14	d	501	CLA	C4B-NB	3.09	1.41	1.37
14	e	1129	CLA	MG-NB	-3.09	1.99	2.05
14	c	511	CLA	C4D-ND	-3.09	1.33	1.37
14	s	507	CLA	C4D-ND	-3.09	1.33	1.37
14	1	507	CLA	C4B-NB	3.09	1.41	1.37
14	H	1236	CLA	C1D-ND	3.09	1.41	1.37
14	6	512	CLA	C4D-ND	-3.09	1.33	1.37
14	B	1213	CLA	C1D-ND	3.09	1.41	1.37
14	r	512	CLA	C1D-ND	3.09	1.41	1.37
21	H	1852	SQD	O48-C23	3.09	1.42	1.33
14	b	501	CLA	C4D-ND	-3.09	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	f	1852	SQD	O48-C23	3.09	1.42	1.33
14	d	506	CLA	C4D-ND	-3.09	1.33	1.37
14	u	518	CLA	C4D-ND	-3.09	1.33	1.37
14	1	501	CLA	C4B-NB	3.09	1.41	1.37
14	u	518	CLA	C4B-NB	3.09	1.41	1.37
14	6	518	CLA	C4D-ND	-3.09	1.33	1.37
14	H	1219	CLA	C4D-ND	-3.09	1.33	1.37
14	4	512	CLA	C4B-NB	3.09	1.41	1.37
14	G	1114	CLA	C3B-C4B	3.09	1.50	1.42
14	2	502	CLA	C4D-ND	-3.09	1.33	1.37
14	d	512	CLA	C4D-ND	-3.09	1.33	1.37
14	v	518	CLA	C4D-ND	-3.09	1.33	1.37
14	6	507	CLA	C4B-NB	3.09	1.41	1.37
14	u	511	CLA	C4D-ND	-3.09	1.33	1.37
14	e	1237	CLA	CMB-C2B	-3.09	1.44	1.50
14	2	517	CLA	C4B-NB	3.09	1.41	1.37
14	A	1112	CLA	C1D-ND	3.09	1.41	1.37
14	T	1303	CLA	C4D-ND	-3.08	1.33	1.37
14	A	1136	CLA	C3B-C4B	3.08	1.50	1.42
14	d	504	CLA	C4D-ND	-3.08	1.33	1.37
14	q	517	CLA	C4D-ND	-3.08	1.33	1.37
14	Y	510	CLA	C4B-NB	3.08	1.41	1.37
14	s	509	CLA	C4B-NB	3.08	1.41	1.37
14	d	517	CLA	C4D-ND	-3.08	1.33	1.37
14	5	511	CLA	C4B-NB	3.08	1.41	1.37
14	e	1118	CLA	C1D-ND	3.08	1.41	1.37
14	5	518	CLA	C4D-ND	-3.08	1.33	1.37
14	H	1213	CLA	C1D-ND	3.08	1.41	1.37
14	v	519	CLA	C4B-NB	3.08	1.41	1.37
14	b	502	CLA	C4D-ND	-3.08	1.33	1.37
14	q	510	CLA	C4D-ND	-3.08	1.33	1.37
14	r	517	CLA	C4D-ND	-3.08	1.33	1.37
14	d	518	CLA	C4D-ND	-3.08	1.33	1.37
14	t	508	CLA	C4B-NB	3.08	1.41	1.37
14	5	511	CLA	C4D-ND	-3.08	1.33	1.37
14	t	509	CLA	C4D-ND	-3.08	1.33	1.37
14	A	1801	CLA	C1D-ND	3.08	1.41	1.37
14	f	1021	CLA	CMD-C2D	-3.08	1.44	1.50
14	3	502	CLA	C4D-ND	-3.08	1.33	1.37
14	4	513	CLA	C4D-ND	-3.08	1.33	1.37
14	B	1209	CLA	C4D-ND	-3.08	1.33	1.37
14	4	509	CLA	C4D-ND	-3.08	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1227	CLA	C1D-ND	3.08	1.41	1.37
14	G	1107	CLA	CMB-C2B	-3.08	1.44	1.50
14	l	1303	CLA	C4D-ND	-3.08	1.33	1.37
14	Y	512	CLA	C4B-NB	3.08	1.41	1.37
14	J	1303	CLA	C4D-ND	-3.08	1.33	1.37
14	4	519	CLA	C4B-NB	3.08	1.41	1.37
14	a	501	CLA	C4B-NB	3.08	1.41	1.37
14	G	1136	CLA	C3B-C4B	3.07	1.50	1.42
14	c	502	CLA	C4D-ND	-3.07	1.33	1.37
14	t	511	CLA	C4D-ND	-3.07	1.33	1.37
14	G	1112	CLA	C1D-ND	3.07	1.41	1.37
14	d	508	CLA	C4B-NB	3.07	1.41	1.37
14	2	512	CLA	C4D-ND	-3.07	1.33	1.37
14	6	504	CLA	C4D-ND	-3.07	1.33	1.37
14	f	1219	CLA	C4D-ND	-3.07	1.33	1.37
14	A	1140	CLA	C1D-ND	3.07	1.41	1.37
14	3	512	CLA	C4D-ND	-3.07	1.33	1.37
14	H	1209	CLA	C4D-ND	-3.07	1.33	1.37
14	s	505	CLA	C4D-ND	-3.07	1.33	1.37
14	u	503	CLA	C4D-ND	-3.07	1.33	1.37
14	G	1801	CLA	C1D-ND	3.07	1.41	1.37
14	Y	503	CLA	C4B-NB	3.07	1.41	1.37
14	t	501	CLA	C4D-ND	-3.07	1.33	1.37
14	2	512	CLA	C1D-ND	3.07	1.41	1.37
14	f	1209	CLA	C4D-ND	-3.07	1.33	1.37
14	Y	507	CLA	C4B-NB	3.07	1.41	1.37
14	3	505	CLA	C4D-ND	-3.07	1.33	1.37
14	4	518	CLA	C4D-ND	-3.07	1.33	1.37
14	H	1227	CLA	C1D-ND	3.07	1.41	1.37
14	G	1237	CLA	CMB-C2B	-3.07	1.44	1.50
14	3	502	CLA	C4B-NB	3.07	1.41	1.37
14	4	505	CLA	C4B-NB	3.07	1.41	1.37
14	c	511	CLA	C4B-NB	3.07	1.41	1.37
14	d	519	CLA	C4D-ND	-3.07	1.33	1.37
14	s	512	CLA	C3B-C4B	3.07	1.49	1.42
14	A	1108	CLA	C1D-ND	3.07	1.41	1.37
14	1	512	CLA	C4B-NB	3.07	1.41	1.37
14	e	1117	CLA	C1D-ND	3.07	1.41	1.37
14	f	1213	CLA	C1D-ND	3.07	1.41	1.37
14	u	511	CLA	C4B-NB	3.07	1.41	1.37
14	v	508	CLA	C4B-NB	3.07	1.41	1.37
14	V	1501	CLA	C4B-NB	3.07	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1226	CLA	C1B-NB	-3.07	1.34	1.37
14	2	511	CLA	C4D-ND	-3.07	1.33	1.37
14	b	505	CLA	C4B-NB	3.06	1.41	1.37
14	r	519	CLA	C4B-NB	3.06	1.41	1.37
14	v	507	CLA	C4B-NB	3.06	1.41	1.37
14	A	1237	CLA	CMB-C2B	-3.06	1.44	1.50
14	v	513	CLA	C3B-C4B	3.06	1.49	1.42
14	c	518	CLA	C4D-ND	-3.06	1.33	1.37
14	2	504	CLA	C4D-ND	-3.06	1.33	1.37
14	r	512	CLA	C4D-ND	-3.06	1.33	1.37
14	6	513	CLA	C3B-C4B	3.06	1.49	1.42
14	4	501	CLA	C4D-ND	-3.06	1.33	1.37
14	q	513	CLA	C4D-ND	-3.06	1.33	1.37
14	G	1109	CLA	C1D-ND	3.06	1.41	1.37
14	B	1205	CLA	C1D-ND	3.06	1.41	1.37
14	6	519	CLA	C4B-NB	3.06	1.41	1.37
14	r	504	CLA	C4D-ND	-3.06	1.33	1.37
14	1	503	CLA	C4B-NB	3.06	1.41	1.37
14	q	512	CLA	C4B-NB	3.06	1.41	1.37
14	Z	512	CLA	C4D-ND	-3.06	1.33	1.37
14	1	517	CLA	C4B-NB	3.06	1.41	1.37
14	3	511	CLA	C4B-NB	3.06	1.41	1.37
14	d	502	CLA	C4B-NB	3.06	1.41	1.37
14	e	1139	CLA	C1D-ND	3.06	1.41	1.37
14	2	519	CLA	C4B-NB	3.06	1.41	1.37
14	e	1104	CLA	C1D-ND	3.06	1.41	1.37
14	e	1121	CLA	C1D-ND	3.06	1.41	1.37
14	t	505	CLA	C4B-NB	3.06	1.41	1.37
14	c	513	CLA	C4D-ND	-3.06	1.33	1.37
14	A	1128	CLA	C1B-NB	-3.06	1.34	1.37
14	c	516	CLA	C4D-ND	-3.05	1.33	1.37
14	u	516	CLA	C4D-ND	-3.05	1.33	1.37
14	6	504	CLA	C4B-NB	3.05	1.41	1.37
14	6	518	CLA	C4B-NB	3.05	1.41	1.37
14	Z	517	CLA	C4B-NB	3.05	1.41	1.37
14	5	516	CLA	C4D-ND	-3.05	1.33	1.37
14	G	1108	CLA	C1D-ND	3.05	1.41	1.37
14	t	519	CLA	C4B-NB	3.05	1.41	1.37
14	B	1021	CLA	CMD-C2D	-3.05	1.44	1.50
14	5	518	CLA	C4B-NB	3.05	1.41	1.37
14	e	1108	CLA	C1D-ND	3.05	1.41	1.37
14	A	1114	CLA	C3B-C4B	3.05	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1226	CLA	C1B-NB	-3.05	1.34	1.37
14	e	1114	CLA	C3B-C4B	3.05	1.49	1.42
14	G	1135	CLA	CMD-C2D	-3.05	1.44	1.50
14	s	502	CLA	C4B-NB	3.05	1.41	1.37
14	Z	511	CLA	C4D-ND	-3.05	1.33	1.37
14	b	508	CLA	C4B-NB	3.05	1.41	1.37
14	d	519	CLA	C4B-NB	3.05	1.41	1.37
14	1	512	CLA	C4D-ND	-3.05	1.33	1.37
14	s	508	CLA	C4B-NB	3.05	1.41	1.37
14	5	502	CLA	C4D-ND	-3.05	1.33	1.37
14	5	513	CLA	C4D-ND	-3.05	1.33	1.37
14	a	512	CLA	C4D-ND	-3.05	1.33	1.37
14	r	502	CLA	C4D-ND	-3.05	1.33	1.37
14	f	1226	CLA	C1B-NB	-3.05	1.34	1.37
14	s	507	CLA	C4B-NB	3.05	1.41	1.37
14	A	1135	CLA	CMD-C2D	-3.05	1.44	1.50
14	3	508	CLA	C4B-NB	3.05	1.41	1.37
14	4	508	CLA	C4B-NB	3.05	1.41	1.37
14	u	501	CLA	C4B-NB	3.05	1.41	1.37
14	c	512	CLA	C4D-ND	-3.05	1.33	1.37
14	e	1115	CLA	C1D-ND	3.05	1.41	1.37
14	q	512	CLA	C4D-ND	-3.04	1.33	1.37
14	f	1209	CLA	C4B-NB	3.04	1.41	1.37
14	v	512	CLA	C4D-ND	-3.04	1.33	1.37
14	G	1138	CLA	C3B-C4B	3.04	1.49	1.42
14	1	513	CLA	C4D-ND	-3.04	1.33	1.37
14	s	516	CLA	C4B-NB	3.04	1.41	1.37
14	u	508	CLA	C4B-NB	3.04	1.41	1.37
14	G	1104	CLA	C1D-ND	3.04	1.41	1.37
14	v	504	CLA	C4D-ND	-3.04	1.33	1.37
14	a	508	CLA	C4B-NB	3.04	1.41	1.37
14	d	513	CLA	C3B-C4B	3.04	1.49	1.42
14	e	1106	CLA	C1D-ND	3.04	1.41	1.37
14	A	1140	CLA	C3B-C4B	3.04	1.49	1.42
14	e	1135	CLA	CMD-C2D	-3.04	1.44	1.50
14	H	1209	CLA	C4B-NB	3.04	1.41	1.37
14	Y	502	CLA	C4B-NB	3.04	1.41	1.37
14	t	518	CLA	C4B-NB	3.04	1.41	1.37
14	A	1138	CLA	C3B-C4B	3.04	1.49	1.42
14	t	506	CLA	C4D-ND	-3.04	1.33	1.37
14	t	512	CLA	C4D-ND	-3.04	1.33	1.37
14	H	1216	CLA	C4B-NB	3.03	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	511	CLA	C4D-ND	-3.03	1.33	1.37
14	A	1115	CLA	C1D-ND	3.03	1.41	1.37
14	e	1140	CLA	C1D-ND	3.03	1.41	1.37
14	e	1140	CLA	C3B-C4B	3.03	1.49	1.42
14	3	516	CLA	C4B-NB	3.03	1.41	1.37
14	q	517	CLA	C4B-NB	3.03	1.41	1.37
14	H	1021	CLA	CMD-C2D	-3.03	1.44	1.50
14	b	513	CLA	C4D-ND	-3.03	1.33	1.37
14	6	503	CLA	C4B-NB	3.03	1.41	1.37
14	H	1206	CLA	C1D-ND	3.03	1.41	1.37
14	d	504	CLA	C4B-NB	3.03	1.41	1.37
14	B	1209	CLA	C4B-NB	3.03	1.41	1.37
14	f	1220	CLA	C1D-ND	3.03	1.41	1.37
14	c	508	CLA	C4B-NB	3.03	1.41	1.37
14	c	518	CLA	C4B-NB	3.03	1.41	1.37
14	q	502	CLA	C4B-NB	3.03	1.41	1.37
14	4	506	CLA	C4D-ND	-3.03	1.33	1.37
14	q	509	CLA	C4B-NB	3.03	1.41	1.37
14	Y	512	CLA	C4D-ND	-3.03	1.33	1.37
14	Y	513	CLA	C4D-ND	-3.03	1.33	1.37
14	A	1109	CLA	C1D-ND	3.03	1.41	1.37
14	B	1216	CLA	C4B-NB	3.03	1.41	1.37
14	a	511	CLA	C4B-NB	3.03	1.41	1.37
14	v	518	CLA	C4B-NB	3.03	1.41	1.37
14	5	501	CLA	C4B-NB	3.03	1.41	1.37
14	A	1139	CLA	C1D-ND	3.02	1.41	1.37
14	G	1140	CLA	C3B-C4B	3.02	1.49	1.42
14	4	518	CLA	C4B-NB	3.02	1.41	1.37
14	5	508	CLA	C4B-NB	3.02	1.41	1.37
14	A	1117	CLA	C1D-ND	3.02	1.41	1.37
14	3	503	CLA	C4B-NB	3.02	1.41	1.37
14	a	516	CLA	C4B-NB	3.02	1.41	1.37
14	e	1119	CLA	CMB-C2B	-3.02	1.44	1.50
14	5	512	CLA	C4D-ND	-3.02	1.33	1.37
14	q	503	CLA	C4B-NB	3.02	1.41	1.37
14	r	502	CLA	C4B-NB	3.02	1.41	1.37
14	s	502	CLA	C4D-ND	-3.02	1.33	1.37
14	2	511	CLA	C4B-NB	3.02	1.41	1.37
14	c	509	CLA	C4B-NB	3.02	1.41	1.37
14	H	1205	CLA	C1D-ND	3.02	1.41	1.37
14	v	502	CLA	C4B-NB	3.02	1.41	1.37
14	G	1106	CLA	C1D-ND	3.02	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1117	CLA	C1D-ND	3.02	1.41	1.37
14	G	1105	CLA	C1D-ND	3.02	1.41	1.37
14	Z	519	CLA	C4B-NB	3.02	1.41	1.37
14	n	1501	CLA	C4B-NB	3.02	1.41	1.37
14	B	1220	CLA	C1D-ND	3.02	1.41	1.37
14	B	1240	CLA	C4B-NB	3.02	1.41	1.37
14	2	502	CLA	C4B-NB	3.02	1.41	1.37
14	Z	511	CLA	C4B-NB	3.02	1.41	1.37
14	d	507	CLA	C4B-NB	3.02	1.41	1.37
14	f	1240	CLA	C4B-NB	3.02	1.41	1.37
14	Z	509	CLA	C4B-NB	3.01	1.41	1.37
14	f	1216	CLA	C4B-NB	3.01	1.41	1.37
14	A	1104	CLA	C1D-ND	3.01	1.41	1.37
14	s	511	CLA	C4D-ND	-3.01	1.33	1.37
14	b	506	CLA	C4D-ND	-3.01	1.33	1.37
14	a	511	CLA	C4D-ND	-3.01	1.33	1.37
14	e	1105	CLA	C1D-ND	3.01	1.41	1.37
14	b	518	CLA	C4B-NB	3.01	1.41	1.37
14	u	512	CLA	C4D-ND	-3.01	1.33	1.37
14	L	1501	CLA	C4B-NB	3.01	1.41	1.37
14	d	503	CLA	C4B-NB	3.01	1.41	1.37
14	e	1138	CLA	C3B-C4B	3.01	1.49	1.42
14	d	518	CLA	C4B-NB	3.01	1.41	1.37
14	G	1013	CLA	C1B-NB	-3.01	1.34	1.37
14	q	506	CLA	C3B-C4B	3.01	1.49	1.42
14	v	517	CLA	C4B-NB	3.01	1.41	1.37
14	1	502	CLA	C4B-NB	3.01	1.41	1.37
14	f	1205	CLA	C1D-ND	3.01	1.41	1.37
14	Z	513	CLA	C3B-C4B	3.01	1.49	1.42
14	A	1106	CLA	C1D-ND	3.00	1.41	1.37
14	5	509	CLA	C4B-NB	3.00	1.41	1.37
14	4	502	CLA	C4D-ND	-3.00	1.33	1.37
14	4	512	CLA	C4D-ND	-3.00	1.33	1.37
14	c	507	CLA	C4D-ND	-3.00	1.33	1.37
14	t	504	CLA	C4D-ND	-3.00	1.33	1.37
14	e	1013	CLA	C1B-NB	-3.00	1.34	1.37
14	r	508	CLA	C4B-NB	3.00	1.41	1.37
14	3	511	CLA	C4D-ND	-3.00	1.33	1.37
14	R	1302	CLA	C4B-NB	3.00	1.41	1.37
14	G	1121	CLA	C1D-ND	3.00	1.41	1.37
14	A	1121	CLA	C1D-ND	3.00	1.41	1.37
14	5	512	CLA	C4B-NB	3.00	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	u	513	CLA	C4D-ND	-3.00	1.33	1.37
14	2	501	CLA	C4B-NB	3.00	1.41	1.37
14	G	1128	CLA	C4B-NB	3.00	1.41	1.37
14	s	510	CLA	C4B-NB	3.00	1.41	1.37
14	u	507	CLA	C4B-NB	3.00	1.41	1.37
14	f	1023	CLA	CMC-C2C	-3.00	1.44	1.50
14	c	512	CLA	C4B-NB	3.00	1.41	1.37
14	s	513	CLA	C4D-ND	-3.00	1.33	1.37
14	t	502	CLA	C4D-ND	-3.00	1.33	1.37
14	t	510	CLA	C4D-ND	-3.00	1.33	1.37
14	R	1301	CLA	C3B-C4B	3.00	1.49	1.42
14	r	513	CLA	C3B-C4B	3.00	1.49	1.42
14	3	504	CLA	C4D-ND	-3.00	1.33	1.37
14	Z	508	CLA	C4B-NB	2.99	1.41	1.37
14	2	509	CLA	C4B-NB	2.99	1.41	1.37
14	Z	502	CLA	C4B-NB	2.99	1.41	1.37
15	f	2002	PQN	C5-C4	-2.99	1.42	1.48
14	A	1119	CLA	CMB-C2B	-2.99	1.44	1.50
14	c	501	CLA	C4B-NB	2.99	1.41	1.37
14	2	508	CLA	C4B-NB	2.99	1.41	1.37
14	A	1105	CLA	C1D-ND	2.99	1.41	1.37
14	6	502	CLA	C4B-NB	2.99	1.41	1.37
14	u	509	CLA	C4B-NB	2.99	1.41	1.37
14	Y	507	CLA	C4D-ND	-2.99	1.33	1.37
14	G	1139	CLA	C1D-ND	2.99	1.41	1.37
14	r	501	CLA	C4B-NB	2.99	1.41	1.37
14	r	511	CLA	C4B-NB	2.99	1.41	1.37
14	5	506	CLA	C4B-NB	2.99	1.41	1.37
14	v	503	CLA	C4B-NB	2.99	1.41	1.37
14	1	509	CLA	C4B-NB	2.99	1.41	1.37
14	a	503	CLA	C4B-NB	2.99	1.41	1.37
14	B	1206	CLA	C1D-ND	2.99	1.41	1.37
14	a	504	CLA	C4D-ND	-2.98	1.33	1.37
14	j	1301	CLA	C3B-C4B	2.98	1.49	1.42
14	5	507	CLA	C4B-NB	2.98	1.41	1.37
14	H	1220	CLA	C1D-ND	2.98	1.41	1.37
14	e	1102	CLA	C3B-C4B	2.98	1.49	1.42
14	3	507	CLA	C4B-NB	2.98	1.41	1.37
14	F	1301	CLA	C3B-C4B	2.98	1.49	1.42
14	G	1129	CLA	CMD-C2D	-2.98	1.44	1.50
14	5	505	CLA	C4B-NB	2.98	1.41	1.37
14	H	1218	CLA	C4B-NB	2.98	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1124	CLA	C1D-ND	2.98	1.41	1.37
14	1	506	CLA	C3B-C4B	2.98	1.49	1.42
14	G	1102	CLA	C3B-C4B	2.98	1.49	1.42
14	B	1023	CLA	CMC-C2C	-2.98	1.44	1.50
14	s	503	CLA	C4B-NB	2.98	1.41	1.37
14	G	1115	CLA	C1D-ND	2.98	1.41	1.37
14	Y	505	CLA	C4B-NB	2.97	1.41	1.37
14	4	504	CLA	C4D-ND	-2.97	1.33	1.37
14	b	512	CLA	C4D-ND	-2.97	1.33	1.37
14	a	519	CLA	C4B-NB	2.97	1.41	1.37
14	Y	506	CLA	C3B-C4B	2.97	1.49	1.42
14	G	1119	CLA	CMB-C2B	-2.97	1.44	1.50
14	c	507	CLA	C4B-NB	2.97	1.41	1.37
14	e	1109	CLA	C1D-ND	2.97	1.41	1.37
14	q	511	CLA	C4B-NB	2.97	1.41	1.37
14	u	512	CLA	C4B-NB	2.97	1.41	1.37
14	a	507	CLA	C4B-NB	2.97	1.41	1.37
14	c	505	CLA	C4B-NB	2.97	1.41	1.37
14	A	1013	CLA	C1B-NB	-2.97	1.34	1.37
14	e	1013	CLA	CMD-C2D	-2.97	1.44	1.50
14	A	1126	CLA	C1D-ND	2.97	1.41	1.37
14	b	511	CLA	C4D-ND	-2.97	1.33	1.37
14	H	1023	CLA	CMC-C2C	-2.97	1.44	1.50
14	Z	510	CLA	C4B-NB	2.97	1.41	1.37
14	c	506	CLA	C4B-NB	2.97	1.41	1.37
14	J	1302	CLA	C4B-NB	2.97	1.41	1.37
14	c	510	CLA	C4B-NB	2.97	1.41	1.37
15	B	2002	PQN	C5-C4	-2.97	1.42	1.48
14	1	505	CLA	C4B-NB	2.97	1.41	1.37
14	B	1226	CLA	MG-NB	-2.97	1.99	2.05
14	A	1102	CLA	C3B-C4B	2.97	1.49	1.42
14	d	513	CLA	C4D-ND	-2.97	1.33	1.37
14	v	513	CLA	C4D-ND	-2.97	1.33	1.37
14	H	1240	CLA	C4B-NB	2.97	1.41	1.37
14	f	1206	CLA	C1D-ND	2.97	1.41	1.37
14	2	510	CLA	C4B-NB	2.96	1.41	1.37
14	q	505	CLA	C4B-NB	2.96	1.41	1.37
14	u	505	CLA	C4B-NB	2.96	1.41	1.37
14	3	510	CLA	C4B-NB	2.96	1.41	1.37
14	G	1126	CLA	C1D-ND	2.96	1.41	1.37
14	f	1221	CLA	C1D-ND	2.96	1.41	1.37
14	e	1128	CLA	C4B-NB	2.96	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1221	CLA	C1D-ND	2.96	1.41	1.37
14	e	1129	CLA	CMD-C2D	-2.96	1.44	1.50
14	2	513	CLA	C3B-C4B	2.96	1.49	1.42
14	a	510	CLA	C4B-NB	2.96	1.41	1.37
14	u	510	CLA	C4B-NB	2.96	1.41	1.37
14	B	1226	CLA	C4B-NB	2.96	1.41	1.37
14	4	510	CLA	C4D-ND	-2.96	1.33	1.37
14	b	504	CLA	C4D-ND	-2.96	1.33	1.37
14	6	513	CLA	C4D-ND	-2.96	1.33	1.37
14	e	1126	CLA	C1D-ND	2.96	1.41	1.37
14	G	1124	CLA	C1D-ND	2.95	1.41	1.37
14	J	1302	CLA	C4D-ND	-2.95	1.33	1.37
14	Y	509	CLA	C4B-NB	2.95	1.41	1.37
14	H	1221	CLA	C1D-ND	2.95	1.41	1.37
14	3	513	CLA	C4D-ND	-2.95	1.33	1.37
14	f	1230	CLA	C4B-NB	2.95	1.41	1.37
14	A	1129	CLA	CMD-C2D	-2.95	1.44	1.50
14	B	1230	CLA	C1D-ND	2.95	1.41	1.37
14	6	517	CLA	C4B-NB	2.95	1.41	1.37
14	u	507	CLA	C4D-ND	-2.95	1.33	1.37
14	A	1013	CLA	CMD-C2D	-2.95	1.44	1.50
14	u	506	CLA	C4B-NB	2.95	1.41	1.37
14	f	1226	CLA	MG-NB	-2.95	1.99	2.05
14	Z	501	CLA	C4B-NB	2.95	1.41	1.37
14	r	509	CLA	C4B-NB	2.95	1.41	1.37
15	H	2002	PQN	C5-C4	-2.95	1.42	1.48
14	A	1124	CLA	C1D-ND	2.95	1.41	1.37
14	B	1218	CLA	C4B-NB	2.95	1.41	1.37
14	f	1012	CLA	C3B-C4B	2.94	1.49	1.42
18	G	5001	LHG	O7-C5	-2.94	1.39	1.46
14	f	1213	CLA	C4B-NB	2.94	1.41	1.37
14	H	1012	CLA	C3B-C4B	2.94	1.49	1.42
14	s	504	CLA	C4D-ND	-2.94	1.33	1.37
14	F	1302	CLA	C4B-NB	2.94	1.41	1.37
14	b	510	CLA	C4D-ND	-2.94	1.33	1.37
14	f	1230	CLA	C1D-ND	2.94	1.41	1.37
14	q	508	CLA	C4B-NB	2.94	1.41	1.37
18	A	5001	LHG	O7-C5	-2.94	1.39	1.46
14	G	1128	CLA	MG-NB	-2.94	2.00	2.05
14	5	510	CLA	C4B-NB	2.94	1.41	1.37
14	H	1230	CLA	C1D-ND	2.94	1.41	1.37
14	e	1130	CLA	C1D-ND	2.94	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	n	4219	BCR	C10-C9	-2.94	1.31	1.35
14	H	1226	CLA	MG-NB	-2.94	2.00	2.05
14	B	1012	CLA	C3B-C4B	2.94	1.49	1.42
14	1	507	CLA	C4D-ND	-2.94	1.33	1.37
14	e	1022	CLA	C1D-ND	2.94	1.41	1.37
14	6	505	CLA	C4B-NB	2.94	1.41	1.37
14	1	508	CLA	C4B-NB	2.94	1.41	1.37
14	f	1201	CLA	C4B-NB	2.94	1.41	1.37
14	H	1209	CLA	C3B-C4B	2.94	1.49	1.42
14	a	513	CLA	C4D-ND	-2.93	1.33	1.37
14	T	1302	CLA	C4B-NB	2.93	1.41	1.37
14	e	1116	CLA	C4B-NB	2.93	1.41	1.37
14	A	1128	CLA	MG-NB	-2.93	2.00	2.05
14	b	507	CLA	C4D-ND	-2.93	1.33	1.37
14	G	1108	CLA	C4B-NB	2.93	1.41	1.37
17	L	4219	BCR	C10-C9	-2.93	1.31	1.35
14	A	1134	CLA	C4B-NB	2.93	1.41	1.37
14	1	511	CLA	C4B-NB	2.93	1.41	1.37
14	l	1302	CLA	C4B-NB	2.93	1.41	1.37
14	v	505	CLA	C4B-NB	2.93	1.41	1.37
14	H	1217	CLA	C4D-ND	-2.93	1.33	1.37
14	d	505	CLA	C4B-NB	2.93	1.41	1.37
14	a	518	CLA	C4B-NB	2.93	1.41	1.37
14	e	1128	CLA	MG-NB	-2.93	2.00	2.05
14	A	1022	CLA	C1D-ND	2.93	1.41	1.37
14	e	1134	CLA	C4B-NB	2.92	1.41	1.37
14	5	507	CLA	C4D-ND	-2.92	1.33	1.37
14	A	1128	CLA	C4B-NB	2.92	1.41	1.37
14	Y	508	CLA	C4B-NB	2.92	1.41	1.37
14	B	1209	CLA	C3B-C4B	2.92	1.49	1.42
14	s	518	CLA	C4B-NB	2.92	1.41	1.37
14	e	1119	CLA	CMC-C2C	-2.92	1.44	1.50
14	B	1217	CLA	C4D-ND	-2.92	1.33	1.37
14	4	510	CLA	C4B-NB	2.92	1.41	1.37
14	r	503	CLA	C4B-NB	2.92	1.41	1.37
14	A	1130	CLA	C1D-ND	2.92	1.41	1.37
21	s	822	SQD	O47-C7	2.92	1.42	1.34
14	f	1218	CLA	C4B-NB	2.92	1.41	1.37
14	r	504	CLA	C3B-C4B	2.92	1.49	1.42
14	H	1201	CLA	C4B-NB	2.92	1.41	1.37
14	Y	511	CLA	C4B-NB	2.92	1.41	1.37
14	3	518	CLA	C4B-NB	2.92	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	517	CLA	C4B-NB	2.91	1.41	1.37
14	f	1209	CLA	C3B-C4B	2.91	1.49	1.42
14	A	1108	CLA	C4B-NB	2.91	1.41	1.37
14	3	519	CLA	C4B-NB	2.91	1.41	1.37
14	H	1230	CLA	C4B-NB	2.91	1.41	1.37
15	H	2002	PQN	C10-C5	-2.91	1.35	1.40
14	4	507	CLA	C4D-ND	-2.91	1.33	1.37
14	f	1236	CLA	C3B-C4B	2.91	1.49	1.42
14	B	1213	CLA	C4B-NB	2.91	1.41	1.37
14	B	1236	CLA	C3B-C4B	2.91	1.49	1.42
14	B	1201	CLA	C4B-NB	2.91	1.41	1.37
14	Z	518	CLA	C4B-NB	2.91	1.41	1.37
18	e	5001	LHG	O7-C5	-2.91	1.39	1.46
15	B	2002	PQN	C10-C5	-2.91	1.35	1.40
14	Z	504	CLA	C3B-C4B	2.91	1.49	1.42
14	v	510	CLA	C3B-C4B	2.91	1.49	1.42
14	H	1214	CLA	C4B-NB	2.91	1.41	1.37
14	2	504	CLA	C3B-C4B	2.91	1.49	1.42
14	m	1401	CLA	C4B-NB	2.90	1.41	1.37
15	G	2001	PQN	C11-C12	2.90	1.54	1.50
14	H	1210	CLA	C3B-C4B	2.90	1.49	1.42
14	B	1214	CLA	C4B-NB	2.90	1.41	1.37
14	G	1116	CLA	C4B-NB	2.90	1.41	1.37
14	G	1022	CLA	C1D-ND	2.90	1.41	1.37
14	T	1302	CLA	C4D-ND	-2.90	1.33	1.37
14	e	1108	CLA	C4B-NB	2.90	1.41	1.37
14	s	519	CLA	C4B-NB	2.90	1.41	1.37
14	v	507	CLA	C4D-ND	-2.90	1.33	1.37
14	G	1013	CLA	CMD-C2D	-2.90	1.44	1.50
17	V	4219	BCR	C10-C9	-2.90	1.31	1.35
14	l	1302	CLA	C4D-ND	-2.90	1.33	1.37
21	a	822	SQD	O47-C7	2.90	1.42	1.34
14	r	510	CLA	C4B-NB	2.90	1.41	1.37
14	B	1239	CLA	CMB-C2B	-2.90	1.44	1.50
14	B	1208	CLA	C4B-NB	2.90	1.41	1.37
14	2	503	CLA	C4B-NB	2.90	1.41	1.37
14	H	1239	CLA	CMB-C2B	-2.90	1.44	1.50
14	b	508	CLA	CMB-C2B	-2.90	1.44	1.50
14	b	516	CLA	C4D-ND	-2.90	1.33	1.37
14	e	1013	CLA	CMC-C2C	-2.90	1.44	1.50
14	4	516	CLA	C4D-ND	-2.89	1.33	1.37
14	G	1130	CLA	C1D-ND	2.89	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	2001	PQN	C3-C2	2.89	1.40	1.35
14	t	503	CLA	C4D-ND	-2.89	1.33	1.37
14	f	1210	CLA	C3B-C4B	2.89	1.49	1.42
14	B	1210	CLA	C3B-C4B	2.89	1.49	1.42
14	q	507	CLA	C4D-ND	-2.89	1.33	1.37
14	H	1213	CLA	C4B-NB	2.89	1.41	1.37
14	e	1129	CLA	CMB-C2B	-2.89	1.44	1.50
20	f	5002	LMG	O8-C9	-2.89	1.38	1.45
15	G	2001	PQN	C3-C2	2.89	1.40	1.35
14	H	1236	CLA	C3B-C4B	2.89	1.49	1.42
14	H	1225	CLA	C1D-ND	2.89	1.41	1.37
14	t	516	CLA	C4D-ND	-2.89	1.33	1.37
14	e	1127	CLA	C1D-ND	2.89	1.41	1.37
14	A	1013	CLA	CMC-C2C	-2.89	1.44	1.50
14	B	1225	CLA	C1D-ND	2.89	1.41	1.37
14	6	507	CLA	C4D-ND	-2.89	1.33	1.37
14	A	1127	CLA	C1D-ND	2.89	1.41	1.37
14	G	1134	CLA	C4B-NB	2.89	1.41	1.37
14	Z	503	CLA	C4B-NB	2.89	1.41	1.37
14	f	1208	CLA	C4B-NB	2.89	1.41	1.37
14	f	1226	CLA	C4B-NB	2.89	1.41	1.37
14	A	1116	CLA	C4B-NB	2.89	1.41	1.37
15	f	2002	PQN	C10-C5	-2.89	1.35	1.40
14	4	503	CLA	C4D-ND	-2.89	1.33	1.37
14	A	1129	CLA	CMB-C2B	-2.89	1.44	1.50
14	L	1501	CLA	CMB-C2B	-2.89	1.44	1.50
14	A	1119	CLA	CMC-C2C	-2.89	1.44	1.50
14	G	1022	CLA	CMB-C2B	-2.88	1.44	1.50
14	t	507	CLA	C4D-ND	-2.88	1.33	1.37
14	2	518	CLA	C4B-NB	2.88	1.41	1.37
14	j	1302	CLA	C4B-NB	2.88	1.41	1.37
14	B	1230	CLA	C4B-NB	2.88	1.41	1.37
14	H	1208	CLA	C4B-NB	2.88	1.41	1.37
21	3	822	SQD	O47-C7	2.88	1.42	1.34
14	f	1239	CLA	CMB-C2B	-2.88	1.44	1.50
21	n	5216	SQD	O48-C23	2.88	1.41	1.33
14	V	1501	CLA	CMB-C2B	-2.88	1.44	1.50
14	t	501	CLA	C3B-C4B	2.88	1.49	1.42
20	B	5002	LMG	O8-C9	-2.88	1.38	1.45
14	K	1401	CLA	C4B-NB	2.88	1.41	1.37
14	A	1022	CLA	CMB-C2B	-2.88	1.44	1.50
14	G	1119	CLA	CMC-C2C	-2.88	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	508	CLA	CMB-C2B	-2.88	1.44	1.50
14	G	1013	CLA	CMC-C2C	-2.88	1.44	1.50
15	A	2001	PQN	C3-C2	2.88	1.40	1.35
14	q	516	CLA	C4B-NB	2.88	1.41	1.37
14	4	501	CLA	C3B-C4B	2.88	1.49	1.42
14	f	1225	CLA	C1D-ND	2.88	1.41	1.37
14	3	509	CLA	C3B-C4B	2.87	1.49	1.42
14	H	1226	CLA	C4B-NB	2.87	1.41	1.37
14	e	1139	CLA	C4B-NB	2.87	1.41	1.37
14	a	509	CLA	C3B-C4B	2.87	1.49	1.42
14	b	519	CLA	C3B-C4B	2.87	1.49	1.42
14	t	519	CLA	C3B-C4B	2.87	1.49	1.42
14	e	1022	CLA	CMB-C2B	-2.87	1.44	1.50
14	1	516	CLA	C4B-NB	2.87	1.41	1.37
14	b	510	CLA	C4B-NB	2.87	1.41	1.37
14	t	510	CLA	C4B-NB	2.87	1.41	1.37
14	6	510	CLA	C3B-C4B	2.87	1.49	1.42
14	G	1011	CLA	CMD-C2D	-2.87	1.44	1.50
14	d	507	CLA	C4D-ND	-2.87	1.33	1.37
21	r	822	SQD	O47-C7	2.87	1.42	1.34
14	4	519	CLA	C3B-C4B	2.87	1.49	1.42
14	b	501	CLA	C3B-C4B	2.87	1.49	1.42
20	H	5002	LMG	O8-C9	-2.87	1.38	1.45
14	A	1121	CLA	CMD-C2D	-2.87	1.44	1.50
14	G	1121	CLA	CMD-C2D	-2.87	1.44	1.50
14	G	1112	CLA	C3B-C4B	2.87	1.49	1.42
14	b	513	CLA	C3B-C4B	2.87	1.49	1.42
14	e	1011	CLA	CMD-C2D	-2.87	1.44	1.50
14	n	1501	CLA	CMB-C2B	-2.87	1.44	1.50
14	t	507	CLA	C4B-NB	2.86	1.41	1.37
14	G	1102	CLA	C4B-NB	2.86	1.41	1.37
14	G	1102	CLA	C1D-ND	2.86	1.41	1.37
14	d	504	CLA	C3B-C4B	2.86	1.49	1.42
14	d	510	CLA	C3B-C4B	2.86	1.49	1.42
14	e	1112	CLA	C3B-C4B	2.86	1.49	1.42
14	t	508	CLA	CMB-C2B	-2.86	1.44	1.50
14	c	513	CLA	C3B-C4B	2.86	1.49	1.42
14	G	1139	CLA	C3B-C4B	2.86	1.49	1.42
14	u	513	CLA	C3B-C4B	2.86	1.49	1.42
14	e	1121	CLA	CMD-C2D	-2.86	1.44	1.50
14	f	1217	CLA	C4D-ND	-2.86	1.33	1.37
14	Y	510	CLA	C3B-C4B	2.86	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	5216	SQD	O48-C23	2.86	1.41	1.33
14	H	1226	CLA	MG-ND	-2.86	2.00	2.05
14	d	506	CLA	C3B-C4B	2.86	1.49	1.42
14	r	518	CLA	C4B-NB	2.86	1.41	1.37
14	c	509	CLA	C3B-C4B	2.86	1.49	1.42
14	G	1129	CLA	CMB-C2B	-2.86	1.44	1.50
14	5	513	CLA	C3B-C4B	2.86	1.49	1.42
14	G	1013	CLA	C3B-C4B	2.86	1.49	1.42
14	a	503	CLA	C3B-C4B	2.86	1.49	1.42
14	4	507	CLA	C4B-NB	2.86	1.41	1.37
14	U	1401	CLA	C4B-NB	2.86	1.41	1.37
14	e	1102	CLA	C4B-NB	2.86	1.41	1.37
21	V	5216	SQD	O48-C23	2.85	1.41	1.33
15	A	2001	PQN	C11-C12	2.85	1.54	1.50
15	B	2002	PQN	C3-C2	2.85	1.40	1.35
14	A	1112	CLA	C3B-C4B	2.85	1.49	1.42
14	6	504	CLA	C3B-C4B	2.85	1.49	1.42
14	A	1102	CLA	C1D-ND	2.85	1.41	1.37
21	2	822	SQD	O47-C7	2.85	1.42	1.34
14	3	517	CLA	C3B-C4B	2.85	1.49	1.42
14	Y	516	CLA	C4B-NB	2.85	1.41	1.37
14	a	517	CLA	C3B-C4B	2.85	1.49	1.42
14	s	503	CLA	C3B-C4B	2.85	1.49	1.42
14	A	1102	CLA	C4B-NB	2.85	1.41	1.37
14	A	1140	CLA	C4B-NB	2.85	1.41	1.37
14	b	509	CLA	C3B-C4B	2.85	1.49	1.42
14	A	1011	CLA	CMD-C2D	-2.85	1.44	1.50
14	H	1224	CLA	C4B-NB	2.85	1.41	1.37
14	A	1139	CLA	C4B-NB	2.85	1.41	1.37
14	f	1214	CLA	C4B-NB	2.85	1.41	1.37
14	B	1201	CLA	C3B-C4B	2.85	1.49	1.42
15	H	2002	PQN	C3-C2	2.85	1.40	1.35
14	3	503	CLA	C3B-C4B	2.85	1.49	1.42
14	4	513	CLA	C3B-C4B	2.85	1.49	1.42
14	B	1205	CLA	CMD-C2D	-2.84	1.44	1.50
14	e	1102	CLA	C1D-ND	2.84	1.41	1.37
14	q	510	CLA	C3B-C4B	2.84	1.49	1.42
14	t	513	CLA	C3B-C4B	2.84	1.49	1.42
14	6	506	CLA	C3B-C4B	2.84	1.49	1.42
14	2	507	CLA	C4B-NB	2.84	1.41	1.37
21	Z	822	SQD	O47-C7	2.84	1.42	1.34
21	q	822	SQD	O47-C7	2.84	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1226	CLA	MG-ND	-2.84	2.00	2.05
14	5	517	CLA	C3B-C4B	2.84	1.49	1.42
14	s	517	CLA	C3B-C4B	2.84	1.49	1.42
14	Z	509	CLA	C3B-C4B	2.84	1.49	1.42
14	B	1226	CLA	MG-ND	-2.84	2.00	2.05
14	4	509	CLA	C3B-C4B	2.84	1.49	1.42
14	s	509	CLA	C3B-C4B	2.84	1.49	1.42
14	e	1022	CLA	MG-NB	-2.84	2.00	2.05
14	5	509	CLA	C3B-C4B	2.84	1.49	1.42
14	1	510	CLA	C3B-C4B	2.84	1.49	1.42
14	u	517	CLA	C3B-C4B	2.84	1.49	1.42
14	H	1235	CLA	C4B-NB	2.84	1.41	1.37
14	3	506	CLA	C3B-C4B	2.84	1.49	1.42
14	B	1224	CLA	C4B-NB	2.84	1.41	1.37
15	e	2001	PQN	C11-C12	2.84	1.54	1.50
14	H	1201	CLA	C3B-C4B	2.84	1.49	1.42
14	a	501	CLA	C3B-C4B	2.84	1.49	1.42
14	b	503	CLA	C4D-ND	-2.84	1.33	1.37
14	A	1133	CLA	C1D-ND	2.84	1.41	1.37
14	G	1139	CLA	C4B-NB	2.83	1.41	1.37
14	A	1139	CLA	C3B-C4B	2.83	1.49	1.42
14	G	1140	CLA	C4B-NB	2.83	1.41	1.37
14	t	509	CLA	C3B-C4B	2.83	1.49	1.42
14	G	1127	CLA	C1D-ND	2.83	1.41	1.37
14	f	1205	CLA	CMD-C2D	-2.83	1.44	1.50
21	B	1852	SQD	O2-C2	-2.83	1.36	1.43
14	A	1013	CLA	C3B-C4B	2.83	1.49	1.42
21	1	822	SQD	O47-C7	2.83	1.42	1.34
14	H	1205	CLA	CMD-C2D	-2.83	1.44	1.50
14	e	1139	CLA	C3B-C4B	2.83	1.49	1.42
14	G	1129	CLA	C1D-ND	2.82	1.41	1.37
14	b	507	CLA	C4B-NB	2.82	1.41	1.37
21	H	1852	SQD	O2-C2	-2.82	1.36	1.43
14	e	1114	CLA	CMB-C2B	-2.82	1.44	1.50
14	H	1240	CLA	C3B-C4B	2.82	1.49	1.42
14	f	1201	CLA	C3B-C4B	2.82	1.49	1.42
14	v	506	CLA	C3B-C4B	2.82	1.49	1.42
14	v	512	CLA	C3B-C4B	2.82	1.49	1.42
14	v	509	CLA	C3B-C4B	2.82	1.49	1.42
14	f	1222	CLA	C3B-C4B	2.82	1.49	1.42
14	G	1133	CLA	C1D-ND	2.82	1.41	1.37
14	Z	507	CLA	C4B-NB	2.82	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	516	CLA	C3B-C4B	2.82	1.49	1.42
21	Y	822	SQD	O47-C7	2.82	1.42	1.34
14	v	504	CLA	C3B-C4B	2.82	1.49	1.42
14	3	501	CLA	C3B-C4B	2.82	1.49	1.42
14	H	1222	CLA	C3B-C4B	2.82	1.49	1.42
14	u	509	CLA	C3B-C4B	2.82	1.49	1.42
14	A	1114	CLA	CMB-C2B	-2.82	1.44	1.50
14	r	507	CLA	C4B-NB	2.82	1.41	1.37
14	e	1110	CLA	C4B-NB	2.82	1.41	1.37
14	e	1013	CLA	C3B-C4B	2.82	1.49	1.42
14	A	1107	CLA	MG-NB	-2.81	2.00	2.05
14	f	1232	CLA	C3B-C4B	2.81	1.49	1.42
14	4	516	CLA	C3B-C4B	2.81	1.49	1.42
14	s	506	CLA	C3B-C4B	2.81	1.49	1.42
14	f	1218	CLA	C3B-C4B	2.81	1.49	1.42
14	e	1107	CLA	MG-NB	-2.81	2.00	2.05
14	Y	512	CLA	C3B-C4B	2.81	1.49	1.42
14	Y	519	CLA	C3B-C4B	2.81	1.49	1.42
14	c	517	CLA	C3B-C4B	2.81	1.49	1.42
14	5	512	CLA	C3B-C4B	2.81	1.49	1.42
21	f	1852	SQD	O2-C2	-2.81	1.36	1.43
14	a	506	CLA	C3B-C4B	2.81	1.49	1.42
14	b	503	CLA	C3B-C4B	2.81	1.49	1.42
15	f	2002	PQN	C3-C2	2.81	1.40	1.35
14	e	1140	CLA	C4B-NB	2.81	1.41	1.37
14	A	1022	CLA	MG-NB	-2.81	2.00	2.05
14	B	1232	CLA	C3B-C4B	2.81	1.49	1.42
14	f	1221	CLA	C3B-C4B	2.81	1.49	1.42
14	B	1221	CLA	C3B-C4B	2.81	1.49	1.42
14	4	503	CLA	C3B-C4B	2.80	1.49	1.42
14	2	509	CLA	C3B-C4B	2.80	1.49	1.42
14	r	509	CLA	C3B-C4B	2.80	1.49	1.42
14	G	1111	CLA	CMC-C2C	-2.80	1.44	1.50
14	G	1120	CLA	C1D-ND	2.80	1.41	1.37
14	H	1232	CLA	C3B-C4B	2.80	1.49	1.42
14	A	1111	CLA	CMC-C2C	-2.80	1.44	1.50
14	G	1022	CLA	MG-NB	-2.80	2.00	2.05
14	q	519	CLA	C3B-C4B	2.80	1.49	1.42
14	1	519	CLA	C3B-C4B	2.80	1.49	1.42
14	f	1232	CLA	C4B-NB	2.80	1.41	1.37
14	G	1114	CLA	CMB-C2B	-2.80	1.44	1.50
14	B	1222	CLA	C3B-C4B	2.80	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1229	CLA	C3B-C4B	2.80	1.49	1.42
14	1	512	CLA	C3B-C4B	2.80	1.49	1.42
14	d	509	CLA	C3B-C4B	2.80	1.49	1.42
14	t	503	CLA	C3B-C4B	2.80	1.49	1.42
14	B	1235	CLA	C4B-NB	2.80	1.41	1.37
14	f	1224	CLA	C4B-NB	2.80	1.41	1.37
14	6	509	CLA	C3B-C4B	2.80	1.49	1.42
14	U	1401	CLA	C3B-C4B	2.80	1.49	1.42
14	f	1240	CLA	C3B-C4B	2.80	1.49	1.42
14	G	1101	CLA	C1D-ND	2.80	1.41	1.37
14	s	501	CLA	C3B-C4B	2.80	1.49	1.42
14	t	516	CLA	C3B-C4B	2.80	1.49	1.42
14	e	1111	CLA	CMC-C2C	-2.79	1.44	1.50
14	b	504	CLA	C3B-C4B	2.79	1.49	1.42
14	e	1138	CLA	C4B-NB	2.79	1.41	1.37
14	u	512	CLA	C3B-C4B	2.79	1.49	1.42
14	e	1133	CLA	C1D-ND	2.79	1.41	1.37
14	q	512	CLA	C3B-C4B	2.79	1.49	1.42
14	f	1229	CLA	C3B-C4B	2.79	1.49	1.42
14	m	1401	CLA	C3B-C4B	2.79	1.49	1.42
14	f	1227	CLA	C4B-NB	2.79	1.41	1.37
14	B	1240	CLA	C3B-C4B	2.79	1.49	1.42
14	c	512	CLA	C3B-C4B	2.79	1.49	1.42
14	v	503	CLA	C3B-C4B	2.79	1.49	1.42
14	K	1401	CLA	C3B-C4B	2.79	1.49	1.42
14	a	505	CLA	C4B-NB	2.79	1.41	1.37
14	s	505	CLA	C4B-NB	2.79	1.41	1.37
14	A	1101	CLA	C1D-ND	2.79	1.41	1.37
14	V	1502	CLA	C1D-ND	2.79	1.41	1.37
14	m	1105	CLA	C4D-ND	-2.79	1.33	1.37
14	3	505	CLA	C4B-NB	2.79	1.41	1.37
14	a	508	CLA	CMB-C2B	-2.78	1.44	1.50
14	u	516	CLA	C3B-C4B	2.78	1.49	1.42
14	f	1228	CLA	C3B-C4B	2.78	1.49	1.42
14	H	1218	CLA	C3B-C4B	2.78	1.49	1.42
14	t	511	CLA	C3B-C4B	2.78	1.49	1.42
14	H	1221	CLA	C3B-C4B	2.78	1.49	1.42
14	4	504	CLA	C3B-C4B	2.78	1.49	1.42
14	4	511	CLA	C3B-C4B	2.78	1.49	1.42
14	a	516	CLA	C3B-C4B	2.78	1.49	1.42
14	s	504	CLA	C3B-C4B	2.78	1.49	1.42
14	B	1218	CLA	C3B-C4B	2.78	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1107	CLA	MG-NB	-2.78	2.00	2.05
14	A	1120	CLA	C1D-ND	2.78	1.41	1.37
14	e	1101	CLA	C1D-ND	2.78	1.41	1.37
14	4	517	CLA	C3B-C4B	2.78	1.49	1.42
14	A	1129	CLA	C1D-ND	2.78	1.41	1.37
14	K	1105	CLA	C4D-ND	-2.77	1.33	1.37
14	B	1204	CLA	C1D-ND	2.77	1.41	1.37
14	B	1206	CLA	C4B-NB	2.77	1.41	1.37
14	B	1228	CLA	C3B-C4B	2.77	1.49	1.42
14	a	504	CLA	C3B-C4B	2.77	1.49	1.42
14	L	1502	CLA	C3B-C4B	2.77	1.49	1.42
14	q	513	CLA	C3B-C4B	2.77	1.49	1.42
14	U	1105	CLA	C4D-ND	-2.77	1.33	1.37
14	H	1228	CLA	C3B-C4B	2.77	1.49	1.42
14	B	1229	CLA	C3B-C4B	2.77	1.49	1.42
14	6	512	CLA	C3B-C4B	2.77	1.49	1.42
14	5	506	CLA	C3B-C4B	2.77	1.49	1.42
14	f	1235	CLA	C4B-NB	2.77	1.41	1.37
14	3	516	CLA	C3B-C4B	2.77	1.49	1.42
14	5	516	CLA	C3B-C4B	2.77	1.49	1.42
14	6	505	CLA	C3B-C4B	2.77	1.49	1.42
14	b	511	CLA	C3B-C4B	2.77	1.49	1.42
14	e	1123	CLA	C4B-NB	2.77	1.41	1.37
14	H	1232	CLA	C4B-NB	2.77	1.41	1.37
14	1	508	CLA	CMB-C2B	-2.76	1.44	1.50
14	Y	508	CLA	CMB-C2B	-2.76	1.44	1.50
14	A	1115	CLA	C4B-NB	2.76	1.41	1.37
21	n	5216	SQD	O47-C7	2.76	1.42	1.34
14	G	1117	CLA	CMB-C2B	-2.76	1.44	1.50
14	t	512	CLA	C3B-C4B	2.76	1.49	1.42
14	e	1119	CLA	MG-NB	-2.76	2.00	2.05
14	t	517	CLA	C3B-C4B	2.76	1.49	1.42
14	c	506	CLA	C3B-C4B	2.76	1.49	1.42
14	q	501	CLA	C3B-C4B	2.76	1.49	1.42
14	t	504	CLA	C3B-C4B	2.76	1.49	1.42
14	B	1239	CLA	C4B-NB	2.76	1.41	1.37
14	G	1013	CLA	MG-NB	-2.76	2.00	2.05
14	f	1206	CLA	C4B-NB	2.76	1.41	1.37
14	3	504	CLA	C3B-C4B	2.76	1.49	1.42
14	d	516	CLA	C3B-C4B	2.76	1.49	1.42
14	A	1119	CLA	MG-NB	-2.76	2.00	2.05
14	6	503	CLA	C3B-C4B	2.76	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	V	1502	CLA	C3B-C4B	2.76	1.49	1.42
14	Y	513	CLA	C3B-C4B	2.76	1.49	1.42
14	b	512	CLA	C3B-C4B	2.76	1.49	1.42
14	u	506	CLA	C3B-C4B	2.76	1.49	1.42
14	v	505	CLA	C3B-C4B	2.76	1.49	1.42
14	d	503	CLA	C3B-C4B	2.76	1.49	1.42
14	A	1137	CLA	C3B-C4B	2.76	1.49	1.42
14	H	1227	CLA	C4B-NB	2.76	1.41	1.37
14	3	508	CLA	CMB-C2B	-2.76	1.45	1.50
14	1	513	CLA	C3B-C4B	2.76	1.49	1.42
14	f	1204	CLA	C1D-ND	2.75	1.41	1.37
14	G	1137	CLA	C3B-C4B	2.75	1.49	1.42
14	F	1301	CLA	C4B-NB	2.75	1.41	1.37
14	q	508	CLA	CMB-C2B	-2.75	1.45	1.50
14	H	1239	CLA	C4B-NB	2.75	1.41	1.37
14	d	512	CLA	C3B-C4B	2.75	1.49	1.42
14	B	1227	CLA	C4B-NB	2.75	1.41	1.37
14	B	1232	CLA	C4B-NB	2.75	1.41	1.37
14	G	1133	CLA	CMB-C2B	-2.75	1.45	1.50
14	B	1229	CLA	C4B-NB	2.75	1.41	1.37
14	H	1204	CLA	C1D-ND	2.75	1.41	1.37
14	A	1103	CLA	CMC-C2C	-2.75	1.45	1.50
14	e	1013	CLA	MG-NB	-2.75	2.00	2.05
14	Z	501	CLA	C3B-C4B	2.75	1.49	1.42
14	4	512	CLA	C3B-C4B	2.75	1.49	1.42
14	4	518	CLA	C3B-C4B	2.75	1.49	1.42
14	b	517	CLA	C3B-C4B	2.75	1.49	1.42
14	s	516	CLA	C3B-C4B	2.75	1.49	1.42
14	A	1128	CLA	C1D-ND	2.75	1.41	1.37
14	B	1221	CLA	C4B-NB	2.75	1.41	1.37
14	2	501	CLA	C3B-C4B	2.75	1.49	1.42
14	e	1237	CLA	C1D-ND	2.75	1.41	1.37
14	H	1229	CLA	C4B-NB	2.75	1.41	1.37
14	e	1115	CLA	C4B-NB	2.75	1.41	1.37
14	G	1134	CLA	C3B-C4B	2.75	1.49	1.42
14	c	516	CLA	C3B-C4B	2.75	1.49	1.42
14	e	1107	CLA	C4B-NB	2.75	1.41	1.37
14	e	1133	CLA	CMB-C2B	-2.75	1.45	1.50
14	Y	501	CLA	C3B-C4B	2.75	1.49	1.42
14	6	516	CLA	C3B-C4B	2.74	1.49	1.42
14	A	1107	CLA	C4B-NB	2.74	1.41	1.37
14	G	1115	CLA	C4B-NB	2.74	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	u	518	CLA	C3B-C4B	2.74	1.49	1.42
15	A	2001	PQN	C10-C5	-2.74	1.36	1.40
15	e	2001	PQN	C10-C5	-2.74	1.36	1.40
14	A	1013	CLA	MG-NB	-2.74	2.00	2.05
14	f	1225	CLA	MG-NB	-2.74	2.00	2.05
14	4	510	CLA	C3B-C4B	2.74	1.49	1.42
14	r	510	CLA	C3B-C4B	2.74	1.49	1.42
14	n	1502	CLA	C1D-ND	2.74	1.41	1.37
14	b	518	CLA	C3B-C4B	2.74	1.49	1.42
21	L	5216	SQD	O47-C7	2.74	1.42	1.34
14	Z	510	CLA	C3B-C4B	2.74	1.49	1.42
14	A	1110	CLA	C4B-NB	2.74	1.41	1.37
14	e	1129	CLA	C1D-ND	2.74	1.41	1.37
14	1	501	CLA	C3B-C4B	2.74	1.49	1.42
15	G	2001	PQN	C10-C5	-2.74	1.36	1.40
14	G	1119	CLA	MG-NB	-2.74	2.00	2.05
14	G	1107	CLA	C4B-NB	2.74	1.41	1.37
14	e	1128	CLA	C1D-ND	2.74	1.41	1.37
14	e	1137	CLA	C3B-C4B	2.74	1.49	1.42
14	B	1234	CLA	MG-NB	-2.74	2.00	2.05
14	H	1206	CLA	C4B-NB	2.74	1.41	1.37
14	f	1202	CLA	C4B-NB	2.74	1.41	1.37
14	2	510	CLA	C3B-C4B	2.74	1.49	1.42
14	r	501	CLA	C3B-C4B	2.74	1.49	1.42
14	H	1234	CLA	MG-NB	-2.74	2.00	2.05
14	e	1113	CLA	C3B-C4B	2.73	1.49	1.42
14	s	511	CLA	C3B-C4B	2.73	1.49	1.42
14	Z	505	CLA	C4B-NB	2.73	1.41	1.37
14	A	1123	CLA	C4B-NB	2.73	1.41	1.37
14	Y	516	CLA	C1D-ND	2.73	1.41	1.37
14	e	1120	CLA	C1D-ND	2.73	1.41	1.37
14	s	508	CLA	CMB-C2B	-2.73	1.45	1.50
14	t	510	CLA	C3B-C4B	2.73	1.49	1.42
14	u	511	CLA	C3B-C4B	2.73	1.49	1.42
14	5	518	CLA	C3B-C4B	2.73	1.49	1.42
14	d	505	CLA	C3B-C4B	2.73	1.49	1.42
14	t	518	CLA	C3B-C4B	2.73	1.49	1.42
14	c	504	CLA	C3B-C4B	2.73	1.49	1.42
14	2	505	CLA	C4B-NB	2.73	1.41	1.37
14	A	1134	CLA	C3B-C4B	2.73	1.49	1.42
14	G	1110	CLA	C3B-C4B	2.73	1.49	1.42
14	U	1103	CLA	C4B-NB	2.73	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1021	CLA	C4B-NB	2.73	1.41	1.37
14	d	501	CLA	C3B-C4B	2.73	1.49	1.42
14	G	1103	CLA	CMC-C2C	-2.73	1.45	1.50
14	H	1234	CLA	C3B-C4B	2.73	1.49	1.42
14	B	1202	CLA	C4B-NB	2.73	1.41	1.37
14	A	1113	CLA	C3B-C4B	2.73	1.49	1.42
14	d	511	CLA	C3B-C4B	2.73	1.49	1.42
14	B	1234	CLA	C3B-C4B	2.73	1.49	1.42
14	n	1502	CLA	C3B-C4B	2.73	1.49	1.42
14	q	504	CLA	C3B-C4B	2.73	1.49	1.42
14	B	1215	CLA	C4B-NB	2.73	1.41	1.37
14	B	1228	CLA	C4B-NB	2.73	1.41	1.37
14	G	1123	CLA	C4B-NB	2.73	1.41	1.37
14	H	1228	CLA	C4B-NB	2.73	1.41	1.37
14	n	1502	CLA	C4B-NB	2.73	1.41	1.37
21	V	5216	SQD	O47-C7	2.73	1.42	1.34
14	c	518	CLA	C3B-C4B	2.73	1.49	1.42
14	r	505	CLA	C4B-NB	2.72	1.41	1.37
14	b	510	CLA	C3B-C4B	2.72	1.49	1.42
14	K	1103	CLA	C4B-NB	2.72	1.41	1.37
14	f	1228	CLA	C4B-NB	2.72	1.41	1.37
14	3	511	CLA	C3B-C4B	2.72	1.49	1.42
14	A	1133	CLA	CMB-C2B	-2.72	1.45	1.50
14	e	1103	CLA	CMC-C2C	-2.72	1.45	1.50
14	A	1237	CLA	C1D-ND	2.72	1.41	1.37
14	B	1207	CLA	C4B-NB	2.72	1.41	1.37
14	G	1103	CLA	C1D-ND	2.72	1.41	1.37
14	q	516	CLA	C1D-ND	2.72	1.41	1.37
14	G	1110	CLA	C4B-NB	2.72	1.41	1.37
14	G	1115	CLA	CMC-C2C	-2.72	1.45	1.50
14	v	501	CLA	C3B-C4B	2.72	1.49	1.42
14	G	1138	CLA	C4B-NB	2.72	1.41	1.37
14	H	1012	CLA	C1D-ND	2.72	1.41	1.37
14	6	508	CLA	C3B-C4B	2.72	1.49	1.42
14	d	508	CLA	C3B-C4B	2.72	1.49	1.42
14	H	1221	CLA	C4B-NB	2.72	1.41	1.37
14	B	1217	CLA	C3B-C4B	2.72	1.49	1.42
14	6	511	CLA	C3B-C4B	2.72	1.49	1.42
14	A	1138	CLA	C4B-NB	2.72	1.41	1.37
14	f	1012	CLA	C1D-ND	2.72	1.41	1.37
14	5	504	CLA	C3B-C4B	2.72	1.49	1.42
14	f	1221	CLA	C4B-NB	2.72	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1117	CLA	CMB-C2B	-2.72	1.45	1.50
14	A	1115	CLA	CMC-C2C	-2.72	1.45	1.50
14	2	508	CLA	CMB-C2B	-2.72	1.45	1.50
14	v	516	CLA	C3B-C4B	2.72	1.49	1.42
14	L	1502	CLA	C4B-NB	2.72	1.41	1.37
14	m	1103	CLA	C4B-NB	2.72	1.41	1.37
14	f	1217	CLA	C3B-C4B	2.72	1.49	1.42
14	A	1135	CLA	MG-ND	-2.72	2.00	2.05
14	Z	508	CLA	CMB-C2B	-2.72	1.45	1.50
14	j	1301	CLA	C4B-NB	2.72	1.41	1.37
14	G	1113	CLA	C3B-C4B	2.71	1.49	1.42
14	6	501	CLA	C3B-C4B	2.71	1.49	1.42
14	f	1207	CLA	C3B-C4B	2.71	1.49	1.42
14	j	1302	CLA	C3B-C4B	2.71	1.49	1.42
14	H	1202	CLA	C4B-NB	2.71	1.41	1.37
14	f	1239	CLA	C4B-NB	2.71	1.41	1.37
14	c	511	CLA	C3B-C4B	2.71	1.49	1.42
14	t	505	CLA	C3B-C4B	2.71	1.49	1.42
14	G	1135	CLA	C1B-NB	-2.71	1.34	1.37
14	u	504	CLA	C3B-C4B	2.71	1.49	1.42
14	1	504	CLA	C3B-C4B	2.71	1.49	1.42
14	H	1207	CLA	C3B-C4B	2.71	1.49	1.42
14	e	1104	CLA	C4B-NB	2.71	1.41	1.37
14	H	1216	CLA	C3B-C4B	2.71	1.49	1.42
14	H	1217	CLA	C3B-C4B	2.71	1.49	1.42
14	e	1130	CLA	C3B-C4B	2.71	1.49	1.42
14	v	508	CLA	C3B-C4B	2.71	1.49	1.42
14	b	502	CLA	C1B-C2B	2.71	1.49	1.43
14	f	1215	CLA	CMB-C2B	-2.71	1.45	1.50
14	a	513	CLA	C3B-C4B	2.71	1.49	1.42
14	a	511	CLA	C3B-C4B	2.71	1.49	1.42
14	u	502	CLA	C1B-C2B	2.71	1.49	1.43
14	A	1133	CLA	MG-NB	-2.71	2.00	2.05
14	A	1130	CLA	C3B-C4B	2.71	1.49	1.42
14	f	1234	CLA	MG-NB	-2.71	2.00	2.05
14	G	1237	CLA	C1D-ND	2.71	1.41	1.37
14	H	1205	CLA	C3B-C4B	2.71	1.49	1.42
14	f	1221	CLA	C1B-NB	-2.71	1.34	1.37
14	f	1229	CLA	C4B-NB	2.71	1.41	1.37
14	1	516	CLA	C1D-ND	2.71	1.41	1.37
14	H	1225	CLA	MG-NB	-2.71	2.00	2.05
14	e	1133	CLA	MG-NB	-2.71	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1021	CLA	C4B-NB	2.71	1.41	1.37
14	A	1110	CLA	C3B-C4B	2.70	1.49	1.42
14	L	1502	CLA	C1D-ND	2.70	1.41	1.37
14	B	1207	CLA	C3B-C4B	2.70	1.49	1.42
14	G	1130	CLA	C3B-C4B	2.70	1.49	1.42
14	H	1215	CLA	C4B-NB	2.70	1.41	1.37
14	R	1301	CLA	C4B-NB	2.70	1.41	1.37
14	A	1135	CLA	C1B-NB	-2.70	1.34	1.37
14	e	1107	CLA	C1D-ND	2.70	1.41	1.37
14	c	510	CLA	C3B-C4B	2.70	1.49	1.42
14	A	1103	CLA	C1D-ND	2.70	1.41	1.37
14	Y	504	CLA	C3B-C4B	2.70	1.49	1.42
14	e	1110	CLA	C3B-C4B	2.70	1.49	1.42
14	5	510	CLA	C3B-C4B	2.70	1.49	1.42
14	Z	503	CLA	C3B-C4B	2.70	1.49	1.42
14	e	1116	CLA	C3B-C4B	2.70	1.49	1.42
14	V	1502	CLA	C4B-NB	2.70	1.41	1.37
14	5	511	CLA	C3B-C4B	2.70	1.49	1.42
14	G	1106	CLA	C4B-NB	2.70	1.41	1.37
14	B	1206	CLA	MG-NB	-2.70	2.00	2.05
14	B	1225	CLA	MG-NB	-2.70	2.00	2.05
14	G	1116	CLA	C3B-C4B	2.70	1.49	1.42
14	G	1801	CLA	C3B-C4B	2.70	1.49	1.42
14	f	1234	CLA	C3B-C4B	2.70	1.49	1.42
14	u	510	CLA	C3B-C4B	2.70	1.49	1.42
14	a	507	CLA	C3B-C4B	2.70	1.49	1.42
14	t	506	CLA	C3B-C4B	2.70	1.49	1.42
14	f	1221	CLA	CMD-C2D	-2.70	1.45	1.50
14	e	1117	CLA	CMB-C2B	-2.69	1.45	1.50
14	d	518	CLA	C3B-C4B	2.69	1.49	1.42
14	B	1012	CLA	C1D-ND	2.69	1.41	1.37
14	4	502	CLA	C1B-C2B	2.69	1.49	1.43
14	f	1216	CLA	C3B-C4B	2.69	1.49	1.42
14	B	1215	CLA	CMB-C2B	-2.69	1.45	1.50
14	e	1134	CLA	C3B-C4B	2.69	1.49	1.42
14	f	1206	CLA	MG-NB	-2.69	2.00	2.05
14	H	1215	CLA	CMB-C2B	-2.69	1.45	1.50
14	u	503	CLA	C3B-C4B	2.69	1.49	1.42
14	f	1207	CLA	C4B-NB	2.69	1.41	1.37
14	e	1106	CLA	C4B-NB	2.69	1.41	1.37
14	G	1133	CLA	MG-NB	-2.69	2.00	2.05
14	B	1216	CLA	C3B-C4B	2.69	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	1302	CLA	C3B-C4B	2.69	1.49	1.42
14	G	1128	CLA	C1D-ND	2.69	1.41	1.37
14	f	1215	CLA	C4B-NB	2.69	1.41	1.37
14	4	506	CLA	C3B-C4B	2.69	1.49	1.42
14	f	1205	CLA	CMC-C2C	-2.69	1.45	1.50
14	R	1302	CLA	C3B-C4B	2.69	1.49	1.42
14	G	1135	CLA	MG-ND	-2.69	2.00	2.05
14	H	1213	CLA	C3B-C4B	2.69	1.49	1.42
14	v	511	CLA	C3B-C4B	2.69	1.49	1.42
14	A	1104	CLA	C4B-NB	2.69	1.41	1.37
14	1	517	CLA	C3B-C4B	2.69	1.49	1.42
14	c	502	CLA	C1B-C2B	2.69	1.49	1.43
14	H	1206	CLA	MG-NB	-2.69	2.00	2.05
14	5	502	CLA	C1B-C2B	2.69	1.49	1.43
14	3	513	CLA	C3B-C4B	2.68	1.49	1.42
14	5	503	CLA	C3B-C4B	2.68	1.49	1.42
14	A	1106	CLA	C4B-NB	2.68	1.41	1.37
14	s	507	CLA	C3B-C4B	2.68	1.49	1.42
14	A	1116	CLA	C3B-C4B	2.68	1.49	1.42
14	u	519	CLA	C3B-C4B	2.68	1.49	1.42
14	r	508	CLA	CMB-C2B	-2.68	1.45	1.50
14	c	503	CLA	C3B-C4B	2.68	1.49	1.42
14	Z	516	CLA	C3B-C4B	2.68	1.49	1.42
14	B	1221	CLA	C1B-NB	-2.68	1.34	1.37
14	3	507	CLA	C3B-C4B	2.68	1.49	1.42
14	A	1107	CLA	C1D-ND	2.68	1.41	1.37
14	A	1801	CLA	C3B-C4B	2.68	1.49	1.42
14	G	1120	CLA	C3B-C4B	2.68	1.49	1.42
14	G	1129	CLA	MG-ND	-2.68	2.00	2.05
14	e	1135	CLA	MG-ND	-2.68	2.00	2.05
14	e	1103	CLA	C1D-ND	2.68	1.41	1.37
14	G	1124	CLA	CMD-C2D	-2.68	1.45	1.50
14	e	1103	CLA	CMD-C2D	-2.68	1.45	1.50
14	2	503	CLA	C3B-C4B	2.68	1.49	1.42
14	Y	507	CLA	C3B-C4B	2.68	1.49	1.42
14	H	1202	CLA	C3B-C4B	2.68	1.49	1.42
14	v	507	CLA	C3B-C4B	2.68	1.49	1.42
14	e	1115	CLA	CMC-C2C	-2.68	1.45	1.50
14	e	1124	CLA	CMD-C2D	-2.68	1.45	1.50
14	f	1220	CLA	CMC-C2C	-2.68	1.45	1.50
14	1	508	CLA	C3B-C4B	2.68	1.49	1.42
14	e	1101	CLA	CMD-C2D	-2.68	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1104	CLA	C4B-NB	2.67	1.41	1.37
14	Y	508	CLA	C3B-C4B	2.67	1.49	1.42
14	c	505	CLA	C3B-C4B	2.67	1.49	1.42
14	Y	505	CLA	C1B-C2B	2.67	1.49	1.43
14	A	1120	CLA	C3B-C4B	2.67	1.49	1.42
14	d	519	CLA	C3B-C4B	2.67	1.49	1.42
14	G	1103	CLA	CMD-C2D	-2.67	1.45	1.50
14	L	1503	CLA	C4B-NB	2.67	1.41	1.37
14	3	518	CLA	C3B-C4B	2.67	1.49	1.42
14	Y	517	CLA	C3B-C4B	2.67	1.49	1.42
14	a	518	CLA	C3B-C4B	2.67	1.49	1.42
14	c	519	CLA	C3B-C4B	2.67	1.49	1.42
14	4	505	CLA	C3B-C4B	2.67	1.49	1.42
14	G	1111	CLA	C1D-ND	2.67	1.41	1.37
14	e	1135	CLA	C1B-NB	-2.67	1.34	1.37
14	G	1121	CLA	CMB-C2B	-2.67	1.45	1.50
14	Z	518	CLA	C3B-C4B	2.67	1.49	1.42
14	A	1124	CLA	CMD-C2D	-2.67	1.45	1.50
14	H	1207	CLA	C4B-NB	2.67	1.41	1.37
14	B	1213	CLA	C3B-C4B	2.67	1.49	1.42
14	H	1229	CLA	C1D-ND	2.67	1.41	1.37
14	2	518	CLA	C3B-C4B	2.67	1.49	1.42
14	4	517	CLA	C1B-C2B	2.67	1.49	1.43
14	H	1220	CLA	CMC-C2C	-2.67	1.45	1.50
14	e	1131	CLA	MG-NB	-2.67	2.00	2.05
14	6	518	CLA	C3B-C4B	2.67	1.49	1.42
14	B	1205	CLA	C3B-C4B	2.67	1.49	1.42
14	q	507	CLA	C3B-C4B	2.67	1.49	1.42
14	e	1801	CLA	C3B-C4B	2.67	1.49	1.42
14	u	505	CLA	C3B-C4B	2.67	1.49	1.42
14	e	1120	CLA	C3B-C4B	2.67	1.49	1.42
14	5	505	CLA	C3B-C4B	2.66	1.49	1.42
14	2	516	CLA	C3B-C4B	2.66	1.49	1.42
14	Y	516	CLA	C3B-C4B	2.66	1.49	1.42
14	1	505	CLA	C1B-C2B	2.66	1.49	1.43
14	B	1205	CLA	CMC-C2C	-2.66	1.45	1.50
14	1	516	CLA	C3B-C4B	2.66	1.49	1.42
14	6	519	CLA	C3B-C4B	2.66	1.49	1.42
14	r	503	CLA	C3B-C4B	2.66	1.49	1.42
14	b	506	CLA	C3B-C4B	2.66	1.49	1.42
14	n	1503	CLA	C4B-NB	2.66	1.41	1.37
14	e	1121	CLA	CMB-C2B	-2.66	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	506	CLA	C3B-C4B	2.66	1.49	1.42
14	5	519	CLA	C3B-C4B	2.66	1.49	1.42
14	q	516	CLA	C3B-C4B	2.66	1.49	1.42
14	1	507	CLA	C3B-C4B	2.66	1.49	1.42
14	6	507	CLA	C3B-C4B	2.66	1.49	1.42
14	q	517	CLA	C3B-C4B	2.66	1.49	1.42
14	v	519	CLA	C3B-C4B	2.66	1.49	1.42
14	e	1127	CLA	MG-NB	-2.66	2.00	2.05
14	A	1111	CLA	C1D-ND	2.66	1.41	1.37
14	s	518	CLA	C3B-C4B	2.66	1.49	1.42
14	Z	506	CLA	C3B-C4B	2.66	1.49	1.42
14	B	1221	CLA	CMD-C2D	-2.66	1.45	1.50
14	t	502	CLA	C1B-C2B	2.66	1.49	1.43
14	c	501	CLA	C3B-C4B	2.66	1.49	1.42
14	H	1205	CLA	CMC-C2C	-2.66	1.45	1.50
14	A	1103	CLA	CMD-C2D	-2.66	1.45	1.50
14	H	1220	CLA	C4B-NB	2.66	1.41	1.37
14	r	518	CLA	C3B-C4B	2.66	1.49	1.42
14	A	1121	CLA	CMB-C2B	-2.66	1.45	1.50
14	m	1103	CLA	C1B-C2B	2.66	1.49	1.43
14	b	507	CLA	C1B-C2B	2.66	1.49	1.43
14	u	501	CLA	C3B-C4B	2.66	1.49	1.42
14	v	518	CLA	C3B-C4B	2.66	1.49	1.42
14	H	1221	CLA	C1B-NB	-2.66	1.34	1.37
14	s	505	CLA	C1B-C2B	2.65	1.49	1.43
14	A	1103	CLA	C3B-C4B	2.65	1.49	1.42
14	5	501	CLA	C3B-C4B	2.65	1.49	1.42
14	s	513	CLA	C3B-C4B	2.65	1.49	1.42
14	K	1103	CLA	C1B-C2B	2.65	1.49	1.43
14	a	518	CLA	C1B-C2B	2.65	1.49	1.43
14	B	1202	CLA	C3B-C4B	2.65	1.49	1.42
14	H	1223	CLA	C3B-C4B	2.65	1.49	1.42
14	f	1202	CLA	C3B-C4B	2.65	1.49	1.42
14	a	505	CLA	C1B-C2B	2.65	1.49	1.43
14	q	508	CLA	C3B-C4B	2.65	1.49	1.42
14	r	506	CLA	C3B-C4B	2.65	1.49	1.42
14	J	1303	CLA	C3B-C4B	2.65	1.49	1.42
14	U	1103	CLA	C1B-C2B	2.65	1.49	1.43
14	r	505	CLA	C3B-C4B	2.65	1.49	1.42
14	A	1101	CLA	CMD-C2D	-2.65	1.45	1.50
14	4	507	CLA	C1B-C2B	2.65	1.49	1.43
14	H	1021	CLA	C4B-NB	2.65	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	505	CLA	C1B-C2B	2.65	1.49	1.43
14	e	1103	CLA	C3B-C4B	2.65	1.49	1.42
14	f	1213	CLA	C3B-C4B	2.65	1.49	1.42
14	t	507	CLA	C1B-C2B	2.65	1.49	1.43
14	c	508	CLA	C3B-C4B	2.65	1.49	1.42
14	A	1127	CLA	MG-NB	-2.65	2.00	2.05
14	H	1217	CLA	C1B-C2B	2.65	1.49	1.43
14	B	1220	CLA	CMC-C2C	-2.65	1.45	1.50
14	d	507	CLA	C3B-C4B	2.65	1.49	1.42
14	f	1214	CLA	C3B-C4B	2.65	1.49	1.42
14	G	1107	CLA	C1D-ND	2.65	1.41	1.37
14	G	1101	CLA	CMD-C2D	-2.65	1.45	1.50
14	q	505	CLA	C1B-C2B	2.65	1.49	1.43
14	l	1303	CLA	C3B-C4B	2.65	1.49	1.42
14	2	505	CLA	C3B-C4B	2.65	1.49	1.42
14	G	1103	CLA	C3B-C4B	2.65	1.49	1.42
14	t	502	CLA	C3B-C4B	2.65	1.49	1.42
14	A	1129	CLA	MG-ND	-2.65	2.00	2.05
14	e	1129	CLA	MG-ND	-2.65	2.00	2.05
14	H	1211	CLA	CMD-C2D	-2.64	1.45	1.50
14	G	1127	CLA	MG-NB	-2.64	2.00	2.05
14	e	1124	CLA	MG-NB	-2.64	2.00	2.05
14	A	1131	CLA	MG-NB	-2.64	2.00	2.05
14	t	504	CLA	C1B-C2B	2.64	1.49	1.43
14	H	1205	CLA	C4B-NB	2.64	1.41	1.37
14	t	517	CLA	C1B-C2B	2.64	1.49	1.43
14	V	1503	CLA	C4B-NB	2.64	1.41	1.37
14	f	1215	CLA	MG-NB	-2.64	2.00	2.05
14	Y	518	CLA	C3B-C4B	2.64	1.48	1.42
14	Z	517	CLA	C3B-C4B	2.64	1.48	1.42
14	f	1205	CLA	C3B-C4B	2.64	1.48	1.42
14	A	1137	CLA	C4B-NB	2.64	1.41	1.37
14	J	1302	CLA	C3B-C4B	2.64	1.48	1.42
14	f	1211	CLA	C3B-C4B	2.64	1.48	1.42
14	4	502	CLA	C3B-C4B	2.64	1.48	1.42
14	l	1302	CLA	C3B-C4B	2.64	1.48	1.42
14	1	518	CLA	C3B-C4B	2.64	1.48	1.42
14	b	505	CLA	C3B-C4B	2.64	1.48	1.42
14	u	508	CLA	CMB-C2B	-2.64	1.45	1.50
14	b	516	CLA	C1B-C2B	2.64	1.49	1.43
14	A	1131	CLA	C1D-ND	2.64	1.41	1.37
14	Z	503	CLA	C1B-C2B	2.64	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	518	CLA	C1B-C2B	2.64	1.49	1.43
14	b	502	CLA	C3B-C4B	2.64	1.48	1.42
14	Z	507	CLA	C3B-C4B	2.64	1.48	1.42
14	f	1212	CLA	C4B-NB	2.64	1.41	1.37
14	f	1229	CLA	C1D-ND	2.64	1.41	1.37
14	B	1211	CLA	C3B-C4B	2.64	1.48	1.42
14	f	1220	CLA	C3B-C4B	2.64	1.48	1.42
14	f	1224	CLA	C3B-C4B	2.64	1.48	1.42
14	B	1215	CLA	MG-NB	-2.64	2.00	2.05
14	4	504	CLA	C1B-C2B	2.63	1.49	1.43
14	e	1137	CLA	C4B-NB	2.63	1.41	1.37
14	c	508	CLA	CMB-C2B	-2.63	1.45	1.50
14	T	1303	CLA	C3B-C4B	2.63	1.48	1.42
14	b	504	CLA	C1B-C2B	2.63	1.49	1.43
18	V	5218	LHG	O7-C5	-2.63	1.40	1.46
14	s	502	CLA	C1B-C2B	2.63	1.49	1.43
14	2	517	CLA	C3B-C4B	2.63	1.48	1.42
14	B	1229	CLA	C1D-ND	2.63	1.41	1.37
14	c	505	CLA	C1B-C2B	2.63	1.49	1.43
14	6	502	CLA	C1B-C2B	2.63	1.49	1.43
14	G	1123	CLA	C3B-C4B	2.63	1.48	1.42
14	5	508	CLA	C3B-C4B	2.63	1.48	1.42
18	e	5003	LHG	O7-C5	-2.63	1.40	1.46
14	3	516	CLA	C1B-C2B	2.63	1.49	1.43
14	s	502	CLA	C3B-C4B	2.63	1.48	1.42
14	1	518	CLA	C1B-C2B	2.63	1.49	1.43
14	r	517	CLA	C1B-C2B	2.63	1.49	1.43
14	b	517	CLA	C1B-C2B	2.63	1.49	1.43
14	B	1205	CLA	C4B-NB	2.63	1.41	1.37
14	q	503	CLA	C3B-C4B	2.63	1.48	1.42
14	s	518	CLA	C1B-C2B	2.63	1.49	1.43
14	Y	509	CLA	C3B-C4B	2.63	1.48	1.42
14	A	1124	CLA	MG-NB	-2.63	2.00	2.05
14	H	1221	CLA	CMD-C2D	-2.63	1.45	1.50
14	H	1227	CLA	CMB-C2B	-2.63	1.45	1.50
14	B	1223	CLA	C3B-C4B	2.63	1.48	1.42
14	Z	505	CLA	C3B-C4B	2.63	1.48	1.42
14	5	508	CLA	CMB-C2B	-2.63	1.45	1.50
14	4	513	CLA	C1B-C2B	2.63	1.49	1.43
14	v	506	CLA	C1B-C2B	2.63	1.49	1.43
14	r	516	CLA	C3B-C4B	2.63	1.48	1.42
14	2	507	CLA	C3B-C4B	2.63	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1123	CLA	C3B-C4B	2.63	1.48	1.42
14	d	502	CLA	C1B-C2B	2.63	1.49	1.43
14	A	1117	CLA	C4B-NB	2.63	1.41	1.37
14	e	1123	CLA	C3B-C4B	2.63	1.48	1.42
14	Y	518	CLA	C1B-C2B	2.63	1.49	1.43
14	e	1022	CLA	CMD-C2D	-2.63	1.45	1.50
14	B	1214	CLA	C3B-C4B	2.63	1.48	1.42
14	f	1203	CLA	C3B-C4B	2.62	1.48	1.42
14	G	1131	CLA	C1D-ND	2.62	1.41	1.37
14	B	1217	CLA	C1B-C2B	2.62	1.49	1.43
14	r	517	CLA	C3B-C4B	2.62	1.48	1.42
14	B	1203	CLA	C3B-C4B	2.62	1.48	1.42
14	H	1220	CLA	C3B-C4B	2.62	1.48	1.42
14	G	1117	CLA	C4B-NB	2.62	1.41	1.37
14	5	505	CLA	C1B-C2B	2.62	1.49	1.43
14	t	516	CLA	C1B-C2B	2.62	1.49	1.43
14	b	513	CLA	C1B-C2B	2.62	1.49	1.43
14	B	1211	CLA	CMD-C2D	-2.62	1.45	1.50
14	1	503	CLA	C3B-C4B	2.62	1.48	1.42
14	e	1139	CLA	MG-NB	-2.62	2.00	2.05
14	f	1205	CLA	C4B-NB	2.62	1.41	1.37
14	5	518	CLA	C1B-C2B	2.62	1.49	1.43
14	f	1021	CLA	MG-NB	-2.62	2.00	2.05
14	q	505	CLA	C3B-C4B	2.62	1.48	1.42
14	H	1215	CLA	MG-NB	-2.62	2.00	2.05
14	Z	519	CLA	C1B-C2B	2.62	1.49	1.43
14	q	518	CLA	C1B-C2B	2.62	1.49	1.43
14	v	502	CLA	C1B-C2B	2.62	1.49	1.43
21	f	1852	SQD	O47-C7	2.62	1.41	1.34
14	s	516	CLA	C1B-C2B	2.62	1.49	1.43
14	G	1237	CLA	MG-NB	-2.62	2.00	2.05
14	r	507	CLA	C3B-C4B	2.62	1.48	1.42
14	G	1130	CLA	MG-NB	-2.62	2.00	2.05
14	v	508	CLA	CMB-C2B	-2.62	1.45	1.50
14	B	1220	CLA	C3B-C4B	2.62	1.48	1.42
14	1	505	CLA	C3B-C4B	2.62	1.48	1.42
14	T	1302	CLA	C3B-C4B	2.62	1.48	1.42
14	Y	503	CLA	C3B-C4B	2.62	1.48	1.42
14	q	518	CLA	C3B-C4B	2.62	1.48	1.42
14	G	1105	CLA	MG-NB	-2.62	2.00	2.05
14	s	513	CLA	C1B-C2B	2.62	1.49	1.43
14	u	505	CLA	C1B-C2B	2.62	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1231	CLA	C3B-C4B	2.62	1.48	1.42
14	a	507	CLA	C1B-C2B	2.62	1.49	1.43
21	H	1852	SQD	O47-C7	2.61	1.41	1.34
14	A	1022	CLA	CMD-C2D	-2.61	1.45	1.50
14	B	1220	CLA	C4B-NB	2.61	1.41	1.37
14	f	1220	CLA	C4B-NB	2.61	1.41	1.37
14	B	1231	CLA	C3B-C4B	2.61	1.48	1.42
14	r	511	CLA	C3B-C4B	2.61	1.48	1.42
14	G	1124	CLA	MG-NB	-2.61	2.00	2.05
14	H	1203	CLA	C3B-C4B	2.61	1.48	1.42
18	L	5218	LHG	O7-C5	-2.61	1.40	1.46
14	H	1021	CLA	MG-NB	-2.61	2.00	2.05
14	G	1111	CLA	C3B-C4B	2.61	1.48	1.42
14	G	1131	CLA	MG-NB	-2.61	2.00	2.05
14	f	1211	CLA	CMD-C2D	-2.61	1.45	1.50
14	H	1211	CLA	C3B-C4B	2.61	1.48	1.42
14	u	508	CLA	C3B-C4B	2.61	1.48	1.42
14	H	1021	CLA	C1D-ND	2.61	1.41	1.37
14	c	518	CLA	C1B-C2B	2.61	1.49	1.43
18	A	5003	LHG	O7-C5	-2.61	1.40	1.46
14	6	508	CLA	CMB-C2B	-2.61	1.45	1.50
14	Y	505	CLA	C3B-C4B	2.61	1.48	1.42
14	e	1111	CLA	C1D-ND	2.61	1.41	1.37
14	3	513	CLA	C1B-C2B	2.61	1.49	1.43
14	a	516	CLA	C1B-C2B	2.61	1.49	1.43
14	f	1217	CLA	C1B-C2B	2.61	1.49	1.43
14	A	1237	CLA	MG-NB	-2.61	2.00	2.05
14	f	1223	CLA	C3B-C4B	2.61	1.48	1.42
14	t	513	CLA	C1B-C2B	2.61	1.49	1.43
14	1	509	CLA	C3B-C4B	2.61	1.48	1.42
14	A	1125	CLA	MG-NB	-2.61	2.00	2.05
18	G	5003	LHG	O7-C5	-2.61	1.40	1.46
14	B	1224	CLA	C3B-C4B	2.61	1.48	1.42
21	B	1852	SQD	O47-C7	2.60	1.41	1.34
18	n	5218	LHG	O7-C5	-2.60	1.40	1.46
14	3	502	CLA	C1B-C2B	2.60	1.49	1.43
14	4	516	CLA	C1B-C2B	2.60	1.49	1.43
14	G	1125	CLA	MG-NB	-2.60	2.00	2.05
14	2	511	CLA	C3B-C4B	2.60	1.48	1.42
14	B	1227	CLA	CMB-C2B	-2.60	1.45	1.50
14	a	510	CLA	C3B-C4B	2.60	1.48	1.42
14	Z	511	CLA	C3B-C4B	2.60	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1106	CLA	C3B-C4B	2.60	1.48	1.42
14	2	503	CLA	C1B-C2B	2.60	1.49	1.43
14	Y	502	CLA	C1B-C2B	2.60	1.49	1.43
14	B	1021	CLA	MG-NB	-2.60	2.00	2.05
14	d	506	CLA	C1B-C2B	2.60	1.49	1.43
14	H	1231	CLA	C3B-C4B	2.60	1.48	1.42
14	d	517	CLA	C3B-C4B	2.60	1.48	1.42
14	3	510	CLA	C3B-C4B	2.60	1.48	1.42
14	r	503	CLA	C1B-C2B	2.60	1.49	1.43
14	d	508	CLA	CMB-C2B	-2.60	1.45	1.50
14	e	1105	CLA	C3B-C4B	2.60	1.48	1.42
14	6	506	CLA	C1B-C2B	2.60	1.49	1.43
14	u	518	CLA	C1B-C2B	2.60	1.49	1.43
14	B	1021	CLA	C1D-ND	2.60	1.41	1.37
14	e	1131	CLA	C3B-C4B	2.60	1.48	1.42
14	G	1022	CLA	CMD-C2D	-2.59	1.45	1.50
14	3	507	CLA	C1B-C2B	2.59	1.49	1.43
14	3	502	CLA	C3B-C4B	2.59	1.48	1.42
14	4	505	CLA	C1B-C2B	2.59	1.49	1.43
14	B	1212	CLA	C3B-C4B	2.59	1.48	1.42
14	A	1139	CLA	MG-NB	-2.59	2.00	2.05
14	A	1130	CLA	MG-NB	-2.59	2.00	2.05
14	Z	518	CLA	C1B-C2B	2.59	1.49	1.43
14	K	1105	CLA	C3B-C4B	2.59	1.48	1.42
14	v	517	CLA	C3B-C4B	2.59	1.48	1.42
14	v	511	CLA	C1B-C2B	2.59	1.49	1.43
14	H	1214	CLA	C3B-C4B	2.59	1.48	1.42
14	e	1117	CLA	C4B-NB	2.59	1.41	1.37
14	m	1105	CLA	C3B-C4B	2.59	1.48	1.42
14	G	1136	CLA	C4B-NB	2.59	1.41	1.37
14	4	503	CLA	C1B-C2B	2.59	1.49	1.43
14	2	519	CLA	C1B-C2B	2.59	1.49	1.43
14	f	1210	CLA	CMC-C2C	-2.59	1.45	1.50
14	f	1212	CLA	C3B-C4B	2.59	1.48	1.42
14	f	1227	CLA	C3B-C4B	2.59	1.48	1.42
14	A	1136	CLA	C4B-NB	2.59	1.41	1.37
14	1	502	CLA	C1B-C2B	2.59	1.49	1.43
14	A	1105	CLA	MG-NB	-2.59	2.00	2.05
14	B	1227	CLA	C3B-C4B	2.59	1.48	1.42
14	Z	508	CLA	C3B-C4B	2.59	1.48	1.42
14	U	1105	CLA	C3B-C4B	2.59	1.48	1.42
14	Z	519	CLA	C3B-C4B	2.59	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	511	CLA	C1B-C2B	2.59	1.49	1.43
14	H	1221	CLA	MG-NB	-2.59	2.00	2.05
14	r	519	CLA	C3B-C4B	2.59	1.48	1.42
14	t	505	CLA	C1B-C2B	2.59	1.49	1.43
14	H	1216	CLA	MG-NB	-2.59	2.00	2.05
14	H	1208	CLA	C3B-C4B	2.59	1.48	1.42
14	q	509	CLA	C3B-C4B	2.58	1.48	1.42
14	H	1212	CLA	C3B-C4B	2.58	1.48	1.42
14	e	1125	CLA	MG-NB	-2.58	2.00	2.05
14	b	505	CLA	C1B-C2B	2.58	1.49	1.43
14	H	1227	CLA	C3B-C4B	2.58	1.48	1.42
14	6	511	CLA	C1B-C2B	2.58	1.49	1.43
14	6	517	CLA	C3B-C4B	2.58	1.48	1.42
14	e	1131	CLA	C1D-ND	2.58	1.41	1.37
14	H	1224	CLA	C3B-C4B	2.58	1.48	1.42
14	2	517	CLA	C1B-C2B	2.58	1.49	1.43
14	s	510	CLA	C3B-C4B	2.58	1.48	1.42
14	e	1131	CLA	C4B-NB	2.58	1.41	1.37
14	s	507	CLA	C1B-C2B	2.58	1.49	1.43
14	A	1111	CLA	C3B-C4B	2.58	1.48	1.42
14	G	1139	CLA	MG-NB	-2.58	2.00	2.05
14	a	502	CLA	C1B-C2B	2.58	1.49	1.43
14	e	1105	CLA	MG-NB	-2.58	2.00	2.05
14	e	1130	CLA	MG-NB	-2.58	2.00	2.05
14	c	503	CLA	C1B-C2B	2.58	1.49	1.43
14	q	517	CLA	C1B-C2B	2.58	1.49	1.43
14	e	1237	CLA	MG-NB	-2.58	2.00	2.05
14	A	1106	CLA	C3B-C4B	2.58	1.48	1.42
14	f	1208	CLA	C3B-C4B	2.58	1.48	1.42
14	H	1210	CLA	CMC-C2C	-2.58	1.45	1.50
14	e	1140	CLA	CMC-C2C	-2.58	1.45	1.50
14	u	516	CLA	C1B-C2B	2.58	1.49	1.43
14	G	1137	CLA	C4B-NB	2.58	1.41	1.37
14	1	501	CLA	C1B-C2B	2.58	1.49	1.43
14	2	508	CLA	C3B-C4B	2.58	1.48	1.42
14	f	1203	CLA	MG-NB	-2.58	2.00	2.05
14	1	517	CLA	C1B-C2B	2.58	1.49	1.43
14	B	1212	CLA	CMC-C2C	-2.58	1.45	1.50
14	f	1238	CLA	CMD-C2D	-2.58	1.45	1.50
14	a	505	CLA	C3B-C4B	2.57	1.48	1.42
14	B	1216	CLA	MG-NB	-2.57	2.00	2.05
14	a	513	CLA	C1B-C2B	2.57	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1105	CLA	C3B-C4B	2.57	1.48	1.42
14	a	502	CLA	C3B-C4B	2.57	1.48	1.42
14	t	503	CLA	C1B-C2B	2.57	1.49	1.43
14	H	1203	CLA	MG-NB	-2.57	2.00	2.05
14	2	519	CLA	C3B-C4B	2.57	1.48	1.42
14	A	1107	CLA	C1B-NB	-2.57	1.34	1.37
14	G	1107	CLA	C1B-NB	-2.57	1.34	1.37
14	Y	501	CLA	C1B-C2B	2.57	1.49	1.43
14	A	1131	CLA	C3B-C4B	2.57	1.48	1.42
14	B	1208	CLA	C3B-C4B	2.57	1.48	1.42
14	A	1140	CLA	CMC-C2C	-2.57	1.45	1.50
14	G	1140	CLA	CMC-C2C	-2.57	1.45	1.50
14	q	501	CLA	C1B-C2B	2.57	1.49	1.43
14	b	503	CLA	C1B-C2B	2.57	1.49	1.43
14	G	1124	CLA	CMB-C2B	-2.57	1.45	1.50
14	q	502	CLA	C1B-C2B	2.57	1.49	1.43
14	a	501	CLA	C1B-C2B	2.57	1.49	1.43
14	H	1212	CLA	CMC-C2C	-2.57	1.45	1.50
14	m	1105	CLA	C1B-C2B	2.57	1.49	1.43
14	v	502	CLA	C3B-C4B	2.57	1.48	1.42
14	L	1501	CLA	MG-NB	-2.57	2.00	2.05
14	c	507	CLA	C1B-C2B	2.57	1.49	1.43
14	5	503	CLA	C1B-C2B	2.57	1.49	1.43
14	5	507	CLA	C1B-C2B	2.57	1.49	1.43
14	6	502	CLA	C3B-C4B	2.57	1.48	1.42
14	r	519	CLA	C1B-C2B	2.57	1.49	1.43
14	A	1124	CLA	C4B-NB	2.57	1.40	1.37
14	H	1212	CLA	C4B-NB	2.57	1.40	1.37
14	2	518	CLA	C1B-C2B	2.57	1.49	1.43
14	B	1203	CLA	MG-NB	-2.56	2.00	2.05
14	e	1111	CLA	C3B-C4B	2.56	1.48	1.42
14	b	518	CLA	C1B-C2B	2.56	1.49	1.43
14	d	513	CLA	C1B-C2B	2.56	1.49	1.43
14	A	1124	CLA	CMB-C2B	-2.56	1.45	1.50
14	a	519	CLA	C3B-C4B	2.56	1.48	1.42
14	A	1120	CLA	C4B-NB	2.56	1.40	1.37
14	f	1227	CLA	CMB-C2B	-2.56	1.45	1.50
14	1	507	CLA	C1B-C2B	2.56	1.49	1.43
14	Y	517	CLA	C1B-C2B	2.56	1.49	1.43
14	G	1131	CLA	C3B-C4B	2.56	1.48	1.42
14	B	1212	CLA	C4B-NB	2.56	1.40	1.37
14	5	506	CLA	C1B-C2B	2.56	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1210	CLA	CMC-C2C	-2.56	1.45	1.50
14	e	1124	CLA	CMB-C2B	-2.56	1.45	1.50
14	Y	507	CLA	C1B-C2B	2.56	1.49	1.43
14	Z	517	CLA	C1B-C2B	2.56	1.49	1.43
14	G	1108	CLA	C3B-C4B	2.56	1.48	1.42
14	3	501	CLA	C1B-C2B	2.56	1.49	1.43
14	G	1118	CLA	CMD-C2D	-2.56	1.45	1.50
14	4	512	CLA	C1B-C2B	2.56	1.49	1.43
14	K	1105	CLA	C1B-C2B	2.56	1.49	1.43
14	r	512	CLA	MG-NB	-2.56	2.00	2.05
14	b	510	CLA	C1B-C2B	2.56	1.49	1.43
14	e	1120	CLA	C4B-NB	2.56	1.40	1.37
14	r	518	CLA	C1B-C2B	2.56	1.49	1.43
14	f	1223	CLA	CMC-C2C	-2.56	1.45	1.50
14	G	1130	CLA	C4B-NB	2.56	1.40	1.37
14	u	504	CLA	C1B-C2B	2.56	1.49	1.43
14	6	513	CLA	C1B-C2B	2.56	1.49	1.43
14	3	505	CLA	C3B-C4B	2.56	1.48	1.42
14	c	506	CLA	C1B-C2B	2.56	1.49	1.43
14	4	518	CLA	C1B-C2B	2.55	1.49	1.43
14	5	516	CLA	C1B-C2B	2.55	1.49	1.43
14	A	1105	CLA	C3B-C4B	2.55	1.48	1.42
14	n	1501	CLA	MG-NB	-2.55	2.00	2.05
14	s	505	CLA	C3B-C4B	2.55	1.48	1.42
14	f	1212	CLA	CMC-C2C	-2.55	1.45	1.50
14	v	516	CLA	C1B-C2B	2.55	1.49	1.43
14	G	1106	CLA	C3B-C4B	2.55	1.48	1.42
14	G	1117	CLA	C3B-C4B	2.55	1.48	1.42
14	H	1204	CLA	C4B-NB	2.55	1.40	1.37
14	B	1223	CLA	CMC-C2C	-2.55	1.45	1.50
14	H	1238	CLA	CMD-C2D	-2.55	1.45	1.50
14	t	512	CLA	C1B-C2B	2.55	1.49	1.43
14	a	519	CLA	C1B-C2B	2.55	1.49	1.43
14	f	1232	CLA	MG-NB	-2.55	2.00	2.05
14	s	501	CLA	C1B-C2B	2.55	1.49	1.43
14	t	510	CLA	C1B-C2B	2.55	1.49	1.43
14	e	1139	CLA	CMD-C2D	-2.55	1.45	1.50
14	e	1124	CLA	C4B-NB	2.55	1.40	1.37
14	e	1130	CLA	C4B-NB	2.55	1.40	1.37
14	s	519	CLA	C3B-C4B	2.55	1.48	1.42
14	f	1012	CLA	MG-NB	-2.55	2.00	2.05
14	G	1115	CLA	C3B-C4B	2.55	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	u	507	CLA	C1B-C2B	2.55	1.49	1.43
14	A	1103	CLA	C4B-NB	2.55	1.40	1.37
14	d	502	CLA	C3B-C4B	2.55	1.48	1.42
14	u	503	CLA	C1B-C2B	2.55	1.49	1.43
14	u	506	CLA	C1B-C2B	2.55	1.49	1.43
14	H	1230	CLA	C3B-C4B	2.55	1.48	1.42
14	B	1238	CLA	CMD-C2D	-2.55	1.45	1.50
14	e	1011	CLA	CMB-C2B	-2.55	1.45	1.50
14	f	1216	CLA	MG-NB	-2.55	2.00	2.05
14	e	1117	CLA	C3B-C4B	2.55	1.48	1.42
14	e	1136	CLA	C4B-NB	2.55	1.40	1.37
14	4	510	CLA	C1B-C2B	2.55	1.49	1.43
14	A	1131	CLA	C4B-NB	2.55	1.40	1.37
14	U	1105	CLA	C1B-C2B	2.55	1.49	1.43
14	f	1227	CLA	MG-NB	-2.55	2.00	2.05
14	B	1222	CLA	C4B-NB	2.55	1.40	1.37
14	G	1131	CLA	C4B-NB	2.55	1.40	1.37
14	r	508	CLA	C3B-C4B	2.55	1.48	1.42
14	2	504	CLA	C1B-C2B	2.55	1.49	1.43
14	q	507	CLA	C1B-C2B	2.55	1.49	1.43
14	f	1021	CLA	C1D-ND	2.55	1.40	1.37
14	v	513	CLA	C1B-C2B	2.54	1.49	1.43
14	H	1227	CLA	MG-NB	-2.54	2.00	2.05
14	A	1108	CLA	C3B-C4B	2.54	1.48	1.42
14	d	509	CLA	C1B-C2B	2.54	1.49	1.43
14	B	1219	CLA	CMD-C2D	-2.54	1.45	1.50
14	G	1117	CLA	MG-NB	-2.54	2.00	2.05
14	V	1501	CLA	MG-NB	-2.54	2.00	2.05
14	B	1221	CLA	MG-NB	-2.54	2.00	2.05
14	t	508	CLA	MG-NB	-2.54	2.00	2.05
14	u	502	CLA	C3B-C4B	2.54	1.48	1.42
14	A	1013	CLA	CMB-C2B	-2.54	1.45	1.50
14	b	512	CLA	C1B-C2B	2.54	1.49	1.43
14	A	1124	CLA	C3B-C4B	2.54	1.48	1.42
14	B	1204	CLA	C3B-C4B	2.54	1.48	1.42
14	3	519	CLA	C3B-C4B	2.54	1.48	1.42
14	6	509	CLA	C1B-C2B	2.54	1.49	1.43
14	V	1501	CLA	C1B-NB	-2.54	1.34	1.37
14	1	511	CLA	C3B-C4B	2.54	1.48	1.42
14	A	1117	CLA	MG-NB	-2.54	2.00	2.05
14	b	508	CLA	MG-NB	-2.54	2.00	2.05
14	G	1124	CLA	C4B-NB	2.54	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1013	CLA	CMB-C2B	-2.54	1.45	1.50
14	B	1230	CLA	C3B-C4B	2.54	1.48	1.42
14	q	511	CLA	C3B-C4B	2.54	1.48	1.42
14	G	1119	CLA	C1B-NB	-2.54	1.34	1.37
14	e	1107	CLA	C1B-NB	-2.54	1.34	1.37
14	B	1232	CLA	MG-NB	-2.54	2.00	2.05
14	G	1103	CLA	C4B-NB	2.54	1.40	1.37
14	6	501	CLA	C1B-C2B	2.54	1.49	1.43
14	H	1223	CLA	CMC-C2C	-2.54	1.45	1.50
14	Y	511	CLA	C3B-C4B	2.54	1.48	1.42
14	5	510	CLA	C1B-C2B	2.54	1.49	1.43
14	c	516	CLA	C1B-C2B	2.54	1.49	1.43
14	v	509	CLA	C1B-C2B	2.54	1.49	1.43
14	A	1117	CLA	C3B-C4B	2.54	1.48	1.42
14	G	1120	CLA	MG-NB	-2.54	2.00	2.05
14	e	1124	CLA	C3B-C4B	2.54	1.48	1.42
14	t	518	CLA	C1B-C2B	2.53	1.49	1.43
14	f	1238	CLA	MG-NB	-2.53	2.00	2.05
14	2	502	CLA	C1B-C2B	2.53	1.49	1.43
14	n	1501	CLA	C3B-C4B	2.53	1.48	1.42
14	b	519	CLA	C1B-C2B	2.53	1.49	1.43
14	1	502	CLA	C3B-C4B	2.53	1.48	1.42
14	5	504	CLA	C1B-C2B	2.53	1.49	1.43
14	A	1130	CLA	C1B-NB	-2.53	1.34	1.37
14	5	502	CLA	C3B-C4B	2.53	1.48	1.42
14	A	1139	CLA	CMD-C2D	-2.53	1.45	1.50
14	G	1139	CLA	CMD-C2D	-2.53	1.45	1.50
14	A	1011	CLA	CMB-C2B	-2.53	1.45	1.50
14	G	1237	CLA	CMD-C2D	-2.53	1.45	1.50
14	d	516	CLA	C1B-C2B	2.53	1.49	1.43
14	f	1204	CLA	C3B-C4B	2.53	1.48	1.42
14	A	1237	CLA	CMD-C2D	-2.53	1.45	1.50
14	A	1120	CLA	MG-NB	-2.53	2.00	2.05
14	s	512	CLA	MG-NB	-2.53	2.00	2.05
14	e	1119	CLA	C3B-C4B	2.53	1.48	1.42
14	G	1101	CLA	CMC-C2C	-2.53	1.45	1.50
14	e	1108	CLA	C3B-C4B	2.53	1.48	1.42
14	5	519	CLA	C1B-C2B	2.53	1.49	1.43
14	Z	504	CLA	C1B-C2B	2.53	1.49	1.43
14	r	504	CLA	C1B-C2B	2.53	1.49	1.43
14	A	1118	CLA	CMD-C2D	-2.53	1.45	1.50
14	4	508	CLA	MG-NB	-2.53	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1117	CLA	MG-NB	-2.53	2.00	2.05
14	G	1124	CLA	C3B-C4B	2.53	1.48	1.42
14	Y	502	CLA	C3B-C4B	2.53	1.48	1.42
14	q	502	CLA	C3B-C4B	2.53	1.48	1.42
14	G	1011	CLA	CMB-C2B	-2.53	1.45	1.50
14	s	519	CLA	C1B-C2B	2.53	1.49	1.43
14	A	1130	CLA	C4B-NB	2.53	1.40	1.37
14	G	1102	CLA	CHC-C1C	2.53	1.43	1.38
14	4	519	CLA	C1B-C2B	2.53	1.49	1.43
14	6	516	CLA	C1B-C2B	2.53	1.49	1.43
14	v	501	CLA	C1B-C2B	2.53	1.49	1.43
14	a	505	CLA	CMD-C2D	-2.53	1.45	1.50
14	H	1204	CLA	C3B-C4B	2.52	1.48	1.42
14	3	519	CLA	C1B-C2B	2.52	1.49	1.43
14	G	1011	CLA	MG-NB	-2.52	2.00	2.05
14	H	1235	CLA	MG-NB	-2.52	2.00	2.05
14	A	1104	CLA	C3B-C4B	2.52	1.48	1.42
14	H	1219	CLA	CMD-C2D	-2.52	1.45	1.50
14	e	1104	CLA	C3B-C4B	2.52	1.48	1.42
14	H	1012	CLA	CHC-C1C	2.52	1.43	1.38
14	B	1227	CLA	MG-NB	-2.52	2.00	2.05
14	f	1204	CLA	MG-NB	-2.52	2.00	2.05
14	A	1119	CLA	C1B-NB	-2.52	1.34	1.37
14	A	1101	CLA	CMC-C2C	-2.52	1.45	1.50
14	f	1219	CLA	CMD-C2D	-2.52	1.45	1.50
14	A	1115	CLA	C3B-C4B	2.52	1.48	1.42
14	e	1013	CLA	CMB-C2B	-2.52	1.45	1.50
14	c	502	CLA	C3B-C4B	2.52	1.48	1.42
14	G	1119	CLA	C3B-C4B	2.52	1.48	1.42
14	2	505	CLA	C1B-C2B	2.52	1.49	1.43
14	H	1222	CLA	C4B-NB	2.52	1.40	1.37
14	Z	505	CLA	C1B-C2B	2.52	1.49	1.43
14	r	502	CLA	C1B-C2B	2.52	1.49	1.43
14	2	512	CLA	MG-NB	-2.52	2.00	2.05
14	e	1237	CLA	CMD-C2D	-2.52	1.45	1.50
14	u	510	CLA	C1B-C2B	2.52	1.49	1.43
14	q	516	CLA	MG-NB	-2.52	2.00	2.05
14	G	1801	CLA	MG-NB	-2.52	2.00	2.05
14	H	1231	CLA	C1B-C2B	2.52	1.49	1.43
14	v	518	CLA	C1B-C2B	2.52	1.49	1.43
14	G	1131	CLA	CMB-C2B	-2.52	1.45	1.50
14	e	1130	CLA	C1B-NB	-2.52	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1119	CLA	C3B-C4B	2.52	1.48	1.42
14	3	512	CLA	MG-NB	-2.52	2.00	2.05
14	e	1126	CLA	MG-NB	-2.52	2.00	2.05
14	d	517	CLA	C1B-C2B	2.52	1.49	1.43
14	4	508	CLA	C3B-C4B	2.52	1.48	1.42
14	G	1121	CLA	C4B-NB	2.52	1.40	1.37
14	3	505	CLA	CMD-C2D	-2.52	1.45	1.50
14	u	519	CLA	C1B-C2B	2.52	1.49	1.43
14	c	504	CLA	C1B-C2B	2.52	1.49	1.43
14	H	1240	CLA	CMD-C2D	-2.51	1.45	1.50
14	B	1231	CLA	C1B-C2B	2.51	1.49	1.43
14	d	501	CLA	C1B-C2B	2.51	1.49	1.43
14	a	512	CLA	MG-NB	-2.51	2.00	2.05
14	e	1116	CLA	MG-NB	-2.51	2.00	2.05
14	e	1120	CLA	MG-NB	-2.51	2.00	2.05
14	n	1501	CLA	C1B-NB	-2.51	1.34	1.37
14	e	1102	CLA	CHC-C1C	2.51	1.43	1.38
14	G	1104	CLA	C3B-C4B	2.51	1.48	1.42
14	t	508	CLA	C3B-C4B	2.51	1.48	1.42
14	6	518	CLA	C1B-C2B	2.51	1.49	1.43
14	Z	512	CLA	MG-NB	-2.51	2.00	2.05
14	G	1116	CLA	MG-NB	-2.51	2.00	2.05
14	A	1121	CLA	C4B-NB	2.51	1.40	1.37
14	B	1238	CLA	MG-NB	-2.51	2.00	2.05
14	G	1102	CLA	MG-NB	-2.51	2.00	2.05
21	f	1852	SQD	O47-C45	-2.51	1.40	1.46
14	e	1106	CLA	MG-NB	-2.51	2.00	2.05
14	A	1801	CLA	MG-NB	-2.51	2.00	2.05
14	H	1238	CLA	MG-NB	-2.51	2.00	2.05
14	f	1230	CLA	C3B-C4B	2.51	1.48	1.42
14	B	1012	CLA	MG-NB	-2.51	2.00	2.05
14	f	1234	CLA	MG-ND	-2.51	2.00	2.05
14	G	1127	CLA	C3B-C4B	2.51	1.48	1.42
14	e	1118	CLA	CMD-C2D	-2.51	1.45	1.50
14	6	517	CLA	C1B-C2B	2.51	1.49	1.43
14	v	504	CLA	C1B-C2B	2.51	1.49	1.43
14	f	1234	CLA	C1B-NB	-2.51	1.34	1.37
14	L	1501	CLA	C3B-C4B	2.51	1.48	1.42
14	b	508	CLA	C3B-C4B	2.51	1.48	1.42
14	Y	503	CLA	C1B-C2B	2.51	1.49	1.43
14	c	509	CLA	C1B-C2B	2.51	1.49	1.43
14	c	510	CLA	C1B-C2B	2.51	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1012	CLA	CHC-C1C	2.51	1.43	1.38
14	c	519	CLA	C1B-C2B	2.51	1.49	1.43
14	e	1115	CLA	C3B-C4B	2.51	1.48	1.42
14	f	1221	CLA	MG-NB	-2.51	2.00	2.05
14	B	1240	CLA	CMD-C2D	-2.50	1.45	1.50
14	e	1011	CLA	MG-NB	-2.50	2.00	2.05
14	e	1022	CLA	C4B-NB	2.50	1.40	1.37
14	a	503	CLA	C1B-C2B	2.50	1.49	1.43
14	e	1127	CLA	C3B-C4B	2.50	1.48	1.42
14	3	503	CLA	C1B-C2B	2.50	1.49	1.43
14	B	1206	CLA	C1B-NB	-2.50	1.34	1.37
14	Z	516	CLA	C1B-C2B	2.50	1.49	1.43
14	t	501	CLA	C1B-C2B	2.50	1.49	1.43
14	1	516	CLA	MG-NB	-2.50	2.00	2.05
14	e	1136	CLA	CMD-C2D	-2.50	1.45	1.50
14	B	1235	CLA	C3B-C4B	2.50	1.48	1.42
14	H	1204	CLA	MG-NB	-2.50	2.00	2.05
14	G	1120	CLA	C4B-NB	2.50	1.40	1.37
14	G	1130	CLA	C1B-NB	-2.50	1.34	1.37
14	t	519	CLA	C1B-C2B	2.50	1.49	1.43
14	G	1137	CLA	MG-NB	-2.50	2.00	2.05
14	f	1215	CLA	C3B-C4B	2.50	1.48	1.42
14	H	1012	CLA	MG-NB	-2.50	2.00	2.05
14	H	1232	CLA	MG-NB	-2.50	2.00	2.05
14	4	501	CLA	C1B-C2B	2.50	1.49	1.43
14	d	510	CLA	C1B-C2B	2.50	1.49	1.43
14	H	1205	CLA	CMB-C2B	-2.50	1.45	1.50
14	B	1204	CLA	C4B-NB	2.50	1.40	1.37
14	f	1231	CLA	C1B-C2B	2.50	1.49	1.43
14	a	508	CLA	MG-NB	-2.50	2.00	2.05
14	G	1123	CLA	CMD-C2D	-2.50	1.45	1.50
14	H	1215	CLA	C3B-C4B	2.50	1.48	1.42
14	A	1106	CLA	MG-NB	-2.50	2.00	2.05
14	5	509	CLA	C1B-C2B	2.50	1.49	1.43
14	B	1204	CLA	MG-NB	-2.50	2.00	2.05
14	B	1235	CLA	MG-NB	-2.50	2.00	2.05
14	3	508	CLA	MG-NB	-2.50	2.00	2.05
14	R	1301	CLA	MG-NB	-2.50	2.00	2.05
14	6	504	CLA	C1B-C2B	2.50	1.49	1.43
14	d	505	CLA	C1B-C2B	2.50	1.49	1.43
14	Z	502	CLA	C1B-C2B	2.50	1.49	1.43
14	B	1205	CLA	CMB-C2B	-2.50	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	s	505	CLA	CMD-C2D	-2.50	1.45	1.50
14	H	1218	CLA	C1B-C2B	2.50	1.49	1.43
14	f	1219	CLA	C3B-C4B	2.50	1.48	1.42
14	A	1116	CLA	MG-NB	-2.50	2.00	2.05
14	F	1301	CLA	MG-NB	-2.50	2.00	2.05
14	e	1101	CLA	CMC-C2C	-2.50	1.45	1.50
14	G	1124	CLA	C1B-NB	-2.50	1.34	1.37
14	T	1303	CLA	C1B-C2B	2.50	1.49	1.43
14	A	1011	CLA	MG-NB	-2.50	2.00	2.05
14	H	1234	CLA	C1B-NB	-2.49	1.34	1.37
14	L	1503	CLA	C1B-C2B	2.49	1.49	1.43
14	s	503	CLA	C1B-C2B	2.49	1.49	1.43
14	H	1210	CLA	MG-NB	-2.49	2.00	2.05
14	A	1112	CLA	C4B-NB	2.49	1.40	1.37
14	A	1102	CLA	CHC-C1C	2.49	1.43	1.38
14	A	1126	CLA	MG-NB	-2.49	2.00	2.05
14	G	1109	CLA	MG-NB	-2.49	2.00	2.05
14	G	1118	CLA	MG-NB	-2.49	2.00	2.05
14	A	1131	CLA	CMB-C2B	-2.49	1.45	1.50
14	b	506	CLA	C1B-C2B	2.49	1.49	1.43
14	A	1127	CLA	C3B-C4B	2.49	1.48	1.42
14	d	503	CLA	C1B-C2B	2.49	1.49	1.43
14	f	1012	CLA	CHC-C1C	2.49	1.43	1.38
14	r	505	CLA	C1B-C2B	2.49	1.49	1.43
14	A	1137	CLA	MG-NB	-2.49	2.00	2.05
14	B	1234	CLA	MG-ND	-2.49	2.00	2.05
14	G	1106	CLA	MG-NB	-2.49	2.00	2.05
14	e	1801	CLA	MG-NB	-2.49	2.00	2.05
14	f	1012	CLA	C4B-NB	2.49	1.40	1.37
14	2	507	CLA	C1B-C2B	2.49	1.49	1.43
14	s	511	CLA	C1B-C2B	2.49	1.49	1.43
14	e	1136	CLA	CMB-C2B	-2.49	1.45	1.50
14	G	1109	CLA	CMD-C2D	-2.49	1.45	1.50
14	U	1103	CLA	C3B-C4B	2.49	1.48	1.42
14	G	1132	CLA	MG-NB	-2.49	2.00	2.05
14	1	503	CLA	C1B-C2B	2.49	1.49	1.43
14	4	506	CLA	C1B-C2B	2.49	1.49	1.43
14	d	518	CLA	C1B-C2B	2.49	1.49	1.43
15	A	2001	PQN	C10-C1	-2.49	1.43	1.48
14	f	1204	CLA	C1B-C2B	2.49	1.49	1.43
14	e	1128	CLA	MG-ND	-2.49	2.00	2.05
14	G	1131	CLA	CMD-C2D	-2.49	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1128	CLA	MG-ND	-2.49	2.00	2.05
14	e	1121	CLA	MG-NB	-2.49	2.00	2.05
14	q	503	CLA	C1B-C2B	2.49	1.49	1.43
14	H	1226	CLA	C1D-ND	2.49	1.40	1.37
14	e	1103	CLA	C4B-NB	2.49	1.40	1.37
14	e	1119	CLA	C1B-NB	-2.49	1.34	1.37
14	H	1230	CLA	CMC-C2C	-2.49	1.45	1.50
14	H	1235	CLA	C3B-C4B	2.49	1.48	1.42
21	B	1852	SQD	O47-C45	-2.49	1.40	1.46
14	B	1215	CLA	C3B-C4B	2.49	1.48	1.42
14	r	506	CLA	C1B-C2B	2.49	1.49	1.43
14	u	509	CLA	C1B-C2B	2.49	1.49	1.43
14	H	1206	CLA	C1B-NB	-2.49	1.34	1.37
14	6	510	CLA	C1B-C2B	2.49	1.49	1.43
14	v	517	CLA	C1B-C2B	2.49	1.49	1.43
14	B	1214	CLA	CMC-C2C	-2.49	1.45	1.50
14	G	1125	CLA	C3B-C4B	2.49	1.48	1.42
14	K	1103	CLA	C3B-C4B	2.48	1.48	1.42
14	Y	506	CLA	C1B-C2B	2.48	1.49	1.43
14	e	1127	CLA	CMD-C2D	-2.48	1.45	1.50
14	c	507	CLA	C3B-C4B	2.48	1.48	1.42
14	f	1218	CLA	C1B-C2B	2.48	1.49	1.43
14	A	1102	CLA	MG-NB	-2.48	2.00	2.05
14	e	1137	CLA	MG-NB	-2.48	2.00	2.05
14	V	1503	CLA	C1B-C2B	2.48	1.49	1.43
14	A	1128	CLA	MG-ND	-2.48	2.00	2.05
14	f	1235	CLA	C3B-C4B	2.48	1.48	1.42
14	H	1214	CLA	CMC-C2C	-2.48	1.45	1.50
14	b	505	CLA	CMD-C2D	-2.48	1.45	1.50
14	H	1234	CLA	MG-ND	-2.48	2.00	2.05
14	H	1214	CLA	CMB-C2B	-2.48	1.45	1.50
14	e	1122	CLA	C4B-NB	2.48	1.40	1.37
14	Y	516	CLA	MG-NB	-2.48	2.00	2.05
14	A	1136	CLA	CMB-C2B	-2.48	1.45	1.50
14	d	504	CLA	C1B-C2B	2.48	1.49	1.43
14	G	1237	CLA	C4B-NB	2.48	1.40	1.37
14	f	1240	CLA	CMD-C2D	-2.48	1.45	1.50
14	a	511	CLA	C1B-C2B	2.48	1.49	1.43
14	q	504	CLA	C1B-C2B	2.48	1.49	1.43
14	a	508	CLA	C3B-C4B	2.48	1.48	1.42
14	A	1109	CLA	MG-NB	-2.48	2.00	2.05
14	B	1214	CLA	CMB-C2B	-2.48	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1123	CLA	CMD-C2D	-2.48	1.45	1.50
14	3	511	CLA	C1B-C2B	2.48	1.49	1.43
14	Z	507	CLA	C1B-C2B	2.48	1.49	1.43
14	G	1022	CLA	C4B-NB	2.48	1.40	1.37
14	V	1501	CLA	C3B-C4B	2.48	1.48	1.42
17	n	4219	BCR	C21-C22	-2.48	1.32	1.35
14	G	1126	CLA	MG-NB	-2.48	2.00	2.05
14	s	508	CLA	MG-NB	-2.48	2.00	2.05
14	e	1124	CLA	C1B-NB	-2.48	1.34	1.37
21	H	1852	SQD	O47-C45	-2.48	1.40	1.46
14	2	516	CLA	C1B-C2B	2.48	1.49	1.43
14	A	1118	CLA	C4B-NB	2.48	1.40	1.37
14	e	1119	CLA	C4B-NB	2.48	1.40	1.37
14	f	1204	CLA	C4B-NB	2.48	1.40	1.37
14	A	1121	CLA	MG-NB	-2.48	2.00	2.05
14	q	511	CLA	MG-NB	-2.48	2.00	2.05
14	4	505	CLA	CMD-C2D	-2.48	1.45	1.50
14	G	1122	CLA	CMC-C2C	-2.48	1.45	1.50
14	A	1124	CLA	C1B-NB	-2.48	1.34	1.37
14	f	1222	CLA	C4B-NB	2.48	1.40	1.37
14	n	1503	CLA	C1B-C2B	2.48	1.49	1.43
14	e	1107	CLA	MG-ND	-2.48	2.00	2.05
14	e	1109	CLA	MG-NB	-2.48	2.00	2.05
14	A	1125	CLA	C3B-C4B	2.48	1.48	1.42
14	Z	506	CLA	C1B-C2B	2.48	1.49	1.43
14	v	510	CLA	C1B-C2B	2.48	1.49	1.43
14	B	1210	CLA	MG-NB	-2.48	2.00	2.05
14	G	1118	CLA	C4B-NB	2.48	1.40	1.37
14	f	1214	CLA	CMB-C2B	-2.47	1.45	1.50
14	1	506	CLA	C1B-C2B	2.47	1.49	1.43
14	u	507	CLA	C3B-C4B	2.47	1.48	1.42
14	H	1234	CLA	C4B-NB	2.47	1.40	1.37
14	5	501	CLA	C1B-C2B	2.47	1.49	1.43
14	e	1123	CLA	MG-NB	-2.47	2.00	2.05
14	f	1235	CLA	MG-NB	-2.47	2.00	2.05
14	B	1218	CLA	C1B-C2B	2.47	1.49	1.43
14	r	507	CLA	C1B-C2B	2.47	1.49	1.43
14	f	1223	CLA	C4B-NB	2.47	1.40	1.37
14	A	1123	CLA	CMD-C2D	-2.47	1.45	1.50
14	f	1214	CLA	CMC-C2C	-2.47	1.45	1.50
14	B	1204	CLA	C1B-C2B	2.47	1.49	1.43
14	2	510	CLA	C1B-C2B	2.47	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	u	501	CLA	C1B-C2B	2.47	1.49	1.43
14	5	507	CLA	C3B-C4B	2.47	1.48	1.42
14	A	1113	CLA	C4B-NB	2.47	1.40	1.37
14	6	505	CLA	C1B-C2B	2.47	1.49	1.43
14	v	519	CLA	C1B-C2B	2.47	1.49	1.43
14	e	1131	CLA	CMB-C2B	-2.47	1.45	1.50
14	G	1108	CLA	MG-NB	-2.47	2.00	2.05
14	G	1801	CLA	C4B-NB	2.47	1.40	1.37
14	2	506	CLA	C1B-C2B	2.47	1.49	1.43
14	Y	513	CLA	C1B-C2B	2.47	1.49	1.43
14	c	512	CLA	MG-NB	-2.47	2.00	2.05
14	B	1238	CLA	C3B-C4B	2.47	1.48	1.42
14	A	1131	CLA	CMD-C2D	-2.47	1.45	1.50
14	b	501	CLA	C1B-C2B	2.47	1.49	1.43
14	A	1122	CLA	CMC-C2C	-2.47	1.45	1.50
14	d	512	CLA	MG-NB	-2.47	2.00	2.05
14	q	510	CLA	C1B-C2B	2.47	1.49	1.43
14	t	505	CLA	CMD-C2D	-2.47	1.45	1.50
14	H	1238	CLA	C3B-C4B	2.47	1.48	1.42
14	f	1205	CLA	CMB-C2B	-2.47	1.45	1.50
14	6	503	CLA	C1B-C2B	2.47	1.49	1.43
14	H	1231	CLA	C4B-NB	2.47	1.40	1.37
14	m	1103	CLA	C3B-C4B	2.47	1.48	1.42
14	e	1122	CLA	CMC-C2C	-2.47	1.45	1.50
14	A	1118	CLA	MG-NB	-2.47	2.00	2.05
15	G	2001	PQN	C10-C1	-2.47	1.43	1.48
14	v	505	CLA	C1B-C2B	2.47	1.49	1.43
14	B	1230	CLA	CMC-C2C	-2.47	1.45	1.50
14	B	1219	CLA	C3B-C4B	2.47	1.48	1.42
14	Z	502	CLA	C3B-C4B	2.47	1.48	1.42
14	A	1022	CLA	C4B-NB	2.47	1.40	1.37
14	u	513	CLA	C1B-C2B	2.47	1.49	1.43
14	A	1136	CLA	CMD-C2D	-2.47	1.45	1.50
14	e	1113	CLA	C4B-NB	2.47	1.40	1.37
14	l	1303	CLA	C1B-C2B	2.47	1.49	1.43
14	d	507	CLA	C1B-C2B	2.46	1.49	1.43
14	s	517	CLA	C1B-C2B	2.46	1.49	1.43
14	Y	511	CLA	MG-NB	-2.46	2.00	2.05
14	G	1112	CLA	C4B-NB	2.46	1.40	1.37
14	Z	510	CLA	C1B-C2B	2.46	1.49	1.43
14	e	1111	CLA	MG-NB	-2.46	2.00	2.05
14	G	1136	CLA	CMB-C2B	-2.46	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	1303	CLA	C1B-C2B	2.46	1.49	1.43
14	H	1223	CLA	C4B-NB	2.46	1.40	1.37
14	e	1112	CLA	C4B-NB	2.46	1.40	1.37
14	5	512	CLA	MG-NB	-2.46	2.00	2.05
14	5	501	CLA	CMC-C2C	-2.46	1.45	1.50
14	B	1223	CLA	C4B-NB	2.46	1.40	1.37
14	B	1234	CLA	C1B-NB	-2.46	1.34	1.37
14	B	1225	CLA	MG-ND	-2.46	2.00	2.05
14	c	513	CLA	C1B-C2B	2.46	1.49	1.43
14	v	507	CLA	C1B-C2B	2.46	1.49	1.43
14	j	1301	CLA	MG-NB	-2.46	2.00	2.05
14	A	1117	CLA	C1B-NB	-2.46	1.34	1.37
14	G	1113	CLA	C4B-NB	2.46	1.40	1.37
14	6	507	CLA	C1B-C2B	2.46	1.49	1.43
14	q	513	CLA	C1B-C2B	2.46	1.49	1.43
14	q	506	CLA	C1B-C2B	2.46	1.49	1.43
14	A	1801	CLA	C4B-NB	2.46	1.40	1.37
14	B	1226	CLA	C1D-ND	2.46	1.40	1.37
14	e	1111	CLA	C4B-NB	2.46	1.40	1.37
14	Y	510	CLA	C1B-C2B	2.46	1.49	1.43
14	t	506	CLA	C1B-C2B	2.46	1.49	1.43
14	r	510	CLA	C1B-C2B	2.46	1.49	1.43
14	G	1136	CLA	CMD-C2D	-2.46	1.45	1.50
14	G	1107	CLA	MG-ND	-2.46	2.00	2.05
14	c	501	CLA	C1B-C2B	2.46	1.49	1.43
14	A	1109	CLA	CMD-C2D	-2.46	1.45	1.50
14	G	1122	CLA	C4B-NB	2.46	1.40	1.37
14	6	512	CLA	MG-NB	-2.46	2.00	2.05
14	u	512	CLA	MG-NB	-2.46	2.00	2.05
14	a	510	CLA	C1B-C2B	2.46	1.49	1.43
14	A	1109	CLA	CMC-C2C	-2.46	1.45	1.50
14	A	1132	CLA	MG-NB	-2.46	2.00	2.05
14	G	1121	CLA	MG-NB	-2.46	2.00	2.05
14	H	1207	CLA	CMD-C2D	-2.46	1.45	1.50
14	Y	516	CLA	C1B-C2B	2.46	1.49	1.43
14	a	517	CLA	C1B-C2B	2.46	1.49	1.43
14	e	1109	CLA	CMD-C2D	-2.46	1.45	1.50
14	e	1131	CLA	CMD-C2D	-2.46	1.45	1.50
14	B	1207	CLA	CMD-C2D	-2.46	1.45	1.50
14	1	504	CLA	C1B-C2B	2.46	1.49	1.43
14	L	1501	CLA	C1B-NB	-2.46	1.34	1.37
14	B	1230	CLA	C1B-C2B	2.46	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1119	CLA	C4B-NB	2.46	1.40	1.37
14	s	508	CLA	C3B-C4B	2.46	1.48	1.42
14	e	1119	CLA	CMD-C2D	-2.46	1.45	1.50
14	G	1113	CLA	MG-NB	-2.46	2.00	2.05
14	e	1102	CLA	MG-NB	-2.45	2.00	2.05
14	H	1219	CLA	C3B-C4B	2.45	1.48	1.42
14	Z	513	CLA	C1B-C2B	2.45	1.49	1.43
14	c	501	CLA	CMC-C2C	-2.45	1.45	1.50
14	A	1107	CLA	MG-ND	-2.45	2.00	2.05
14	1	510	CLA	C1B-C2B	2.45	1.49	1.43
14	n	1503	CLA	CMC-C2C	-2.45	1.45	1.50
14	G	1117	CLA	C1B-NB	-2.45	1.34	1.37
14	e	1112	CLA	MG-NB	-2.45	2.00	2.05
14	f	1238	CLA	C3B-C4B	2.45	1.48	1.42
14	r	516	CLA	C1B-C2B	2.45	1.49	1.43
14	H	1210	CLA	C4B-NB	2.45	1.40	1.37
14	6	519	CLA	C1B-C2B	2.45	1.49	1.43
14	q	516	CLA	C1B-C2B	2.45	1.49	1.43
14	A	1127	CLA	CMD-C2D	-2.45	1.45	1.50
14	G	1127	CLA	CMD-C2D	-2.45	1.45	1.50
14	u	511	CLA	C1B-C2B	2.45	1.49	1.43
14	2	502	CLA	C3B-C4B	2.45	1.48	1.42
14	3	508	CLA	C3B-C4B	2.45	1.48	1.42
14	H	1230	CLA	MG-NB	-2.45	2.00	2.05
14	f	1238	CLA	C4B-NB	2.45	1.40	1.37
14	A	1123	CLA	MG-NB	-2.45	2.00	2.05
14	G	1104	CLA	MG-NB	-2.45	2.00	2.05
14	1	519	CLA	C1B-C2B	2.45	1.49	1.43
14	V	1503	CLA	CMC-C2C	-2.45	1.45	1.50
14	s	510	CLA	C1B-C2B	2.45	1.49	1.43
14	f	1210	CLA	MG-NB	-2.45	2.00	2.05
14	B	1021	CLA	CMC-C2C	-2.45	1.45	1.50
14	e	1125	CLA	C3B-C4B	2.45	1.48	1.42
14	A	1119	CLA	CMD-C2D	-2.45	1.45	1.50
17	V	4219	BCR	C21-C22	-2.45	1.32	1.35
14	H	1225	CLA	MG-ND	-2.45	2.00	2.05
14	G	1119	CLA	C4B-NB	2.45	1.40	1.37
14	e	1121	CLA	C4B-NB	2.45	1.40	1.37
14	3	510	CLA	C1B-C2B	2.45	1.49	1.43
14	c	511	CLA	C1B-C2B	2.45	1.49	1.43
14	G	1126	CLA	C3B-C4B	2.45	1.48	1.42
14	2	505	CLA	CMD-C2D	-2.45	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	513	CLA	C1B-C2B	2.45	1.49	1.43
14	e	1132	CLA	MG-NB	-2.45	2.00	2.05
14	e	1136	CLA	MG-NB	-2.45	2.00	2.05
14	H	1219	CLA	C1B-C2B	2.45	1.49	1.43
14	b	507	CLA	C3B-C4B	2.45	1.48	1.42
14	f	1021	CLA	CMC-C2C	-2.45	1.45	1.50
14	H	1204	CLA	C1B-C2B	2.45	1.49	1.43
14	1	511	CLA	MG-NB	-2.45	2.00	2.05
14	u	501	CLA	CMC-C2C	-2.44	1.45	1.50
14	A	1108	CLA	MG-NB	-2.44	2.00	2.05
14	v	503	CLA	C1B-C2B	2.44	1.49	1.43
14	G	1119	CLA	CMD-C2D	-2.44	1.45	1.50
14	f	1207	CLA	CMD-C2D	-2.44	1.45	1.50
14	3	517	CLA	C1B-C2B	2.44	1.49	1.43
14	5	517	CLA	C1B-C2B	2.44	1.49	1.43
14	Y	504	CLA	C1B-C2B	2.44	1.49	1.43
14	A	1113	CLA	MG-NB	-2.44	2.00	2.05
14	f	1222	CLA	MG-NB	-2.44	2.00	2.05
14	r	505	CLA	CMD-C2D	-2.44	1.45	1.50
14	f	1230	CLA	CMC-C2C	-2.44	1.45	1.50
14	f	1021	CLA	C1B-C2B	2.44	1.49	1.43
14	3	504	CLA	C1B-C2B	2.44	1.49	1.43
14	Y	512	CLA	MG-NB	-2.44	2.00	2.05
14	5	511	CLA	C1B-C2B	2.44	1.49	1.43
14	B	1210	CLA	C4B-NB	2.44	1.40	1.37
14	A	1237	CLA	C4B-NB	2.44	1.40	1.37
14	A	1126	CLA	C3B-C4B	2.44	1.48	1.42
14	B	1222	CLA	MG-NB	-2.44	2.00	2.05
14	H	1230	CLA	CMD-C2D	-2.44	1.45	1.50
14	f	1219	CLA	C1B-C2B	2.44	1.49	1.43
15	e	2001	PQN	C10-C1	-2.44	1.43	1.48
14	Z	505	CLA	CMD-C2D	-2.44	1.45	1.50
14	r	502	CLA	CMB-C2B	-2.44	1.45	1.50
14	Y	519	CLA	C1B-C2B	2.44	1.49	1.43
14	q	511	CLA	C1B-C2B	2.44	1.49	1.43
14	f	1235	CLA	CMB-C2B	-2.44	1.45	1.50
14	B	1219	CLA	C1B-C2B	2.44	1.49	1.43
14	f	1230	CLA	C1B-C2B	2.44	1.49	1.43
14	q	519	CLA	C1B-C2B	2.44	1.49	1.43
14	1	511	CLA	C1B-C2B	2.44	1.49	1.43
14	G	1115	CLA	MG-NB	-2.44	2.01	2.05
14	A	1122	CLA	C4B-NB	2.44	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	516	CLA	C1B-C2B	2.44	1.49	1.43
14	q	508	CLA	MG-NB	-2.44	2.01	2.05
14	G	1123	CLA	MG-NB	-2.44	2.01	2.05
14	e	1118	CLA	MG-NB	-2.44	2.01	2.05
14	L	1503	CLA	CMC-C2C	-2.44	1.45	1.50
14	A	1115	CLA	MG-NB	-2.44	2.01	2.05
14	G	1138	CLA	MG-NB	-2.44	2.01	2.05
14	e	1126	CLA	C3B-C4B	2.44	1.48	1.42
14	e	1107	CLA	CMC-C2C	-2.44	1.45	1.50
14	c	517	CLA	C1B-C2B	2.44	1.49	1.43
14	1	508	CLA	MG-NB	-2.43	2.01	2.05
14	e	1108	CLA	MG-NB	-2.43	2.01	2.05
14	A	1107	CLA	CMC-C2C	-2.43	1.45	1.50
14	H	1230	CLA	C1B-C2B	2.43	1.49	1.43
14	u	517	CLA	C1B-C2B	2.43	1.49	1.43
14	1	512	CLA	MG-NB	-2.43	2.01	2.05
14	m	1103	CLA	CMD-C2D	-2.43	1.45	1.50
14	r	511	CLA	C1B-C2B	2.43	1.49	1.43
14	G	1109	CLA	CMC-C2C	-2.43	1.45	1.50
14	e	1113	CLA	CMC-C2C	-2.43	1.45	1.50
14	B	1231	CLA	C4B-NB	2.43	1.40	1.37
14	G	1113	CLA	CMC-C2C	-2.43	1.45	1.50
17	L	4219	BCR	C21-C22	-2.43	1.32	1.35
14	s	504	CLA	C1B-C2B	2.43	1.49	1.43
14	d	519	CLA	C1B-C2B	2.43	1.49	1.43
14	G	1136	CLA	MG-NB	-2.43	2.01	2.05
14	2	502	CLA	CMB-C2B	-2.43	1.45	1.50
14	n	1502	CLA	MG-NB	-2.43	2.01	2.05
14	r	502	CLA	C3B-C4B	2.43	1.48	1.42
14	f	1225	CLA	MG-ND	-2.43	2.01	2.05
14	B	1230	CLA	CMB-C2B	-2.43	1.45	1.50
14	G	1123	CLA	C1B-NB	-2.43	1.34	1.37
14	A	1022	CLA	MG-ND	-2.43	2.01	2.05
14	5	513	CLA	C1B-C2B	2.43	1.49	1.43
14	f	1210	CLA	C4B-NB	2.43	1.40	1.37
14	A	1113	CLA	CMC-C2C	-2.43	1.45	1.50
14	G	1128	CLA	CMD-C2D	-2.43	1.45	1.50
14	f	1021	CLA	CMB-C2B	-2.43	1.45	1.50
14	e	1138	CLA	MG-NB	-2.43	2.01	2.05
14	Y	511	CLA	C1B-C2B	2.43	1.49	1.43
14	e	1801	CLA	C4B-NB	2.43	1.40	1.37
14	H	1207	CLA	CMC-C2C	-2.43	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	511	CLA	C1B-C2B	2.43	1.49	1.43
14	f	1206	CLA	C1B-NB	-2.43	1.34	1.37
14	B	1021	CLA	CMB-C2B	-2.43	1.45	1.50
14	B	1212	CLA	C1B-C2B	2.43	1.49	1.43
14	e	1115	CLA	MG-NB	-2.43	2.01	2.05
14	f	1226	CLA	C1D-ND	2.43	1.40	1.37
14	B	1235	CLA	CMB-C2B	-2.43	1.45	1.50
14	H	1225	CLA	CMC-C2C	-2.43	1.45	1.50
14	e	1109	CLA	CMC-C2C	-2.43	1.45	1.50
14	Z	511	CLA	C1B-C2B	2.43	1.49	1.43
14	u	505	CLA	CMD-C2D	-2.43	1.45	1.50
14	B	1234	CLA	C4B-NB	2.43	1.40	1.37
14	e	1118	CLA	C4B-NB	2.43	1.40	1.37
14	Y	508	CLA	MG-NB	-2.43	2.01	2.05
14	G	1107	CLA	CMC-C2C	-2.42	1.45	1.50
14	c	505	CLA	CMD-C2D	-2.42	1.45	1.50
14	G	1111	CLA	MG-NB	-2.42	2.01	2.05
14	G	1121	CLA	C1B-C2B	2.42	1.49	1.43
14	f	1230	CLA	CMB-C2B	-2.42	1.45	1.50
14	A	1127	CLA	C1B-NB	-2.42	1.34	1.37
14	A	1136	CLA	MG-NB	-2.42	2.01	2.05
14	f	1225	CLA	C3B-C4B	2.42	1.48	1.42
14	r	513	CLA	C1B-C2B	2.42	1.49	1.43
14	A	1112	CLA	MG-NB	-2.42	2.01	2.05
14	A	1237	CLA	CMC-C2C	-2.42	1.45	1.50
14	e	1237	CLA	CMC-C2C	-2.42	1.45	1.50
14	e	1022	CLA	MG-ND	-2.42	2.01	2.05
14	A	1130	CLA	CMC-C2C	-2.42	1.45	1.50
14	H	1224	CLA	C1B-C2B	2.42	1.49	1.43
14	G	1127	CLA	C1B-NB	-2.42	1.34	1.37
14	H	1021	CLA	CMB-C2B	-2.42	1.45	1.50
14	A	1104	CLA	MG-NB	-2.42	2.01	2.05
18	B	1842	LHG	O8-C6	-2.42	1.39	1.45
14	5	505	CLA	CMD-C2D	-2.42	1.45	1.50
14	4	507	CLA	C3B-C4B	2.42	1.48	1.42
14	e	1104	CLA	MG-NB	-2.42	2.01	2.05
14	B	1238	CLA	C4B-NB	2.42	1.40	1.37
14	a	504	CLA	C1B-C2B	2.42	1.49	1.43
14	H	1229	CLA	MG-NB	-2.42	2.01	2.05
14	G	1130	CLA	CMC-C2C	-2.42	1.45	1.50
14	G	1022	CLA	MG-ND	-2.42	2.01	2.05
14	e	1113	CLA	MG-NB	-2.42	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1230	CLA	MG-NB	-2.42	2.01	2.05
14	e	1117	CLA	C1B-NB	-2.42	1.34	1.37
14	H	1239	CLA	C1B-C2B	2.42	1.48	1.43
14	f	1212	CLA	C1B-C2B	2.42	1.48	1.43
14	A	1121	CLA	C1B-C2B	2.42	1.48	1.43
14	f	1234	CLA	C4B-NB	2.42	1.40	1.37
14	A	1111	CLA	MG-NB	-2.42	2.01	2.05
14	H	1021	CLA	CMC-C2C	-2.42	1.45	1.50
14	4	509	CLA	C1B-C2B	2.42	1.48	1.43
14	e	1121	CLA	C1B-C2B	2.42	1.48	1.43
14	B	1209	CLA	CMC-C2C	-2.42	1.45	1.50
14	K	1103	CLA	CMD-C2D	-2.42	1.45	1.50
14	Y	502	CLA	MG-NB	-2.42	2.01	2.05
14	r	511	CLA	MG-NB	-2.42	2.01	2.05
14	A	1128	CLA	CMD-C2D	-2.41	1.45	1.50
14	f	1230	CLA	CMD-C2D	-2.41	1.45	1.50
14	G	1133	CLA	C4B-NB	2.41	1.40	1.37
14	e	1122	CLA	MG-NB	-2.41	2.01	2.05
14	v	512	CLA	MG-NB	-2.41	2.01	2.05
14	B	1230	CLA	CMD-C2D	-2.41	1.45	1.50
14	e	1134	CLA	C1B-C2B	2.41	1.48	1.43
14	Z	502	CLA	CMB-C2B	-2.41	1.45	1.50
18	H	1842	LHG	O8-C6	-2.41	1.39	1.45
14	V	1502	CLA	MG-NB	-2.41	2.01	2.05
14	2	513	CLA	C1B-C2B	2.41	1.48	1.43
14	G	1111	CLA	C4B-NB	2.41	1.40	1.37
14	H	1238	CLA	C1B-NB	-2.41	1.34	1.37
14	t	507	CLA	C3B-C4B	2.41	1.48	1.42
14	A	1111	CLA	C4B-NB	2.41	1.40	1.37
14	B	1225	CLA	C3B-C4B	2.41	1.48	1.42
14	e	1126	CLA	CMD-C2D	-2.41	1.45	1.50
14	e	1130	CLA	CMC-C2C	-2.41	1.45	1.50
14	A	1122	CLA	MG-NB	-2.41	2.01	2.05
14	3	506	CLA	C1B-C2B	2.41	1.48	1.43
14	t	509	CLA	C1B-C2B	2.41	1.48	1.43
14	B	1207	CLA	CMC-C2C	-2.41	1.45	1.50
14	f	1203	CLA	CMC-C2C	-2.41	1.45	1.50
14	B	1224	CLA	C1B-C2B	2.41	1.48	1.43
14	f	1209	CLA	CMC-C2C	-2.41	1.45	1.50
14	H	1212	CLA	C1B-C2B	2.41	1.48	1.43
14	q	512	CLA	MG-NB	-2.41	2.01	2.05
14	B	1012	CLA	C4B-NB	2.41	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1127	CLA	C1B-NB	-2.41	1.34	1.37
14	B	1229	CLA	MG-NB	-2.41	2.01	2.05
14	H	1240	CLA	C1B-C2B	2.41	1.48	1.43
14	H	1209	CLA	CMC-C2C	-2.41	1.45	1.50
14	G	1112	CLA	MG-NB	-2.41	2.01	2.05
14	A	1126	CLA	CMD-C2D	-2.41	1.45	1.50
14	H	1203	CLA	CMC-C2C	-2.41	1.45	1.50
14	e	1130	CLA	CMB-C2B	-2.41	1.45	1.50
14	A	1107	CLA	C3B-C4B	2.41	1.48	1.42
14	a	509	CLA	C1B-C2B	2.41	1.48	1.43
14	f	1220	CLA	C1B-C2B	2.41	1.48	1.43
14	B	1239	CLA	C1B-C2B	2.41	1.48	1.43
14	e	1013	CLA	C4B-NB	2.40	1.40	1.37
14	A	1138	CLA	MG-NB	-2.40	2.01	2.05
14	f	1224	CLA	C1B-C2B	2.40	1.48	1.43
14	s	506	CLA	C1B-C2B	2.40	1.48	1.43
14	L	1502	CLA	MG-NB	-2.40	2.01	2.05
14	A	1134	CLA	C1B-C2B	2.40	1.48	1.43
14	f	1232	CLA	C1B-NB	-2.40	1.34	1.37
14	G	1134	CLA	C1B-C2B	2.40	1.48	1.43
14	s	509	CLA	C1B-C2B	2.40	1.48	1.43
14	G	1237	CLA	CMC-C2C	-2.40	1.45	1.50
14	q	502	CLA	MG-NB	-2.40	2.01	2.05
14	a	506	CLA	C1B-C2B	2.40	1.48	1.43
14	q	509	CLA	C1B-C2B	2.40	1.48	1.43
14	H	1225	CLA	C3B-C4B	2.40	1.48	1.42
14	B	1203	CLA	CMC-C2C	-2.40	1.45	1.50
14	H	1230	CLA	CMB-C2B	-2.40	1.45	1.50
14	H	1023	CLA	MG-NB	-2.40	2.01	2.05
14	d	517	CLA	MG-NB	-2.40	2.01	2.05
14	B	1021	CLA	C1B-C2B	2.40	1.48	1.43
15	e	2001	PQN	C5-C4	-2.40	1.43	1.48
14	G	1122	CLA	MG-NB	-2.40	2.01	2.05
14	q	512	CLA	C1B-C2B	2.40	1.48	1.43
14	G	1132	CLA	CMD-C2D	-2.40	1.45	1.50
14	U	1103	CLA	CMD-C2D	-2.40	1.45	1.50
14	H	1238	CLA	C4B-NB	2.40	1.40	1.37
14	f	1023	CLA	MG-NB	-2.40	2.01	2.05
14	1	502	CLA	MG-NB	-2.40	2.01	2.05
14	2	511	CLA	MG-NB	-2.40	2.01	2.05
14	e	1121	CLA	MG-ND	-2.40	2.01	2.05
14	A	1123	CLA	C1B-NB	-2.40	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	512	CLA	C1B-C2B	2.40	1.48	1.43
15	H	2002	PQN	C11-C12	2.40	1.54	1.50
14	f	1239	CLA	C1B-C2B	2.40	1.48	1.43
14	A	1121	CLA	MG-ND	-2.40	2.01	2.05
14	r	508	CLA	MG-NB	-2.40	2.01	2.05
14	e	1237	CLA	C4B-NB	2.40	1.40	1.37
14	G	1119	CLA	MG-ND	-2.40	2.01	2.05
14	A	1118	CLA	C1B-C2B	2.40	1.48	1.43
14	G	1123	CLA	C1B-C2B	2.40	1.48	1.43
14	B	1230	CLA	MG-NB	-2.40	2.01	2.05
14	f	1225	CLA	CMB-C2B	-2.40	1.45	1.50
14	Z	511	CLA	MG-NB	-2.40	2.01	2.05
14	b	509	CLA	C1B-C2B	2.40	1.48	1.43
14	f	1225	CLA	CMC-C2C	-2.40	1.45	1.50
14	1	508	CLA	C1B-NB	-2.39	1.34	1.37
14	A	1132	CLA	CMD-C2D	-2.39	1.45	1.50
21	f	1852	SQD	O4-C4	-2.39	1.37	1.43
15	A	2001	PQN	C5-C4	-2.39	1.43	1.48
14	G	1138	CLA	CMB-C2B	-2.39	1.45	1.50
14	B	1023	CLA	C3B-C4B	2.39	1.48	1.42
14	B	1235	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	1123	CLA	C1B-C2B	2.39	1.48	1.43
14	f	1023	CLA	C3B-C4B	2.39	1.48	1.42
14	H	1219	CLA	MG-NB	-2.39	2.01	2.05
14	B	1220	CLA	C1B-C2B	2.39	1.48	1.43
14	f	1221	CLA	MG-ND	-2.39	2.01	2.05
14	B	1225	CLA	CMC-C2C	-2.39	1.45	1.50
14	e	1128	CLA	CMD-C2D	-2.39	1.45	1.50
14	H	1231	CLA	MG-NB	-2.39	2.01	2.05
14	r	501	CLA	C1B-C2B	2.39	1.48	1.43
14	G	1107	CLA	C3B-C4B	2.39	1.48	1.42
14	B	1023	CLA	MG-NB	-2.39	2.01	2.05
14	B	1221	CLA	CMB-C2B	-2.39	1.45	1.50
14	G	1121	CLA	MG-ND	-2.39	2.01	2.05
18	f	1842	LHG	O8-C6	-2.39	1.39	1.45
14	e	1119	CLA	MG-ND	-2.39	2.01	2.05
14	e	1132	CLA	CMD-C2D	-2.39	1.45	1.50
14	B	1213	CLA	C1B-C2B	2.39	1.48	1.43
14	f	1207	CLA	CMC-C2C	-2.39	1.45	1.50
14	H	1021	CLA	C1B-C2B	2.39	1.48	1.43
14	A	1130	CLA	CMB-C2B	-2.39	1.45	1.50
14	H	1235	CLA	CMB-C2B	-2.39	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	v	502	CLA	MG-NB	-2.39	2.01	2.05
14	e	1237	CLA	MG-ND	-2.39	2.01	2.05
14	f	1223	CLA	MG-NB	-2.39	2.01	2.05
14	e	1123	CLA	C1B-C2B	2.39	1.48	1.43
14	U	1401	CLA	MG-NB	-2.39	2.01	2.05
14	e	1123	CLA	C1B-NB	-2.39	1.34	1.37
14	G	1104	CLA	C1B-C2B	2.39	1.48	1.43
14	e	1138	CLA	CMB-C2B	-2.39	1.45	1.50
14	G	1140	CLA	CMD-C2D	-2.38	1.45	1.50
14	G	1118	CLA	C1B-C2B	2.38	1.48	1.43
14	A	1119	CLA	MG-ND	-2.38	2.01	2.05
14	f	1229	CLA	MG-NB	-2.38	2.01	2.05
14	G	1122	CLA	CMB-C2B	-2.38	1.45	1.50
14	v	512	CLA	C1B-C2B	2.38	1.48	1.43
14	G	1125	CLA	C1B-NB	-2.38	1.34	1.37
14	f	1240	CLA	C1B-C2B	2.38	1.48	1.43
14	H	1222	CLA	MG-NB	-2.38	2.01	2.05
14	6	512	CLA	C1B-C2B	2.38	1.48	1.43
14	A	1104	CLA	C1B-C2B	2.38	1.48	1.43
14	f	1213	CLA	C1B-C2B	2.38	1.48	1.43
14	m	1401	CLA	MG-NB	-2.38	2.01	2.05
14	e	1107	CLA	C3B-C4B	2.38	1.48	1.42
14	H	1220	CLA	C1B-C2B	2.38	1.48	1.43
14	e	1104	CLA	C1B-C2B	2.38	1.48	1.43
14	H	1211	CLA	C4B-NB	2.38	1.40	1.37
14	H	1223	CLA	MG-NB	-2.38	2.01	2.05
14	F	1302	CLA	C1B-C2B	2.38	1.48	1.43
14	A	1013	CLA	C4B-NB	2.38	1.40	1.37
14	G	1126	CLA	CMD-C2D	-2.38	1.45	1.50
14	1	509	CLA	C1B-C2B	2.38	1.48	1.43
14	t	505	CLA	MG-NB	-2.38	2.01	2.05
14	l	1302	CLA	C1B-C2B	2.38	1.48	1.43
14	v	517	CLA	MG-NB	-2.38	2.01	2.05
14	e	1125	CLA	C1B-NB	-2.38	1.34	1.37
14	c	510	CLA	MG-NB	-2.38	2.01	2.05
14	d	502	CLA	MG-NB	-2.38	2.01	2.05
14	u	512	CLA	C1B-C2B	2.38	1.48	1.43
14	B	1240	CLA	C1B-C2B	2.38	1.48	1.43
14	G	1108	CLA	C1B-C2B	2.38	1.48	1.43
14	H	1213	CLA	C1B-C2B	2.38	1.48	1.43
14	H	1012	CLA	C4B-NB	2.38	1.40	1.37
14	G	1130	CLA	CMB-C2B	-2.38	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	r	509	CLA	C1B-C2B	2.38	1.48	1.43
14	A	1011	CLA	C4B-NB	2.38	1.40	1.37
14	f	1231	CLA	C4B-NB	2.38	1.40	1.37
14	Z	501	CLA	C1B-C2B	2.38	1.48	1.43
14	j	1302	CLA	C1B-C2B	2.38	1.48	1.43
14	A	1133	CLA	C4B-NB	2.38	1.40	1.37
14	G	1112	CLA	CMC-C2C	-2.37	1.45	1.50
14	6	517	CLA	MG-NB	-2.37	2.01	2.05
14	H	1224	CLA	MG-NB	-2.37	2.01	2.05
14	3	509	CLA	C1B-C2B	2.37	1.48	1.43
14	e	1140	CLA	CMD-C2D	-2.37	1.45	1.50
14	H	1225	CLA	CMB-C2B	-2.37	1.45	1.50
14	H	1235	CLA	CMD-C2D	-2.37	1.45	1.50
14	e	1138	CLA	CMD-C2D	-2.37	1.45	1.50
14	2	501	CLA	C1B-C2B	2.37	1.48	1.43
14	A	1237	CLA	MG-ND	-2.37	2.01	2.05
14	A	1138	CLA	CMB-C2B	-2.37	1.45	1.50
14	e	1112	CLA	CMC-C2C	-2.37	1.45	1.50
14	B	1223	CLA	MG-NB	-2.37	2.01	2.05
14	f	1219	CLA	MG-NB	-2.37	2.01	2.05
14	e	1126	CLA	CMC-C2C	-2.37	1.45	1.50
14	H	1232	CLA	C1B-NB	-2.37	1.34	1.37
14	5	512	CLA	C1B-C2B	2.37	1.48	1.43
14	e	1237	CLA	C1B-C2B	2.37	1.48	1.43
14	B	1206	CLA	CMD-C2D	-2.37	1.45	1.50
14	B	1225	CLA	CMB-C2B	-2.37	1.45	1.50
14	2	501	CLA	CMC-C2C	-2.37	1.45	1.50
14	G	1132	CLA	CMC-C2C	-2.37	1.45	1.50
14	e	1110	CLA	CMB-C2B	-2.37	1.45	1.50
14	f	1221	CLA	CMB-C2B	-2.37	1.45	1.50
14	f	1235	CLA	CMD-C2D	-2.37	1.45	1.50
14	H	1221	CLA	CMB-C2B	-2.37	1.45	1.50
14	B	1207	CLA	MG-NB	-2.37	2.01	2.05
14	u	511	CLA	MG-NB	-2.37	2.01	2.05
14	Y	512	CLA	C1B-C2B	2.37	1.48	1.43
14	e	1118	CLA	C1B-C2B	2.37	1.48	1.43
15	B	2002	PQN	C11-C12	2.37	1.54	1.50
14	r	509	CLA	MG-NB	-2.37	2.01	2.05
14	e	1122	CLA	C3B-C4B	2.37	1.48	1.42
14	B	1219	CLA	MG-NB	-2.37	2.01	2.05
14	B	1231	CLA	MG-NB	-2.37	2.01	2.05
21	B	1852	SQD	O4-C4	-2.37	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1112	CLA	CMC-C2C	-2.37	1.45	1.50
14	H	1023	CLA	C3B-C4B	2.37	1.48	1.42
14	B	1224	CLA	MG-NB	-2.37	2.01	2.05
14	c	508	CLA	MG-NB	-2.37	2.01	2.05
14	J	1302	CLA	C1B-C2B	2.37	1.48	1.43
14	Y	508	CLA	C1B-NB	-2.37	1.34	1.37
14	2	508	CLA	MG-NB	-2.37	2.01	2.05
14	H	1206	CLA	CMD-C2D	-2.37	1.45	1.50
14	Y	509	CLA	C1B-C2B	2.37	1.48	1.43
14	e	1122	CLA	C1B-C2B	2.37	1.48	1.43
14	Z	501	CLA	CMC-C2C	-2.37	1.45	1.50
14	q	516	CLA	CMD-C2D	-2.37	1.45	1.50
14	B	1221	CLA	MG-ND	-2.37	2.01	2.05
14	G	1109	CLA	C3B-C4B	2.36	1.48	1.42
14	G	1134	CLA	CMB-C2B	-2.36	1.45	1.50
14	H	1201	CLA	CMD-C2D	-2.36	1.45	1.50
14	A	1122	CLA	C1B-C2B	2.36	1.48	1.43
14	K	1401	CLA	MG-NB	-2.36	2.01	2.05
14	r	501	CLA	CMC-C2C	-2.36	1.45	1.50
14	f	1207	CLA	MG-NB	-2.36	2.01	2.05
14	u	502	CLA	CMB-C2B	-2.36	1.45	1.50
14	G	1013	CLA	C4B-NB	2.36	1.40	1.37
14	H	1021	CLA	C3B-C4B	2.36	1.48	1.42
14	A	1134	CLA	CMB-C2B	-2.36	1.45	1.50
14	1	516	CLA	CMD-C2D	-2.36	1.45	1.50
14	e	1109	CLA	C3B-C4B	2.36	1.48	1.42
14	A	1106	CLA	CMB-C2B	-2.36	1.45	1.50
14	G	1122	CLA	C1B-C2B	2.36	1.48	1.43
14	R	1302	CLA	C1B-C2B	2.36	1.48	1.43
14	u	510	CLA	MG-NB	-2.36	2.01	2.05
14	V	1503	CLA	C3B-C4B	2.36	1.48	1.42
14	2	502	CLA	MG-NB	-2.36	2.01	2.05
14	H	1226	CLA	CMC-C2C	-2.36	1.45	1.50
14	G	1011	CLA	C4B-NB	2.36	1.40	1.37
14	G	1111	CLA	CMD-C2D	-2.36	1.45	1.50
14	e	1134	CLA	CMB-C2B	-2.36	1.45	1.50
14	2	509	CLA	MG-NB	-2.36	2.01	2.05
14	G	1110	CLA	CMB-C2B	-2.36	1.45	1.50
14	e	1140	CLA	CMB-C2B	-2.36	1.45	1.50
14	B	1205	CLA	MG-NB	-2.36	2.01	2.05
14	c	512	CLA	C1B-C2B	2.36	1.48	1.43
14	G	1122	CLA	C3B-C4B	2.36	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1236	CLA	MG-NB	-2.36	2.01	2.05
14	5	510	CLA	MG-NB	-2.36	2.01	2.05
14	A	1237	CLA	C1B-C2B	2.36	1.48	1.43
14	A	1132	CLA	C3B-C4B	2.36	1.48	1.42
14	A	1126	CLA	CMC-C2C	-2.36	1.45	1.50
14	H	1221	CLA	MG-ND	-2.36	2.01	2.05
14	T	1302	CLA	C1B-C2B	2.36	1.48	1.43
14	u	508	CLA	MG-NB	-2.36	2.01	2.05
14	d	512	CLA	C1B-C2B	2.36	1.48	1.43
14	G	1126	CLA	CMC-C2C	-2.36	1.45	1.50
14	Y	516	CLA	CMD-C2D	-2.36	1.45	1.50
14	H	1214	CLA	MG-NB	-2.36	2.01	2.05
14	L	1503	CLA	C3B-C4B	2.36	1.48	1.42
14	A	1136	CLA	C1B-NB	-2.36	1.34	1.37
14	A	1140	CLA	CMD-C2D	-2.36	1.45	1.50
14	G	1140	CLA	CMB-C2B	-2.36	1.45	1.50
14	f	1238	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	1108	CLA	C1B-C2B	2.35	1.48	1.43
14	Z	508	CLA	MG-NB	-2.35	2.01	2.05
14	4	505	CLA	MG-NB	-2.35	2.01	2.05
14	r	510	CLA	MG-NB	-2.35	2.01	2.05
15	G	2001	PQN	C5-C4	-2.35	1.43	1.48
14	5	508	CLA	MG-NB	-2.35	2.01	2.05
14	2	509	CLA	C1B-C2B	2.35	1.48	1.43
14	A	1110	CLA	CMB-C2B	-2.35	1.45	1.50
14	A	1122	CLA	CMB-C2B	-2.35	1.45	1.50
14	e	1139	CLA	CMB-C2B	-2.35	1.45	1.50
14	Z	506	CLA	MG-NB	-2.35	2.01	2.05
14	H	1202	CLA	CMD-C2D	-2.35	1.45	1.50
14	f	1201	CLA	CMD-C2D	-2.35	1.45	1.50
14	H	1239	CLA	MG-NB	-2.35	2.01	2.05
14	H	1236	CLA	CMB-C2B	-2.35	1.45	1.50
14	Z	509	CLA	C1B-C2B	2.35	1.48	1.43
14	n	1503	CLA	C3B-C4B	2.35	1.48	1.42
14	f	1202	CLA	CMD-C2D	-2.35	1.45	1.50
14	f	1205	CLA	MG-NB	-2.35	2.01	2.05
14	5	502	CLA	CMB-C2B	-2.35	1.45	1.50
14	A	1139	CLA	CMB-C2B	-2.35	1.45	1.50
14	v	505	CLA	CMD-C2D	-2.35	1.45	1.50
14	B	1214	CLA	MG-NB	-2.35	2.01	2.05
14	G	1237	CLA	MG-ND	-2.35	2.01	2.05
14	A	1122	CLA	C3B-C4B	2.35	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	2002	PQN	C11-C3	2.35	1.55	1.51
14	F	1302	CLA	MG-NB	-2.35	2.01	2.05
14	G	1108	CLA	CMB-C2B	-2.35	1.45	1.50
14	G	1139	CLA	CMB-C2B	-2.35	1.45	1.50
14	H	1236	CLA	MG-NB	-2.35	2.01	2.05
14	e	1108	CLA	CMB-C2B	-2.35	1.45	1.50
14	A	1111	CLA	CMD-C2D	-2.35	1.45	1.50
14	6	502	CLA	MG-NB	-2.35	2.01	2.05
14	H	1208	CLA	MG-NB	-2.35	2.01	2.05
14	H	1208	CLA	C1B-C2B	2.35	1.48	1.43
14	B	1238	CLA	C1B-NB	-2.35	1.34	1.37
14	q	508	CLA	C1B-NB	-2.35	1.34	1.37
14	R	1302	CLA	MG-NB	-2.34	2.01	2.05
14	A	1140	CLA	CMB-C2B	-2.34	1.45	1.50
17	G	4003	BCR	C30-C25	-2.34	1.50	1.53
14	B	1239	CLA	MG-NB	-2.34	2.01	2.05
14	Z	509	CLA	MG-NB	-2.34	2.01	2.05
14	A	1132	CLA	CMC-C2C	-2.34	1.45	1.50
14	d	505	CLA	CMD-C2D	-2.34	1.45	1.50
14	e	1111	CLA	CMD-C2D	-2.34	1.45	1.50
14	2	518	CLA	MG-NB	-2.34	2.01	2.05
14	6	505	CLA	CMD-C2D	-2.34	1.45	1.50
14	a	519	CLA	MG-NB	-2.34	2.01	2.05
21	H	1852	SQD	O4-C4	-2.34	1.37	1.43
14	A	1125	CLA	C1B-NB	-2.34	1.34	1.37
14	H	1203	CLA	C4B-NB	2.34	1.40	1.37
14	A	1109	CLA	C3B-C4B	2.34	1.48	1.42
15	e	2001	PQN	C11-C3	2.34	1.55	1.51
14	G	1106	CLA	CMB-C2B	-2.34	1.45	1.50
14	2	510	CLA	MG-NB	-2.34	2.01	2.05
14	a	510	CLA	MG-NB	-2.34	2.01	2.05
14	4	502	CLA	CMB-C2B	-2.34	1.45	1.50
14	j	1302	CLA	MG-NB	-2.34	2.01	2.05
15	f	2002	PQN	C11-C12	2.34	1.54	1.50
14	Z	510	CLA	MG-NB	-2.34	2.01	2.05
14	e	1103	CLA	CMB-C2B	-2.34	1.45	1.50
14	f	1201	CLA	CMC-C2C	-2.34	1.45	1.50
14	u	518	CLA	CMD-C2D	-2.34	1.45	1.50
14	B	1201	CLA	CMC-C2C	-2.34	1.45	1.50
14	B	1226	CLA	CMC-C2C	-2.34	1.45	1.50
14	f	1231	CLA	MG-NB	-2.34	2.01	2.05
14	f	1239	CLA	MG-NB	-2.34	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1105	CLA	C1B-NB	-2.34	1.34	1.37
14	B	1219	CLA	CMB-C2B	-2.34	1.45	1.50
14	G	1132	CLA	C3B-C4B	2.34	1.48	1.42
14	b	512	CLA	MG-NB	-2.34	2.01	2.05
14	2	502	CLA	CMD-C2D	-2.34	1.45	1.50
14	v	502	CLA	CMB-C2B	-2.34	1.45	1.50
14	5	511	CLA	MG-NB	-2.34	2.01	2.05
14	B	1202	CLA	CMD-C2D	-2.34	1.45	1.50
14	H	1205	CLA	MG-NB	-2.34	2.01	2.05
14	e	1130	CLA	MG-ND	-2.34	2.01	2.05
14	A	1108	CLA	CMB-C2B	-2.34	1.45	1.50
14	6	502	CLA	CMB-C2B	-2.34	1.45	1.50
14	A	1117	CLA	CMC-C2C	-2.34	1.45	1.50
14	q	509	CLA	CMB-C2B	-2.34	1.45	1.50
14	B	1208	CLA	MG-NB	-2.34	2.01	2.05
14	c	518	CLA	CMD-C2D	-2.33	1.45	1.50
14	G	1237	CLA	C1B-C2B	2.33	1.48	1.43
14	e	1133	CLA	C4B-NB	2.33	1.40	1.37
14	e	1132	CLA	CMC-C2C	-2.33	1.45	1.50
14	B	1021	CLA	C3B-C4B	2.33	1.48	1.42
14	Z	502	CLA	MG-NB	-2.33	2.01	2.05
14	Z	502	CLA	CMD-C2D	-2.33	1.45	1.50
14	e	1113	CLA	CMD-C2D	-2.33	1.45	1.50
14	U	1103	CLA	MG-NB	-2.33	2.01	2.05
14	f	1208	CLA	MG-NB	-2.33	2.01	2.05
14	r	506	CLA	MG-NB	-2.33	2.01	2.05
14	A	1105	CLA	C1B-NB	-2.33	1.34	1.37
14	B	1211	CLA	C4B-NB	2.33	1.40	1.37
14	G	1136	CLA	C1B-NB	-2.33	1.34	1.37
14	b	511	CLA	C1B-C2B	2.33	1.48	1.43
14	H	1238	CLA	CMB-C2B	-2.33	1.45	1.50
14	H	1201	CLA	CMC-C2C	-2.33	1.45	1.50
14	e	1122	CLA	CMB-C2B	-2.33	1.45	1.50
14	2	506	CLA	MG-NB	-2.33	2.01	2.05
14	H	1213	CLA	MG-NB	-2.33	2.01	2.05
14	A	1138	CLA	CMD-C2D	-2.33	1.45	1.50
14	G	1113	CLA	CMD-C2D	-2.33	1.45	1.50
14	d	502	CLA	CMB-C2B	-2.33	1.45	1.50
14	e	1128	CLA	CMC-C2C	-2.33	1.45	1.50
14	f	1206	CLA	CMD-C2D	-2.33	1.45	1.50
14	t	511	CLA	C1B-C2B	2.33	1.48	1.43
14	e	1132	CLA	C3B-C4B	2.33	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1113	CLA	CMD-C2D	-2.33	1.45	1.50
14	f	1214	CLA	MG-NB	-2.33	2.01	2.05
14	f	1238	CLA	C1B-NB	-2.33	1.34	1.37
14	c	502	CLA	CMB-C2B	-2.33	1.45	1.50
14	f	1226	CLA	CMC-C2C	-2.33	1.45	1.50
14	r	518	CLA	MG-NB	-2.33	2.01	2.05
14	f	1206	CLA	CMC-C2C	-2.33	1.45	1.50
14	A	1127	CLA	C4B-NB	2.33	1.40	1.37
14	G	1103	CLA	C1B-NB	-2.33	1.34	1.37
14	G	1138	CLA	CMD-C2D	-2.33	1.45	1.50
14	K	1103	CLA	MG-NB	-2.33	2.01	2.05
14	t	518	CLA	MG-NB	-2.33	2.01	2.05
14	A	1103	CLA	CMB-C2B	-2.33	1.45	1.50
14	B	1238	CLA	CMB-C2B	-2.33	1.45	1.50
14	f	1216	CLA	CMC-C2C	-2.33	1.45	1.50
14	e	1127	CLA	C4B-NB	2.33	1.40	1.37
14	s	502	CLA	CMD-C2D	-2.33	1.45	1.50
14	c	511	CLA	MG-NB	-2.33	2.01	2.05
14	B	1234	CLA	CMC-C2C	-2.33	1.45	1.50
14	H	1234	CLA	CMC-C2C	-2.33	1.45	1.50
14	b	502	CLA	CMB-C2B	-2.33	1.45	1.50
14	f	1224	CLA	MG-NB	-2.33	2.01	2.05
14	4	511	CLA	C1B-C2B	2.33	1.48	1.43
14	e	1011	CLA	C1B-C2B	2.32	1.48	1.43
14	a	509	CLA	MG-NB	-2.32	2.01	2.05
14	e	1108	CLA	C1B-C2B	2.32	1.48	1.43
14	Z	519	CLA	MG-NB	-2.32	2.01	2.05
14	4	512	CLA	MG-NB	-2.32	2.01	2.05
14	G	1103	CLA	CMB-C2B	-2.32	1.45	1.50
17	B	4017	BCR	C10-C9	-2.32	1.32	1.35
14	b	505	CLA	MG-NB	-2.32	2.01	2.05
14	B	1232	CLA	C1B-NB	-2.32	1.34	1.37
14	A	1120	CLA	C1B-C2B	2.32	1.48	1.43
14	4	511	CLA	CMD-C2D	-2.32	1.45	1.50
14	G	1105	CLA	C1B-NB	-2.32	1.34	1.37
14	q	511	CLA	CMB-C2B	-2.32	1.45	1.50
14	f	1208	CLA	C1B-C2B	2.32	1.48	1.43
15	H	2002	PQN	C11-C3	2.32	1.55	1.51
14	f	1211	CLA	C4B-NB	2.32	1.40	1.37
20	l	5104	LMG	O7-C8	-2.32	1.40	1.46
17	f	4017	BCR	C10-C9	-2.32	1.32	1.35
14	G	1109	CLA	CMB-C2B	-2.32	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1117	CLA	CMC-C2C	-2.32	1.45	1.50
14	s	513	CLA	MG-NB	-2.32	2.01	2.05
14	t	512	CLA	MG-NB	-2.32	2.01	2.05
14	B	1208	CLA	C1B-C2B	2.32	1.48	1.43
14	5	518	CLA	CMD-C2D	-2.32	1.45	1.50
14	A	1105	CLA	C4B-NB	2.32	1.40	1.37
14	G	1127	CLA	C4B-NB	2.32	1.40	1.37
14	v	518	CLA	MG-NB	-2.32	2.01	2.05
14	6	518	CLA	MG-NB	-2.32	2.01	2.05
14	u	519	CLA	MG-NB	-2.32	2.01	2.05
20	T	5104	LMG	O7-C8	-2.32	1.40	1.46
14	B	1201	CLA	CMD-C2D	-2.32	1.45	1.50
14	Y	503	CLA	CMD-C2D	-2.32	1.45	1.50
14	e	1106	CLA	CMB-C2B	-2.32	1.45	1.50
14	m	1401	CLA	C1B-C2B	2.32	1.48	1.43
20	J	5104	LMG	O7-C8	-2.32	1.40	1.46
14	A	1140	CLA	MG-NB	-2.32	2.01	2.05
14	A	1130	CLA	MG-ND	-2.32	2.01	2.05
14	e	1109	CLA	CMB-C2B	-2.32	1.45	1.50
15	A	2001	PQN	C11-C3	2.32	1.55	1.51
14	f	1236	CLA	MG-NB	-2.32	2.01	2.05
14	e	1126	CLA	C1B-NB	-2.32	1.34	1.37
14	G	1110	CLA	CMD-C2D	-2.32	1.45	1.50
14	A	1109	CLA	C1B-C2B	2.32	1.48	1.43
14	G	1109	CLA	C1B-C2B	2.32	1.48	1.43
15	B	2002	PQN	C11-C3	2.32	1.55	1.51
14	H	1209	CLA	CMB-C2B	-2.32	1.45	1.50
14	G	1120	CLA	C1B-C2B	2.32	1.48	1.43
14	B	1236	CLA	CMB-C2B	-2.32	1.45	1.50
14	f	1216	CLA	CMD-C2D	-2.32	1.45	1.50
14	G	1126	CLA	C1B-NB	-2.31	1.34	1.37
14	b	511	CLA	MG-NB	-2.31	2.01	2.05
14	r	502	CLA	MG-NB	-2.31	2.01	2.05
14	3	502	CLA	CMD-C2D	-2.31	1.45	1.50
14	3	519	CLA	MG-NB	-2.31	2.01	2.05
14	G	1140	CLA	MG-NB	-2.31	2.01	2.05
14	A	1126	CLA	C1B-NB	-2.31	1.34	1.37
14	H	1215	CLA	CMD-C2D	-2.31	1.45	1.50
14	b	511	CLA	CMD-C2D	-2.31	1.45	1.50
14	f	1213	CLA	CMD-C2D	-2.31	1.45	1.50
14	f	1215	CLA	CMD-C2D	-2.31	1.45	1.50
14	A	1127	CLA	CMB-C2B	-2.31	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	s	506	CLA	CMC-C2C	-2.31	1.45	1.50
14	B	1213	CLA	MG-NB	-2.31	2.01	2.05
14	A	1103	CLA	C1B-NB	-2.31	1.34	1.37
14	B	1209	CLA	CMB-C2B	-2.31	1.45	1.50
14	t	502	CLA	CMB-C2B	-2.31	1.45	1.50
14	B	1021	CLA	MG-ND	-2.31	2.01	2.05
14	e	1114	CLA	MG-NB	-2.31	2.01	2.05
14	j	1302	CLA	CMB-C2B	-2.31	1.45	1.50
14	H	1207	CLA	MG-NB	-2.31	2.01	2.05
14	Z	518	CLA	MG-NB	-2.31	2.01	2.05
14	s	510	CLA	MG-NB	-2.31	2.01	2.05
14	H	1216	CLA	CMC-C2C	-2.31	1.45	1.50
14	F	1302	CLA	CMB-C2B	-2.31	1.45	1.50
14	G	1127	CLA	CMB-C2B	-2.31	1.45	1.50
14	u	502	CLA	CMD-C2D	-2.31	1.45	1.50
15	G	2001	PQN	C11-C3	2.31	1.55	1.51
14	A	1114	CLA	MG-NB	-2.31	2.01	2.05
14	5	519	CLA	MG-NB	-2.31	2.01	2.05
14	f	1213	CLA	MG-NB	-2.31	2.01	2.05
14	q	509	CLA	MG-NB	-2.31	2.01	2.05
14	B	1216	CLA	CMC-C2C	-2.31	1.45	1.50
14	e	1133	CLA	C3B-C4B	2.31	1.48	1.42
17	H	4017	BCR	C10-C9	-2.31	1.32	1.35
14	6	519	CLA	MG-NB	-2.31	2.01	2.05
14	G	1133	CLA	MG-ND	-2.31	2.01	2.05
14	f	1021	CLA	MG-ND	-2.31	2.01	2.05
14	e	1120	CLA	C1B-C2B	2.31	1.48	1.43
14	A	1011	CLA	C1B-C2B	2.31	1.48	1.43
14	A	1135	CLA	C1D-ND	2.31	1.40	1.37
14	A	1128	CLA	CMC-C2C	-2.31	1.45	1.50
17	A	4003	BCR	C30-C25	-2.31	1.50	1.53
14	Z	516	CLA	MG-NB	-2.31	2.01	2.05
14	Y	511	CLA	CMB-C2B	-2.31	1.45	1.50
14	3	510	CLA	MG-NB	-2.31	2.01	2.05
14	Y	513	CLA	MG-NB	-2.31	2.01	2.05
14	H	1202	CLA	C1B-C2B	2.31	1.48	1.43
14	A	1109	CLA	CMB-C2B	-2.31	1.45	1.50
14	b	518	CLA	MG-NB	-2.31	2.01	2.05
14	H	1023	CLA	MG-ND	-2.31	2.01	2.05
14	Z	513	CLA	MG-NB	-2.31	2.01	2.05
14	e	1140	CLA	MG-NB	-2.31	2.01	2.05
14	2	507	CLA	MG-NB	-2.31	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1232	CLA	CMB-C2B	-2.31	1.45	1.50
14	1	503	CLA	MG-NB	-2.31	2.01	2.05
14	d	519	CLA	MG-NB	-2.31	2.01	2.05
14	A	1118	CLA	C3B-C4B	2.31	1.48	1.42
14	K	1401	CLA	C1B-C2B	2.31	1.48	1.43
14	H	1216	CLA	CMD-C2D	-2.30	1.45	1.50
14	B	1203	CLA	C4B-NB	2.30	1.40	1.37
14	G	1120	CLA	CMC-C2C	-2.30	1.45	1.50
14	f	1219	CLA	CMB-C2B	-2.30	1.45	1.50
14	2	513	CLA	MG-NB	-2.30	2.01	2.05
14	s	519	CLA	MG-NB	-2.30	2.01	2.05
14	B	1206	CLA	CMC-C2C	-2.30	1.45	1.50
14	f	1234	CLA	CMC-C2C	-2.30	1.45	1.50
14	H	1215	CLA	C1B-NB	-2.30	1.35	1.37
14	e	1109	CLA	C1B-C2B	2.30	1.48	1.43
14	e	1137	CLA	CMB-C2B	-2.30	1.45	1.50
14	A	1120	CLA	CMC-C2C	-2.30	1.45	1.50
14	R	1302	CLA	CMB-C2B	-2.30	1.45	1.50
14	G	1123	CLA	MG-ND	-2.30	2.01	2.05
14	U	1401	CLA	C1B-C2B	2.30	1.48	1.43
14	1	511	CLA	CMB-C2B	-2.30	1.45	1.50
14	e	1108	CLA	CMD-C2D	-2.30	1.45	1.50
14	f	1202	CLA	C1B-C2B	2.30	1.48	1.43
14	m	1103	CLA	MG-NB	-2.30	2.01	2.05
14	H	1219	CLA	CMB-C2B	-2.30	1.45	1.50
14	Z	517	CLA	CMC-C2C	-2.30	1.45	1.50
14	G	1105	CLA	CMD-C2D	-2.30	1.45	1.50
14	e	1117	CLA	CMC-C2C	-2.30	1.45	1.50
14	B	1216	CLA	CMD-C2D	-2.30	1.45	1.50
14	f	1236	CLA	CMB-C2B	-2.30	1.45	1.50
14	2	519	CLA	MG-NB	-2.30	2.01	2.05
14	r	507	CLA	MG-NB	-2.30	2.01	2.05
14	H	1225	CLA	C4B-NB	2.30	1.40	1.37
14	H	1208	CLA	CMB-C2B	-2.30	1.45	1.50
14	Z	511	CLA	CMB-C2B	-2.30	1.45	1.50
14	t	503	CLA	CMD-C2D	-2.30	1.45	1.50
14	j	1302	CLA	CMD-C2D	-2.30	1.45	1.50
14	4	518	CLA	MG-NB	-2.30	2.01	2.05
14	Y	509	CLA	MG-NB	-2.30	2.01	2.05
14	c	519	CLA	MG-NB	-2.30	2.01	2.05
14	2	516	CLA	MG-NB	-2.30	2.01	2.05
14	3	509	CLA	MG-NB	-2.30	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1118	CLA	C3B-C4B	2.30	1.48	1.42
14	B	1232	CLA	CMB-C2B	-2.30	1.45	1.50
14	e	1137	CLA	CMD-C2D	-2.30	1.45	1.50
14	f	1021	CLA	C3B-C4B	2.30	1.48	1.42
14	t	511	CLA	MG-NB	-2.30	2.01	2.05
14	e	1105	CLA	C4B-NB	2.30	1.40	1.37
14	G	1130	CLA	CMD-C2D	-2.30	1.45	1.50
14	a	502	CLA	CMD-C2D	-2.30	1.45	1.50
14	A	1133	CLA	MG-ND	-2.30	2.01	2.05
14	t	511	CLA	CMD-C2D	-2.30	1.45	1.50
14	B	1202	CLA	C1B-C2B	2.30	1.48	1.43
14	G	1022	CLA	CMC-C2C	-2.30	1.45	1.50
14	r	502	CLA	CMD-C2D	-2.30	1.45	1.50
14	G	1135	CLA	C1D-ND	2.29	1.40	1.37
14	G	1114	CLA	MG-NB	-2.29	2.01	2.05
14	e	1110	CLA	MG-NB	-2.29	2.01	2.05
14	r	519	CLA	MG-NB	-2.29	2.01	2.05
14	B	1220	CLA	CMD-C2D	-2.29	1.45	1.50
14	G	1133	CLA	C3B-C4B	2.29	1.48	1.42
14	B	1023	CLA	MG-ND	-2.29	2.01	2.05
14	f	1023	CLA	MG-ND	-2.29	2.01	2.05
14	B	1213	CLA	CMD-C2D	-2.29	1.45	1.50
14	Z	503	CLA	MG-NB	-2.29	2.01	2.05
14	v	519	CLA	MG-NB	-2.29	2.01	2.05
14	A	1108	CLA	CMD-C2D	-2.29	1.45	1.50
14	n	1503	CLA	MG-NB	-2.29	2.01	2.05
14	Z	512	CLA	CMD-C2D	-2.29	1.45	1.50
14	e	1112	CLA	CMD-C2D	-2.29	1.45	1.50
14	1	509	CLA	MG-NB	-2.29	2.01	2.05
14	e	1110	CLA	C1B-C2B	2.29	1.48	1.43
14	d	502	CLA	CMD-C2D	-2.29	1.45	1.50
14	e	1117	CLA	CMD-C2D	-2.29	1.45	1.50
14	f	1203	CLA	C4B-NB	2.29	1.40	1.37
14	A	1125	CLA	CMD-C2D	-2.29	1.45	1.50
14	A	1136	CLA	CMC-C2C	-2.29	1.45	1.50
14	1	502	CLA	CMB-C2B	-2.29	1.45	1.50
14	e	1135	CLA	C1D-ND	2.29	1.40	1.37
14	2	511	CLA	CMB-C2B	-2.29	1.45	1.50
14	H	1213	CLA	CMD-C2D	-2.29	1.45	1.50
14	f	1012	CLA	CMD-C2D	-2.29	1.45	1.50
14	Z	507	CLA	MG-NB	-2.29	2.01	2.05
14	3	506	CLA	CMC-C2C	-2.29	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	502	CLA	MG-NB	-2.29	2.01	2.05
14	G	1118	CLA	C3B-C4B	2.29	1.48	1.42
14	A	1130	CLA	CMD-C2D	-2.29	1.45	1.50
14	G	1125	CLA	CMD-C2D	-2.29	1.45	1.50
14	Y	503	CLA	MG-NB	-2.29	2.01	2.05
14	f	1209	CLA	CMB-C2B	-2.29	1.45	1.50
14	f	1218	CLA	MG-NB	-2.29	2.01	2.05
14	r	513	CLA	MG-NB	-2.29	2.01	2.05
14	B	1215	CLA	C1B-NB	-2.29	1.35	1.37
14	1	509	CLA	CMB-C2B	-2.29	1.45	1.50
14	4	503	CLA	CMD-C2D	-2.29	1.45	1.50
14	6	502	CLA	CMD-C2D	-2.29	1.45	1.50
14	H	1220	CLA	CMD-C2D	-2.29	1.45	1.50
14	Y	509	CLA	CMB-C2B	-2.29	1.45	1.50
14	e	1127	CLA	CMB-C2B	-2.29	1.45	1.50
14	r	511	CLA	CMB-C2B	-2.29	1.45	1.50
14	G	1011	CLA	C1B-C2B	2.29	1.48	1.43
14	3	513	CLA	MG-NB	-2.29	2.01	2.05
14	6	501	CLA	MG-NB	-2.29	2.01	2.05
14	H	1211	CLA	MG-NB	-2.29	2.01	2.05
14	Y	504	CLA	MG-NB	-2.29	2.01	2.05
14	B	1215	CLA	CMD-C2D	-2.29	1.46	1.50
14	e	1011	CLA	C4B-NB	2.29	1.40	1.37
14	H	1218	CLA	MG-NB	-2.29	2.01	2.05
14	d	518	CLA	MG-NB	-2.29	2.01	2.05
14	j	1301	CLA	CMB-C2B	-2.29	1.46	1.50
14	e	1103	CLA	C1B-NB	-2.29	1.35	1.37
14	B	1222	CLA	CHC-C1C	2.29	1.43	1.38
14	A	1133	CLA	C3B-C4B	2.29	1.48	1.42
17	V	4219	BCR	C17-C18	-2.29	1.32	1.35
14	q	503	CLA	MG-NB	-2.29	2.01	2.05
14	r	508	CLA	CMC-C2C	-2.29	1.46	1.50
14	G	1129	CLA	C1B-NB	-2.29	1.35	1.37
14	f	1225	CLA	C4B-NB	2.29	1.40	1.37
14	e	1133	CLA	MG-ND	-2.29	2.01	2.05
14	2	512	CLA	CMD-C2D	-2.29	1.46	1.50
14	q	502	CLA	CMD-C2D	-2.29	1.46	1.50
14	Z	506	CLA	CMC-C2C	-2.29	1.46	1.50
14	e	1120	CLA	CMC-C2C	-2.29	1.46	1.50
14	e	1022	CLA	CMC-C2C	-2.29	1.46	1.50
14	r	517	CLA	CMC-C2C	-2.29	1.46	1.50
14	B	1207	CLA	C1B-C2B	2.28	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	501	CLA	MG-NB	-2.28	2.01	2.05
14	v	501	CLA	MG-NB	-2.28	2.01	2.05
14	q	502	CLA	CMB-C2B	-2.28	1.46	1.50
14	r	517	CLA	MG-NB	-2.28	2.01	2.05
14	H	1207	CLA	C1B-C2B	2.28	1.48	1.43
14	a	512	CLA	C1B-C2B	2.28	1.48	1.43
14	H	1222	CLA	CHC-C1C	2.28	1.43	1.38
14	A	1110	CLA	CMD-C2D	-2.28	1.46	1.50
14	G	1128	CLA	CMC-C2C	-2.28	1.46	1.50
14	G	1101	CLA	CMB-C2B	-2.28	1.46	1.50
14	G	1110	CLA	MG-NB	-2.28	2.01	2.05
14	a	517	CLA	MG-NB	-2.28	2.01	2.05
14	s	512	CLA	C1B-C2B	2.28	1.48	1.43
14	f	1220	CLA	CMD-C2D	-2.28	1.46	1.50
14	s	502	CLA	CMB-C2B	-2.28	1.46	1.50
14	s	509	CLA	MG-NB	-2.28	2.01	2.05
14	v	516	CLA	MG-NB	-2.28	2.01	2.05
14	G	1108	CLA	CMD-C2D	-2.28	1.46	1.50
14	e	1105	CLA	CMD-C2D	-2.28	1.46	1.50
14	1	502	CLA	CMD-C2D	-2.28	1.46	1.50
14	Y	502	CLA	CMD-C2D	-2.28	1.46	1.50
14	t	518	CLA	CMD-C2D	-2.28	1.46	1.50
14	H	1021	CLA	MG-ND	-2.28	2.01	2.05
14	f	1222	CLA	CHC-C1C	2.28	1.43	1.38
14	V	1502	CLA	CMC-C2C	-2.28	1.46	1.50
14	A	1105	CLA	CMD-C2D	-2.28	1.46	1.50
14	H	1206	CLA	CMC-C2C	-2.28	1.46	1.50
14	Y	502	CLA	CMB-C2B	-2.28	1.46	1.50
14	B	1225	CLA	C4B-NB	2.28	1.40	1.37
14	e	1136	CLA	C1B-NB	-2.28	1.35	1.37
14	b	503	CLA	CMD-C2D	-2.28	1.46	1.50
14	G	1105	CLA	C4B-NB	2.28	1.40	1.37
14	4	511	CLA	MG-NB	-2.28	2.01	2.05
21	n	5216	SQD	O2-C2	-2.28	1.37	1.43
14	L	1503	CLA	MG-NB	-2.28	2.01	2.05
14	q	519	CLA	MG-NB	-2.28	2.01	2.05
14	s	517	CLA	MG-NB	-2.28	2.01	2.05
22	X	170	FMN	C10-N1	2.28	1.37	1.33
14	2	517	CLA	CMC-C2C	-2.28	1.46	1.50
14	A	1110	CLA	MG-NB	-2.28	2.01	2.05
14	B	1240	CLA	MG-NB	-2.28	2.01	2.05
14	2	503	CLA	MG-NB	-2.28	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	m	1105	CLA	MG-NB	-2.28	2.01	2.05
14	A	1133	CLA	CMD-C2D	-2.28	1.46	1.50
14	U	1105	CLA	CMD-C2D	-2.28	1.46	1.50
14	r	512	CLA	CMD-C2D	-2.28	1.46	1.50
14	G	1103	CLA	MG-NB	-2.28	2.01	2.05
14	Y	518	CLA	MG-NB	-2.28	2.01	2.05
14	A	1022	CLA	CMC-C2C	-2.28	1.46	1.50
14	A	1112	CLA	CMD-C2D	-2.28	1.46	1.50
14	G	1110	CLA	CMC-C2C	-2.28	1.46	1.50
14	f	1208	CLA	CMB-C2B	-2.28	1.46	1.50
14	r	516	CLA	MG-NB	-2.28	2.01	2.05
14	s	502	CLA	MG-NB	-2.28	2.01	2.05
14	1	513	CLA	MG-NB	-2.28	2.01	2.05
14	3	517	CLA	MG-NB	-2.28	2.01	2.05
14	n	1502	CLA	CMC-C2C	-2.27	1.46	1.50
14	G	1110	CLA	C1B-C2B	2.27	1.48	1.43
14	A	1137	CLA	CMD-C2D	-2.27	1.46	1.50
14	5	502	CLA	CMD-C2D	-2.27	1.46	1.50
14	G	1136	CLA	CMC-C2C	-2.27	1.46	1.50
14	q	503	CLA	CMD-C2D	-2.27	1.46	1.50
14	f	1012	CLA	CMC-C2C	-2.27	1.46	1.50
14	A	1110	CLA	C1B-C2B	2.27	1.48	1.43
14	A	1115	CLA	CMD-C2D	-2.27	1.46	1.50
14	e	1115	CLA	CMD-C2D	-2.27	1.46	1.50
14	5	505	CLA	MG-NB	-2.27	2.01	2.05
14	3	512	CLA	C1B-C2B	2.27	1.48	1.43
14	G	1130	CLA	MG-ND	-2.27	2.01	2.05
14	f	1220	CLA	MG-NB	-2.27	2.01	2.05
14	e	1104	CLA	CMC-C2C	-2.27	1.46	1.50
14	A	1013	CLA	MG-ND	-2.27	2.01	2.05
14	d	516	CLA	MG-NB	-2.27	2.01	2.05
14	e	1125	CLA	CMD-C2D	-2.27	1.46	1.50
14	n	1503	CLA	CMD-C2D	-2.27	1.46	1.50
14	G	1132	CLA	C1B-C2B	2.27	1.48	1.43
14	B	1218	CLA	MG-NB	-2.27	2.01	2.05
14	1	504	CLA	MG-NB	-2.27	2.01	2.05
14	B	1208	CLA	CMB-C2B	-2.27	1.46	1.50
14	G	1112	CLA	CMD-C2D	-2.27	1.46	1.50
14	G	1137	CLA	CMD-C2D	-2.27	1.46	1.50
14	a	513	CLA	MG-NB	-2.27	2.01	2.05
14	3	509	CLA	CMC-C2C	-2.27	1.46	1.50
14	b	517	CLA	MG-NB	-2.27	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	517	CLA	MG-NB	-2.27	2.01	2.05
14	G	1125	CLA	CMB-C2B	-2.27	1.46	1.50
14	6	516	CLA	MG-NB	-2.27	2.01	2.05
14	B	1235	CLA	C1B-C2B	2.27	1.48	1.43
14	A	1104	CLA	CMC-C2C	-2.27	1.46	1.50
14	1	503	CLA	CMD-C2D	-2.27	1.46	1.50
14	f	1232	CLA	CMB-C2B	-2.27	1.46	1.50
14	q	506	CLA	MG-NB	-2.27	2.01	2.05
22	P	170	FMN	C10-N1	2.27	1.37	1.33
14	B	1222	CLA	CMC-C2C	-2.27	1.46	1.50
14	G	1129	CLA	CMC-C2C	-2.27	1.46	1.50
14	B	1211	CLA	MG-NB	-2.27	2.01	2.05
14	c	513	CLA	MG-NB	-2.27	2.01	2.05
14	u	518	CLA	MG-NB	-2.27	2.01	2.05
22	p	170	FMN	C10-N1	2.27	1.37	1.33
14	A	1110	CLA	CMC-C2C	-2.27	1.46	1.50
14	e	1125	CLA	CMB-C2B	-2.27	1.46	1.50
14	A	1123	CLA	MG-ND	-2.27	2.01	2.05
14	q	504	CLA	MG-NB	-2.27	2.01	2.05
14	q	513	CLA	MG-NB	-2.27	2.01	2.05
14	H	1223	CLA	C1B-C2B	2.27	1.48	1.43
17	e	4003	BCR	C30-C25	-2.27	1.50	1.53
14	u	507	CLA	MG-NB	-2.27	2.01	2.05
14	f	1209	CLA	CMD-C2D	-2.27	1.46	1.50
14	B	1012	CLA	CMD-C2D	-2.27	1.46	1.50
14	f	1210	CLA	CMB-C2B	-2.27	1.46	1.50
14	f	1235	CLA	C1B-C2B	2.27	1.48	1.43
14	t	507	CLA	MG-NB	-2.27	2.01	2.05
17	H	4017	BCR	C21-C22	-2.27	1.32	1.35
14	A	1137	CLA	CMB-C2B	-2.27	1.46	1.50
14	e	1136	CLA	CMC-C2C	-2.27	1.46	1.50
14	Z	517	CLA	MG-NB	-2.27	2.01	2.05
14	A	1801	CLA	CMC-C2C	-2.27	1.46	1.50
14	e	1110	CLA	CMC-C2C	-2.27	1.46	1.50
14	H	1222	CLA	CMC-C2C	-2.26	1.46	1.50
14	a	506	CLA	CMC-C2C	-2.26	1.46	1.50
14	H	1240	CLA	MG-NB	-2.26	2.01	2.05
14	G	1104	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	502	CLA	MG-NB	-2.26	2.01	2.05
14	f	1240	CLA	MG-NB	-2.26	2.01	2.05
14	K	1105	CLA	CMD-C2D	-2.26	1.46	1.50
14	d	518	CLA	CMD-C2D	-2.26	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	q	512	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	1104	CLA	CMD-C2D	-2.26	1.46	1.50
14	Z	508	CLA	CMC-C2C	-2.26	1.46	1.50
14	q	505	CLA	CMD-C2D	-2.26	1.46	1.50
14	H	1210	CLA	CMB-C2B	-2.26	1.46	1.50
14	e	1801	CLA	CMC-C2C	-2.26	1.46	1.50
21	V	5216	SQD	O2-C2	-2.26	1.37	1.43
14	F	1302	CLA	CMD-C2D	-2.26	1.46	1.50
14	1	518	CLA	MG-NB	-2.26	2.01	2.05
14	5	518	CLA	MG-NB	-2.26	2.01	2.05
14	B	1210	CLA	CMB-C2B	-2.26	1.46	1.50
14	L	1502	CLA	CMC-C2C	-2.26	1.46	1.50
14	4	518	CLA	CMD-C2D	-2.26	1.46	1.50
14	G	1013	CLA	MG-ND	-2.26	2.01	2.05
14	V	1503	CLA	MG-NB	-2.26	2.01	2.05
14	f	1207	CLA	C1B-C2B	2.26	1.48	1.43
14	A	1116	CLA	CMC-C2C	-2.26	1.46	1.50
14	q	516	CLA	MG-ND	-2.26	2.01	2.05
14	r	501	CLA	MG-NB	-2.26	2.01	2.05
14	F	1301	CLA	CMB-C2B	-2.26	1.46	1.50
14	e	1130	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	1103	CLA	MG-NB	-2.26	2.01	2.05
14	Y	519	CLA	MG-NB	-2.26	2.01	2.05
14	s	509	CLA	CMC-C2C	-2.26	1.46	1.50
14	6	508	CLA	MG-NB	-2.26	2.01	2.05
14	4	517	CLA	MG-NB	-2.26	2.01	2.05
14	e	1103	CLA	MG-NB	-2.26	2.01	2.05
14	A	1129	CLA	CMC-C2C	-2.26	1.46	1.50
14	G	1137	CLA	CMB-C2B	-2.26	1.46	1.50
21	L	5216	SQD	O2-C2	-2.26	1.37	1.43
14	f	1223	CLA	C1B-C2B	2.26	1.48	1.43
14	G	1133	CLA	CMD-C2D	-2.26	1.46	1.50
14	2	505	CLA	MG-NB	-2.26	2.01	2.05
14	e	1123	CLA	MG-ND	-2.26	2.01	2.05
14	f	1222	CLA	CMC-C2C	-2.26	1.46	1.50
14	Y	505	CLA	MG-NB	-2.26	2.01	2.05
14	m	1105	CLA	CMD-C2D	-2.26	1.46	1.50
14	G	1103	CLA	MG-ND	-2.26	2.01	2.05
14	c	505	CLA	MG-NB	-2.26	2.01	2.05
14	B	1223	CLA	C1B-C2B	2.26	1.48	1.43
14	Y	512	CLA	CMD-C2D	-2.26	1.46	1.50
14	e	1116	CLA	CMC-C2C	-2.26	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1101	CLA	CMB-C2B	-2.26	1.46	1.50
20	H	5002	LMG	O7-C8	-2.26	1.41	1.46
14	G	1116	CLA	C1B-C2B	2.26	1.48	1.43
14	q	518	CLA	MG-NB	-2.26	2.01	2.05
14	A	1118	CLA	MG-ND	-2.26	2.01	2.05
14	Y	511	CLA	CMD-C2D	-2.26	1.46	1.50
14	b	518	CLA	CMD-C2D	-2.26	1.46	1.50
14	f	1227	CLA	CMD-C2D	-2.26	1.46	1.50
14	G	1115	CLA	CMD-C2D	-2.26	1.46	1.50
14	e	1135	CLA	CMB-C2B	-2.25	1.46	1.50
14	v	502	CLA	CMD-C2D	-2.25	1.46	1.50
17	n	4219	BCR	C17-C18	-2.25	1.32	1.35
14	u	506	CLA	MG-NB	-2.25	2.01	2.05
20	B	5002	LMG	O7-C8	-2.25	1.41	1.46
14	a	504	CLA	MG-NB	-2.25	2.01	2.05
14	e	1118	CLA	MG-ND	-2.25	2.01	2.05
14	R	1302	CLA	CMD-C2D	-2.25	1.46	1.50
14	e	1133	CLA	CMD-C2D	-2.25	1.46	1.50
14	G	1801	CLA	C1B-C2B	2.25	1.48	1.43
20	f	5002	LMG	O7-C8	-2.25	1.41	1.46
14	e	1116	CLA	C1B-C2B	2.25	1.48	1.43
14	2	508	CLA	CMC-C2C	-2.25	1.46	1.50
14	r	506	CLA	CMB-C2B	-2.25	1.46	1.50
14	2	517	CLA	MG-NB	-2.25	2.01	2.05
14	u	513	CLA	MG-NB	-2.25	2.01	2.05
14	a	509	CLA	CMC-C2C	-2.25	1.46	1.50
17	L	4219	BCR	C17-C18	-2.25	1.32	1.35
14	G	1801	CLA	CMC-C2C	-2.25	1.46	1.50
14	H	1012	CLA	CMD-C2D	-2.25	1.46	1.50
14	H	1209	CLA	CMD-C2D	-2.25	1.46	1.50
14	5	508	CLA	CMC-C2C	-2.25	1.46	1.50
14	a	507	CLA	MG-NB	-2.25	2.01	2.05
14	L	1503	CLA	CMD-C2D	-2.25	1.46	1.50
14	R	1301	CLA	CMB-C2B	-2.25	1.46	1.50
14	v	505	CLA	MG-NB	-2.25	2.01	2.05
14	2	506	CLA	CMC-C2C	-2.25	1.46	1.50
14	c	508	CLA	CMC-C2C	-2.25	1.46	1.50
14	A	1132	CLA	C1B-C2B	2.25	1.48	1.43
14	1	512	CLA	CMD-C2D	-2.25	1.46	1.50
14	H	1228	CLA	MG-NB	-2.25	2.01	2.05
14	B	1227	CLA	CMD-C2D	-2.25	1.46	1.50
14	f	1217	CLA	CMD-C2D	-2.25	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1236	CLA	C1B-C2B	2.25	1.48	1.43
14	c	518	CLA	MG-NB	-2.25	2.01	2.05
14	Z	506	CLA	CMB-C2B	-2.25	1.46	1.50
14	d	503	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	1217	CLA	CMD-C2D	-2.25	1.46	1.50
14	4	519	CLA	MG-NB	-2.25	2.01	2.05
14	5	513	CLA	MG-NB	-2.25	2.01	2.05
14	r	505	CLA	MG-NB	-2.25	2.01	2.05
14	v	511	CLA	MG-NB	-2.25	2.01	2.05
14	B	1225	CLA	C1B-NB	-2.25	1.35	1.37
14	s	507	CLA	MG-NB	-2.25	2.01	2.05
14	B	1201	CLA	CHC-C1C	2.25	1.43	1.38
14	A	1138	CLA	CMC-C2C	-2.25	1.46	1.50
14	A	1101	CLA	CMB-C2B	-2.25	1.46	1.50
14	2	503	CLA	CMD-C2D	-2.25	1.46	1.50
14	6	504	CLA	MG-NB	-2.25	2.01	2.05
14	e	1103	CLA	MG-ND	-2.25	2.01	2.05
14	t	510	CLA	MG-NB	-2.25	2.01	2.05
14	H	1236	CLA	C1B-C2B	2.25	1.48	1.43
14	f	1215	CLA	C1B-NB	-2.25	1.35	1.37
14	Z	503	CLA	CMD-C2D	-2.25	1.46	1.50
14	c	502	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	1220	CLA	MG-NB	-2.25	2.01	2.05
14	4	507	CLA	MG-NB	-2.25	2.01	2.05
14	f	1236	CLA	C1B-C2B	2.25	1.48	1.43
14	1	511	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	1117	CLA	CMD-C2D	-2.25	1.46	1.50
14	r	503	CLA	CMD-C2D	-2.25	1.46	1.50
14	K	1401	CLA	CHC-C1C	2.25	1.43	1.38
14	A	1124	CLA	MG-ND	-2.25	2.01	2.05
14	d	508	CLA	MG-NB	-2.24	2.01	2.05
14	f	1211	CLA	MG-NB	-2.24	2.01	2.05
14	n	1501	CLA	CMD-C2D	-2.24	1.46	1.50
14	H	1239	CLA	C3B-C4B	2.24	1.48	1.42
14	V	1503	CLA	CMD-C2D	-2.24	1.46	1.50
14	f	1201	CLA	CHC-C1C	2.24	1.43	1.38
14	1	519	CLA	MG-NB	-2.24	2.01	2.05
14	2	501	CLA	MG-NB	-2.24	2.01	2.05
14	G	1124	CLA	MG-ND	-2.24	2.01	2.05
14	3	502	CLA	CMB-C2B	-2.24	1.46	1.50
14	f	1234	CLA	CHC-C1C	2.24	1.43	1.38
17	B	4017	BCR	C21-C22	-2.24	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	f	4017	BCR	C21-C22	-2.24	1.32	1.35
14	3	504	CLA	MG-NB	-2.24	2.01	2.05
14	Y	516	CLA	MG-ND	-2.24	2.01	2.05
14	u	501	CLA	MG-NB	-2.24	2.01	2.05
14	B	1023	CLA	CMD-C2D	-2.24	1.46	1.50
14	e	1104	CLA	CMD-C2D	-2.24	1.46	1.50
14	H	1235	CLA	C1B-C2B	2.24	1.48	1.43
14	5	506	CLA	MG-NB	-2.24	2.01	2.05
14	Y	507	CLA	MG-NB	-2.24	2.01	2.05
14	Z	505	CLA	MG-NB	-2.24	2.01	2.05
14	G	1116	CLA	CMC-C2C	-2.24	1.46	1.50
14	e	1138	CLA	CMC-C2C	-2.24	1.46	1.50
14	B	1239	CLA	C3B-C4B	2.24	1.48	1.42
14	B	1012	CLA	CMC-C2C	-2.24	1.46	1.50
14	f	1023	CLA	CMD-C2D	-2.24	1.46	1.50
14	A	1125	CLA	CMB-C2B	-2.24	1.46	1.50
14	5	501	CLA	MG-NB	-2.24	2.01	2.05
14	H	1220	CLA	MG-NB	-2.24	2.01	2.05
14	A	1801	CLA	C1B-C2B	2.24	1.48	1.43
14	Z	512	CLA	C1B-C2B	2.24	1.48	1.43
14	u	502	CLA	MG-NB	-2.24	2.01	2.05
14	e	1132	CLA	C1B-C2B	2.24	1.48	1.43
14	G	1114	CLA	CMD-C2D	-2.24	1.46	1.50
14	3	507	CLA	MG-NB	-2.24	2.01	2.05
14	d	505	CLA	MG-NB	-2.24	2.01	2.05
14	f	1239	CLA	C3B-C4B	2.24	1.48	1.42
14	B	1203	CLA	CMD-C2D	-2.24	1.46	1.50
14	V	1502	CLA	CMD-C2D	-2.24	1.46	1.50
14	v	508	CLA	MG-NB	-2.24	2.01	2.05
14	6	518	CLA	CMD-C2D	-2.24	1.46	1.50
14	G	1104	CLA	CMC-C2C	-2.24	1.46	1.50
14	v	517	CLA	CMD-C2D	-2.24	1.46	1.50
14	B	1209	CLA	CMD-C2D	-2.24	1.46	1.50
14	v	504	CLA	MG-NB	-2.24	2.01	2.05
14	v	508	CLA	C1B-C2B	2.24	1.48	1.43
14	A	1129	CLA	C1B-NB	-2.24	1.35	1.37
14	G	1138	CLA	CMC-C2C	-2.24	1.46	1.50
14	H	1217	CLA	CMD-C2D	-2.24	1.46	1.50
14	r	503	CLA	MG-NB	-2.24	2.01	2.05
14	t	513	CLA	MG-NB	-2.24	2.01	2.05
14	6	517	CLA	CMD-C2D	-2.24	1.46	1.50
14	G	1117	CLA	CMD-C2D	-2.24	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	509	CLA	CMD-C2D	-2.24	1.46	1.50
14	u	508	CLA	CMC-C2C	-2.24	1.46	1.50
14	e	1801	CLA	C1B-C2B	2.24	1.48	1.43
14	a	502	CLA	CMB-C2B	-2.24	1.46	1.50
14	A	1103	CLA	MG-ND	-2.24	2.01	2.05
14	1	506	CLA	MG-NB	-2.24	2.01	2.05
14	G	1135	CLA	CMB-C2B	-2.24	1.46	1.50
14	H	1234	CLA	CHC-C1C	2.24	1.43	1.38
14	r	512	CLA	C1B-C2B	2.24	1.48	1.43
14	G	1129	CLA	C4B-NB	2.24	1.40	1.37
14	A	1135	CLA	CMB-C2B	-2.24	1.46	1.50
14	1	505	CLA	MG-NB	-2.23	2.01	2.05
14	1	516	CLA	MG-ND	-2.23	2.01	2.05
14	T	1303	CLA	MG-NB	-2.23	2.01	2.05
14	s	511	CLA	MG-NB	-2.23	2.01	2.05
14	B	1234	CLA	CHC-C1C	2.23	1.43	1.38
14	Y	519	CLA	CHC-C1C	2.23	1.43	1.38
21	H	1852	SQD	O3-C3	-2.23	1.37	1.43
14	b	507	CLA	MG-NB	-2.23	2.01	2.05
14	s	504	CLA	MG-NB	-2.23	2.01	2.05
14	u	505	CLA	MG-NB	-2.23	2.01	2.05
21	2	822	SQD	O2-C2	-2.23	1.37	1.43
14	H	1210	CLA	CMD-C2D	-2.23	1.46	1.50
17	n	4219	BCR	C1-C6	-2.23	1.50	1.53
14	q	505	CLA	MG-NB	-2.23	2.01	2.05
14	r	506	CLA	CMC-C2C	-2.23	1.46	1.50
14	J	1303	CLA	MG-NB	-2.23	2.01	2.05
14	G	1022	CLA	C3B-C4B	2.23	1.48	1.42
14	3	506	CLA	MG-NB	-2.23	2.01	2.05
18	A	5005	LHG	O7-C5	-2.23	1.41	1.46
18	G	5005	LHG	O7-C5	-2.23	1.41	1.46
14	a	512	CLA	CMB-C2B	-2.23	1.46	1.50
14	f	1234	CLA	CMD-C2D	-2.23	1.46	1.50
14	m	1401	CLA	CMC-C2C	-2.23	1.46	1.50
14	a	516	CLA	MG-NB	-2.23	2.01	2.05
14	v	510	CLA	MG-NB	-2.23	2.01	2.05
14	G	1106	CLA	C1B-C2B	2.23	1.48	1.43
14	G	1106	CLA	CMC-C2C	-2.23	1.46	1.50
14	c	506	CLA	MG-NB	-2.23	2.01	2.05
18	e	5005	LHG	O7-C5	-2.23	1.41	1.46
14	6	505	CLA	MG-NB	-2.23	2.01	2.05
14	A	1116	CLA	C1B-C2B	2.23	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1114	CLA	CMD-C2D	-2.23	1.46	1.50
14	1	505	CLA	CMD-C2D	-2.23	1.46	1.50
14	4	510	CLA	MG-NB	-2.23	2.01	2.05
14	b	510	CLA	MG-NB	-2.23	2.01	2.05
14	A	1106	CLA	C1B-C2B	2.23	1.48	1.43
14	e	1110	CLA	CMD-C2D	-2.23	1.46	1.50
21	B	1852	SQD	O3-C3	-2.23	1.37	1.43
14	q	506	CLA	CHC-C1C	2.23	1.43	1.38
14	2	512	CLA	C1B-C2B	2.23	1.48	1.43
14	5	507	CLA	MG-NB	-2.23	2.01	2.05
14	R	1301	CLA	CMD-C2D	-2.23	1.46	1.50
14	f	1212	CLA	CMD-C2D	-2.23	1.46	1.50
14	f	1235	CLA	CMC-C2C	-2.23	1.46	1.50
14	q	517	CLA	MG-NB	-2.23	2.01	2.05
14	B	1204	CLA	CMD-C2D	-2.23	1.46	1.50
14	H	1225	CLA	C1B-NB	-2.23	1.35	1.37
14	H	1201	CLA	CHC-C1C	2.23	1.43	1.38
14	B	1234	CLA	CMB-C2B	-2.23	1.46	1.50
14	H	1203	CLA	CMD-C2D	-2.23	1.46	1.50
14	n	1502	CLA	CMD-C2D	-2.23	1.46	1.50
14	K	1105	CLA	MG-NB	-2.23	2.01	2.05
14	t	519	CLA	MG-NB	-2.23	2.01	2.05
14	G	1125	CLA	CMC-C2C	-2.23	1.46	1.50
14	f	1231	CLA	CMD-C2D	-2.23	1.46	1.50
14	6	503	CLA	CMD-C2D	-2.23	1.46	1.50
14	s	506	CLA	MG-NB	-2.23	2.01	2.05
14	B	1234	CLA	CMD-C2D	-2.23	1.46	1.50
14	F	1301	CLA	CMD-C2D	-2.23	1.46	1.50
14	m	1401	CLA	CHC-C1C	2.23	1.43	1.38
14	1	506	CLA	CMC-C2C	-2.23	1.46	1.50
14	H	1221	CLA	CMC-C2C	-2.23	1.46	1.50
14	v	518	CLA	CMD-C2D	-2.23	1.46	1.50
14	B	1228	CLA	MG-NB	-2.23	2.01	2.05
14	e	1104	CLA	C1B-NB	-2.23	1.35	1.37
14	A	1106	CLA	CMC-C2C	-2.23	1.46	1.50
14	f	1203	CLA	CMD-C2D	-2.23	1.46	1.50
14	U	1401	CLA	CHC-C1C	2.22	1.43	1.38
14	L	1502	CLA	CMB-C2B	-2.22	1.46	1.50
14	H	1234	CLA	CMB-C2B	-2.22	1.46	1.50
14	e	1124	CLA	MG-ND	-2.22	2.01	2.05
14	Y	505	CLA	CMD-C2D	-2.22	1.46	1.50
14	d	517	CLA	CMD-C2D	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1129	CLA	CMC-C2C	-2.22	1.46	1.50
14	f	1213	CLA	CMC-C2C	-2.22	1.46	1.50
14	v	506	CLA	CMC-C2C	-2.22	1.46	1.50
14	c	517	CLA	MG-NB	-2.22	2.01	2.05
14	d	504	CLA	MG-NB	-2.22	2.01	2.05
14	6	511	CLA	MG-NB	-2.22	2.01	2.05
14	H	1203	CLA	C1B-C2B	2.22	1.48	1.43
14	Y	506	CLA	CMC-C2C	-2.22	1.46	1.50
14	v	512	CLA	CMB-C2B	-2.22	1.46	1.50
14	H	1226	CLA	C3B-C4B	2.22	1.48	1.42
14	A	1110	CLA	C1B-NB	-2.22	1.35	1.37
14	6	510	CLA	MG-NB	-2.22	2.01	2.05
14	e	1013	CLA	MG-ND	-2.22	2.01	2.05
14	G	1111	CLA	C1B-C2B	2.22	1.48	1.43
14	c	502	CLA	MG-NB	-2.22	2.01	2.05
14	s	518	CLA	MG-NB	-2.22	2.01	2.05
14	q	519	CLA	CHC-C1C	2.22	1.43	1.38
14	u	508	CLA	C1B-NB	-2.22	1.35	1.37
14	3	516	CLA	MG-NB	-2.22	2.01	2.05
14	c	501	CLA	MG-NB	-2.22	2.01	2.05
14	1	507	CLA	CMD-C2D	-2.22	1.46	1.50
14	q	506	CLA	CMC-C2C	-2.22	1.46	1.50
14	d	508	CLA	C1B-C2B	2.22	1.48	1.43
14	1	517	CLA	MG-NB	-2.22	2.01	2.05
14	s	501	CLA	MG-NB	-2.22	2.01	2.05
14	H	1012	CLA	CMC-C2C	-2.22	1.46	1.50
14	e	1114	CLA	CMD-C2D	-2.22	1.46	1.50
21	r	822	SQD	O2-C2	-2.22	1.37	1.43
21	u	822	SQD	O2-C2	-2.22	1.37	1.43
14	Y	501	CLA	MG-NB	-2.22	2.01	2.05
21	Z	822	SQD	O2-C2	-2.22	1.37	1.43
14	A	1109	CLA	C4B-NB	2.22	1.40	1.37
14	H	1234	CLA	CMD-C2D	-2.22	1.46	1.50
14	Y	507	CLA	CMD-C2D	-2.22	1.46	1.50
14	u	517	CLA	CMC-C2C	-2.22	1.46	1.50
14	1	507	CLA	MG-NB	-2.22	2.01	2.05
14	Y	506	CLA	MG-NB	-2.22	2.01	2.05
14	j	1301	CLA	CMD-C2D	-2.22	1.46	1.50
14	H	1206	CLA	MG-ND	-2.22	2.01	2.05
21	5	822	SQD	O2-C2	-2.22	1.37	1.43
14	e	1129	CLA	C1B-NB	-2.22	1.35	1.37
14	t	508	CLA	CMC-C2C	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	506	CLA	MG-NB	-2.22	2.01	2.05
14	A	1125	CLA	CMC-C2C	-2.22	1.46	1.50
14	B	1235	CLA	CMC-C2C	-2.22	1.46	1.50
14	K	1401	CLA	CMC-C2C	-2.22	1.46	1.50
14	f	1211	CLA	CMC-C2C	-2.22	1.46	1.50
14	q	501	CLA	MG-NB	-2.22	2.01	2.05
14	q	507	CLA	MG-NB	-2.22	2.01	2.05
14	6	508	CLA	C1B-C2B	2.22	1.48	1.43
14	H	1240	CLA	CHC-C1C	2.22	1.43	1.38
14	n	1503	CLA	CMB-C2B	-2.22	1.46	1.50
14	B	1240	CLA	CHC-C1C	2.22	1.43	1.38
14	L	1502	CLA	CMD-C2D	-2.22	1.46	1.50
14	s	505	CLA	MG-NB	-2.21	2.01	2.05
14	2	506	CLA	CMB-C2B	-2.21	1.46	1.50
14	1	501	CLA	MG-NB	-2.21	2.01	2.05
14	e	1132	CLA	MG-ND	-2.21	2.01	2.05
14	G	1118	CLA	CMB-C2B	-2.21	1.46	1.50
14	H	1023	CLA	CMD-C2D	-2.21	1.46	1.50
14	H	1223	CLA	CMD-C2D	-2.21	1.46	1.50
14	H	1224	CLA	CMD-C2D	-2.21	1.46	1.50
14	e	1120	CLA	CMD-C2D	-2.21	1.46	1.50
14	e	1125	CLA	CMC-C2C	-2.21	1.46	1.50
14	A	1111	CLA	C1B-C2B	2.21	1.48	1.43
14	L	1501	CLA	CMD-C2D	-2.21	1.46	1.50
14	G	1102	CLA	CMC-C2C	-2.21	1.46	1.50
14	G	1120	CLA	CMD-C2D	-2.21	1.46	1.50
14	A	1022	CLA	C3B-C4B	2.21	1.48	1.42
17	V	4219	BCR	C1-C6	-2.21	1.50	1.53
14	b	519	CLA	MG-NB	-2.21	2.01	2.05
14	5	502	CLA	MG-NB	-2.21	2.01	2.05
14	H	1212	CLA	MG-NB	-2.21	2.01	2.05
14	U	1105	CLA	MG-NB	-2.21	2.01	2.05
14	f	1228	CLA	MG-NB	-2.21	2.01	2.05
14	2	509	CLA	CMD-C2D	-2.21	1.46	1.50
14	H	1227	CLA	CMD-C2D	-2.21	1.46	1.50
14	A	1132	CLA	MG-ND	-2.21	2.01	2.05
14	f	1216	CLA	MG-ND	-2.21	2.01	2.05
14	H	1231	CLA	CMD-C2D	-2.21	1.46	1.50
14	Y	506	CLA	CHC-C1C	2.21	1.43	1.38
14	l	1303	CLA	MG-NB	-2.21	2.01	2.05
14	f	1226	CLA	C3B-C4B	2.21	1.47	1.42
14	e	1110	CLA	C1B-NB	-2.21	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	c	509	CLA	MG-NB	-2.21	2.01	2.05
14	s	516	CLA	MG-NB	-2.21	2.01	2.05
14	e	1102	CLA	CMD-C2D	-2.21	1.46	1.50
14	3	512	CLA	CMB-C2B	-2.21	1.46	1.50
14	G	1118	CLA	MG-ND	-2.21	2.01	2.05
14	G	1132	CLA	MG-ND	-2.21	2.01	2.05
17	n	4219	BCR	C14-C13	-2.21	1.32	1.35
14	H	1228	CLA	CHC-C1C	2.21	1.43	1.38
14	f	1240	CLA	CHC-C1C	2.21	1.43	1.38
14	a	506	CLA	MG-NB	-2.21	2.01	2.05
14	B	1231	CLA	CMD-C2D	-2.21	1.46	1.50
14	f	1228	CLA	CHC-C1C	2.21	1.43	1.38
14	d	510	CLA	MG-NB	-2.21	2.01	2.05
14	d	511	CLA	MG-NB	-2.21	2.01	2.05
14	f	1211	CLA	C1B-C2B	2.21	1.48	1.43
14	A	1101	CLA	C1B-NB	-2.21	1.35	1.37
14	B	1202	CLA	CMC-C2C	-2.21	1.46	1.50
14	3	509	CLA	CMD-C2D	-2.21	1.46	1.50
14	Y	508	CLA	CMC-C2C	-2.21	1.46	1.50
14	v	501	CLA	CMC-C2C	-2.21	1.46	1.50
14	B	1217	CLA	MG-NB	-2.21	2.01	2.05
14	5	517	CLA	CMC-C2C	-2.21	1.46	1.50
14	6	512	CLA	CMB-C2B	-2.21	1.46	1.50
14	H	1202	CLA	CMC-C2C	-2.21	1.46	1.50
14	e	1101	CLA	C1B-NB	-2.21	1.35	1.37
14	b	513	CLA	MG-NB	-2.21	2.01	2.05
14	H	1212	CLA	CMD-C2D	-2.21	1.46	1.50
21	f	1852	SQD	O3-C3	-2.21	1.37	1.43
14	e	1116	CLA	CHC-C1C	2.21	1.43	1.38
21	d	822	SQD	O2-C2	-2.21	1.37	1.43
14	A	1104	CLA	C1B-NB	-2.21	1.35	1.37
14	f	1203	CLA	C1B-C2B	2.21	1.48	1.43
14	B	1226	CLA	C3B-C4B	2.21	1.47	1.42
14	3	501	CLA	MG-NB	-2.21	2.01	2.05
14	5	509	CLA	MG-NB	-2.21	2.01	2.05
14	3	505	CLA	MG-NB	-2.21	2.01	2.05
14	b	519	CLA	CHC-C1C	2.21	1.43	1.38
14	1	508	CLA	CMC-C2C	-2.21	1.46	1.50
14	f	1202	CLA	CMC-C2C	-2.21	1.46	1.50
14	1	506	CLA	CHC-C1C	2.21	1.43	1.38
14	G	1104	CLA	C1B-NB	-2.20	1.35	1.37
14	6	503	CLA	MG-NB	-2.20	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	503	CLA	CMD-C2D	-2.20	1.46	1.50
14	q	507	CLA	CMD-C2D	-2.20	1.46	1.50
14	f	1023	CLA	C4B-NB	2.20	1.40	1.37
14	f	1211	CLA	CMB-C2B	-2.20	1.46	1.50
14	B	1203	CLA	C1B-C2B	2.20	1.48	1.43
14	v	503	CLA	CMD-C2D	-2.20	1.46	1.50
14	b	502	CLA	MG-NB	-2.20	2.01	2.05
14	A	1126	CLA	C4B-NB	2.20	1.40	1.37
14	e	1109	CLA	C4B-NB	2.20	1.40	1.37
14	e	1102	CLA	CMC-C2C	-2.20	1.46	1.50
14	3	511	CLA	MG-NB	-2.20	2.01	2.05
14	n	1502	CLA	CMB-C2B	-2.20	1.46	1.50
14	3	518	CLA	MG-NB	-2.20	2.01	2.05
14	H	1235	CLA	CMC-C2C	-2.20	1.46	1.50
14	T	1302	CLA	CMB-C2B	-2.20	1.46	1.50
14	V	1502	CLA	CMB-C2B	-2.20	1.46	1.50
14	Y	517	CLA	MG-NB	-2.20	2.01	2.05
14	H	1023	CLA	C4B-NB	2.20	1.40	1.37
14	Y	510	CLA	MG-NB	-2.20	2.01	2.05
14	Z	509	CLA	CMD-C2D	-2.20	1.46	1.50
14	f	1204	CLA	CMD-C2D	-2.20	1.46	1.50
14	H	1216	CLA	MG-ND	-2.20	2.01	2.05
17	A	4008	BCR	C10-C9	-2.20	1.32	1.35
14	G	1125	CLA	C4B-NB	2.20	1.40	1.37
14	f	1211	CLA	C1B-NB	-2.20	1.35	1.37
14	f	1225	CLA	C1B-NB	-2.20	1.35	1.37
14	a	512	CLA	CMD-C2D	-2.20	1.46	1.50
14	d	501	CLA	CMC-C2C	-2.20	1.46	1.50
21	c	822	SQD	O2-C2	-2.20	1.37	1.43
18	A	5002	LHG	O7-C5	-2.20	1.41	1.46
14	B	1216	CLA	MG-ND	-2.20	2.01	2.05
14	f	1234	CLA	CMB-C2B	-2.20	1.46	1.50
14	e	1126	CLA	C4B-NB	2.20	1.40	1.37
14	c	507	CLA	MG-NB	-2.20	2.01	2.05
14	A	1118	CLA	CMB-C2B	-2.20	1.46	1.50
14	4	508	CLA	CMC-C2C	-2.20	1.46	1.50
14	H	1213	CLA	CMC-C2C	-2.20	1.46	1.50
14	U	1401	CLA	CMC-C2C	-2.20	1.46	1.50
14	U	1103	CLA	CMC-C2C	-2.20	1.46	1.50
14	G	1112	CLA	CHC-C1C	2.20	1.43	1.38
14	4	513	CLA	MG-NB	-2.20	2.01	2.05
14	d	503	CLA	MG-NB	-2.20	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	507	CLA	MG-NB	-2.20	2.01	2.05
14	A	1120	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	1212	CLA	CMD-C2D	-2.20	1.46	1.50
14	Z	501	CLA	MG-NB	-2.20	2.01	2.05
14	A	1129	CLA	C4B-NB	2.20	1.40	1.37
14	G	1101	CLA	C1B-NB	-2.20	1.35	1.37
14	q	508	CLA	CMC-C2C	-2.20	1.46	1.50
14	e	1106	CLA	C1B-C2B	2.20	1.48	1.43
14	B	1221	CLA	CMC-C2C	-2.20	1.46	1.50
14	4	519	CLA	CHC-C1C	2.20	1.43	1.38
14	e	1129	CLA	C4B-NB	2.20	1.40	1.37
14	H	1218	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	1215	CLA	CAC-C3C	-2.20	1.45	1.51
14	G	1135	CLA	CMC-C2C	-2.20	1.46	1.50
14	f	1217	CLA	MG-NB	-2.20	2.01	2.05
14	1	519	CLA	CHC-C1C	2.20	1.43	1.38
14	4	512	CLA	CMD-C2D	-2.20	1.46	1.50
14	V	1501	CLA	CMD-C2D	-2.20	1.46	1.50
21	6	822	SQD	O2-C2	-2.20	1.37	1.43
14	3	518	CLA	CMD-C2D	-2.20	1.46	1.50
14	5	509	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	1210	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	1223	CLA	CMD-C2D	-2.19	1.46	1.50
14	3	503	CLA	CMD-C2D	-2.19	1.46	1.50
14	G	1102	CLA	CMD-C2D	-2.19	1.46	1.50
14	b	512	CLA	CMD-C2D	-2.19	1.46	1.50
14	a	511	CLA	MG-NB	-2.19	2.01	2.05
14	f	1215	CLA	CAC-C3C	-2.19	1.45	1.51
14	A	1135	CLA	CMC-C2C	-2.19	1.46	1.50
14	e	1135	CLA	CMC-C2C	-2.19	1.46	1.50
14	f	1210	CLA	CMD-C2D	-2.19	1.46	1.50
14	A	1115	CLA	C1B-C2B	2.19	1.48	1.43
14	B	1206	CLA	MG-ND	-2.19	2.01	2.05
14	H	1023	CLA	CHC-C1C	2.19	1.43	1.38
14	B	1211	CLA	C1B-C2B	2.19	1.48	1.43
14	A	1127	CLA	MG-ND	-2.19	2.01	2.05
14	6	506	CLA	MG-NB	-2.19	2.01	2.05
17	f	4010	BCR	C17-C18	-2.19	1.32	1.35
14	s	504	CLA	CMD-C2D	-2.19	1.46	1.50
18	e	5002	LHG	O7-C5	-2.19	1.41	1.46
14	4	506	CLA	MG-NB	-2.19	2.01	2.05
14	a	518	CLA	MG-NB	-2.19	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1023	CLA	C4B-NB	2.19	1.40	1.37
21	v	822	SQD	O2-C2	-2.19	1.37	1.43
14	T	1302	CLA	MG-NB	-2.19	2.01	2.05
14	u	517	CLA	MG-NB	-2.19	2.01	2.05
14	B	1224	CLA	CMD-C2D	-2.19	1.46	1.50
14	a	504	CLA	CMD-C2D	-2.19	1.46	1.50
14	q	511	CLA	CMD-C2D	-2.19	1.46	1.50
14	f	1206	CLA	MG-ND	-2.19	2.01	2.05
17	S	4018	BCR	C1-C6	-2.19	1.50	1.53
14	Z	504	CLA	MG-NB	-2.19	2.01	2.05
14	B	1213	CLA	CMC-C2C	-2.19	1.46	1.50
14	3	512	CLA	CMD-C2D	-2.19	1.46	1.50
14	s	512	CLA	CMD-C2D	-2.19	1.46	1.50
14	b	508	CLA	CMC-C2C	-2.19	1.46	1.50
14	K	1103	CLA	CMC-C2C	-2.19	1.46	1.50
14	L	1503	CLA	CMB-C2B	-2.19	1.46	1.50
14	1	501	CLA	CMC-C2C	-2.19	1.46	1.50
14	b	501	CLA	CHC-C1C	2.19	1.43	1.38
14	H	1215	CLA	CMC-C2C	-2.19	1.46	1.50
14	G	1126	CLA	C4B-NB	2.19	1.40	1.37
14	H	1204	CLA	CMD-C2D	-2.19	1.46	1.50
14	d	506	CLA	CMC-C2C	-2.19	1.46	1.50
14	e	1106	CLA	CMC-C2C	-2.19	1.46	1.50
14	J	1302	CLA	CMB-C2B	-2.19	1.46	1.50
14	H	1228	CLA	CMD-C2D	-2.19	1.46	1.50
14	Z	519	CLA	CMB-C2B	-2.19	1.46	1.50
14	c	509	CLA	CMD-C2D	-2.19	1.46	1.50
14	t	519	CLA	CHC-C1C	2.19	1.43	1.38
14	H	1211	CLA	C1B-C2B	2.19	1.48	1.43
14	u	512	CLA	CMD-C2D	-2.19	1.46	1.50
21	a	822	SQD	O2-C2	-2.19	1.37	1.43
17	L	4219	BCR	C1-C6	-2.19	1.50	1.53
14	B	1228	CLA	CMD-C2D	-2.19	1.46	1.50
14	6	506	CLA	CMC-C2C	-2.19	1.46	1.50
14	c	512	CLA	CMD-C2D	-2.19	1.46	1.50
14	6	501	CLA	CMC-C2C	-2.19	1.46	1.50
14	e	1118	CLA	CMB-C2B	-2.19	1.46	1.50
14	f	1223	CLA	CMD-C2D	-2.19	1.46	1.50
14	s	506	CLA	CMB-C2B	-2.19	1.46	1.50
14	t	501	CLA	CHC-C1C	2.19	1.43	1.38
14	u	509	CLA	MG-NB	-2.19	2.01	2.05
14	s	509	CLA	CMD-C2D	-2.19	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	507	CLA	MG-NB	-2.19	2.01	2.05
14	e	1022	CLA	C3B-C4B	2.19	1.47	1.42
14	e	1116	CLA	CMD-C2D	-2.19	1.46	1.50
14	Z	512	CLA	MG-ND	-2.18	2.01	2.05
17	B	4010	BCR	C17-C18	-2.18	1.32	1.35
14	f	1212	CLA	MG-NB	-2.18	2.01	2.05
14	r	512	CLA	MG-ND	-2.18	2.01	2.05
14	5	512	CLA	CMD-C2D	-2.18	1.46	1.50
14	s	512	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	1229	CLA	CHC-C1C	2.18	1.43	1.38
14	V	1503	CLA	CMB-C2B	-2.18	1.46	1.50
14	f	1221	CLA	CMC-C2C	-2.18	1.46	1.50
14	e	1111	CLA	C1B-C2B	2.18	1.48	1.43
14	f	1228	CLA	C1B-C2B	2.18	1.48	1.43
14	R	1301	CLA	MG-ND	-2.18	2.01	2.05
14	A	1102	CLA	CMD-C2D	-2.18	1.46	1.50
14	c	517	CLA	CMC-C2C	-2.18	1.46	1.50
14	A	1116	CLA	CHC-C1C	2.18	1.43	1.38
14	B	1212	CLA	MG-NB	-2.18	2.01	2.05
14	v	503	CLA	MG-NB	-2.18	2.01	2.05
14	v	512	CLA	CMD-C2D	-2.18	1.46	1.50
14	f	1218	CLA	CMD-C2D	-2.18	1.46	1.50
14	A	1102	CLA	CMC-C2C	-2.18	1.46	1.50
14	4	501	CLA	CHC-C1C	2.18	1.43	1.38
14	a	508	CLA	CMC-C2C	-2.18	1.46	1.50
14	t	506	CLA	MG-NB	-2.18	2.01	2.05
14	d	512	CLA	CMB-C2B	-2.18	1.46	1.50
14	f	1238	CLA	CMC-C2C	-2.18	1.46	1.50
14	r	509	CLA	CMD-C2D	-2.18	1.46	1.50
14	u	506	CLA	CMC-C2C	-2.18	1.46	1.50
14	J	1302	CLA	MG-NB	-2.18	2.01	2.05
14	2	512	CLA	MG-ND	-2.18	2.01	2.05
17	H	4010	BCR	C17-C18	-2.18	1.32	1.35
14	2	507	CLA	CMD-C2D	-2.18	1.46	1.50
14	e	1134	CLA	CMD-C2D	-2.18	1.46	1.50
21	t	822	SQD	O3-C3	-2.18	1.37	1.43
14	G	1115	CLA	C1B-C2B	2.18	1.48	1.43
14	Z	509	CLA	CMB-C2B	-2.18	1.46	1.50
14	v	519	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	1214	CLA	CMD-C2D	-2.18	1.46	1.50
14	H	1208	CLA	CMD-C2D	-2.18	1.46	1.50
14	3	512	CLA	MG-ND	-2.18	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1127	CLA	MG-ND	-2.18	2.01	2.05
14	e	1134	CLA	MG-NB	-2.18	2.01	2.05
14	e	1237	CLA	C1B-NB	-2.18	1.35	1.37
14	Y	501	CLA	CMC-C2C	-2.18	1.46	1.50
21	q	822	SQD	O2-C2	-2.18	1.37	1.43
14	j	1301	CLA	MG-ND	-2.18	2.01	2.05
14	B	1023	CLA	CHC-C1C	2.18	1.42	1.38
14	f	1208	CLA	CMD-C2D	-2.18	1.46	1.50
14	f	1236	CLA	CMC-C2C	-2.18	1.46	1.50
14	s	503	CLA	CMD-C2D	-2.18	1.46	1.50
14	v	506	CLA	MG-NB	-2.18	2.01	2.05
14	m	1103	CLA	CMC-C2C	-2.18	1.46	1.50
14	B	1218	CLA	CMD-C2D	-2.18	1.46	1.50
14	G	1131	CLA	MG-ND	-2.18	2.01	2.05
17	G	4008	BCR	C10-C9	-2.18	1.32	1.35
14	B	1201	CLA	C1B-C2B	2.18	1.48	1.43
14	s	518	CLA	CMD-C2D	-2.18	1.46	1.50
14	G	1109	CLA	C4B-NB	2.18	1.40	1.37
14	H	1201	CLA	C1B-C2B	2.18	1.48	1.43
14	5	517	CLA	MG-NB	-2.18	2.01	2.05
14	a	512	CLA	MG-ND	-2.18	2.01	2.05
14	f	1218	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	1228	CLA	C1B-C2B	2.18	1.48	1.43
14	H	1217	CLA	MG-NB	-2.18	2.01	2.05
14	s	512	CLA	MG-ND	-2.18	2.01	2.05
14	A	1116	CLA	CMD-C2D	-2.18	1.46	1.50
14	B	1231	CLA	CMB-C2B	-2.18	1.46	1.50
14	H	1205	CLA	C1B-NB	-2.18	1.35	1.37
14	4	506	CLA	CMB-C2B	-2.17	1.46	1.50
14	G	1111	CLA	CMB-C2B	-2.17	1.46	1.50
14	A	1111	CLA	CMB-C2B	-2.17	1.46	1.50
14	2	519	CLA	CMB-C2B	-2.17	1.46	1.50
14	e	1105	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	505	CLA	MG-NB	-2.17	2.01	2.05
14	t	502	CLA	MG-NB	-2.17	2.01	2.05
14	u	513	CLA	CHC-C1C	2.17	1.42	1.38
14	4	502	CLA	MG-NB	-2.17	2.01	2.05
14	H	1209	CLA	MG-NB	-2.17	2.01	2.05
14	a	501	CLA	CHC-C1C	2.17	1.42	1.38
14	A	1118	CLA	CMC-C2C	-2.17	1.46	1.50
14	G	1116	CLA	CMD-C2D	-2.17	1.46	1.50
14	e	1112	CLA	CHC-C1C	2.17	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1211	CLA	CMC-C2C	-2.17	1.46	1.50
14	b	506	CLA	MG-NB	-2.17	2.01	2.05
14	H	1228	CLA	C1B-C2B	2.17	1.48	1.43
14	A	1106	CLA	CMD-C2D	-2.17	1.46	1.50
14	G	1132	CLA	CMB-C2B	-2.17	1.46	1.50
14	1	510	CLA	MG-NB	-2.17	2.01	2.05
14	2	509	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	1228	CLA	CHC-C1C	2.17	1.42	1.38
14	3	508	CLA	CMC-C2C	-2.17	1.46	1.50
14	H	1224	CLA	CMC-C2C	-2.17	1.46	1.50
14	f	1224	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	1208	CLA	CMD-C2D	-2.17	1.46	1.50
14	6	519	CLA	CMB-C2B	-2.17	1.46	1.50
14	H	1236	CLA	CMC-C2C	-2.17	1.46	1.50
14	c	503	CLA	CMD-C2D	-2.17	1.46	1.50
14	q	501	CLA	CMC-C2C	-2.17	1.46	1.50
14	A	1133	CLA	CMC-C2C	-2.17	1.46	1.50
14	B	1236	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	501	CLA	MG-NB	-2.17	2.01	2.05
14	G	1116	CLA	CHC-C1C	2.17	1.42	1.38
14	v	509	CLA	CHC-C1C	2.17	1.42	1.38
14	H	1203	CLA	CMB-C2B	-2.17	1.46	1.50
14	H	1224	CLA	CMB-C2B	-2.17	1.46	1.50
14	l	1302	CLA	CMB-C2B	-2.17	1.46	1.50
17	k	4018	BCR	C30-C25	-2.17	1.50	1.53
14	G	1102	CLA	C1B-NB	-2.17	1.35	1.37
14	B	1230	CLA	MG-ND	-2.17	2.01	2.05
14	H	1215	CLA	CAC-C3C	-2.17	1.45	1.51
14	H	1222	CLA	CMD-C2D	-2.17	1.46	1.50
14	s	518	CLA	CMB-C2B	-2.17	1.46	1.50
14	f	1023	CLA	CHC-C1C	2.17	1.42	1.38
14	H	1236	CLA	CMD-C2D	-2.17	1.46	1.50
14	e	1115	CLA	CMB-C2B	-2.17	1.46	1.50
14	l	1302	CLA	MG-NB	-2.17	2.01	2.05
14	u	504	CLA	MG-NB	-2.17	2.01	2.05
14	v	509	CLA	MG-NB	-2.17	2.01	2.05
14	A	1134	CLA	CMD-C2D	-2.17	1.46	1.50
17	L	4219	BCR	C14-C13	-2.17	1.32	1.35
14	B	1236	CLA	CMD-C2D	-2.17	1.46	1.50
14	G	1110	CLA	C1B-NB	-2.17	1.35	1.37
14	G	1128	CLA	CHC-C4B	-2.17	1.34	1.39
14	B	1211	CLA	CMB-C2B	-2.17	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	1231	CLA	CMB-C2B	-2.17	1.46	1.50
17	e	4008	BCR	C10-C9	-2.17	1.32	1.35
14	B	1218	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	1222	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	1201	CLA	MG-NB	-2.17	2.01	2.05
17	I	4018	BCR	C1-C6	-2.17	1.50	1.53
14	H	1231	CLA	CMB-C2B	-2.17	1.46	1.50
14	Y	504	CLA	CMB-C2B	-2.17	1.46	1.50
14	A	1112	CLA	CHC-C1C	2.17	1.42	1.38
17	I	4018	BCR	C30-C25	-2.16	1.50	1.53
14	A	1122	CLA	CMD-C2D	-2.16	1.46	1.50
14	3	501	CLA	CHC-C1C	2.16	1.42	1.38
14	d	509	CLA	MG-NB	-2.16	2.01	2.05
18	G	5002	LHG	O7-C5	-2.16	1.41	1.46
14	e	1122	CLA	CMD-C2D	-2.16	1.46	1.50
14	s	501	CLA	CHC-C1C	2.16	1.42	1.38
14	G	1118	CLA	CMC-C2C	-2.16	1.46	1.50
14	Z	513	CLA	CMD-C2D	-2.16	1.46	1.50
21	3	822	SQD	O2-C2	-2.16	1.37	1.43
14	B	1207	CLA	CHC-C1C	2.16	1.42	1.38
21	4	822	SQD	O3-C3	-2.16	1.37	1.43
14	G	1122	CLA	CMD-C2D	-2.16	1.46	1.50
14	e	1106	CLA	CMD-C2D	-2.16	1.46	1.50
14	6	510	CLA	CHC-C1C	2.16	1.42	1.38
21	b	822	SQD	O3-C3	-2.16	1.37	1.43
14	3	504	CLA	CMD-C2D	-2.16	1.46	1.50
14	3	506	CLA	CMB-C2B	-2.16	1.46	1.50
14	r	507	CLA	CMD-C2D	-2.16	1.46	1.50
14	f	1222	CLA	CMD-C2D	-2.16	1.46	1.50
14	l	1303	CLA	CMD-C2D	-2.16	1.46	1.50
21	d	822	SQD	O4-C4	-2.16	1.37	1.43
14	Y	513	CLA	CHC-C1C	2.16	1.42	1.38
14	G	1127	CLA	CMC-C2C	-2.16	1.46	1.50
14	Y	516	CLA	CMB-C2B	-2.16	1.46	1.50
14	G	1113	CLA	C1B-C2B	2.16	1.48	1.43
14	Z	512	CLA	C1B-NB	-2.16	1.35	1.37
14	B	1224	CLA	CMC-C2C	-2.16	1.46	1.50
14	B	1229	CLA	C1B-C2B	2.16	1.48	1.43
14	u	518	CLA	CHC-C1C	2.16	1.42	1.38
14	e	1129	CLA	C3B-C4B	2.16	1.47	1.42
14	B	1215	CLA	CMC-C2C	-2.16	1.46	1.50
14	6	512	CLA	CMD-C2D	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	512	CLA	CMB-C2B	-2.16	1.46	1.50
14	e	1118	CLA	CMC-C2C	-2.16	1.46	1.50
14	r	512	CLA	CMB-C2B	-2.16	1.46	1.50
14	B	1205	CLA	C1B-NB	-2.16	1.35	1.37
14	H	1229	CLA	CHC-C1C	2.16	1.42	1.38
14	H	1203	CLA	MG-ND	-2.16	2.01	2.05
14	f	1230	CLA	MG-ND	-2.16	2.01	2.05
14	c	506	CLA	CMC-C2C	-2.16	1.46	1.50
14	e	1124	CLA	CMC-C2C	-2.16	1.46	1.50
14	e	1125	CLA	C4B-NB	2.16	1.40	1.37
14	6	509	CLA	MG-NB	-2.16	2.01	2.05
21	1	822	SQD	O2-C2	-2.16	1.37	1.43
14	B	1238	CLA	CMC-C2C	-2.16	1.46	1.50
14	G	1106	CLA	CMD-C2D	-2.16	1.46	1.50
14	B	1203	CLA	MG-ND	-2.16	2.01	2.05
14	r	519	CLA	CMB-C2B	-2.16	1.46	1.50
14	e	1101	CLA	MG-NB	-2.16	2.01	2.05
14	b	506	CLA	CMB-C2B	-2.16	1.46	1.50
14	d	507	CLA	CMD-C2D	-2.16	1.46	1.50
14	q	510	CLA	CMB-C2B	-2.16	1.46	1.50
14	5	504	CLA	MG-NB	-2.16	2.01	2.05
14	b	504	CLA	MG-NB	-2.16	2.01	2.05
14	G	1121	CLA	C1B-NB	-2.16	1.35	1.37
14	B	1226	CLA	CHC-C4B	-2.16	1.34	1.39
14	G	1115	CLA	CMB-C2B	-2.16	1.46	1.50
14	f	1232	CLA	CMD-C2D	-2.16	1.46	1.50
14	5	506	CLA	CMC-C2C	-2.16	1.46	1.50
14	e	1111	CLA	CMB-C2B	-2.16	1.46	1.50
14	f	1214	CLA	CMD-C2D	-2.16	1.46	1.50
14	B	1224	CLA	CMB-C2B	-2.16	1.46	1.50
14	4	512	CLA	CMB-C2B	-2.16	1.46	1.50
14	a	501	CLA	CMC-C2C	-2.16	1.46	1.50
14	b	511	CLA	CMB-C2B	-2.16	1.46	1.50
14	3	503	CLA	MG-NB	-2.16	2.01	2.05
14	f	1229	CLA	CHC-C1C	2.16	1.42	1.38
14	u	513	CLA	CMD-C2D	-2.16	1.46	1.50
14	H	1205	CLA	C1B-C2B	2.16	1.48	1.43
14	A	1011	CLA	CMC-C2C	-2.16	1.46	1.50
14	A	1132	CLA	CMB-C2B	-2.16	1.46	1.50
14	A	1131	CLA	MG-ND	-2.16	2.01	2.05
14	f	1203	CLA	MG-ND	-2.16	2.01	2.05
14	b	519	CLA	CMC-C2C	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1011	CLA	CMC-C2C	-2.16	1.46	1.50
14	e	1127	CLA	CMC-C2C	-2.16	1.46	1.50
14	f	1236	CLA	CMD-C2D	-2.16	1.46	1.50
14	q	504	CLA	CMB-C2B	-2.16	1.46	1.50
14	F	1301	CLA	MG-ND	-2.15	2.01	2.05
14	a	503	CLA	MG-NB	-2.15	2.01	2.05
14	B	1214	CLA	C1B-C2B	2.15	1.48	1.43
14	u	509	CLA	CMD-C2D	-2.15	1.46	1.50
14	e	1128	CLA	CHC-C4B	-2.15	1.34	1.39
21	r	822	SQD	O4-C4	-2.15	1.37	1.43
14	A	1134	CLA	MG-NB	-2.15	2.01	2.05
14	2	504	CLA	MG-NB	-2.15	2.01	2.05
14	f	1201	CLA	C1B-C2B	2.15	1.48	1.43
14	f	1229	CLA	C1B-C2B	2.15	1.48	1.43
14	5	513	CLA	CHC-C1C	2.15	1.42	1.38
14	u	503	CLA	MG-NB	-2.15	2.01	2.05
14	A	1124	CLA	CMC-C2C	-2.15	1.46	1.50
14	a	506	CLA	CMB-C2B	-2.15	1.46	1.50
14	f	1226	CLA	CHC-C4B	-2.15	1.34	1.39
14	5	503	CLA	CMD-C2D	-2.15	1.46	1.50
14	6	507	CLA	CMD-C2D	-2.15	1.46	1.50
14	e	1137	CLA	CMC-C2C	-2.15	1.46	1.50
14	m	1103	CLA	CMB-C2B	-2.15	1.46	1.50
14	H	1207	CLA	CHC-C1C	2.15	1.42	1.38
14	A	1101	CLA	MG-NB	-2.15	2.01	2.05
14	f	1209	CLA	MG-NB	-2.15	2.01	2.05
14	r	509	CLA	CMB-C2B	-2.15	1.46	1.50
14	v	511	CLA	CMB-C2B	-2.15	1.46	1.50
14	1	513	CLA	CHC-C1C	2.15	1.42	1.38
14	f	1214	CLA	C1B-C2B	2.15	1.48	1.43
14	5	503	CLA	MG-NB	-2.15	2.01	2.05
14	A	1115	CLA	CMB-C2B	-2.15	1.46	1.50
14	G	1133	CLA	CMC-C2C	-2.15	1.46	1.50
14	r	518	CLA	CMD-C2D	-2.15	1.46	1.50
14	s	517	CLA	CMC-C2C	-2.15	1.46	1.50
14	2	512	CLA	C1B-NB	-2.15	1.35	1.37
14	K	1103	CLA	CMB-C2B	-2.15	1.46	1.50
14	r	501	CLA	CMB-C2B	-2.15	1.46	1.50
14	e	1115	CLA	C1B-C2B	2.15	1.48	1.43
14	2	519	CLA	CMC-C2C	-2.15	1.46	1.50
14	f	1228	CLA	CMD-C2D	-2.15	1.46	1.50
14	q	510	CLA	MG-NB	-2.15	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1125	CLA	C4B-NB	2.15	1.40	1.37
14	5	508	CLA	C1B-NB	-2.15	1.35	1.37
14	r	519	CLA	CMC-C2C	-2.15	1.46	1.50
14	s	511	CLA	CMD-C2D	-2.15	1.46	1.50
14	u	511	CLA	CMB-C2B	-2.15	1.46	1.50
14	e	1125	CLA	MG-ND	-2.15	2.01	2.05
21	Y	822	SQD	O2-C2	-2.15	1.37	1.43
14	5	508	CLA	C1B-C2B	2.15	1.48	1.43
14	A	1121	CLA	C1B-NB	-2.15	1.35	1.37
14	B	1211	CLA	C1B-NB	-2.15	1.35	1.37
14	5	513	CLA	CMD-C2D	-2.15	1.46	1.50
14	G	1126	CLA	MG-ND	-2.15	2.01	2.05
14	G	1101	CLA	MG-NB	-2.15	2.01	2.05
14	r	504	CLA	MG-NB	-2.15	2.01	2.05
17	A	4002	BCR	C30-C25	-2.15	1.50	1.53
14	A	1129	CLA	C3B-C4B	2.15	1.47	1.42
14	A	1105	CLA	CMC-C2C	-2.15	1.46	1.50
14	t	512	CLA	CMD-C2D	-2.15	1.46	1.50
14	6	508	CLA	CMC-C2C	-2.15	1.46	1.50
14	H	1239	CLA	CMD-C2D	-2.15	1.46	1.50
14	U	1103	CLA	CMB-C2B	-2.15	1.46	1.50
14	s	519	CLA	CMB-C2B	-2.15	1.46	1.50
14	G	1127	CLA	MG-ND	-2.15	2.01	2.05
14	f	1207	CLA	CHC-C1C	2.15	1.42	1.38
14	G	1134	CLA	CMD-C2D	-2.15	1.46	1.50
14	d	519	CLA	CMB-C2B	-2.15	1.46	1.50
14	r	513	CLA	CMD-C2D	-2.15	1.46	1.50
14	f	1209	CLA	C1B-NB	-2.15	1.35	1.37
14	B	1203	CLA	CMB-C2B	-2.15	1.46	1.50
14	H	1232	CLA	CMD-C2D	-2.15	1.46	1.50
14	v	507	CLA	CMD-C2D	-2.15	1.46	1.50
14	A	1125	CLA	MG-ND	-2.15	2.01	2.05
14	B	1232	CLA	CMD-C2D	-2.15	1.46	1.50
14	f	1201	CLA	MG-NB	-2.15	2.01	2.05
14	A	1127	CLA	CMC-C2C	-2.15	1.46	1.50
14	2	512	CLA	CMB-C2B	-2.15	1.46	1.50
14	t	506	CLA	CMB-C2B	-2.15	1.46	1.50
14	j	1301	CLA	C1B-C2B	2.15	1.48	1.43
14	4	503	CLA	MG-NB	-2.15	2.01	2.05
14	t	503	CLA	MG-NB	-2.15	2.01	2.05
14	c	513	CLA	CHC-C1C	2.15	1.42	1.38
21	s	822	SQD	O2-C2	-2.15	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1220	CLA	CMB-C2B	-2.15	1.46	1.50
14	3	511	CLA	CMD-C2D	-2.15	1.46	1.50
14	a	518	CLA	CMD-C2D	-2.15	1.46	1.50
14	e	1133	CLA	CMC-C2C	-2.15	1.46	1.50
14	q	510	CLA	CMD-C2D	-2.15	1.46	1.50
14	G	1124	CLA	CMC-C2C	-2.15	1.46	1.50
14	H	1229	CLA	C1B-C2B	2.15	1.48	1.43
14	3	517	CLA	CMC-C2C	-2.15	1.46	1.50
14	H	1211	CLA	CMB-C2B	-2.15	1.46	1.50
14	e	1112	CLA	CMB-C2B	-2.15	1.46	1.50
14	f	1023	CLA	CMB-C2B	-2.15	1.46	1.50
14	c	508	CLA	C1B-C2B	2.15	1.48	1.43
14	c	517	CLA	CHC-C1C	2.14	1.42	1.38
14	e	1106	CLA	C1B-NB	-2.14	1.35	1.37
14	u	516	CLA	MG-NB	-2.14	2.01	2.05
14	Y	510	CLA	CMD-C2D	-2.14	1.46	1.50
14	a	511	CLA	CMD-C2D	-2.14	1.46	1.50
14	H	1214	CLA	CMD-C2D	-2.14	1.46	1.50
14	Z	519	CLA	CMC-C2C	-2.14	1.46	1.50
14	f	1220	CLA	CMB-C2B	-2.14	1.46	1.50
14	t	513	CLA	CHC-C1C	2.14	1.42	1.38
14	s	501	CLA	CMC-C2C	-2.14	1.46	1.50
14	s	508	CLA	CMC-C2C	-2.14	1.46	1.50
14	A	1139	CLA	MG-ND	-2.14	2.01	2.05
14	r	513	CLA	CHC-C1C	2.14	1.42	1.38
14	f	1224	CLA	CMB-C2B	-2.14	1.46	1.50
14	d	509	CLA	CHC-C1C	2.14	1.42	1.38
14	B	1209	CLA	MG-NB	-2.14	2.01	2.05
14	H	1201	CLA	MG-NB	-2.14	2.01	2.05
14	H	1210	CLA	C1B-C2B	2.14	1.48	1.43
14	u	508	CLA	C1B-C2B	2.14	1.48	1.43
14	H	1023	CLA	CMB-C2B	-2.14	1.46	1.50
14	q	504	CLA	CMC-C2C	-2.14	1.46	1.50
14	6	504	CLA	CHC-C1C	2.14	1.42	1.38
14	e	1131	CLA	MG-ND	-2.14	2.01	2.05
14	2	501	CLA	CMB-C2B	-2.14	1.46	1.50
14	c	503	CLA	MG-NB	-2.14	2.01	2.05
14	H	1023	CLA	C1B-NB	-2.14	1.35	1.37
14	a	518	CLA	CMB-C2B	-2.14	1.46	1.50
14	r	509	CLA	CMC-C2C	-2.14	1.46	1.50
14	q	513	CLA	CHC-C1C	2.14	1.42	1.38
21	6	822	SQD	O4-C4	-2.14	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	5216	SQD	O4-C4	-2.14	1.37	1.43
14	G	1129	CLA	C3B-C4B	2.14	1.47	1.42
14	G	1134	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	519	CLA	CMB-C2B	-2.14	1.46	1.50
14	b	509	CLA	CMB-C2B	-2.14	1.46	1.50
14	b	512	CLA	CMB-C2B	-2.14	1.46	1.50
14	e	1116	CLA	CMB-C2B	-2.14	1.46	1.50
14	e	1131	CLA	CMC-C2C	-2.14	1.46	1.50
14	f	1203	CLA	CMB-C2B	-2.14	1.46	1.50
14	G	1139	CLA	MG-ND	-2.14	2.01	2.05
14	3	519	CLA	CMB-C2B	-2.14	1.46	1.50
18	B	1855	LHG	P-O6	2.14	1.68	1.59
14	4	516	CLA	MG-NB	-2.14	2.01	2.05
14	t	516	CLA	MG-NB	-2.14	2.01	2.05
14	1	504	CLA	CMB-C2B	-2.14	1.46	1.50
14	Z	507	CLA	CMD-C2D	-2.14	1.46	1.50
14	d	508	CLA	CMC-C2C	-2.14	1.46	1.50
14	f	1224	CLA	CMC-C2C	-2.14	1.46	1.50
14	A	1103	CLA	C1B-C2B	2.14	1.48	1.43
14	A	1102	CLA	MG-ND	-2.14	2.01	2.05
14	t	504	CLA	MG-NB	-2.14	2.01	2.05
14	v	507	CLA	MG-NB	-2.14	2.01	2.05
14	2	513	CLA	CMD-C2D	-2.14	1.46	1.50
14	G	1801	CLA	CMB-C2B	-2.14	1.46	1.50
14	f	1228	CLA	CMC-C2C	-2.14	1.46	1.50
14	f	1012	CLA	MG-ND	-2.14	2.01	2.05
17	e	4002	BCR	C30-C25	-2.14	1.50	1.53
14	A	1113	CLA	C1B-C2B	2.14	1.48	1.43
14	5	507	CLA	CMD-C2D	-2.14	1.46	1.50
14	R	1301	CLA	CMC-C2C	-2.14	1.46	1.50
14	u	513	CLA	CMB-C2B	-2.14	1.46	1.50
14	c	518	CLA	CHC-C1C	2.14	1.42	1.38
14	A	1111	CLA	MG-ND	-2.14	2.01	2.05
14	e	1102	CLA	MG-ND	-2.14	2.01	2.05
14	A	1116	CLA	CMB-C2B	-2.14	1.46	1.50
14	A	1128	CLA	CHC-C4B	-2.14	1.34	1.39
14	B	1202	CLA	CHC-C1C	2.14	1.42	1.38
14	5	518	CLA	CHC-C1C	2.14	1.42	1.38
14	v	510	CLA	CHC-C1C	2.14	1.42	1.38
14	G	1112	CLA	MG-ND	-2.14	2.01	2.05
14	A	1137	CLA	CMC-C2C	-2.14	1.46	1.50
14	3	518	CLA	CMC-C2C	-2.14	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1134	CLA	CMC-C2C	-2.14	1.46	1.50
14	f	1202	CLA	CHC-C1C	2.14	1.42	1.38
14	b	509	CLA	MG-NB	-2.14	2.01	2.05
14	j	1302	CLA	CMC-C2C	-2.14	1.46	1.50
14	G	1011	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	517	CLA	CMC-C2C	-2.14	1.46	1.50
14	b	509	CLA	CMD-C2D	-2.14	1.46	1.50
14	B	1023	CLA	C1B-NB	-2.14	1.35	1.37
14	H	1202	CLA	CHC-C1C	2.14	1.42	1.38
14	A	1112	CLA	CMB-C2B	-2.14	1.46	1.50
14	B	1023	CLA	CMB-C2B	-2.14	1.46	1.50
14	3	518	CLA	CMB-C2B	-2.14	1.46	1.50
21	2	822	SQD	O4-C4	-2.14	1.37	1.43
14	H	1218	CLA	CMB-C2B	-2.14	1.46	1.50
14	f	1205	CLA	C1B-C2B	2.14	1.48	1.43
14	f	1221	CLA	CHC-C1C	2.14	1.42	1.38
18	H	1855	LHG	P-O6	2.14	1.67	1.59
21	Z	822	SQD	O4-C4	-2.14	1.37	1.43
14	G	1103	CLA	C1B-C2B	2.14	1.48	1.43
14	A	1109	CLA	MG-ND	-2.14	2.01	2.05
14	A	1102	CLA	C1B-NB	-2.14	1.35	1.37
14	B	1221	CLA	CHC-C1C	2.14	1.42	1.38
21	v	822	SQD	O4-C4	-2.13	1.37	1.43
14	H	1238	CLA	CMC-C2C	-2.13	1.46	1.50
14	d	509	CLA	CMD-C2D	-2.13	1.46	1.50
14	R	1301	CLA	C1B-C2B	2.13	1.48	1.43
14	H	1232	CLA	MG-ND	-2.13	2.01	2.05
21	L	5216	SQD	O4-C4	-2.13	1.37	1.43
14	B	1228	CLA	CMC-C2C	-2.13	1.46	1.50
14	v	508	CLA	CMC-C2C	-2.13	1.46	1.50
14	e	1102	CLA	C1B-NB	-2.13	1.35	1.37
14	4	504	CLA	MG-NB	-2.13	2.01	2.05
14	G	1125	CLA	MG-ND	-2.13	2.01	2.05
14	d	510	CLA	CHC-C1C	2.13	1.42	1.38
14	B	1205	CLA	C1B-C2B	2.13	1.48	1.43
14	G	1138	CLA	CHC-C1C	2.13	1.42	1.38
18	f	1855	LHG	P-O6	2.13	1.67	1.59
21	t	822	SQD	O2-C2	-2.13	1.38	1.43
14	A	1126	CLA	MG-ND	-2.13	2.01	2.05
14	H	1221	CLA	CHC-C1C	2.13	1.42	1.38
14	4	509	CLA	CMB-C2B	-2.13	1.46	1.50
14	B	1209	CLA	C1B-C2B	2.13	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	1301	CLA	C1B-C2B	2.13	1.48	1.43
14	s	503	CLA	MG-NB	-2.13	2.01	2.05
17	k	4018	BCR	C1-C6	-2.13	1.50	1.53
14	2	518	CLA	CMD-C2D	-2.13	1.46	1.50
14	G	1112	CLA	CMB-C2B	-2.13	1.46	1.50
14	Y	504	CLA	CMD-C2D	-2.13	1.46	1.50
14	c	507	CLA	CMD-C2D	-2.13	1.46	1.50
21	4	822	SQD	O2-C2	-2.13	1.38	1.43
14	H	1214	CLA	C1B-C2B	2.13	1.48	1.43
14	e	1113	CLA	C1B-C2B	2.13	1.48	1.43
14	A	1801	CLA	CMB-C2B	-2.13	1.46	1.50
14	u	517	CLA	CMD-C2D	-2.13	1.46	1.50
14	b	516	CLA	MG-NB	-2.13	2.01	2.05
14	4	519	CLA	CMC-C2C	-2.13	1.46	1.50
14	c	513	CLA	CMD-C2D	-2.13	1.46	1.50
14	e	1103	CLA	C1B-C2B	2.13	1.48	1.43
14	f	1205	CLA	C1B-NB	-2.13	1.35	1.37
14	5	516	CLA	MG-NB	-2.13	2.01	2.05
21	Z	822	SQD	O3-C3	-2.13	1.38	1.43
14	c	513	CLA	CMB-C2B	-2.13	1.46	1.50
14	s	518	CLA	CMC-C2C	-2.13	1.46	1.50
14	3	503	CLA	CHC-C1C	2.13	1.42	1.38
14	d	506	CLA	CHC-C1C	2.13	1.42	1.38
14	A	1237	CLA	C1B-NB	-2.13	1.35	1.37
14	1	510	CLA	CMD-C2D	-2.13	1.46	1.50
14	4	509	CLA	MG-NB	-2.13	2.01	2.05
14	G	1109	CLA	MG-ND	-2.13	2.01	2.05
14	t	509	CLA	MG-NB	-2.13	2.01	2.05
14	e	1139	CLA	CHC-C1C	2.13	1.42	1.38
14	G	1128	CLA	C3B-C4B	2.13	1.47	1.42
14	f	1215	CLA	CMC-C2C	-2.13	1.46	1.50
14	r	508	CLA	CMD-C2D	-2.13	1.46	1.50
14	H	1209	CLA	CHC-C1C	2.13	1.42	1.38
14	d	518	CLA	CMB-C2B	-2.13	1.46	1.50
14	H	1230	CLA	MG-ND	-2.13	2.01	2.05
14	1	504	CLA	CMD-C2D	-2.13	1.46	1.50
14	q	504	CLA	CMD-C2D	-2.13	1.46	1.50
14	v	504	CLA	CHC-C1C	2.13	1.42	1.38
14	1	510	CLA	CMB-C2B	-2.13	1.46	1.50
14	f	1211	CLA	MG-ND	-2.13	2.01	2.05
17	V	4020	BCR	C21-C22	-2.13	1.33	1.35
14	B	1210	CLA	C1B-C2B	2.13	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	509	CLA	CHC-C1C	2.13	1.42	1.38
14	d	512	CLA	CMD-C2D	-2.13	1.46	1.50
14	t	511	CLA	CMB-C2B	-2.13	1.46	1.50
14	Z	513	CLA	CMB-C2B	-2.13	1.46	1.50
14	a	518	CLA	CMC-C2C	-2.13	1.46	1.50
14	f	1209	CLA	CHC-C1C	2.13	1.42	1.38
14	f	1213	CLA	CHC-C1C	2.13	1.42	1.38
14	f	1210	CLA	C1B-C2B	2.13	1.48	1.43
14	3	511	CLA	CMB-C2B	-2.13	1.46	1.50
14	4	511	CLA	CMB-C2B	-2.13	1.46	1.50
14	Y	517	CLA	CMB-C2B	-2.13	1.46	1.50
14	a	510	CLA	CMD-C2D	-2.13	1.46	1.50
14	Z	509	CLA	C1B-NB	-2.13	1.35	1.37
21	b	822	SQD	O2-C2	-2.13	1.38	1.43
14	e	1139	CLA	MG-ND	-2.13	2.01	2.05
14	J	1303	CLA	CMD-C2D	-2.13	1.46	1.50
14	2	504	CLA	CMB-C2B	-2.13	1.46	1.50
14	b	513	CLA	CHC-C1C	2.12	1.42	1.38
18	V	5220	LHG	O7-C5	-2.12	1.41	1.46
14	A	1131	CLA	CMC-C2C	-2.12	1.46	1.50
14	3	501	CLA	CMC-C2C	-2.12	1.46	1.50
14	Y	510	CLA	CMB-C2B	-2.12	1.46	1.50
14	Z	518	CLA	CMD-C2D	-2.12	1.46	1.50
14	G	1133	CLA	C1B-C2B	2.12	1.48	1.43
14	Z	508	CLA	MG-ND	-2.12	2.01	2.05
14	c	516	CLA	MG-NB	-2.12	2.01	2.05
14	c	518	CLA	CMB-C2B	-2.12	1.46	1.50
17	A	4008	BCR	C21-C22	-2.12	1.33	1.35
14	e	1132	CLA	CMB-C2B	-2.12	1.46	1.50
14	v	509	CLA	CMC-C2C	-2.12	1.46	1.50
14	B	1012	CLA	MG-ND	-2.12	2.01	2.05
14	2	510	CLA	CMD-C2D	-2.12	1.46	1.50
14	f	1204	CLA	CMB-C2B	-2.12	1.46	1.50
18	n	5220	LHG	O7-C5	-2.12	1.41	1.46
14	A	1801	CLA	CMD-C2D	-2.12	1.46	1.50
14	1	516	CLA	CMB-C2B	-2.12	1.46	1.50
14	2	508	CLA	CMD-C2D	-2.12	1.46	1.50
14	6	511	CLA	CMB-C2B	-2.12	1.46	1.50
14	G	1105	CLA	CMC-C2C	-2.12	1.46	1.50
14	a	509	CLA	CMB-C2B	-2.12	1.46	1.50
14	A	1128	CLA	C3B-C4B	2.12	1.47	1.42
14	H	1220	CLA	CMB-C2B	-2.12	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1122	CLA	MG-ND	-2.12	2.01	2.05
14	t	501	CLA	MG-NB	-2.12	2.01	2.05
14	5	517	CLA	CHC-C1C	2.12	1.42	1.38
14	B	1218	CLA	CMC-C2C	-2.12	1.46	1.50
14	t	509	CLA	CMB-C2B	-2.12	1.46	1.50
14	v	513	CLA	MG-NB	-2.12	2.01	2.05
14	5	511	CLA	CMB-C2B	-2.12	1.46	1.50
14	H	1211	CLA	CMC-C2C	-2.12	1.46	1.50
14	u	508	CLA	CMD-C2D	-2.12	1.46	1.50
14	G	1237	CLA	C1B-NB	-2.12	1.35	1.37
14	t	519	CLA	CMC-C2C	-2.12	1.46	1.50
14	H	1226	CLA	CHC-C4B	-2.12	1.34	1.39
14	B	1209	CLA	CHC-C1C	2.12	1.42	1.38
14	G	1139	CLA	C1B-C2B	2.12	1.48	1.43
14	2	513	CLA	CMB-C2B	-2.12	1.46	1.50
14	G	1123	CLA	CMC-C2C	-2.12	1.46	1.50
14	Z	508	CLA	CMD-C2D	-2.12	1.46	1.50
14	e	1801	CLA	CMB-C2B	-2.12	1.46	1.50
14	q	516	CLA	CMB-C2B	-2.12	1.46	1.50
14	u	507	CLA	CMD-C2D	-2.12	1.46	1.50
14	A	1237	CLA	CAC-C3C	-2.12	1.45	1.51
14	H	1209	CLA	C1B-C2B	2.12	1.48	1.43
14	e	1111	CLA	MG-ND	-2.12	2.01	2.05
14	F	1302	CLA	CMC-C2C	-2.12	1.46	1.50
14	5	517	CLA	CMD-C2D	-2.12	1.46	1.50
14	q	513	CLA	CMC-C2C	-2.12	1.46	1.50
14	t	512	CLA	CMB-C2B	-2.12	1.46	1.50
14	6	506	CLA	CHC-C1C	2.12	1.42	1.38
14	A	1112	CLA	MG-ND	-2.12	2.01	2.05
14	F	1301	CLA	CMC-C2C	-2.12	1.46	1.50
14	G	1104	CLA	CMB-C2B	-2.12	1.46	1.50
14	u	513	CLA	CMC-C2C	-2.12	1.46	1.50
18	L	5220	LHG	O7-C5	-2.12	1.41	1.46
14	H	1206	CLA	CAC-C3C	-2.12	1.45	1.51
14	f	1206	CLA	CAC-C3C	-2.12	1.45	1.51
14	G	1134	CLA	MG-NB	-2.12	2.01	2.05
14	R	1302	CLA	CMC-C2C	-2.12	1.46	1.50
14	c	509	CLA	CMB-C2B	-2.12	1.46	1.50
14	s	511	CLA	CMB-C2B	-2.12	1.46	1.50
14	G	1139	CLA	CHC-C1C	2.12	1.42	1.38
14	A	1104	CLA	CMB-C2B	-2.12	1.46	1.50
14	6	509	CLA	CMD-C2D	-2.12	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1104	CLA	CMB-C2B	-2.12	1.46	1.50
14	f	1239	CLA	CMD-C2D	-2.12	1.46	1.50
17	L	4020	BCR	C21-C22	-2.12	1.33	1.35
14	j	1301	CLA	CMC-C2C	-2.12	1.46	1.50
14	3	517	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	1239	CLA	CMD-C2D	-2.12	1.46	1.50
14	Y	519	CLA	CMB-C2B	-2.12	1.46	1.50
14	c	517	CLA	CMD-C2D	-2.12	1.46	1.50
14	A	1114	CLA	C1B-NB	-2.11	1.35	1.37
14	s	503	CLA	CHC-C1C	2.11	1.42	1.38
14	5	513	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	1106	CLA	C1B-NB	-2.11	1.35	1.37
14	H	1012	CLA	C1B-NB	-2.11	1.35	1.37
14	4	509	CLA	CMD-C2D	-2.11	1.46	1.50
14	2	508	CLA	MG-ND	-2.11	2.01	2.05
14	b	503	CLA	MG-NB	-2.11	2.01	2.05
14	5	508	CLA	CMD-C2D	-2.11	1.46	1.50
14	U	1401	CLA	CMD-C2D	-2.11	1.46	1.50
14	u	503	CLA	CMD-C2D	-2.11	1.46	1.50
14	G	1114	CLA	C1B-NB	-2.11	1.35	1.37
14	G	1118	CLA	C1B-NB	-2.11	1.35	1.37
14	B	1211	CLA	MG-ND	-2.11	2.01	2.05
14	c	504	CLA	MG-NB	-2.11	2.01	2.05
14	B	1206	CLA	CAC-C3C	-2.11	1.45	1.51
14	e	1116	CLA	MG-ND	-2.11	2.01	2.05
14	1	519	CLA	CMB-C2B	-2.11	1.46	1.50
14	3	509	CLA	CMB-C2B	-2.11	1.46	1.50
14	G	1116	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	1134	CLA	CMC-C2C	-2.11	1.46	1.50
14	T	1303	CLA	CMD-C2D	-2.11	1.46	1.50
14	d	511	CLA	CMB-C2B	-2.11	1.46	1.50
14	r	504	CLA	CMD-C2D	-2.11	1.46	1.50
14	f	1209	CLA	C1B-C2B	2.11	1.48	1.43
14	e	1106	CLA	MG-ND	-2.11	2.01	2.05
14	e	1237	CLA	CAC-C3C	-2.11	1.45	1.51
14	A	1139	CLA	CHC-C1C	2.11	1.42	1.38
14	s	509	CLA	CMB-C2B	-2.11	1.46	1.50
14	f	1210	CLA	MG-ND	-2.11	2.01	2.05
14	4	501	CLA	CMB-C2B	-2.11	1.46	1.50
14	6	518	CLA	CMB-C2B	-2.11	1.46	1.50
14	Z	501	CLA	CMB-C2B	-2.11	1.46	1.50
14	G	1111	CLA	MG-ND	-2.11	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1114	CLA	C1B-NB	-2.11	1.35	1.37
17	V	4219	BCR	C14-C13	-2.11	1.33	1.35
14	A	1138	CLA	CHC-C1C	2.11	1.42	1.38
14	T	1303	CLA	CMC-C2C	-2.11	1.46	1.50
14	c	508	CLA	CMD-C2D	-2.11	1.46	1.50
14	G	1116	CLA	MG-ND	-2.11	2.01	2.05
14	H	1205	CLA	MG-ND	-2.11	2.01	2.05
14	H	1211	CLA	MG-ND	-2.11	2.01	2.05
17	n	4020	BCR	C21-C22	-2.11	1.33	1.35
14	1	513	CLA	CMC-C2C	-2.11	1.46	1.50
14	Z	509	CLA	CMC-C2C	-2.11	1.46	1.50
14	v	501	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	1013	CLA	CHC-C1C	2.11	1.42	1.38
14	2	513	CLA	CHC-C1C	2.11	1.42	1.38
21	n	5216	SQD	O4-C4	-2.11	1.38	1.43
14	r	508	CLA	C1B-NB	-2.11	1.35	1.37
14	Z	504	CLA	CMB-C2B	-2.11	1.46	1.50
14	b	510	CLA	CMD-C2D	-2.11	1.46	1.50
14	e	1126	CLA	MG-ND	-2.11	2.01	2.05
14	Z	513	CLA	CHC-C1C	2.11	1.42	1.38
14	e	1138	CLA	CHC-C1C	2.11	1.42	1.38
14	K	1401	CLA	CMD-C2D	-2.11	1.46	1.50
14	b	508	CLA	CMD-C2D	-2.11	1.46	1.50
14	H	1012	CLA	MG-ND	-2.11	2.01	2.05
14	j	1301	CLA	C1B-NB	-2.11	1.35	1.37
14	u	512	CLA	CMB-C2B	-2.11	1.46	1.50
14	G	1114	CLA	CMC-C2C	-2.11	1.46	1.50
14	H	1204	CLA	CMB-C2B	-2.11	1.46	1.50
14	b	516	CLA	CMD-C2D	-2.11	1.46	1.50
14	e	1140	CLA	C1B-C2B	2.11	1.48	1.43
14	m	1105	CLA	C3C-C2C	2.11	1.41	1.36
14	B	1205	CLA	MG-ND	-2.11	2.01	2.05
14	4	516	CLA	CMD-C2D	-2.11	1.46	1.50
14	b	501	CLA	CMB-C2B	-2.11	1.46	1.50
14	G	1120	CLA	C1B-NB	-2.11	1.35	1.37
14	e	1120	CLA	C1B-NB	-2.11	1.35	1.37
14	4	513	CLA	CHC-C1C	2.11	1.42	1.38
14	t	509	CLA	CHC-C1C	2.11	1.42	1.38
14	2	511	CLA	CMD-C2D	-2.10	1.46	1.50
14	6	509	CLA	CMC-C2C	-2.10	1.46	1.50
14	Z	510	CLA	CMD-C2D	-2.10	1.46	1.50
14	3	510	CLA	CMD-C2D	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5	518	CLA	CMB-C2B	-2.10	1.46	1.50
14	G	1112	CLA	C1B-NB	-2.10	1.35	1.37
14	e	1121	CLA	C1B-NB	-2.10	1.35	1.37
14	H	1213	CLA	CHC-C1C	2.10	1.42	1.38
14	5	513	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	504	CLA	CMB-C2B	-2.10	1.46	1.50
14	r	510	CLA	CMD-C2D	-2.10	1.46	1.50
14	f	1205	CLA	MG-ND	-2.10	2.01	2.05
14	G	1140	CLA	C1B-C2B	2.10	1.48	1.43
14	t	509	CLA	C1B-NB	-2.10	1.35	1.37
14	B	1229	CLA	CMC-C2C	-2.10	1.46	1.50
14	G	1137	CLA	CMC-C2C	-2.10	1.46	1.50
14	r	508	CLA	MG-ND	-2.10	2.01	2.05
14	B	1204	CLA	CMB-C2B	-2.10	1.46	1.50
14	H	1229	CLA	CMC-C2C	-2.10	1.46	1.50
14	c	511	CLA	CMB-C2B	-2.10	1.46	1.50
14	e	1801	CLA	CMD-C2D	-2.10	1.46	1.50
14	3	504	CLA	CMB-C2B	-2.10	1.46	1.50
14	5	509	CLA	CMB-C2B	-2.10	1.46	1.50
14	t	511	CLA	CHC-C1C	2.10	1.42	1.38
14	H	1204	CLA	CMC-C2C	-2.10	1.46	1.50
14	u	516	CLA	CMD-C2D	-2.10	1.46	1.50
14	A	1120	CLA	C1B-NB	-2.10	1.35	1.37
14	R	1301	CLA	C1B-NB	-2.10	1.35	1.37
14	G	1237	CLA	CAC-C3C	-2.10	1.45	1.51
17	G	4002	BCR	C30-C25	-2.10	1.50	1.53
14	A	1139	CLA	C1B-C2B	2.10	1.48	1.43
14	H	1206	CLA	C3B-C4B	2.10	1.47	1.42
14	B	1213	CLA	CHC-C1C	2.10	1.42	1.38
14	6	513	CLA	MG-NB	-2.10	2.01	2.05
14	J	1303	CLA	CMC-C2C	-2.10	1.46	1.50
14	s	510	CLA	CMD-C2D	-2.10	1.46	1.50
14	B	1222	CLA	C1B-C2B	2.10	1.48	1.43
14	A	1116	CLA	MG-ND	-2.10	2.01	2.05
14	G	1106	CLA	MG-ND	-2.10	2.01	2.05
14	H	1218	CLA	CMC-C2C	-2.10	1.46	1.50
14	b	502	CLA	CMC-C2C	-2.10	1.46	1.50
14	t	516	CLA	CMD-C2D	-2.10	1.46	1.50
14	v	516	CLA	CHC-C1C	2.10	1.42	1.38
14	G	1121	CLA	CMC-C2C	-2.10	1.46	1.50
14	m	1401	CLA	CMD-C2D	-2.10	1.46	1.50
14	e	1117	CLA	MG-ND	-2.10	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	e	4008	BCR	C21-C22	-2.10	1.33	1.35
14	A	1105	CLA	CMB-C2B	-2.10	1.46	1.50
14	Z	504	CLA	CMD-C2D	-2.10	1.46	1.50
14	e	1105	CLA	CMB-C2B	-2.10	1.46	1.50
14	v	519	CLA	CMC-C2C	-2.10	1.46	1.50
14	e	1115	CLA	MG-ND	-2.10	2.01	2.05
14	f	1222	CLA	C1B-C2B	2.10	1.48	1.43
14	6	501	CLA	CMB-C2B	-2.10	1.46	1.50
14	n	1501	CLA	CMC-C2C	-2.10	1.46	1.50
14	K	1105	CLA	C3C-C2C	2.10	1.41	1.36
14	4	501	CLA	MG-NB	-2.10	2.01	2.05
21	n	5216	SQD	O3-C3	-2.10	1.38	1.43
14	f	1023	CLA	C1B-C2B	2.10	1.48	1.43
14	a	504	CLA	CHC-C1C	2.10	1.42	1.38
14	1	517	CLA	CMD-C2D	-2.10	1.46	1.50
14	e	1237	CLA	C3B-C4B	2.10	1.47	1.42
14	G	1130	CLA	CHC-C1C	2.10	1.42	1.38
14	1	517	CLA	CMB-C2B	-2.10	1.46	1.50
17	S	4018	BCR	C30-C25	-2.10	1.50	1.53
14	B	1204	CLA	CMC-C2C	-2.10	1.46	1.50
14	1	504	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	519	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	503	CLA	CHC-C1C	2.10	1.42	1.38
14	A	1115	CLA	MG-ND	-2.10	2.01	2.05
14	a	511	CLA	CMB-C2B	-2.10	1.46	1.50
14	A	1106	CLA	MG-ND	-2.10	2.01	2.05
14	2	504	CLA	CMD-C2D	-2.10	1.46	1.50
14	G	1105	CLA	CMB-C2B	-2.10	1.46	1.50
14	H	1231	CLA	CMC-C2C	-2.10	1.46	1.50
14	e	1121	CLA	CMC-C2C	-2.10	1.46	1.50
14	t	501	CLA	CMB-C2B	-2.10	1.46	1.50
14	c	506	CLA	CHC-C1C	2.10	1.42	1.38
14	f	1217	CLA	CHC-C1C	2.10	1.42	1.38
14	e	1109	CLA	MG-ND	-2.10	2.01	2.05
14	f	1223	CLA	MG-ND	-2.10	2.01	2.05
14	B	1023	CLA	C1B-C2B	2.10	1.48	1.43
14	Y	510	CLA	CHC-C1C	2.10	1.42	1.38
21	s	822	SQD	O3-C3	-2.10	1.38	1.43
14	2	509	CLA	CMC-C2C	-2.10	1.46	1.50
14	6	510	CLA	CMB-C2B	-2.10	1.46	1.50
21	L	5216	SQD	O3-C3	-2.10	1.38	1.43
14	G	1125	CLA	C1B-C2B	2.09	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1222	CLA	C1B-C2B	2.09	1.48	1.43
14	d	511	CLA	CHC-C1C	2.09	1.42	1.38
14	s	511	CLA	CHC-C1C	2.09	1.42	1.38
14	f	1216	CLA	C1B-NB	-2.09	1.35	1.37
14	r	512	CLA	C1B-NB	-2.09	1.35	1.37
14	G	1102	CLA	MG-ND	-2.09	2.01	2.05
14	f	1218	CLA	CMC-C2C	-2.09	1.46	1.50
14	e	1128	CLA	C3B-C4B	2.09	1.47	1.42
14	d	501	CLA	CMD-C2D	-2.09	1.46	1.50
14	d	510	CLA	CMB-C2B	-2.09	1.46	1.50
14	f	1240	CLA	CMB-C2B	-2.09	1.46	1.50
20	J	5104	LMG	O8-C9	-2.09	1.40	1.45
14	f	1204	CLA	CMC-C2C	-2.09	1.46	1.50
14	e	1122	CLA	C1B-NB	-2.09	1.35	1.37
14	a	509	CLA	CHC-C1C	2.09	1.42	1.38
14	B	1206	CLA	C3B-C4B	2.09	1.47	1.42
14	H	1228	CLA	CMC-C2C	-2.09	1.46	1.50
14	Z	511	CLA	CMD-C2D	-2.09	1.46	1.50
14	e	1133	CLA	C1B-C2B	2.09	1.48	1.43
14	A	1117	CLA	MG-ND	-2.09	2.01	2.05
14	G	1131	CLA	CMC-C2C	-2.09	1.46	1.50
14	Y	513	CLA	CMB-C2B	-2.09	1.46	1.50
14	u	510	CLA	CMD-C2D	-2.09	1.46	1.50
14	v	516	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	1217	CLA	CHC-C1C	2.09	1.42	1.38
14	v	506	CLA	CHC-C1C	2.09	1.42	1.38
14	B	1227	CLA	CMC-C2C	-2.09	1.46	1.50
14	r	504	CLA	CMB-C2B	-2.09	1.46	1.50
14	b	501	CLA	MG-NB	-2.09	2.01	2.05
21	2	822	SQD	O3-C3	-2.09	1.38	1.43
14	G	1112	CLA	C1B-C2B	2.09	1.48	1.43
20	T	5104	LMG	O8-C9	-2.09	1.40	1.45
14	r	513	CLA	CMB-C2B	-2.09	1.46	1.50
17	n	4020	BCR	C10-C9	-2.09	1.33	1.35
14	A	1140	CLA	C1B-C2B	2.09	1.48	1.43
20	l	5104	LMG	O8-C9	-2.09	1.40	1.45
14	e	1112	CLA	MG-ND	-2.09	2.01	2.05
14	e	1125	CLA	C1B-C2B	2.09	1.48	1.43
17	G	4008	BCR	C21-C22	-2.09	1.33	1.35
14	6	501	CLA	CMD-C2D	-2.09	1.46	1.50
14	a	517	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	1125	CLA	C1B-C2B	2.09	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	d	504	CLA	CHC-C1C	2.09	1.42	1.38
14	3	508	CLA	CMD-C2D	-2.09	1.46	1.50
14	5	512	CLA	CMB-C2B	-2.09	1.46	1.50
14	q	519	CLA	CMB-C2B	-2.09	1.46	1.50
14	r	516	CLA	CMD-C2D	-2.09	1.46	1.50
14	G	1106	CLA	C1B-NB	-2.09	1.35	1.37
14	q	513	CLA	CMD-C2D	-2.09	1.46	1.50
14	v	518	CLA	CMB-C2B	-2.09	1.46	1.50
14	F	1301	CLA	C1B-NB	-2.09	1.35	1.37
14	H	1211	CLA	C1B-NB	-2.09	1.35	1.37
14	5	509	CLA	CHC-C1C	2.09	1.42	1.38
14	4	504	CLA	CMB-C2B	-2.09	1.46	1.50
14	e	1114	CLA	CMC-C2C	-2.09	1.46	1.50
14	e	1139	CLA	C1B-C2B	2.09	1.48	1.43
21	r	822	SQD	O3-C3	-2.09	1.38	1.43
14	3	519	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	508	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	1209	CLA	C1B-NB	-2.09	1.35	1.37
14	A	1123	CLA	CMC-C2C	-2.09	1.46	1.50
14	r	511	CLA	CMD-C2D	-2.09	1.46	1.50
14	v	509	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	1113	CLA	CMB-C2B	-2.09	1.46	1.50
14	L	1501	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	507	CLA	CMD-C2D	-2.09	1.46	1.50
14	s	504	CLA	CMB-C2B	-2.09	1.46	1.50
14	e	1118	CLA	C1B-NB	-2.09	1.35	1.37
14	T	1302	CLA	CMC-C2C	-2.09	1.46	1.50
14	t	509	CLA	CMD-C2D	-2.09	1.46	1.50
14	2	508	CLA	C1B-NB	-2.09	1.35	1.37
14	4	509	CLA	CHC-C1C	2.09	1.42	1.38
14	G	1013	CLA	CHC-C1C	2.09	1.42	1.38
14	Y	513	CLA	CMC-C2C	-2.09	1.46	1.50
14	f	1231	CLA	CMC-C2C	-2.09	1.46	1.50
14	v	508	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	1133	CLA	C1B-C2B	2.09	1.48	1.43
14	A	1114	CLA	CMC-C2C	-2.09	1.46	1.50
14	3	513	CLA	CMB-C2B	-2.09	1.46	1.50
14	a	517	CLA	CHC-C1C	2.09	1.42	1.38
14	c	509	CLA	CHC-C1C	2.09	1.42	1.38
14	V	1502	CLA	C1B-NB	-2.09	1.35	1.37
14	Y	504	CLA	CMC-C2C	-2.09	1.46	1.50
14	Y	517	CLA	CMD-C2D	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	e	1113	CLA	CMB-C2B	-2.09	1.46	1.50
14	q	501	CLA	CMB-C2B	-2.09	1.46	1.50
14	u	501	CLA	CMD-C2D	-2.09	1.46	1.50
14	s	508	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	1232	CLA	MG-ND	-2.08	2.01	2.05
14	Z	508	CLA	C1B-C2B	2.08	1.48	1.43
14	c	506	CLA	CMD-C2D	-2.08	1.46	1.50
14	d	519	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	1112	CLA	C1B-C2B	2.08	1.48	1.43
14	u	517	CLA	CHC-C1C	2.08	1.42	1.38
14	J	1302	CLA	CMC-C2C	-2.08	1.46	1.50
14	Y	503	CLA	CMB-C2B	-2.08	1.46	1.50
14	a	508	CLA	C1B-NB	-2.08	1.35	1.37
14	e	1132	CLA	C1B-NB	-2.08	1.35	1.37
14	4	511	CLA	CHC-C1C	2.08	1.42	1.38
14	f	1206	CLA	CHC-C4B	-2.08	1.34	1.39
14	A	1022	CLA	O2D-CED	-2.08	1.40	1.45
14	6	519	CLA	CMD-C2D	-2.08	1.46	1.50
14	G	1801	CLA	CMD-C2D	-2.08	1.46	1.50
14	s	517	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	1132	CLA	C1B-NB	-2.08	1.35	1.37
14	c	508	CLA	C1B-NB	-2.08	1.35	1.37
14	e	1022	CLA	O2D-CED	-2.08	1.40	1.45
14	f	1229	CLA	CMC-C2C	-2.08	1.46	1.50
14	H	1223	CLA	MG-ND	-2.08	2.01	2.05
14	e	1123	CLA	CMC-C2C	-2.08	1.46	1.50
14	n	1502	CLA	CHC-C1C	2.08	1.42	1.38
14	s	508	CLA	MG-ND	-2.08	2.01	2.05
14	4	508	CLA	C1B-NB	-2.08	1.35	1.37
14	G	1111	CLA	C1B-NB	-2.08	1.35	1.37
14	d	509	CLA	CMB-C2B	-2.08	1.46	1.50
21	4	822	SQD	O4-C4	-2.08	1.38	1.43
14	3	509	CLA	CHC-C1C	2.08	1.42	1.38
14	B	1223	CLA	MG-ND	-2.08	2.01	2.05
14	Y	501	CLA	CMB-C2B	-2.08	1.46	1.50
14	a	513	CLA	CMB-C2B	-2.08	1.46	1.50
14	H	1023	CLA	C1B-C2B	2.08	1.48	1.43
14	A	1130	CLA	CHC-C1C	2.08	1.42	1.38
14	b	511	CLA	CHC-C1C	2.08	1.42	1.38
14	b	516	CLA	CHC-C1C	2.08	1.42	1.38
14	n	1503	CLA	MG-ND	-2.08	2.01	2.05
14	Z	506	CLA	CMD-C2D	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	c	507	CLA	CMB-C2B	-2.08	1.46	1.50
14	u	518	CLA	CMB-C2B	-2.08	1.46	1.50
14	L	1502	CLA	CHC-C1C	2.08	1.42	1.38
14	c	505	CLA	CHC-C1C	2.08	1.42	1.38
14	e	1801	CLA	CHC-C1C	2.08	1.42	1.38
21	a	822	SQD	O3-C3	-2.08	1.38	1.43
14	A	1237	CLA	C3B-C4B	2.08	1.47	1.42
14	H	1210	CLA	CHC-C1C	2.08	1.42	1.38
14	B	1210	CLA	MG-ND	-2.08	2.01	2.05
14	G	1115	CLA	MG-ND	-2.08	2.01	2.05
21	t	822	SQD	O4-C4	-2.08	1.38	1.43
14	2	508	CLA	C1B-C2B	2.08	1.48	1.43
14	A	1102	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	1231	CLA	CMC-C2C	-2.08	1.46	1.50
14	1	501	CLA	CMB-C2B	-2.08	1.46	1.50
14	G	1139	CLA	CMC-C2C	-2.08	1.46	1.50
14	v	504	CLA	CMD-C2D	-2.08	1.46	1.50
14	c	504	CLA	CHC-C1C	2.08	1.42	1.38
14	c	512	CLA	CMB-C2B	-2.08	1.46	1.50
14	G	1121	CLA	C3B-C4B	2.08	1.47	1.42
14	f	1023	CLA	C1B-NB	-2.08	1.35	1.37
14	B	1206	CLA	CHC-C4B	-2.08	1.34	1.39
14	d	504	CLA	CMD-C2D	-2.08	1.46	1.50
14	H	1210	CLA	MG-ND	-2.08	2.01	2.05
14	J	1302	CLA	CMD-C2D	-2.08	1.46	1.50
14	q	513	CLA	CMB-C2B	-2.08	1.46	1.50
14	q	518	CLA	CMD-C2D	-2.08	1.46	1.50
14	b	508	CLA	C1B-NB	-2.08	1.35	1.37
14	5	505	CLA	CHC-C1C	2.08	1.42	1.38
14	B	1240	CLA	CMB-C2B	-2.08	1.46	1.50
14	a	510	CLA	O2A-CGA	2.08	1.37	1.30
14	2	517	CLA	CMD-C2D	-2.08	1.46	1.50
14	c	513	CLA	CMC-C2C	-2.08	1.46	1.50
14	v	501	CLA	CMD-C2D	-2.08	1.46	1.50
14	1	509	CLA	CMD-C2D	-2.08	1.46	1.50
14	3	507	CLA	CMD-C2D	-2.08	1.46	1.50
14	Y	510	CLA	CMC-C2C	-2.08	1.46	1.50
14	t	507	CLA	CMD-C2D	-2.08	1.46	1.50
14	e	1104	CLA	CHC-C1C	2.08	1.42	1.38
14	u	505	CLA	CHC-C1C	2.08	1.42	1.38
14	A	1118	CLA	C1B-NB	-2.08	1.35	1.37
21	V	5216	SQD	O3-C3	-2.08	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	513	CLA	CMB-C2B	-2.08	1.46	1.50
14	d	509	CLA	CMC-C2C	-2.08	1.46	1.50
14	u	509	CLA	CMB-C2B	-2.08	1.46	1.50
14	H	1204	CLA	MG-ND	-2.08	2.01	2.05
14	e	1013	CLA	CHC-C1C	2.07	1.42	1.38
14	d	519	CLA	CMD-C2D	-2.07	1.46	1.50
14	5	510	CLA	CMB-C2B	-2.07	1.46	1.50
14	v	510	CLA	CMB-C2B	-2.07	1.46	1.50
14	v	501	CLA	CHC-C1C	2.07	1.42	1.38
14	3	510	CLA	O2A-CGA	2.07	1.37	1.30
14	A	1111	CLA	C1B-NB	-2.07	1.35	1.37
14	H	1227	CLA	C1B-NB	-2.07	1.35	1.37
14	f	1210	CLA	C1B-NB	-2.07	1.35	1.37
14	a	506	CLA	CMD-C2D	-2.07	1.46	1.50
14	d	516	CLA	CHC-C1C	2.07	1.42	1.38
14	f	1210	CLA	CHC-C1C	2.07	1.42	1.38
14	s	510	CLA	O2A-CGA	2.07	1.37	1.30
14	U	1105	CLA	C3C-C2C	2.07	1.41	1.36
14	A	1126	CLA	CMB-C2B	-2.07	1.46	1.50
14	4	513	CLA	CMD-C2D	-2.07	1.46	1.50
14	q	517	CLA	CMB-C2B	-2.07	1.46	1.50
14	f	1206	CLA	C3B-C4B	2.07	1.47	1.42
21	u	822	SQD	O4-C4	-2.07	1.38	1.43
14	6	519	CLA	CMC-C2C	-2.07	1.46	1.50
14	d	501	CLA	CMB-C2B	-2.07	1.46	1.50
14	t	502	CLA	CMC-C2C	-2.07	1.46	1.50
14	6	516	CLA	CHC-C1C	2.07	1.42	1.38
17	V	4020	BCR	C10-C9	-2.07	1.33	1.35
14	G	1237	CLA	C3B-C4B	2.07	1.47	1.42
14	4	508	CLA	CMD-C2D	-2.07	1.46	1.50
14	H	1240	CLA	CMB-C2B	-2.07	1.46	1.50
14	b	518	CLA	CMB-C2B	-2.07	1.46	1.50
14	d	510	CLA	CMC-C2C	-2.07	1.46	1.50
14	e	1102	CLA	CMB-C2B	-2.07	1.46	1.50
14	A	1121	CLA	CMC-C2C	-2.07	1.46	1.50
14	4	510	CLA	CMD-C2D	-2.07	1.46	1.50
14	G	1126	CLA	CMB-C2B	-2.07	1.46	1.50
14	d	508	CLA	CMD-C2D	-2.07	1.46	1.50
14	e	1126	CLA	CMB-C2B	-2.07	1.46	1.50
14	t	504	CLA	CMB-C2B	-2.07	1.46	1.50
21	c	822	SQD	O4-C4	-2.07	1.38	1.43
14	e	1111	CLA	C1B-NB	-2.07	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	513	CLA	CMD-C2D	-2.07	1.46	1.50
14	b	509	CLA	CHC-C1C	2.07	1.42	1.38
14	s	517	CLA	CHC-C1C	2.07	1.42	1.38
21	5	822	SQD	O4-C4	-2.07	1.38	1.43
14	B	1202	CLA	MG-NB	-2.07	2.01	2.05
14	L	1502	CLA	C1B-NB	-2.07	1.35	1.37
14	H	1206	CLA	CHC-C4B	-2.07	1.34	1.39
14	A	1122	CLA	MG-ND	-2.07	2.01	2.05
14	5	503	CLA	CMB-C2B	-2.07	1.46	1.50
14	q	517	CLA	CMD-C2D	-2.07	1.46	1.50
21	Y	822	SQD	O3-C3	-2.07	1.38	1.43
14	l	1303	CLA	CMC-C2C	-2.07	1.46	1.50
14	b	505	CLA	MG-ND	-2.07	2.01	2.05
14	1	510	CLA	CHC-C1C	2.07	1.42	1.38
14	f	1208	CLA	CHC-C1C	2.07	1.42	1.38
14	1	503	CLA	CMB-C2B	-2.07	1.46	1.50
14	s	509	CLA	CHC-C1C	2.07	1.42	1.38
14	t	508	CLA	CMD-C2D	-2.07	1.46	1.50
14	t	518	CLA	CMB-C2B	-2.07	1.46	1.50
14	A	1112	CLA	C1B-NB	-2.07	1.35	1.37
14	G	1117	CLA	MG-ND	-2.07	2.01	2.05
14	G	1022	CLA	O2D-CED	-2.07	1.40	1.45
14	q	512	CLA	C1B-NB	-2.07	1.35	1.37
14	A	1104	CLA	MG-ND	-2.07	2.01	2.05
14	2	506	CLA	CMD-C2D	-2.07	1.46	1.50
14	6	504	CLA	CMD-C2D	-2.07	1.46	1.50
14	f	1202	CLA	MG-NB	-2.07	2.01	2.05
14	Z	510	CLA	CHC-C1C	2.07	1.42	1.38
14	q	510	CLA	CHC-C1C	2.07	1.42	1.38
18	n	5218	LHG	P-O6	2.07	1.67	1.59
14	d	513	CLA	CMD-C2D	-2.07	1.46	1.50
14	b	508	CLA	MG-ND	-2.07	2.01	2.05
14	3	517	CLA	CHC-C1C	2.07	1.42	1.38
14	6	503	CLA	CMB-C2B	-2.07	1.46	1.50
14	T	1302	CLA	CMD-C2D	-2.07	1.46	1.50
14	c	519	CLA	CMB-C2B	-2.07	1.46	1.50
14	B	1210	CLA	C1B-NB	-2.07	1.35	1.37
14	B	1210	CLA	CHC-C1C	2.07	1.42	1.38
14	f	1227	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	1227	CLA	CHC-C1C	2.07	1.42	1.38
14	H	1208	CLA	CHC-C1C	2.07	1.42	1.38
18	L	5218	LHG	P-O6	2.07	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	d	822	SQD	O3-C3	-2.07	1.38	1.43
14	3	504	CLA	CHC-C1C	2.07	1.42	1.38
14	3	510	CLA	CHC-C1C	2.07	1.42	1.38
14	4	518	CLA	CMB-C2B	-2.07	1.46	1.50
14	r	517	CLA	CMB-C2B	-2.07	1.46	1.50
14	t	508	CLA	C1B-NB	-2.07	1.35	1.37
14	H	1202	CLA	MG-NB	-2.07	2.01	2.05
14	G	1115	CLA	CHC-C1C	2.07	1.42	1.38
14	4	502	CLA	CMD-C2D	-2.07	1.46	1.50
14	G	1104	CLA	CHC-C1C	2.06	1.42	1.38
14	H	1217	CLA	CMB-C2B	-2.06	1.46	1.50
14	d	510	CLA	CMD-C2D	-2.06	1.46	1.50
14	v	519	CLA	CMD-C2D	-2.06	1.46	1.50
14	m	1103	CLA	C1B-NB	-2.06	1.35	1.37
14	f	1220	CLA	MG-ND	-2.06	2.01	2.05
14	B	1217	CLA	CMB-C2B	-2.06	1.46	1.50
14	Y	513	CLA	CMD-C2D	-2.06	1.46	1.50
14	b	519	CLA	CMD-C2D	-2.06	1.46	1.50
14	u	510	CLA	CMB-C2B	-2.06	1.46	1.50
14	u	503	CLA	CHC-C1C	2.06	1.42	1.38
14	1	513	CLA	CMD-C2D	-2.06	1.46	1.50
14	4	519	CLA	CMD-C2D	-2.06	1.46	1.50
14	5	501	CLA	CMB-C2B	-2.06	1.46	1.50
14	t	519	CLA	CMD-C2D	-2.06	1.46	1.50
18	V	5218	LHG	P-O6	2.06	1.67	1.59
18	e	5008	LHG	P-O6	2.06	1.67	1.59
14	6	508	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	1104	CLA	CHC-C1C	2.06	1.42	1.38
14	e	1104	CLA	CAC-C3C	-2.06	1.45	1.51
21	b	822	SQD	O4-C4	-2.06	1.38	1.43
14	B	1212	CLA	CMB-C2B	-2.06	1.46	1.50
14	Z	519	CLA	CMD-C2D	-2.06	1.46	1.50
14	u	504	CLA	CMB-C2B	-2.06	1.46	1.50
14	5	507	CLA	CMB-C2B	-2.06	1.46	1.50
14	2	510	CLA	CHC-C1C	2.06	1.42	1.38
14	s	504	CLA	CHC-C1C	2.06	1.42	1.38
14	c	510	CLA	CMB-C2B	-2.06	1.46	1.50
14	t	513	CLA	CMD-C2D	-2.06	1.46	1.50
14	n	1501	CLA	MG-ND	-2.06	2.01	2.05
14	A	1139	CLA	CMC-C2C	-2.06	1.46	1.50
14	5	516	CLA	CMD-C2D	-2.06	1.46	1.50
14	Z	517	CLA	CMD-C2D	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	s	519	CLA	CMC-C2C	-2.06	1.46	1.50
14	V	1502	CLA	CHC-C1C	2.06	1.42	1.38
14	B	1012	CLA	C1B-NB	-2.06	1.35	1.37
14	3	508	CLA	C1B-NB	-2.06	1.35	1.37
14	d	516	CLA	CMD-C2D	-2.06	1.46	1.50
14	r	510	CLA	CMB-C2B	-2.06	1.46	1.50
14	v	513	CLA	CMD-C2D	-2.06	1.46	1.50
14	3	511	CLA	CHC-C1C	2.06	1.42	1.38
14	b	506	CLA	CHC-C1C	2.06	1.42	1.38
14	5	510	CLA	CMD-C2D	-2.06	1.46	1.50
14	b	504	CLA	CMB-C2B	-2.06	1.46	1.50
14	H	1239	CLA	C1B-NB	-2.06	1.35	1.37
14	J	1303	CLA	CHC-C1C	2.06	1.42	1.38
14	Y	512	CLA	MG-ND	-2.06	2.01	2.05
14	a	508	CLA	MG-ND	-2.06	2.01	2.05
14	H	1227	CLA	CHC-C1C	2.06	1.42	1.38
14	d	513	CLA	MG-NB	-2.06	2.01	2.05
14	q	508	CLA	MG-ND	-2.06	2.01	2.05
14	f	1012	CLA	C1B-NB	-2.06	1.35	1.37
21	Y	822	SQD	O4-C4	-2.06	1.38	1.43
14	a	505	CLA	CMC-C2C	-2.06	1.46	1.50
14	d	503	CLA	CMB-C2B	-2.06	1.46	1.50
14	B	1204	CLA	MG-ND	-2.06	2.01	2.05
21	q	822	SQD	O4-C4	-2.06	1.38	1.43
14	3	505	CLA	CMC-C2C	-2.06	1.46	1.50
14	c	501	CLA	CMB-C2B	-2.06	1.46	1.50
14	c	510	CLA	CMD-C2D	-2.06	1.46	1.50
14	f	1202	CLA	C1B-NB	-2.06	1.35	1.37
14	s	512	CLA	C1B-NB	-2.06	1.35	1.37
14	f	1238	CLA	C1B-C2B	2.06	1.48	1.43
14	6	509	CLA	CMB-C2B	-2.06	1.46	1.50
14	G	1113	CLA	CMB-C2B	-2.06	1.46	1.50
14	H	1212	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	5008	LHG	P-O6	2.06	1.67	1.59
14	5	512	CLA	CHC-C1C	2.06	1.42	1.38
21	1	822	SQD	O4-C4	-2.06	1.38	1.43
14	L	1503	CLA	MG-ND	-2.06	2.01	2.05
14	H	1220	CLA	MG-ND	-2.06	2.01	2.05
14	c	503	CLA	CMB-C2B	-2.06	1.46	1.50
14	e	1139	CLA	CMC-C2C	-2.06	1.46	1.50
14	r	513	CLA	CMC-C2C	-2.06	1.46	1.50
14	s	513	CLA	CMB-C2B	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	506	CLA	CHC-C1C	2.06	1.42	1.38
14	4	516	CLA	CHC-C1C	2.06	1.42	1.38
14	1	508	CLA	CMD-C2D	-2.06	1.46	1.50
14	3	506	CLA	CMD-C2D	-2.06	1.46	1.50
14	4	502	CLA	CMC-C2C	-2.06	1.46	1.50
14	A	1123	CLA	CMB-C2B	-2.06	1.46	1.50
14	f	1012	CLA	CMB-C2B	-2.06	1.46	1.50
14	r	506	CLA	CMD-C2D	-2.06	1.46	1.50
21	6	822	SQD	O3-C3	-2.06	1.38	1.43
14	G	1801	CLA	CHC-C1C	2.06	1.42	1.38
14	V	1501	CLA	MG-ND	-2.06	2.01	2.05
14	u	510	CLA	CMC-C2C	-2.06	1.46	1.50
17	f	4017	BCR	C30-C25	-2.06	1.50	1.53
14	4	508	CLA	MG-ND	-2.06	2.01	2.05
14	G	1102	CLA	CMB-C2B	-2.06	1.46	1.50
14	r	517	CLA	CMD-C2D	-2.06	1.46	1.50
21	3	822	SQD	O3-C3	-2.06	1.38	1.43
14	r	508	CLA	C1B-C2B	2.06	1.48	1.43
14	5	506	CLA	CHC-C1C	2.06	1.42	1.38
14	Y	509	CLA	CMD-C2D	-2.06	1.46	1.50
14	a	517	CLA	CMB-C2B	-2.06	1.46	1.50
14	f	1212	CLA	CMB-C2B	-2.06	1.46	1.50
14	f	1227	CLA	CHC-C1C	2.06	1.42	1.38
14	l	1303	CLA	CHC-C1C	2.06	1.42	1.38
14	2	513	CLA	CMC-C2C	-2.06	1.46	1.50
14	G	1120	CLA	CMB-C2B	-2.06	1.46	1.50
14	q	519	CLA	CMD-C2D	-2.06	1.46	1.50
14	s	507	CLA	CMD-C2D	-2.06	1.46	1.50
14	b	505	CLA	CHC-C1C	2.05	1.42	1.38
14	e	1130	CLA	CHC-C1C	2.05	1.42	1.38
14	5	501	CLA	CMD-C2D	-2.05	1.46	1.50
14	V	1501	CLA	CMC-C2C	-2.05	1.46	1.50
14	s	513	CLA	CMD-C2D	-2.05	1.46	1.50
14	B	1220	CLA	MG-ND	-2.05	2.01	2.05
14	4	505	CLA	MG-ND	-2.05	2.01	2.05
14	a	511	CLA	CHC-C1C	2.05	1.42	1.38
14	1	518	CLA	CMD-C2D	-2.05	1.46	1.50
14	v	505	CLA	CHC-C1C	2.05	1.42	1.38
14	6	516	CLA	CMD-C2D	-2.05	1.46	1.50
14	q	510	CLA	CMC-C2C	-2.05	1.46	1.50
14	1	508	CLA	MG-ND	-2.05	2.01	2.05
14	t	508	CLA	MG-ND	-2.05	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1232	CLA	CMC-C2C	-2.05	1.46	1.50
14	3	508	CLA	MG-ND	-2.05	2.01	2.05
14	G	1132	CLA	C1B-NB	-2.05	1.35	1.37
14	U	1103	CLA	C1B-NB	-2.05	1.35	1.37
14	e	1112	CLA	C1B-C2B	2.05	1.48	1.43
14	A	1104	CLA	CAC-C3C	-2.05	1.45	1.51
14	u	512	CLA	CHC-C1C	2.05	1.42	1.38
14	H	1228	CLA	CMB-C2B	-2.05	1.46	1.50
14	6	519	CLA	CHC-C1C	2.05	1.42	1.38
14	1	510	CLA	CMC-C2C	-2.05	1.46	1.50
14	c	517	CLA	CMB-C2B	-2.05	1.46	1.50
14	f	1204	CLA	MG-ND	-2.05	2.01	2.05
14	f	1235	CLA	MG-ND	-2.05	2.01	2.05
18	G	5008	LHG	P-O6	2.05	1.67	1.59
14	H	1213	CLA	C1B-NB	-2.05	1.35	1.37
14	K	1401	CLA	CMB-C2B	-2.05	1.46	1.50
14	Z	516	CLA	CMD-C2D	-2.05	1.46	1.50
14	l	1302	CLA	CMC-C2C	-2.05	1.46	1.50
14	q	505	CLA	CMC-C2C	-2.05	1.46	1.50
14	6	511	CLA	CHC-C1C	2.05	1.42	1.38
14	c	512	CLA	CHC-C1C	2.05	1.42	1.38
14	e	1104	CLA	MG-ND	-2.05	2.01	2.05
14	e	1122	CLA	MG-ND	-2.05	2.01	2.05
14	f	1232	CLA	MG-ND	-2.05	2.01	2.05
14	2	516	CLA	CMD-C2D	-2.05	1.46	1.50
14	L	1501	CLA	MG-ND	-2.05	2.01	2.05
14	c	516	CLA	CMD-C2D	-2.05	1.46	1.50
14	a	510	CLA	CHC-C1C	2.05	1.42	1.38
14	G	1104	CLA	MG-ND	-2.05	2.01	2.05
14	U	1401	CLA	CMB-C2B	-2.05	1.46	1.50
14	5	504	CLA	CHC-C1C	2.05	1.42	1.38
14	r	510	CLA	CHC-C1C	2.05	1.42	1.38
14	v	519	CLA	CHC-C1C	2.05	1.42	1.38
21	q	822	SQD	O3-C3	-2.05	1.38	1.43
14	1	519	CLA	CMC-C2C	-2.05	1.46	1.50
14	5	519	CLA	CMB-C2B	-2.05	1.46	1.50
14	b	513	CLA	CMD-C2D	-2.05	1.46	1.50
14	q	519	CLA	CMC-C2C	-2.05	1.46	1.50
14	e	1121	CLA	C3B-C4B	2.05	1.47	1.42
14	t	503	CLA	CHC-C1C	2.05	1.42	1.38
17	H	4017	BCR	C30-C25	-2.05	1.50	1.53
14	Y	519	CLA	CMC-C2C	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	r	511	CLA	CMC-C2C	-2.05	1.46	1.50
14	H	1216	CLA	C1B-NB	-2.05	1.35	1.37
14	u	509	CLA	CHC-C1C	2.05	1.42	1.38
17	L	4020	BCR	C10-C9	-2.05	1.33	1.35
14	A	1140	CLA	MG-ND	-2.05	2.01	2.05
14	B	1228	CLA	CMB-C2B	-2.05	1.46	1.50
14	H	1227	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	510	CLA	CMB-C2B	-2.05	1.46	1.50
14	v	516	CLA	CMB-C2B	-2.05	1.46	1.50
14	H	1217	CLA	CHC-C1C	2.05	1.42	1.38
14	t	518	CLA	CHC-C1C	2.05	1.42	1.38
14	G	1123	CLA	CMB-C2B	-2.05	1.46	1.50
14	Z	513	CLA	CMC-C2C	-2.05	1.46	1.50
14	s	510	CLA	CHC-C1C	2.05	1.42	1.38
14	e	1123	CLA	CMB-C2B	-2.05	1.46	1.50
14	f	1228	CLA	CMB-C2B	-2.05	1.46	1.50
14	G	1140	CLA	MG-ND	-2.05	2.01	2.05
14	A	1801	CLA	CHC-C1C	2.05	1.42	1.38
14	e	1120	CLA	CHC-C1C	2.05	1.42	1.38
14	A	1121	CLA	C3B-C4B	2.05	1.47	1.42
14	3	513	CLA	CMD-C2D	-2.05	1.46	1.50
14	b	516	CLA	CMB-C2B	-2.05	1.46	1.50
14	e	1120	CLA	CMB-C2B	-2.05	1.46	1.50
14	G	1104	CLA	CAC-C3C	-2.05	1.45	1.51
14	Y	508	CLA	MG-ND	-2.05	2.01	2.05
14	b	518	CLA	CHC-C1C	2.05	1.42	1.38
21	s	822	SQD	O4-C4	-2.05	1.38	1.43
14	1	505	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	506	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	507	CLA	CMB-C2B	-2.05	1.46	1.50
14	f	1232	CLA	CMC-C2C	-2.05	1.46	1.50
14	q	503	CLA	CMB-C2B	-2.05	1.46	1.50
14	t	510	CLA	CMB-C2B	-2.05	1.46	1.50
14	G	1101	CLA	MG-ND	-2.05	2.01	2.05
14	s	506	CLA	CMD-C2D	-2.05	1.46	1.50
14	d	519	CLA	CHC-C1C	2.05	1.42	1.38
14	u	516	CLA	CHC-C1C	2.05	1.42	1.38
14	B	1012	CLA	CMB-C2B	-2.05	1.46	1.50
14	6	513	CLA	CMD-C2D	-2.05	1.46	1.50
14	b	502	CLA	CMD-C2D	-2.05	1.46	1.50
14	q	509	CLA	CMD-C2D	-2.05	1.46	1.50
14	t	510	CLA	CMD-C2D	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	510	CLA	CHC-C1C	2.05	1.42	1.38
14	l	1303	CLA	CMB-C2B	-2.05	1.46	1.50
14	t	517	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	1227	CLA	MG-ND	-2.04	2.01	2.05
14	e	1132	CLA	C4B-NB	2.04	1.40	1.37
14	H	1012	CLA	CMB-C2B	-2.04	1.46	1.50
14	r	507	CLA	CMC-C2C	-2.04	1.46	1.50
14	H	1222	CLA	MG-ND	-2.04	2.01	2.05
14	V	1503	CLA	MG-ND	-2.04	2.01	2.05
14	2	519	CLA	CMD-C2D	-2.04	1.46	1.50
21	a	822	SQD	O4-C4	-2.04	1.38	1.43
14	2	509	CLA	C1B-NB	-2.04	1.35	1.37
14	2	517	CLA	CMB-C2B	-2.04	1.46	1.50
14	e	1140	CLA	MG-ND	-2.04	2.01	2.05
21	3	822	SQD	O4-C4	-2.04	1.38	1.43
14	s	508	CLA	C1B-NB	-2.04	1.35	1.37
14	5	506	CLA	CMB-C2B	-2.04	1.46	1.50
14	u	509	CLA	CMC-C2C	-2.04	1.46	1.50
14	q	512	CLA	MG-ND	-2.04	2.01	2.05
14	A	1115	CLA	CHC-C1C	2.04	1.42	1.38
14	B	1208	CLA	CHC-C1C	2.04	1.42	1.38
18	G	5006	LHG	O7-C5	-2.04	1.41	1.46
14	B	1229	CLA	CMD-C2D	-2.04	1.46	1.50
14	Y	518	CLA	CMD-C2D	-2.04	1.46	1.50
14	m	1401	CLA	CMB-C2B	-2.04	1.46	1.50
14	u	504	CLA	CHC-C1C	2.04	1.42	1.38
14	f	1229	CLA	CMD-C2D	-2.04	1.46	1.50
14	r	519	CLA	CMD-C2D	-2.04	1.46	1.50
14	b	503	CLA	CHC-C1C	2.04	1.42	1.38
14	q	508	CLA	CMD-C2D	-2.04	1.46	1.50
14	5	503	CLA	CHC-C1C	2.04	1.42	1.38
14	5	506	CLA	CMD-C2D	-2.04	1.46	1.50
14	a	501	CLA	CMB-C2B	-2.04	1.46	1.50
14	B	1216	CLA	C1B-NB	-2.04	1.35	1.37
21	v	822	SQD	O3-C3	-2.04	1.38	1.43
14	3	508	CLA	C1B-C2B	2.04	1.48	1.43
14	1	512	CLA	MG-ND	-2.04	2.01	2.05
14	f	1227	CLA	MG-ND	-2.04	2.01	2.05
14	H	1229	CLA	CMD-C2D	-2.04	1.46	1.50
14	T	1303	CLA	CMB-C2B	-2.04	1.46	1.50
14	t	510	CLA	CHC-C1C	2.04	1.42	1.38
14	f	1235	CLA	C1B-NB	-2.04	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	507	CLA	CMD-C2D	-2.04	1.46	1.50
14	H	1202	CLA	CMB-C2B	-2.04	1.46	1.50
14	B	1235	CLA	MG-ND	-2.04	2.01	2.05
14	u	516	CLA	CMB-C2B	-2.04	1.46	1.50
14	d	501	CLA	CHC-C1C	2.04	1.42	1.38
14	B	1222	CLA	MG-ND	-2.04	2.01	2.05
21	u	822	SQD	O3-C3	-2.04	1.38	1.43
14	A	1120	CLA	CMB-C2B	-2.04	1.46	1.50
14	t	519	CLA	CMB-C2B	-2.04	1.46	1.50
14	H	1238	CLA	C1B-C2B	2.04	1.48	1.43
14	f	1219	CLA	MG-ND	-2.04	2.01	2.05
14	1	519	CLA	CMD-C2D	-2.04	1.46	1.50
14	6	510	CLA	CMD-C2D	-2.04	1.46	1.50
14	Z	503	CLA	CMB-C2B	-2.04	1.46	1.50
14	b	517	CLA	CMC-C2C	-2.04	1.46	1.50
14	l	1302	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	1132	CLA	C4B-NB	2.04	1.40	1.37
14	4	518	CLA	CHC-C1C	2.04	1.42	1.38
14	Y	516	CLA	O2A-CGA	2.04	1.37	1.30
14	4	507	CLA	CMB-C2B	-2.04	1.46	1.50
14	5	510	CLA	CMC-C2C	-2.04	1.46	1.50
14	b	519	CLA	CMB-C2B	-2.04	1.46	1.50
14	v	506	CLA	CMB-C2B	-2.04	1.46	1.50
14	G	1126	CLA	C1B-C2B	2.04	1.48	1.43
14	B	1239	CLA	C1B-NB	-2.04	1.35	1.37
14	G	1122	CLA	C1B-NB	-2.04	1.35	1.37
14	c	501	CLA	CMD-C2D	-2.04	1.46	1.50
14	u	501	CLA	CHC-C1C	2.04	1.42	1.38
14	b	503	CLA	CMB-C2B	-2.04	1.46	1.50
14	G	1237	CLA	CHC-C4B	-2.04	1.34	1.39
21	c	822	SQD	O3-C3	-2.04	1.38	1.43
14	H	1219	CLA	MG-ND	-2.04	2.01	2.05
14	4	517	CLA	CMC-C2C	-2.04	1.46	1.50
14	H	1209	CLA	C1B-NB	-2.04	1.35	1.37
14	a	516	CLA	CHC-C1C	2.04	1.42	1.38
14	4	519	CLA	CMB-C2B	-2.03	1.46	1.50
14	u	506	CLA	CMD-C2D	-2.03	1.46	1.50
14	u	517	CLA	CMB-C2B	-2.03	1.46	1.50
14	c	516	CLA	CHC-C1C	2.03	1.42	1.38
14	5	504	CLA	CMB-C2B	-2.03	1.46	1.50
14	u	501	CLA	CMB-C2B	-2.03	1.46	1.50
14	u	504	CLA	CMD-C2D	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	v	504	CLA	CMC-C2C	-2.03	1.46	1.50
14	5	516	CLA	CHC-C1C	2.03	1.42	1.38
14	c	503	CLA	CHC-C1C	2.03	1.42	1.38
21	5	822	SQD	O3-C3	-2.03	1.38	1.43
17	B	4017	BCR	C30-C25	-2.03	1.51	1.53
17	c	523	BCR	C1-C6	-2.03	1.51	1.53
14	r	509	CLA	C1B-NB	-2.03	1.35	1.37
14	v	503	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	1120	CLA	CAC-C3C	-2.03	1.45	1.51
14	e	1115	CLA	CHC-C1C	2.03	1.42	1.38
14	2	501	CLA	CMD-C2D	-2.03	1.46	1.50
14	4	516	CLA	CMB-C2B	-2.03	1.46	1.50
14	4	505	CLA	CHC-C1C	2.03	1.42	1.38
14	s	516	CLA	CHC-C1C	2.03	1.42	1.38
14	2	510	CLA	CMB-C2B	-2.03	1.46	1.50
14	q	512	CLA	CMB-C2B	-2.03	1.46	1.50
14	q	516	CLA	O2A-CGA	2.03	1.37	1.30
14	Y	505	CLA	CMC-C2C	-2.03	1.46	1.50
14	f	1217	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	1101	CLA	MG-ND	-2.03	2.01	2.05
14	r	507	CLA	MG-ND	-2.03	2.01	2.05
14	e	1103	CLA	CAC-C3C	-2.03	1.45	1.51
14	Z	511	CLA	CMC-C2C	-2.03	1.46	1.50
14	c	504	CLA	CMD-C2D	-2.03	1.46	1.50
14	s	501	CLA	CMD-C2D	-2.03	1.46	1.50
14	e	1801	CLA	C1B-NB	-2.03	1.35	1.37
14	a	505	CLA	MG-ND	-2.03	2.01	2.05
14	6	501	CLA	CHC-C1C	2.03	1.42	1.38
14	d	516	CLA	CMB-C2B	-2.03	1.46	1.50
14	3	512	CLA	C1B-NB	-2.03	1.35	1.37
14	s	509	CLA	C1B-NB	-2.03	1.35	1.37
14	H	1235	CLA	MG-ND	-2.03	2.01	2.05
14	v	509	CLA	CMB-C2B	-2.03	1.46	1.50
14	a	512	CLA	C1B-NB	-2.03	1.35	1.37
14	t	506	CLA	CHC-C1C	2.03	1.42	1.38
14	G	1132	CLA	C4B-NB	2.03	1.40	1.37
21	1	822	SQD	O3-C3	-2.03	1.38	1.43
14	t	505	CLA	MG-ND	-2.03	2.01	2.05
14	a	508	CLA	C1B-C2B	2.03	1.48	1.43
14	B	1213	CLA	CMB-C2B	-2.03	1.46	1.50
14	2	511	CLA	CMC-C2C	-2.03	1.46	1.50
14	Y	508	CLA	CMD-C2D	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	501	CLA	CHC-C1C	2.03	1.42	1.38
14	b	510	CLA	CHC-C1C	2.03	1.42	1.38
14	f	1235	CLA	CHC-C1C	2.03	1.42	1.38
14	5	517	CLA	CMB-C2B	-2.03	1.46	1.50
14	6	516	CLA	CMB-C2B	-2.03	1.46	1.50
14	b	507	CLA	CMD-C2D	-2.03	1.46	1.50
14	v	505	CLA	CMC-C2C	-2.03	1.46	1.50
14	3	516	CLA	CHC-C1C	2.03	1.42	1.38
14	6	505	CLA	CHC-C1C	2.03	1.42	1.38
14	T	1303	CLA	CHC-C1C	2.03	1.42	1.38
14	Y	519	CLA	CMD-C2D	-2.03	1.46	1.50
14	f	1202	CLA	CMB-C2B	-2.03	1.46	1.50
14	f	1213	CLA	CMB-C2B	-2.03	1.46	1.50
14	t	502	CLA	CMD-C2D	-2.03	1.46	1.50
14	H	1232	CLA	CMC-C2C	-2.03	1.46	1.50
14	Z	507	CLA	CMB-C2B	-2.03	1.46	1.50
14	v	510	CLA	CMD-C2D	-2.03	1.46	1.50
14	4	503	CLA	CHC-C1C	2.03	1.42	1.38
14	B	1227	CLA	C1B-NB	-2.03	1.35	1.37
14	4	509	CLA	C1B-NB	-2.03	1.35	1.37
14	Y	517	CLA	CMC-C2C	-2.03	1.46	1.50
14	u	503	CLA	CMB-C2B	-2.03	1.46	1.50
14	u	505	CLA	MG-ND	-2.03	2.01	2.05
14	q	501	CLA	CMD-C2D	-2.03	1.46	1.50
14	f	1201	CLA	C1B-NB	-2.03	1.35	1.37
14	L	1502	CLA	C1B-C2B	2.03	1.48	1.43
14	B	1219	CLA	MG-ND	-2.03	2.01	2.05
18	e	5006	LHG	O7-C5	-2.02	1.41	1.46
14	4	503	CLA	CMB-C2B	-2.02	1.46	1.50
14	4	510	CLA	CMB-C2B	-2.02	1.46	1.50
14	Y	507	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	1801	CLA	C1B-NB	-2.02	1.35	1.37
14	B	1235	CLA	C1B-NB	-2.02	1.35	1.37
14	e	1135	CLA	C1B-C2B	2.02	1.48	1.43
14	u	506	CLA	CMB-C2B	-2.02	1.46	1.50
14	v	517	CLA	CMB-C2B	-2.02	1.46	1.50
14	c	505	CLA	MG-ND	-2.02	2.01	2.05
20	H	5002	LMG	O1-C7	-2.02	1.40	1.43
14	u	506	CLA	CHC-C1C	2.02	1.42	1.38
14	V	1501	CLA	C1B-C2B	2.02	1.48	1.43
14	t	516	CLA	CMB-C2B	-2.02	1.46	1.50
14	q	501	CLA	CHC-C1C	2.02	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	508	CLA	C1B-NB	-2.02	1.35	1.37
14	2	507	CLA	CMB-C2B	-2.02	1.46	1.50
14	5	509	CLA	CMC-C2C	-2.02	1.46	1.50
14	Z	501	CLA	CMD-C2D	-2.02	1.46	1.50
14	c	510	CLA	CMC-C2C	-2.02	1.46	1.50
14	t	504	CLA	CMD-C2D	-2.02	1.46	1.50
14	G	1126	CLA	CHC-C1C	2.02	1.42	1.38
14	e	1126	CLA	C1B-C2B	2.02	1.48	1.43
14	2	507	CLA	CMC-C2C	-2.02	1.46	1.50
14	3	501	CLA	CMD-C2D	-2.02	1.46	1.50
14	3	510	CLA	CMB-C2B	-2.02	1.46	1.50
14	6	510	CLA	CMC-C2C	-2.02	1.46	1.50
14	t	507	CLA	CMB-C2B	-2.02	1.46	1.50
14	e	1101	CLA	MG-ND	-2.02	2.01	2.05
14	B	1238	CLA	C1B-C2B	2.02	1.48	1.43
14	1	508	CLA	C1B-C2B	2.02	1.48	1.43
14	1	517	CLA	CMC-C2C	-2.02	1.46	1.50
14	Z	517	CLA	CMB-C2B	-2.02	1.46	1.50
14	Y	509	CLA	MG-ND	-2.02	2.01	2.05
14	1	516	CLA	O2A-CGA	2.02	1.37	1.30
14	5	504	CLA	CMD-C2D	-2.02	1.46	1.50
14	Y	506	CLA	CMD-C2D	-2.02	1.46	1.50
14	5	501	CLA	CHC-C1C	2.02	1.42	1.38
14	d	505	CLA	CHC-C1C	2.02	1.42	1.38
14	c	504	CLA	CMB-C2B	-2.02	1.46	1.50
14	t	505	CLA	CMC-C2C	-2.02	1.46	1.50
14	v	513	CLA	CMB-C2B	-2.02	1.46	1.50
14	b	517	CLA	CMD-C2D	-2.02	1.46	1.50
14	A	1237	CLA	CHC-C4B	-2.02	1.34	1.39
14	G	1133	CLA	C1B-NB	-2.02	1.35	1.37
14	A	1120	CLA	CHC-C1C	2.02	1.42	1.38
14	s	508	CLA	C1B-C2B	2.02	1.48	1.43
14	d	513	CLA	CMB-C2B	-2.02	1.46	1.50
14	u	519	CLA	CMB-C2B	-2.02	1.46	1.50
17	5	523	BCR	C1-C6	-2.02	1.51	1.53
14	c	519	CLA	CHC-C1C	2.02	1.42	1.38
14	Z	502	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	1113	CLA	C1B-NB	-2.02	1.35	1.37
14	e	1102	CLA	C1B-C2B	2.02	1.48	1.43
14	t	505	CLA	CHC-C1C	2.02	1.42	1.38
14	r	518	CLA	CMB-C2B	-2.02	1.46	1.50
14	B	1229	CLA	C1B-NB	-2.02	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	510	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	5006	LHG	O7-C5	-2.02	1.41	1.46
14	a	501	CLA	CMD-C2D	-2.02	1.46	1.50
14	Y	512	CLA	C1B-NB	-2.02	1.35	1.37
14	A	1126	CLA	CHC-C1C	2.02	1.42	1.38
14	a	504	CLA	CMC-C2C	-2.02	1.46	1.50
14	G	1120	CLA	CAC-C3C	-2.02	1.45	1.51
14	1	509	CLA	MG-ND	-2.02	2.01	2.05
14	4	506	CLA	CMC-C2C	-2.02	1.46	1.50
14	v	517	CLA	CMC-C2C	-2.02	1.46	1.50
14	H	1227	CLA	MG-ND	-2.02	2.01	2.05
14	4	504	CLA	CMD-C2D	-2.02	1.46	1.50
14	s	510	CLA	CMB-C2B	-2.02	1.46	1.50
14	s	517	CLA	CMB-C2B	-2.02	1.46	1.50
14	s	518	CLA	CHC-C1C	2.02	1.42	1.38
14	q	508	CLA	C1B-C2B	2.02	1.48	1.43
14	L	1501	CLA	C1B-C2B	2.02	1.48	1.43
14	6	506	CLA	CMB-C2B	-2.02	1.46	1.50
14	a	507	CLA	CMB-C2B	-2.02	1.46	1.50
14	f	1223	CLA	C1B-NB	-2.02	1.35	1.37
14	1	518	CLA	CHC-C1C	2.02	1.42	1.38
14	G	1120	CLA	CHC-C1C	2.02	1.42	1.38
14	H	1216	CLA	CHC-C1C	2.02	1.42	1.38
14	2	516	CLA	CMB-C2B	-2.02	1.46	1.50
14	3	517	CLA	CMB-C2B	-2.02	1.46	1.50
14	H	1208	CLA	CMC-C2C	-2.02	1.46	1.50
14	1	512	CLA	C1B-NB	-2.02	1.35	1.37
14	n	1502	CLA	C1B-C2B	2.02	1.48	1.43
14	B	1202	CLA	CMB-C2B	-2.02	1.46	1.50
14	6	504	CLA	CMC-C2C	-2.02	1.46	1.50
14	s	501	CLA	CMB-C2B	-2.02	1.46	1.50
14	s	505	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	1108	CLA	CHC-C1C	2.02	1.42	1.38
14	q	509	CLA	MG-ND	-2.02	2.01	2.05
14	b	501	CLA	CMD-C2D	-2.01	1.46	1.50
14	v	510	CLA	CMC-C2C	-2.01	1.46	1.50
14	c	501	CLA	CHC-C1C	2.01	1.42	1.38
14	2	507	CLA	MG-ND	-2.01	2.01	2.05
14	f	1222	CLA	MG-ND	-2.01	2.01	2.05
14	A	1103	CLA	CAC-C3C	-2.01	1.45	1.51
14	5	516	CLA	CMB-C2B	-2.01	1.46	1.50
14	d	504	CLA	CMC-C2C	-2.01	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	r	501	CLA	CMD-C2D	-2.01	1.46	1.50
14	v	506	CLA	CMD-C2D	-2.01	1.46	1.50
14	u	519	CLA	CHC-C1C	2.01	1.42	1.38
14	3	501	CLA	CMB-C2B	-2.01	1.46	1.50
14	Z	510	CLA	CMC-C2C	-2.01	1.46	1.50
14	e	1112	CLA	C1B-NB	-2.01	1.35	1.37
14	4	517	CLA	CMD-C2D	-2.01	1.46	1.50
14	Y	501	CLA	CMD-C2D	-2.01	1.46	1.50
14	Y	512	CLA	CMB-C2B	-2.01	1.46	1.50
14	c	509	CLA	CMC-C2C	-2.01	1.46	1.50
14	r	505	CLA	CMC-C2C	-2.01	1.46	1.50
14	t	501	CLA	CMD-C2D	-2.01	1.46	1.50
14	t	506	CLA	CMD-C2D	-2.01	1.46	1.50
14	V	1502	CLA	C1B-C2B	2.01	1.48	1.43
17	H	4017	BCR	C17-C18	-2.01	1.33	1.35
14	B	1223	CLA	C1B-NB	-2.01	1.35	1.37
14	Z	518	CLA	CMB-C2B	-2.01	1.46	1.50
14	b	509	CLA	CMC-C2C	-2.01	1.46	1.50
14	5	519	CLA	CHC-C1C	2.01	1.42	1.38
14	A	1013	CLA	CAC-C3C	-2.01	1.45	1.51
14	A	1105	CLA	MG-ND	-2.01	2.01	2.05
14	q	507	CLA	CMC-C2C	-2.01	1.46	1.50
14	r	518	CLA	CMC-C2C	-2.01	1.46	1.50
14	e	1113	CLA	CHC-C1C	2.01	1.42	1.38
14	c	506	CLA	CMB-C2B	-2.01	1.46	1.50
14	d	506	CLA	CMD-C2D	-2.01	1.46	1.50
14	d	507	CLA	CMB-C2B	-2.01	1.46	1.50
14	u	507	CLA	CMB-C2B	-2.01	1.46	1.50
14	B	1232	CLA	CHC-C1C	2.01	1.42	1.38
14	1	506	CLA	CMD-C2D	-2.01	1.46	1.50
14	2	505	CLA	CMC-C2C	-2.01	1.46	1.50
14	4	513	CLA	CMC-C2C	-2.01	1.46	1.50
14	6	505	CLA	CMC-C2C	-2.01	1.46	1.50
14	Z	518	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	1124	CLA	CHC-C1C	2.01	1.42	1.38
14	5	510	CLA	CHC-C1C	2.01	1.42	1.38
14	v	513	CLA	CHC-C1C	2.01	1.42	1.38
14	2	503	CLA	CMB-C2B	-2.01	1.46	1.50
14	3	504	CLA	CMC-C2C	-2.01	1.46	1.50
14	6	517	CLA	CMC-C2C	-2.01	1.46	1.50
14	b	511	CLA	CMC-C2C	-2.01	1.46	1.50
14	G	1109	CLA	C1B-NB	-2.01	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1229	CLA	C1B-NB	-2.01	1.35	1.37
14	d	513	CLA	CHC-C1C	2.01	1.42	1.38
14	b	506	CLA	CMD-C2D	-2.01	1.46	1.50
20	B	5002	LMG	O1-C7	-2.01	1.40	1.43
14	t	508	CLA	C1B-C2B	2.01	1.48	1.43
14	G	1801	CLA	C1B-NB	-2.01	1.35	1.37
14	e	1113	CLA	C1B-NB	-2.01	1.35	1.37
14	u	504	CLA	CMC-C2C	-2.01	1.46	1.50
14	6	512	CLA	CHC-C1C	2.01	1.42	1.38
14	e	1126	CLA	CHC-C1C	2.01	1.42	1.38
14	e	1237	CLA	CHC-C4B	-2.01	1.34	1.39
14	Z	516	CLA	CMB-C2B	-2.01	1.46	1.50
14	G	1013	CLA	CAC-C3C	-2.01	1.46	1.51
14	a	502	CLA	CMC-C2C	-2.01	1.46	1.50
14	5	505	CLA	MG-ND	-2.01	2.01	2.05
14	H	1239	CLA	CHC-C4B	-2.01	1.34	1.39
14	q	518	CLA	CHC-C1C	2.01	1.42	1.38
14	2	502	CLA	CMC-C2C	-2.01	1.46	1.50
14	c	510	CLA	CHC-C1C	2.01	1.42	1.38
14	q	517	CLA	CHC-C1C	2.01	1.42	1.38
14	4	511	CLA	CMC-C2C	-2.01	1.46	1.50
14	v	512	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	1126	CLA	C1B-C2B	2.01	1.48	1.43
14	Y	508	CLA	C1B-C2B	2.01	1.48	1.43
14	e	1013	CLA	CAC-C3C	-2.01	1.46	1.51
17	f	4014	BCR	C10-C9	-2.01	1.33	1.35
14	4	504	CLA	CHC-C1C	2.01	1.42	1.38
14	c	516	CLA	CMB-C2B	-2.01	1.46	1.50
14	e	1120	CLA	CAC-C3C	-2.01	1.46	1.51
14	e	1127	CLA	C1B-C2B	2.01	1.48	1.43
14	A	1109	CLA	C1B-NB	-2.01	1.35	1.37
14	A	1122	CLA	C1B-NB	-2.01	1.35	1.37
14	n	1502	CLA	C1B-NB	-2.01	1.35	1.37
14	2	518	CLA	CMB-C2B	-2.01	1.46	1.50
14	4	509	CLA	CMC-C2C	-2.01	1.46	1.50
14	q	502	CLA	CMC-C2C	-2.01	1.46	1.50
14	v	507	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	1136	CLA	MG-ND	-2.01	2.01	2.05
14	1	512	CLA	CMB-C2B	-2.01	1.46	1.50
14	d	512	CLA	CHC-C1C	2.01	1.42	1.38
14	H	1222	CLA	C1B-NB	-2.01	1.35	1.37
14	A	1135	CLA	C1B-C2B	2.01	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1103	CLA	CAC-C3C	-2.01	1.46	1.51
14	J	1303	CLA	CMB-C2B	-2.01	1.46	1.50
14	1	502	CLA	CMC-C2C	-2.01	1.46	1.50
14	6	507	CLA	CMB-C2B	-2.01	1.46	1.50
14	Z	507	CLA	CMC-C2C	-2.01	1.46	1.50
14	d	506	CLA	CMB-C2B	-2.01	1.46	1.50
14	t	503	CLA	CMB-C2B	-2.01	1.46	1.50
14	t	509	CLA	CMC-C2C	-2.01	1.46	1.50
14	3	506	CLA	CHC-C1C	2.01	1.42	1.38
14	f	1229	CLA	C1B-NB	-2.01	1.35	1.37
14	2	510	CLA	CMC-C2C	-2.00	1.46	1.50
14	3	503	CLA	CMB-C2B	-2.00	1.46	1.50
14	t	506	CLA	CMC-C2C	-2.00	1.46	1.50
14	G	1124	CLA	CHC-C1C	2.00	1.42	1.38
14	6	506	CLA	CMD-C2D	-2.00	1.46	1.50
14	d	512	CLA	CMC-C2C	-2.00	1.46	1.50
14	e	1124	CLA	CHC-C1C	2.00	1.42	1.38
14	A	1102	CLA	C1B-C2B	2.00	1.48	1.43
14	6	513	CLA	CMB-C2B	-2.00	1.46	1.50
14	f	1219	CLA	CMC-C2C	-2.00	1.46	1.50
14	e	1105	CLA	MG-ND	-2.00	2.01	2.05
14	H	1232	CLA	CHC-C1C	2.00	1.42	1.38
14	r	509	CLA	CHC-C1C	2.00	1.42	1.38
14	t	516	CLA	CHC-C1C	2.00	1.42	1.38
14	q	509	CLA	C1B-NB	-2.00	1.35	1.37
14	1	507	CLA	CMC-C2C	-2.00	1.46	1.50
14	b	513	CLA	CMB-C2B	-2.00	1.46	1.50
14	B	1223	CLA	CMB-C2B	-2.00	1.46	1.50
14	4	505	CLA	CMC-C2C	-2.00	1.46	1.50
14	r	516	CLA	CMB-C2B	-2.00	1.46	1.50
14	1	512	CLA	CHC-C1C	2.00	1.42	1.38
14	2	505	CLA	CMB-C2B	-2.00	1.46	1.50
14	H	1213	CLA	CMB-C2B	-2.00	1.46	1.50
14	H	1219	CLA	CMC-C2C	-2.00	1.46	1.50
14	G	1108	CLA	CMC-C2C	-2.00	1.46	1.50
14	H	1235	CLA	C1B-NB	-2.00	1.35	1.37
14	G	1108	CLA	CHC-C1C	2.00	1.42	1.38
14	3	505	CLA	MG-ND	-2.00	2.01	2.05
14	e	1109	CLA	C1B-NB	-2.00	1.35	1.37
14	f	1239	CLA	C1B-NB	-2.00	1.35	1.37
14	A	1108	CLA	CMC-C2C	-2.00	1.46	1.50
14	3	507	CLA	CMB-C2B	-2.00	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Y	502	CLA	CMC-C2C	-2.00	1.46	1.50
14	d	505	CLA	CMC-C2C	-2.00	1.46	1.50
14	q	511	CLA	CMC-C2C	-2.00	1.46	1.50
14	r	507	CLA	CMB-C2B	-2.00	1.46	1.50
14	r	510	CLA	CMC-C2C	-2.00	1.46	1.50
17	B	4014	BCR	C10-C9	-2.00	1.33	1.35
14	s	502	CLA	CMC-C2C	-2.00	1.46	1.50
14	G	1113	CLA	C1B-NB	-2.00	1.35	1.37
14	H	1202	CLA	C1B-NB	-2.00	1.35	1.37
14	f	1213	CLA	C1B-NB	-2.00	1.35	1.37

All (7290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1023	CLA	C4A-NA-C1A	9.67	111.06	106.71
14	B	1023	CLA	C4A-NA-C1A	9.59	111.02	106.71
14	f	1023	CLA	C4A-NA-C1A	9.53	110.99	106.71
15	G	2001	PQN	C11-C12-C13	-9.51	110.96	126.79
15	A	2001	PQN	C11-C12-C13	-9.50	110.98	126.79
15	e	2001	PQN	C11-C12-C13	-9.49	110.99	126.79
15	f	2002	PQN	C11-C12-C13	-9.11	111.63	126.79
15	B	2002	PQN	C11-C12-C13	-9.10	111.64	126.79
15	H	2002	PQN	C11-C12-C13	-9.09	111.67	126.79
14	e	1103	CLA	C4A-NA-C1A	8.34	110.46	106.71
17	G	4008	BCR	C24-C23-C22	-8.34	113.63	126.23
17	e	4008	BCR	C24-C23-C22	-8.32	113.66	126.23
17	A	4008	BCR	C24-C23-C22	-8.32	113.66	126.23
14	A	1103	CLA	C4A-NA-C1A	8.32	110.45	106.71
14	G	1103	CLA	C4A-NA-C1A	8.31	110.44	106.71
14	f	1239	CLA	C4A-NA-C1A	8.20	110.39	106.71
14	H	1239	CLA	C4A-NA-C1A	8.14	110.37	106.71
14	B	1239	CLA	C4A-NA-C1A	8.12	110.36	106.71
14	G	1109	CLA	C4A-NA-C1A	7.99	110.30	106.71
14	A	1109	CLA	C4A-NA-C1A	7.99	110.30	106.71
14	G	1101	CLA	C4A-NA-C1A	7.97	110.29	106.71
14	H	1214	CLA	C4A-NA-C1A	7.94	110.28	106.71
14	n	1503	CLA	C4A-NA-C1A	7.93	110.27	106.71
14	Z	502	CLA	C4A-NA-C1A	7.91	110.26	106.71
14	e	1109	CLA	C4A-NA-C1A	7.91	110.26	106.71
14	L	1503	CLA	C4A-NA-C1A	7.88	110.25	106.71
14	B	1214	CLA	C4A-NA-C1A	7.87	110.25	106.71
14	e	1101	CLA	C4A-NA-C1A	7.87	110.25	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1115	CLA	C4A-NA-C1A	7.86	110.24	106.71
14	f	1214	CLA	C4A-NA-C1A	7.85	110.24	106.71
14	B	1205	CLA	C4A-NA-C1A	7.85	110.24	106.71
14	s	502	CLA	C4A-NA-C1A	7.85	110.23	106.71
14	V	1503	CLA	C4A-NA-C1A	7.85	110.23	106.71
14	2	502	CLA	C4A-NA-C1A	7.83	110.22	106.71
14	f	1205	CLA	C4A-NA-C1A	7.82	110.22	106.71
14	G	1115	CLA	C4A-NA-C1A	7.81	110.22	106.71
14	r	502	CLA	C4A-NA-C1A	7.81	110.22	106.71
14	A	1101	CLA	C4A-NA-C1A	7.81	110.22	106.71
14	3	502	CLA	C4A-NA-C1A	7.79	110.21	106.71
14	B	1201	CLA	C4A-NA-C1A	7.78	110.20	106.71
14	a	502	CLA	C4A-NA-C1A	7.78	110.20	106.71
14	t	502	CLA	C4A-NA-C1A	7.78	110.20	106.71
14	f	1201	CLA	C4A-NA-C1A	7.77	110.20	106.71
14	e	1115	CLA	C4A-NA-C1A	7.77	110.20	106.71
14	H	1205	CLA	C4A-NA-C1A	7.76	110.19	106.71
14	q	508	CLA	C4A-NA-C1A	7.76	110.19	106.71
14	G	1137	CLA	C4A-NA-C1A	7.74	110.19	106.71
14	f	1215	CLA	C4A-NA-C1A	7.74	110.18	106.71
14	A	1137	CLA	C4A-NA-C1A	7.72	110.18	106.71
14	H	1201	CLA	C4A-NA-C1A	7.72	110.18	106.71
14	b	502	CLA	C4A-NA-C1A	7.72	110.17	106.71
14	4	502	CLA	C4A-NA-C1A	7.70	110.17	106.71
14	e	1237	CLA	C4A-NA-C1A	7.70	110.17	106.71
14	Z	501	CLA	C4A-NA-C1A	7.68	110.16	106.71
14	e	1137	CLA	C4A-NA-C1A	7.68	110.16	106.71
14	5	502	CLA	C4A-NA-C1A	7.67	110.15	106.71
14	B	1215	CLA	C4A-NA-C1A	7.66	110.15	106.71
14	f	1213	CLA	C4A-NA-C1A	7.66	110.15	106.71
14	H	1215	CLA	C4A-NA-C1A	7.63	110.14	106.71
14	1	508	CLA	C4A-NA-C1A	7.63	110.14	106.71
14	G	1104	CLA	C4A-NA-C1A	7.63	110.14	106.71
14	A	1120	CLA	C4A-NA-C1A	7.62	110.13	106.71
14	A	1237	CLA	C4A-NA-C1A	7.62	110.13	106.71
14	G	1237	CLA	C4A-NA-C1A	7.61	110.13	106.71
14	B	1213	CLA	C4A-NA-C1A	7.60	110.12	106.71
14	H	1212	CLA	C4A-NA-C1A	7.60	110.12	106.71
14	A	1122	CLA	C4A-NA-C1A	7.60	110.12	106.71
14	Y	508	CLA	C4A-NA-C1A	7.60	110.12	106.71
14	2	501	CLA	C4A-NA-C1A	7.60	110.12	106.71
14	H	1213	CLA	C4A-NA-C1A	7.60	110.12	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1104	CLA	C4A-NA-C1A	7.59	110.12	106.71
14	r	501	CLA	C4A-NA-C1A	7.58	110.11	106.71
14	c	502	CLA	C4A-NA-C1A	7.58	110.11	106.71
14	l	1303	CLA	C4A-NA-C1A	7.58	110.11	106.71
14	A	1104	CLA	C4A-NA-C1A	7.57	110.11	106.71
14	1	502	CLA	C4A-NA-C1A	7.56	110.10	106.71
14	u	502	CLA	C4A-NA-C1A	7.55	110.10	106.71
14	G	1120	CLA	C4A-NA-C1A	7.54	110.10	106.71
14	e	1120	CLA	C4A-NA-C1A	7.54	110.10	106.71
14	q	502	CLA	C4A-NA-C1A	7.54	110.10	106.71
14	H	1218	CLA	C4A-NA-C1A	7.54	110.10	106.71
14	e	1122	CLA	C4A-NA-C1A	7.54	110.09	106.71
14	d	502	CLA	C4A-NA-C1A	7.53	110.09	106.71
14	v	501	CLA	C4A-NA-C1A	7.52	110.09	106.71
14	G	1133	CLA	C4A-NA-C1A	7.52	110.08	106.71
14	f	1212	CLA	C4A-NA-C1A	7.52	110.08	106.71
14	e	1133	CLA	C4A-NA-C1A	7.50	110.08	106.71
14	G	1122	CLA	C4A-NA-C1A	7.50	110.08	106.71
14	G	1118	CLA	C4A-NA-C1A	7.50	110.08	106.71
14	f	1223	CLA	C4A-NA-C1A	7.50	110.08	106.71
14	J	1303	CLA	C4A-NA-C1A	7.49	110.07	106.71
14	Y	502	CLA	C4A-NA-C1A	7.49	110.07	106.71
14	e	1118	CLA	C4A-NA-C1A	7.49	110.07	106.71
14	6	502	CLA	C4A-NA-C1A	7.48	110.07	106.71
14	u	508	CLA	C4A-NA-C1A	7.48	110.07	106.71
14	B	1212	CLA	C4A-NA-C1A	7.48	110.07	106.71
14	T	1303	CLA	C4A-NA-C1A	7.47	110.06	106.71
14	6	501	CLA	C4A-NA-C1A	7.47	110.06	106.71
14	d	501	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	A	1118	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	Y	518	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	B	1223	CLA	C4A-NA-C1A	7.45	110.06	106.71
14	A	1133	CLA	C4A-NA-C1A	7.45	110.06	106.71
14	u	501	CLA	C4A-NA-C1A	7.45	110.06	106.71
14	b	517	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	f	1218	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	A	1112	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	4	517	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	v	502	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	5	508	CLA	C4A-NA-C1A	7.43	110.05	106.71
14	5	501	CLA	C4A-NA-C1A	7.41	110.04	106.71
14	e	1112	CLA	C4A-NA-C1A	7.40	110.03	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1220	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	B	1218	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	c	508	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	v	503	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	H	1223	CLA	C4A-NA-C1A	7.38	110.03	106.71
14	G	1134	CLA	C4A-NA-C1A	7.38	110.02	106.71
14	Y	501	CLA	C4A-NA-C1A	7.38	110.02	106.71
14	6	503	CLA	C4A-NA-C1A	7.37	110.02	106.71
14	t	517	CLA	C4A-NA-C1A	7.37	110.02	106.71
14	1	501	CLA	C4A-NA-C1A	7.36	110.02	106.71
14	1	518	CLA	C4A-NA-C1A	7.36	110.01	106.71
14	H	1211	CLA	C4A-NA-C1A	7.36	110.01	106.71
14	A	1140	CLA	C4A-NA-C1A	7.35	110.01	106.71
15	B	2002	PQN	C15-C13-C12	-7.34	106.26	121.12
14	B	1220	CLA	C4A-NA-C1A	7.34	110.01	106.71
14	G	1112	CLA	C4A-NA-C1A	7.34	110.01	106.71
15	H	2002	PQN	C15-C13-C12	-7.34	106.26	121.12
14	H	1228	CLA	C4A-NA-C1A	7.34	110.00	106.71
14	B	1228	CLA	C4A-NA-C1A	7.34	110.00	106.71
14	f	1211	CLA	C4A-NA-C1A	7.33	110.00	106.71
14	f	1228	CLA	C4A-NA-C1A	7.33	110.00	106.71
14	J	1302	CLA	C4A-NA-C1A	7.32	110.00	106.71
14	4	501	CLA	C4A-NA-C1A	7.32	110.00	106.71
14	e	1134	CLA	C4A-NA-C1A	7.32	110.00	106.71
15	f	2002	PQN	C15-C13-C12	-7.32	106.30	121.12
14	A	1134	CLA	C4A-NA-C1A	7.32	110.00	106.71
14	A	1119	CLA	C4A-NA-C1A	7.32	110.00	106.71
14	n	1502	CLA	C4A-NA-C1A	7.31	109.99	106.71
14	e	1126	CLA	C4A-NA-C1A	7.31	109.99	106.71
14	q	501	CLA	C4A-NA-C1A	7.31	109.99	106.71
14	5	504	CLA	C4A-NA-C1A	7.31	109.99	106.71
14	c	501	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	f	1220	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	l	1302	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	t	501	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	e	1119	CLA	C4A-NA-C1A	7.29	109.98	106.71
14	e	1140	CLA	C4A-NA-C1A	7.29	109.98	106.71
14	G	1126	CLA	C4A-NA-C1A	7.29	109.98	106.71
14	4	509	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	G	1119	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	d	503	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	f	1204	CLA	C4A-NA-C1A	7.28	109.98	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1140	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	T	1302	CLA	C4A-NA-C1A	7.27	109.98	106.71
14	a	509	CLA	C4A-NA-C1A	7.27	109.97	106.71
14	B	1211	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	r	517	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	q	518	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	b	501	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	3	509	CLA	C4A-NA-C1A	7.25	109.97	106.71
14	L	1502	CLA	C4A-NA-C1A	7.25	109.97	106.71
14	A	1126	CLA	C4A-NA-C1A	7.25	109.96	106.71
14	c	504	CLA	C4A-NA-C1A	7.25	109.96	106.71
14	Y	505	CLA	C4A-NA-C1A	7.24	109.96	106.71
14	H	1204	CLA	C4A-NA-C1A	7.24	109.96	106.71
14	2	517	CLA	C4A-NA-C1A	7.23	109.96	106.71
14	5	507	CLA	C4A-NA-C1A	7.23	109.96	106.71
17	n	4019	BCR	C24-C23-C22	-7.23	115.31	126.23
14	B	1204	CLA	C4A-NA-C1A	7.23	109.95	106.71
14	Z	519	CLA	C4A-NA-C1A	7.21	109.95	106.71
17	L	4019	BCR	C24-C23-C22	-7.20	115.35	126.23
17	V	4019	BCR	C24-C23-C22	-7.20	115.35	126.23
14	u	504	CLA	C4A-NA-C1A	7.20	109.94	106.71
14	s	509	CLA	C4A-NA-C1A	7.20	109.94	106.71
14	t	509	CLA	C4A-NA-C1A	7.20	109.94	106.71
14	1	505	CLA	C4A-NA-C1A	7.19	109.94	106.71
14	Z	517	CLA	C4A-NA-C1A	7.19	109.94	106.71
14	u	507	CLA	C4A-NA-C1A	7.18	109.93	106.71
14	b	509	CLA	C4A-NA-C1A	7.18	109.93	106.71
14	r	503	CLA	C4A-NA-C1A	7.18	109.93	106.71
14	Z	503	CLA	C4A-NA-C1A	7.17	109.93	106.71
14	2	519	CLA	C4A-NA-C1A	7.17	109.93	106.71
14	V	1502	CLA	C4A-NA-C1A	7.16	109.92	106.71
14	u	503	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	4	513	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	r	506	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	a	506	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	c	507	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	t	519	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	2	503	CLA	C4A-NA-C1A	7.13	109.91	106.71
14	b	518	CLA	C4A-NA-C1A	7.13	109.91	106.71
14	4	519	CLA	C4A-NA-C1A	7.13	109.91	106.71
14	Y	507	CLA	C4A-NA-C1A	7.13	109.91	106.71
14	c	519	CLA	C4A-NA-C1A	7.12	109.91	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	d	506	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	4	506	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	f	1206	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	t	518	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	s	519	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	c	503	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	e	1113	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	A	1113	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	4	518	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	a	513	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	b	513	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	r	519	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	H	1206	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	q	505	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	e	1013	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	B	1206	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	a	501	CLA	C4A-NA-C1A	7.09	109.89	106.71
14	q	507	CLA	C4A-NA-C1A	7.09	109.89	106.71
14	2	506	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	b	506	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	e	1108	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	e	1125	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	s	501	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	G	1013	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	t	513	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	A	1125	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	b	519	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	c	505	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	s	504	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	H	1238	CLA	C4A-NA-C1A	7.07	109.88	106.71
14	e	1111	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	5	503	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	6	506	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	A	1111	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	B	1202	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	3	519	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	3	504	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	3	513	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	d	511	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	1	507	CLA	C4A-NA-C1A	7.05	109.87	106.71
14	3	506	CLA	C4A-NA-C1A	7.05	109.87	106.71
14	5	519	CLA	C4A-NA-C1A	7.04	109.87	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Z	505	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	a	507	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	f	1202	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	4	503	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	t	510	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	G	1113	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	t	503	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	A	1013	CLA	C4A-NA-C1A	7.03	109.87	106.71
14	A	1138	CLA	C4A-NA-C1A	7.03	109.87	106.71
14	b	503	CLA	C4A-NA-C1A	7.03	109.87	106.71
14	A	1108	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	G	1138	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	6	511	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	a	519	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	B	1217	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	G	1111	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	Z	506	CLA	C4A-NA-C1A	7.01	109.86	106.71
14	v	506	CLA	C4A-NA-C1A	7.01	109.86	106.71
14	v	511	CLA	C4A-NA-C1A	7.01	109.86	106.71
14	5	505	CLA	C4A-NA-C1A	7.00	109.86	106.71
14	G	1125	CLA	C4A-NA-C1A	7.00	109.85	106.71
14	s	506	CLA	C4A-NA-C1A	7.00	109.85	106.71
14	u	519	CLA	C4A-NA-C1A	7.00	109.85	106.71
14	t	507	CLA	C4A-NA-C1A	7.00	109.85	106.71
14	t	506	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	f	1238	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	Z	504	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	K	1103	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	3	501	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	2	505	CLA	C4A-NA-C1A	6.98	109.85	106.71
14	Y	504	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	Y	511	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	a	504	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	3	507	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	U	1103	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	d	518	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	f	1217	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	q	504	CLA	C4A-NA-C1A	6.97	109.84	106.71
14	s	513	CLA	C4A-NA-C1A	6.97	109.84	106.71
14	d	509	CLA	C4A-NA-C1A	6.97	109.84	106.71
14	6	509	CLA	C4A-NA-C1A	6.96	109.84	106.71
14	s	511	CLA	C4A-NA-C1A	6.96	109.84	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1217	CLA	C4A-NA-C1A	6.96	109.83	106.71
14	r	518	CLA	C4A-NA-C1A	6.96	109.83	106.71
14	3	511	CLA	C4A-NA-C1A	6.96	109.83	106.71
14	s	507	CLA	C4A-NA-C1A	6.96	109.83	106.71
14	H	1202	CLA	C4A-NA-C1A	6.95	109.83	106.71
14	H	1231	CLA	C4A-NA-C1A	6.95	109.83	106.71
14	G	1108	CLA	C4A-NA-C1A	6.95	109.83	106.71
14	Y	517	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	v	508	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	a	511	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	b	507	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	u	506	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	B	1238	CLA	C4A-NA-C1A	6.94	109.82	106.71
14	r	504	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	1	504	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	4	510	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	6	508	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	f	1235	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	B	1231	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	3	518	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	G	1110	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	1	511	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	Z	518	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	2	518	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	m	1103	CLA	C4A-NA-C1A	6.91	109.81	106.71
14	4	507	CLA	C4A-NA-C1A	6.91	109.81	106.71
14	t	512	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	d	508	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	u	509	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	b	512	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	6	518	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	e	1138	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	s	505	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	u	505	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	2	504	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	6	504	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	f	1231	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	B	1235	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	5	506	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	Z	509	CLA	C4A-NA-C1A	6.87	109.80	106.71
14	v	509	CLA	C4A-NA-C1A	6.87	109.80	106.71
14	a	505	CLA	C4A-NA-C1A	6.86	109.79	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1209	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	r	505	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	b	510	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	v	518	CLA	C4A-NA-C1A	6.85	109.79	106.71
14	4	512	CLA	C4A-NA-C1A	6.85	109.79	106.71
14	a	518	CLA	C4A-NA-C1A	6.85	109.79	106.71
14	3	505	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	q	517	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	B	1224	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	4	504	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	6	513	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	d	504	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	f	1229	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	d	507	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	v	504	CLA	C4A-NA-C1A	6.83	109.78	106.71
14	v	517	CLA	C4A-NA-C1A	6.83	109.78	106.71
14	1	517	CLA	C4A-NA-C1A	6.83	109.78	106.71
14	6	517	CLA	C4A-NA-C1A	6.83	109.78	106.71
14	B	1229	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	H	1221	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	u	510	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	2	509	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	Y	503	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	s	518	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	A	1110	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	5	509	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	1	503	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	H	1235	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	q	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	v	513	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	B	1209	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	d	517	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	H	1229	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	c	506	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	H	1240	CLA	C4A-NA-C1A	6.80	109.76	106.71
14	t	504	CLA	C4A-NA-C1A	6.80	109.76	106.71
14	Z	516	CLA	C4A-NA-C1A	6.80	109.76	106.71
14	r	509	CLA	C4A-NA-C1A	6.79	109.76	106.71
14	a	516	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	6	507	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	B	1221	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	e	1110	CLA	C4A-NA-C1A	6.78	109.75	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1224	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	q	503	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	Y	510	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	c	510	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	q	513	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	Y	513	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	c	509	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	B	1240	CLA	C4A-NA-C1A	6.76	109.75	106.71
14	6	505	CLA	C4A-NA-C1A	6.76	109.75	106.71
14	Z	508	CLA	C4A-NA-C1A	6.76	109.75	106.71
14	b	504	CLA	C4A-NA-C1A	6.76	109.75	106.71
14	v	519	CLA	C4A-NA-C1A	6.76	109.74	106.71
14	H	1209	CLA	C4A-NA-C1A	6.76	109.74	106.71
14	f	1221	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	v	507	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	H	1224	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	B	1230	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	1	513	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	2	508	CLA	C4A-NA-C1A	6.74	109.74	106.71
14	d	505	CLA	C4A-NA-C1A	6.74	109.74	106.71
14	5	510	CLA	C4A-NA-C1A	6.74	109.74	106.71
14	R	1302	CLA	C4A-NA-C1A	6.74	109.73	106.71
14	V	1501	CLA	C4A-NA-C1A	6.73	109.73	106.71
14	d	513	CLA	C4A-NA-C1A	6.72	109.73	106.71
14	1	510	CLA	C4A-NA-C1A	6.72	109.73	106.71
14	u	518	CLA	C4A-NA-C1A	6.72	109.73	106.71
14	f	1240	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	v	505	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	2	516	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	6	519	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	d	519	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	f	1236	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	Y	509	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	3	516	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	G	1121	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	A	1136	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	e	1132	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	s	516	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	n	1501	CLA	C4A-NA-C1A	6.69	109.71	106.71
14	G	1132	CLA	C4A-NA-C1A	6.69	109.71	106.71
14	A	1121	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	f	1230	CLA	C4A-NA-C1A	6.68	109.71	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	1501	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	q	516	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	q	510	CLA	C4A-NA-C1A	6.67	109.71	106.71
14	v	510	CLA	C4A-NA-C1A	6.67	109.70	106.71
14	r	508	CLA	C4A-NA-C1A	6.67	109.70	106.71
14	G	1106	CLA	C4A-NA-C1A	6.67	109.70	106.71
14	U	1105	CLA	C4A-NA-C1A	6.67	109.70	106.71
14	A	1106	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	e	1136	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	2	507	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	A	1132	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	Y	516	CLA	C4A-NA-C1A	6.65	109.70	106.71
14	K	1105	CLA	C4A-NA-C1A	6.65	109.69	106.71
14	6	510	CLA	C4A-NA-C1A	6.65	109.69	106.71
14	H	1230	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	B	1236	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	F	1302	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	H	1236	CLA	C4A-NA-C1A	6.63	109.69	106.71
14	1	506	CLA	C4A-NA-C1A	6.63	109.69	106.71
14	q	509	CLA	C4A-NA-C1A	6.63	109.69	106.71
14	3	503	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	B	1021	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	f	1021	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	j	1302	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	m	1105	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	r	516	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	q	506	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	G	1136	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	b	508	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	d	510	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	a	510	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	e	1106	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	e	1121	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	r	507	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	5	518	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	r	511	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	H	1207	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	a	503	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	c	518	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	s	503	CLA	C4A-NA-C1A	6.60	109.67	106.71
17	f	4006	BCR	C7-C8-C9	-6.59	116.27	126.23
14	1	509	CLA	C4A-NA-C1A	6.59	109.67	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Y	506	CLA	C4A-NA-C1A	6.59	109.67	106.71
17	V	4022	BCR	C7-C8-C9	-6.59	116.28	126.23
14	Z	507	CLA	C4A-NA-C1A	6.59	109.67	106.71
14	e	1123	CLA	C4A-NA-C1A	6.59	109.67	106.71
14	f	1207	CLA	C4A-NA-C1A	6.59	109.67	106.71
14	2	511	CLA	C4A-NA-C1A	6.59	109.67	106.71
17	L	4022	BCR	C7-C8-C9	-6.59	116.28	126.23
14	H	1021	CLA	C4A-NA-C1A	6.58	109.67	106.71
14	1	516	CLA	C4A-NA-C1A	6.58	109.66	106.71
14	4	508	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	Z	511	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	A	1123	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	B	1207	CLA	C4A-NA-C1A	6.57	109.66	106.71
17	H	4006	BCR	C7-C8-C9	-6.57	116.31	126.23
14	5	516	CLA	C4A-NA-C1A	6.56	109.66	106.71
14	c	516	CLA	C4A-NA-C1A	6.56	109.66	106.71
17	B	4006	BCR	C7-C8-C9	-6.56	116.32	126.23
17	n	4022	BCR	C7-C8-C9	-6.56	116.32	126.23
14	3	508	CLA	C4A-NA-C1A	6.56	109.65	106.71
14	f	1203	CLA	C4A-NA-C1A	6.56	109.65	106.71
14	3	510	CLA	C4A-NA-C1A	6.55	109.65	106.71
14	H	1203	CLA	C4A-NA-C1A	6.55	109.65	106.71
14	a	508	CLA	C4A-NA-C1A	6.55	109.65	106.71
14	t	508	CLA	C4A-NA-C1A	6.54	109.65	106.71
14	f	1227	CLA	C4A-NA-C1A	6.54	109.65	106.71
14	B	1203	CLA	C4A-NA-C1A	6.54	109.64	106.71
14	q	519	CLA	C4A-NA-C1A	6.52	109.64	106.71
14	G	1123	CLA	C4A-NA-C1A	6.52	109.64	106.71
14	u	516	CLA	C4A-NA-C1A	6.51	109.64	106.71
14	G	1114	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	c	511	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	u	511	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	c	513	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	5	511	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	s	510	CLA	C4A-NA-C1A	6.50	109.63	106.71
14	t	516	CLA	C4A-NA-C1A	6.50	109.63	106.71
14	s	508	CLA	C4A-NA-C1A	6.49	109.63	106.71
14	B	1227	CLA	C4A-NA-C1A	6.49	109.62	106.71
14	4	516	CLA	C4A-NA-C1A	6.49	109.62	106.71
14	e	1105	CLA	C4A-NA-C1A	6.49	109.62	106.71
14	b	516	CLA	C4A-NA-C1A	6.48	109.62	106.71
14	A	1114	CLA	C4A-NA-C1A	6.48	109.62	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	s	517	CLA	C4A-NA-C1A	6.47	109.61	106.71
14	e	1114	CLA	C4A-NA-C1A	6.47	109.61	106.71
14	G	1801	CLA	C4A-NA-C1A	6.45	109.61	106.71
14	A	1105	CLA	C4A-NA-C1A	6.44	109.60	106.71
14	5	513	CLA	C4A-NA-C1A	6.44	109.60	106.71
14	t	505	CLA	C4A-NA-C1A	6.44	109.60	106.71
14	4	505	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	6	516	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	1	519	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	u	517	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	d	516	CLA	C4A-NA-C1A	6.42	109.59	106.71
14	r	513	CLA	C4A-NA-C1A	6.42	109.59	106.71
14	H	1227	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	B	1232	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	f	1232	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	b	505	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	G	1105	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	a	517	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	v	516	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	2	513	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	u	513	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	A	1801	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	H	1232	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	3	517	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	A	4007	BCR	C3-C4-C5	-6.38	102.68	114.08
17	G	4007	BCR	C3-C4-C5	-6.38	102.69	114.08
17	e	4007	BCR	C3-C4-C5	-6.37	102.69	114.08
14	e	1801	CLA	C4A-NA-C1A	6.37	109.57	106.71
14	A	1131	CLA	C4A-NA-C1A	6.37	109.57	106.71
14	Z	513	CLA	C4A-NA-C1A	6.37	109.57	106.71
14	Y	519	CLA	C4A-NA-C1A	6.36	109.57	106.71
14	c	517	CLA	C4A-NA-C1A	6.36	109.56	106.71
14	5	517	CLA	C4A-NA-C1A	6.34	109.56	106.71
14	j	1301	CLA	C4A-NA-C1A	6.34	109.56	106.71
14	6	512	CLA	C4A-NA-C1A	6.33	109.55	106.71
14	G	1131	CLA	C4A-NA-C1A	6.33	109.55	106.71
14	r	510	CLA	C4A-NA-C1A	6.31	109.54	106.71
14	2	510	CLA	C4A-NA-C1A	6.31	109.54	106.71
14	e	1131	CLA	C4A-NA-C1A	6.31	109.54	106.71
14	G	1107	CLA	C4A-NA-C1A	6.29	109.54	106.71
14	B	1219	CLA	C4A-NA-C1A	6.28	109.53	106.71
14	f	1219	CLA	C4A-NA-C1A	6.28	109.53	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1102	CLA	C4A-NA-C1A	6.28	109.53	106.71
14	F	1301	CLA	C4A-NA-C1A	6.26	109.52	106.71
14	G	1102	CLA	C4A-NA-C1A	6.25	109.52	106.71
14	Z	510	CLA	C4A-NA-C1A	6.25	109.52	106.71
14	R	1301	CLA	C4A-NA-C1A	6.25	109.52	106.71
14	v	512	CLA	C4A-NA-C1A	6.24	109.51	106.71
15	A	2001	PQN	C15-C13-C12	-6.24	108.50	121.12
15	G	2001	PQN	C15-C13-C12	-6.24	108.50	121.12
15	e	2001	PQN	C15-C13-C12	-6.23	108.51	121.12
14	d	512	CLA	C4A-NA-C1A	6.22	109.50	106.71
14	H	1208	CLA	C4A-NA-C1A	6.20	109.50	106.71
14	e	1102	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	A	1107	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	e	1107	CLA	C4A-NA-C1A	6.18	109.48	106.71
14	e	1127	CLA	C4A-NA-C1A	6.17	109.48	106.71
14	H	1219	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	H	1210	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	f	1208	CLA	C4A-NA-C1A	6.14	109.47	106.71
14	c	512	CLA	C4A-NA-C1A	6.12	109.46	106.71
14	A	1127	CLA	C4A-NA-C1A	6.12	109.46	106.71
14	B	1210	CLA	C4A-NA-C1A	6.12	109.46	106.71
17	A	4011	BCR	C7-C8-C9	-6.12	116.99	126.23
17	G	4011	BCR	C7-C8-C9	-6.12	116.99	126.23
14	B	1208	CLA	C4A-NA-C1A	6.11	109.45	106.71
14	Y	512	CLA	C4A-NA-C1A	6.11	109.45	106.71
14	u	512	CLA	C4A-NA-C1A	6.11	109.45	106.71
14	1	512	CLA	C4A-NA-C1A	6.11	109.45	106.71
14	f	1210	CLA	C4A-NA-C1A	6.09	109.44	106.71
17	e	4011	BCR	C7-C8-C9	-6.09	117.03	126.23
14	r	512	CLA	C4A-NA-C1A	6.08	109.44	106.71
14	H	1216	CLA	C4A-NA-C1A	6.07	109.44	106.71
14	5	512	CLA	C4A-NA-C1A	6.06	109.43	106.71
14	G	1116	CLA	C4A-NA-C1A	6.05	109.43	106.71
14	G	1127	CLA	C4A-NA-C1A	6.05	109.43	106.71
14	2	512	CLA	C4A-NA-C1A	6.03	109.42	106.71
14	B	1222	CLA	C4A-NA-C1A	6.01	109.41	106.71
14	q	512	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	f	1222	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	A	1116	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	A	1135	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	H	1222	CLA	C4A-NA-C1A	5.98	109.40	106.71
14	G	1135	CLA	C4A-NA-C1A	5.98	109.39	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	511	CLA	C4A-NA-C1A	5.97	109.39	106.71
14	H	1226	CLA	C4A-NA-C1A	5.97	109.39	106.71
14	e	1116	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	H	1226	CLA	CMB-C2B-C1B	-5.95	116.31	125.37
14	B	1216	CLA	C4A-NA-C1A	5.94	109.38	106.71
14	f	1226	CLA	CMB-C2B-C1B	-5.93	116.34	125.37
14	B	1226	CLA	CMB-C2B-C1B	-5.92	116.35	125.37
14	Z	512	CLA	C4A-NA-C1A	5.91	109.36	106.71
14	4	511	CLA	C4A-NA-C1A	5.88	109.35	106.71
17	f	4010	BCR	C20-C21-C22	-5.88	118.92	127.31
17	H	4010	BCR	C20-C21-C22	-5.88	118.92	127.31
17	B	4010	BCR	C20-C21-C22	-5.87	118.93	127.31
17	V	4219	BCR	C15-C14-C13	-5.87	118.93	127.31
17	L	4219	BCR	C15-C14-C13	-5.87	118.93	127.31
14	f	1216	CLA	C4A-NA-C1A	5.87	109.34	106.71
14	e	1135	CLA	C4A-NA-C1A	5.85	109.34	106.71
17	n	4219	BCR	C15-C14-C13	-5.85	118.97	127.31
14	A	1117	CLA	C4A-NA-C1A	5.84	109.33	106.71
14	A	1128	CLA	C4A-NA-C1A	5.84	109.33	106.71
17	T	4013	BCR	C20-C21-C22	-5.83	118.99	127.31
14	t	511	CLA	C4A-NA-C1A	5.83	109.33	106.71
17	J	4013	BCR	C20-C21-C22	-5.82	119.01	127.31
14	B	1226	CLA	C4A-NA-C1A	5.81	109.32	106.71
14	e	1128	CLA	C4A-NA-C1A	5.81	109.32	106.71
14	e	1117	CLA	C4A-NA-C1A	5.80	109.31	106.71
17	l	4013	BCR	C20-C21-C22	-5.79	119.04	127.31
14	G	1011	CLA	C4A-NA-C1A	5.79	109.31	106.71
14	G	1128	CLA	C4A-NA-C1A	5.79	109.31	106.71
14	e	1011	CLA	C4A-NA-C1A	5.79	109.31	106.71
14	A	1011	CLA	C4A-NA-C1A	5.78	109.30	106.71
14	K	1401	CLA	C4A-NA-C1A	5.77	109.30	106.71
14	f	1226	CLA	C4A-NA-C1A	5.76	109.30	106.71
17	H	4010	BCR	C15-C14-C13	-5.76	119.09	127.31
14	G	1117	CLA	C4A-NA-C1A	5.76	109.29	106.71
17	f	4010	BCR	C15-C14-C13	-5.75	119.10	127.31
17	B	4010	BCR	C15-C14-C13	-5.75	119.11	127.31
14	G	1129	CLA	C4A-NA-C1A	5.74	109.29	106.71
14	f	1225	CLA	C4A-NA-C1A	5.74	109.28	106.71
14	m	1401	CLA	C4A-NA-C1A	5.72	109.28	106.71
14	G	1013	CLA	CMB-C2B-C1B	-5.72	116.66	125.37
14	A	1013	CLA	CMB-C2B-C1B	-5.71	116.67	125.37
14	e	1013	CLA	CMB-C2B-C1B	-5.70	116.68	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1124	CLA	C4A-NA-C1A	5.70	109.27	106.71
14	a	512	CLA	C4A-NA-C1A	5.69	109.27	106.71
14	A	1124	CLA	C4A-NA-C1A	5.69	109.26	106.71
14	A	1129	CLA	C4A-NA-C1A	5.69	109.26	106.71
14	G	1124	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	U	1401	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	B	1225	CLA	C4A-NA-C1A	5.66	109.25	106.71
14	e	1129	CLA	C4A-NA-C1A	5.62	109.23	106.71
14	H	1225	CLA	C4A-NA-C1A	5.60	109.22	106.71
14	f	1234	CLA	C4A-NA-C1A	5.60	109.22	106.71
17	v	524	BCR	C7-C8-C9	-5.58	117.80	126.23
17	d	524	BCR	C7-C8-C9	-5.58	117.81	126.23
17	6	524	BCR	C7-C8-C9	-5.57	117.81	126.23
14	3	512	CLA	C4A-NA-C1A	5.57	109.21	106.71
14	s	512	CLA	C4A-NA-C1A	5.53	109.19	106.71
14	B	1234	CLA	C4A-NA-C1A	5.48	109.17	106.71
14	H	1234	CLA	C4A-NA-C1A	5.48	109.17	106.71
17	F	4016	BCR	C15-C14-C13	-5.45	119.54	127.31
17	R	4016	BCR	C15-C14-C13	-5.44	119.55	127.31
17	j	4016	BCR	C15-C14-C13	-5.42	119.57	127.31
14	e	1011	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	G	1011	CLA	O2D-CGD-CBD	5.42	120.89	111.27
14	A	1011	CLA	O2D-CGD-CBD	5.41	120.89	111.27
21	f	1852	SQD	O5-C5-C4	5.40	119.50	109.69
21	B	1852	SQD	O5-C5-C4	5.40	119.49	109.69
15	H	2002	PQN	C14-C13-C12	-5.38	109.87	123.68
14	A	1139	CLA	C4A-NA-C1A	5.38	109.13	106.71
14	e	1139	CLA	C4A-NA-C1A	5.38	109.12	106.71
15	B	2002	PQN	C14-C13-C12	-5.37	109.89	123.68
14	H	1226	CLA	C2D-C1D-ND	-5.37	106.15	110.10
21	H	1852	SQD	O5-C5-C4	5.37	119.44	109.69
15	f	2002	PQN	C14-C13-C12	-5.36	109.92	123.68
14	f	1226	CLA	C2D-C1D-ND	-5.36	106.16	110.10
14	B	1226	CLA	C2D-C1D-ND	-5.35	106.17	110.10
14	G	1139	CLA	C4A-NA-C1A	5.34	109.11	106.71
15	G	2001	PQN	C14-C13-C12	-5.28	110.12	123.68
17	e	4011	BCR	C20-C21-C22	-5.28	119.77	127.31
15	A	2001	PQN	C14-C13-C12	-5.28	110.14	123.68
17	A	4011	BCR	C20-C21-C22	-5.27	119.78	127.31
15	e	2001	PQN	C14-C13-C12	-5.27	110.15	123.68
17	G	4011	BCR	C20-C21-C22	-5.27	119.79	127.31
14	A	1128	CLA	CMB-C2B-C1B	-5.25	117.37	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1128	CLA	CMB-C2B-C1B	-5.24	117.39	125.37
17	s	522	BCR	C11-C10-C9	-5.23	119.85	127.31
14	G	1128	CLA	CMB-C2B-C1B	-5.23	117.41	125.37
17	3	522	BCR	C11-C10-C9	-5.21	119.88	127.31
17	a	522	BCR	C11-C10-C9	-5.19	119.91	127.31
17	J	4012	BCR	C20-C21-C22	-5.13	119.99	127.31
17	T	4012	BCR	C20-C21-C22	-5.12	120.00	127.31
17	l	4012	BCR	C20-C21-C22	-5.11	120.01	127.31
17	A	4007	BCR	C28-C27-C26	-5.08	105.01	114.08
17	G	4007	BCR	C28-C27-C26	-5.07	105.02	114.08
17	e	4007	BCR	C28-C27-C26	-5.07	105.03	114.08
14	f	1012	CLA	C4A-NA-C1A	5.05	108.98	106.71
14	B	1012	CLA	C4A-NA-C1A	5.05	108.97	106.71
14	e	1022	CLA	C4A-NA-C1A	5.04	108.97	106.71
14	3	516	CLA	CAC-C3C-C4C	5.03	131.33	124.81
14	s	516	CLA	CAC-C3C-C4C	5.02	131.33	124.81
14	a	516	CLA	CAC-C3C-C4C	5.01	131.31	124.81
14	A	1022	CLA	C4A-NA-C1A	4.99	108.95	106.71
17	3	521	BCR	C20-C21-C22	-4.99	120.19	127.31
17	a	521	BCR	C20-C21-C22	-4.98	120.20	127.31
17	j	4016	BCR	C11-C10-C9	-4.97	120.22	127.31
14	G	1022	CLA	C4A-NA-C1A	4.97	108.94	106.71
14	G	1130	CLA	CMB-C2B-C1B	-4.96	117.81	125.37
17	G	4008	BCR	C20-C21-C22	-4.96	120.23	127.31
17	e	4008	BCR	C20-C21-C22	-4.96	120.23	127.31
17	s	521	BCR	C20-C21-C22	-4.96	120.23	127.31
17	R	4016	BCR	C11-C10-C9	-4.96	120.23	127.31
17	F	4016	BCR	C11-C10-C9	-4.96	120.24	127.31
17	T	4015	BCR	C7-C8-C9	-4.95	118.75	126.23
17	B	4006	BCR	C24-C23-C22	-4.95	118.75	126.23
14	A	1130	CLA	CMB-C2B-C1B	-4.95	117.84	125.37
17	A	4008	BCR	C20-C21-C22	-4.95	120.25	127.31
17	J	4013	BCR	C24-C23-C22	-4.94	118.76	126.23
17	l	4013	BCR	C24-C23-C22	-4.94	118.76	126.23
14	e	1130	CLA	CMB-C2B-C1B	-4.94	117.84	125.37
17	l	4015	BCR	C7-C8-C9	-4.94	118.77	126.23
14	H	1012	CLA	C4A-NA-C1A	4.93	108.92	106.71
14	G	1130	CLA	C4A-NA-C1A	4.93	108.92	106.71
17	H	4006	BCR	C24-C23-C22	-4.93	118.79	126.23
17	J	4015	BCR	C7-C8-C9	-4.93	118.79	126.23
17	e	4001	BCR	C16-C17-C18	-4.92	120.28	127.31
17	T	4013	BCR	C24-C23-C22	-4.92	118.79	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4001	BCR	C16-C17-C18	-4.92	120.29	127.31
17	f	4006	BCR	C24-C23-C22	-4.92	118.81	126.23
17	G	4001	BCR	C16-C17-C18	-4.90	120.31	127.31
17	n	4219	BCR	C1-C6-C5	-4.90	115.72	122.61
17	L	4219	BCR	C1-C6-C5	-4.89	115.73	122.61
17	e	4002	BCR	C16-C17-C18	-4.88	120.34	127.31
17	A	4002	BCR	C16-C17-C18	-4.88	120.34	127.31
17	V	4219	BCR	C1-C6-C5	-4.88	115.74	122.61
17	G	4002	BCR	C16-C17-C18	-4.88	120.35	127.31
17	e	4002	BCR	C7-C8-C9	-4.87	118.87	126.23
14	A	1130	CLA	C4A-NA-C1A	4.87	108.89	106.71
17	A	4002	BCR	C7-C8-C9	-4.85	118.91	126.23
17	G	4002	BCR	C7-C8-C9	-4.83	118.94	126.23
17	e	4008	BCR	C15-C14-C13	-4.81	120.44	127.31
17	A	4008	BCR	C15-C14-C13	-4.81	120.44	127.31
17	s	523	BCR	C15-C14-C13	-4.81	120.45	127.31
17	a	523	BCR	C15-C14-C13	-4.80	120.45	127.31
17	3	523	BCR	C15-C14-C13	-4.80	120.46	127.31
17	H	4004	BCR	C20-C21-C22	-4.80	120.46	127.31
17	B	4004	BCR	C20-C21-C22	-4.79	120.47	127.31
17	G	4008	BCR	C15-C14-C13	-4.78	120.49	127.31
17	f	4004	BCR	C20-C21-C22	-4.77	120.50	127.31
21	f	1852	SQD	O7-S-C6	4.77	112.61	106.94
21	B	1852	SQD	O7-S-C6	4.77	112.61	106.94
14	e	1130	CLA	C4A-NA-C1A	4.75	108.84	106.71
21	H	1852	SQD	O7-S-C6	4.74	112.57	106.94
17	B	4017	BCR	C15-C14-C13	-4.73	120.56	127.31
17	H	4017	BCR	C15-C14-C13	-4.72	120.58	127.31
21	Y	822	SQD	O5-C5-C4	4.71	118.25	109.69
17	b	522	BCR	C15-C16-C17	-4.71	113.82	123.47
21	1	822	SQD	O5-C5-C4	4.71	118.24	109.69
17	l	4013	BCR	C16-C17-C18	-4.71	120.59	127.31
17	f	4017	BCR	C15-C14-C13	-4.70	120.60	127.31
17	t	522	BCR	C15-C16-C17	-4.70	113.84	123.47
17	4	522	BCR	C15-C16-C17	-4.70	113.85	123.47
21	q	822	SQD	O5-C5-C4	4.70	118.23	109.69
17	J	4013	BCR	C16-C17-C18	-4.67	120.64	127.31
17	s	522	BCR	C3-C4-C5	-4.67	105.74	114.08
17	3	522	BCR	C3-C4-C5	-4.66	105.75	114.08
14	K	1401	CLA	CAA-C2A-C3A	-4.66	100.02	112.78
17	a	522	BCR	C3-C4-C5	-4.66	105.76	114.08
14	U	1401	CLA	CAA-C2A-C3A	-4.66	100.02	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	4013	BCR	C16-C17-C18	-4.66	120.66	127.31
14	m	1401	CLA	CAA-C2A-C3A	-4.66	100.03	112.78
17	V	4219	BCR	C16-C17-C18	-4.64	120.69	127.31
17	t	523	BCR	C15-C14-C13	-4.63	120.70	127.31
17	b	523	BCR	C15-C14-C13	-4.63	120.70	127.31
17	d	522	BCR	C15-C14-C13	-4.63	120.70	127.31
17	L	4219	BCR	C16-C17-C18	-4.63	120.71	127.31
17	5	522	BCR	C15-C14-C13	-4.62	120.71	127.31
17	3	524	BCR	C15-C14-C13	-4.62	120.72	127.31
17	e	4008	BCR	C16-C17-C18	-4.62	120.72	127.31
17	n	4219	BCR	C16-C17-C18	-4.62	120.72	127.31
17	B	4010	BCR	C15-C16-C17	-4.61	114.02	123.47
17	a	524	BCR	C15-C14-C13	-4.61	120.73	127.31
17	f	4010	BCR	C15-C16-C17	-4.61	114.03	123.47
17	H	4010	BCR	C15-C16-C17	-4.61	114.03	123.47
17	4	523	BCR	C15-C14-C13	-4.61	120.73	127.31
17	H	4004	BCR	C16-C17-C18	-4.61	120.74	127.31
17	s	524	BCR	C15-C14-C13	-4.61	120.74	127.31
17	u	522	BCR	C15-C14-C13	-4.60	120.74	127.31
17	c	522	BCR	C15-C14-C13	-4.60	120.75	127.31
17	f	4004	BCR	C16-C17-C18	-4.60	120.75	127.31
17	G	4008	BCR	C16-C17-C18	-4.59	120.76	127.31
17	B	4004	BCR	C16-C17-C18	-4.59	120.76	127.31
17	L	4219	BCR	C15-C16-C17	-4.59	114.07	123.47
17	V	4219	BCR	C15-C16-C17	-4.59	114.08	123.47
17	6	522	BCR	C15-C14-C13	-4.59	120.77	127.31
17	A	4008	BCR	C16-C17-C18	-4.59	120.77	127.31
17	v	522	BCR	C15-C14-C13	-4.58	120.77	127.31
17	5	522	BCR	C11-C10-C9	-4.58	120.77	127.31
17	n	4219	BCR	C15-C16-C17	-4.58	114.09	123.47
17	u	522	BCR	C11-C10-C9	-4.58	120.78	127.31
17	Z	522	BCR	C15-C14-C13	-4.57	120.78	127.31
17	c	522	BCR	C11-C10-C9	-4.57	120.79	127.31
17	B	4010	BCR	C3-C4-C5	-4.56	105.94	114.08
17	f	4010	BCR	C3-C4-C5	-4.55	105.96	114.08
17	H	4010	BCR	C3-C4-C5	-4.54	105.98	114.08
17	2	522	BCR	C15-C14-C13	-4.53	120.84	127.31
17	5	521	BCR	C15-C14-C13	-4.52	120.85	127.31
17	f	4017	BCR	C16-C17-C18	-4.51	120.87	127.31
17	q	522	BCR	C11-C10-C9	-4.51	120.87	127.31
17	c	521	BCR	C15-C14-C13	-4.51	120.87	127.31
17	Y	522	BCR	C11-C10-C9	-4.51	120.88	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	u	521	BCR	C15-C14-C13	-4.51	120.88	127.31
17	Y	524	BCR	C16-C17-C18	-4.50	120.89	127.31
17	q	524	BCR	C16-C17-C18	-4.50	120.89	127.31
17	r	522	BCR	C15-C14-C13	-4.50	120.89	127.31
17	1	524	BCR	C16-C17-C18	-4.50	120.89	127.31
17	H	4017	BCR	C16-C17-C18	-4.50	120.89	127.31
17	a	522	BCR	C15-C14-C13	-4.50	120.89	127.31
17	1	522	BCR	C11-C10-C9	-4.49	120.90	127.31
17	v	524	BCR	C15-C14-C13	-4.49	120.90	127.31
17	B	4017	BCR	C16-C17-C18	-4.49	120.90	127.31
14	B	1023	CLA	CAC-C3C-C4C	4.48	130.63	124.81
17	d	524	BCR	C15-C14-C13	-4.48	120.92	127.31
17	3	522	BCR	C15-C14-C13	-4.47	120.93	127.31
17	s	522	BCR	C15-C14-C13	-4.47	120.93	127.31
14	H	1023	CLA	CAC-C3C-C4C	4.47	130.60	124.81
17	6	524	BCR	C15-C14-C13	-4.46	120.94	127.31
14	f	1023	CLA	CAC-C3C-C4C	4.46	130.59	124.81
17	3	521	BCR	C15-C14-C13	-4.45	120.97	127.31
17	a	521	BCR	C15-C14-C13	-4.44	120.97	127.31
17	r	521	BCR	C28-C27-C26	-4.44	106.15	114.08
17	R	4016	BCR	C7-C8-C9	-4.44	119.53	126.23
17	s	521	BCR	C15-C14-C13	-4.43	120.99	127.31
14	f	1232	CLA	CMB-C2B-C1B	-4.43	118.62	125.37
21	c	822	SQD	O7-S-C6	4.43	112.20	106.94
17	2	521	BCR	C28-C27-C26	-4.42	106.18	114.08
21	5	822	SQD	O7-S-C6	4.42	112.19	106.94
17	Z	521	BCR	C28-C27-C26	-4.42	106.19	114.08
17	j	4016	BCR	C7-C8-C9	-4.41	119.56	126.23
17	F	4016	BCR	C7-C8-C9	-4.41	119.57	126.23
21	u	822	SQD	O7-S-C6	4.41	112.18	106.94
21	b	822	SQD	O47-C7-C8	4.41	119.20	111.09
14	B	1232	CLA	CMB-C2B-C1B	-4.41	118.65	125.37
21	4	822	SQD	O47-C7-C8	4.41	119.20	111.09
21	t	822	SQD	O47-C7-C8	4.41	119.20	111.09
18	B	1842	LHG	O4-P-O5	4.40	134.00	112.24
18	H	1842	LHG	O4-P-O5	4.40	134.00	112.24
18	f	1842	LHG	O4-P-O5	4.40	133.99	112.24
14	H	1232	CLA	CMB-C2B-C1B	-4.40	118.67	125.37
14	H	1234	CLA	CMB-C2B-C1B	-4.39	118.68	125.37
14	B	1234	CLA	CMB-C2B-C1B	-4.38	118.69	125.37
17	r	524	BCR	C15-C14-C13	-4.38	121.06	127.31
17	5	524	BCR	C15-C14-C13	-4.37	121.07	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1234	CLA	CMB-C2B-C1B	-4.37	118.71	125.37
17	2	524	BCR	C15-C14-C13	-4.36	121.09	127.31
17	u	524	BCR	C15-C14-C13	-4.35	121.10	127.31
17	t	524	BCR	C16-C17-C18	-4.35	121.11	127.31
17	c	524	BCR	C15-C14-C13	-4.34	121.11	127.31
17	4	524	BCR	C16-C17-C18	-4.34	121.12	127.31
17	b	524	BCR	C16-C17-C18	-4.33	121.13	127.31
17	Z	524	BCR	C15-C14-C13	-4.33	121.13	127.31
17	2	521	BCR	C24-C23-C22	-4.33	119.69	126.23
17	t	521	BCR	C7-C8-C9	-4.33	119.69	126.23
17	r	521	BCR	C24-C23-C22	-4.33	119.70	126.23
17	Z	521	BCR	C24-C23-C22	-4.33	119.70	126.23
17	f	4004	BCR	C24-C23-C22	-4.32	119.71	126.23
17	Y	524	BCR	C15-C14-C13	-4.32	121.15	127.31
17	4	521	BCR	C7-C8-C9	-4.32	119.71	126.23
17	s	522	BCR	C7-C8-C9	-4.32	119.71	126.23
17	K	4104	BCR	C7-C8-C9	-4.31	119.72	126.23
17	n	4022	BCR	C11-C10-C9	-4.31	121.16	127.31
17	r	521	BCR	C20-C21-C22	-4.31	121.16	127.31
17	1	524	BCR	C15-C14-C13	-4.30	121.17	127.31
17	3	522	BCR	C7-C8-C9	-4.30	119.74	126.23
17	U	4104	BCR	C7-C8-C9	-4.30	119.74	126.23
17	2	521	BCR	C20-C21-C22	-4.30	121.18	127.31
17	t	524	BCR	C11-C10-C9	-4.29	121.18	127.31
17	B	4004	BCR	C24-C23-C22	-4.29	119.75	126.23
17	H	4004	BCR	C24-C23-C22	-4.29	119.75	126.23
17	b	524	BCR	C11-C10-C9	-4.29	121.18	127.31
17	m	4104	BCR	C7-C8-C9	-4.29	119.76	126.23
17	Z	523	BCR	C15-C14-C13	-4.29	121.19	127.31
17	q	524	BCR	C15-C14-C13	-4.29	121.19	127.31
14	e	1128	CLA	CHB-C1B-NB	4.29	128.79	124.26
17	4	524	BCR	C11-C10-C9	-4.29	121.19	127.31
21	Y	822	SQD	O7-S-C6	4.28	112.03	106.94
17	r	523	BCR	C15-C14-C13	-4.27	121.21	127.31
17	Z	521	BCR	C20-C21-C22	-4.27	121.21	127.31
17	b	521	BCR	C7-C8-C9	-4.27	119.79	126.23
17	a	522	BCR	C7-C8-C9	-4.27	119.79	126.23
21	v	822	SQD	O47-C7-C8	4.27	118.94	111.09
17	L	4022	BCR	C11-C10-C9	-4.27	121.22	127.31
17	2	523	BCR	C15-C14-C13	-4.27	121.22	127.31
14	A	1128	CLA	CHB-C1B-NB	4.26	128.77	124.26
18	e	5008	LHG	O4-P-O5	4.26	133.31	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Y	504	CLA	O2D-CGD-O1D	-4.26	115.50	123.84
17	V	4022	BCR	C11-C10-C9	-4.26	121.23	127.31
21	1	822	SQD	O7-S-C6	4.26	112.00	106.94
18	A	5008	LHG	O4-P-O5	4.26	133.29	112.24
18	e	5002	LHG	O4-P-O5	4.26	133.28	112.24
17	u	523	BCR	C15-C14-C13	-4.26	121.24	127.31
17	S	4018	BCR	C16-C17-C18	-4.25	121.24	127.31
21	6	822	SQD	O47-C7-C8	4.25	118.91	111.09
18	A	5004	LHG	O4-P-O5	4.25	133.25	112.24
18	G	5002	LHG	O4-P-O5	4.25	133.25	112.24
14	G	1128	CLA	CHB-C1B-NB	4.25	128.76	124.26
18	A	5002	LHG	O4-P-O5	4.25	133.25	112.24
18	G	5008	LHG	O4-P-O5	4.25	133.25	112.24
18	G	5004	LHG	O4-P-O5	4.25	133.24	112.24
21	q	822	SQD	O7-S-C6	4.25	111.99	106.94
17	k	4018	BCR	C16-C17-C18	-4.25	121.25	127.31
14	q	504	CLA	O2D-CGD-O1D	-4.25	115.54	123.84
17	W	4021	BCR	C24-C23-C22	-4.24	119.82	126.23
14	1	504	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
21	d	822	SQD	O47-C7-C8	4.24	118.89	111.09
18	e	5004	LHG	O4-P-O5	4.24	133.20	112.24
17	M	4021	BCR	C24-C23-C22	-4.23	119.84	126.23
17	1	521	BCR	C24-C23-C22	-4.23	119.84	126.23
17	q	521	BCR	C24-C23-C22	-4.22	119.85	126.23
18	k	5001	LHG	O4-P-O5	4.22	133.11	112.24
17	I	4018	BCR	C16-C17-C18	-4.22	121.29	127.31
17	o	4021	BCR	C24-C23-C22	-4.22	119.86	126.23
18	S	5001	LHG	O4-P-O5	4.22	133.10	112.24
17	1	522	BCR	C15-C14-C13	-4.22	121.29	127.31
18	I	5001	LHG	O4-P-O5	4.22	133.09	112.24
17	q	522	BCR	C15-C14-C13	-4.22	121.29	127.31
17	s	521	BCR	C16-C17-C18	-4.21	121.30	127.31
17	Y	521	BCR	C24-C23-C22	-4.21	119.87	126.23
18	G	5003	LHG	O4-P-O5	4.21	133.06	112.24
18	A	5003	LHG	O4-P-O5	4.21	133.03	112.24
17	3	521	BCR	C16-C17-C18	-4.20	121.31	127.31
17	Y	522	BCR	C15-C14-C13	-4.20	121.31	127.31
17	5	523	BCR	C15-C14-C13	-4.20	121.31	127.31
18	e	5003	LHG	O4-P-O5	4.20	133.02	112.24
17	S	4018	BCR	C15-C16-C17	-4.20	114.87	123.47
17	a	521	BCR	C16-C17-C18	-4.20	121.32	127.31
17	c	523	BCR	C15-C14-C13	-4.20	121.32	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	e	5006	LHG	O4-P-O5	4.19	132.97	112.24
17	S	4018	BCR	C24-C23-C22	-4.19	119.90	126.23
17	k	4018	BCR	C15-C16-C17	-4.19	114.89	123.47
18	G	5006	LHG	O4-P-O5	4.19	132.96	112.24
18	A	5006	LHG	O4-P-O5	4.19	132.95	112.24
17	k	4018	BCR	C24-C23-C22	-4.19	119.91	126.23
17	I	4018	BCR	C15-C16-C17	-4.19	114.90	123.47
14	G	1011	CLA	C1D-ND-C4D	-4.18	103.37	106.33
17	I	4018	BCR	C24-C23-C22	-4.18	119.92	126.23
18	G	5007	LHG	O4-P-O5	4.17	132.86	112.24
18	n	5221	LHG	O4-P-O5	4.17	132.86	112.24
18	L	5221	LHG	O4-P-O5	4.17	132.84	112.24
18	A	5007	LHG	O4-P-O5	4.17	132.84	112.24
18	V	5221	LHG	O4-P-O5	4.17	132.83	112.24
14	A	1134	CLA	CAA-C2A-C3A	-4.17	101.37	112.78
14	e	1134	CLA	CAA-C2A-C3A	-4.16	101.38	112.78
17	H	4010	BCR	C11-C10-C9	-4.16	121.37	127.31
18	n	5220	LHG	O4-P-O5	4.16	132.82	112.24
18	e	5007	LHG	O4-P-O5	4.16	132.81	112.24
18	V	5220	LHG	O4-P-O5	4.16	132.80	112.24
18	L	5220	LHG	O4-P-O5	4.16	132.79	112.24
17	e	4001	BCR	C3-C4-C5	-4.15	106.67	114.08
17	n	4019	BCR	C7-C8-C9	-4.15	119.96	126.23
18	G	5001	LHG	O4-P-O5	4.15	132.75	112.24
18	e	5001	LHG	O4-P-O5	4.15	132.75	112.24
18	G	5009	LHG	O4-P-O5	4.15	132.75	112.24
14	G	1134	CLA	CAA-C2A-C3A	-4.15	101.42	112.78
18	A	5001	LHG	O4-P-O5	4.15	132.74	112.24
14	e	1011	CLA	C1D-ND-C4D	-4.15	103.39	106.33
18	e	5009	LHG	O4-P-O5	4.14	132.73	112.24
14	A	1011	CLA	CGD-CBD-CAD	4.14	124.16	110.73
18	A	5009	LHG	O4-P-O5	4.14	132.72	112.24
17	A	4001	BCR	C3-C4-C5	-4.14	106.68	114.08
17	B	4010	BCR	C11-C10-C9	-4.14	121.40	127.31
17	L	4019	BCR	C7-C8-C9	-4.14	119.98	126.23
18	n	5218	LHG	O4-P-O5	4.14	132.71	112.24
14	e	1011	CLA	CGD-CBD-CAD	4.14	124.14	110.73
18	V	5218	LHG	O4-P-O5	4.14	132.70	112.24
17	Z	521	BCR	C16-C17-C18	-4.14	121.41	127.31
18	L	5218	LHG	O4-P-O5	4.14	132.69	112.24
17	V	4019	BCR	C7-C8-C9	-4.14	119.99	126.23
17	G	4001	BCR	C3-C4-C5	-4.13	106.70	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1011	CLA	CGD-CBD-CAD	4.13	124.11	110.73
17	f	4010	BCR	C11-C10-C9	-4.12	121.43	127.31
17	e	4003	BCR	C3-C4-C5	-4.12	106.72	114.08
17	2	521	BCR	C16-C17-C18	-4.12	121.44	127.31
18	e	5005	LHG	O4-P-O5	4.11	132.57	112.24
14	A	1011	CLA	C1D-ND-C4D	-4.11	103.42	106.33
17	s	523	BCR	C11-C10-C9	-4.11	121.45	127.31
18	A	5005	LHG	O4-P-O5	4.11	132.54	112.24
17	A	4003	BCR	C3-C4-C5	-4.10	106.75	114.08
18	G	5005	LHG	O4-P-O5	4.10	132.53	112.24
14	H	1226	CLA	CHB-C1B-NB	4.10	128.60	124.26
17	r	521	BCR	C16-C17-C18	-4.09	121.47	127.31
17	a	523	BCR	C11-C10-C9	-4.09	121.48	127.31
21	c	822	SQD	O47-C7-C8	4.08	118.60	111.09
17	G	4003	BCR	C3-C4-C5	-4.08	106.79	114.08
17	3	523	BCR	C11-C10-C9	-4.07	121.50	127.31
21	u	822	SQD	O47-C7-C8	4.07	118.58	111.09
14	f	1209	CLA	O2D-CGD-CBD	4.07	118.50	111.27
21	5	822	SQD	O47-C7-C8	4.07	118.57	111.09
17	j	4016	BCR	C24-C23-C22	-4.07	120.09	126.23
17	q	522	BCR	C7-C8-C9	-4.06	120.10	126.23
21	n	5216	SQD	O7-S-C6	4.06	111.77	106.94
21	L	5216	SQD	O7-S-C6	4.06	111.77	106.94
17	L	4022	BCR	C20-C21-C22	-4.06	121.52	127.31
17	W	4021	BCR	C15-C14-C13	-4.06	121.52	127.31
14	f	1226	CLA	CHB-C1B-NB	4.05	128.55	124.26
14	B	1209	CLA	O2D-CGD-CBD	4.05	118.47	111.27
17	1	522	BCR	C7-C8-C9	-4.04	120.12	126.23
21	V	5216	SQD	O7-S-C6	4.04	111.75	106.94
18	f	1855	LHG	O4-P-O5	4.04	132.23	112.24
14	H	1209	CLA	O2D-CGD-CBD	4.04	118.45	111.27
18	B	1855	LHG	O4-P-O5	4.04	132.22	112.24
14	B	1226	CLA	CHB-C1B-NB	4.04	128.53	124.26
17	Y	522	BCR	C7-C8-C9	-4.04	120.13	126.23
17	V	4022	BCR	C20-C21-C22	-4.04	121.55	127.31
17	F	4016	BCR	C24-C23-C22	-4.04	120.13	126.23
17	n	4022	BCR	C20-C21-C22	-4.03	121.55	127.31
18	H	1855	LHG	O4-P-O5	4.03	132.18	112.24
17	t	521	BCR	C20-C21-C22	-4.03	121.55	127.31
17	Z	522	BCR	C11-C10-C9	-4.03	121.56	127.31
17	6	523	BCR	C15-C14-C13	-4.03	121.56	127.31
17	v	523	BCR	C15-C14-C13	-4.03	121.56	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	R	4016	BCR	C24-C23-C22	-4.03	120.15	126.23
17	4	521	BCR	C20-C21-C22	-4.03	121.56	127.31
17	e	4003	BCR	C20-C21-C22	-4.03	121.56	127.31
17	o	4021	BCR	C15-C14-C13	-4.03	121.56	127.31
17	b	521	BCR	C20-C21-C22	-4.03	121.56	127.31
17	M	4021	BCR	C15-C14-C13	-4.02	121.57	127.31
21	q	822	SQD	C1-O5-C5	4.02	121.58	113.69
17	b	524	BCR	C15-C14-C13	-4.02	121.58	127.31
17	m	4104	BCR	C20-C21-C22	-4.02	121.58	127.31
21	Y	822	SQD	C1-O5-C5	4.02	121.57	113.69
17	2	522	BCR	C11-C10-C9	-4.01	121.58	127.31
17	d	523	BCR	C15-C14-C13	-4.01	121.58	127.31
21	1	822	SQD	C1-O5-C5	4.01	121.56	113.69
17	e	4003	BCR	C16-C17-C18	-4.01	121.59	127.31
17	t	524	BCR	C15-C14-C13	-4.01	121.59	127.31
17	4	524	BCR	C15-C14-C13	-4.01	121.59	127.31
17	6	524	BCR	C16-C17-C18	-4.01	121.59	127.31
17	A	4003	BCR	C20-C21-C22	-4.01	121.59	127.31
14	A	1129	CLA	C3B-C4B-NB	-4.00	106.80	110.52
14	G	1129	CLA	C3B-C4B-NB	-4.00	106.80	110.52
17	G	4003	BCR	C16-C17-C18	-4.00	121.60	127.31
17	U	4104	BCR	C20-C21-C22	-4.00	121.60	127.31
17	b	522	BCR	C15-C14-C13	-4.00	121.61	127.31
17	M	4021	BCR	C20-C21-C22	-4.00	121.61	127.31
17	4	522	BCR	C15-C14-C13	-4.00	121.61	127.31
17	K	4104	BCR	C20-C21-C22	-3.99	121.62	127.31
14	e	1129	CLA	C3B-C4B-NB	-3.99	106.81	110.52
17	H	4005	BCR	C7-C8-C9	-3.99	120.21	126.23
17	d	524	BCR	C16-C17-C18	-3.99	121.62	127.31
17	o	4021	BCR	C20-C21-C22	-3.99	121.62	127.31
17	A	4003	BCR	C16-C17-C18	-3.98	121.63	127.31
17	5	521	BCR	C20-C21-C22	-3.98	121.63	127.31
17	c	521	BCR	C20-C21-C22	-3.98	121.63	127.31
17	t	522	BCR	C15-C14-C13	-3.98	121.63	127.31
17	v	524	BCR	C16-C17-C18	-3.98	121.64	127.31
17	r	522	BCR	C11-C10-C9	-3.97	121.64	127.31
17	u	521	BCR	C20-C21-C22	-3.97	121.64	127.31
17	V	4019	BCR	C11-C10-C9	-3.97	121.65	127.31
17	f	4014	BCR	C16-C17-C18	-3.97	121.65	127.31
17	G	4003	BCR	C20-C21-C22	-3.97	121.65	127.31
17	W	4021	BCR	C20-C21-C22	-3.97	121.65	127.31
17	B	4005	BCR	C7-C8-C9	-3.97	120.24	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	r	521	BCR	C15-C14-C13	-3.97	121.65	127.31
17	B	4009	BCR	C11-C10-C9	-3.96	121.65	127.31
17	L	4019	BCR	C11-C10-C9	-3.96	121.65	127.31
17	1	523	BCR	C15-C14-C13	-3.96	121.66	127.31
17	U	4104	BCR	C16-C17-C18	-3.96	121.66	127.31
17	B	4014	BCR	C16-C17-C18	-3.96	121.66	127.31
17	B	4017	BCR	C24-C23-C22	-3.96	120.26	126.23
17	1	521	BCR	C20-C21-C22	-3.96	121.66	127.31
17	H	4017	BCR	C24-C23-C22	-3.95	120.26	126.23
17	q	523	BCR	C15-C14-C13	-3.95	121.67	127.31
17	Y	521	BCR	C3-C4-C5	-3.95	107.02	114.08
17	f	4005	BCR	C7-C8-C9	-3.95	120.26	126.23
17	2	521	BCR	C15-C14-C13	-3.95	121.67	127.31
17	H	4014	BCR	C16-C17-C18	-3.95	121.67	127.31
17	m	4104	BCR	C16-C17-C18	-3.95	121.68	127.31
17	K	4104	BCR	C16-C17-C18	-3.95	121.68	127.31
17	1	521	BCR	C3-C4-C5	-3.95	107.03	114.08
17	q	521	BCR	C3-C4-C5	-3.94	107.03	114.08
17	Y	521	BCR	C20-C21-C22	-3.94	121.68	127.31
17	f	4006	BCR	C15-C14-C13	-3.94	121.68	127.31
17	n	4019	BCR	C11-C10-C9	-3.94	121.68	127.31
17	f	4017	BCR	C24-C23-C22	-3.94	120.28	126.23
17	H	4006	BCR	C15-C14-C13	-3.94	121.69	127.31
17	H	4009	BCR	C11-C10-C9	-3.94	121.69	127.31
17	q	521	BCR	C20-C21-C22	-3.94	121.69	127.31
17	v	522	BCR	C11-C10-C9	-3.94	121.69	127.31
17	M	4021	BCR	C15-C16-C17	-3.94	115.41	123.47
17	Y	523	BCR	C15-C14-C13	-3.94	121.69	127.31
17	f	4009	BCR	C11-C10-C9	-3.94	121.69	127.31
17	Z	521	BCR	C15-C14-C13	-3.93	121.70	127.31
17	B	4006	BCR	C15-C14-C13	-3.93	121.70	127.31
17	6	522	BCR	C11-C10-C9	-3.93	121.70	127.31
17	G	4002	BCR	C20-C21-C22	-3.93	121.70	127.31
14	H	1221	CLA	CMB-C2B-C1B	-3.92	119.39	125.37
17	d	522	BCR	C11-C10-C9	-3.92	121.71	127.31
17	B	4014	BCR	C20-C19-C18	-3.92	115.40	126.42
21	s	822	SQD	O7-S-C6	3.92	111.60	106.94
17	W	4021	BCR	C15-C16-C17	-3.92	115.45	123.47
17	A	4002	BCR	C20-C21-C22	-3.92	121.72	127.31
17	f	4014	BCR	C20-C19-C18	-3.92	115.41	126.42
14	B	1221	CLA	CMB-C2B-C1B	-3.92	119.41	125.37
17	o	4021	BCR	C15-C16-C17	-3.91	115.46	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	521	BCR	C16-C17-C18	-3.91	121.73	127.31
17	H	4014	BCR	C20-C19-C18	-3.91	115.44	126.42
14	f	1221	CLA	CMB-C2B-C1B	-3.91	119.42	125.37
17	c	521	BCR	C16-C17-C18	-3.91	121.73	127.31
17	u	521	BCR	C16-C17-C18	-3.90	121.74	127.31
14	B	1209	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
14	H	1209	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
21	3	822	SQD	O7-S-C6	3.90	111.57	106.94
17	e	4002	BCR	C20-C21-C22	-3.90	121.75	127.31
14	f	1209	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
17	G	4003	BCR	C15-C14-C13	-3.89	121.76	127.31
17	T	4012	BCR	C3-C4-C5	-3.89	107.13	114.08
17	H	4006	BCR	C34-C9-C10	-3.89	117.48	122.92
17	U	4104	BCR	C38-C26-C25	-3.89	120.17	124.53
21	a	822	SQD	O7-S-C6	3.88	111.56	106.94
17	3	524	BCR	C16-C17-C18	-3.88	121.77	127.31
17	G	4007	BCR	C15-C14-C13	-3.88	121.78	127.31
14	e	1011	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
17	m	4104	BCR	C38-C26-C25	-3.88	120.17	124.53
21	Z	822	SQD	O7-S-C6	3.88	111.55	106.94
17	e	4003	BCR	C15-C14-C13	-3.88	121.78	127.31
17	f	4006	BCR	C34-C9-C10	-3.87	117.50	122.92
17	a	524	BCR	C16-C17-C18	-3.87	121.78	127.31
17	J	4012	BCR	C3-C4-C5	-3.87	107.16	114.08
17	A	4003	BCR	C15-C14-C13	-3.87	121.78	127.31
17	s	524	BCR	C16-C17-C18	-3.87	121.78	127.31
17	A	4007	BCR	C15-C14-C13	-3.86	121.80	127.31
14	A	1011	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
14	G	1011	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
17	K	4104	BCR	C38-C26-C25	-3.86	120.20	124.53
17	B	4006	BCR	C34-C9-C10	-3.86	117.52	122.92
21	2	822	SQD	O7-S-C6	3.86	111.52	106.94
14	A	1013	CLA	CMB-C2B-C3B	3.85	135.92	126.59
14	G	1013	CLA	CMB-C2B-C3B	3.85	135.92	126.59
17	l	4012	BCR	C3-C4-C5	-3.85	107.20	114.08
17	e	4001	BCR	C20-C21-C22	-3.85	121.81	127.31
17	u	523	BCR	C7-C8-C9	-3.85	120.42	126.23
17	A	4001	BCR	C20-C21-C22	-3.84	121.82	127.31
17	L	4219	BCR	C33-C5-C6	-3.84	120.21	124.53
14	e	1013	CLA	CMB-C2B-C3B	3.84	135.90	126.59
17	n	4219	BCR	C33-C5-C6	-3.84	120.21	124.53
17	G	4001	BCR	C20-C21-C22	-3.84	121.83	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	r	822	SQD	O7-S-C6	3.84	111.50	106.94
17	H	4006	BCR	C33-C5-C6	-3.83	120.22	124.53
17	e	4007	BCR	C15-C14-C13	-3.83	121.84	127.31
17	B	4006	BCR	C33-C5-C6	-3.82	120.23	124.53
17	T	4015	BCR	C15-C14-C13	-3.82	121.85	127.31
17	d	523	BCR	C16-C17-C18	-3.82	121.85	127.31
17	V	4219	BCR	C33-C5-C6	-3.82	120.24	124.53
17	5	523	BCR	C7-C8-C9	-3.82	120.46	126.23
17	B	4017	BCR	C10-C11-C12	-3.82	111.30	123.22
17	f	4006	BCR	C33-C5-C6	-3.82	120.24	124.53
17	H	4017	BCR	C10-C11-C12	-3.82	111.30	123.22
17	f	4017	BCR	C10-C11-C12	-3.82	111.30	123.22
17	1	521	BCR	C15-C14-C13	-3.82	121.86	127.31
17	6	521	BCR	C24-C23-C22	-3.82	120.47	126.23
17	q	521	BCR	C15-C14-C13	-3.81	121.87	127.31
17	Y	521	BCR	C15-C14-C13	-3.81	121.87	127.31
17	J	4015	BCR	C15-C14-C13	-3.80	121.88	127.31
17	c	523	BCR	C7-C8-C9	-3.80	120.49	126.23
17	d	521	BCR	C24-C23-C22	-3.80	120.49	126.23
21	d	822	SQD	O9-S-O7	-3.80	100.80	113.95
17	v	521	BCR	C24-C23-C22	-3.80	120.50	126.23
17	f	4010	BCR	C8-C7-C6	-3.80	116.54	127.20
17	6	523	BCR	C16-C17-C18	-3.80	121.89	127.31
21	6	822	SQD	O9-S-O7	-3.79	100.82	113.95
17	l	4015	BCR	C15-C14-C13	-3.79	121.90	127.31
21	v	822	SQD	O9-S-O7	-3.79	100.83	113.95
17	b	524	BCR	C33-C5-C6	-3.79	120.27	124.53
17	B	4010	BCR	C8-C7-C6	-3.79	116.56	127.20
14	G	1135	CLA	C1-C2-C3	-3.79	119.49	126.04
14	e	1135	CLA	C1-C2-C3	-3.79	119.49	126.04
17	4	524	BCR	C33-C5-C6	-3.78	120.28	124.53
14	A	1135	CLA	C1-C2-C3	-3.78	119.50	126.04
17	H	4010	BCR	C8-C7-C6	-3.78	116.59	127.20
17	d	521	BCR	C28-C27-C26	-3.78	107.33	114.08
17	v	521	BCR	C16-C17-C18	-3.78	121.92	127.31
17	a	522	BCR	C24-C23-C22	-3.77	120.53	126.23
17	G	4002	BCR	C11-C10-C9	-3.77	121.92	127.31
17	2	524	BCR	C33-C5-C6	-3.77	120.30	124.53
17	6	521	BCR	C28-C27-C26	-3.77	107.35	114.08
21	1	822	SQD	O9-S-O7	-3.76	100.92	113.95
17	6	521	BCR	C16-C17-C18	-3.76	121.94	127.31
17	J	4012	BCR	C11-C10-C9	-3.76	121.94	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	4004	BCR	C11-C10-C9	-3.76	121.94	127.31
14	B	1227	CLA	C3B-C4B-NB	-3.76	107.03	110.52
14	H	1227	CLA	C3B-C4B-NB	-3.76	107.03	110.52
14	A	1121	CLA	CAA-C2A-C3A	-3.76	102.48	112.78
17	r	524	BCR	C33-C5-C6	-3.76	120.31	124.53
21	Y	822	SQD	O9-S-O7	-3.76	100.93	113.95
17	v	521	BCR	C28-C27-C26	-3.76	107.36	114.08
21	n	5216	SQD	O9-S-O7	-3.76	100.94	113.95
17	l	4012	BCR	C11-C10-C9	-3.76	121.95	127.31
21	u	822	SQD	O9-S-O7	-3.76	100.95	113.95
17	d	521	BCR	C16-C17-C18	-3.76	121.95	127.31
17	Z	524	BCR	C33-C5-C6	-3.76	120.31	124.53
21	L	5216	SQD	O6-C1-C2	3.75	114.17	108.30
21	q	822	SQD	O9-S-O7	-3.75	100.95	113.95
14	G	1121	CLA	CAA-C2A-C3A	-3.75	102.50	112.78
14	H	1211	CLA	CHB-C4A-NA	3.75	129.70	124.51
17	3	522	BCR	C24-C23-C22	-3.75	120.56	126.23
21	V	5216	SQD	O9-S-O7	-3.75	100.96	113.95
21	L	5216	SQD	O9-S-O7	-3.75	100.97	113.95
17	H	4004	BCR	C11-C10-C9	-3.75	121.96	127.31
14	e	1121	CLA	CAA-C2A-C3A	-3.75	102.51	112.78
21	b	822	SQD	O9-S-C6	3.75	111.40	106.94
17	B	4004	BCR	C11-C10-C9	-3.75	121.96	127.31
17	T	4012	BCR	C11-C10-C9	-3.75	121.96	127.31
17	Z	524	BCR	C16-C17-C18	-3.75	121.96	127.31
17	A	4002	BCR	C11-C10-C9	-3.75	121.96	127.31
17	B	4009	BCR	C21-C20-C19	-3.75	111.52	123.22
14	f	1227	CLA	C3B-C4B-NB	-3.75	107.04	110.52
21	5	822	SQD	O9-S-O7	-3.75	100.98	113.95
14	f	1211	CLA	CHB-C4A-NA	3.74	129.69	124.51
17	H	4009	BCR	C21-C20-C19	-3.74	111.53	123.22
17	2	524	BCR	C16-C17-C18	-3.74	121.97	127.31
17	r	524	BCR	C16-C17-C18	-3.74	121.97	127.31
17	v	523	BCR	C16-C17-C18	-3.74	121.97	127.31
17	t	524	BCR	C33-C5-C6	-3.74	120.33	124.53
21	c	822	SQD	O9-S-O7	-3.74	101.01	113.95
17	f	4009	BCR	C21-C20-C19	-3.74	111.55	123.22
17	e	4002	BCR	C11-C10-C9	-3.74	121.98	127.31
17	v	523	BCR	C7-C8-C9	-3.74	120.59	126.23
21	4	822	SQD	O9-S-C6	3.74	111.38	106.94
17	d	523	BCR	C7-C8-C9	-3.73	120.60	126.23
17	Z	521	BCR	C11-C10-C9	-3.73	121.99	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	t	822	SQD	O9-S-C6	3.73	111.37	106.94
21	V	5216	SQD	C4-C3-C2	3.73	117.33	110.82
17	s	522	BCR	C24-C23-C22	-3.73	120.60	126.23
17	2	521	BCR	C11-C10-C9	-3.72	122.00	127.31
21	b	822	SQD	O9-S-O7	-3.72	101.06	113.95
17	M	4021	BCR	C28-C27-C26	-3.72	107.43	114.08
17	6	523	BCR	C7-C8-C9	-3.72	120.61	126.23
19	e	1849	LMU	O5'-C5'-C4'	3.72	116.45	109.69
21	n	5216	SQD	O6-C1-C2	3.72	114.11	108.30
17	W	4021	BCR	C28-C27-C26	-3.72	107.43	114.08
21	V	5216	SQD	O6-C1-C2	3.72	114.11	108.30
17	t	524	BCR	C7-C8-C9	-3.72	120.61	126.23
17	H	4010	BCR	C24-C23-C22	-3.72	120.62	126.23
14	f	1021	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
17	r	521	BCR	C11-C10-C9	-3.72	122.00	127.31
14	B	1211	CLA	CHB-C4A-NA	3.72	129.65	124.51
21	4	822	SQD	O9-S-O7	-3.72	101.09	113.95
17	m	4104	BCR	C24-C23-C22	-3.71	120.62	126.23
21	t	822	SQD	O9-S-O7	-3.71	101.10	113.95
14	B	1021	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
19	A	1849	LMU	O5'-C5'-C4'	3.71	116.43	109.69
17	U	4104	BCR	C24-C23-C22	-3.71	120.63	126.23
17	f	4010	BCR	C24-C23-C22	-3.71	120.63	126.23
17	B	4010	BCR	C24-C23-C22	-3.70	120.64	126.23
21	L	5216	SQD	C4-C3-C2	3.70	117.29	110.82
17	H	4009	BCR	C15-C14-C13	-3.70	122.03	127.31
14	l	1302	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
17	B	4009	BCR	C15-C14-C13	-3.70	122.03	127.31
17	t	523	BCR	C24-C23-C22	-3.70	120.64	126.23
17	o	4021	BCR	C28-C27-C26	-3.70	107.47	114.08
21	n	5216	SQD	C4-C3-C2	3.70	117.28	110.82
17	l	4015	BCR	C16-C17-C18	-3.70	122.03	127.31
17	K	4104	BCR	C24-C23-C22	-3.70	120.65	126.23
14	H	1021	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
17	I	4018	BCR	C7-C8-C9	-3.70	120.65	126.23
17	4	524	BCR	C7-C8-C9	-3.69	120.65	126.23
17	4	523	BCR	C24-C23-C22	-3.69	120.65	126.23
14	J	1302	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
17	H	4004	BCR	C15-C14-C13	-3.69	122.05	127.31
17	k	4018	BCR	C7-C8-C9	-3.69	120.66	126.23
21	3	822	SQD	O9-S-O7	-3.69	101.19	113.95
19	G	1849	LMU	O5'-C5'-C4'	3.69	116.39	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	S	4018	BCR	C7-C8-C9	-3.69	120.66	126.23
14	G	1131	CLA	C3B-C4B-NB	-3.69	107.09	110.52
17	f	4009	BCR	C15-C14-C13	-3.69	122.05	127.31
17	b	523	BCR	C24-C23-C22	-3.68	120.67	126.23
17	t	521	BCR	C24-C23-C22	-3.68	120.67	126.23
17	b	522	BCR	C20-C21-C22	-3.68	122.05	127.31
21	s	822	SQD	O9-S-O7	-3.68	101.20	113.95
14	T	1302	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
17	Z	523	BCR	C16-C17-C18	-3.68	122.06	127.31
14	e	1101	CLA	C3B-C4B-NB	-3.68	107.10	110.52
17	T	4015	BCR	C16-C17-C18	-3.68	122.06	127.31
17	t	522	BCR	C20-C21-C22	-3.68	122.06	127.31
17	J	4015	BCR	C16-C17-C18	-3.68	122.06	127.31
17	v	521	BCR	C15-C14-C13	-3.67	122.07	127.31
17	b	524	BCR	C7-C8-C9	-3.67	120.68	126.23
17	4	521	BCR	C24-C23-C22	-3.67	120.68	126.23
21	a	822	SQD	O9-S-O7	-3.67	101.24	113.95
17	4	522	BCR	C20-C21-C22	-3.67	122.07	127.31
21	H	1852	SQD	O48-C23-C24	3.67	123.43	111.91
17	B	4004	BCR	C15-C14-C13	-3.67	122.08	127.31
17	q	521	BCR	C16-C17-C18	-3.67	122.08	127.31
21	Z	822	SQD	O47-C7-C8	3.67	119.40	111.50
17	Z	522	BCR	C7-C8-C9	-3.67	120.70	126.23
17	6	521	BCR	C15-C14-C13	-3.66	122.08	127.31
17	1	521	BCR	C16-C17-C18	-3.66	122.08	127.31
17	r	523	BCR	C16-C17-C18	-3.66	122.08	127.31
21	2	822	SQD	O47-C7-C8	3.66	119.39	111.50
17	6	524	BCR	C11-C10-C9	-3.66	122.08	127.31
17	W	4021	BCR	C10-C11-C12	-3.66	111.80	123.22
17	v	524	BCR	C11-C10-C9	-3.66	122.09	127.31
21	r	822	SQD	O47-C7-C8	3.66	119.39	111.50
17	Y	521	BCR	C16-C17-C18	-3.66	122.09	127.31
21	Z	822	SQD	O9-S-O7	-3.66	101.29	113.95
17	2	523	BCR	C16-C17-C18	-3.66	122.09	127.31
14	A	1131	CLA	C3B-C4B-NB	-3.66	107.12	110.52
21	B	1852	SQD	O48-C23-C24	3.66	123.38	111.91
17	M	4021	BCR	C10-C11-C12	-3.66	111.81	123.22
17	f	4004	BCR	C15-C14-C13	-3.66	122.09	127.31
21	f	1852	SQD	O48-C23-C24	3.65	123.38	111.91
17	I	4018	BCR	C27-C26-C25	-3.65	117.42	122.73
14	e	1131	CLA	C3B-C4B-NB	-3.65	107.13	110.52
21	2	822	SQD	O9-S-O7	-3.65	101.31	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	d	521	BCR	C15-C14-C13	-3.65	122.10	127.31
17	b	521	BCR	C24-C23-C22	-3.65	120.72	126.23
17	B	4006	BCR	C20-C21-C22	-3.65	122.11	127.31
21	r	822	SQD	O9-S-O7	-3.65	101.33	113.95
17	d	524	BCR	C11-C10-C9	-3.65	122.11	127.31
21	B	1852	SQD	O9-S-O7	-3.65	101.33	113.95
21	H	1852	SQD	C1-O5-C5	3.64	120.84	113.69
17	k	4018	BCR	C27-C26-C25	-3.64	117.44	122.73
14	A	1101	CLA	C3B-C4B-NB	-3.64	107.14	110.52
14	G	1101	CLA	C3B-C4B-NB	-3.64	107.14	110.52
14	K	1105	CLA	CBC-CAC-C3C	3.64	122.47	112.43
17	b	521	BCR	C11-C10-C9	-3.64	122.12	127.31
17	o	4021	BCR	C10-C11-C12	-3.64	111.86	123.22
17	a	521	BCR	C28-C27-C26	-3.64	107.58	114.08
17	s	521	BCR	C28-C27-C26	-3.64	107.59	114.08
17	1	524	BCR	C33-C5-C6	-3.63	120.45	124.53
21	H	1852	SQD	O9-S-O7	-3.63	101.38	113.95
21	f	1852	SQD	O9-S-O7	-3.63	101.38	113.95
14	U	1105	CLA	CBC-CAC-C3C	3.63	122.44	112.43
17	2	522	BCR	C7-C8-C9	-3.63	120.75	126.23
14	m	1105	CLA	CBC-CAC-C3C	3.63	122.44	112.43
17	S	4018	BCR	C27-C26-C25	-3.63	117.46	122.73
17	Y	523	BCR	C16-C17-C18	-3.63	122.13	127.31
17	f	4006	BCR	C20-C21-C22	-3.63	122.13	127.31
14	G	1132	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
17	3	521	BCR	C28-C27-C26	-3.62	107.61	114.08
17	H	4005	BCR	C15-C14-C13	-3.62	122.14	127.31
17	q	524	BCR	C33-C5-C6	-3.62	120.46	124.53
17	H	4006	BCR	C20-C21-C22	-3.62	122.14	127.31
17	Y	524	BCR	C33-C5-C6	-3.62	120.46	124.53
14	A	1132	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
14	e	1132	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
21	B	1852	SQD	C1-O5-C5	3.62	120.78	113.69
17	V	4219	BCR	C10-C11-C12	-3.61	111.94	123.22
17	L	4219	BCR	C10-C11-C12	-3.61	111.94	123.22
14	G	1129	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
21	f	1852	SQD	C1-O5-C5	3.61	120.77	113.69
17	H	4017	BCR	C34-C9-C8	3.61	123.76	118.08
17	b	522	BCR	C24-C23-C22	-3.61	120.78	126.23
17	r	522	BCR	C7-C8-C9	-3.61	120.78	126.23
17	4	521	BCR	C11-C10-C9	-3.60	122.17	127.31
14	A	1129	CLA	O2D-CGD-O1D	-3.60	116.80	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1129	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
17	n	4219	BCR	C10-C11-C12	-3.60	111.99	123.22
17	1	523	BCR	C16-C17-C18	-3.60	122.18	127.31
17	5	521	BCR	C28-C27-C26	-3.60	107.66	114.08
17	B	4017	BCR	C34-C9-C8	3.59	123.74	118.08
17	f	4017	BCR	C34-C9-C8	3.59	123.73	118.08
17	H	4009	BCR	C24-C23-C22	-3.59	120.81	126.23
17	f	4009	BCR	C24-C23-C22	-3.59	120.81	126.23
17	B	4009	BCR	C24-C23-C22	-3.59	120.81	126.23
17	B	4005	BCR	C15-C14-C13	-3.59	122.19	127.31
17	f	4017	BCR	C8-C9-C10	-3.59	113.44	118.94
17	c	521	BCR	C28-C27-C26	-3.59	107.67	114.08
14	e	1135	CLA	CMB-C2B-C1B	-3.59	119.91	125.37
14	G	1130	CLA	CHB-C1B-NB	3.58	128.05	124.26
17	4	522	BCR	C24-C23-C22	-3.58	120.82	126.23
17	t	521	BCR	C11-C10-C9	-3.58	122.20	127.31
14	A	1130	CLA	CMB-C2B-C3B	3.58	135.26	126.59
14	e	1130	CLA	CMB-C2B-C3B	3.58	135.26	126.59
17	H	4017	BCR	C8-C9-C10	-3.58	113.45	118.94
14	G	1130	CLA	CMB-C2B-C3B	3.58	135.26	126.59
14	A	1130	CLA	CHB-C1B-NB	3.58	128.04	124.26
17	5	524	BCR	C33-C5-C6	-3.58	120.51	124.53
17	u	524	BCR	C33-C5-C6	-3.58	120.51	124.53
17	u	521	BCR	C28-C27-C26	-3.58	107.69	114.08
14	A	1135	CLA	CMB-C2B-C1B	-3.57	119.93	125.37
17	f	4005	BCR	C15-C14-C13	-3.57	122.21	127.31
17	t	522	BCR	C24-C23-C22	-3.57	120.85	126.23
17	v	521	BCR	C20-C21-C22	-3.56	122.22	127.31
17	q	523	BCR	C16-C17-C18	-3.56	122.22	127.31
17	c	524	BCR	C33-C5-C6	-3.56	120.53	124.53
17	L	4219	BCR	C28-C27-C26	-3.56	107.72	114.08
17	6	521	BCR	C20-C21-C22	-3.56	122.23	127.31
17	V	4219	BCR	C28-C27-C26	-3.56	107.72	114.08
17	B	4017	BCR	C8-C9-C10	-3.56	113.48	118.94
17	6	522	BCR	C7-C8-C9	-3.56	120.86	126.23
17	H	4010	BCR	C38-C26-C25	-3.56	120.53	124.53
14	H	1220	CLA	CAA-C2A-C1A	-3.56	100.32	111.97
14	G	1135	CLA	CMB-C2B-C1B	-3.56	119.95	125.37
17	L	4019	BCR	C15-C14-C13	-3.56	122.23	127.31
17	v	521	BCR	C3-C4-C5	-3.56	107.73	114.08
14	B	1220	CLA	CAA-C2A-C1A	-3.55	100.34	111.97
17	s	523	BCR	C7-C8-C9	-3.55	120.87	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1220	CLA	CAA-C2A-C1A	-3.55	100.35	111.97
17	n	4219	BCR	C28-C27-C26	-3.55	107.74	114.08
17	B	4009	BCR	C7-C8-C9	-3.54	120.88	126.23
17	V	4019	BCR	C15-C14-C13	-3.54	122.25	127.31
14	B	1216	CLA	O2A-CGA-O1A	-3.54	114.65	123.59
17	d	522	BCR	C7-C8-C9	-3.54	120.88	126.23
17	v	522	BCR	C7-C8-C9	-3.54	120.88	126.23
14	f	1216	CLA	O2A-CGA-O1A	-3.54	114.65	123.59
14	H	1216	CLA	O2A-CGA-O1A	-3.54	114.66	123.59
17	d	521	BCR	C20-C21-C22	-3.54	122.26	127.31
17	6	521	BCR	C3-C4-C5	-3.54	107.76	114.08
17	3	523	BCR	C7-C8-C9	-3.54	120.89	126.23
17	f	4009	BCR	C7-C8-C9	-3.54	120.89	126.23
14	G	1013	CLA	CAA-C2A-C1A	-3.54	100.39	111.97
14	e	1013	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
14	e	1130	CLA	CHB-C1B-NB	3.54	128.00	124.26
17	d	521	BCR	C3-C4-C5	-3.54	107.76	114.08
17	Z	524	BCR	C11-C10-C9	-3.53	122.27	127.31
17	n	4019	BCR	C15-C14-C13	-3.53	122.27	127.31
14	m	1105	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
17	H	4009	BCR	C7-C8-C9	-3.53	120.90	126.23
17	f	4010	BCR	C38-C26-C25	-3.53	120.56	124.53
14	A	1013	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
14	A	1013	CLA	CAA-C2A-C1A	-3.53	100.41	111.97
14	e	1013	CLA	CAA-C2A-C1A	-3.53	100.41	111.97
17	1	521	BCR	C11-C10-C9	-3.53	122.28	127.31
17	r	524	BCR	C11-C10-C9	-3.53	122.28	127.31
14	G	1013	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
17	B	4010	BCR	C38-C26-C25	-3.52	120.57	124.53
14	K	1105	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
14	G	1123	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
14	f	1207	CLA	C3B-C4B-NB	-3.52	107.25	110.52
14	H	1206	CLA	CMB-C2B-C1B	-3.52	120.02	125.37
14	A	1123	CLA	O2D-CGD-O1D	-3.52	116.97	123.84
14	f	1206	CLA	CMB-C2B-C1B	-3.51	120.02	125.37
17	a	523	BCR	C7-C8-C9	-3.51	120.92	126.23
17	c	521	BCR	C3-C4-C5	-3.51	107.80	114.08
14	B	1206	CLA	CMB-C2B-C1B	-3.51	120.02	125.37
17	2	524	BCR	C11-C10-C9	-3.51	122.30	127.31
14	U	1105	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
14	H	1207	CLA	C3B-C4B-NB	-3.51	107.26	110.52
14	e	1123	CLA	O2D-CGD-O1D	-3.50	116.99	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1102	CLA	CMB-C2B-C1B	-3.50	120.03	125.37
21	s	822	SQD	O9-S-C6	3.50	111.10	106.94
17	5	521	BCR	C3-C4-C5	-3.50	107.83	114.08
17	u	521	BCR	C3-C4-C5	-3.50	107.83	114.08
17	q	521	BCR	C11-C10-C9	-3.50	122.32	127.31
21	3	822	SQD	O9-S-C6	3.50	111.09	106.94
17	f	4014	BCR	C16-C15-C14	-3.49	116.31	123.47
17	n	4219	BCR	C3-C4-C5	-3.49	107.84	114.08
17	Y	521	BCR	C11-C10-C9	-3.49	122.32	127.31
17	A	4007	BCR	C11-C10-C9	-3.49	122.32	127.31
17	H	4014	BCR	C16-C15-C14	-3.49	116.32	123.47
14	d	501	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
17	G	4007	BCR	C11-C10-C9	-3.49	122.33	127.31
17	t	522	BCR	C28-C27-C26	-3.49	107.84	114.08
17	4	523	BCR	C15-C16-C17	-3.49	116.33	123.47
15	f	2002	PQN	C14-C13-C15	-3.49	109.40	115.27
17	b	523	BCR	C15-C16-C17	-3.49	116.33	123.47
14	B	1207	CLA	C3B-C4B-NB	-3.49	107.28	110.52
14	6	501	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
21	d	822	SQD	O9-S-C6	3.49	111.08	106.94
21	a	822	SQD	O9-S-C6	3.48	111.08	106.94
21	r	822	SQD	O9-S-C6	3.48	111.08	106.94
17	5	524	BCR	C7-C8-C9	-3.48	120.97	126.23
17	H	4005	BCR	C24-C23-C22	-3.48	120.97	126.23
17	B	4014	BCR	C16-C15-C14	-3.48	116.34	123.47
17	1	521	BCR	C28-C27-C26	-3.48	107.86	114.08
17	c	524	BCR	C7-C8-C9	-3.48	120.97	126.23
21	Z	822	SQD	O9-S-C6	3.48	111.08	106.94
17	t	523	BCR	C15-C16-C17	-3.48	116.34	123.47
17	q	521	BCR	C28-C27-C26	-3.48	107.86	114.08
15	B	2002	PQN	C14-C13-C15	-3.48	109.42	115.27
17	e	4007	BCR	C16-C17-C18	-3.48	122.34	127.31
21	6	822	SQD	O9-S-C6	3.48	111.07	106.94
14	f	1216	CLA	CHB-C1B-NB	3.48	127.94	124.26
15	H	2002	PQN	C14-C13-C15	-3.48	109.42	115.27
17	G	4007	BCR	C16-C17-C18	-3.47	122.35	127.31
14	B	1216	CLA	CHB-C1B-NB	3.47	127.93	124.26
14	v	501	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
17	b	522	BCR	C28-C27-C26	-3.47	107.88	114.08
17	Y	521	BCR	C28-C27-C26	-3.47	107.88	114.08
17	L	4219	BCR	C3-C4-C5	-3.47	107.88	114.08
17	B	4005	BCR	C24-C23-C22	-3.47	120.99	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	v	822	SQD	O7-S-C6	3.47	111.06	106.94
21	2	822	SQD	O9-S-C6	3.47	111.06	106.94
17	Z	523	BCR	C7-C8-C9	-3.47	121.00	126.23
14	A	1102	CLA	CMB-C2B-C1B	-3.47	120.09	125.37
17	e	4007	BCR	C24-C23-C22	-3.46	121.00	126.23
17	A	4002	BCR	C24-C23-C22	-3.46	121.00	126.23
14	q	508	CLA	CMB-C2B-C1B	-3.46	120.09	125.37
17	u	524	BCR	C7-C8-C9	-3.46	121.00	126.23
17	A	4007	BCR	C24-C23-C22	-3.46	121.00	126.23
17	6	524	BCR	C33-C5-C6	-3.46	120.64	124.53
17	2	523	BCR	C7-C8-C9	-3.46	121.01	126.23
14	G	1102	CLA	CMB-C2B-C1B	-3.46	120.10	125.37
14	G	1126	CLA	CMB-C2B-C1B	-3.46	120.10	125.37
21	d	822	SQD	O7-S-C6	3.46	111.05	106.94
17	4	522	BCR	C28-C27-C26	-3.46	107.90	114.08
17	A	4007	BCR	C16-C17-C18	-3.46	122.37	127.31
17	G	4002	BCR	C24-C23-C22	-3.46	121.01	126.23
21	v	822	SQD	O9-S-C6	3.46	111.05	106.94
17	e	4007	BCR	C11-C10-C9	-3.46	122.38	127.31
17	T	4013	BCR	C3-C4-C5	-3.46	107.90	114.08
17	f	4005	BCR	C24-C23-C22	-3.46	121.01	126.23
17	V	4219	BCR	C3-C4-C5	-3.45	107.91	114.08
17	J	4012	BCR	C7-C8-C9	-3.45	121.02	126.23
17	T	4012	BCR	C7-C8-C9	-3.45	121.02	126.23
17	a	524	BCR	C11-C10-C9	-3.45	122.39	127.31
17	3	522	BCR	C28-C27-C26	-3.45	107.92	114.08
14	Y	508	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
17	V	4219	BCR	C33-C5-C4	3.45	120.24	113.62
17	G	4007	BCR	C24-C23-C22	-3.45	121.02	126.23
14	A	1138	CLA	C3B-C4B-NB	-3.45	107.32	110.52
17	a	522	BCR	C28-C27-C26	-3.45	107.92	114.08
14	G	1116	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
21	1	822	SQD	O47-C7-C8	3.45	118.93	111.50
17	s	524	BCR	C11-C10-C9	-3.45	122.39	127.31
21	6	822	SQD	O7-S-C6	3.44	111.03	106.94
17	b	522	BCR	C7-C8-C9	-3.44	121.03	126.23
17	e	4002	BCR	C24-C23-C22	-3.44	121.03	126.23
17	J	4013	BCR	C3-C4-C5	-3.44	107.93	114.08
14	H	1220	CLA	CAA-CBA-CGA	-3.44	103.19	113.25
17	l	4012	BCR	C7-C8-C9	-3.44	121.03	126.23
17	L	4219	BCR	C33-C5-C4	3.44	120.23	113.62
14	H	1228	CLA	CMB-C2B-C1B	-3.44	120.13	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	4001	BCR	C15-C16-C17	-3.44	116.42	123.47
17	3	524	BCR	C11-C10-C9	-3.44	122.40	127.31
14	1	508	CLA	CMB-C2B-C1B	-3.44	120.13	125.37
14	G	1139	CLA	C3B-C4B-NB	-3.44	107.33	110.52
17	L	4020	BCR	C16-C17-C18	-3.44	122.41	127.31
17	V	4019	BCR	C16-C17-C18	-3.44	122.41	127.31
17	A	4001	BCR	C15-C16-C17	-3.44	116.44	123.47
17	n	4219	BCR	C33-C5-C4	3.43	120.21	113.62
21	Y	822	SQD	O47-C7-C8	3.43	118.90	111.50
17	l	4013	BCR	C3-C4-C5	-3.43	107.95	114.08
17	J	4015	BCR	C11-C10-C9	-3.43	122.41	127.31
17	n	4020	BCR	C16-C17-C18	-3.43	122.41	127.31
14	B	1220	CLA	CAA-CBA-CGA	-3.43	103.22	113.25
14	A	1139	CLA	C3B-C4B-NB	-3.43	107.33	110.52
17	d	524	BCR	C33-C5-C6	-3.43	120.67	124.53
14	A	1126	CLA	CMB-C2B-C1B	-3.43	120.14	125.37
14	e	1126	CLA	CMB-C2B-C1B	-3.43	120.14	125.37
17	G	4007	BCR	C27-C26-C25	-3.43	117.75	122.73
21	q	822	SQD	O47-C7-C8	3.43	118.89	111.50
17	r	523	BCR	C7-C8-C9	-3.43	121.05	126.23
17	A	4002	BCR	C16-C15-C14	-3.43	116.45	123.47
17	G	4002	BCR	C16-C15-C14	-3.43	116.45	123.47
14	f	1220	CLA	CAA-CBA-CGA	-3.43	103.23	113.25
17	T	4015	BCR	C11-C10-C9	-3.43	122.42	127.31
14	e	1116	CLA	CMB-C2B-C1B	-3.43	120.15	125.37
17	v	524	BCR	C33-C5-C6	-3.43	120.68	124.53
14	e	1138	CLA	C3B-C4B-NB	-3.43	107.34	110.52
14	f	1238	CLA	CMB-C2B-C1B	-3.43	120.15	125.37
17	s	522	BCR	C28-C27-C26	-3.42	107.96	114.08
17	e	4007	BCR	C27-C26-C25	-3.42	117.76	122.73
14	G	1138	CLA	C3B-C4B-NB	-3.42	107.34	110.52
17	a	524	BCR	C33-C5-C6	-3.42	120.69	124.53
14	B	1238	CLA	CMB-C2B-C1B	-3.42	120.16	125.37
14	H	1216	CLA	CHB-C1B-NB	3.42	127.88	124.26
17	l	4015	BCR	C11-C10-C9	-3.42	122.43	127.31
17	V	4020	BCR	C16-C17-C18	-3.42	122.43	127.31
14	H	1238	CLA	CMB-C2B-C1B	-3.42	120.16	125.37
17	e	4002	BCR	C16-C15-C14	-3.42	116.47	123.47
17	3	524	BCR	C33-C5-C6	-3.42	120.69	124.53
17	G	4001	BCR	C15-C16-C17	-3.41	116.48	123.47
14	t	507	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
17	4	522	BCR	C7-C8-C9	-3.41	121.08	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1139	CLA	C3B-C4B-NB	-3.41	107.35	110.52
14	H	1204	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
17	A	4007	BCR	C27-C26-C25	-3.41	117.78	122.73
17	3	524	BCR	C24-C23-C22	-3.41	121.09	126.23
21	Y	822	SQD	C4-C3-C2	3.41	116.77	110.82
21	1	822	SQD	C4-C3-C2	3.41	116.77	110.82
14	B	1228	CLA	CMB-C2B-C1B	-3.41	120.18	125.37
17	s	524	BCR	C24-C23-C22	-3.40	121.09	126.23
17	L	4019	BCR	C16-C17-C18	-3.40	122.45	127.31
14	b	507	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
14	e	1117	CLA	CMB-C2B-C1B	-3.40	120.19	125.37
17	3	523	BCR	C16-C17-C18	-3.40	122.45	127.31
14	A	1116	CLA	CMB-C2B-C1B	-3.40	120.19	125.37
14	B	1012	CLA	CMB-C2B-C1B	-3.40	120.19	125.37
17	n	4019	BCR	C16-C17-C18	-3.40	122.45	127.31
14	e	1103	CLA	CHB-C4A-NA	3.40	129.22	124.51
14	4	507	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
17	q	523	BCR	C28-C27-C26	-3.40	108.01	114.08
14	f	1228	CLA	CMB-C2B-C1B	-3.40	120.19	125.37
17	c	523	BCR	C16-C17-C18	-3.40	122.46	127.31
14	f	1204	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
17	s	524	BCR	C33-C5-C6	-3.40	120.71	124.53
17	a	523	BCR	C16-C17-C18	-3.40	122.46	127.31
14	A	1103	CLA	CHB-C4A-NA	3.40	129.21	124.51
17	t	522	BCR	C7-C8-C9	-3.40	121.10	126.23
17	a	524	BCR	C24-C23-C22	-3.40	121.10	126.23
17	1	523	BCR	C28-C27-C26	-3.39	108.02	114.08
17	Y	523	BCR	C28-C27-C26	-3.39	108.02	114.08
14	G	1136	CLA	C3B-C4B-NB	-3.39	107.37	110.52
21	q	822	SQD	C4-C3-C2	3.39	116.74	110.82
14	e	1140	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
14	f	1012	CLA	CMB-C2B-C1B	-3.39	120.21	125.37
17	f	4005	BCR	C16-C17-C18	-3.39	122.47	127.31
14	B	1204	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
14	G	1124	CLA	CAA-C2A-C1A	-3.39	100.88	111.97
14	A	1140	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
14	H	1012	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
21	q	822	SQD	C3-C4-C5	3.38	116.27	110.24
17	u	522	BCR	C7-C8-C9	-3.38	121.12	126.23
14	e	1102	CLA	C3B-C4B-NB	-3.38	107.38	110.52
14	G	1140	CLA	CAA-C2A-C3A	-3.38	103.52	112.78
14	A	1112	CLA	CHB-C4A-NA	3.38	129.19	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1021	CLA	C3B-C4B-NB	-3.38	107.38	110.52
19	G	1849	LMU	C1'-O5'-C5'	3.38	120.32	113.69
21	1	822	SQD	C3-C4-C5	3.38	116.27	110.24
14	f	1229	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
17	A	4002	BCR	C15-C14-C13	-3.38	122.49	127.31
19	A	1849	LMU	C1'-O5'-C5'	3.38	120.32	113.69
17	s	523	BCR	C16-C17-C18	-3.38	122.49	127.31
17	c	522	BCR	C28-C27-C26	-3.38	108.05	114.08
14	A	1136	CLA	C3B-C4B-NB	-3.38	107.38	110.52
17	5	523	BCR	C16-C17-C18	-3.38	122.49	127.31
17	G	4002	BCR	C15-C14-C13	-3.37	122.50	127.31
14	G	1112	CLA	CHB-C4A-NA	3.37	129.18	124.51
14	e	1106	CLA	O2A-CGA-O1A	-3.37	115.08	123.59
21	L	5216	SQD	O9-S-C6	3.37	110.95	106.94
19	e	1849	LMU	C1'-O5'-C5'	3.37	120.31	113.69
17	c	524	BCR	C16-C17-C18	-3.37	122.50	127.31
14	A	1117	CLA	CMB-C2B-C1B	-3.37	120.23	125.37
17	5	522	BCR	C7-C8-C9	-3.37	121.14	126.23
17	u	522	BCR	C28-C27-C26	-3.37	108.06	114.08
14	G	1103	CLA	CHB-C4A-NA	3.37	129.17	124.51
14	A	1124	CLA	CAA-C2A-C1A	-3.37	100.93	111.97
14	H	1229	CLA	CMB-C2B-C1B	-3.37	120.24	125.37
14	e	1112	CLA	CHB-C4A-NA	3.37	129.17	124.51
17	5	524	BCR	C16-C17-C18	-3.37	122.50	127.31
14	G	1106	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
14	B	1221	CLA	CHB-C4A-NA	3.37	129.17	124.51
17	a	523	BCR	C20-C21-C22	-3.37	122.50	127.31
14	f	1221	CLA	CHB-C4A-NA	3.37	129.17	124.51
17	e	4002	BCR	C15-C14-C13	-3.37	122.50	127.31
21	V	5216	SQD	O9-S-C6	3.37	110.94	106.94
17	B	4005	BCR	C16-C17-C18	-3.37	122.51	127.31
14	H	1221	CLA	CHB-C4A-NA	3.36	129.16	124.51
17	c	522	BCR	C7-C8-C9	-3.36	121.15	126.23
14	B	1229	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
14	A	1106	CLA	O2A-CGA-O1A	-3.36	115.10	123.59
14	e	1124	CLA	CAA-C2A-C1A	-3.36	100.95	111.97
14	G	1117	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
17	n	4022	BCR	C16-C15-C14	-3.36	116.59	123.47
14	H	1234	CLA	CMB-C2B-C3B	3.36	134.73	126.59
17	H	4017	BCR	C21-C20-C19	-3.36	112.73	123.22
17	u	523	BCR	C16-C17-C18	-3.36	122.51	127.31
17	5	522	BCR	C28-C27-C26	-3.36	108.08	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1234	CLA	CMB-C2B-C3B	3.36	134.72	126.59
21	Y	822	SQD	C3-C4-C5	3.36	116.23	110.24
14	f	1216	CLA	C3B-C4B-NB	-3.36	107.40	110.52
14	H	1216	CLA	C3B-C4B-NB	-3.36	107.40	110.52
17	B	4017	BCR	C21-C20-C19	-3.36	112.74	123.22
17	u	524	BCR	C16-C17-C18	-3.35	122.52	127.31
14	A	1102	CLA	C3B-C4B-NB	-3.35	107.41	110.52
14	f	1234	CLA	CMB-C2B-C3B	3.35	134.70	126.59
17	d	522	BCR	C28-C27-C26	-3.35	108.09	114.08
17	d	522	BCR	C24-C23-C22	-3.35	121.17	126.23
17	3	523	BCR	C20-C21-C22	-3.35	122.53	127.31
14	B	1021	CLA	C3B-C4B-NB	-3.35	107.41	110.52
17	L	4022	BCR	C16-C15-C14	-3.34	116.62	123.47
14	H	1215	CLA	CMB-C2B-C1B	-3.34	120.28	125.37
21	n	5216	SQD	O9-S-C6	3.34	110.91	106.94
14	e	1136	CLA	C3B-C4B-NB	-3.34	107.41	110.52
14	H	1223	CLA	CMB-C2B-C1B	-3.34	120.28	125.37
17	f	4017	BCR	C21-C20-C19	-3.34	112.78	123.22
17	H	4005	BCR	C16-C17-C18	-3.34	122.54	127.31
14	f	1215	CLA	CMB-C2B-C1B	-3.34	120.28	125.37
17	6	522	BCR	C28-C27-C26	-3.34	108.11	114.08
14	G	1138	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
14	H	1012	CLA	C3B-C4B-NB	-3.34	107.42	110.52
17	G	4011	BCR	C16-C17-C18	-3.34	122.55	127.31
14	G	1102	CLA	C3B-C4B-NB	-3.34	107.42	110.52
14	f	1223	CLA	CMB-C2B-C1B	-3.34	120.29	125.37
17	u	523	BCR	C10-C11-C12	-3.33	112.81	123.22
17	V	4022	BCR	C16-C15-C14	-3.33	116.65	123.47
17	v	522	BCR	C24-C23-C22	-3.33	121.20	126.23
19	l	5105	LMU	O5'-C1'-C2'	3.33	117.40	110.35
17	n	4020	BCR	C20-C21-C22	-3.33	122.56	127.31
14	B	1012	CLA	C3B-C4B-NB	-3.33	107.43	110.52
19	T	5105	LMU	O5'-C1'-C2'	3.33	117.40	110.35
17	s	523	BCR	C20-C21-C22	-3.33	122.56	127.31
17	V	4020	BCR	C20-C21-C22	-3.33	122.56	127.31
19	J	5105	LMU	O5'-C1'-C2'	3.33	117.39	110.35
17	5	523	BCR	C10-C11-C12	-3.33	112.83	123.22
14	A	1138	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
14	B	1215	CLA	CMB-C2B-C1B	-3.32	120.31	125.37
17	n	4022	BCR	C15-C14-C13	-3.32	122.57	127.31
14	B	1223	CLA	CMB-C2B-C1B	-3.32	120.31	125.37
14	G	1113	CLA	CMB-C2B-C1B	-3.32	120.31	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1216	CLA	C3B-C4B-NB	-3.32	107.43	110.52
17	A	4011	BCR	C16-C17-C18	-3.32	122.57	127.31
17	c	523	BCR	C10-C11-C12	-3.32	112.86	123.22
17	L	4020	BCR	C20-C21-C22	-3.32	122.57	127.31
17	6	522	BCR	C24-C23-C22	-3.32	121.22	126.23
14	f	1021	CLA	C3B-C4B-NB	-3.31	107.44	110.52
14	e	1113	CLA	CMB-C2B-C1B	-3.31	120.32	125.37
14	e	1102	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
19	T	5105	LMU	C1'-O5'-C5'	3.31	120.19	113.69
14	e	1138	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
17	v	522	BCR	C28-C27-C26	-3.31	108.16	114.08
14	f	1012	CLA	C3B-C4B-NB	-3.31	107.44	110.52
21	s	822	SQD	O48-C23-C24	3.31	120.07	111.38
14	G	1102	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
14	H	1239	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
14	A	1102	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
14	G	1105	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
14	e	1125	CLA	C6-C5-C3	3.31	122.13	113.45
14	L	1502	CLA	C3B-C4B-NB	-3.31	107.44	110.52
14	f	1239	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
14	A	1113	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
17	e	4011	BCR	C16-C17-C18	-3.31	122.59	127.31
14	A	1105	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
14	B	1239	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
14	G	1125	CLA	C6-C5-C3	3.31	122.12	113.45
14	F	1301	CLA	C3B-C4B-NB	-3.31	107.45	110.52
17	v	522	BCR	C15-C16-C17	-3.31	116.70	123.47
17	r	523	BCR	C20-C21-C22	-3.31	122.59	127.31
21	3	822	SQD	O48-C23-C24	3.30	120.05	111.38
21	a	822	SQD	O48-C23-C24	3.30	120.04	111.38
17	L	4022	BCR	C15-C14-C13	-3.30	122.59	127.31
19	J	5105	LMU	C1'-O5'-C5'	3.30	120.17	113.69
14	A	1125	CLA	C6-C5-C3	3.30	122.11	113.45
14	G	1120	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
17	f	4005	BCR	C20-C21-C22	-3.30	122.60	127.31
14	e	1119	CLA	CMB-C2B-C1B	-3.30	120.35	125.37
21	Y	822	SQD	C44-O6-C1	3.30	120.18	113.74
14	2	516	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
14	A	1112	CLA	C3B-C4B-NB	-3.30	107.46	110.52
14	e	1112	CLA	C3B-C4B-NB	-3.30	107.46	110.52
14	G	1132	CLA	O2D-CGD-CBD	3.29	117.12	111.27
17	V	4022	BCR	C15-C14-C13	-3.29	122.61	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	522	BCR	C28-C27-C26	-3.29	108.20	114.08
14	Z	516	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
14	j	1301	CLA	C3B-C4B-NB	-3.29	107.46	110.52
14	e	1105	CLA	CMB-C2B-C1B	-3.29	120.36	125.37
21	q	822	SQD	C44-O6-C1	3.29	120.17	113.74
17	B	4005	BCR	C20-C21-C22	-3.29	122.62	127.31
17	b	522	BCR	C11-C10-C9	-3.29	122.62	127.31
17	1	522	BCR	C28-C27-C26	-3.29	108.21	114.08
14	r	516	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
17	t	523	BCR	C20-C21-C22	-3.29	122.62	127.31
17	q	522	BCR	C28-C27-C26	-3.29	108.21	114.08
14	e	1120	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
14	G	1112	CLA	C3B-C4B-NB	-3.29	107.47	110.52
14	A	1119	CLA	CMB-C2B-C1B	-3.29	120.36	125.37
17	b	521	BCR	C16-C17-C18	-3.29	122.62	127.31
21	d	822	SQD	C1-O5-C5	3.29	120.14	113.69
17	Z	522	BCR	C24-C23-C22	-3.29	121.27	126.23
14	f	1206	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
17	2	523	BCR	C20-C21-C22	-3.28	122.62	127.31
14	B	1229	CLA	CHD-C1D-ND	-3.28	121.44	124.45
14	R	1301	CLA	C3B-C4B-NB	-3.28	107.47	110.52
14	V	1502	CLA	C3B-C4B-NB	-3.28	107.47	110.52
17	b	523	BCR	C33-C5-C6	-3.28	120.84	124.53
14	A	1120	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
19	l	5105	LMU	C1'-O5'-C5'	3.28	120.13	113.69
21	b	822	SQD	C44-O6-C1	3.28	120.15	113.74
21	6	822	SQD	C1-O5-C5	3.28	120.13	113.69
21	v	822	SQD	C1-O5-C5	3.28	120.13	113.69
14	H	1205	CLA	O2A-CGA-O1A	-3.28	115.31	123.59
17	4	523	BCR	C33-C5-C6	-3.28	120.85	124.53
17	J	4013	BCR	C15-C14-C13	-3.28	122.63	127.31
17	c	523	BCR	C28-C27-C26	-3.28	108.22	114.08
14	e	1118	CLA	CHB-C4A-NA	3.28	129.04	124.51
14	f	1229	CLA	CHD-C1D-ND	-3.28	121.44	124.45
14	f	1205	CLA	O2A-CGA-O1A	-3.28	115.32	123.59
14	A	1132	CLA	O2D-CGD-CBD	3.28	117.09	111.27
17	6	522	BCR	C15-C16-C17	-3.28	116.76	123.47
21	1	822	SQD	C44-O6-C1	3.28	120.14	113.74
17	o	4021	BCR	C38-C26-C25	-3.28	120.85	124.53
14	B	1205	CLA	O2A-CGA-O1A	-3.28	115.33	123.59
21	t	822	SQD	C44-O6-C1	3.27	120.14	113.74
17	4	522	BCR	C11-C10-C9	-3.27	122.64	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	j	4016	BCR	C16-C17-C18	-3.27	122.64	127.31
14	e	1013	CLA	CHB-C1B-NB	3.27	127.72	124.26
17	Z	523	BCR	C20-C21-C22	-3.27	122.64	127.31
17	d	522	BCR	C15-C16-C17	-3.27	116.77	123.47
17	5	524	BCR	C11-C10-C9	-3.27	122.64	127.31
17	5	523	BCR	C28-C27-C26	-3.27	108.24	114.08
17	n	4019	BCR	C20-C21-C22	-3.27	122.64	127.31
17	t	523	BCR	C33-C5-C6	-3.27	120.86	124.53
17	F	4016	BCR	C16-C17-C18	-3.27	122.65	127.31
17	4	521	BCR	C16-C17-C18	-3.27	122.65	127.31
14	G	1119	CLA	CMB-C2B-C1B	-3.27	120.39	125.37
14	Z	512	CLA	C3B-C4B-NB	-3.27	107.48	110.52
17	T	4013	BCR	C15-C14-C13	-3.27	122.65	127.31
17	4	523	BCR	C20-C21-C22	-3.27	122.65	127.31
17	u	524	BCR	C11-C10-C9	-3.26	122.65	127.31
17	u	523	BCR	C28-C27-C26	-3.26	108.25	114.08
21	4	822	SQD	C44-O6-C1	3.26	120.11	113.74
17	R	4016	BCR	C16-C17-C18	-3.26	122.65	127.31
17	t	521	BCR	C16-C17-C18	-3.26	122.65	127.31
14	e	1132	CLA	O2D-CGD-CBD	3.26	117.07	111.27
17	H	4005	BCR	C20-C21-C22	-3.26	122.65	127.31
17	4	521	BCR	C3-C4-C5	-3.26	108.25	114.08
17	t	521	BCR	C3-C4-C5	-3.26	108.25	114.08
17	L	4019	BCR	C20-C21-C22	-3.26	122.66	127.31
17	c	522	BCR	C24-C23-C22	-3.26	121.31	126.23
14	G	1118	CLA	CHB-C4A-NA	3.26	129.02	124.51
14	e	1127	CLA	CMB-C2B-C1B	-3.26	120.41	125.37
14	B	1234	CLA	CHB-C1B-NB	3.26	127.71	124.26
14	U	1401	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
17	t	522	BCR	C11-C10-C9	-3.26	122.66	127.31
14	H	1023	CLA	CHB-C4A-NA	3.26	129.02	124.51
14	G	1127	CLA	CMB-C2B-C1B	-3.26	120.41	125.37
17	u	522	BCR	C24-C23-C22	-3.26	121.31	126.23
14	B	1206	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
14	2	507	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
14	A	1118	CLA	CHB-C4A-NA	3.26	129.01	124.51
14	e	1119	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
17	W	4021	BCR	C38-C26-C25	-3.25	120.87	124.53
17	l	4013	BCR	C15-C14-C13	-3.25	122.67	127.31
14	A	1119	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
17	b	521	BCR	C3-C4-C5	-3.25	108.27	114.08
17	t	524	BCR	C1-C6-C5	-3.25	118.03	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1206	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
17	3	521	BCR	C3-C4-C5	-3.25	108.27	114.08
14	A	1013	CLA	CHB-C1B-NB	3.25	127.70	124.26
17	4	524	BCR	C1-C6-C5	-3.25	118.04	122.61
14	f	1234	CLA	CHB-C1B-NB	3.25	127.70	124.26
17	2	522	BCR	C24-C23-C22	-3.25	121.33	126.23
14	K	1401	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
14	H	1229	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	5	522	BCR	C24-C23-C22	-3.25	121.33	126.23
17	b	523	BCR	C20-C21-C22	-3.25	122.67	127.31
17	c	524	BCR	C11-C10-C9	-3.25	122.68	127.31
17	M	4021	BCR	C38-C26-C25	-3.25	120.88	124.53
14	Z	507	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
14	G	1119	CLA	O2D-CGD-O1D	-3.24	117.49	123.84
14	G	1013	CLA	CHB-C1B-NB	3.24	127.69	124.26
14	n	1502	CLA	C3B-C4B-NB	-3.24	107.51	110.52
17	V	4019	BCR	C20-C21-C22	-3.24	122.68	127.31
17	s	521	BCR	C3-C4-C5	-3.24	108.29	114.08
14	A	1127	CLA	CMB-C2B-C1B	-3.24	120.43	125.37
14	r	507	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	f	4005	BCR	C11-C10-C9	-3.24	122.69	127.31
17	G	4007	BCR	C7-C8-C9	-3.24	121.34	126.23
14	G	1106	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
14	A	1022	CLA	CMB-C2B-C1B	-3.24	120.44	125.37
17	a	521	BCR	C3-C4-C5	-3.23	108.30	114.08
14	f	1023	CLA	CHB-C4A-NA	3.23	128.99	124.51
14	B	1023	CLA	CHB-C4A-NA	3.23	128.98	124.51
17	f	4014	BCR	C3-C4-C5	-3.23	108.30	114.08
17	H	4014	BCR	C3-C4-C5	-3.23	108.30	114.08
14	A	1106	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
14	f	1202	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
21	t	822	SQD	C4-C3-C2	3.23	116.47	110.82
14	A	1105	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
21	b	822	SQD	C4-C3-C2	3.23	116.46	110.82
14	m	1401	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
14	G	1115	CLA	C3B-C4B-NB	-3.23	107.52	110.52
14	e	1115	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
17	r	522	BCR	C24-C23-C22	-3.23	121.36	126.23
14	t	509	CLA	CHB-C4A-NA	3.23	128.97	124.51
21	4	822	SQD	C4-C3-C2	3.23	116.46	110.82
14	B	1202	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
14	G	1105	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	l	1303	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
17	b	524	BCR	C1-C6-C5	-3.23	118.07	122.61
17	6	522	BCR	C3-C4-C5	-3.23	108.32	114.08
17	d	522	BCR	C3-C4-C5	-3.23	108.32	114.08
17	B	4014	BCR	C3-C4-C5	-3.22	108.32	114.08
14	H	1234	CLA	CHB-C1B-NB	3.22	127.67	124.26
14	T	1303	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
14	G	1138	CLA	CHB-C4A-NA	3.22	128.97	124.51
14	H	1202	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
17	e	4007	BCR	C7-C8-C9	-3.22	121.37	126.23
21	Z	822	SQD	C1-O5-C5	3.22	120.01	113.69
14	4	509	CLA	CHB-C4A-NA	3.22	128.96	124.51
17	B	4005	BCR	C11-C10-C9	-3.22	122.72	127.31
14	e	1106	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
14	b	509	CLA	CHB-C4A-NA	3.22	128.96	124.51
14	f	1232	CLA	CMB-C2B-C3B	3.22	134.38	126.59
14	e	1105	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
17	M	4021	BCR	C20-C19-C18	-3.21	117.39	126.42
17	Y	522	BCR	C24-C23-C22	-3.21	121.38	126.23
17	o	4021	BCR	C20-C19-C18	-3.21	117.39	126.42
17	t	523	BCR	C28-C27-C26	-3.21	108.34	114.08
17	A	4007	BCR	C7-C8-C9	-3.21	121.38	126.23
14	2	512	CLA	C3B-C4B-NB	-3.21	107.54	110.52
14	f	1214	CLA	C3B-C4B-NB	-3.21	107.54	110.52
14	J	1303	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
17	t	521	BCR	C28-C27-C26	-3.21	108.34	114.08
14	e	1022	CLA	CMB-C2B-C1B	-3.21	120.48	125.37
14	A	1115	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
17	H	4004	BCR	C33-C5-C6	-3.21	120.92	124.53
17	1	522	BCR	C24-C23-C22	-3.21	121.39	126.23
17	4	521	BCR	C28-C27-C26	-3.21	108.35	114.08
14	A	1138	CLA	CHB-C4A-NA	3.21	128.94	124.51
17	L	4019	BCR	C28-C27-C26	-3.21	108.35	114.08
17	n	4019	BCR	C28-C27-C26	-3.21	108.35	114.08
14	G	1115	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
14	a	512	CLA	C3B-C4B-NB	-3.20	107.54	110.52
14	B	1232	CLA	CMB-C2B-C3B	3.20	134.35	126.59
14	G	1022	CLA	CMB-C2B-C1B	-3.20	120.49	125.37
14	H	1232	CLA	CMB-C2B-C3B	3.20	134.35	126.59
17	V	4019	BCR	C28-C27-C26	-3.20	108.36	114.08
17	H	4005	BCR	C11-C10-C9	-3.20	122.74	127.31
14	r	512	CLA	C3B-C4B-NB	-3.20	107.55	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	v	522	BCR	C3-C4-C5	-3.20	108.36	114.08
17	q	522	BCR	C24-C23-C22	-3.20	121.40	126.23
21	2	822	SQD	C1-O5-C5	3.20	119.97	113.69
21	d	822	SQD	C44-O6-C1	3.20	119.99	113.74
17	Y	521	BCR	C7-C8-C9	-3.20	121.40	126.23
17	W	4021	BCR	C20-C19-C18	-3.20	117.43	126.42
21	b	822	SQD	O7-S-C6	3.20	110.74	106.94
21	r	822	SQD	C1-O5-C5	3.20	119.96	113.69
17	c	521	BCR	C11-C10-C9	-3.20	122.75	127.31
17	b	521	BCR	C28-C27-C26	-3.20	108.37	114.08
17	B	4004	BCR	C33-C5-C6	-3.20	120.94	124.53
17	4	523	BCR	C28-C27-C26	-3.20	108.37	114.08
17	2	522	BCR	C28-C27-C26	-3.19	108.38	114.08
17	G	4001	BCR	C24-C23-C22	-3.19	121.41	126.23
17	s	521	BCR	C11-C10-C9	-3.19	122.76	127.31
14	3	512	CLA	C3B-C4B-NB	-3.19	107.56	110.52
14	e	1115	CLA	C3B-C4B-NB	-3.19	107.56	110.52
17	3	521	BCR	C11-C10-C9	-3.19	122.76	127.31
17	G	4007	BCR	C20-C21-C22	-3.19	122.76	127.31
17	1	524	BCR	C8-C7-C6	-3.19	118.25	127.20
14	H	1205	CLA	CBA-CAA-C2A	3.19	123.27	113.86
14	G	1103	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
14	f	1205	CLA	CBA-CAA-C2A	3.19	123.27	113.86
21	4	822	SQD	O7-S-C6	3.19	110.72	106.94
17	5	521	BCR	C11-C10-C9	-3.19	122.76	127.31
14	A	1103	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
17	r	522	BCR	C28-C27-C26	-3.18	108.39	114.08
17	Z	522	BCR	C28-C27-C26	-3.18	108.39	114.08
17	Y	524	BCR	C11-C10-C9	-3.18	122.77	127.31
17	u	521	BCR	C11-C10-C9	-3.18	122.77	127.31
14	e	1106	CLA	C1-C2-C3	-3.18	120.54	126.04
17	Y	524	BCR	C8-C7-C6	-3.18	118.27	127.20
21	6	822	SQD	C44-O6-C1	3.18	119.95	113.74
14	B	1205	CLA	CBA-CAA-C2A	3.18	123.25	113.86
17	Y	523	BCR	C21-C20-C19	-3.18	113.29	123.22
17	s	522	BCR	C11-C12-C13	-3.18	117.48	126.42
14	B	1214	CLA	C3B-C4B-NB	-3.18	107.56	110.52
14	s	512	CLA	C3B-C4B-NB	-3.18	107.56	110.52
17	q	524	BCR	C8-C7-C6	-3.18	118.27	127.20
14	A	1115	CLA	C3B-C4B-NB	-3.18	107.57	110.52
17	S	4018	BCR	C11-C10-C9	-3.18	122.77	127.31
17	A	4001	BCR	C24-C23-C22	-3.18	121.43	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	523	BCR	C21-C20-C19	-3.18	113.30	123.22
17	b	523	BCR	C28-C27-C26	-3.18	108.40	114.08
17	1	521	BCR	C7-C8-C9	-3.18	121.44	126.23
14	u	508	CLA	CHB-C4A-NA	3.18	128.90	124.51
17	q	523	BCR	C21-C20-C19	-3.17	113.31	123.22
14	e	1123	CLA	CMB-C2B-C1B	-3.17	120.53	125.37
17	q	524	BCR	C11-C10-C9	-3.17	122.78	127.31
14	G	1106	CLA	C1-C2-C3	-3.17	120.56	126.04
17	A	4007	BCR	C20-C21-C22	-3.17	122.78	127.31
17	1	524	BCR	C11-C10-C9	-3.17	122.78	127.31
17	f	4004	BCR	C33-C5-C6	-3.17	120.97	124.53
17	H	4009	BCR	C3-C4-C5	-3.17	108.42	114.08
21	v	822	SQD	C44-O6-C1	3.17	119.93	113.74
17	5	521	BCR	C24-C23-C22	-3.17	121.45	126.23
14	f	1221	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
17	c	521	BCR	C24-C23-C22	-3.16	121.45	126.23
14	e	1103	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
17	e	4001	BCR	C24-C23-C22	-3.16	121.46	126.23
17	s	523	BCR	C24-C23-C22	-3.16	121.46	126.23
14	A	1106	CLA	C1-C2-C3	-3.16	120.58	126.04
14	H	1214	CLA	C3B-C4B-NB	-3.16	107.58	110.52
21	t	822	SQD	O7-S-C6	3.16	110.69	106.94
14	A	1123	CLA	CMB-C2B-C1B	-3.16	120.56	125.37
14	q	508	CLA	CHB-C4A-NA	3.16	128.88	124.51
17	k	4018	BCR	C11-C10-C9	-3.16	122.80	127.31
17	e	4007	BCR	C20-C21-C22	-3.16	122.80	127.31
17	3	522	BCR	C11-C12-C13	-3.16	117.55	126.42
14	B	1202	CLA	CHB-C4A-NA	3.16	128.88	124.51
17	a	522	BCR	C11-C12-C13	-3.16	117.55	126.42
17	f	4009	BCR	C3-C4-C5	-3.16	108.44	114.08
14	G	1123	CLA	CMB-C2B-C1B	-3.15	120.56	125.37
17	B	4009	BCR	C3-C4-C5	-3.15	108.44	114.08
14	e	1138	CLA	CHB-C4A-NA	3.15	128.87	124.51
14	B	1023	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
14	B	1221	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
14	H	1023	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
14	f	1202	CLA	CHB-C4A-NA	3.15	128.87	124.51
17	a	521	BCR	C11-C10-C9	-3.15	122.81	127.31
17	q	521	BCR	C7-C8-C9	-3.15	121.47	126.23
14	H	1221	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
14	5	508	CLA	CHB-C4A-NA	3.15	128.87	124.51
14	n	1502	CLA	CHB-C4A-NA	3.15	128.87	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	523	BCR	C24-C23-C22	-3.15	121.48	126.23
14	a	516	CLA	CBC-CAC-C3C	3.15	121.11	112.43
14	Z	501	CLA	CHB-C4A-NA	3.15	128.86	124.51
17	I	4018	BCR	C11-C10-C9	-3.15	122.82	127.31
14	G	1108	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
14	3	516	CLA	CBC-CAC-C3C	3.14	121.10	112.43
14	A	1013	CLA	CAA-CBA-CGA	-3.14	104.07	113.25
14	e	1013	CLA	CAA-CBA-CGA	-3.14	104.07	113.25
14	G	1801	CLA	CMB-C2B-C1B	-3.14	120.58	125.37
14	f	1023	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
14	K	1105	CLA	CMC-C2C-C1C	-3.14	120.25	125.04
14	U	1105	CLA	CMC-C2C-C1C	-3.14	120.25	125.04
14	V	1502	CLA	CHD-C1D-ND	-3.14	121.57	124.45
14	G	1101	CLA	CHB-C4A-NA	3.14	128.85	124.51
20	H	5002	LMG	O6-C1-O1	-3.14	102.54	109.97
14	e	1101	CLA	CHB-C4A-NA	3.14	128.85	124.51
17	I	4018	BCR	C1-C6-C5	-3.14	118.20	122.61
21	Z	822	SQD	O5-C5-C4	3.14	115.39	109.69
14	f	1213	CLA	CHB-C4A-NA	3.13	128.85	124.51
17	f	4006	BCR	C16-C17-C18	-3.13	122.84	127.31
17	Z	521	BCR	C7-C8-C9	-3.13	121.50	126.23
14	G	1013	CLA	CAA-CBA-CGA	-3.13	104.10	113.25
14	B	1205	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	a	523	BCR	C24-C23-C22	-3.13	121.50	126.23
21	2	822	SQD	O5-C5-C4	3.13	115.38	109.69
14	A	1801	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
14	B	1213	CLA	CHB-C4A-NA	3.13	128.84	124.51
14	2	501	CLA	CHB-C4A-NA	3.13	128.84	124.51
14	f	1205	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	u	521	BCR	C24-C23-C22	-3.13	121.51	126.23
14	m	1105	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
20	B	5002	LMG	O6-C1-O1	-3.13	102.56	109.97
14	s	516	CLA	CBC-CAC-C3C	3.13	121.05	112.43
17	k	4018	BCR	C1-C6-C5	-3.13	118.21	122.61
21	r	822	SQD	O5-C5-C4	3.13	115.37	109.69
14	n	1502	CLA	CHD-C1D-ND	-3.13	121.58	124.45
17	S	4018	BCR	C20-C21-C22	-3.13	122.85	127.31
14	a	502	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	A	1108	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
14	L	1502	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	1	508	CLA	CHB-C4A-NA	3.12	128.83	124.51
17	Y	524	BCR	C7-C8-C9	-3.12	121.52	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	4013	BCR	C2-C1-C6	3.12	115.29	110.48
14	e	1137	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	H	1205	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
17	2	521	BCR	C7-C8-C9	-3.12	121.52	126.23
14	L	1502	CLA	CHD-C1D-ND	-3.12	121.58	124.45
14	A	1107	CLA	CHB-C1B-NB	3.12	127.56	124.26
14	B	1201	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	Y	508	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	c	508	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	r	501	CLA	CHB-C4A-NA	3.12	128.83	124.51
20	f	5002	LMG	O6-C1-O1	-3.12	102.58	109.97
17	m	4104	BCR	C11-C10-C9	-3.12	122.86	127.31
17	1	524	BCR	C7-C8-C9	-3.12	121.52	126.23
14	e	1108	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
14	A	1101	CLA	CHB-C4A-NA	3.12	128.82	124.51
17	q	524	BCR	C7-C8-C9	-3.12	121.53	126.23
14	1	504	CLA	O2D-CGD-CBD	3.11	116.80	111.27
14	H	1213	CLA	CHB-C4A-NA	3.11	128.82	124.51
17	I	4018	BCR	C20-C21-C22	-3.11	122.87	127.31
14	V	1502	CLA	CHB-C4A-NA	3.11	128.81	124.51
14	q	504	CLA	O2D-CGD-CBD	3.11	116.80	111.27
14	f	1201	CLA	CHB-C4A-NA	3.11	128.81	124.51
14	G	1237	CLA	C4-C3-C5	3.11	120.50	115.27
17	T	4015	BCR	C20-C21-C22	-3.11	122.87	127.31
14	H	1202	CLA	CHB-C4A-NA	3.11	128.81	124.51
14	e	1135	CLA	CMB-C2B-C3B	3.11	134.12	126.59
17	r	521	BCR	C7-C8-C9	-3.11	121.54	126.23
17	H	4009	BCR	C16-C17-C18	-3.11	122.87	127.31
14	H	1201	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
17	d	524	BCR	C15-C16-C17	-3.11	117.11	123.47
14	3	502	CLA	CHB-C4A-NA	3.11	128.81	124.51
14	A	1132	CLA	CAC-C3C-C4C	3.11	128.84	124.81
14	e	1801	CLA	CMB-C2B-C1B	-3.11	120.64	125.37
17	k	4018	BCR	C20-C21-C22	-3.11	122.88	127.31
21	3	822	SQD	O47-C7-C8	3.11	119.46	110.80
17	l	4013	BCR	C2-C1-C6	3.11	115.26	110.48
14	L	1503	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
17	B	4006	BCR	C16-C17-C18	-3.10	122.88	127.31
14	Y	504	CLA	O2D-CGD-CBD	3.10	116.78	111.27
17	B	4006	BCR	C31-C1-C6	-3.10	105.26	110.30
14	B	1201	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
14	n	1503	CLA	O2D-CGD-O1D	-3.10	117.77	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	s	502	CLA	CHB-C4A-NA	3.10	128.80	124.51
17	6	524	BCR	C15-C16-C17	-3.10	117.12	123.47
17	J	4013	BCR	C2-C1-C6	3.10	115.26	110.48
14	e	1132	CLA	CAC-C3C-C4C	3.10	128.84	124.81
21	a	822	SQD	O47-C7-C8	3.10	119.45	110.80
14	G	1137	CLA	CHB-C4A-NA	3.10	128.80	124.51
17	G	4001	BCR	C11-C10-C9	-3.10	122.88	127.31
17	f	4006	BCR	C31-C1-C6	-3.10	105.27	110.30
14	A	1137	CLA	CHB-C4A-NA	3.10	128.80	124.51
14	V	1503	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
14	H	1201	CLA	CMB-C2B-C1B	-3.10	120.65	125.37
14	t	508	CLA	CHB-C1B-NB	3.10	127.54	124.26
17	e	4001	BCR	C11-C10-C9	-3.10	122.89	127.31
21	V	5216	SQD	O47-C7-C8	3.10	118.17	111.50
14	e	1237	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
14	f	1201	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
14	4	508	CLA	CHB-C1B-NB	3.10	127.53	124.26
17	V	4219	BCR	C11-C10-C9	-3.10	122.89	127.31
14	H	1201	CLA	CHB-C4A-NA	3.10	128.79	124.51
14	H	1220	CLA	C3B-C4B-NB	-3.10	107.64	110.52
17	J	4015	BCR	C20-C21-C22	-3.10	122.89	127.31
21	s	822	SQD	O47-C7-C8	3.10	119.43	110.80
17	t	523	BCR	C10-C11-C12	-3.10	113.56	123.22
17	S	4018	BCR	C1-C6-C5	-3.09	118.25	122.61
14	A	1135	CLA	CMB-C2B-C3B	3.09	134.08	126.59
21	L	5216	SQD	O47-C7-C8	3.09	118.17	111.50
14	e	1107	CLA	CHB-C1B-NB	3.09	127.53	124.26
17	L	4219	BCR	C11-C10-C9	-3.09	122.90	127.31
14	G	1132	CLA	CAC-C3C-C4C	3.09	128.82	124.81
17	4	523	BCR	C10-C11-C12	-3.09	113.57	123.22
14	f	1236	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
17	H	4006	BCR	C31-C1-C6	-3.09	105.29	110.30
17	A	4001	BCR	C11-C10-C9	-3.09	122.90	127.31
17	b	523	BCR	C10-C11-C12	-3.09	113.58	123.22
14	A	1237	CLA	C4-C3-C5	3.09	120.46	115.27
14	f	1215	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
17	H	4006	BCR	C16-C17-C18	-3.09	122.91	127.31
17	Z	523	BCR	C28-C27-C26	-3.09	108.57	114.08
14	G	1135	CLA	CMB-C2B-C3B	3.09	134.06	126.59
14	A	1140	CLA	C3B-C4B-NB	-3.09	107.65	110.52
17	U	4104	BCR	C15-C14-C13	-3.08	122.91	127.31
21	u	822	SQD	O6-C1-C2	3.08	113.12	108.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1140	CLA	C3B-C4B-NB	-3.08	107.66	110.52
21	5	822	SQD	O6-C1-C2	3.08	113.11	108.30
21	n	5216	SQD	O47-C7-C8	3.08	118.14	111.50
17	v	524	BCR	C15-C16-C17	-3.08	117.16	123.47
17	m	4104	BCR	C15-C14-C13	-3.08	122.91	127.31
17	B	4009	BCR	C16-C17-C18	-3.08	122.92	127.31
17	K	4104	BCR	C11-C10-C9	-3.08	122.92	127.31
17	A	4011	BCR	C20-C19-C18	-3.08	117.77	126.42
18	G	5003	LHG	O8-C23-C24	3.08	121.57	111.91
17	2	523	BCR	C28-C27-C26	-3.08	108.58	114.08
14	e	1114	CLA	CHB-C1B-NB	3.08	127.51	124.26
14	A	1237	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
18	A	5003	LHG	O8-C23-C24	3.07	121.55	111.91
17	e	4011	BCR	C20-C19-C18	-3.07	117.78	126.42
17	r	523	BCR	C28-C27-C26	-3.07	108.59	114.08
14	A	1131	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
14	G	1107	CLA	CHB-C1B-NB	3.07	127.51	124.26
17	G	4008	BCR	C10-C11-C12	-3.07	113.63	123.22
14	B	1220	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	e	5003	LHG	O8-C23-C24	3.07	121.54	111.91
21	c	822	SQD	O6-C1-C2	3.07	113.09	108.30
17	f	4009	BCR	C16-C17-C18	-3.07	122.93	127.31
17	n	4219	BCR	C11-C10-C9	-3.07	122.93	127.31
14	b	508	CLA	CHB-C1B-NB	3.07	127.51	124.26
14	G	1131	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
17	K	4104	BCR	C15-C14-C13	-3.07	122.93	127.31
14	e	1237	CLA	C4-C3-C5	3.07	120.43	115.27
17	G	4011	BCR	C20-C19-C18	-3.07	117.80	126.42
14	B	1201	CLA	CMB-C2B-C1B	-3.07	120.70	125.37
14	B	1236	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
17	U	4104	BCR	C11-C10-C9	-3.06	122.94	127.31
17	l	4015	BCR	C20-C21-C22	-3.06	122.94	127.31
17	2	521	BCR	C3-C4-C5	-3.06	108.61	114.08
14	A	1011	CLA	CHC-C4B-NB	3.06	127.50	124.26
14	G	1011	CLA	CHC-C4B-NB	3.06	127.50	124.26
14	v	519	CLA	C3B-C4B-NB	-3.06	107.67	110.52
14	G	1237	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
17	r	521	BCR	C3-C4-C5	-3.06	108.61	114.08
14	H	1202	CLA	CMB-C2B-C1B	-3.06	120.71	125.37
14	H	1230	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
17	W	4021	BCR	C11-C10-C9	-3.06	122.94	127.31
14	G	1101	CLA	O2D-CGD-O1D	-3.06	117.86	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1011	CLA	CHC-C4B-NB	3.06	127.50	124.26
14	e	1131	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
17	Z	521	BCR	C3-C4-C5	-3.06	108.62	114.08
14	2	509	CLA	CHB-C4A-NA	3.06	128.74	124.51
17	e	4008	BCR	C10-C11-C12	-3.06	113.68	123.22
17	t	521	BCR	C15-C14-C13	-3.06	122.95	127.31
14	H	1228	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
17	A	4008	BCR	C10-C11-C12	-3.06	113.68	123.22
21	1	822	SQD	O8-S-C6	3.05	110.61	105.74
14	e	1101	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
17	R	4016	BCR	C28-C27-C26	-3.05	108.63	114.08
14	G	1114	CLA	CHB-C1B-NB	3.05	127.49	124.26
14	B	1215	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	B	1230	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	t	505	CLA	C3B-C4B-NB	-3.05	107.68	110.52
17	M	4021	BCR	C11-C10-C9	-3.05	122.95	127.31
14	A	1114	CLA	CHB-C1B-NB	3.05	127.49	124.26
17	G	4008	BCR	C11-C10-C9	-3.05	122.96	127.31
14	Z	509	CLA	CHB-C4A-NA	3.05	128.73	124.51
14	G	1124	CLA	CMB-C2B-C1B	-3.05	120.72	125.37
14	f	1221	CLA	C3B-C4B-NB	-3.05	107.69	110.52
14	b	519	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	B	1228	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	A	1101	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	B	1202	CLA	CMB-C2B-C1B	-3.05	120.73	125.37
17	L	4219	BCR	C37-C22-C23	3.05	122.88	118.08
14	f	1227	CLA	CHB-C4A-NA	3.05	128.72	124.51
17	T	4012	BCR	C16-C17-C18	-3.05	122.96	127.31
14	f	1228	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
17	n	4219	BCR	C37-C22-C23	3.05	122.88	118.08
21	q	822	SQD	O8-S-C6	3.04	110.59	105.74
17	B	4010	BCR	C33-C5-C4	3.04	119.47	113.62
14	H	1228	CLA	CHB-C4A-NA	3.04	128.72	124.51
14	r	509	CLA	CHB-C4A-NA	3.04	128.72	124.51
17	j	4016	BCR	C28-C27-C26	-3.04	108.64	114.08
14	2	501	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	t	519	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	r	522	BCR	C15-C16-C17	-3.04	117.24	123.47
17	H	4010	BCR	C33-C5-C4	3.04	119.46	113.62
17	F	4016	BCR	C28-C27-C26	-3.04	108.64	114.08
14	f	1230	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
21	Y	822	SQD	O8-S-C6	3.04	110.59	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	4010	BCR	C33-C5-C4	3.04	119.46	113.62
14	G	1115	CLA	CHB-C4A-NA	3.04	128.72	124.51
14	e	1130	CLA	C3B-C4B-NB	-3.04	107.69	110.52
14	H	1236	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	v	512	CLA	C3B-C4B-NB	-3.04	107.69	110.52
14	G	1135	CLA	CHC-C4B-NB	3.04	127.48	124.26
17	b	521	BCR	C15-C14-C13	-3.04	122.97	127.31
17	f	4014	BCR	C28-C27-C26	-3.04	108.65	114.08
14	Y	512	CLA	C3B-C4B-NB	-3.04	107.69	110.52
14	f	1220	CLA	C3B-C4B-NB	-3.04	107.69	110.52
14	r	501	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	H	1227	CLA	CHB-C4A-NA	3.04	128.72	124.51
14	a	509	CLA	CHB-C4A-NA	3.04	128.72	124.51
14	e	1124	CLA	CMB-C2B-C1B	-3.04	120.74	125.37
14	f	1201	CLA	CMB-C2B-C1B	-3.04	120.74	125.37
17	c	523	BCR	C24-C23-C22	-3.04	121.64	126.23
14	4	505	CLA	C3B-C4B-NB	-3.04	107.70	110.52
14	H	1203	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
14	e	1129	CLA	CHB-C1B-NB	3.04	127.47	124.26
17	4	521	BCR	C15-C14-C13	-3.04	122.98	127.31
21	b	822	SQD	O8-S-C6	3.04	110.58	105.74
14	4	519	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
17	v	523	BCR	C24-C23-C22	-3.03	121.65	126.23
21	t	822	SQD	O8-S-C6	3.03	110.58	105.74
14	B	1227	CLA	CHB-C4A-NA	3.03	128.71	124.51
17	B	4005	BCR	C33-C5-C6	-3.03	121.12	124.53
14	f	1229	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	b	505	CLA	C3B-C4B-NB	-3.03	107.70	110.52
17	B	4014	BCR	C28-C27-C26	-3.03	108.66	114.08
17	V	4219	BCR	C37-C22-C23	3.03	122.86	118.08
14	H	1215	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	G	1140	CLA	C3B-C4B-NB	-3.03	107.70	110.52
14	e	1116	CLA	C3B-C4B-NB	-3.03	107.70	110.52
14	H	1235	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	A	1124	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
14	e	1130	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	Y	503	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	Z	501	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	e	1107	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
14	e	1112	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
17	H	4014	BCR	C28-C27-C26	-3.03	108.67	114.08
21	u	822	SQD	O8-S-C6	3.03	110.56	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	4008	BCR	C11-C10-C9	-3.03	122.99	127.31
14	J	1302	CLA	CHB-C4A-NA	3.03	128.70	124.51
14	R	1302	CLA	C3B-C4B-NB	-3.03	107.71	110.52
21	4	822	SQD	O8-S-C6	3.03	110.56	105.74
19	l	5105	LMU	O5'-C5'-C4'	3.03	115.19	109.69
17	J	4012	BCR	C33-C5-C6	-3.03	121.13	124.53
14	G	1107	CLA	CMB-C2B-C1B	-3.02	120.76	125.37
17	2	522	BCR	C15-C16-C17	-3.02	117.28	123.47
14	e	1013	CLA	C3B-C4B-NB	-3.02	107.71	110.52
17	H	4005	BCR	C33-C5-C6	-3.02	121.13	124.53
14	G	1130	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	J	4012	BCR	C16-C17-C18	-3.02	123.00	127.31
17	o	4021	BCR	C11-C10-C9	-3.02	123.00	127.31
14	A	1115	CLA	CHB-C4A-NA	3.02	128.69	124.51
14	1	503	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	u	523	BCR	C24-C23-C22	-3.02	121.67	126.23
14	H	1232	CLA	CHB-C1B-NB	3.02	127.45	124.26
14	G	1116	CLA	C3B-C4B-NB	-3.02	107.71	110.52
17	Z	522	BCR	C15-C16-C17	-3.02	117.29	123.47
14	H	1216	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
14	B	1228	CLA	CHB-C4A-NA	3.02	128.69	124.51
14	A	1129	CLA	CHB-C1B-NB	3.02	127.45	124.26
14	A	1136	CLA	CHB-C1B-NB	3.02	127.45	124.26
14	e	1136	CLA	CHB-C1B-NB	3.02	127.45	124.26
14	6	519	CLA	C3B-C4B-NB	-3.02	107.71	110.52
14	G	1129	CLA	CHB-C1B-NB	3.02	127.45	124.26
17	v	521	BCR	C11-C10-C9	-3.02	123.00	127.31
18	e	5004	LHG	O8-C23-C24	3.02	121.38	111.91
14	B	1234	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
14	A	1135	CLA	CHC-C4B-NB	3.02	127.45	124.26
17	T	4012	BCR	C33-C5-C6	-3.02	121.14	124.53
17	l	4012	BCR	C16-C17-C18	-3.02	123.00	127.31
14	B	1231	CLA	CMB-C2B-C1B	-3.02	120.77	125.37
14	B	1235	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
17	n	4020	BCR	C10-C11-C12	-3.02	113.80	123.22
14	t	508	CLA	CMB-C2B-C1B	-3.02	120.77	125.37
17	6	523	BCR	C24-C23-C22	-3.02	121.68	126.23
17	T	4015	BCR	C24-C23-C22	-3.02	121.68	126.23
14	B	1216	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
14	f	1203	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
21	q	822	SQD	O9-S-C6	3.02	110.52	106.94
14	B	1023	CLA	C3B-C4B-NB	-3.01	107.72	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1221	CLA	C3B-C4B-NB	-3.01	107.72	110.52
17	S	4018	BCR	C21-C20-C19	-3.01	113.81	123.22
17	A	4008	BCR	C11-C10-C9	-3.01	123.01	127.31
14	e	1119	CLA	CHB-C1B-NB	3.01	127.45	124.26
14	e	1115	CLA	CHB-C4A-NA	3.01	128.68	124.51
14	B	1203	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
17	I	4018	BCR	C21-C20-C19	-3.01	113.81	123.22
14	A	1130	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	q	503	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	A	1119	CLA	CHB-C1B-NB	3.01	127.45	124.26
14	e	1135	CLA	CHC-C4B-NB	3.01	127.45	124.26
14	3	509	CLA	CHB-C4A-NA	3.01	128.68	124.51
14	s	504	CLA	CHB-C4A-NA	3.01	128.68	124.51
14	e	1110	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	A	1140	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
17	J	4015	BCR	C24-C23-C22	-3.01	121.69	126.23
14	f	1234	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	f	1852	SQD	O9-S-C6	3.01	110.52	106.94
20	H	5002	LMG	O1-C7-C8	-3.01	103.64	110.90
19	J	5105	LMU	O5'-C5'-C4'	3.01	115.16	109.69
14	Z	508	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
14	e	1103	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
18	G	5004	LHG	O8-C23-C24	3.01	121.35	111.91
14	H	1215	CLA	CHB-C4A-NA	3.01	128.67	124.51
21	5	822	SQD	O8-S-C6	3.01	110.53	105.74
14	G	1140	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	f	1235	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	A	1103	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
20	B	5002	LMG	O1-C7-C8	-3.01	103.64	110.90
14	l	1302	CLA	CHB-C4A-NA	3.01	128.67	124.51
17	L	4020	BCR	C10-C11-C12	-3.01	113.83	123.22
20	f	5002	LMG	O1-C7-C8	-3.01	103.64	110.90
17	a	524	BCR	C7-C8-C9	-3.01	121.69	126.23
14	f	1231	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
17	l	4012	BCR	C33-C5-C6	-3.01	121.15	124.53
18	A	5004	LHG	O8-C23-C24	3.01	121.34	111.91
14	f	1216	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
17	f	4005	BCR	C33-C5-C6	-3.01	121.15	124.53
14	f	1228	CLA	CHB-C4A-NA	3.01	128.67	124.51
14	B	1229	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
14	G	1133	CLA	C3B-C4B-NB	-3.01	107.73	110.52
14	A	1130	CLA	C3B-C4B-NB	-3.00	107.73	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1226	CLA	CMB-C2B-C3B	3.00	133.86	126.59
14	f	1202	CLA	CMB-C2B-C1B	-3.00	120.79	125.37
17	k	4018	BCR	C21-C20-C19	-3.00	113.84	123.22
17	V	4020	BCR	C10-C11-C12	-3.00	113.84	123.22
14	v	518	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	G	1103	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
17	5	523	BCR	C24-C23-C22	-3.00	121.70	126.23
14	B	1215	CLA	CHB-C4A-NA	3.00	128.66	124.51
14	1	512	CLA	C3B-C4B-NB	-3.00	107.73	110.52
17	d	523	BCR	C24-C23-C22	-3.00	121.70	126.23
17	v	522	BCR	C20-C21-C22	-3.00	123.03	127.31
17	6	522	BCR	C20-C21-C22	-3.00	123.03	127.31
21	c	822	SQD	O8-S-C6	3.00	110.52	105.74
17	T	4013	BCR	C7-C8-C9	-3.00	121.70	126.23
14	e	1140	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	F	1302	CLA	C3B-C4B-NB	-3.00	107.73	110.52
14	H	1229	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	A	1107	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
17	3	524	BCR	C7-C8-C9	-3.00	121.70	126.23
22	P	170	FMN	C4-N3-C2	-3.00	120.10	125.64
17	d	522	BCR	C20-C21-C22	-3.00	123.03	127.31
14	A	1112	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
22	p	170	FMN	C4-N3-C2	-3.00	120.10	125.64
14	G	1130	CLA	C3B-C4B-NB	-3.00	107.73	110.52
14	H	1222	CLA	C3B-C4B-NB	-3.00	107.73	110.52
18	A	5002	LHG	O8-C23-C24	3.00	121.31	111.91
19	T	5105	LMU	O5'-C5'-C4'	3.00	115.14	109.69
14	T	1302	CLA	CHB-C4A-NA	3.00	128.66	124.51
14	F	1301	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
14	H	1234	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
18	G	5002	LHG	O8-C23-C24	3.00	121.31	111.91
14	3	504	CLA	CHB-C4A-NA	2.99	128.65	124.51
14	A	1013	CLA	C3B-C4B-NB	-2.99	107.74	110.52
14	G	1119	CLA	CHB-C1B-NB	2.99	127.43	124.26
14	4	508	CLA	CMB-C2B-C1B	-2.99	120.81	125.37
17	s	524	BCR	C7-C8-C9	-2.99	121.71	126.23
14	G	1136	CLA	CHB-C1B-NB	2.99	127.43	124.26
14	B	1225	CLA	C3B-C4B-NB	-2.99	107.74	110.52
21	H	1852	SQD	O9-S-C6	2.99	110.50	106.94
14	G	1112	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
14	B	1226	CLA	CMB-C2B-C3B	2.99	133.83	126.59
14	A	1116	CLA	C3B-C4B-NB	-2.99	107.74	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1023	CLA	C3B-C4B-NB	-2.99	107.74	110.52
14	f	1023	CLA	C3B-C4B-NB	-2.99	107.74	110.52
17	I	4018	BCR	C10-C11-C12	-2.99	113.88	123.22
14	e	1104	CLA	CHB-C4A-NA	2.99	128.65	124.51
18	e	5002	LHG	O8-C23-C24	2.99	121.29	111.91
14	s	509	CLA	CHB-C4A-NA	2.99	128.65	124.51
17	k	4018	BCR	C10-C11-C12	-2.99	113.89	123.22
14	e	1133	CLA	C3B-C4B-NB	-2.99	107.74	110.52
14	j	1302	CLA	C3B-C4B-NB	-2.99	107.74	110.52
17	S	4018	BCR	C10-C11-C12	-2.99	113.89	123.22
14	5	519	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
17	H	4006	BCR	C8-C9-C10	2.99	123.53	118.94
14	s	507	CLA	CHB-C4A-NA	2.99	128.64	124.51
14	H	1231	CLA	CMB-C2B-C1B	-2.99	120.82	125.37
14	f	1215	CLA	CHB-C4A-NA	2.99	128.64	124.51
14	6	518	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
14	f	1232	CLA	CHB-C1B-NB	2.99	127.42	124.26
14	d	518	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
14	H	1226	CLA	CMB-C2B-C3B	2.99	133.82	126.59
14	a	507	CLA	CHB-C4A-NA	2.99	128.64	124.51
17	c	521	BCR	C30-C25-C26	-2.99	118.41	122.61
17	J	4013	BCR	C16-C15-C14	-2.98	117.36	123.47
14	c	519	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
14	B	1012	CLA	CMB-C2B-C3B	2.98	133.81	126.59
14	d	519	CLA	C3B-C4B-NB	-2.98	107.75	110.52
21	1	822	SQD	O9-S-C6	2.98	110.48	106.94
21	5	822	SQD	O9-S-C6	2.98	110.48	106.94
17	b	523	BCR	C16-C17-C18	-2.98	123.05	127.31
14	A	1110	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
14	q	512	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	j	1301	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	l	4015	BCR	C24-C23-C22	-2.98	121.73	126.23
14	B	1208	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
14	b	508	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
14	6	512	CLA	C3B-C4B-NB	-2.98	107.75	110.52
17	5	521	BCR	C30-C25-C26	-2.98	118.41	122.61
21	d	822	SQD	O8-S-C6	2.98	110.49	105.74
14	e	1124	CLA	CHB-C1B-NB	2.98	127.41	124.26
17	l	4013	BCR	C16-C15-C14	-2.98	117.37	123.47
17	s	521	BCR	C24-C23-C22	-2.98	121.73	126.23
22	X	170	FMN	C4-N3-C2	-2.98	120.14	125.64
14	f	1225	CLA	C3B-C4B-NB	-2.98	107.75	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	508	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
14	s	508	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
21	B	1852	SQD	O9-S-C6	2.98	110.48	106.94
14	H	1225	CLA	C3B-C4B-NB	-2.98	107.75	110.52
17	d	521	BCR	C11-C10-C9	-2.98	123.06	127.31
14	e	1121	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
14	f	1208	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
14	c	503	CLA	CHB-C4A-NA	2.98	128.63	124.51
17	6	521	BCR	C11-C10-C9	-2.98	123.06	127.31
17	A	4011	BCR	C34-C9-C10	-2.98	118.75	122.92
14	G	1013	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	a	504	CLA	CHB-C4A-NA	2.98	128.63	124.51
14	v	503	CLA	CHB-C4A-NA	2.98	128.63	124.51
17	l	4015	BCR	C2-C1-C6	2.98	115.06	110.48
21	v	822	SQD	O8-S-C6	2.98	110.48	105.74
17	a	524	BCR	C8-C7-C6	-2.97	118.85	127.20
14	B	1232	CLA	CHB-C1B-NB	2.97	127.41	124.26
14	R	1301	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	f	1012	CLA	CMB-C2B-C3B	2.97	133.79	126.59
17	G	4011	BCR	C34-C9-C10	-2.97	118.76	122.92
17	a	524	BCR	C15-C16-C17	-2.97	117.39	123.47
14	u	509	CLA	CHB-C4A-NA	2.97	128.62	124.51
14	H	1213	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
17	T	4013	BCR	C16-C15-C14	-2.97	117.39	123.47
14	B	1213	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	G	1117	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	Y	822	SQD	O9-S-C6	2.97	110.47	106.94
17	J	4013	BCR	C7-C8-C9	-2.97	121.75	126.23
14	A	1124	CLA	CHB-C1B-NB	2.97	127.40	124.26
14	A	1104	CLA	CHB-C4A-NA	2.97	128.62	124.51
17	a	521	BCR	C24-C23-C22	-2.97	121.75	126.23
17	3	524	BCR	C15-C16-C17	-2.97	117.39	123.47
14	3	507	CLA	CHB-C4A-NA	2.97	128.62	124.51
21	u	822	SQD	O9-S-C6	2.97	110.47	106.94
17	3	521	BCR	C24-C23-C22	-2.97	121.75	126.23
17	u	523	BCR	C20-C21-C22	-2.97	123.07	127.31
14	u	509	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
17	u	521	BCR	C30-C25-C26	-2.97	118.44	122.61
17	B	4006	BCR	C8-C9-C10	2.97	123.49	118.94
14	H	1222	CLA	CAA-C2A-C1A	-2.97	102.25	111.97
17	s	524	BCR	C15-C16-C17	-2.97	117.40	123.47
17	c	521	BCR	C38-C26-C27	2.97	119.31	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	822	SQD	O9-S-C6	2.97	110.46	106.94
14	f	1210	CLA	C3B-C4B-NB	-2.97	107.76	110.52
14	c	509	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
14	H	1012	CLA	CMB-C2B-C3B	2.96	133.77	126.59
14	A	1133	CLA	C3B-C4B-NB	-2.96	107.77	110.52
14	d	512	CLA	C3B-C4B-NB	-2.96	107.77	110.52
17	s	524	BCR	C8-C7-C6	-2.96	118.88	127.20
14	G	1110	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
14	Z	502	CLA	CHB-C4A-NA	2.96	128.61	124.51
14	u	501	CLA	CHB-C4A-NA	2.96	128.61	124.51
14	r	508	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
14	A	1121	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	u	519	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	5	501	CLA	CHB-C4A-NA	2.96	128.61	124.51
17	3	524	BCR	C8-C7-C6	-2.96	118.88	127.20
17	l	4013	BCR	C7-C8-C9	-2.96	121.76	126.23
14	H	1208	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	A	1111	CLA	CHB-C4A-NA	2.96	128.61	124.51
14	2	508	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
17	f	4006	BCR	C8-C9-C10	2.96	123.48	118.94
14	H	1207	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
21	6	822	SQD	O8-S-C6	2.96	110.46	105.74
14	G	1126	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
17	H	4010	BCR	C38-C26-C27	2.96	119.30	113.62
14	a	508	CLA	CHB-C1B-NB	2.96	127.39	124.26
14	H	1223	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	H	1023	CLA	CBC-CAC-C3C	2.96	120.59	112.43
14	d	507	CLA	CHB-C4A-NA	2.96	128.60	124.51
14	f	1222	CLA	CAA-C2A-C1A	-2.96	102.28	111.97
14	B	1222	CLA	CAA-C2A-C1A	-2.96	102.28	111.97
14	G	1104	CLA	CHB-C4A-NA	2.96	128.60	124.51
19	e	1848	LMU	C1B-O1B-C4'	-2.96	110.65	117.96
14	f	1213	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	f	1023	CLA	CBC-CAC-C3C	2.96	120.58	112.43
14	G	1111	CLA	CHB-C4A-NA	2.95	128.60	124.51
14	u	503	CLA	CHB-C4A-NA	2.95	128.60	124.51
14	v	507	CLA	CHB-C4A-NA	2.95	128.60	124.51
14	G	1140	CLA	CBA-CAA-C2A	2.95	122.58	113.86
14	A	1109	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
14	f	1223	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
17	u	521	BCR	C38-C26-C27	2.95	119.29	113.62
17	5	521	BCR	C38-C26-C27	2.95	119.29	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	J	4015	BCR	C2-C1-C6	2.95	115.03	110.48
14	v	513	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	2	502	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	6	503	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	a	509	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
14	A	1140	CLA	CBA-CAA-C2A	2.95	122.57	113.86
14	Z	518	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	s	504	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
17	l	4015	BCR	C32-C1-C6	-2.95	105.52	110.30
14	n	1502	CLA	O2D-CGD-CBD	2.95	116.51	111.27
14	e	1105	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	5	509	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
17	t	523	BCR	C16-C17-C18	-2.95	123.10	127.31
17	b	524	BCR	C33-C5-C4	2.95	119.28	113.62
14	c	509	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	f	1222	CLA	C3B-C4B-NB	-2.95	107.78	110.52
14	V	1501	CLA	CHB-C1B-NB	2.95	127.38	124.26
17	4	523	BCR	C16-C17-C18	-2.95	123.10	127.31
17	B	4010	BCR	C38-C26-C27	2.95	119.28	113.62
17	T	4015	BCR	C2-C1-C6	2.95	115.02	110.48
14	G	1124	CLA	CHB-C1B-NB	2.95	127.38	124.26
17	b	524	BCR	C20-C21-C22	-2.95	123.11	127.31
14	3	508	CLA	CHB-C1B-NB	2.95	127.38	124.26
14	H	1211	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
14	H	1225	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
14	B	1023	CLA	CBC-CAC-C3C	2.95	120.55	112.43
19	A	1848	LMU	C1B-O1B-C4'	-2.95	110.67	117.96
14	U	1103	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
19	G	1848	LMU	C1B-O1B-C4'	-2.94	110.68	117.96
14	H	1221	CLA	C3B-C4B-NB	-2.94	107.78	110.52
14	e	1140	CLA	CBA-CAA-C2A	2.94	122.55	113.86
14	A	1117	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
14	b	519	CLA	C3B-C4B-NB	-2.94	107.78	110.52
14	a	508	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
14	A	1126	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
14	B	1223	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
14	5	503	CLA	CHB-C4A-NA	2.94	128.58	124.51
17	F	4016	BCR	C20-C21-C22	-2.94	123.11	127.31
17	5	523	BCR	C20-C21-C22	-2.94	123.11	127.31
17	c	523	BCR	C20-C21-C22	-2.94	123.11	127.31
14	L	1502	CLA	O2D-CGD-CBD	2.94	116.50	111.27
17	e	4011	BCR	C34-C9-C10	-2.94	118.80	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1222	CLA	C3B-C4B-NB	-2.94	107.79	110.52
14	m	1401	CLA	C3B-C4B-NB	-2.94	107.79	110.52
14	B	1207	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	e	1117	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	f	1207	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	4	524	BCR	C20-C21-C22	-2.94	123.11	127.31
14	r	502	CLA	CHB-C4A-NA	2.94	128.58	124.51
14	B	1234	CLA	C3B-C4B-NB	-2.94	107.79	110.52
17	f	4010	BCR	C38-C26-C27	2.94	119.26	113.62
14	H	1201	CLA	C3B-C4B-NB	-2.94	107.79	110.52
14	e	1109	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	6	507	CLA	CHB-C4A-NA	2.94	128.57	124.51
14	H	1222	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
14	f	1221	CLA	CMB-C2B-C3B	2.94	133.70	126.59
14	5	509	CLA	CHB-C4A-NA	2.94	128.57	124.51
14	H	1221	CLA	CMB-C2B-C3B	2.94	133.70	126.59
14	G	1121	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
14	4	503	CLA	CHB-C4A-NA	2.94	128.57	124.51
14	K	1103	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
14	s	508	CLA	CHB-C1B-NB	2.94	127.36	124.26
14	A	1105	CLA	CHB-C4A-NA	2.94	128.57	124.51
14	K	1401	CLA	C3B-C4B-NB	-2.94	107.79	110.52
14	d	513	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
14	G	1109	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
14	B	1221	CLA	CMB-C2B-C3B	2.93	133.69	126.59
14	B	1210	CLA	C3B-C4B-NB	-2.93	107.79	110.52
17	R	4016	BCR	C20-C21-C22	-2.93	123.12	127.31
14	5	502	CLA	CHB-C4A-NA	2.93	128.57	124.51
14	4	519	CLA	C3B-C4B-NB	-2.93	107.80	110.52
14	H	1234	CLA	C3B-C4B-NB	-2.93	107.80	110.52
17	Y	523	BCR	C10-C11-C12	-2.93	114.07	123.22
14	c	501	CLA	CHB-C4A-NA	2.93	128.57	124.51
14	t	503	CLA	CHB-C4A-NA	2.93	128.56	124.51
14	f	1201	CLA	C3B-C4B-NB	-2.93	107.80	110.52
14	G	1139	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	L	1501	CLA	CHB-C1B-NB	2.93	127.36	124.26
14	V	1502	CLA	O2D-CGD-CBD	2.93	116.47	111.27
14	f	1222	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
17	j	4016	BCR	C20-C21-C22	-2.93	123.13	127.31
17	4	524	BCR	C33-C5-C4	2.93	119.24	113.62
14	e	1111	CLA	CHB-C4A-NA	2.93	128.56	124.51
14	B	1225	CLA	CMB-C2B-C1B	-2.93	120.91	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1222	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
14	d	502	CLA	CHB-C4A-NA	2.93	128.56	124.51
17	1	523	BCR	C10-C11-C12	-2.92	114.09	123.22
17	J	4015	BCR	C32-C1-C6	-2.92	105.56	110.30
14	s	509	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
14	G	1105	CLA	CHB-C4A-NA	2.92	128.56	124.51
14	Z	513	CLA	C3B-C4B-NB	-2.92	107.80	110.52
14	3	509	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
17	q	523	BCR	C10-C11-C12	-2.92	114.09	123.22
14	H	1210	CLA	C3B-C4B-NB	-2.92	107.80	110.52
14	e	1120	CLA	CHB-C4A-NA	2.92	128.55	124.51
14	A	1120	CLA	CHB-C4A-NA	2.92	128.55	124.51
17	5	524	BCR	C33-C5-C4	2.92	119.23	113.62
17	t	524	BCR	C33-C5-C4	2.92	119.23	113.62
14	f	1225	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
17	L	4219	BCR	C7-C8-C9	-2.92	121.82	126.23
14	H	1214	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
14	d	503	CLA	CHB-C4A-NA	2.92	128.55	124.51
14	m	1103	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
14	6	513	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
14	H	1214	CLA	CHB-C4A-NA	2.92	128.55	124.51
14	J	1302	CLA	C3B-C4B-NB	-2.92	107.81	110.52
14	f	1234	CLA	C3B-C4B-NB	-2.92	107.81	110.52
17	1	522	BCR	C3-C4-C5	-2.92	108.87	114.08
14	B	1201	CLA	C3B-C4B-NB	-2.92	107.81	110.52
14	B	1209	CLA	CHB-C4A-NA	2.92	128.54	124.51
14	e	1126	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
14	t	519	CLA	C3B-C4B-NB	-2.92	107.81	110.52
14	q	507	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
14	c	512	CLA	C3B-C4B-NB	-2.91	107.81	110.52
17	c	522	BCR	C38-C26-C25	-2.91	121.25	124.53
14	f	1214	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
14	B	1211	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
17	f	4010	BCR	C7-C8-C9	-2.91	121.83	126.23
14	u	502	CLA	CHB-C4A-NA	2.91	128.54	124.51
17	n	4219	BCR	C7-C8-C9	-2.91	121.83	126.23
14	Y	507	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
14	n	1501	CLA	CHB-C1B-NB	2.91	127.34	124.26
17	5	522	BCR	C38-C26-C25	-2.91	121.26	124.53
17	c	524	BCR	C33-C5-C4	2.91	119.21	113.62
14	2	518	CLA	CHB-C4A-NA	2.91	128.54	124.51
17	t	524	BCR	C20-C21-C22	-2.91	123.16	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1139	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	q	522	BCR	C3-C4-C5	-2.91	108.88	114.08
14	3	504	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	V	4219	BCR	C21-C20-C19	-2.91	114.14	123.22
14	c	502	CLA	CHB-C4A-NA	2.91	128.53	124.51
14	A	1139	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
14	f	1211	CLA	CMB-C2B-C1B	-2.91	120.94	125.37
14	f	1211	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	u	524	BCR	C33-C5-C4	2.91	119.20	113.62
14	B	1229	CLA	CMB-C2B-C3B	2.91	133.63	126.59
14	b	503	CLA	CHB-C4A-NA	2.90	128.53	124.51
17	B	4010	BCR	C7-C8-C9	-2.90	121.85	126.23
17	H	4010	BCR	C7-C8-C9	-2.90	121.85	126.23
17	Y	522	BCR	C3-C4-C5	-2.90	108.89	114.08
14	H	1229	CLA	CMB-C2B-C3B	2.90	133.62	126.59
14	B	1214	CLA	CHB-C4A-NA	2.90	128.53	124.51
14	t	502	CLA	CHB-C4A-NA	2.90	128.53	124.51
17	T	4015	BCR	C32-C1-C6	-2.90	105.59	110.30
14	5	504	CLA	CHB-C4A-NA	2.90	128.52	124.51
14	a	516	CLA	CHB-C4A-NA	2.90	128.52	124.51
14	f	1209	CLA	CHB-C4A-NA	2.90	128.52	124.51
14	a	504	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	v	502	CLA	CHB-C4A-NA	2.90	128.52	124.51
14	e	1118	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	G	1139	CLA	CHB-C1B-NB	2.90	127.33	124.26
14	r	513	CLA	C3B-C4B-NB	-2.90	107.83	110.52
14	r	519	CLA	C3B-C4B-NB	-2.90	107.83	110.52
17	m	4104	BCR	C38-C26-C27	2.90	119.18	113.62
17	a	523	BCR	C15-C16-C17	-2.90	117.54	123.47
14	B	1214	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	r	511	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	r	518	CLA	CHB-C4A-NA	2.90	128.52	124.51
14	2	519	CLA	C3B-C4B-NB	-2.90	107.83	110.52
14	5	512	CLA	C3B-C4B-NB	-2.90	107.83	110.52
14	3	517	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	s	517	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	6	502	CLA	CHB-C4A-NA	2.90	128.52	124.51
14	Y	509	CLA	CHB-C4A-NA	2.89	128.51	124.51
17	U	4104	BCR	C38-C26-C27	2.89	119.18	113.62
14	3	519	CLA	CHB-C4A-NA	2.89	128.51	124.51
14	B	1211	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
14	1	507	CLA	O2D-CGD-O1D	-2.89	118.18	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1229	CLA	CMB-C2B-C3B	2.89	133.59	126.59
17	B	4009	BCR	C33-C5-C6	-2.89	121.28	124.53
17	V	4219	BCR	C7-C8-C9	-2.89	121.87	126.23
14	G	1120	CLA	CHB-C4A-NA	2.89	128.51	124.51
17	H	4014	BCR	C10-C11-C12	-2.89	114.19	123.22
14	f	1214	CLA	CHB-C4A-NA	2.89	128.51	124.51
14	q	509	CLA	CHB-C4A-NA	2.89	128.51	124.51
14	t	507	CLA	CHB-C4A-NA	2.89	128.51	124.51
17	n	4219	BCR	C21-C20-C19	-2.89	114.20	123.22
14	a	517	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	G	1121	CLA	CHB-C4A-NA	2.89	128.51	124.51
17	K	4104	BCR	C38-C26-C27	2.89	119.17	113.62
14	U	1401	CLA	C3B-C4B-NB	-2.89	107.83	110.52
17	f	4014	BCR	C10-C11-C12	-2.89	114.20	123.22
14	b	519	CLA	CHB-C4A-NA	2.89	128.50	124.51
14	Z	517	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	f	1222	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
14	H	1203	CLA	C3B-C4B-NB	-2.89	107.84	110.52
14	2	511	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	H	1209	CLA	CHB-C4A-NA	2.89	128.50	124.51
14	a	519	CLA	CHB-C4A-NA	2.89	128.50	124.51
17	G	4002	BCR	C3-C4-C5	-2.89	108.92	114.08
14	b	507	CLA	CHB-C4A-NA	2.89	128.50	124.51
14	e	1125	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	l	1302	CLA	C3B-C4B-NB	-2.88	107.84	110.52
14	c	508	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
17	5	522	BCR	C38-C26-C27	2.88	119.16	113.62
14	4	507	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	r	504	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	b	518	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	A	1118	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	A	1122	CLA	CHB-C4A-NA	2.88	128.50	124.51
17	L	4219	BCR	C21-C20-C19	-2.88	114.22	123.22
17	q	524	BCR	C33-C5-C4	2.88	119.15	113.62
17	Y	523	BCR	C15-C16-C17	-2.88	117.57	123.47
14	A	1125	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	Z	504	CLA	CHB-C4A-NA	2.88	128.50	124.51
17	B	4014	BCR	C10-C11-C12	-2.88	114.22	123.22
14	G	1125	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	s	519	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	G	1126	CLA	CMB-C2B-C3B	2.88	133.57	126.59
17	H	4004	BCR	C28-C27-C26	-2.88	108.94	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1212	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	A	1139	CLA	CHB-C1B-NB	2.88	127.31	124.26
14	2	517	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	5	511	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	s	523	BCR	C15-C16-C17	-2.88	117.58	123.47
17	1	524	BCR	C33-C5-C4	2.88	119.14	113.62
17	Y	524	BCR	C33-C5-C4	2.88	119.14	113.62
14	Z	519	CLA	C3B-C4B-NB	-2.88	107.84	110.52
14	B	1222	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
17	v	521	BCR	C7-C8-C9	-2.88	121.89	126.23
14	2	513	CLA	C3B-C4B-NB	-2.88	107.85	110.52
14	5	510	CLA	C3B-C4B-NB	-2.88	107.85	110.52
17	B	4004	BCR	C28-C27-C26	-2.88	108.94	114.08
17	c	522	BCR	C38-C26-C27	2.88	119.14	113.62
17	H	4009	BCR	C33-C5-C6	-2.88	121.30	124.53
17	t	522	BCR	C38-C26-C25	-2.88	121.30	124.53
14	c	511	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
14	s	516	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	t	518	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	c	504	CLA	CHB-C4A-NA	2.87	128.49	124.51
14	q	516	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	c	523	BCR	C15-C16-C17	-2.87	117.59	123.47
14	e	1119	CLA	CHB-C4A-NA	2.87	128.49	124.51
14	t	519	CLA	CHB-C4A-NA	2.87	128.49	124.51
17	4	522	BCR	C38-C26-C25	-2.87	121.30	124.53
14	c	504	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
14	A	1137	CLA	C3B-C4B-NB	-2.87	107.85	110.52
14	b	502	CLA	CHB-C4A-NA	2.87	128.48	124.51
17	e	4002	BCR	C3-C4-C5	-2.87	108.95	114.08
14	4	501	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	Z	511	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	A	4002	BCR	C3-C4-C5	-2.87	108.95	114.08
14	B	1234	CLA	CBC-CAC-C3C	2.87	120.35	112.43
14	4	519	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	f	1212	CLA	CHB-C4A-NA	2.87	128.48	124.51
17	3	523	BCR	C15-C16-C17	-2.87	117.59	123.47
17	5	523	BCR	C15-C16-C17	-2.87	117.59	123.47
14	u	510	CLA	C3B-C4B-NB	-2.87	107.85	110.52
14	u	512	CLA	C3B-C4B-NB	-2.87	107.85	110.52
14	e	1135	CLA	O2A-C1-C2	2.87	116.18	108.64
17	u	522	BCR	C38-C26-C25	-2.87	121.31	124.53
14	e	1122	CLA	CHB-C4A-NA	2.87	128.48	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1217	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	A	1135	CLA	O2A-C1-C2	2.87	116.18	108.64
14	L	1502	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	f	1012	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
17	s	524	BCR	C33-C5-C4	2.87	119.13	113.62
14	1	509	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	H	1222	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
18	G	5003	LHG	C11-C10-C9	-2.87	99.86	114.42
14	B	1203	CLA	C3B-C4B-NB	-2.87	107.85	110.52
14	G	1125	CLA	C3B-C4B-NB	-2.87	107.85	110.52
14	3	516	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	q	507	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	t	501	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	H	1234	CLA	CBC-CAC-C3C	2.87	120.34	112.43
17	H	4010	BCR	C4-C5-C6	-2.87	118.57	122.73
14	G	1122	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	G	1118	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	c	510	CLA	C3B-C4B-NB	-2.87	107.86	110.52
14	H	1211	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	s	511	CLA	CHB-C4A-NA	2.87	128.48	124.51
17	1	523	BCR	C15-C16-C17	-2.87	117.60	123.47
14	f	1234	CLA	CBC-CAC-C3C	2.87	120.33	112.43
14	A	1119	CLA	CHB-C4A-NA	2.87	128.47	124.51
14	u	504	CLA	CHB-C4A-NA	2.87	128.47	124.51
14	e	1126	CLA	CMB-C2B-C3B	2.87	133.53	126.59
18	A	5003	LHG	C11-C10-C9	-2.87	99.88	114.42
14	t	501	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	A	1126	CLA	CMB-C2B-C3B	2.86	133.52	126.59
17	q	523	BCR	C15-C16-C17	-2.86	117.61	123.47
14	1	508	CLA	CHB-C1B-NB	2.86	127.29	124.26
14	G	1107	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	T	1302	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	A	1121	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	n	1502	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
14	1	507	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	Y	507	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	e	1139	CLA	CHB-C1B-NB	2.86	127.29	124.26
14	A	1107	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	e	1013	CLA	CHB-C4A-NA	2.86	128.47	124.51
18	k	5001	LHG	O8-C23-C24	2.86	120.88	111.91
14	Y	508	CLA	CHB-C1B-NB	2.86	127.28	124.26
14	G	1119	CLA	CHB-C4A-NA	2.86	128.47	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	e	5003	LHG	C11-C10-C9	-2.86	99.91	114.42
18	n	5220	LHG	O8-C23-C24	2.86	120.88	111.91
14	4	502	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	6	504	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	5	508	CLA	CMB-C2B-C1B	-2.86	121.02	125.37
14	4	518	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	v	511	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	Z	519	CLA	CHB-C4A-NA	2.86	128.46	124.51
17	L	4022	BCR	C3-C4-C5	-2.86	108.97	114.08
14	V	1502	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	b	510	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	B	1236	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	G	1136	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
17	u	522	BCR	C38-C26-C27	2.86	119.10	113.62
17	f	4004	BCR	C28-C27-C26	-2.86	108.98	114.08
17	V	4022	BCR	C16-C17-C18	-2.86	123.23	127.31
14	B	1217	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	1	516	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	G	1135	CLA	O2A-C1-C2	2.86	116.14	108.64
17	3	524	BCR	C33-C5-C4	2.86	119.10	113.62
17	n	4020	BCR	C34-C9-C8	2.86	122.58	118.08
17	u	523	BCR	C15-C16-C17	-2.86	117.62	123.47
14	H	1228	CLA	CMB-C2B-C3B	2.85	133.50	126.59
14	q	508	CLA	CHB-C1B-NB	2.85	127.28	124.26
14	r	517	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	L	5220	LHG	O8-C23-C24	2.85	120.86	111.91
14	3	511	CLA	CHB-C4A-NA	2.85	128.46	124.51
14	u	511	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	H	1012	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	f	1203	CLA	C3B-C4B-NB	-2.85	107.87	110.52
14	5	507	CLA	CHB-C4A-NA	2.85	128.46	124.51
14	H	1226	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	Y	516	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
17	L	4020	BCR	C34-C9-C8	2.85	122.57	118.08
14	B	1228	CLA	CMB-C2B-C3B	2.85	133.49	126.59
14	f	1223	CLA	CHB-C4A-NA	2.85	128.45	124.51
17	b	522	BCR	C38-C26-C25	-2.85	121.33	124.53
18	I	5001	LHG	O8-C23-C24	2.85	120.85	111.91
18	S	5001	LHG	O8-C23-C24	2.85	120.85	111.91
14	q	502	CLA	CHB-C4A-NA	2.85	128.45	124.51
17	a	524	BCR	C33-C5-C4	2.85	119.09	113.62
14	B	1212	CLA	CHB-C4A-NA	2.85	128.45	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	510	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	B	1012	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	d	507	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	H	1236	CLA	C3B-C4B-NB	-2.85	107.87	110.52
17	B	4010	BCR	C4-C5-C6	-2.85	118.60	122.73
14	2	519	CLA	CHB-C4A-NA	2.85	128.45	124.51
14	v	504	CLA	CHB-C4A-NA	2.85	128.45	124.51
14	e	1137	CLA	C3B-C4B-NB	-2.85	107.87	110.52
17	d	521	BCR	C7-C8-C9	-2.85	121.93	126.23
14	t	510	CLA	CHB-C4A-NA	2.85	128.45	124.51
17	e	4001	BCR	C2-C1-C6	2.85	114.86	110.48
14	B	1226	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
17	G	4001	BCR	C2-C1-C6	2.85	114.86	110.48
14	2	504	CLA	CHB-C4A-NA	2.84	128.45	124.51
14	f	1228	CLA	CMB-C2B-C3B	2.84	133.48	126.59
14	a	511	CLA	CHB-C4A-NA	2.84	128.44	124.51
14	d	504	CLA	CHB-C4A-NA	2.84	128.44	124.51
21	d	822	SQD	O5-C5-C4	2.84	114.86	109.69
14	G	1133	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	d	511	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	V	5220	LHG	O8-C23-C24	2.84	120.83	111.91
14	5	504	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
17	n	4022	BCR	C3-C4-C5	-2.84	109.00	114.08
17	L	4022	BCR	C16-C17-C18	-2.84	123.25	127.31
14	u	508	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
14	B	1221	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
14	e	1133	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
17	6	521	BCR	C7-C8-C9	-2.84	121.94	126.23
14	1	502	CLA	CHB-C4A-NA	2.84	128.44	124.51
14	H	1221	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
14	e	1124	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
14	e	1136	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
14	v	517	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	A	1136	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
14	f	1226	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	f	1221	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
17	Y	523	BCR	C37-C22-C23	2.84	122.55	118.08
17	V	4022	BCR	C3-C4-C5	-2.84	109.01	114.08
14	A	1133	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	e	1101	CLA	C7-C6-C5	-2.84	105.66	113.36
17	u	524	BCR	C21-C20-C19	-2.84	114.37	123.22
14	b	506	CLA	O2D-CGD-O1D	-2.84	118.29	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	501	CLA	CHB-C4A-NA	2.84	128.43	124.51
17	A	4001	BCR	C2-C1-C6	2.84	114.85	110.48
14	u	504	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
14	4	506	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	l	1303	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	6	822	SQD	O5-C5-C4	2.83	114.84	109.69
17	f	4010	BCR	C4-C5-C6	-2.83	118.62	122.73
17	G	4008	BCR	C15-C16-C17	-2.83	117.67	123.47
17	1	523	BCR	C37-C22-C23	2.83	122.54	118.08
21	v	822	SQD	C4-C3-C2	2.83	115.77	110.82
21	6	822	SQD	C4-C3-C2	2.83	115.77	110.82
14	e	1122	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	t	510	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	6	511	CLA	CHB-C4A-NA	2.83	128.43	124.51
14	u	507	CLA	CHB-C4A-NA	2.83	128.43	124.51
17	A	4008	BCR	C15-C16-C17	-2.83	117.67	123.47
17	f	4009	BCR	C33-C5-C6	-2.83	121.35	124.53
14	e	1107	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	B	1223	CLA	CHB-C4A-NA	2.83	128.43	124.51
17	5	524	BCR	C21-C20-C19	-2.83	114.38	123.22
14	e	1134	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	Y	505	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	f	1212	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	t	522	BCR	C38-C26-C27	2.83	119.05	113.62
17	n	4022	BCR	C16-C17-C18	-2.83	123.27	127.31
14	t	506	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	e	4008	BCR	C15-C16-C17	-2.83	117.68	123.47
14	3	510	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	G	1137	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	G	1122	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	r	524	BCR	C7-C8-C9	-2.83	121.96	126.23
14	6	507	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	f	1217	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	H	1239	CLA	CMC-C2C-C3C	2.83	133.79	126.12
14	A	1013	CLA	CHB-C4A-NA	2.83	128.42	124.51
14	H	1223	CLA	CHB-C4A-NA	2.83	128.42	124.51
14	a	513	CLA	CHB-C4A-NA	2.83	128.42	124.51
14	a	510	CLA	CHB-C4A-NA	2.83	128.42	124.51
14	G	1801	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	q	505	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	4	522	BCR	C38-C26-C27	2.83	119.04	113.62
21	v	822	SQD	O5-C5-C4	2.82	114.82	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1212	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
17	r	521	BCR	C33-C5-C6	-2.82	121.36	124.53
14	Y	518	CLA	CHB-C4A-NA	2.82	128.42	124.51
14	B	1239	CLA	CMC-C2C-C3C	2.82	133.78	126.12
14	A	1124	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
14	4	501	CLA	C3B-C4B-NB	-2.82	107.90	110.52
17	Y	523	BCR	C33-C5-C6	-2.82	121.36	124.53
14	6	517	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
14	v	507	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
14	H	1203	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	A	1134	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
14	H	1239	CLA	C16-C15-C13	-2.82	106.80	115.92
14	B	1224	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
17	V	4020	BCR	C34-C9-C8	2.82	122.52	118.08
14	G	1124	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
14	s	510	CLA	C3B-C4B-NB	-2.82	107.90	110.52
14	s	503	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	e	1136	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	u	521	BCR	C38-C26-C25	-2.82	121.36	124.53
21	d	822	SQD	C4-C3-C2	2.82	115.74	110.82
14	G	1136	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	4	510	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	1	505	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	H	1224	CLA	CMB-C2B-C1B	-2.82	121.08	125.37
14	b	510	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	r	519	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	A	1114	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	e	1114	CLA	C3B-C4B-NB	-2.82	107.90	110.52
17	c	524	BCR	C21-C20-C19	-2.82	114.43	123.22
14	c	507	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	H	1212	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	A	1101	CLA	C7-C6-C5	-2.82	105.71	113.36
14	A	1109	CLA	O2A-CGA-O1A	-2.82	116.49	123.59
14	e	1137	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	G	1116	CLA	CMB-C2B-C3B	2.81	133.41	126.59
17	q	523	BCR	C37-C22-C23	2.81	122.51	118.08
14	e	1114	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
14	f	1236	CLA	C3B-C4B-NB	-2.81	107.90	110.52
14	B	1239	CLA	C16-C15-C13	-2.81	106.82	115.92
17	2	521	BCR	C33-C5-C6	-2.81	121.37	124.53
14	f	1239	CLA	CMC-C2C-C3C	2.81	133.76	126.12
14	G	1013	CLA	CHB-C4A-NA	2.81	128.40	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1122	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	5	521	BCR	C38-C26-C25	-2.81	121.37	124.53
14	f	1239	CLA	C16-C15-C13	-2.81	106.83	115.92
14	A	1136	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	t	509	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	e	1109	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
14	R	1302	CLA	CHB-C4A-NA	2.81	128.40	124.51
14	b	501	CLA	C3B-C4B-NB	-2.81	107.91	110.52
14	A	1128	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	b	504	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	Z	524	BCR	C7-C8-C9	-2.81	121.99	126.23
14	e	1117	CLA	CHB-C1B-NB	2.81	127.23	124.26
14	G	1134	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	A	1801	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	e	1128	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	t	504	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	f	1215	CLA	C1-C2-C3	-2.81	121.19	126.04
17	2	524	BCR	C7-C8-C9	-2.81	121.99	126.23
14	n	1503	CLA	CHB-C4A-NA	2.81	128.39	124.51
14	a	510	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	L	5216	SQD	O8-S-C6	2.81	110.21	105.74
17	Y	522	BCR	C33-C5-C6	-2.81	121.38	124.53
14	G	1101	CLA	C7-C6-C5	-2.81	105.74	113.36
14	Z	508	CLA	CHB-C1B-NB	2.81	127.23	124.26
14	T	1303	CLA	CHB-C4A-NA	2.81	128.39	124.51
14	e	1102	CLA	CMB-C2B-C3B	2.81	133.38	126.59
14	G	1114	CLA	C3B-C4B-NB	-2.80	107.91	110.52
21	u	822	SQD	C1-O5-C5	2.80	119.19	113.69
14	A	1125	CLA	C3B-C4B-NB	-2.80	107.91	110.52
14	3	510	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
14	3	519	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	c	521	BCR	C38-C26-C25	-2.80	121.38	124.53
14	3	513	CLA	CHB-C4A-NA	2.80	128.39	124.51
14	G	1117	CLA	CHB-C1B-NB	2.80	127.22	124.26
14	A	1114	CLA	C3B-C4B-NB	-2.80	107.92	110.52
17	R	4016	BCR	C16-C15-C14	-2.80	117.73	123.47
14	e	1116	CLA	CMB-C2B-C3B	2.80	133.38	126.59
21	n	5216	SQD	O8-S-C6	2.80	110.21	105.74
14	e	1129	CLA	O2D-CGD-CBD	2.80	116.25	111.27
14	f	1224	CLA	CMB-C2B-C1B	-2.80	121.10	125.37
14	G	1134	CLA	CHB-C4A-NA	2.80	128.39	124.51
14	e	1121	CLA	CHB-C4A-NA	2.80	128.39	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	522	BCR	C38-C26-C27	2.80	119.00	113.62
14	s	519	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
14	A	1102	CLA	CHB-C4A-NA	2.80	128.38	124.51
17	r	524	BCR	C20-C21-C22	-2.80	123.31	127.31
17	U	4104	BCR	C10-C11-C12	-2.80	114.48	123.22
14	G	1114	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
14	a	519	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
14	F	1302	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	Y	503	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	b	508	CLA	CHB-C4A-NA	2.80	128.38	124.51
17	K	4104	BCR	C3-C4-C5	-2.80	109.08	114.08
14	J	1303	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	1	518	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	e	1124	CLA	C3B-C4B-NB	-2.80	107.92	110.52
14	2	508	CLA	CHB-C1B-NB	2.80	127.22	124.26
14	Y	502	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	A	1137	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	4	509	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	1	523	BCR	C33-C5-C6	-2.80	121.39	124.53
14	6	510	CLA	C3B-C4B-NB	-2.80	107.92	110.52
14	v	510	CLA	C3B-C4B-NB	-2.80	107.92	110.52
14	1	507	CLA	C2A-C1A-CHA	2.80	128.75	123.86
14	A	1102	CLA	CMB-C2B-C3B	2.80	133.36	126.59
14	2	509	CLA	CMB-C2B-C1B	-2.80	121.11	125.37
14	s	510	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	4	504	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	A	1116	CLA	CMB-C2B-C3B	2.79	133.36	126.59
17	Z	521	BCR	C33-C5-C6	-2.79	121.39	124.53
14	3	510	CLA	CHB-C4A-NA	2.79	128.38	124.51
14	G	1128	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	m	4104	BCR	C10-C11-C12	-2.79	114.50	123.22
14	B	1203	CLA	CHB-C4A-NA	2.79	128.38	124.51
14	e	1102	CLA	CHB-C4A-NA	2.79	128.38	124.51
14	G	1129	CLA	O2D-CGD-CBD	2.79	116.23	111.27
14	f	1215	CLA	O2D-CGD-CBD	2.79	116.23	111.27
14	s	516	CLA	CAC-C3C-C2C	-2.79	122.75	127.53
14	f	1240	CLA	C3B-C4B-NB	-2.79	107.92	110.52
14	3	503	CLA	CHB-C4A-NA	2.79	128.37	124.51
17	H	4014	BCR	C36-C18-C19	2.79	122.48	118.08
17	U	4104	BCR	C3-C4-C5	-2.79	109.09	114.08
14	s	505	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	K	4104	BCR	C10-C11-C12	-2.79	114.50	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1124	CLA	C3B-C4B-NB	-2.79	107.92	110.52
14	H	1240	CLA	C3B-C4B-NB	-2.79	107.92	110.52
17	Y	522	BCR	C38-C26-C25	-2.79	121.39	124.53
14	A	1117	CLA	CHB-C1B-NB	2.79	127.21	124.26
14	d	517	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	V	5220	LHG	C11-C10-C9	-2.79	100.26	114.42
14	r	509	CLA	CMB-C2B-C1B	-2.79	121.12	125.37
14	3	516	CLA	CAC-C3C-C2C	-2.79	122.76	127.53
14	j	1302	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	q	507	CLA	C2A-C1A-CHA	2.79	128.74	123.86
17	n	4219	BCR	C1-C6-C7	2.79	123.67	115.78
14	L	1503	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	b	517	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	f	1203	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	A	1129	CLA	O2D-CGD-CBD	2.79	116.22	111.27
14	G	1109	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
14	e	1101	CLA	CAA-CBA-CGA	-2.79	105.11	113.25
14	H	1205	CLA	C3B-C4B-NB	-2.79	107.93	110.52
15	G	2001	PQN	C14-C13-C15	-2.79	110.58	115.27
14	2	519	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	A	1134	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	c	519	CLA	CHB-C4A-NA	2.79	128.37	124.51
17	B	4014	BCR	C36-C18-C19	2.79	122.47	118.08
14	H	1219	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	c	507	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
17	2	524	BCR	C20-C21-C22	-2.79	123.33	127.31
21	V	5216	SQD	O8-S-C6	2.79	110.18	105.74
14	3	505	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	b	509	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	G	1102	CLA	CMB-C2B-C3B	2.79	133.33	126.59
14	q	518	CLA	CHB-C4A-NA	2.78	128.36	124.51
21	5	822	SQD	C1-O5-C5	2.78	119.15	113.69
17	F	4016	BCR	C16-C15-C14	-2.78	117.77	123.47
14	f	1219	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
14	G	1101	CLA	O2D-CGD-CBD	2.78	116.22	111.27
14	e	1801	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
14	B	1215	CLA	C1-C2-C3	-2.78	121.23	126.04
14	B	1217	CLA	CHB-C4A-NA	2.78	128.36	124.51
15	A	2001	PQN	C14-C13-C15	-2.78	110.59	115.27
17	L	4219	BCR	C1-C6-C7	2.78	123.65	115.78
14	c	503	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	B	1240	CLA	C3B-C4B-NB	-2.78	107.93	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1111	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	b	508	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	L	5220	LHG	C11-C10-C9	-2.78	100.30	114.42
14	H	1222	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	v	506	CLA	CHB-C4A-NA	2.78	128.36	124.51
14	A	1101	CLA	CAA-CBA-CGA	-2.78	105.13	113.25
14	G	1137	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	r	519	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	t	508	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	Y	507	CLA	C2A-C1A-CHA	2.78	128.72	123.86
14	e	1134	CLA	CHB-C4A-NA	2.78	128.36	124.51
17	V	4219	BCR	C1-C6-C7	2.78	123.64	115.78
14	c	517	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
15	e	2001	PQN	C14-C13-C15	-2.78	110.59	115.27
14	4	508	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	s	510	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
17	j	4016	BCR	C16-C15-C14	-2.78	117.78	123.47
14	d	510	CLA	C3B-C4B-NB	-2.78	107.94	110.52
14	e	1101	CLA	O2D-CGD-CBD	2.78	116.21	111.27
17	A	4011	BCR	C10-C11-C12	-2.78	114.55	123.22
17	m	4104	BCR	C3-C4-C5	-2.78	109.12	114.08
14	5	507	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
14	G	1135	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
14	A	1101	CLA	O2D-CGD-CBD	2.78	116.20	111.27
14	G	1110	CLA	CHB-C4A-NA	2.78	128.35	124.51
14	s	513	CLA	CHB-C4A-NA	2.78	128.35	124.51
17	c	522	BCR	C23-C24-C25	-2.78	119.40	127.20
17	e	4011	BCR	C10-C11-C12	-2.78	114.55	123.22
14	4	517	CLA	CHB-C4A-NA	2.78	128.35	124.51
14	G	1102	CLA	CHB-C4A-NA	2.78	128.35	124.51
14	e	1125	CLA	C3B-C4B-NB	-2.78	107.94	110.52
14	H	1215	CLA	C1-C2-C3	-2.78	121.24	126.04
14	6	509	CLA	CHB-C4A-NA	2.78	128.35	124.51
14	l	1303	CLA	C3B-C4B-NB	-2.78	107.94	110.52
14	f	1227	CLA	O2A-CGA-O1A	-2.78	116.59	123.59
21	c	822	SQD	C1-O5-C5	2.78	119.14	113.69
14	G	1101	CLA	CAA-CBA-CGA	-2.77	105.14	113.25
17	3	523	BCR	C33-C5-C6	-2.77	121.41	124.53
14	e	1135	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
18	n	5220	LHG	C11-C10-C9	-2.77	100.34	114.42
14	Y	501	CLA	CHB-C4A-NA	2.77	128.35	124.51
17	1	522	BCR	C33-C5-C6	-2.77	121.41	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	4014	BCR	C36-C18-C19	2.77	122.45	118.08
14	A	1111	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	Y	511	CLA	CHB-C4A-NA	2.77	128.35	124.51
14	d	509	CLA	CHB-C4A-NA	2.77	128.35	124.51
17	Z	524	BCR	C33-C5-C4	2.77	118.94	113.62
14	H	1217	CLA	C3B-C4B-NB	-2.77	107.94	110.52
14	b	502	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	d	506	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	Z	509	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
14	A	1135	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	B	1215	CLA	O2D-CGD-CBD	2.77	116.19	111.27
14	Z	503	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	q	519	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
17	5	522	BCR	C23-C24-C25	-2.77	119.42	127.20
14	H	1216	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	e	1109	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	5	503	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
17	q	523	BCR	C33-C5-C6	-2.77	121.42	124.53
17	Z	524	BCR	C20-C21-C22	-2.77	123.36	127.31
17	u	522	BCR	C16-C17-C18	-2.77	123.36	127.31
14	Y	517	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	Z	519	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	e	1110	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	v	509	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	a	516	CLA	CAC-C3C-C2C	-2.77	122.79	127.53
14	G	1113	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	c	510	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	H	1217	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	A	1135	CLA	C3B-C4B-NB	-2.77	107.95	110.52
14	B	1240	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
17	G	4003	BCR	C7-C8-C9	-2.77	122.05	126.23
14	H	1240	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	a	503	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	v	519	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	e	5001	LHG	C20-C19-C18	-2.77	100.38	114.42
21	3	822	SQD	C44-O6-C1	2.77	119.14	113.74
14	H	1215	CLA	O2D-CGD-CBD	2.77	116.19	111.27
14	B	1219	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	5	505	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	f	1240	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	1	503	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	e	1133	CLA	CHB-C4A-NA	2.77	128.34	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	c	513	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	u	510	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	e	1113	CLA	CHB-C4A-NA	2.77	128.34	124.51
17	G	4011	BCR	C10-C11-C12	-2.77	114.59	123.22
14	5	517	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	G	1109	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	5	510	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	G	1124	CLA	C3B-C4B-NB	-2.76	107.95	110.52
14	t	502	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
17	c	522	BCR	C16-C17-C18	-2.76	123.36	127.31
17	u	522	BCR	C23-C24-C25	-2.76	119.44	127.20
14	1	508	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
14	v	501	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	e	1118	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	A	5001	LHG	C20-C19-C18	-2.76	100.40	114.42
17	e	4008	BCR	C33-C5-C6	-2.76	121.42	124.53
14	1	501	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	2	503	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	4	508	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	B	1222	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	T	1303	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	G	5001	LHG	C20-C19-C18	-2.76	100.40	114.42
14	d	519	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	5	519	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	B	1217	CLA	C3B-C4B-NB	-2.76	107.95	110.52
14	H	1218	CLA	C3B-C4B-NB	-2.76	107.95	110.52
17	G	4008	BCR	C38-C26-C25	-2.76	121.43	124.53
17	s	523	BCR	C33-C5-C6	-2.76	121.43	124.53
14	1	517	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	A	1109	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	G	1133	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	1	519	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	A	1106	CLA	O2D-CGD-CBD	2.76	116.17	111.27
14	A	1118	CLA	C3B-C4B-NB	-2.76	107.95	110.52
14	a	510	CLA	C3B-C4B-NB	-2.76	107.95	110.52
21	r	822	SQD	C44-O6-C1	2.76	119.13	113.74
14	Y	508	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	r	503	CLA	CHB-C4A-NA	2.76	128.33	124.51
17	r	524	BCR	C33-C5-C4	2.76	118.92	113.62
14	u	507	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	B	1227	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
17	a	523	BCR	C33-C5-C6	-2.76	121.43	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	u	519	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	a	505	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	u	505	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	s	524	BCR	C21-C20-C19	-2.76	114.61	123.22
14	4	502	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	B	1216	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	f	1217	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	A	1114	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
14	B	1205	CLA	C3B-C4B-NB	-2.76	107.96	110.52
14	G	1127	CLA	C3B-C4B-NB	-2.76	107.96	110.52
17	2	524	BCR	C33-C5-C4	2.76	118.92	113.62
14	G	1113	CLA	CMB-C2B-C3B	2.76	133.27	126.59
14	A	1128	CLA	C2B-C1B-NB	-2.76	108.38	110.23
14	e	1113	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
14	v	519	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
17	H	4010	BCR	C36-C18-C19	2.76	122.42	118.08
21	c	822	SQD	O5-C5-C4	2.76	114.70	109.69
14	6	519	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
14	B	1227	CLA	CHB-C1B-NB	2.76	127.18	124.26
14	t	508	CLA	CHB-C4A-NA	2.76	128.32	124.51
14	B	1239	CLA	C6-C7-C8	-2.76	107.01	115.92
14	H	1239	CLA	C6-C7-C8	-2.76	107.01	115.92
14	H	1227	CLA	CHB-C1B-NB	2.76	127.17	124.26
14	e	1111	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
14	e	1113	CLA	CMB-C2B-C3B	2.76	133.26	126.59
17	q	522	BCR	C33-C5-C6	-2.76	121.43	124.53
17	B	4009	BCR	C33-C5-C4	2.76	118.91	113.62
17	q	524	BCR	C21-C20-C19	-2.76	114.62	123.22
14	e	1114	CLA	CAA-C2A-C3A	-2.75	105.23	112.78
14	G	1114	CLA	CAA-C2A-C3A	-2.75	105.23	112.78
14	H	1220	CLA	CHB-C4A-NA	2.75	128.32	124.51
17	1	522	BCR	C38-C26-C25	-2.75	121.44	124.53
17	G	4008	BCR	C33-C5-C6	-2.75	121.44	124.53
14	q	508	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
14	A	1113	CLA	CMB-C2B-C3B	2.75	133.26	126.59
14	u	511	CLA	CHB-C4A-NA	2.75	128.32	124.51
14	c	505	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
17	H	4009	BCR	C33-C5-C4	2.75	118.91	113.62
17	a	524	BCR	C21-C20-C19	-2.75	114.63	123.22
14	V	1503	CLA	CHB-C4A-NA	2.75	128.32	124.51
14	e	1123	CLA	CHB-C4A-NA	2.75	128.32	124.51
17	3	524	BCR	C21-C20-C19	-2.75	114.63	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1113	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	G	1135	CLA	C3B-C4B-NB	-2.75	107.96	110.52
17	Y	524	BCR	C21-C20-C19	-2.75	114.63	123.22
14	G	1107	CLA	C2D-C1D-ND	-2.75	108.08	110.10
14	e	1110	CLA	C1-C2-C3	-2.75	121.28	126.04
14	H	1238	CLA	CHB-C4A-NA	2.75	128.32	124.51
14	6	506	CLA	CHB-C4A-NA	2.75	128.32	124.51
14	e	1131	CLA	CHB-C4A-NA	2.75	128.32	124.51
14	e	1104	CLA	C3B-C4B-NB	-2.75	107.96	110.52
14	6	506	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	f	1239	CLA	C6-C7-C8	-2.75	107.03	115.92
14	A	1131	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	t	513	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	A	1105	CLA	CMB-C2B-C3B	2.75	133.25	126.59
14	e	1135	CLA	C3B-C4B-NB	-2.75	107.96	110.52
17	1	523	BCR	C23-C24-C25	-2.75	119.48	127.20
17	q	523	BCR	C23-C24-C25	-2.75	119.48	127.20
14	d	506	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
17	1	524	BCR	C21-C20-C19	-2.75	114.64	123.22
14	e	1106	CLA	O2D-CGD-CBD	2.75	116.15	111.27
14	H	1229	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	r	516	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	J	1303	CLA	C3B-C4B-NB	-2.75	107.97	110.52
14	u	513	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	r	524	BCR	C8-C7-C6	-2.75	119.49	127.20
14	2	516	CLA	CHB-C4A-NA	2.75	128.31	124.51
21	Z	822	SQD	C44-O6-C1	2.75	119.11	113.74
14	G	1105	CLA	CMB-C2B-C3B	2.75	133.24	126.59
14	e	1105	CLA	CMB-C2B-C3B	2.75	133.24	126.59
14	H	1227	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
14	r	508	CLA	CHB-C1B-NB	2.75	127.17	124.26
17	f	4010	BCR	C36-C18-C19	2.75	122.41	118.08
14	A	1133	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	Y	513	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	H	1239	CLA	O2A-C1-C2	-2.75	101.42	108.64
14	1	511	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	q	501	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	q	517	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
14	t	511	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
21	2	822	SQD	C44-O6-C1	2.75	119.10	113.74
14	6	519	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	f	1231	CLA	O2D-CGD-O1D	-2.75	118.47	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4008	BCR	C33-C5-C6	-2.74	121.45	124.53
14	5	513	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	Z	503	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	G	1120	CLA	O2D-CGD-CBD	2.74	116.14	111.27
14	r	503	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	B	1239	CLA	O2A-C1-C2	-2.74	101.42	108.64
17	5	522	BCR	C16-C17-C18	-2.74	123.39	127.31
17	2	523	BCR	C15-C16-C17	-2.74	117.86	123.47
14	4	511	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	Y	519	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	b	516	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	v	506	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	f	4017	BCR	C20-C21-C22	-2.74	123.40	127.31
14	f	1239	CLA	O2A-C1-C2	-2.74	101.43	108.64
14	4	506	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	H	1231	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	u	517	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	G	1131	CLA	CHB-C4A-NA	2.74	128.30	124.51
17	e	4003	BCR	C7-C8-C9	-2.74	122.09	126.23
17	Z	523	BCR	C15-C16-C17	-2.74	117.86	123.47
14	e	1128	CLA	C2B-C1B-NB	-2.74	108.39	110.23
14	A	1113	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	6	501	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	d	519	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	B	4010	BCR	C36-C18-C19	2.74	122.39	118.08
17	l	4013	BCR	C10-C11-C12	-2.74	114.67	123.22
14	U	1401	CLA	O2D-CGD-CBD	2.74	116.14	111.27
14	f	1223	CLA	CMB-C2B-C3B	2.74	133.22	126.59
14	A	1123	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	d	501	CLA	CHB-C4A-NA	2.74	128.30	124.51
21	a	822	SQD	C44-O6-C1	2.74	119.09	113.74
21	5	822	SQD	O5-C5-C4	2.74	114.67	109.69
14	A	1110	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	4	513	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	f	1239	CLA	CHB-C4A-NA	2.74	128.30	124.51
21	s	822	SQD	C44-O6-C1	2.74	119.09	113.74
17	A	4003	BCR	C7-C8-C9	-2.74	122.10	126.23
14	d	512	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	u	503	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	B	1223	CLA	CMB-C2B-C3B	2.74	133.22	126.59
14	Z	516	CLA	CHB-C4A-NA	2.74	128.30	124.51
17	H	4004	BCR	C16-C15-C14	-2.74	117.87	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	s	522	BCR	C33-C5-C6	-2.74	121.45	124.53
14	f	1227	CLA	CHB-C1B-NB	2.74	127.15	124.26
14	1	513	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	t	517	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	2	503	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
14	t	516	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
14	G	1106	CLA	O2D-CGD-CBD	2.74	116.13	111.27
14	H	1223	CLA	CMB-C2B-C3B	2.74	133.22	126.59
14	f	1205	CLA	C3B-C4B-NB	-2.74	107.98	110.52
14	1	506	CLA	CHB-C4A-NA	2.74	128.29	124.51
17	Y	523	BCR	C23-C24-C25	-2.74	119.52	127.20
14	f	1229	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	n	1501	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	q	503	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	e	4008	BCR	C38-C26-C25	-2.73	121.46	124.53
17	r	523	BCR	C15-C16-C17	-2.73	117.87	123.47
17	2	522	BCR	C1-C6-C5	-2.73	118.76	122.61
14	4	516	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
14	e	1107	CLA	C2D-C1D-ND	-2.73	108.09	110.10
14	b	506	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	B	4017	BCR	C20-C21-C22	-2.73	123.41	127.31
17	r	522	BCR	C1-C6-C5	-2.73	118.76	122.61
14	f	1217	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	A	5009	LHG	O8-C23-C24	2.73	120.49	111.91
14	f	1216	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	6	512	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
17	f	4004	BCR	C16-C15-C14	-2.73	117.88	123.47
17	f	4009	BCR	C33-C5-C4	2.73	118.86	113.62
14	1	516	CLA	CAC-C3C-C4C	2.73	128.35	124.81
14	6	517	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	G	1110	CLA	C1-C2-C3	-2.73	121.32	126.04
14	e	1106	CLA	C3B-C4B-NB	-2.73	107.98	110.52
14	B	1220	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	6	513	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	J	4013	BCR	C20-C19-C18	-2.73	118.74	126.42
17	Z	522	BCR	C1-C6-C5	-2.73	118.77	122.61
17	G	4007	BCR	C15-C16-C17	-2.73	117.88	123.47
14	B	1231	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
14	u	508	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
14	V	1501	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	q	513	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	e	5009	LHG	O8-C23-C24	2.73	120.48	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1216	CLA	O2A-CGA-CBA	2.73	120.47	111.91
18	G	5009	LHG	O8-C23-C24	2.73	120.47	111.91
14	L	1501	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	T	4013	BCR	C10-C11-C12	-2.73	114.70	123.22
17	J	4013	BCR	C10-C11-C12	-2.73	114.70	123.22
17	A	4008	BCR	C38-C26-C25	-2.73	121.46	124.53
14	b	513	CLA	CHB-C4A-NA	2.73	128.28	124.51
14	B	1216	CLA	O2A-CGA-CBA	2.73	120.47	111.91
17	Z	524	BCR	C8-C7-C6	-2.73	119.54	127.20
17	L	4019	BCR	C38-C26-C25	-2.73	121.47	124.53
17	R	4016	BCR	C11-C12-C13	-2.73	118.75	126.42
14	Y	504	CLA	CHB-C4A-NA	2.73	128.28	124.51
14	f	1235	CLA	CHB-C4A-NA	2.73	128.28	124.51
17	q	522	BCR	C38-C26-C25	-2.73	121.47	124.53
14	H	1213	CLA	O2D-CGD-CBD	2.73	116.11	111.27
17	B	4004	BCR	C16-C15-C14	-2.73	117.89	123.47
14	Y	510	CLA	CHB-C4A-NA	2.73	128.28	124.51
21	u	822	SQD	O5-C5-C4	2.73	114.64	109.69
14	f	1222	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
14	f	1238	CLA	CHB-C4A-NA	2.73	128.28	124.51
14	q	516	CLA	CAC-C3C-C4C	2.73	128.35	124.81
14	A	1110	CLA	C1-C2-C3	-2.73	121.33	126.04
17	n	4019	BCR	C38-C26-C25	-2.72	121.47	124.53
14	Y	506	CLA	CHB-C4A-NA	2.72	128.28	124.51
14	e	1126	CLA	O2D-CGD-CBD	2.72	116.11	111.27
17	2	524	BCR	C8-C7-C6	-2.72	119.55	127.20
14	5	511	CLA	CHB-C4A-NA	2.72	128.28	124.51
14	v	517	CLA	CHB-C4A-NA	2.72	128.28	124.51
14	d	508	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
17	3	522	BCR	C15-C16-C17	-2.72	117.89	123.47
17	s	522	BCR	C15-C16-C17	-2.72	117.89	123.47
14	c	505	CLA	CHB-C4A-NA	2.72	128.28	124.51
14	B	1213	CLA	O2D-CGD-CBD	2.72	116.11	111.27
14	b	505	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
14	b	518	CLA	C3B-C4B-NB	-2.72	107.99	110.52
14	q	504	CLA	CHB-C4A-NA	2.72	128.28	124.51
14	5	508	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	c	508	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
17	c	524	BCR	C15-C16-C17	-2.72	117.90	123.47
14	H	1216	CLA	O2A-CGA-CBA	2.72	120.45	111.91
14	t	513	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	K	1401	CLA	O2D-CGD-CBD	2.72	116.11	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	522	BCR	C15-C16-C17	-2.72	117.90	123.47
14	B	1238	CLA	CHB-C4A-NA	2.72	128.28	124.51
17	v	523	BCR	C28-C27-C26	-2.72	109.22	114.08
14	4	505	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	r	504	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	u	510	CLA	CHB-C4A-NA	2.72	128.27	124.51
14	r	505	CLA	C1-C2-C3	-2.72	121.34	126.04
17	5	524	BCR	C15-C16-C17	-2.72	117.90	123.47
17	T	4013	BCR	C20-C19-C18	-2.72	118.78	126.42
14	H	1239	CLA	CMC-C2C-C1C	-2.72	120.90	125.04
14	Z	505	CLA	C1-C2-C3	-2.72	121.34	126.04
14	A	1120	CLA	O2D-CGD-CBD	2.72	116.10	111.27
17	j	4016	BCR	C11-C12-C13	-2.72	118.78	126.42
14	1	501	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	q	506	CLA	CHB-C4A-NA	2.72	128.27	124.51
14	e	1127	CLA	CMB-C2B-C3B	2.72	133.17	126.59
17	6	523	BCR	C28-C27-C26	-2.72	109.22	114.08
14	v	513	CLA	CHB-C4A-NA	2.72	128.27	124.51
14	A	1127	CLA	CMB-C2B-C3B	2.72	133.17	126.59
17	l	4013	BCR	C20-C19-C18	-2.72	118.78	126.42
14	A	1106	CLA	C3B-C4B-NB	-2.72	107.99	110.52
14	f	1213	CLA	O2D-CGD-CBD	2.72	116.10	111.27
14	c	511	CLA	CHB-C4A-NA	2.72	128.27	124.51
17	F	4016	BCR	C11-C12-C13	-2.72	118.78	126.42
14	G	1127	CLA	CMB-C2B-C3B	2.72	133.17	126.59
14	A	1107	CLA	C2D-C1D-ND	-2.72	108.10	110.10
14	G	1801	CLA	CMB-C2B-C3B	2.72	133.17	126.59
14	5	510	CLA	CHB-C4A-NA	2.72	128.27	124.51
21	4	822	SQD	C1-O5-C5	2.72	119.02	113.69
14	Z	504	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
21	3	822	SQD	O8-S-C6	2.72	110.07	105.74
14	B	1218	CLA	C3B-C4B-NB	-2.72	108.00	110.52
17	n	4219	BCR	C23-C22-C21	-2.71	114.78	118.94
14	A	1127	CLA	C3B-C4B-NB	-2.71	108.00	110.52
14	e	1120	CLA	O2D-CGD-CBD	2.71	116.09	111.27
14	U	1103	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	5	512	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
14	t	505	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
14	m	1401	CLA	O2D-CGD-CBD	2.71	116.09	111.27
17	V	4019	BCR	C38-C26-C25	-2.71	121.48	124.53
14	2	504	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
14	Y	501	CLA	O2D-CGD-O1D	-2.71	118.53	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	v	508	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	q	510	CLA	C3B-C4B-NB	-2.71	108.00	110.52
14	B	1229	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	H	1239	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	v	512	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
17	H	4017	BCR	C20-C21-C22	-2.71	123.44	127.31
14	6	508	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	G	1128	CLA	C2B-C1B-NB	-2.71	108.42	110.23
14	G	1118	CLA	C3B-C4B-NB	-2.71	108.00	110.52
17	A	4007	BCR	C15-C16-C17	-2.71	117.92	123.47
17	L	4219	BCR	C23-C22-C21	-2.71	114.78	118.94
17	v	522	BCR	C38-C26-C25	-2.71	121.49	124.53
14	1	510	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	r	506	CLA	CHB-C4A-NA	2.71	128.26	124.51
17	e	4007	BCR	C15-C16-C17	-2.71	117.92	123.47
14	A	1801	CLA	CMB-C2B-C3B	2.71	133.15	126.59
14	1	510	CLA	C3B-C4B-NB	-2.71	108.00	110.52
14	f	1220	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	A	1104	CLA	C3B-C4B-NB	-2.71	108.00	110.52
14	G	1123	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	A	1126	CLA	O2D-CGD-CBD	2.71	116.08	111.27
14	r	513	CLA	CHB-C4A-NA	2.71	128.25	124.51
14	6	508	CLA	CMB-C2B-C1B	-2.71	121.25	125.37
17	a	522	BCR	C16-C17-C18	-2.71	123.45	127.31
14	B	1239	CLA	CHB-C4A-NA	2.71	128.25	124.51
14	t	516	CLA	CHB-C4A-NA	2.71	128.25	124.51
17	V	4219	BCR	C23-C22-C21	-2.71	114.79	118.94
17	Y	523	BCR	C23-C22-C21	-2.71	114.79	118.94
14	t	501	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
14	u	512	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
14	2	507	CLA	CHB-C4A-NA	2.71	128.25	124.51
14	G	1106	CLA	CHB-C4A-NA	2.71	128.25	124.51
14	b	511	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
14	G	1126	CLA	O2D-CGD-CBD	2.71	116.08	111.27
17	u	524	BCR	C15-C16-C17	-2.70	117.93	123.47
14	Y	517	CLA	CHB-C4A-NA	2.70	128.25	124.51
14	Y	516	CLA	CAC-C3C-C4C	2.70	128.32	124.81
14	B	1235	CLA	CHB-C4A-NA	2.70	128.25	124.51
17	d	523	BCR	C28-C27-C26	-2.70	109.25	114.08
17	d	522	BCR	C38-C26-C25	-2.70	121.49	124.53
14	a	511	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
14	Z	505	CLA	CHB-C4A-NA	2.70	128.25	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Z	513	CLA	CHB-C4A-NA	2.70	128.25	124.51
14	d	513	CLA	CHB-C4A-NA	2.70	128.25	124.51
14	e	1127	CLA	C3B-C4B-NB	-2.70	108.01	110.52
14	4	501	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	4	513	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	A	1140	CLA	CHB-C4A-NA	2.70	128.25	124.51
21	t	822	SQD	C1-O5-C5	2.70	118.99	113.69
14	G	1113	CLA	CHB-C4A-NA	2.70	128.25	124.51
14	b	513	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	3	511	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	v	508	CLA	CMB-C2B-C1B	-2.70	121.26	125.37
21	b	822	SQD	C1-O5-C5	2.70	118.99	113.69
14	a	513	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	s	506	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	t	506	CLA	CHB-C4A-NA	2.70	128.25	124.51
14	2	505	CLA	C1-C2-C3	-2.70	121.38	126.04
14	G	1140	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	b	511	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	6	507	CLA	C2A-C1A-CHA	2.70	128.58	123.86
14	v	511	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	v	507	CLA	C2A-C1A-CHA	2.70	128.58	123.86
14	6	511	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
17	V	4020	BCR	C16-C15-C14	-2.70	117.95	123.47
14	d	516	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
17	3	522	BCR	C33-C5-C6	-2.70	121.50	124.53
14	2	513	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	Y	505	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	Z	507	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	d	517	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	4	518	CLA	C3B-C4B-NB	-2.70	108.01	110.52
14	t	512	CLA	C3B-C4B-NB	-2.70	108.01	110.52
14	f	1221	CLA	CHB-C1B-NB	2.70	127.11	124.26
14	f	1023	CLA	CMB-C2B-C1B	-2.70	121.26	125.37
14	q	501	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
14	3	513	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
14	1	504	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	2	505	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	Z	507	CLA	C2A-C1A-CHA	2.70	128.57	123.86
14	K	1103	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	b	501	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
14	c	502	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
21	V	5216	SQD	O5-C5-C4	2.69	114.59	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1022	CLA	CMB-C2B-C3B	2.69	133.11	126.59
14	B	1239	CLA	CMC-C2C-C1C	-2.69	120.94	125.04
14	c	510	CLA	CHB-C4A-NA	2.69	128.24	124.51
14	G	1106	CLA	C3B-C4B-NB	-2.69	108.02	110.52
17	n	4020	BCR	C16-C15-C14	-2.69	117.96	123.47
17	H	4010	BCR	C31-C1-C6	-2.69	105.93	110.30
14	n	1501	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
14	u	506	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
17	6	522	BCR	C38-C26-C25	-2.69	121.50	124.53
14	B	1220	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
14	c	513	CLA	CHB-C4A-NA	2.69	128.24	124.51
17	L	4020	BCR	C16-C15-C14	-2.69	117.96	123.47
17	1	523	BCR	C23-C22-C21	-2.69	114.81	118.94
14	4	512	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	B	1023	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
17	3	522	BCR	C16-C17-C18	-2.69	123.47	127.31
14	5	505	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	q	511	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	c	512	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	a	519	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	e	1120	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	e	1801	CLA	CMB-C2B-C3B	2.69	133.10	126.59
21	n	5216	SQD	O48-C23-O10	-2.69	116.81	123.59
17	f	4017	BCR	C15-C16-C17	-2.69	117.97	123.47
14	s	513	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	L	5216	SQD	O5-C5-C4	2.69	114.58	109.69
14	f	1220	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	G	1128	CLA	C7-C6-C5	-2.69	106.06	113.36
14	A	1011	CLA	C2A-C1A-CHA	2.69	128.56	123.86
14	L	1501	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	Z	511	CLA	CHB-C4A-NA	2.69	128.23	124.51
17	c	521	BCR	C23-C24-C25	-2.69	119.66	127.20
21	a	822	SQD	O8-S-C6	2.69	110.02	105.74
14	c	504	CLA	C3B-C4B-NB	-2.69	108.02	110.52
17	Y	522	BCR	C38-C26-C27	2.69	118.78	113.62
14	3	506	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
14	H	1220	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
14	2	506	CLA	CHB-C4A-NA	2.69	128.22	124.51
17	f	4014	BCR	C2-C1-C6	2.68	114.61	110.48
14	U	1105	CLA	CAC-C3C-C2C	2.68	132.12	127.53
14	s	511	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	1	505	CLA	CHB-C4A-NA	2.68	128.22	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	516	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	H	1227	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	V	1501	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	m	1105	CLA	CAC-C3C-C2C	2.68	132.12	127.53
14	2	507	CLA	C2A-C1A-CHA	2.68	128.55	123.86
17	5	521	BCR	C23-C24-C25	-2.68	119.67	127.20
17	G	4011	BCR	C38-C26-C25	-2.68	121.52	124.53
14	2	511	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	f	1238	CLA	CMB-C2B-C3B	2.68	133.09	126.59
14	c	506	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	V	4020	BCR	C36-C18-C19	2.68	122.30	118.08
14	v	516	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	f	1218	CLA	C3B-C4B-NB	-2.68	108.03	110.52
14	d	511	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	e	1124	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	A	1106	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	q	510	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	A	4011	BCR	C38-C26-C25	-2.68	121.52	124.53
21	n	5216	SQD	O5-C5-C4	2.68	114.56	109.69
17	q	522	BCR	C38-C26-C27	2.68	118.77	113.62
17	s	522	BCR	C16-C17-C18	-2.68	123.48	127.31
14	G	1119	CLA	CMC-C2C-C1C	-2.68	120.96	125.04
14	H	1023	CLA	CMB-C2B-C1B	-2.68	121.29	125.37
21	s	822	SQD	O8-S-C6	2.68	110.01	105.74
17	6	523	BCR	C20-C21-C22	-2.68	123.48	127.31
14	u	516	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	B	1230	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
14	r	508	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	d	507	CLA	C2A-C1A-CHA	2.68	128.54	123.86
14	H	1238	CLA	CMB-C2B-C3B	2.68	133.08	126.59
14	q	517	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	r	511	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	q	522	BCR	C11-C12-C13	-2.68	118.89	126.42
14	Y	510	CLA	C3B-C4B-NB	-2.68	108.03	110.52
14	2	508	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	d	508	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	f	1239	CLA	CMC-C2C-C1C	-2.68	120.96	125.04
14	f	1230	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
21	V	5216	SQD	O48-C23-O10	-2.68	116.83	123.59
17	Y	522	BCR	C11-C12-C13	-2.68	118.89	126.42
14	5	506	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	A	1124	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1128	CLA	C7-C6-C5	-2.68	106.09	113.36
14	Y	518	CLA	C3B-C4B-NB	-2.68	108.03	110.52
14	t	518	CLA	C3B-C4B-NB	-2.68	108.03	110.52
17	v	523	BCR	C20-C21-C22	-2.68	123.49	127.31
14	Z	508	CLA	CHB-C4A-NA	2.68	128.21	124.51
17	H	4017	BCR	C15-C16-C17	-2.68	117.99	123.47
14	5	516	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
14	e	1022	CLA	CMB-C2B-C3B	2.68	133.07	126.59
14	B	1205	CLA	CHB-C4A-NA	2.67	128.21	124.51
14	H	1230	CLA	CAA-C2A-C3A	-2.67	105.45	112.78
21	L	5216	SQD	O48-C23-O10	-2.67	116.84	123.59
17	1	522	BCR	C11-C12-C13	-2.67	118.90	126.42
14	G	1022	CLA	CMB-C2B-C3B	2.67	133.06	126.59
17	v	522	BCR	C16-C17-C18	-2.67	123.49	127.31
17	4	524	BCR	C24-C23-C22	-2.67	122.19	126.23
14	5	507	CLA	C2A-C1A-CHA	2.67	128.53	123.86
17	1	522	BCR	C38-C26-C27	2.67	118.75	113.62
14	c	507	CLA	C2A-C1A-CHA	2.67	128.53	123.86
17	b	524	BCR	C24-C23-C22	-2.67	122.20	126.23
17	5	522	BCR	C33-C5-C6	-2.67	121.53	124.53
17	n	4020	BCR	C38-C26-C25	2.67	127.53	124.53
14	m	1103	CLA	CHB-C4A-NA	2.67	128.21	124.51
14	5	502	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
14	a	506	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
14	3	518	CLA	CHB-C4A-NA	2.67	128.21	124.51
14	H	1235	CLA	CHB-C4A-NA	2.67	128.21	124.51
14	A	1136	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
14	H	1221	CLA	CHB-C1B-NB	2.67	127.08	124.26
22	p	170	FMN	C4A-C4-N3	2.67	119.97	113.19
14	r	507	CLA	C2A-C1A-CHA	2.67	128.53	123.86
14	f	1209	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	e	1140	CLA	CHB-C4A-NA	2.67	128.20	124.51
17	B	4017	BCR	C15-C16-C17	-2.67	118.00	123.47
17	f	4010	BCR	C31-C1-C6	-2.67	105.97	110.30
14	K	1105	CLA	CAC-C3C-C2C	2.67	132.09	127.53
14	e	1136	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
14	B	1238	CLA	CMB-C2B-C3B	2.67	133.05	126.59
17	u	521	BCR	C23-C24-C25	-2.67	119.71	127.20
14	5	513	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	G	1124	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
14	e	1011	CLA	C2A-C1A-CHA	2.67	128.53	123.86
14	r	507	CLA	CHB-C4A-NA	2.67	128.20	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	u	513	CLA	CHB-C4A-NA	2.67	128.20	124.51
14	Z	513	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
14	v	504	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	5	522	BCR	C15-C16-C17	-2.67	118.01	123.47
14	G	1120	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	f	1227	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	a	523	BCR	C28-C27-C26	-2.67	109.31	114.08
14	B	1227	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	a	522	BCR	C33-C5-C6	-2.67	121.53	124.53
14	f	1205	CLA	CHB-C4A-NA	2.67	128.20	124.51
17	3	523	BCR	C28-C27-C26	-2.67	109.31	114.08
17	u	522	BCR	C15-C16-C17	-2.67	118.01	123.47
14	1	518	CLA	C3B-C4B-NB	-2.67	108.04	110.52
17	L	4020	BCR	C36-C18-C19	2.67	122.28	118.08
14	r	517	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	X	170	FMN	C4A-C4-N3	2.67	119.96	113.19
14	A	1120	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	e	1237	CLA	C11-C12-C13	-2.67	107.30	115.92
14	3	508	CLA	CHB-C4A-NA	2.67	128.20	124.51
17	c	522	BCR	C15-C16-C17	-2.67	118.01	123.47
14	G	1136	CLA	O2A-CGA-O1A	-2.67	116.87	123.59
14	5	506	CLA	CHB-C4A-NA	2.66	128.20	124.51
14	a	518	CLA	CHB-C4A-NA	2.66	128.20	124.51
14	e	1128	CLA	C7-C6-C5	-2.66	106.12	113.36
14	e	1131	CLA	C1-C2-C3	-2.66	121.44	126.04
14	e	1106	CLA	CHB-C4A-NA	2.66	128.20	124.51
17	B	4014	BCR	C2-C1-C6	2.66	114.58	110.48
17	v	522	BCR	C38-C26-C27	2.66	118.73	113.62
14	b	516	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	B	4010	BCR	C31-C1-C6	-2.66	105.98	110.30
14	H	1213	CLA	C3B-C4B-NB	-2.66	108.05	110.52
14	u	504	CLA	C3B-C4B-NB	-2.66	108.05	110.52
17	f	4005	BCR	C28-C27-C26	-2.66	109.32	114.08
14	A	1011	CLA	C4D-C3D-CAD	-2.66	104.96	108.10
14	H	1238	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
14	s	508	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	6	516	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
14	u	506	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	q	510	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	P	170	FMN	C4A-C4-N3	2.66	119.95	113.19
17	3	524	BCR	C23-C24-C25	-2.66	119.73	127.20
14	1	517	CLA	CHB-C4A-NA	2.66	128.19	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	511	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	a	524	BCR	C23-C24-C25	-2.66	119.73	127.20
14	2	510	CLA	C3B-C4B-NB	-2.66	108.05	110.52
14	f	1213	CLA	C3B-C4B-NB	-2.66	108.05	110.52
17	r	523	BCR	C11-C10-C9	-2.66	123.52	127.31
17	e	4011	BCR	C38-C26-C25	-2.66	121.54	124.53
14	B	1225	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	5	513	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	u	507	CLA	C2A-C1A-CHA	2.66	128.51	123.86
17	n	4020	BCR	C36-C18-C19	2.66	122.27	118.08
14	u	505	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	1	510	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
14	a	508	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	G	1237	CLA	C11-C12-C13	-2.66	107.33	115.92
17	u	522	BCR	C33-C5-C6	-2.66	121.55	124.53
14	B	1213	CLA	C3B-C4B-NB	-2.66	108.05	110.52
14	d	503	CLA	C3B-C4B-NB	-2.66	108.05	110.52
14	u	518	CLA	C3B-C4B-NB	-2.66	108.05	110.52
17	s	524	BCR	C23-C24-C25	-2.66	119.74	127.20
14	d	518	CLA	CHB-C4A-NA	2.66	128.18	124.51
14	2	513	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
14	f	1225	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	d	513	CLA	C3B-C4B-NB	-2.65	108.05	110.52
14	u	513	CLA	C3B-C4B-NB	-2.65	108.05	110.52
17	R	4016	BCR	C33-C5-C6	-2.65	121.55	124.53
14	A	1237	CLA	C11-C12-C13	-2.65	107.34	115.92
17	d	523	BCR	C20-C21-C22	-2.65	123.52	127.31
14	v	512	CLA	CHB-C1B-NB	2.65	127.07	124.26
17	Y	522	BCR	C23-C24-C25	-2.65	119.75	127.20
14	5	516	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	c	506	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	c	516	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	1	522	BCR	C23-C24-C25	-2.65	119.75	127.20
14	A	1119	CLA	CMC-C2C-C1C	-2.65	121.00	125.04
14	B	1209	CLA	C3B-C4B-NB	-2.65	108.05	110.52
14	A	1131	CLA	C1-C2-C3	-2.65	121.45	126.04
14	G	1011	CLA	C2A-C1A-CHA	2.65	128.50	123.86
17	B	4005	BCR	C28-C27-C26	-2.65	109.34	114.08
14	u	502	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
14	4	504	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	e	1125	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	H	4005	BCR	C28-C27-C26	-2.65	109.34	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	l	4015	BCR	C38-C26-C25	-2.65	121.55	124.53
14	3	518	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	a	518	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	q	518	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	B	1221	CLA	CHB-C1B-NB	2.65	127.06	124.26
17	q	522	BCR	C23-C24-C25	-2.65	119.76	127.20
17	q	523	BCR	C23-C22-C21	-2.65	114.87	118.94
17	t	521	BCR	C33-C5-C6	-2.65	121.55	124.53
17	B	4010	BCR	C11-C12-C13	-2.65	118.97	126.42
17	L	4020	BCR	C38-C26-C25	2.65	127.50	124.53
17	H	4014	BCR	C2-C1-C6	2.65	114.56	110.48
14	q	505	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	c	518	CLA	C3B-C4B-NB	-2.65	108.06	110.52
17	H	4010	BCR	C11-C12-C13	-2.65	118.98	126.42
14	t	505	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	H	1205	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	b	512	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	6	504	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
14	f	1232	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
17	s	523	BCR	C28-C27-C26	-2.65	109.35	114.08
14	d	505	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	u	516	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	5	518	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	a	503	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	4	505	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	r	505	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	Z	506	CLA	CHB-C4A-NA	2.65	128.17	124.51
17	J	4015	BCR	C38-C26-C25	-2.64	121.56	124.53
17	j	4016	BCR	C33-C5-C6	-2.64	121.56	124.53
14	G	1237	CLA	C2B-C1B-NB	-2.64	108.46	110.23
17	t	524	BCR	C24-C23-C22	-2.64	122.24	126.23
14	Y	519	CLA	C3B-C4B-NB	-2.64	108.06	110.52
14	H	1231	CLA	CHB-C4A-NA	2.64	128.17	124.51
14	G	1104	CLA	C3B-C4B-NB	-2.64	108.06	110.52
14	6	503	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	Z	522	BCR	C20-C21-C22	-2.64	123.54	127.31
14	c	516	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
21	Z	822	SQD	O8-S-C6	2.64	109.95	105.74
14	A	1237	CLA	C2B-C1B-NB	-2.64	108.46	110.23
14	6	505	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	5	504	CLA	C3B-C4B-NB	-2.64	108.06	110.52
14	B	1221	CLA	O2D-CGD-CBD	2.64	115.96	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1119	CLA	CMC-C2C-C1C	-2.64	121.02	125.04
14	A	1125	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	6	518	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	s	505	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	V	4020	BCR	C38-C26-C25	2.64	127.49	124.53
17	H	4014	BCR	C24-C23-C22	-2.64	122.25	126.23
14	2	517	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	t	511	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	2	523	BCR	C11-C10-C9	-2.64	123.54	127.31
14	3	519	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	s	519	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	Y	510	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	f	1224	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	v	503	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	v	518	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	f	4010	BCR	C11-C12-C13	-2.64	119.01	126.42
14	6	503	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	H	1209	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	B	1230	CLA	CAA-C2A-C1A	-2.64	103.33	111.97
17	f	4014	BCR	C24-C23-C22	-2.64	122.25	126.23
17	6	522	BCR	C38-C26-C27	2.64	118.68	113.62
14	2	510	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	1	519	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	q	519	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	B	1232	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	G	1131	CLA	C1-C2-C3	-2.64	121.48	126.04
14	s	518	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	G	1111	CLA	C3B-C4B-NB	-2.64	108.07	110.52
17	c	522	BCR	C33-C5-C6	-2.64	121.57	124.53
14	A	1135	CLA	CHB-C4A-NA	2.63	128.16	124.51
14	B	1231	CLA	CHB-C4A-NA	2.63	128.16	124.51
14	b	505	CLA	CHB-C4A-NA	2.63	128.16	124.51
14	c	513	CLA	C3B-C4B-NB	-2.63	108.07	110.52
14	2	506	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
17	Z	523	BCR	C11-C10-C9	-2.63	123.55	127.31
14	H	1225	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	2	822	SQD	O8-S-C6	2.63	109.94	105.74
14	r	506	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
17	H	4014	BCR	C34-C9-C8	2.63	122.22	118.08
14	f	1221	CLA	O2D-CGD-CBD	2.63	115.95	111.27
14	f	1229	CLA	C6-C7-C8	-2.63	107.41	115.92
17	6	522	BCR	C16-C17-C18	-2.63	123.55	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1229	CLA	C6-C7-C8	-2.63	107.41	115.92
14	B	1224	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
17	e	4008	BCR	C7-C8-C9	-2.63	122.26	126.23
14	4	517	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	t	517	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	n	1501	CLA	C3B-C4B-NB	-2.63	108.08	110.52
17	B	4014	BCR	C24-C23-C22	-2.63	122.26	126.23
17	F	4016	BCR	C33-C5-C6	-2.63	121.58	124.53
14	B	1238	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	u	501	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	G	1135	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	Z	517	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	f	1205	CLA	O2D-CGD-CBD	2.63	115.94	111.27
14	A	1113	CLA	C3B-C4B-NB	-2.63	108.08	110.52
14	b	517	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	b	521	BCR	C33-C5-C6	-2.63	121.58	124.53
14	f	1230	CLA	CAA-C2A-C1A	-2.63	103.36	111.97
14	v	505	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	r	513	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	e	1104	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
14	e	1101	CLA	CHB-C1B-NB	2.63	127.04	124.26
14	6	505	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	d	504	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	v	513	CLA	C3B-C4B-NB	-2.63	108.08	110.52
14	G	1125	CLA	CHB-C4A-NA	2.63	128.14	124.51
14	f	1231	CLA	CHB-C4A-NA	2.63	128.14	124.51
14	e	1117	CLA	C1-C2-C3	-2.63	121.50	126.04
14	G	1011	CLA	C4D-C3D-CAD	-2.63	105.00	108.10
14	H	1232	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	s	508	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	v	503	CLA	C3B-C4B-NB	-2.63	108.08	110.52
14	t	504	CLA	CHB-C4A-NA	2.63	128.14	124.51
14	H	1225	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	H	1221	CLA	O2D-CGD-CBD	2.63	115.93	111.27
17	d	522	BCR	C38-C26-C27	2.63	118.66	113.62
14	r	510	CLA	C3B-C4B-NB	-2.62	108.08	110.52
17	A	4008	BCR	C7-C8-C9	-2.62	122.27	126.23
14	B	1229	CLA	C6-C7-C8	-2.62	107.44	115.92
14	d	505	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
14	v	505	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
14	A	1117	CLA	C1-C2-C3	-2.62	121.51	126.04
14	e	1011	CLA	C4D-C3D-CAD	-2.62	105.01	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	s	518	CLA	C3B-C4B-NB	-2.62	108.08	110.52
14	Z	510	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
14	e	1237	CLA	C2B-C1B-NB	-2.62	108.47	110.23
14	H	1203	CLA	C1-C2-C3	-2.62	121.51	126.04
14	d	503	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	3	505	CLA	CHB-C4A-NA	2.62	128.13	124.51
14	r	510	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	H	1230	CLA	CAA-C2A-C1A	-2.62	103.39	111.97
14	q	511	CLA	C3B-C4B-NB	-2.62	108.08	110.52
17	4	521	BCR	C33-C5-C6	-2.62	121.59	124.53
14	Z	510	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	Z	506	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	c	501	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	u	518	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	5	512	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
14	G	1117	CLA	C1-C2-C3	-2.62	121.52	126.04
14	6	512	CLA	CHB-C1B-NB	2.62	127.03	124.26
14	3	503	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	d	518	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	e	1113	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	a	508	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	s	501	CLA	CHB-C4A-NA	2.62	128.13	124.51
14	3	508	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	6	513	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	d	517	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	A	1104	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
17	2	522	BCR	C20-C21-C22	-2.62	123.58	127.31
14	A	1101	CLA	CHB-C1B-NB	2.62	127.03	124.26
17	e	4007	BCR	C38-C26-C27	2.62	118.64	113.62
14	A	1104	CLA	CMB-C2B-C1B	-2.62	121.39	125.37
14	f	1235	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	e	1135	CLA	CHB-C4A-NA	2.61	128.13	124.51
14	H	1202	CLA	CMB-C2B-C3B	2.61	132.92	126.59
14	f	1238	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	e	1104	CLA	O2A-CGA-O1A	-2.61	116.99	123.59
21	r	822	SQD	O8-S-C6	2.61	109.91	105.74
14	Y	511	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	q	513	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	B	1205	CLA	O2D-CGD-CBD	2.61	115.91	111.27
14	1	511	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	f	1225	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	b	504	CLA	CHB-C4A-NA	2.61	128.13	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	s	517	CLA	CHB-C4A-NA	2.61	128.13	124.51
17	Z	523	BCR	C24-C23-C22	-2.61	122.29	126.23
14	B	1235	CLA	C3B-C4B-NB	-2.61	108.09	110.52
14	a	505	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	H	1222	CLA	CMB-C2B-C3B	2.61	132.91	126.59
17	A	4007	BCR	C38-C26-C27	2.61	118.63	113.62
14	5	501	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	a	501	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	a	517	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	G	1104	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
14	3	518	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
14	6	517	CLA	C3B-C4B-NB	-2.61	108.09	110.52
14	B	1202	CLA	CMB-C2B-C3B	2.61	132.91	126.59
14	v	510	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	a	518	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
14	f	1222	CLA	CMB-C2B-C3B	2.61	132.91	126.59
14	1	509	CLA	C3B-C4B-NB	-2.61	108.09	110.52
17	d	522	BCR	C16-C17-C18	-2.61	123.59	127.31
17	B	4014	BCR	C34-C9-C8	2.61	122.19	118.08
17	G	4007	BCR	C38-C26-C27	2.61	118.63	113.62
14	B	1222	CLA	CMB-C2B-C3B	2.61	132.91	126.59
14	c	512	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
14	u	512	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
17	o	4021	BCR	C33-C5-C6	-2.61	121.60	124.53
17	r	522	BCR	C20-C21-C22	-2.61	123.59	127.31
14	B	1225	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	Z	502	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	2	501	CLA	C3B-C4B-NB	-2.61	108.10	110.52
14	G	1113	CLA	C3B-C4B-NB	-2.61	108.10	110.52
14	v	504	CLA	C3B-C4B-NB	-2.61	108.10	110.52
14	1	513	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	r	502	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
17	G	4008	BCR	C7-C8-C9	-2.60	122.30	126.23
14	a	506	CLA	CHB-C4A-NA	2.60	128.11	124.51
17	u	523	BCR	C33-C5-C6	-2.60	121.60	124.53
17	f	4014	BCR	C34-C9-C8	2.60	122.18	118.08
14	3	506	CLA	CHB-C4A-NA	2.60	128.11	124.51
14	B	1203	CLA	C1-C2-C3	-2.60	121.54	126.04
14	2	502	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	2	504	CLA	C3B-C4B-NB	-2.60	108.10	110.52
17	s	521	BCR	C33-C5-C6	-2.60	121.61	124.53
14	H	1224	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	c	518	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	d	512	CLA	CHB-C1B-NB	2.60	127.01	124.26
14	5	518	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
17	T	4015	BCR	C38-C26-C25	-2.60	121.61	124.53
19	f	1843	LMU	C1B-O1B-C4'	-2.60	111.53	117.96
14	3	517	CLA	CHB-C4A-NA	2.60	128.11	124.51
14	6	504	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	V	1501	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	G	1137	CLA	CHB-C1B-NB	2.60	127.01	124.26
17	2	523	BCR	C24-C23-C22	-2.60	122.31	126.23
17	3	521	BCR	C33-C5-C6	-2.60	121.61	124.53
17	a	521	BCR	C33-C5-C6	-2.60	121.61	124.53
14	1	511	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	r	504	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	s	518	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
17	H	4006	BCR	C39-C30-C25	-2.60	106.08	110.30
17	5	523	BCR	C33-C5-C6	-2.60	121.61	124.53
14	u	518	CLA	CHB-C4A-NA	2.60	128.10	124.51
14	Z	501	CLA	C3B-C4B-NB	-2.60	108.11	110.52
17	3	524	BCR	C37-C22-C23	2.59	122.17	118.08
19	B	1843	LMU	C1B-O1B-C4'	-2.59	111.54	117.96
14	Y	513	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
17	a	521	BCR	C20-C19-C18	-2.59	119.13	126.42
14	H	1240	CLA	CHB-C4A-NA	2.59	128.10	124.51
14	G	1101	CLA	CHB-C1B-NB	2.59	127.00	124.26
14	G	1104	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
17	a	522	BCR	C20-C21-C22	-2.59	123.61	127.31
14	v	517	CLA	C3B-C4B-NB	-2.59	108.11	110.52
17	f	4014	BCR	C8-C7-C6	-2.59	119.92	127.20
17	3	521	BCR	C20-C19-C18	-2.59	119.14	126.42
14	A	1111	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	L	1501	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	3	501	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	f	1202	CLA	CMB-C2B-C3B	2.59	132.86	126.59
14	A	1011	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	6	518	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	G	1022	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
14	B	1240	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	H	1235	CLA	C3B-C4B-NB	-2.59	108.11	110.52
17	3	522	BCR	C20-C21-C22	-2.59	123.61	127.31
14	6	510	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
14	Z	512	CLA	O2D-CGD-O1D	-2.59	118.78	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	522	BCR	C1-C6-C5	-2.59	118.97	122.61
14	r	510	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	Y	509	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	H	1205	CLA	O2D-CGD-CBD	2.59	115.87	111.27
14	q	511	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
14	v	516	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	r	501	CLA	C3B-C4B-NB	-2.59	108.11	110.52
17	a	523	BCR	C33-C5-C4	2.59	118.58	113.62
14	c	518	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	A	1022	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
14	Y	511	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	e	1237	CLA	C6-C5-C3	2.58	120.23	113.45
14	H	1218	CLA	CHB-C4A-NA	2.58	128.09	124.51
14	f	1240	CLA	CHB-C4A-NA	2.58	128.09	124.51
14	q	516	CLA	CHB-C4A-NA	2.58	128.09	124.51
19	H	1843	LMU	C1B-O1B-C4'	-2.58	111.57	117.96
14	d	510	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
17	B	4017	BCR	C33-C5-C6	-2.58	121.63	124.53
17	U	4104	BCR	C30-C25-C26	-2.58	118.97	122.61
14	A	1237	CLA	C6-C5-C3	2.58	120.23	113.45
17	s	522	BCR	C20-C21-C22	-2.58	123.62	127.31
17	r	522	BCR	C38-C26-C25	-2.58	121.63	124.53
14	s	506	CLA	CHB-C4A-NA	2.58	128.08	124.51
17	d	523	BCR	C10-C11-C12	-2.58	115.16	123.22
14	5	518	CLA	CHB-C4A-NA	2.58	128.08	124.51
17	3	523	BCR	C33-C5-C4	2.58	118.58	113.62
17	s	523	BCR	C33-C5-C4	2.58	118.58	113.62
14	f	1203	CLA	C1-C2-C3	-2.58	121.58	126.04
14	G	1108	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	a	517	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	A	1138	CLA	CHB-C1B-NB	2.58	126.99	124.26
17	G	4003	BCR	C11-C10-C9	-2.58	123.63	127.31
17	s	524	BCR	C37-C22-C23	2.58	122.14	118.08
14	A	1127	CLA	CHB-C4A-NA	2.58	128.08	124.51
14	Y	516	CLA	CHB-C4A-NA	2.58	128.08	124.51
14	G	1237	CLA	C6-C5-C3	2.58	120.22	113.45
14	e	1138	CLA	CHB-C1B-NB	2.58	126.99	124.26
14	e	1111	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	s	503	CLA	C3B-C4B-NB	-2.58	108.12	110.52
17	6	522	BCR	C11-C12-C13	-2.58	119.17	126.42
14	e	1022	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
14	H	1201	CLA	CMB-C2B-C3B	2.58	132.84	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J	5105	LMU	C1'-C2'-C3'	2.58	115.37	110.00
17	B	4006	BCR	C39-C30-C25	-2.58	106.11	110.30
18	n	5221	LHG	C11-C10-C9	-2.58	101.33	114.42
14	b	516	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	H	1239	CLA	C11-C10-C8	-2.58	107.58	115.92
17	d	524	BCR	C21-C20-C19	-2.58	115.17	123.22
17	u	522	BCR	C1-C6-C5	-2.58	118.98	122.61
19	T	5105	LMU	C1'-C2'-C3'	2.58	115.36	110.00
18	e	5002	LHG	C11-C10-C9	-2.58	101.34	114.42
17	3	522	BCR	C38-C26-C27	2.58	118.57	113.62
17	2	522	BCR	C11-C12-C13	-2.58	119.18	126.42
14	e	1119	CLA	CHC-C1C-NC	2.58	128.11	124.20
18	L	5221	LHG	C11-C10-C9	-2.58	101.34	114.42
17	r	523	BCR	C24-C23-C22	-2.58	122.34	126.23
14	r	512	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
17	s	522	BCR	C38-C26-C27	2.58	118.56	113.62
14	B	1239	CLA	C11-C10-C8	-2.58	107.59	115.92
17	B	4014	BCR	C8-C7-C6	-2.58	119.97	127.20
19	l	5105	LMU	C1'-C2'-C3'	2.58	115.36	110.00
14	d	516	CLA	CHB-C4A-NA	2.58	128.07	124.51
17	Z	522	BCR	C11-C12-C13	-2.58	119.18	126.42
18	V	5221	LHG	C11-C10-C9	-2.58	101.35	114.42
17	s	521	BCR	C29-C30-C25	2.58	114.45	110.48
14	Z	518	CLA	C3B-C4B-NB	-2.58	108.13	110.52
14	v	518	CLA	C3B-C4B-NB	-2.58	108.13	110.52
14	6	516	CLA	CHB-C4A-NA	2.58	128.07	124.51
17	t	524	BCR	C8-C7-C6	-2.57	119.97	127.20
14	H	1021	CLA	CHC-C4B-NB	2.57	126.98	124.26
14	f	1239	CLA	C11-C10-C8	-2.57	107.60	115.92
14	1	518	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
17	d	522	BCR	C11-C12-C13	-2.57	119.19	126.42
17	q	524	BCR	C1-C6-C5	-2.57	118.99	122.61
14	e	1011	CLA	C3B-C4B-NB	-2.57	108.13	110.52
14	2	510	CLA	CHB-C4A-NA	2.57	128.07	124.51
17	v	523	BCR	C33-C5-C6	-2.57	121.64	124.53
14	e	1127	CLA	CHB-C4A-NA	2.57	128.07	124.51
14	f	1218	CLA	CHB-C4A-NA	2.57	128.07	124.51
14	t	516	CLA	C3B-C4B-NB	-2.57	108.13	110.52
17	6	523	BCR	C10-C11-C12	-2.57	115.19	123.22
17	c	523	BCR	C33-C5-C6	-2.57	121.64	124.53
17	s	521	BCR	C20-C19-C18	-2.57	119.19	126.42
17	1	524	BCR	C1-C6-C5	-2.57	118.99	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	d	504	CLA	C3B-C4B-NB	-2.57	108.13	110.52
17	6	524	BCR	C21-C20-C19	-2.57	115.19	123.22
17	F	4016	BCR	C21-C20-C19	-2.57	115.20	123.22
17	v	523	BCR	C10-C11-C12	-2.57	115.20	123.22
14	Y	518	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	e	1022	CLA	C2D-C1D-ND	-2.57	108.21	110.10
14	H	1207	CLA	CHB-C4A-NA	2.57	128.06	124.51
14	G	1138	CLA	CHB-C1B-NB	2.57	126.98	124.26
14	2	512	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
17	r	522	BCR	C11-C12-C13	-2.57	119.20	126.42
17	v	522	BCR	C11-C12-C13	-2.57	119.20	126.42
17	R	4016	BCR	C21-C20-C19	-2.57	115.20	123.22
17	M	4021	BCR	C33-C5-C6	-2.57	121.64	124.53
17	H	4017	BCR	C33-C5-C6	-2.57	121.64	124.53
14	B	1201	CLA	CMB-C2B-C3B	2.57	132.81	126.59
17	e	4003	BCR	C11-C10-C9	-2.57	123.64	127.31
14	f	1204	CLA	CHB-C4A-NA	2.57	128.06	124.51
17	j	4016	BCR	C21-C20-C19	-2.57	115.20	123.22
14	q	518	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	B	1224	CLA	CHB-C4A-NA	2.57	128.06	124.51
14	f	1205	CLA	C1-C2-C3	-2.57	121.60	126.04
14	t	518	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
18	A	5002	LHG	C11-C10-C9	-2.57	101.39	114.42
17	a	524	BCR	C37-C22-C23	2.57	122.12	118.08
17	A	4003	BCR	C11-C10-C9	-2.57	123.65	127.31
14	4	516	CLA	C3B-C4B-NB	-2.57	108.14	110.52
14	e	1105	CLA	C3B-C4B-NB	-2.57	108.14	110.52
14	q	509	CLA	C3B-C4B-NB	-2.57	108.14	110.52
17	H	4014	BCR	C8-C7-C6	-2.57	120.00	127.20
17	c	522	BCR	C1-C6-C5	-2.56	119.00	122.61
17	4	524	BCR	C8-C7-C6	-2.56	120.00	127.20
14	G	1137	CLA	CAA-CBA-CGA	-2.56	105.76	113.25
14	f	1232	CLA	CHB-C4A-NA	2.56	128.06	124.51
14	6	511	CLA	C3B-C4B-NB	-2.56	108.14	110.52
17	H	4009	BCR	C29-C30-C25	2.56	114.43	110.48
17	f	4006	BCR	C39-C30-C25	-2.56	106.14	110.30
14	f	1224	CLA	CHB-C4A-NA	2.56	128.06	124.51
18	G	5002	LHG	C11-C10-C9	-2.56	101.42	114.42
17	Y	524	BCR	C1-C6-C5	-2.56	119.00	122.61
14	e	1137	CLA	CAA-CBA-CGA	-2.56	105.77	113.25
17	3	521	BCR	C29-C30-C25	2.56	114.42	110.48
14	1	516	CLA	CHB-C4A-NA	2.56	128.05	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	v	524	BCR	C21-C20-C19	-2.56	115.22	123.22
22	X	170	FMN	C4A-C10-N10	2.56	120.22	116.48
17	m	4104	BCR	C30-C25-C26	-2.56	119.01	122.61
17	2	522	BCR	C38-C26-C25	-2.56	121.65	124.53
17	f	4017	BCR	C33-C5-C6	-2.56	121.65	124.53
17	b	524	BCR	C8-C7-C6	-2.56	120.01	127.20
14	f	1201	CLA	CMB-C2B-C3B	2.56	132.79	126.59
14	A	1137	CLA	CAA-CBA-CGA	-2.56	105.77	113.25
14	b	518	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
17	v	524	BCR	C37-C22-C23	2.56	122.11	118.08
17	H	4014	BCR	C24-C25-C26	2.56	127.66	121.46
14	G	1011	CLA	C3B-C4B-NB	-2.56	108.14	110.52
14	F	1302	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
14	A	1137	CLA	CHB-C1B-NB	2.56	126.97	124.26
14	G	1123	CLA	C2A-C1A-CHA	2.56	128.34	123.86
14	G	1132	CLA	CHB-C4A-NA	2.56	128.05	124.51
14	Z	504	CLA	C3B-C4B-NB	-2.56	108.14	110.52
17	f	4009	BCR	C29-C30-C25	2.56	114.42	110.48
22	P	170	FMN	C4A-C10-N10	2.56	120.22	116.48
14	e	1138	CLA	O2D-CGD-CBD	2.56	115.81	111.27
14	H	1236	CLA	C1-C2-C3	-2.56	122.61	126.75
17	K	4104	BCR	C30-C25-C26	-2.56	119.01	122.61
14	Z	509	CLA	C3B-C4B-NB	-2.56	108.14	110.52
14	4	518	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
14	A	1138	CLA	O2D-CGD-CBD	2.56	115.81	111.27
17	f	4014	BCR	C24-C25-C26	2.56	127.66	121.46
14	G	1124	CLA	C2D-C1D-ND	-2.56	108.22	110.10
14	K	1105	CLA	CMC-C2C-C3C	2.56	133.06	126.12
14	e	1102	CLA	CHB-C1B-NB	2.56	126.96	124.26
14	G	1116	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
14	A	1108	CLA	C3B-C4B-NB	-2.56	108.14	110.52
14	f	1222	CLA	CHB-C4A-NA	2.56	128.05	124.51
17	5	524	BCR	C8-C7-C6	-2.56	120.03	127.20
22	p	170	FMN	C4A-C10-N10	2.56	120.22	116.48
17	c	524	BCR	C8-C7-C6	-2.56	120.03	127.20
14	H	1232	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	e	4008	BCR	C34-C9-C8	2.55	122.10	118.08
14	e	1237	CLA	CHC-C4B-NB	2.55	126.96	124.26
14	A	1132	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	G	1127	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	A	1123	CLA	C2A-C1A-CHA	2.55	128.32	123.86
17	6	523	BCR	C33-C5-C6	-2.55	121.66	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1218	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
14	b	512	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
14	d	509	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
14	e	1237	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	e	1108	CLA	C3B-C4B-NB	-2.55	108.15	110.52
14	v	511	CLA	C3B-C4B-NB	-2.55	108.15	110.52
14	1	506	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	a	521	BCR	C29-C30-C25	2.55	114.41	110.48
14	b	513	CLA	C3B-C4B-NB	-2.55	108.15	110.52
14	q	501	CLA	C3B-C4B-NB	-2.55	108.15	110.52
14	U	1105	CLA	CMC-C2C-C3C	2.55	133.04	126.12
14	a	518	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
21	V	5216	SQD	O48-C23-C24	2.55	119.91	111.91
14	s	501	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
14	v	510	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	d	523	BCR	C33-C5-C6	-2.55	121.66	124.53
17	u	523	BCR	C21-C20-C19	-2.55	115.26	123.22
14	4	512	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	W	4021	BCR	C38-C26-C27	2.55	118.51	113.62
14	m	1105	CLA	CMC-C2C-C3C	2.55	133.04	126.12
14	e	1133	CLA	CHC-C4B-NB	2.55	126.95	124.26
14	e	1123	CLA	C2A-C1A-CHA	2.55	128.31	123.86
14	f	1229	CLA	C3B-C4B-NB	-2.55	108.15	110.52
17	a	522	BCR	C38-C26-C27	2.55	118.51	113.62
14	H	1229	CLA	C3B-C4B-NB	-2.55	108.15	110.52
17	B	4009	BCR	C29-C30-C25	2.55	114.40	110.48
14	B	1207	CLA	CHB-C4A-NA	2.55	128.03	124.51
14	H	1205	CLA	C1-C2-C3	-2.55	121.64	126.04
21	a	822	SQD	C4-C3-C2	2.55	115.27	110.82
14	A	1237	CLA	CHC-C4B-NB	2.55	126.95	124.26
14	B	1218	CLA	CHB-C4A-NA	2.55	128.03	124.51
17	6	524	BCR	C37-C22-C23	2.55	122.09	118.08
14	e	1124	CLA	C2D-C1D-ND	-2.55	108.23	110.10
14	s	518	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
17	B	4014	BCR	C24-C25-C26	2.55	127.63	121.46
17	W	4021	BCR	C33-C5-C6	-2.55	121.67	124.53
17	5	523	BCR	C21-C20-C19	-2.54	115.28	123.22
14	B	1232	CLA	CHB-C4A-NA	2.54	128.03	124.51
17	B	4009	BCR	C16-C15-C14	-2.54	118.26	123.47
17	u	524	BCR	C8-C7-C6	-2.54	120.06	127.20
21	L	5216	SQD	C45-O47-C7	2.54	124.05	117.79
14	3	518	CLA	O2D-CGD-O1D	-2.54	118.86	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	o	4021	BCR	C38-C26-C27	2.54	118.50	113.62
17	H	4009	BCR	C16-C15-C14	-2.54	118.26	123.47
14	H	1204	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	A	1119	CLA	CHC-C1C-NC	2.54	128.06	124.20
14	B	1225	CLA	CHB-C1B-NB	2.54	126.95	124.26
14	f	1225	CLA	CHB-C1B-NB	2.54	126.95	124.26
17	G	4008	BCR	C34-C9-C8	2.54	122.08	118.08
14	t	512	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	F	1301	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	Z	510	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	G	1119	CLA	CHC-C1C-NC	2.54	128.06	124.20
14	A	1022	CLA	C2D-C1D-ND	-2.54	108.23	110.10
14	B	1205	CLA	C1-C2-C3	-2.54	121.65	126.04
14	R	1301	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	j	1301	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	3	822	SQD	C4-C3-C2	2.54	115.26	110.82
14	f	1218	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	Z	522	BCR	C38-C26-C25	-2.54	121.67	124.53
14	f	1207	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	L	5216	SQD	O48-C23-C24	2.54	119.88	111.91
17	b	522	BCR	C23-C24-C25	-2.54	120.07	127.20
14	A	1116	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	L	4022	BCR	C33-C5-C6	-2.54	121.68	124.53
14	5	511	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
14	Y	506	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	G	1237	CLA	CHC-C4B-NB	2.54	126.94	124.26
21	n	5216	SQD	C45-O47-C7	2.54	124.04	117.79
14	6	509	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	L	4022	BCR	C21-C20-C19	-2.54	115.30	123.22
14	H	1219	CLA	C3B-C4B-NB	-2.54	108.16	110.52
14	B	1204	CLA	CHB-C4A-NA	2.54	128.02	124.51
14	H	1224	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	s	822	SQD	C4-C3-C2	2.54	115.25	110.82
14	e	1137	CLA	CHB-C1B-NB	2.54	126.94	124.26
17	4	522	BCR	C23-C24-C25	-2.54	120.07	127.20
17	L	4020	BCR	C8-C9-C10	-2.54	115.05	118.94
17	c	523	BCR	C21-C20-C19	-2.54	115.30	123.22
14	B	1222	CLA	CHB-C4A-NA	2.54	128.02	124.51
14	G	1801	CLA	CHB-C4A-NA	2.54	128.02	124.51
17	A	4008	BCR	C34-C9-C8	2.54	122.08	118.08
14	Z	511	CLA	C3B-C4B-NB	-2.54	108.16	110.52
14	j	1302	CLA	O2D-CGD-O1D	-2.54	118.88	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	4003	BCR	C21-C20-C19	-2.54	115.30	123.22
17	f	4009	BCR	C16-C15-C14	-2.54	118.28	123.47
14	G	1138	CLA	O2D-CGD-CBD	2.54	115.78	111.27
17	G	4008	BCR	C38-C26-C27	2.54	118.49	113.62
17	t	522	BCR	C23-C24-C25	-2.54	120.08	127.20
14	2	511	CLA	C3B-C4B-NB	-2.54	108.16	110.52
14	c	519	CLA	C3B-C4B-NB	-2.54	108.16	110.52
14	u	508	CLA	CHB-C1B-NB	2.54	126.94	124.26
21	V	5216	SQD	C45-O47-C7	2.54	124.03	117.79
14	H	1218	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	c	509	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
17	e	4002	BCR	C23-C24-C25	-2.54	120.08	127.20
17	u	522	BCR	C21-C20-C19	-2.54	115.31	123.22
14	Y	502	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
14	B	1210	CLA	C1-C2-C3	-2.53	121.66	126.04
14	f	1236	CLA	C1-C2-C3	-2.53	122.65	126.75
14	q	502	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
17	c	522	BCR	C21-C20-C19	-2.53	115.31	123.22
17	Y	522	BCR	C20-C21-C22	-2.53	123.69	127.31
14	B	1229	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	d	511	CLA	C3B-C4B-NB	-2.53	108.17	110.52
17	2	524	BCR	C37-C22-C23	2.53	122.07	118.08
14	3	501	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	G	1022	CLA	C2D-C1D-ND	-2.53	108.24	110.10
14	B	1236	CLA	C1-C2-C3	-2.53	122.66	126.75
21	n	5216	SQD	O48-C23-C24	2.53	119.85	111.91
17	Z	524	BCR	C37-C22-C23	2.53	122.07	118.08
17	d	523	BCR	C11-C10-C9	-2.53	123.70	127.31
17	G	4002	BCR	C23-C24-C25	-2.53	120.09	127.20
14	f	1238	CLA	CHB-C1B-NB	2.53	126.94	124.26
18	A	5006	LHG	O8-C23-C24	2.53	119.85	111.91
14	3	517	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	s	517	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	t	511	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	G	5001	LHG	O8-C23-C24	2.53	119.85	111.91
14	u	511	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
14	6	510	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	H	1222	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	5	522	BCR	C21-C20-C19	-2.53	115.32	123.22
14	H	1210	CLA	C1-C2-C3	-2.53	121.67	126.04
17	A	4002	BCR	C23-C24-C25	-2.53	120.10	127.20
14	A	1121	CLA	O2D-CGD-CBD	2.53	115.76	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	r	522	BCR	C33-C5-C6	-2.53	121.69	124.53
14	1	501	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	b	517	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	1	502	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	A	1102	CLA	CHB-C1B-NB	2.53	126.94	124.26
14	e	1121	CLA	O2D-CGD-CBD	2.53	115.76	111.27
17	r	522	BCR	C38-C26-C27	2.53	118.47	113.62
17	n	4020	BCR	C8-C9-C10	-2.53	115.06	118.94
14	f	1219	CLA	C3B-C4B-NB	-2.53	108.17	110.52
17	M	4021	BCR	C38-C26-C27	2.53	118.47	113.62
14	f	1023	CLA	CAA-CBA-CGA	-2.53	105.86	113.25
14	R	1302	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	A	1237	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	K	1401	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	e	1132	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	A	1124	CLA	C2D-C1D-ND	-2.53	108.24	110.10
14	A	1128	CLA	CMB-C2B-C3B	2.53	132.71	126.59
14	H	1023	CLA	CAA-CBA-CGA	-2.53	105.87	113.25
17	m	4104	BCR	C15-C16-C17	-2.53	118.30	123.47
14	4	517	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	B	1231	CLA	CMB-C2B-C3B	2.53	132.71	126.59
14	H	1225	CLA	CMB-C2B-C3B	2.53	132.71	126.59
14	m	1401	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	G	1134	CLA	O2D-CGD-CBD	2.53	115.76	111.27
17	A	4003	BCR	C21-C20-C19	-2.53	115.33	123.22
14	e	1116	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
14	d	509	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
14	H	1231	CLA	CMB-C2B-C3B	2.53	132.71	126.59
17	d	524	BCR	C37-C22-C23	2.53	122.06	118.08
14	f	1231	CLA	CMB-C2B-C3B	2.53	132.71	126.59
14	A	1134	CLA	O2D-CGD-CBD	2.53	115.76	111.27
17	n	4022	BCR	C21-C20-C19	-2.53	115.34	123.22
17	B	4006	BCR	C1-C6-C5	-2.53	119.06	122.61
14	e	1128	CLA	CMB-C2B-C3B	2.52	132.70	126.59
17	q	522	BCR	C20-C21-C22	-2.52	123.71	127.31
14	G	1105	CLA	C3B-C4B-NB	-2.52	108.17	110.52
17	V	4022	BCR	C21-C20-C19	-2.52	115.34	123.22
18	G	5006	LHG	O8-C23-C24	2.52	119.83	111.91
14	G	1105	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
14	t	511	CLA	CHB-C1B-NB	2.52	126.93	124.26
18	e	5001	LHG	O8-C23-C24	2.52	119.83	111.91
14	B	1219	CLA	C3B-C4B-NB	-2.52	108.17	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	511	CLA	C3B-C4B-NB	-2.52	108.17	110.52
17	1	522	BCR	C20-C21-C22	-2.52	123.71	127.31
14	A	1116	CLA	CHB-C1B-NB	2.52	126.93	124.26
14	q	506	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	e	1108	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	B	5002	LMG	O1-C1-C2	-2.52	104.36	108.30
14	5	508	CLA	CHB-C1B-NB	2.52	126.93	124.26
14	u	509	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	q	512	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	H	1225	CLA	CHB-C1B-NB	2.52	126.93	124.26
17	H	4006	BCR	C1-C6-C5	-2.52	119.06	122.61
14	c	511	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
17	e	4008	BCR	C38-C26-C27	2.52	118.46	113.62
14	f	1203	CLA	C11-C12-C13	-2.52	107.77	115.92
20	f	5002	LMG	O1-C1-C2	-2.52	104.37	108.30
14	B	1023	CLA	CAA-CBA-CGA	-2.52	105.89	113.25
14	f	1234	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	e	1116	CLA	CHB-C1B-NB	2.52	126.92	124.26
14	A	1105	CLA	C3B-C4B-NB	-2.52	108.18	110.52
17	V	4022	BCR	C33-C5-C6	-2.52	121.70	124.53
17	T	4015	BCR	C21-C20-C19	-2.52	115.35	123.22
17	n	4022	BCR	C33-C5-C6	-2.52	121.70	124.53
21	v	822	SQD	C45-O47-C7	2.52	122.59	117.90
17	G	4003	BCR	C21-C20-C19	-2.52	115.36	123.22
18	A	5001	LHG	O8-C23-C24	2.52	119.81	111.91
14	2	518	CLA	C3B-C4B-NB	-2.52	108.18	110.52
14	5	509	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
17	L	4219	BCR	C39-C30-C25	-2.52	106.22	110.30
14	H	1211	CLA	CMB-C2B-C3B	2.52	132.69	126.59
14	Y	512	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
21	d	822	SQD	C45-O47-C7	2.52	122.59	117.90
14	e	1134	CLA	O2D-CGD-CBD	2.52	115.74	111.27
14	f	1210	CLA	C1-C2-C3	-2.52	121.69	126.04
17	U	4104	BCR	C15-C16-C17	-2.52	118.32	123.47
17	f	4006	BCR	C1-C6-C5	-2.52	119.07	122.61
14	G	1116	CLA	CHB-C1B-NB	2.52	126.92	124.26
14	4	513	CLA	C3B-C4B-NB	-2.52	108.18	110.52
17	A	4008	BCR	C38-C26-C27	2.51	118.45	113.62
14	B	1210	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	e	5006	LHG	O8-C23-C24	2.51	119.80	111.91
14	v	509	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
14	r	511	CLA	C3B-C4B-NB	-2.51	108.18	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	q	519	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	e	1105	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
17	V	4020	BCR	C8-C9-C10	-2.51	115.08	118.94
14	1	512	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
17	J	4015	BCR	C21-C20-C19	-2.51	115.37	123.22
14	A	1801	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	6	822	SQD	C45-O47-C7	2.51	122.58	117.90
14	A	1105	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
17	2	522	BCR	C38-C26-C27	2.51	118.44	113.62
14	2	518	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
14	B	1234	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	G	1237	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	d	510	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	G	1121	CLA	O2D-CGD-CBD	2.51	115.73	111.27
17	n	4020	BCR	C28-C27-C26	-2.51	109.59	114.08
17	J	4013	BCR	C32-C1-C6	-2.51	106.22	110.30
14	c	508	CLA	CHB-C1B-NB	2.51	126.92	124.26
14	4	510	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	6	509	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
14	v	509	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
17	Y	523	BCR	C34-C9-C8	2.51	122.03	118.08
17	v	523	BCR	C11-C10-C9	-2.51	123.73	127.31
14	d	516	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	A	1126	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	e	5005	LHG	O8-C23-C24	2.51	119.78	111.91
14	B	1211	CLA	CMB-C2B-C3B	2.51	132.67	126.59
14	e	1126	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	f	1211	CLA	CMB-C2B-C3B	2.51	132.66	126.59
14	a	501	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
14	r	518	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	H	1238	CLA	CHB-C1B-NB	2.51	126.91	124.26
14	G	1108	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	H	1203	CLA	C11-C12-C13	-2.51	107.81	115.92
14	A	1134	CLA	C2A-C1A-CHA	2.51	128.24	123.86
17	1	523	BCR	C34-C9-C8	2.51	122.03	118.08
17	K	4104	BCR	C15-C16-C17	-2.51	118.34	123.47
14	G	1128	CLA	CMB-C2B-C3B	2.51	132.66	126.59
14	B	1238	CLA	CHB-C1B-NB	2.51	126.91	124.26
14	H	1234	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	B	1225	CLA	CMB-C2B-C3B	2.51	132.66	126.59
17	B	4014	BCR	C35-C13-C12	2.51	122.03	118.08
14	5	519	CLA	C3B-C4B-NB	-2.51	108.19	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	517	CLA	C3B-C4B-NB	-2.51	108.19	110.52
20	H	5002	LMG	O1-C1-C2	-2.51	104.39	108.30
17	T	4013	BCR	C32-C1-C6	-2.50	106.24	110.30
14	G	1134	CLA	C2A-C1A-CHA	2.50	128.24	123.86
14	G	1133	CLA	CHC-C4B-NB	2.50	126.91	124.26
18	A	5005	LHG	O8-C23-C24	2.50	119.77	111.91
14	f	1215	CLA	CMB-C2B-C3B	2.50	132.65	126.59
14	B	1203	CLA	C11-C12-C13	-2.50	107.83	115.92
17	f	4009	BCR	C8-C7-C6	-2.50	120.17	127.20
14	4	511	CLA	CHB-C1B-NB	2.50	126.91	124.26
14	u	519	CLA	C3B-C4B-NB	-2.50	108.19	110.52
14	A	1108	CLA	CHB-C4A-NA	2.50	127.97	124.51
14	f	1225	CLA	CMB-C2B-C3B	2.50	132.65	126.59
14	Y	501	CLA	C3B-C4B-NB	-2.50	108.19	110.52
14	t	509	CLA	C3B-C4B-NB	-2.50	108.19	110.52
14	f	1219	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
17	q	523	BCR	C34-C9-C8	2.50	122.02	118.08
17	Z	522	BCR	C38-C26-C27	2.50	118.42	113.62
14	B	1219	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
14	B	1021	CLA	CHC-C4B-NB	2.50	126.90	124.26
17	l	4013	BCR	C32-C1-C6	-2.50	106.24	110.30
14	4	511	CLA	C3B-C4B-NB	-2.50	108.20	110.52
14	b	511	CLA	CHB-C1B-NB	2.50	126.90	124.26
14	H	1215	CLA	CMB-C2B-C3B	2.50	132.64	126.59
14	a	503	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	H	1219	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
14	G	1110	CLA	C3B-C4B-NB	-2.50	108.20	110.52
14	t	510	CLA	C3B-C4B-NB	-2.50	108.20	110.52
14	B	1206	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
17	6	523	BCR	C11-C10-C9	-2.50	123.75	127.31
14	1	519	CLA	CHB-C4A-NA	2.50	127.97	124.51
14	2	505	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	e	1134	CLA	C2A-C1A-CHA	2.50	128.23	123.86
14	A	1123	CLA	CMB-C2B-C3B	2.50	132.64	126.59
18	A	5009	LHG	C11-C10-C9	-2.50	101.75	114.42
17	l	4015	BCR	C21-C20-C19	-2.50	115.42	123.22
14	d	509	CLA	C3B-C4B-NB	-2.50	108.20	110.52
17	V	4219	BCR	C39-C30-C25	-2.50	106.25	110.30
17	B	4009	BCR	C8-C7-C6	-2.50	120.19	127.20
17	2	523	BCR	C10-C11-C12	-2.50	115.43	123.22
14	f	1206	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
14	e	1123	CLA	CMB-C2B-C3B	2.50	132.63	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	q	524	BCR	C24-C23-C22	-2.49	122.47	126.23
18	G	5009	LHG	C11-C10-C9	-2.49	101.76	114.42
18	e	5009	LHG	C11-C10-C9	-2.49	101.76	114.42
14	V	1502	CLA	CHB-C1B-NB	2.49	126.90	124.26
18	G	5005	LHG	O8-C23-C24	2.49	119.74	111.91
17	n	4219	BCR	C39-C30-C25	-2.49	106.25	110.30
17	r	524	BCR	C37-C22-C23	2.49	122.01	118.08
14	A	1129	CLA	CHC-C4B-NB	2.49	126.90	124.26
14	e	1801	CLA	CHB-C4A-NA	2.49	127.96	124.51
17	2	522	BCR	C33-C5-C6	-2.49	121.73	124.53
14	q	504	CLA	C3B-C4B-NB	-2.49	108.20	110.52
17	Z	523	BCR	C10-C11-C12	-2.49	115.44	123.22
14	G	1123	CLA	CMB-C2B-C3B	2.49	132.62	126.59
17	L	4020	BCR	C28-C27-C26	-2.49	109.63	114.08
17	d	524	BCR	C20-C21-C22	-2.49	123.75	127.31
17	I	4018	BCR	C33-C5-C4	2.49	118.40	113.62
17	f	4006	BCR	C15-C16-C17	-2.49	118.37	123.47
14	G	1126	CLA	CHB-C4A-NA	2.49	127.96	124.51
14	Y	506	CLA	C3B-C4B-NB	-2.49	108.20	110.52
14	v	509	CLA	C3B-C4B-NB	-2.49	108.20	110.52
14	G	1102	CLA	CHB-C1B-NB	2.49	126.89	124.26
17	r	523	BCR	C10-C11-C12	-2.49	115.45	123.22
14	3	503	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	H	1210	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	3	501	CLA	C3B-C4B-NB	-2.49	108.21	110.52
14	6	516	CLA	C3B-C4B-NB	-2.49	108.21	110.52
14	e	1135	CLA	C2D-C1D-ND	-2.49	108.27	110.10
14	B	1228	CLA	C1-C2-C3	-2.49	121.74	126.04
17	s	521	BCR	C7-C8-C9	-2.49	122.47	126.23
14	s	503	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	e	5003	LHG	C20-C19-C18	-2.49	101.80	114.42
14	B	1215	CLA	CMB-C2B-C3B	2.49	132.61	126.59
14	U	1401	CLA	CHB-C4A-NA	2.49	127.95	124.51
14	u	503	CLA	C3B-C4B-NB	-2.49	108.21	110.52
14	v	516	CLA	C3B-C4B-NB	-2.49	108.21	110.52
17	e	4001	BCR	C21-C20-C19	-2.49	115.46	123.22
14	Z	518	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
14	H	1210	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	f	4014	BCR	C35-C13-C12	2.49	121.99	118.08
17	H	4009	BCR	C8-C7-C6	-2.49	120.22	127.20
18	G	5003	LHG	C20-C19-C18	-2.49	101.81	114.42
14	3	502	CLA	O2D-CGD-O1D	-2.48	118.98	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1210	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
14	r	518	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
17	r	524	BCR	C21-C20-C19	-2.48	115.46	123.22
14	2	509	CLA	C3B-C4B-NB	-2.48	108.21	110.52
14	A	1133	CLA	CHC-C4B-NB	2.48	126.89	124.26
14	B	1210	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
18	A	5003	LHG	C20-C19-C18	-2.48	101.81	114.42
14	l	1303	CLA	O2D-CGD-CBD	2.48	115.68	111.27
17	G	4001	BCR	C21-C20-C19	-2.48	115.47	123.22
17	G	4007	BCR	C10-C11-C12	-2.48	115.47	123.22
17	k	4018	BCR	C33-C5-C4	2.48	118.39	113.62
14	f	1208	CLA	C3B-C4B-NB	-2.48	108.21	110.52
14	t	513	CLA	C3B-C4B-NB	-2.48	108.21	110.52
17	A	4007	BCR	C10-C11-C12	-2.48	115.47	123.22
17	q	524	BCR	C37-C22-C23	2.48	121.99	118.08
14	t	509	CLA	O2A-CGA-O1A	-2.48	117.11	123.30
14	Z	505	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
14	r	505	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
17	V	4020	BCR	C28-C27-C26	-2.48	109.64	114.08
14	T	1303	CLA	O2D-CGD-CBD	2.48	115.68	111.27
14	H	1234	CLA	CAC-C3C-C4C	2.48	128.03	124.81
17	A	4001	BCR	C21-C20-C19	-2.48	115.47	123.22
17	S	4018	BCR	C30-C25-C26	-2.48	119.12	122.61
17	r	523	BCR	C33-C5-C6	-2.48	121.74	124.53
17	Z	524	BCR	C21-C20-C19	-2.48	115.48	123.22
14	b	509	CLA	C3B-C4B-NB	-2.48	108.21	110.52
14	f	1021	CLA	CHC-C4B-NB	2.48	126.88	124.26
14	J	1303	CLA	O2D-CGD-CBD	2.48	115.67	111.27
17	v	524	BCR	C20-C21-C22	-2.48	123.77	127.31
17	e	4007	BCR	C10-C11-C12	-2.48	115.48	123.22
17	t	523	BCR	C34-C9-C8	2.48	121.98	118.08
17	2	524	BCR	C21-C20-C19	-2.48	115.48	123.22
14	v	508	CLA	CHB-C1B-NB	2.48	126.88	124.26
14	H	1230	CLA	C3B-C4B-NB	-2.48	108.22	110.52
14	q	506	CLA	C3B-C4B-NB	-2.48	108.22	110.52
14	s	501	CLA	C3B-C4B-NB	-2.48	108.22	110.52
14	4	509	CLA	O2A-CGA-O1A	-2.48	117.13	123.30
17	S	4018	BCR	C33-C5-C4	2.48	118.37	113.62
17	f	4006	BCR	C33-C5-C4	2.47	118.37	113.62
17	Y	524	BCR	C37-C22-C23	2.47	121.98	118.08
21	f	1852	SQD	O47-C7-C8	2.47	116.83	111.50
17	6	524	BCR	C20-C21-C22	-2.47	123.78	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1228	CLA	C1-C2-C3	-2.47	121.76	126.04
14	s	502	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
17	A	4003	BCR	C24-C23-C22	-2.47	122.50	126.23
18	e	5001	LHG	C11-C10-C9	-2.47	101.87	114.42
17	A	4003	BCR	C38-C26-C25	-2.47	121.75	124.53
14	1	506	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	6	509	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	c	506	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	f	1210	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	Y	524	BCR	C24-C23-C22	-2.47	122.50	126.23
17	H	4014	BCR	C35-C13-C12	2.47	121.97	118.08
14	e	1129	CLA	CHC-C4B-NB	2.47	126.87	124.26
17	B	4006	BCR	C15-C16-C17	-2.47	118.41	123.47
14	b	510	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	s	512	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
17	G	4002	BCR	C10-C11-C12	-2.47	115.51	123.22
14	A	1110	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	5	506	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	d	501	CLA	C3B-C4B-NB	-2.47	108.22	110.52
17	B	4006	BCR	C33-C5-C4	2.47	118.36	113.62
14	3	506	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
17	Y	521	BCR	C33-C5-C6	-2.47	121.75	124.53
17	A	4002	BCR	C10-C11-C12	-2.47	115.51	123.22
18	A	5001	LHG	C11-C10-C9	-2.47	101.89	114.42
17	4	523	BCR	C34-C9-C8	2.47	121.97	118.08
17	3	521	BCR	C7-C8-C9	-2.47	122.50	126.23
14	B	1230	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	A	1121	CLA	CHC-C4B-NB	2.47	126.87	124.26
14	u	517	CLA	CHB-C4A-NA	2.47	127.92	124.51
14	H	1206	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
17	A	4008	BCR	C16-C15-C14	-2.47	118.42	123.47
14	5	503	CLA	C3B-C4B-NB	-2.47	108.23	110.52
17	u	521	BCR	C7-C8-C9	-2.47	122.51	126.23
17	G	4008	BCR	C16-C15-C14	-2.47	118.42	123.47
14	G	1121	CLA	CHC-C4B-NB	2.47	126.87	124.26
14	a	513	CLA	C3B-C4B-NB	-2.47	108.23	110.52
14	G	1105	CLA	CHD-C1D-ND	-2.47	122.19	124.45
14	6	501	CLA	C3B-C4B-NB	-2.47	108.23	110.52
17	H	4006	BCR	C33-C5-C4	2.46	118.35	113.62
14	B	1213	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
17	Z	522	BCR	C33-C5-C6	-2.46	121.76	124.53
14	b	509	CLA	O2A-CGA-O1A	-2.46	117.16	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	e	5009	LHG	C27-C26-C25	-2.46	101.92	114.42
17	e	4008	BCR	C16-C15-C14	-2.46	118.43	123.47
14	Y	519	CLA	CHB-C4A-NA	2.46	127.92	124.51
14	H	1228	CLA	C1-C2-C3	-2.46	121.78	126.04
14	L	1502	CLA	CHB-C1B-NB	2.46	126.86	124.26
17	c	522	BCR	C11-C12-C13	-2.46	119.50	126.42
14	e	1116	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	e	5001	LHG	O8-C23-O10	-2.46	117.38	123.59
17	I	4018	BCR	C30-C25-C26	-2.46	119.14	122.61
18	G	5001	LHG	C11-C10-C9	-2.46	101.92	114.42
17	5	522	BCR	C11-C12-C13	-2.46	119.50	126.42
18	G	5001	LHG	O8-C23-O10	-2.46	117.38	123.59
14	a	501	CLA	C3B-C4B-NB	-2.46	108.23	110.52
14	H	1213	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
17	d	522	BCR	C33-C5-C6	-2.46	121.76	124.53
17	H	4006	BCR	C15-C16-C17	-2.46	118.43	123.47
17	L	4020	BCR	C29-C28-C27	-2.46	105.88	111.38
17	1	524	BCR	C24-C23-C22	-2.46	122.52	126.23
17	a	521	BCR	C7-C8-C9	-2.46	122.52	126.23
14	a	502	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
14	f	1206	CLA	CHB-C4A-NA	2.46	127.92	124.51
14	3	512	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
18	A	5009	LHG	C27-C26-C25	-2.46	101.93	114.42
18	G	5009	LHG	C27-C26-C25	-2.46	101.94	114.42
14	A	1117	CLA	C3B-C4B-NB	-2.46	108.23	110.52
14	1	503	CLA	C3B-C4B-NB	-2.46	108.23	110.52
14	G	1129	CLA	CHC-C4B-NB	2.46	126.86	124.26
17	Z	523	BCR	C33-C5-C6	-2.46	121.77	124.53
14	B	1206	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	t	511	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
14	e	1117	CLA	C3B-C4B-NB	-2.46	108.23	110.52
14	f	1230	CLA	C3B-C4B-NB	-2.46	108.23	110.52
14	u	506	CLA	C3B-C4B-NB	-2.46	108.23	110.52
17	1	521	BCR	C33-C5-C6	-2.46	121.77	124.53
17	e	4003	BCR	C38-C26-C25	-2.46	121.77	124.53
17	q	521	BCR	C33-C5-C6	-2.46	121.77	124.53
17	V	4019	BCR	C16-C15-C14	-2.46	118.44	123.47
14	4	509	CLA	C3B-C4B-NB	-2.46	108.24	110.52
21	B	1852	SQD	O47-C7-C8	2.46	116.79	111.50
14	n	1502	CLA	CHB-C1B-NB	2.46	126.86	124.26
17	u	522	BCR	C11-C12-C13	-2.46	119.52	126.42
14	e	1123	CLA	C3B-C4B-NB	-2.46	108.24	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1121	CLA	CHC-C4B-NB	2.46	126.86	124.26
14	e	1129	CLA	CMB-C2B-C1B	-2.46	121.63	125.37
14	A	1135	CLA	C2D-C1D-ND	-2.45	108.30	110.10
14	B	1234	CLA	CAC-C3C-C4C	2.45	128.00	124.81
17	e	4002	BCR	C10-C11-C12	-2.45	115.56	123.22
14	1	504	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	3	516	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	G	1117	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	a	506	CLA	CMB-C2B-C1B	-2.45	121.63	125.37
14	B	1208	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	Y	517	CLA	C3B-C4B-NB	-2.45	108.24	110.52
20	l	5104	LMG	O6-C1-O1	-2.45	104.16	109.97
14	4	511	CLA	CMB-C2B-C1B	-2.45	121.63	125.37
20	J	5104	LMG	O6-C1-O1	-2.45	104.17	109.97
17	c	521	BCR	C7-C8-C9	-2.45	122.53	126.23
17	u	522	BCR	C33-C5-C4	2.45	118.33	113.62
14	B	1210	CLA	CBC-CAC-C3C	2.45	119.19	112.43
14	H	1210	CLA	CBC-CAC-C3C	2.45	119.19	112.43
14	f	1210	CLA	CBC-CAC-C3C	2.45	119.19	112.43
17	b	523	BCR	C34-C9-C8	2.45	121.94	118.08
17	H	4009	BCR	C15-C16-C17	-2.45	118.45	123.47
17	5	522	BCR	C33-C5-C4	2.45	118.33	113.62
14	G	1133	CLA	CHB-C1B-NB	2.45	126.85	124.26
14	s	506	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
17	v	522	BCR	C33-C5-C6	-2.45	121.78	124.53
14	B	1012	CLA	C16-C15-C13	-2.45	108.00	115.92
14	a	516	CLA	C3B-C4B-NB	-2.45	108.24	110.52
21	a	822	SQD	C1-O5-C5	2.45	118.50	113.69
17	5	521	BCR	C7-C8-C9	-2.45	122.53	126.23
17	A	4001	BCR	C11-C12-C13	-2.45	119.53	126.42
17	1	524	BCR	C37-C22-C23	2.45	121.94	118.08
14	f	1234	CLA	CAC-C3C-C4C	2.45	127.99	124.81
14	d	508	CLA	CHB-C1B-NB	2.45	126.85	124.26
14	j	1301	CLA	CHB-C1B-NB	2.45	126.85	124.26
17	e	4001	BCR	C11-C12-C13	-2.45	119.54	126.42
14	u	501	CLA	C3B-C4B-NB	-2.45	108.24	110.52
18	A	5001	LHG	O8-C23-O10	-2.45	117.42	123.59
21	3	822	SQD	C1-O5-C5	2.45	118.49	113.69
14	r	516	CLA	O2D-CGD-CBD	2.45	115.62	111.27
14	f	1216	CLA	C1-O2A-CGA	2.45	122.86	116.44
14	f	1229	CLA	CHB-C1B-NB	2.45	126.85	124.26
14	H	1206	CLA	CHB-C4A-NA	2.45	127.89	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	503	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
14	r	508	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
14	f	1012	CLA	C16-C15-C13	-2.45	108.02	115.92
14	a	512	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
17	B	4009	BCR	C15-C16-C17	-2.44	118.47	123.47
14	Y	503	CLA	C3B-C4B-NB	-2.44	108.25	110.52
17	n	4020	BCR	C29-C28-C27	-2.44	105.91	111.38
17	G	4003	BCR	C24-C23-C22	-2.44	122.54	126.23
14	5	517	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	b	511	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
14	Y	504	CLA	C3B-C4B-NB	-2.44	108.25	110.52
17	e	4003	BCR	C24-C23-C22	-2.44	122.54	126.23
17	u	521	BCR	C34-C9-C8	2.44	121.93	118.08
17	3	522	BCR	C38-C26-C25	-2.44	121.78	124.53
14	Z	516	CLA	O2D-CGD-CBD	2.44	115.61	111.27
14	c	501	CLA	C3B-C4B-NB	-2.44	108.25	110.52
14	e	1110	CLA	C3B-C4B-NB	-2.44	108.25	110.52
17	G	4003	BCR	C10-C11-C12	-2.44	115.60	123.22
14	Y	509	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
17	2	523	BCR	C33-C5-C6	-2.44	121.79	124.53
17	6	522	BCR	C33-C5-C6	-2.44	121.79	124.53
14	G	1119	CLA	CAC-C3C-C4C	2.44	127.98	124.81
14	H	1216	CLA	C1-O2A-CGA	2.44	122.85	116.44
17	L	4019	BCR	C16-C15-C14	-2.44	118.47	123.47
17	G	4007	BCR	C21-C20-C19	-2.44	115.60	123.22
17	e	4007	BCR	C21-C20-C19	-2.44	115.60	123.22
14	H	1012	CLA	C16-C15-C13	-2.44	108.03	115.92
17	V	4020	BCR	C29-C28-C27	-2.44	105.92	111.38
17	U	4104	BCR	C28-C27-C26	-2.44	109.72	114.08
14	e	1136	CLA	C1-C2-C3	-2.44	121.82	126.04
14	q	503	CLA	C3B-C4B-NB	-2.44	108.25	110.52
20	T	5104	LMG	O6-C1-O1	-2.44	104.20	109.97
20	f	5002	LMG	C42-C41-C40	-2.44	102.05	114.42
14	A	1116	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	a	522	BCR	C38-C26-C25	-2.44	121.79	124.53
14	f	1213	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
17	2	523	BCR	C21-C20-C19	-2.44	115.61	123.22
14	2	516	CLA	O2D-CGD-CBD	2.44	115.60	111.27
17	B	4014	BCR	C37-C22-C23	2.44	121.92	118.08
17	H	4010	BCR	C23-C22-C21	2.44	122.68	118.94
14	B	1216	CLA	C1-O2A-CGA	2.44	122.84	116.44
18	L	5221	LHG	C20-C19-C18	-2.44	102.05	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	r	523	BCR	C21-C20-C19	-2.44	115.61	123.22
17	H	4014	BCR	C37-C22-C23	2.44	121.92	118.08
21	s	822	SQD	C1-O5-C5	2.44	118.47	113.69
14	6	508	CLA	CHB-C1B-NB	2.44	126.84	124.26
14	5	501	CLA	C3B-C4B-NB	-2.44	108.25	110.52
21	H	1852	SQD	O47-C7-C8	2.44	116.75	111.50
17	k	4018	BCR	C30-C25-C26	-2.44	119.18	122.61
17	f	4009	BCR	C15-C16-C17	-2.44	118.48	123.47
14	A	1133	CLA	CHB-C1B-NB	2.44	126.83	124.26
14	6	508	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
17	H	4006	BCR	C3-C4-C5	-2.44	109.73	114.08
14	G	1022	CLA	C3B-C4B-NB	-2.44	108.26	110.52
14	c	503	CLA	C3B-C4B-NB	-2.44	108.26	110.52
14	A	1129	CLA	CMB-C2B-C1B	-2.43	121.66	125.37
14	1	509	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
17	e	4003	BCR	C10-C11-C12	-2.43	115.62	123.22
21	u	822	SQD	C45-O47-C7	2.43	122.43	117.90
17	A	4003	BCR	C10-C11-C12	-2.43	115.62	123.22
14	G	1114	CLA	CHB-C4A-NA	2.43	127.88	124.51
14	R	1301	CLA	CHB-C1B-NB	2.43	126.83	124.26
14	q	509	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
17	n	4019	BCR	C16-C15-C14	-2.43	118.49	123.47
14	H	1208	CLA	C3B-C4B-NB	-2.43	108.26	110.52
17	m	4104	BCR	C28-C27-C26	-2.43	109.73	114.08
14	G	1136	CLA	C1-C2-C3	-2.43	121.84	126.04
17	G	4003	BCR	C38-C26-C25	-2.43	121.80	124.53
14	c	517	CLA	CHB-C4A-NA	2.43	127.88	124.51
17	A	4007	BCR	C21-C20-C19	-2.43	115.63	123.22
17	Z	523	BCR	C21-C20-C19	-2.43	115.63	123.22
14	2	508	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
14	A	1123	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	1	517	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	G	1130	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	m	4104	BCR	C23-C24-C25	-2.43	120.38	127.20
20	B	5002	LMG	C42-C41-C40	-2.43	102.09	114.42
14	B	1210	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
14	d	502	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	r	509	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	u	517	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	A	1136	CLA	C1-C2-C3	-2.43	121.84	126.04
17	f	4014	BCR	C37-C22-C23	2.43	121.91	118.08
14	G	1131	CLA	CHB-C1B-NB	2.43	126.83	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	V	5221	LHG	C20-C19-C18	-2.43	102.09	114.42
14	t	503	CLA	C2D-C1D-ND	-2.43	108.31	110.10
17	s	524	BCR	C27-C26-C25	-2.43	119.20	122.73
14	5	517	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	F	1301	CLA	CHB-C1B-NB	2.43	126.83	124.26
20	H	5002	LMG	C42-C41-C40	-2.43	102.10	114.42
14	G	1129	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
17	5	521	BCR	C34-C9-C8	2.43	121.90	118.08
18	n	5221	LHG	C20-C19-C18	-2.43	102.11	114.42
17	K	4104	BCR	C28-C27-C26	-2.43	109.74	114.08
17	U	4104	BCR	C23-C24-C25	-2.43	120.39	127.20
14	v	502	CLA	C3B-C4B-NB	-2.43	108.26	110.52
17	B	4010	BCR	C23-C22-C21	2.43	122.66	118.94
17	G	4001	BCR	C11-C12-C13	-2.43	119.60	126.42
14	a	504	CLA	C3B-C4B-NB	-2.43	108.27	110.52
14	u	511	CLA	C3B-C4B-NB	-2.43	108.27	110.52
17	K	4104	BCR	C23-C24-C25	-2.43	120.39	127.20
17	B	4006	BCR	C3-C4-C5	-2.42	109.75	114.08
21	5	822	SQD	C45-O47-C7	2.42	122.42	117.90
14	G	1116	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	f	1215	CLA	C3C-C4C-NC	-2.42	107.85	110.57
17	V	4020	BCR	C15-C14-C13	-2.42	123.85	127.31
14	s	516	CLA	C3B-C4B-NB	-2.42	108.27	110.52
17	c	522	BCR	C33-C5-C4	2.42	118.27	113.62
14	A	1106	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
14	d	508	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
14	b	512	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	A	1114	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	f	1210	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
14	e	1127	CLA	C1-C2-C3	-2.42	121.86	126.04
14	v	508	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
14	4	503	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	H	1215	CLA	C3C-C4C-NC	-2.42	107.86	110.57
14	e	1124	CLA	CHD-C1D-ND	-2.42	122.23	124.45
14	s	504	CLA	C3B-C4B-NB	-2.42	108.27	110.52
14	v	501	CLA	C3B-C4B-NB	-2.42	108.27	110.52
14	f	1023	CLA	CMB-C2B-C3B	2.42	132.44	126.59
14	B	1240	CLA	C1-C2-C3	-2.42	121.86	126.04
14	A	1124	CLA	CHD-C1D-ND	-2.42	122.23	124.45
14	s	507	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	t	503	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	e	1106	CLA	CMB-C2B-C1B	-2.42	121.69	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	o	4021	BCR	C36-C18-C19	2.42	121.89	118.08
14	A	1127	CLA	C1-C2-C3	-2.42	121.86	126.04
14	H	1210	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
14	e	1135	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
14	B	1230	CLA	CHB-C4A-NA	2.42	127.85	124.51
14	G	1123	CLA	C3B-C4B-NB	-2.42	108.27	110.52
14	e	1133	CLA	CHB-C1B-NB	2.42	126.81	124.26
17	t	523	BCR	C21-C20-C19	-2.42	115.68	123.22
14	H	1202	CLA	C3B-C4B-NB	-2.42	108.27	110.52
14	c	517	CLA	C3B-C4B-NB	-2.42	108.27	110.52
17	I	4018	BCR	C38-C26-C27	2.42	118.26	113.62
17	G	4002	BCR	C33-C5-C6	-2.42	121.82	124.53
21	5	822	SQD	C4-C3-C2	2.42	115.04	110.82
17	c	521	BCR	C34-C9-C8	2.41	121.88	118.08
14	e	1119	CLA	CAC-C3C-C4C	2.41	127.94	124.81
14	G	1106	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
14	4	503	CLA	C2D-C1D-ND	-2.41	108.33	110.10
14	e	1105	CLA	CHD-C1D-ND	-2.41	122.24	124.45
14	U	1105	CLA	CHB-C4A-NA	2.41	127.85	124.51
21	c	822	SQD	C45-O47-C7	2.41	122.39	117.90
14	3	507	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
14	e	1118	CLA	CHC-C4B-NB	2.41	126.81	124.26
14	e	1114	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	c	511	CLA	C3B-C4B-NB	-2.41	108.28	110.52
18	L	5218	LHG	C27-C26-C25	-2.41	102.18	114.42
14	B	1023	CLA	CMB-C2B-C3B	2.41	132.43	126.59
17	f	4006	BCR	C3-C4-C5	-2.41	109.77	114.08
17	u	522	BCR	C1-C6-C7	2.41	122.60	115.78
14	f	1235	CLA	CHD-C1D-ND	-2.41	122.24	124.45
14	G	1135	CLA	C2D-C1D-ND	-2.41	108.33	110.10
18	I	5001	LHG	C20-C19-C18	-2.41	102.18	114.42
17	f	4014	BCR	C15-C14-C13	-2.41	123.87	127.31
14	A	1136	CLA	CHB-C4A-NA	2.41	127.84	124.51
14	A	1130	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	n	5218	LHG	C27-C26-C25	-2.41	102.19	114.42
14	H	1023	CLA	CMB-C2B-C3B	2.41	132.43	126.59
14	A	1119	CLA	CAC-C3C-C4C	2.41	127.94	124.81
14	6	502	CLA	C3B-C4B-NB	-2.41	108.28	110.52
17	a	522	BCR	C23-C24-C25	-2.41	120.44	127.20
17	5	522	BCR	C1-C6-C7	2.41	122.59	115.78
18	S	5001	LHG	C20-C19-C18	-2.41	102.20	114.42
18	k	5001	LHG	C20-C19-C18	-2.41	102.20	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1136	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	A	4002	BCR	C20-C19-C18	-2.41	119.65	126.42
14	A	1022	CLA	C3B-C4B-NB	-2.41	108.28	110.52
17	e	4002	BCR	C20-C19-C18	-2.41	119.65	126.42
14	a	507	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
14	G	1135	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
17	M	4021	BCR	C36-C18-C19	2.41	121.87	118.08
17	s	522	BCR	C38-C26-C25	-2.41	121.83	124.53
14	Y	513	CLA	C3B-C4B-NB	-2.41	108.28	110.52
14	q	513	CLA	C3B-C4B-NB	-2.41	108.28	110.52
14	A	1105	CLA	CHD-C1D-ND	-2.41	122.24	124.45
14	v	502	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
18	V	5218	LHG	C27-C26-C25	-2.41	102.21	114.42
17	H	4014	BCR	C15-C14-C13	-2.41	123.88	127.31
14	f	1230	CLA	CHB-C4A-NA	2.41	127.84	124.51
14	5	511	CLA	C3B-C4B-NB	-2.41	108.28	110.52
14	f	1222	CLA	CHB-C1B-NB	2.41	126.80	124.26
17	q	522	BCR	C30-C25-C26	-2.41	119.22	122.61
17	e	4002	BCR	C33-C5-C6	-2.41	121.83	124.53
14	G	1136	CLA	CHB-C4A-NA	2.41	127.84	124.51
14	A	1801	CLA	C3B-C4B-NB	-2.40	108.28	110.52
14	G	1801	CLA	C3B-C4B-NB	-2.40	108.28	110.52
17	4	524	BCR	C3-C4-C5	-2.40	109.78	114.08
14	B	1229	CLA	CHB-C1B-NB	2.40	126.80	124.26
17	k	4018	BCR	C38-C26-C27	2.40	118.23	113.62
14	G	1124	CLA	CHD-C1D-ND	-2.40	122.25	124.45
14	A	1120	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
14	r	511	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
14	G	1127	CLA	C1-C2-C3	-2.40	121.89	126.04
21	u	822	SQD	C4-C3-C2	2.40	115.02	110.82
14	G	1117	CLA	C7-C6-C5	-2.40	106.83	113.36
14	t	506	CLA	C3B-C4B-NB	-2.40	108.29	110.52
17	b	524	BCR	C3-C4-C5	-2.40	109.79	114.08
14	Z	508	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
17	e	4001	BCR	C35-C13-C12	2.40	121.86	118.08
17	c	522	BCR	C1-C6-C7	2.40	122.57	115.78
17	6	524	BCR	C23-C24-C25	-2.40	120.46	127.20
17	H	4010	BCR	C20-C19-C18	-2.40	119.67	126.42
14	e	1102	CLA	O2D-CGD-CBD	2.40	115.53	111.27
14	A	1135	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
17	Y	522	BCR	C30-C25-C26	-2.40	119.23	122.61
14	q	517	CLA	C3B-C4B-NB	-2.40	108.29	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	4003	BCR	C16-C15-C14	-2.40	118.56	123.47
17	S	4018	BCR	C38-C26-C27	2.40	118.23	113.62
14	4	512	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	4	523	BCR	C21-C20-C19	-2.40	115.73	123.22
14	3	513	CLA	C3B-C4B-NB	-2.40	108.29	110.52
14	t	512	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	X	170	FMN	O4-C4-C4A	-2.40	120.23	126.60
20	B	5002	LMG	C38-C37-C36	-2.40	102.25	114.42
14	e	1127	CLA	CAA-CBA-CGA	-2.40	106.24	113.25
15	G	2001	PQN	C2M-C2-C3	-2.40	120.49	124.40
14	H	1213	CLA	C11-C10-C8	-2.40	108.17	115.92
14	3	504	CLA	C3B-C4B-NB	-2.40	108.29	110.52
17	f	4010	BCR	C23-C22-C21	2.40	122.62	118.94
17	v	524	BCR	C23-C24-C25	-2.40	120.47	127.20
17	3	522	BCR	C23-C24-C25	-2.40	120.47	127.20
18	G	5006	LHG	C11-C10-C9	-2.40	102.25	114.42
14	3	509	CLA	C3B-C4B-NB	-2.40	108.29	110.52
14	t	504	CLA	C3B-C4B-NB	-2.40	108.29	110.52
17	G	4002	BCR	C20-C19-C18	-2.40	119.68	126.42
17	u	522	BCR	C20-C21-C22	-2.40	123.89	127.31
18	e	5006	LHG	C11-C10-C9	-2.40	102.26	114.42
14	d	502	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
14	B	1213	CLA	C11-C10-C8	-2.40	108.17	115.92
21	c	822	SQD	C4-C3-C2	2.40	115.01	110.82
14	H	1240	CLA	C1-C2-C3	-2.40	121.90	126.04
17	t	522	BCR	C33-C5-C4	2.40	118.22	113.62
14	A	1131	CLA	CHB-C1B-NB	2.40	126.79	124.26
17	B	4014	BCR	C15-C14-C13	-2.40	123.89	127.31
17	L	4020	BCR	C15-C14-C13	-2.40	123.89	127.31
17	f	4010	BCR	C20-C19-C18	-2.40	119.69	126.42
14	f	1240	CLA	C1-C2-C3	-2.40	121.90	126.04
17	B	4010	BCR	C20-C19-C18	-2.40	119.69	126.42
14	f	1236	CLA	O2D-CGD-CBD	2.40	115.52	111.27
17	Z	521	BCR	C29-C30-C25	2.40	114.17	110.48
17	f	4010	BCR	C28-C27-C26	-2.39	109.80	114.08
17	t	524	BCR	C3-C4-C5	-2.39	109.80	114.08
17	1	522	BCR	C30-C25-C26	-2.39	119.24	122.61
17	5	522	BCR	C20-C21-C22	-2.39	123.89	127.31
14	B	1215	CLA	C3C-C4C-NC	-2.39	107.89	110.57
14	B	1222	CLA	CHB-C1B-NB	2.39	126.79	124.26
14	H	1222	CLA	CHB-C1B-NB	2.39	126.79	124.26
18	A	5006	LHG	C11-C10-C9	-2.39	102.28	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1230	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	f	5002	LMG	C38-C37-C36	-2.39	102.28	114.42
14	A	1127	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
14	2	511	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
20	H	5002	LMG	C38-C37-C36	-2.39	102.28	114.42
14	H	1205	CLA	CHB-C1B-NB	2.39	126.79	124.26
14	A	1129	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	A	4001	BCR	C35-C13-C12	2.39	121.84	118.08
17	L	4020	BCR	C11-C10-C9	-2.39	123.90	127.31
14	H	1210	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
14	s	516	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
14	A	1117	CLA	C7-C6-C5	-2.39	106.86	113.36
17	B	4006	BCR	C37-C22-C21	-2.39	119.57	122.92
14	Z	511	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
17	s	522	BCR	C23-C24-C25	-2.39	120.49	127.20
17	Z	522	BCR	C36-C18-C19	2.39	121.84	118.08
14	6	502	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
14	B	1236	CLA	O2D-CGD-CBD	2.39	115.51	111.27
17	4	522	BCR	C1-C6-C5	-2.39	119.25	122.61
17	a	524	BCR	C27-C26-C25	-2.39	119.26	122.73
14	G	1129	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	t	522	BCR	C33-C5-C6	-2.39	121.84	124.53
17	A	4007	BCR	C29-C30-C25	2.39	114.16	110.48
14	A	1102	CLA	O2D-CGD-CBD	2.39	115.51	111.27
17	r	521	BCR	C29-C30-C25	2.39	114.16	110.48
14	f	1213	CLA	C11-C10-C8	-2.39	108.20	115.92
17	4	522	BCR	C33-C5-C4	2.39	118.20	113.62
14	e	1131	CLA	CHB-C1B-NB	2.39	126.78	124.26
14	f	1205	CLA	CHB-C1B-NB	2.39	126.78	124.26
14	3	511	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
17	k	4018	BCR	C4-C5-C6	-2.39	119.27	122.73
17	A	4003	BCR	C16-C15-C14	-2.39	118.58	123.47
14	K	1105	CLA	CHB-C4A-NA	2.39	127.81	124.51
14	6	512	CLA	CHB-C4A-NA	2.39	127.81	124.51
14	G	1107	CLA	CHB-C4A-NA	2.39	127.81	124.51
14	e	1120	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
14	G	1103	CLA	C1-C2-C3	-2.39	121.92	126.04
14	e	1140	CLA	CHB-C1B-NB	2.39	126.78	124.26
17	W	4021	BCR	C36-C18-C19	2.39	121.84	118.08
17	V	4019	BCR	C33-C5-C6	-2.39	121.85	124.53
14	1	513	CLA	C3B-C4B-NB	-2.39	108.30	110.52
14	4	506	CLA	C3B-C4B-NB	-2.39	108.30	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1117	CLA	C7-C6-C5	-2.39	106.88	113.36
17	d	524	BCR	C23-C24-C25	-2.38	120.50	127.20
17	S	4018	BCR	C4-C5-C6	-2.38	119.27	122.73
17	T	4013	BCR	C11-C10-C9	-2.38	123.91	127.31
17	b	523	BCR	C21-C20-C19	-2.38	115.78	123.22
14	e	1129	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	H	1225	CLA	C2D-C1D-ND	-2.38	108.35	110.10
17	e	4007	BCR	C29-C30-C25	2.38	114.15	110.48
14	3	516	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
14	H	1236	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
17	3	524	BCR	C27-C26-C25	-2.38	119.27	122.73
14	a	516	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
15	A	2001	PQN	C2M-C2-C3	-2.38	120.51	124.40
17	l	4015	BCR	C16-C15-C14	-2.38	118.59	123.47
14	d	506	CLA	C3B-C4B-NB	-2.38	108.31	110.52
22	P	170	FMN	O4-C4-C4A	-2.38	120.28	126.60
17	b	522	BCR	C33-C5-C4	2.38	118.19	113.62
14	c	509	CLA	CMB-C2B-C3B	2.38	132.36	126.59
17	4	522	BCR	C33-C5-C6	-2.38	121.85	124.53
14	s	509	CLA	C3B-C4B-NB	-2.38	108.31	110.52
14	G	1103	CLA	CMB-C2B-C3B	2.38	132.35	126.59
17	t	522	BCR	C1-C6-C5	-2.38	119.26	122.61
17	2	521	BCR	C29-C30-C25	2.38	114.15	110.48
14	a	511	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
14	s	511	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
17	G	4007	BCR	C29-C30-C25	2.38	114.14	110.48
14	6	506	CLA	C3B-C4B-NB	-2.38	108.31	110.52
14	e	1117	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
14	f	1236	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
17	n	4020	BCR	C11-C10-C9	-2.38	123.91	127.31
14	H	1224	CLA	CMB-C2B-C3B	2.38	132.35	126.59
17	f	4006	BCR	C37-C22-C21	-2.38	119.59	122.92
14	A	1103	CLA	CMB-C2B-C3B	2.38	132.35	126.59
14	s	513	CLA	C3B-C4B-NB	-2.38	108.31	110.52
17	A	4002	BCR	C33-C5-C6	-2.38	121.86	124.53
17	2	522	BCR	C36-C18-C19	2.38	121.82	118.08
17	B	4010	BCR	C28-C27-C26	-2.38	109.83	114.08
14	G	1127	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
14	e	1022	CLA	C3B-C4B-NB	-2.38	108.31	110.52
14	H	1229	CLA	CHB-C1B-NB	2.38	126.77	124.26
14	b	507	CLA	CHC-C4B-NB	2.38	126.77	124.26
14	e	1103	CLA	CMB-C2B-C3B	2.38	132.34	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	4003	BCR	C16-C15-C14	-2.37	118.61	123.47
14	G	1120	CLA	CMB-C2B-C1B	-2.37	121.75	125.37
14	b	506	CLA	C3B-C4B-NB	-2.37	108.31	110.52
17	H	4010	BCR	C28-C27-C26	-2.37	109.84	114.08
14	T	1303	CLA	O2A-CGA-O1A	-2.37	117.38	123.30
14	e	1130	CLA	CHB-C4A-NA	2.37	127.79	124.51
14	A	1117	CLA	CMB-C2B-C3B	2.37	132.33	126.59
14	f	1210	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
21	3	822	SQD	O5-C5-C4	2.37	114.00	109.69
14	B	1224	CLA	CMB-C2B-C3B	2.37	132.33	126.59
14	5	509	CLA	CMB-C2B-C3B	2.37	132.33	126.59
17	J	4013	BCR	C11-C10-C9	-2.37	123.92	127.31
17	l	4013	BCR	C11-C10-C9	-2.37	123.92	127.31
14	e	1111	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
21	a	822	SQD	O5-C5-C4	2.37	114.00	109.69
14	a	507	CLA	C2A-C1A-CHA	2.37	128.01	123.86
14	4	504	CLA	C3B-C4B-NB	-2.37	108.31	110.52
17	c	522	BCR	C20-C21-C22	-2.37	123.93	127.31
14	u	509	CLA	CMB-C2B-C3B	2.37	132.33	126.59
17	J	4015	BCR	C16-C15-C14	-2.37	118.62	123.47
14	B	1236	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
14	s	507	CLA	C2A-C1A-CHA	2.37	128.00	123.86
22	p	170	FMN	O4-C4-C4A	-2.37	120.31	126.60
17	f	4010	BCR	C33-C5-C6	-2.37	121.87	124.53
17	r	522	BCR	C36-C18-C19	2.37	121.81	118.08
14	G	1120	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
14	m	1105	CLA	CHB-C4A-NA	2.37	127.79	124.51
14	v	512	CLA	CHB-C4A-NA	2.37	127.79	124.51
14	A	1109	CLA	O1D-CGD-CBD	2.37	129.33	124.48
14	H	1236	CLA	O2D-CGD-CBD	2.37	115.48	111.27
17	t	524	BCR	C1-C6-C7	2.37	122.48	115.78
21	s	822	SQD	O5-C5-C4	2.37	114.00	109.69
14	e	1117	CLA	CMB-C2B-C3B	2.37	132.32	126.59
14	u	516	CLA	C3B-C4B-NB	-2.37	108.32	110.52
14	b	503	CLA	C2D-C1D-ND	-2.37	108.36	110.10
14	e	1109	CLA	O1D-CGD-CBD	2.37	129.33	124.48
17	H	4006	BCR	C37-C22-C21	-2.37	119.61	122.92
14	A	1140	CLA	CHB-C1B-NB	2.37	126.76	124.26
14	e	1103	CLA	C1-C2-C3	-2.37	121.95	126.04
14	e	1237	CLA	C3B-C4B-NB	-2.37	108.32	110.52
19	A	1849	LMU	O5'-C1'-C2'	2.37	115.36	110.35
19	G	1849	LMU	O5'-C1'-C2'	2.37	115.36	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1111	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
14	B	1235	CLA	CHD-C1D-ND	-2.37	122.28	124.45
14	e	1104	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
17	n	4020	BCR	C15-C14-C13	-2.37	123.93	127.31
14	G	1117	CLA	CMB-C2B-C3B	2.37	132.32	126.59
17	I	4018	BCR	C4-C5-C6	-2.37	119.30	122.73
17	a	522	BCR	C31-C1-C6	-2.36	106.46	110.30
14	a	509	CLA	C3B-C4B-NB	-2.36	108.32	110.52
14	H	1021	CLA	C11-C12-C13	-2.36	108.28	115.92
14	J	1303	CLA	O2A-CGA-O1A	-2.36	117.41	123.30
14	B	1202	CLA	C3B-C4B-NB	-2.36	108.32	110.52
17	T	4015	BCR	C16-C15-C14	-2.36	118.63	123.47
14	A	1103	CLA	C1-C2-C3	-2.36	121.96	126.04
14	G	1102	CLA	O2D-CGD-CBD	2.36	115.47	111.27
17	V	4020	BCR	C11-C10-C9	-2.36	123.94	127.31
14	A	1107	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	c	521	BCR	C27-C26-C25	-2.36	119.30	122.73
15	e	2001	PQN	C2M-C2-C3	-2.36	120.55	124.40
17	V	4219	BCR	C36-C18-C19	2.36	121.80	118.08
15	B	2002	PQN	C2M-C2-C3	-2.36	120.55	124.40
14	G	1111	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
17	3	522	BCR	C31-C1-C6	-2.36	106.47	110.30
14	e	1107	CLA	CHB-C4A-NA	2.36	127.78	124.51
18	n	5218	LHG	O8-C23-C24	2.36	119.32	111.91
14	A	1118	CLA	CHC-C4B-NB	2.36	126.75	124.26
14	B	1205	CLA	CHB-C1B-NB	2.36	126.75	124.26
14	G	1117	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
14	A	1120	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
19	e	1849	LMU	O5'-C1'-C2'	2.36	115.34	110.35
17	G	4001	BCR	C35-C13-C12	2.36	121.79	118.08
17	2	522	BCR	C3-C4-C5	-2.36	109.86	114.08
14	n	1503	CLA	O2D-CGD-CBD	2.36	115.46	111.27
17	s	522	BCR	C31-C1-C6	-2.36	106.47	110.30
14	A	1104	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
17	B	4014	BCR	C12-C13-C14	-2.36	115.33	118.94
14	2	506	CLA	C3B-C4B-NB	-2.36	108.33	110.52
14	G	1104	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
14	f	1224	CLA	CMB-C2B-C3B	2.36	132.29	126.59
14	n	1501	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
14	G	1118	CLA	CHC-C4B-NB	2.36	126.75	124.26
17	4	524	BCR	C1-C6-C7	2.36	122.44	115.78
14	f	1202	CLA	C3B-C4B-NB	-2.36	108.33	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1210	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
14	A	1117	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
14	B	1021	CLA	C11-C12-C13	-2.35	108.31	115.92
17	L	4019	BCR	C33-C5-C6	-2.35	121.89	124.53
17	b	522	BCR	C33-C5-C6	-2.35	121.89	124.53
17	b	522	BCR	C1-C6-C5	-2.35	119.30	122.61
14	A	1103	CLA	C3B-C4B-NB	-2.35	108.33	110.52
14	Z	506	CLA	C3B-C4B-NB	-2.35	108.33	110.52
18	L	5218	LHG	O8-C23-C24	2.35	119.29	111.91
17	b	524	BCR	C1-C6-C7	2.35	122.43	115.78
14	l	1303	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
14	e	1120	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
14	G	1103	CLA	C3B-C4B-NB	-2.35	108.33	110.52
17	B	4010	BCR	C33-C5-C6	-2.35	121.89	124.53
17	s	523	BCR	C8-C7-C6	-2.35	120.60	127.20
17	r	522	BCR	C3-C4-C5	-2.35	109.88	114.08
14	3	507	CLA	C2A-C1A-CHA	2.35	127.97	123.86
17	v	524	BCR	C10-C11-C12	-2.35	115.89	123.22
14	V	1501	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
17	Z	522	BCR	C23-C24-C25	-2.35	120.60	127.20
21	r	822	SQD	O6-C1-C2	2.35	111.97	108.30
14	L	1501	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
14	d	512	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	v	523	BCR	C21-C20-C19	-2.35	115.89	123.22
14	G	1237	CLA	C3B-C4B-NB	-2.35	108.34	110.52
14	a	502	CLA	C3B-C4B-NB	-2.35	108.34	110.52
14	f	1232	CLA	C3B-C4B-NB	-2.35	108.34	110.52
17	L	4219	BCR	C36-C18-C19	2.35	121.78	118.08
14	B	1204	CLA	CHD-C1D-ND	-2.35	122.30	124.45
14	G	1013	CLA	C3C-C4C-NC	-2.35	107.94	110.57
14	G	1109	CLA	O1D-CGD-CBD	2.35	129.29	124.48
14	c	505	CLA	C3B-C4B-NB	-2.35	108.34	110.52
14	b	508	CLA	C2D-C1D-ND	-2.35	108.38	110.10
14	f	1021	CLA	C11-C12-C13	-2.35	108.34	115.92
17	f	4014	BCR	C15-C16-C17	-2.35	118.67	123.47
14	5	516	CLA	C3B-C4B-NB	-2.35	108.34	110.52
14	e	1801	CLA	C3B-C4B-NB	-2.35	108.34	110.52
17	Z	522	BCR	C3-C4-C5	-2.35	109.89	114.08
18	L	5221	LHG	O8-C23-C24	2.35	119.27	111.91
17	6	523	BCR	C21-C20-C19	-2.34	115.90	123.22
17	d	523	BCR	C21-C20-C19	-2.34	115.90	123.22
18	V	5218	LHG	O8-C23-C24	2.34	119.26	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	t	822	SQD	O5-C5-C4	2.34	113.95	109.69
14	L	1503	CLA	O2D-CGD-CBD	2.34	115.43	111.27
17	3	523	BCR	C8-C7-C6	-2.34	120.62	127.20
17	a	523	BCR	C8-C7-C6	-2.34	120.62	127.20
14	B	1225	CLA	C2D-C1D-ND	-2.34	108.38	110.10
15	f	2002	PQN	C2M-C2-C3	-2.34	120.58	124.40
18	V	5221	LHG	O8-C23-C24	2.34	119.26	111.91
18	n	5221	LHG	O8-C23-C24	2.34	119.26	111.91
14	H	1235	CLA	CHD-C1D-ND	-2.34	122.30	124.45
14	a	509	CLA	CMB-C2B-C3B	2.34	132.26	126.59
14	v	506	CLA	C3B-C4B-NB	-2.34	108.34	110.52
14	Z	513	CLA	CHB-C1B-NB	2.34	126.73	124.26
14	e	1107	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
17	B	4014	BCR	C15-C16-C17	-2.34	118.68	123.47
14	A	1237	CLA	C3B-C4B-NB	-2.34	108.34	110.52
14	4	507	CLA	CHC-C4B-NB	2.34	126.73	124.26
14	G	1115	CLA	CHC-C4B-NB	2.34	126.73	124.26
14	H	1204	CLA	CHD-C1D-ND	-2.34	122.31	124.45
14	f	1203	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
14	4	508	CLA	C2D-C1D-ND	-2.34	108.38	110.10
17	5	523	BCR	C33-C5-C4	2.34	118.11	113.62
17	M	4021	BCR	C3-C4-C5	-2.34	109.90	114.08
17	W	4021	BCR	C3-C4-C5	-2.34	109.90	114.08
17	5	521	BCR	C27-C26-C25	-2.34	119.34	122.73
14	e	1103	CLA	C3B-C4B-NB	-2.34	108.35	110.52
14	u	505	CLA	C3B-C4B-NB	-2.34	108.35	110.52
14	G	1140	CLA	CHB-C1B-NB	2.34	126.73	124.26
14	H	1206	CLA	CHC-C4B-NB	2.34	126.73	124.26
14	B	1203	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
14	H	1203	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
14	f	1211	CLA	O2D-CGD-CBD	2.34	115.42	111.27
14	e	1127	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
14	f	1227	CLA	CHD-C1D-ND	-2.34	122.31	124.45
17	e	4011	BCR	C15-C14-C13	-2.34	123.98	127.31
14	H	1226	CLA	CAC-C3C-C4C	2.34	127.84	124.81
14	B	1209	CLA	CHB-C1B-NB	2.34	126.73	124.26
17	c	523	BCR	C33-C5-C4	2.34	118.10	113.62
17	f	4014	BCR	C12-C13-C14	-2.34	115.36	118.94
14	3	504	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
14	B	1206	CLA	CHC-C4B-NB	2.34	126.73	124.26
14	f	1209	CLA	CHB-C1B-NB	2.34	126.73	124.26
17	H	4014	BCR	C12-C13-C14	-2.33	115.36	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	u	521	BCR	C27-C26-C25	-2.33	119.34	122.73
22	P	170	FMN	C10-C4A-N5	-2.33	119.90	124.86
14	b	504	CLA	C3B-C4B-NB	-2.33	108.35	110.52
17	r	522	BCR	C23-C24-C25	-2.33	120.64	127.20
14	s	509	CLA	CMB-C2B-C3B	2.33	132.24	126.59
17	6	524	BCR	C10-C11-C12	-2.33	115.93	123.22
17	o	4021	BCR	C3-C4-C5	-2.33	109.91	114.08
14	G	1107	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
14	G	1104	CLA	C11-C12-C13	-2.33	108.38	115.92
14	H	1215	CLA	C16-C15-C13	-2.33	108.38	115.92
20	T	5104	LMG	O3-C3-C2	-2.33	104.95	110.35
17	H	4014	BCR	C15-C16-C17	-2.33	118.69	123.47
14	A	1104	CLA	C11-C12-C13	-2.33	108.38	115.92
17	c	524	BCR	C38-C26-C25	-2.33	121.91	124.53
14	A	1107	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
22	X	170	FMN	C10-C4A-N5	-2.33	119.91	124.86
17	H	4004	BCR	C20-C19-C18	-2.33	119.86	126.42
17	A	4011	BCR	C15-C14-C13	-2.33	123.98	127.31
17	H	4010	BCR	C16-C17-C18	-2.33	123.98	127.31
17	a	524	BCR	C20-C21-C22	-2.33	123.98	127.31
17	n	4219	BCR	C36-C18-C19	2.33	121.75	118.08
14	H	1212	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
17	n	4019	BCR	C33-C5-C6	-2.33	121.91	124.53
14	c	516	CLA	C3B-C4B-NB	-2.33	108.35	110.52
20	H	5002	LMG	O3-C3-C2	-2.33	104.96	110.35
14	B	1226	CLA	CAC-C3C-C4C	2.33	127.83	124.81
14	r	509	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
14	s	504	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
17	2	522	BCR	C23-C24-C25	-2.33	120.66	127.20
14	t	511	CLA	C2D-C1D-ND	-2.33	108.39	110.10
17	u	523	BCR	C33-C5-C4	2.33	118.09	113.62
14	A	1137	CLA	C4-C3-C5	2.33	119.19	115.27
14	e	1104	CLA	C11-C12-C13	-2.33	108.39	115.92
14	f	1021	CLA	O2A-C1-C2	-2.33	102.52	108.64
14	B	1215	CLA	C16-C15-C13	-2.33	108.40	115.92
14	3	509	CLA	CMB-C2B-C3B	2.33	132.22	126.59
14	B	1201	CLA	CHB-C1B-NB	2.33	126.72	124.26
14	f	1204	CLA	CHD-C1D-ND	-2.33	122.32	124.45
14	G	1111	CLA	CMB-C2B-C1B	-2.33	121.83	125.37
17	u	524	BCR	C37-C22-C23	2.33	121.74	118.08
17	s	524	BCR	C20-C21-C22	-2.33	123.99	127.31
17	H	4010	BCR	C33-C5-C6	-2.33	121.92	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	524	BCR	C20-C21-C22	-2.32	123.99	127.31
14	A	1127	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
14	e	1137	CLA	C4-C3-C5	2.32	119.18	115.27
17	d	521	BCR	C33-C5-C6	-2.32	121.92	124.53
20	B	5002	LMG	O3-C3-C2	-2.32	104.98	110.35
14	e	1122	CLA	C3B-C4B-NB	-2.32	108.36	110.52
21	2	822	SQD	O6-C1-C2	2.32	111.93	108.30
14	A	1013	CLA	C3C-C4C-NC	-2.32	107.97	110.57
20	f	5002	LMG	O3-C3-C2	-2.32	104.98	110.35
14	f	1226	CLA	CAC-C3C-C4C	2.32	127.82	124.81
14	H	1211	CLA	O2D-CGD-CBD	2.32	115.39	111.27
14	V	1503	CLA	O2D-CGD-CBD	2.32	115.39	111.27
17	a	524	BCR	C1-C6-C5	-2.32	119.34	122.61
14	B	1211	CLA	O2D-CGD-CBD	2.32	115.39	111.27
17	Y	524	BCR	C16-C15-C14	-2.32	118.72	123.47
17	H	4009	BCR	C37-C22-C23	2.32	121.73	118.08
14	B	1202	CLA	O2A-C1-C2	-2.32	102.54	108.64
14	r	506	CLA	C3B-C4B-NB	-2.32	108.36	110.52
14	G	1137	CLA	C4-C3-C5	2.32	119.17	115.27
21	Z	822	SQD	O6-C1-C2	2.32	111.92	108.30
14	2	509	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
17	d	524	BCR	C10-C11-C12	-2.32	115.98	123.22
14	H	1201	CLA	CHB-C1B-NB	2.32	126.71	124.26
21	4	822	SQD	O5-C5-C4	2.32	113.91	109.69
14	B	1232	CLA	C3B-C4B-NB	-2.32	108.36	110.52
14	Y	506	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
17	B	4014	BCR	C38-C26-C25	2.32	127.13	124.53
14	Z	509	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
14	B	1021	CLA	O2A-C1-C2	-2.32	102.54	108.64
14	s	511	CLA	C3B-C4B-NB	-2.32	108.36	110.52
14	2	509	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
20	J	5104	LMG	O3-C3-C2	-2.32	104.99	110.35
14	B	1227	CLA	CHD-C1D-ND	-2.32	122.33	124.45
14	H	1223	CLA	C3B-C4B-NB	-2.32	108.37	110.52
17	u	524	BCR	C38-C26-C25	-2.32	121.93	124.53
17	3	524	BCR	C34-C9-C8	2.32	121.73	118.08
14	q	506	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
14	Z	509	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
14	f	1219	CLA	CHB-C4A-NA	2.32	127.71	124.51
14	H	1021	CLA	O2A-C1-C2	-2.32	102.55	108.64
14	f	1212	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
14	A	1103	CLA	CAA-C2A-C1A	-2.31	104.39	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1117	CLA	CHD-C1D-ND	-2.31	122.33	124.45
14	B	1219	CLA	CHB-C4A-NA	2.31	127.71	124.51
22	p	170	FMN	C10-C4A-N5	-2.31	119.95	124.86
17	d	522	BCR	C23-C24-C25	-2.31	120.70	127.20
14	e	1111	CLA	CMB-C2B-C1B	-2.31	121.84	125.37
14	f	1215	CLA	C16-C15-C13	-2.31	108.44	115.92
17	B	4009	BCR	C37-C22-C23	2.31	121.72	118.08
14	a	504	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
17	B	4004	BCR	C20-C19-C18	-2.31	119.92	126.42
17	u	521	BCR	C20-C19-C18	-2.31	119.92	126.42
14	f	1225	CLA	C1-C2-C3	-2.31	122.04	126.04
14	f	1202	CLA	O2A-C1-C2	-2.31	102.56	108.64
17	6	522	BCR	C36-C18-C19	2.31	121.72	118.08
17	A	4008	BCR	C28-C27-C26	-2.31	109.95	114.08
14	H	1232	CLA	C3B-C4B-NB	-2.31	108.37	110.52
14	f	1225	CLA	C2D-C1D-ND	-2.31	108.40	110.10
14	r	509	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
17	c	521	BCR	C20-C19-C18	-2.31	119.93	126.42
15	H	2002	PQN	C2M-C2-C3	-2.31	120.63	124.40
17	c	521	BCR	C33-C5-C6	-2.31	121.93	124.53
21	b	822	SQD	O5-C5-C4	2.31	113.89	109.69
17	3	524	BCR	C1-C6-C5	-2.31	119.36	122.61
14	e	1103	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
14	r	511	CLA	CHB-C1B-NB	2.31	126.70	124.26
14	B	1212	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
17	5	521	BCR	C20-C19-C18	-2.31	119.93	126.42
17	6	521	BCR	C33-C5-C6	-2.31	121.94	124.53
14	G	1103	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
17	Y	524	BCR	C20-C21-C22	-2.31	124.02	127.31
14	r	513	CLA	CHB-C1B-NB	2.31	126.70	124.26
14	A	1111	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
17	q	524	BCR	C16-C15-C14	-2.31	118.75	123.47
14	3	509	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
17	f	4014	BCR	C38-C26-C25	2.31	127.12	124.53
14	G	1127	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
21	Y	822	SQD	O48-C23-O10	-2.31	117.77	123.59
17	e	4008	BCR	C28-C27-C26	-2.31	109.96	114.08
14	3	508	CLA	C3B-C4B-NB	-2.31	108.38	110.52
14	H	1012	CLA	CHB-C1B-NB	2.31	126.70	124.26
14	1	506	CLA	CMB-C2B-C1B	-2.31	121.86	125.37
17	1	524	BCR	C16-C15-C14	-2.31	118.75	123.47
14	f	1201	CLA	O2A-CGA-O1A	-2.31	117.77	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	4010	BCR	C16-C17-C18	-2.31	124.02	127.31
17	a	524	BCR	C34-C9-C8	2.31	121.71	118.08
14	f	1201	CLA	CHB-C1B-NB	2.31	126.70	124.26
14	f	1206	CLA	CHC-C4B-NB	2.31	126.70	124.26
17	f	4004	BCR	C20-C19-C18	-2.31	119.94	126.42
17	5	524	BCR	C38-C26-C25	-2.31	121.94	124.53
14	A	1123	CLA	CHA-C1A-NA	-2.31	121.12	126.40
14	H	1219	CLA	CHB-C4A-NA	2.31	127.70	124.51
14	n	1502	CLA	CMB-C2B-C1B	-2.31	121.86	125.37
20	l	5104	LMG	O3-C3-C2	-2.31	105.02	110.35
14	b	503	CLA	C3B-C4B-NB	-2.30	108.38	110.52
17	d	522	BCR	C36-C18-C19	2.30	121.71	118.08
21	q	822	SQD	O48-C23-O10	-2.30	117.78	123.59
17	V	4019	BCR	C40-C30-C25	-2.30	106.56	110.30
17	v	521	BCR	C33-C5-C6	-2.30	121.94	124.53
17	v	521	BCR	C16-C15-C14	-2.30	118.76	123.47
14	G	1137	CLA	C2A-C1A-CHA	2.30	127.89	123.86
14	Z	511	CLA	CHB-C1B-NB	2.30	126.69	124.26
17	6	522	BCR	C23-C24-C25	-2.30	120.73	127.20
14	G	1113	CLA	O2A-CGA-O1A	-2.30	117.56	123.30
17	G	4011	BCR	C15-C14-C13	-2.30	124.02	127.31
14	B	1201	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
14	e	1123	CLA	CHA-C1A-NA	-2.30	121.13	126.40
17	s	524	BCR	C34-C9-C8	2.30	121.70	118.08
17	G	4008	BCR	C28-C27-C26	-2.30	109.97	114.08
17	f	4010	BCR	C16-C17-C18	-2.30	124.03	127.31
17	v	522	BCR	C23-C24-C25	-2.30	120.74	127.20
17	q	524	BCR	C20-C21-C22	-2.30	124.03	127.31
14	L	1502	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
14	G	1123	CLA	CHA-C1A-NA	-2.30	121.13	126.40
17	u	521	BCR	C33-C5-C6	-2.30	121.95	124.53
17	6	521	BCR	C16-C15-C14	-2.30	118.76	123.47
14	5	505	CLA	C3B-C4B-NB	-2.30	108.38	110.52
14	c	512	CLA	CHB-C1B-NB	2.30	126.69	124.26
14	s	509	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
14	G	1104	CLA	C1-C2-C3	-2.30	122.07	126.04
14	e	1117	CLA	CHD-C1D-ND	-2.30	122.34	124.45
17	c	524	BCR	C37-C22-C23	2.30	121.70	118.08
17	f	4009	BCR	C37-C22-C23	2.30	121.70	118.08
14	H	1201	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
14	e	1013	CLA	C3C-C4C-NC	-2.30	107.99	110.57
14	H	1202	CLA	O2A-C1-C2	-2.30	102.60	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1302	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
14	2	511	CLA	CHB-C1B-NB	2.30	126.69	124.26
14	B	1225	CLA	C1-C2-C3	-2.30	122.07	126.04
14	H	1225	CLA	C1-C2-C3	-2.30	122.07	126.04
14	3	511	CLA	C3B-C4B-NB	-2.30	108.38	110.52
17	5	521	BCR	C33-C5-C6	-2.30	121.95	124.53
20	H	5002	LMG	O2-C2-C1	-2.30	104.47	110.05
14	a	509	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
14	s	508	CLA	C3B-C4B-NB	-2.30	108.39	110.52
17	H	4014	BCR	C23-C22-C21	-2.30	115.42	118.94
14	G	1117	CLA	CHD-C1D-ND	-2.29	122.34	124.45
14	3	502	CLA	C3B-C4B-NB	-2.29	108.39	110.52
14	a	508	CLA	C3B-C4B-NB	-2.29	108.39	110.52
18	G	5005	LHG	C11-C10-C9	-2.29	102.78	114.42
18	A	5005	LHG	C11-C10-C9	-2.29	102.78	114.42
17	f	4014	BCR	C23-C22-C21	-2.29	115.42	118.94
14	e	1113	CLA	O2A-CGA-O1A	-2.29	117.58	123.30
14	s	512	CLA	CHB-C1B-NB	2.29	126.69	124.26
17	d	521	BCR	C16-C15-C14	-2.29	118.77	123.47
17	e	4002	BCR	C35-C13-C12	2.29	121.69	118.08
20	B	5002	LMG	O2-C2-C1	-2.29	104.47	110.05
17	B	4014	BCR	C23-C22-C21	-2.29	115.42	118.94
14	A	1137	CLA	C2A-C1A-CHA	2.29	127.87	123.86
17	v	522	BCR	C36-C18-C19	2.29	121.69	118.08
14	H	1227	CLA	CHD-C1D-ND	-2.29	122.35	124.45
14	J	1302	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
14	G	1114	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
21	f	1852	SQD	C4-C3-C2	2.29	114.82	110.82
17	5	524	BCR	C37-C22-C23	2.29	121.69	118.08
17	H	4004	BCR	C39-C30-C25	-2.29	106.58	110.30
14	e	1237	CLA	O2D-CGD-CBD	2.29	115.34	111.27
14	H	1239	CLA	CHC-C4B-NB	2.29	126.68	124.26
18	e	5005	LHG	C11-C10-C9	-2.29	102.80	114.42
14	f	1231	CLA	CHD-C1D-ND	-2.29	122.35	124.45
17	f	4004	BCR	C39-C30-C25	-2.29	106.59	110.30
18	A	5004	LHG	C5-O7-C7	-2.29	112.16	117.79
18	e	5004	LHG	C5-O7-C7	-2.29	112.16	117.79
14	l	1302	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
14	Y	504	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
14	A	1104	CLA	C1-C2-C3	-2.29	122.08	126.04
14	B	1223	CLA	C3B-C4B-NB	-2.29	108.39	110.52
21	1	822	SQD	O48-C23-O10	-2.29	117.82	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1119	CLA	C2D-C1D-ND	-2.29	108.42	110.10
14	A	1113	CLA	O2A-CGA-O1A	-2.29	117.60	123.30
14	e	1104	CLA	C1-C2-C3	-2.29	122.09	126.04
21	B	1852	SQD	C4-C3-C2	2.29	114.82	110.82
14	G	1122	CLA	C3B-C4B-NB	-2.29	108.39	110.52
14	f	1238	CLA	C3B-C4B-NB	-2.29	108.39	110.52
14	m	1103	CLA	C3B-C4B-NB	-2.29	108.39	110.52
14	q	504	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
18	G	5007	LHG	C27-C26-C25	-2.29	102.82	114.42
20	T	5104	LMG	O2-C2-C1	-2.29	104.49	110.05
17	t	521	BCR	C29-C30-C25	2.29	114.00	110.48
14	H	1204	CLA	O2D-CGD-CBD	2.29	115.33	111.27
14	A	1115	CLA	CHC-C4B-NB	2.28	126.68	124.26
14	G	1011	CLA	CMD-C2D-C3D	2.28	132.87	127.61
18	G	5007	LHG	C18-C17-C16	-2.28	102.83	114.42
14	2	513	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	s	504	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	t	508	CLA	C2D-C1D-ND	-2.28	108.42	110.10
14	H	1226	CLA	C2B-C1B-NB	-2.28	108.70	110.23
18	B	1842	LHG	O8-C23-C24	2.28	119.07	111.91
18	G	5004	LHG	C5-O7-C7	-2.28	112.17	117.79
17	1	524	BCR	C20-C21-C22	-2.28	124.05	127.31
14	1	504	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
14	2	502	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
14	r	502	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
18	A	5007	LHG	C18-C17-C16	-2.28	102.83	114.42
17	G	4002	BCR	C35-C13-C12	2.28	121.67	118.08
14	H	1012	CLA	CAA-CBA-CGA	-2.28	106.58	113.25
17	q	522	BCR	C1-C6-C7	2.28	122.24	115.78
18	e	5007	LHG	C18-C17-C16	-2.28	102.84	114.42
14	e	1129	CLA	C2D-C1D-ND	-2.28	108.42	110.10
14	G	1105	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	s	502	CLA	C3B-C4B-NB	-2.28	108.40	110.52
17	d	523	BCR	C33-C5-C4	2.28	118.00	113.62
14	4	508	CLA	CHC-C1C-NC	2.28	127.66	124.20
14	3	510	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
14	A	1114	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
18	e	5007	LHG	C27-C26-C25	-2.28	102.85	114.42
14	B	1012	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
14	a	506	CLA	CHB-C1B-NB	2.28	126.67	124.26
17	B	4004	BCR	C39-C30-C25	-2.28	106.60	110.30
17	s	524	BCR	C1-C6-C5	-2.28	119.40	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	n	4019	BCR	C40-C30-C25	-2.28	106.60	110.30
14	f	1012	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
14	4	511	CLA	C2D-C1D-ND	-2.28	108.42	110.10
14	e	1108	CLA	O2D-CGD-CBD	2.28	115.32	111.27
14	t	508	CLA	CHC-C1C-NC	2.28	127.66	124.20
14	r	512	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	Y	522	BCR	C1-C6-C7	2.28	122.22	115.78
14	A	1109	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
14	e	1114	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
14	4	503	CLA	C3B-C4B-NB	-2.28	108.40	110.52
17	1	521	BCR	C2-C1-C6	2.28	113.99	110.48
14	A	1103	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
20	f	5002	LMG	O2-C2-C1	-2.28	104.51	110.05
17	L	4019	BCR	C40-C30-C25	-2.28	106.61	110.30
17	s	522	BCR	C21-C20-C19	-2.28	116.11	123.22
19	G	1849	LMU	C3'-C4'-C5'	2.28	114.30	110.24
14	e	1115	CLA	CHC-C4B-NB	2.28	126.67	124.26
17	1	522	BCR	C1-C6-C7	2.28	122.22	115.78
17	q	521	BCR	C2-C1-C6	2.28	113.98	110.48
17	Z	521	BCR	C20-C19-C18	-2.28	120.02	126.42
18	H	1842	LHG	O8-C23-C24	2.28	119.05	111.91
14	t	507	CLA	CHC-C4B-NB	2.28	126.67	124.26
17	A	4008	BCR	C20-C19-C18	-2.28	120.03	126.42
17	2	521	BCR	C20-C19-C18	-2.28	120.03	126.42
18	A	5007	LHG	C27-C26-C25	-2.27	102.88	114.42
14	a	512	CLA	CHB-C1B-NB	2.27	126.67	124.26
17	3	522	BCR	C21-C20-C19	-2.27	116.12	123.22
18	f	1842	LHG	O8-C23-C24	2.27	119.05	111.91
14	G	1103	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
20	J	5104	LMG	O2-C2-C1	-2.27	104.52	110.05
14	Z	501	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
14	4	509	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
14	u	512	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	r	502	CLA	C3B-C4B-NB	-2.27	108.41	110.52
14	e	1125	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
17	e	4008	BCR	C20-C19-C18	-2.27	120.03	126.42
14	H	1209	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	Z	502	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
14	a	510	CLA	O2A-CGA-O1A	-2.27	117.64	123.30
14	e	1137	CLA	C2A-C1A-CHA	2.27	127.83	123.86
14	G	1108	CLA	O2D-CGD-CBD	2.27	115.30	111.27
17	4	521	BCR	C29-C30-C25	2.27	113.98	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	506	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	B	1012	CLA	C11-C12-C13	-2.27	108.58	115.92
14	V	1502	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
14	H	1239	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
14	A	1119	CLA	C2D-C1D-ND	-2.27	108.43	110.10
14	b	511	CLA	C2D-C1D-ND	-2.27	108.43	110.10
17	6	523	BCR	C33-C5-C4	2.27	117.98	113.62
14	3	512	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	t	503	CLA	C3B-C4B-NB	-2.27	108.41	110.52
14	H	1239	CLA	O2D-CGD-CBD	2.27	115.30	111.27
14	H	1012	CLA	C11-C12-C13	-2.27	108.59	115.92
17	A	4002	BCR	C35-C13-C12	2.27	121.65	118.08
14	f	1012	CLA	C11-C12-C13	-2.27	108.59	115.92
19	A	1849	LMU	C3'-C4'-C5'	2.27	114.28	110.24
14	A	1111	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	A	1134	CLA	C3B-C4B-NB	-2.27	108.41	110.52
14	f	1236	CLA	CHB-C4A-NA	2.27	127.65	124.51
17	Y	521	BCR	C2-C1-C6	2.27	113.97	110.48
14	e	1130	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
17	r	521	BCR	C20-C19-C18	-2.27	120.05	126.42
14	b	508	CLA	CHC-C1C-NC	2.27	127.64	124.20
14	A	1105	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	B	1221	CLA	C2A-C1A-CHA	2.27	127.82	123.86
14	G	1130	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
17	r	524	BCR	C1-C6-C5	-2.27	119.42	122.61
17	c	521	BCR	C15-C16-C17	-2.27	118.83	123.47
14	B	1204	CLA	O2D-CGD-CBD	2.27	115.30	111.27
14	G	1237	CLA	O2D-CGD-CBD	2.27	115.30	111.27
20	l	5104	LMG	O2-C2-C1	-2.27	104.54	110.05
14	A	1129	CLA	C2D-C1D-ND	-2.27	108.43	110.10
17	2	524	BCR	C1-C6-C5	-2.27	119.42	122.61
14	2	501	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
17	H	4014	BCR	C38-C26-C25	2.27	127.07	124.53
17	B	4006	BCR	C28-C27-C26	-2.26	110.03	114.08
14	G	1011	CLA	OBD-CAD-C3D	2.26	133.97	128.52
21	B	1852	SQD	O48-C23-O10	-2.26	117.88	123.59
14	A	1011	CLA	CMD-C2D-C3D	2.26	132.82	127.61
17	G	4008	BCR	C20-C19-C18	-2.26	120.06	126.42
14	3	504	CLA	CHB-C1B-NB	2.26	126.65	124.26
14	r	501	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
14	A	1108	CLA	O2D-CGD-CBD	2.26	115.29	111.27
14	B	1239	CLA	O2D-CGD-CBD	2.26	115.29	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	521	BCR	C29-C30-C25	2.26	113.97	110.48
14	A	1122	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	G	1134	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	G	1109	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
14	e	1103	CLA	CAA-CBA-CGA	-2.26	106.64	113.25
14	B	1238	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	H	1214	CLA	CHB-C1B-NB	2.26	126.65	124.26
17	a	522	BCR	C21-C20-C19	-2.26	116.16	123.22
14	f	1239	CLA	O2D-CGD-CBD	2.26	115.29	111.27
14	s	510	CLA	O2A-CGA-O1A	-2.26	117.66	123.30
14	H	1231	CLA	CHD-C1D-ND	-2.26	122.38	124.45
14	5	512	CLA	CHB-C1B-NB	2.26	126.65	124.26
14	G	1022	CLA	CAA-CBA-CGA	-2.26	106.65	113.25
14	e	1022	CLA	CAA-CBA-CGA	-2.26	106.65	113.25
18	f	1855	LHG	C11-C10-C9	-2.26	102.95	114.42
14	H	1221	CLA	C2A-C1A-CHA	2.26	127.81	123.86
14	e	1011	CLA	CMD-C2D-C3D	2.26	132.81	127.61
14	A	1237	CLA	O2D-CGD-CBD	2.26	115.28	111.27
17	5	521	BCR	C15-C16-C17	-2.26	118.85	123.47
19	e	1849	LMU	C3'-C4'-C5'	2.26	114.27	110.24
14	f	1023	CLA	CMD-C2D-C3D	2.26	132.81	127.61
14	a	511	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	A	1022	CLA	CAA-CBA-CGA	-2.26	106.65	113.25
17	f	4006	BCR	C28-C27-C26	-2.26	110.05	114.08
14	e	1133	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
14	e	1105	CLA	CHB-C1B-NB	2.26	126.65	124.26
14	f	1219	CLA	CHC-C4B-NB	2.26	126.65	124.26
14	U	1103	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	H	1208	CLA	CHB-C4A-NA	2.26	127.63	124.51
21	H	1852	SQD	O48-C23-O10	-2.26	117.90	123.59
14	f	1221	CLA	C2A-C1A-CHA	2.26	127.81	123.86
18	B	1855	LHG	C11-C10-C9	-2.26	102.97	114.42
17	v	523	BCR	C33-C5-C4	2.26	117.95	113.62
21	f	1852	SQD	O48-C23-O10	-2.26	117.90	123.59
17	u	521	BCR	C15-C16-C17	-2.26	118.85	123.47
14	f	1224	CLA	C1-C2-C3	-2.26	122.14	126.04
14	H	1238	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	f	1212	CLA	C3B-C4B-NB	-2.26	108.42	110.52
14	b	509	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
21	H	1852	SQD	O6-C1-C2	2.26	111.83	108.30
17	e	4002	BCR	C38-C26-C27	2.26	117.95	113.62
17	T	4012	BCR	C28-C27-C26	-2.26	110.05	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1214	CLA	CHB-C1B-NB	2.25	126.64	124.26
14	G	1129	CLA	C2D-C1D-ND	-2.25	108.44	110.10
14	H	1224	CLA	C1-C2-C3	-2.25	122.14	126.04
14	G	1107	CLA	CAA-CBA-CGA	-2.25	106.67	113.25
14	f	1204	CLA	O2D-CGD-CBD	2.25	115.27	111.27
14	d	502	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
21	H	1852	SQD	C4-C3-C2	2.25	114.76	110.82
14	2	512	CLA	CHB-C4A-NA	2.25	127.63	124.51
14	V	1501	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
14	q	508	CLA	CMB-C2B-C3B	2.25	132.04	126.59
14	H	1226	CLA	CHC-C1C-NC	2.25	127.62	124.20
14	A	1134	CLA	C4-C3-C5	2.25	119.06	115.27
14	4	508	CLA	C3B-C4B-NB	-2.25	108.43	110.52
18	H	1855	LHG	C11-C10-C9	-2.25	102.99	114.42
14	e	1109	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
17	J	4012	BCR	C28-C27-C26	-2.25	110.06	114.08
15	e	2001	PQN	C21-C20-C18	-2.25	108.64	115.92
14	a	504	CLA	CHB-C1B-NB	2.25	126.64	124.26
14	B	1239	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
14	B	1224	CLA	C1-C2-C3	-2.25	122.15	126.04
14	A	1125	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
17	l	4012	BCR	C28-C27-C26	-2.25	110.06	114.08
17	L	4219	BCR	C24-C23-C22	-2.25	122.83	126.23
14	B	1231	CLA	CHD-C1D-ND	-2.25	122.39	124.45
14	m	1401	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
14	A	1115	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
14	B	1214	CLA	CHB-C1B-NB	2.25	126.64	124.26
14	B	1023	CLA	CMD-C2D-C3D	2.25	132.79	127.61
14	L	1501	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
14	H	1023	CLA	CMD-C2D-C3D	2.25	132.79	127.61
17	n	4219	BCR	C24-C23-C22	-2.25	122.84	126.23
14	6	502	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
14	B	1239	CLA	CHC-C4B-NB	2.25	126.64	124.26
14	G	1111	CLA	CHB-C1B-NB	2.25	126.64	124.26
14	s	506	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	A	2001	PQN	C21-C20-C18	-2.25	108.65	115.92
14	t	508	CLA	C3B-C4B-NB	-2.25	108.43	110.52
17	n	4020	BCR	C21-C20-C19	-2.25	116.20	123.22
14	n	1501	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
14	G	1115	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
14	G	1103	CLA	C3C-C4C-NC	-2.25	108.05	110.57
14	f	1239	CLA	O2A-CGA-O1A	-2.25	117.92	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	q	822	SQD	O48-C23-C24	2.25	118.96	111.91
14	A	1107	CLA	CAA-CBA-CGA	-2.25	106.69	113.25
14	f	1211	CLA	C3B-C4B-NB	-2.25	108.43	110.52
18	H	1855	LHG	C18-C17-C16	-2.25	103.02	114.42
14	G	1134	CLA	C4-C3-C5	2.25	119.05	115.27
14	e	1011	CLA	OBD-CAD-C3D	2.25	133.93	128.52
17	L	4020	BCR	C21-C20-C19	-2.25	116.21	123.22
14	K	1103	CLA	C3B-C4B-NB	-2.25	108.43	110.52
14	f	1223	CLA	C3B-C4B-NB	-2.25	108.43	110.52
14	L	1501	CLA	C2A-C1A-CHA	2.25	127.79	123.86
14	1	508	CLA	CMB-C2B-C3B	2.25	132.03	126.59
17	A	4002	BCR	C38-C26-C27	2.25	117.93	113.62
14	A	1011	CLA	OBD-CAD-C3D	2.25	133.92	128.52
14	t	509	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
17	V	4020	BCR	C21-C20-C19	-2.24	116.21	123.22
14	A	1130	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
17	G	4002	BCR	C38-C26-C27	2.24	117.93	113.62
20	f	5002	LMG	C35-C34-C33	-2.24	103.03	114.42
14	Y	508	CLA	CMB-C2B-C3B	2.24	132.02	126.59
21	Y	822	SQD	O48-C23-C24	2.24	118.95	111.91
14	m	1105	CLA	O2D-CGD-CBD	2.24	115.25	111.27
14	H	1226	CLA	C3B-C2B-C1B	2.24	109.87	107.16
18	f	1855	LHG	C18-C17-C16	-2.24	103.04	114.42
20	B	5002	LMG	C35-C34-C33	-2.24	103.04	114.42
18	B	1855	LHG	C18-C17-C16	-2.24	103.04	114.42
14	A	1121	CLA	C2D-C1D-ND	-2.24	108.45	110.10
14	B	1012	CLA	CHB-C1B-NB	2.24	126.63	124.26
14	H	1219	CLA	CHC-C4B-NB	2.24	126.63	124.26
14	e	1107	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
14	B	1211	CLA	C3B-C4B-NB	-2.24	108.44	110.52
14	H	1211	CLA	C3B-C4B-NB	-2.24	108.44	110.52
17	V	4219	BCR	C24-C23-C22	-2.24	122.85	126.23
14	B	1215	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	G	2001	PQN	C21-C20-C18	-2.24	108.68	115.92
17	H	4014	BCR	C8-C9-C10	-2.24	115.50	118.94
17	H	4006	BCR	C28-C27-C26	-2.24	110.08	114.08
14	s	503	CLA	CAA-CBA-CGA	-2.24	106.56	112.51
14	B	1236	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	p	170	FMN	C9A-C5A-N5	-2.24	120.00	122.43
14	e	1134	CLA	C4-C3-C5	2.24	119.04	115.27
17	d	522	BCR	C21-C20-C19	-2.24	116.23	123.22
14	U	1105	CLA	O2D-CGD-CBD	2.24	115.25	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1852	SQD	O6-C1-C2	2.24	111.80	108.30
17	B	4009	BCR	C1-C6-C5	-2.24	119.46	122.61
14	H	1220	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
22	P	170	FMN	C9A-C5A-N5	-2.24	120.00	122.43
14	Z	502	CLA	C3B-C4B-NB	-2.24	108.44	110.52
14	u	509	CLA	C3B-C4B-NB	-2.24	108.44	110.52
14	B	1226	CLA	CHC-C1C-NC	2.24	127.60	124.20
17	e	4011	BCR	C23-C24-C25	-2.24	120.92	127.20
20	H	5002	LMG	C35-C34-C33	-2.24	103.07	114.42
17	v	522	BCR	C21-C20-C19	-2.24	116.24	123.22
17	Z	524	BCR	C1-C6-C5	-2.24	119.47	122.61
17	6	522	BCR	C21-C20-C19	-2.23	116.24	123.22
14	3	503	CLA	CAA-CBA-CGA	-2.23	106.58	112.51
14	Z	507	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
14	n	1501	CLA	C2A-C1A-CHA	2.23	127.77	123.86
14	Y	508	CLA	CHC-C1C-NC	2.23	127.59	124.20
14	G	1125	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
14	K	1105	CLA	O2D-CGD-CBD	2.23	115.24	111.27
14	e	1134	CLA	C3B-C4B-NB	-2.23	108.44	110.52
14	t	509	CLA	C2A-C1A-CHA	2.23	127.76	123.86
14	f	1226	CLA	C2B-C1B-NB	-2.23	108.73	110.23
17	H	4009	BCR	C1-C6-C5	-2.23	119.47	122.61
14	v	502	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
14	e	1121	CLA	C2A-C1A-CHA	2.23	127.76	123.86
21	1	822	SQD	O48-C23-C24	2.23	118.91	111.91
14	a	513	CLA	CHC-C4B-NB	2.23	126.62	124.26
14	G	1121	CLA	C2D-C1D-ND	-2.23	108.46	110.10
14	G	1128	CLA	C3B-C2B-C1B	2.23	109.86	107.16
17	s	524	BCR	C38-C26-C27	2.23	117.90	113.62
14	2	502	CLA	C3B-C4B-NB	-2.23	108.45	110.52
14	H	1211	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
14	f	1220	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
14	A	1132	CLA	C2D-C1D-ND	-2.23	108.46	110.10
14	A	1121	CLA	C2A-C1A-CHA	2.23	127.76	123.86
14	f	1226	CLA	CHC-C1C-NC	2.23	127.58	124.20
14	2	507	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
17	G	4011	BCR	C23-C24-C25	-2.23	120.94	127.20
17	c	522	BCR	C3-C4-C5	-2.23	110.10	114.08
17	B	4005	BCR	C21-C20-C19	-2.23	116.26	123.22
14	B	1219	CLA	CHC-C4B-NB	2.23	126.62	124.26
14	f	1012	CLA	CHB-C1B-NB	2.23	126.62	124.26
14	u	511	CLA	CHB-C1B-NB	2.23	126.62	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	4006	BCR	C29-C30-C25	2.23	113.91	110.48
14	B	1220	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
17	H	4005	BCR	C21-C20-C19	-2.23	116.27	123.22
14	b	509	CLA	C2A-C1A-CHA	2.23	127.75	123.86
17	A	4011	BCR	C23-C24-C25	-2.23	120.95	127.20
22	X	170	FMN	C9A-C5A-N5	-2.23	120.01	122.43
21	H	1852	SQD	C44-O6-C1	2.23	118.09	113.74
14	e	1115	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
14	A	1135	CLA	CHB-C1B-NB	2.23	126.61	124.26
14	s	507	CLA	O2A-CGA-O1A	-2.23	117.75	123.30
14	A	1133	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
14	V	1501	CLA	C2A-C1A-CHA	2.23	127.75	123.86
14	r	507	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
14	d	511	CLA	CHD-C1D-ND	-2.23	122.41	124.45
14	f	1211	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
14	r	503	CLA	C3B-C4B-NB	-2.22	108.45	110.52
14	5	509	CLA	C3B-C4B-NB	-2.22	108.45	110.52
17	o	4021	BCR	C8-C7-C6	-2.22	120.96	127.20
17	f	4014	BCR	C8-C9-C10	-2.22	115.53	118.94
14	l	1302	CLA	O2D-CGD-CBD	2.22	115.22	111.27
17	Y	522	BCR	C1-C6-C5	-2.22	119.48	122.61
17	5	521	BCR	C31-C1-C6	-2.22	106.69	110.30
17	u	521	BCR	C31-C1-C6	-2.22	106.69	110.30
14	f	1208	CLA	CHB-C4A-NA	2.22	127.59	124.51
14	u	512	CLA	CHB-C4A-NA	2.22	127.59	124.51
14	K	1401	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
14	e	1119	CLA	C2D-C1D-ND	-2.22	108.47	110.10
14	G	1133	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
17	Y	522	BCR	C21-C20-C19	-2.22	116.28	123.22
18	G	5006	LHG	C27-C26-C25	-2.22	103.14	114.42
17	B	4014	BCR	C8-C9-C10	-2.22	115.53	118.94
20	J	5104	LMG	C1-C2-C3	-2.22	105.37	110.00
20	T	5104	LMG	C1-C2-C3	-2.22	105.37	110.00
14	e	1111	CLA	CHB-C1B-NB	2.22	126.61	124.26
14	B	1212	CLA	C3B-C4B-NB	-2.22	108.45	110.52
14	1	508	CLA	CHC-C1C-NC	2.22	127.57	124.20
14	d	504	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
17	f	4005	BCR	C21-C20-C19	-2.22	116.29	123.22
17	H	4006	BCR	C29-C30-C25	2.22	113.90	110.48
14	H	1236	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	c	521	BCR	C31-C1-C6	-2.22	106.70	110.30
14	4	509	CLA	C2A-C1A-CHA	2.22	127.74	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	4009	BCR	C1-C6-C5	-2.22	119.49	122.61
14	G	1121	CLA	C2A-C1A-CHA	2.22	127.74	123.86
14	G	1104	CLA	CHD-C1D-ND	-2.22	122.41	124.45
14	a	503	CLA	CAA-CBA-CGA	-2.22	106.62	112.51
18	e	5006	LHG	C27-C26-C25	-2.22	103.16	114.42
14	c	511	CLA	CHB-C1B-NB	2.22	126.61	124.26
14	e	1135	CLA	CHB-C1B-NB	2.22	126.61	124.26
17	f	4009	BCR	C36-C18-C19	2.22	121.57	118.08
14	6	511	CLA	CHD-C1D-ND	-2.22	122.42	124.45
17	M	4021	BCR	C8-C7-C6	-2.22	120.97	127.20
14	A	1128	CLA	C3B-C2B-C1B	2.22	109.84	107.16
17	b	522	BCR	C11-C12-C13	-2.22	120.19	126.42
18	A	5006	LHG	C27-C26-C25	-2.22	103.17	114.42
17	a	523	BCR	C11-C12-C13	-2.22	120.19	126.42
17	H	4009	BCR	C36-C18-C19	2.22	121.57	118.08
14	s	505	CLA	C2D-C1D-ND	-2.22	108.47	110.10
14	c	512	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	1	522	BCR	C21-C20-C19	-2.22	116.30	123.22
17	q	522	BCR	C21-C20-C19	-2.22	116.30	123.22
20	l	5104	LMG	C1-C2-C3	-2.22	105.38	110.00
14	q	508	CLA	CHC-C1C-NC	2.22	127.57	124.20
14	U	1401	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
14	B	1208	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	t	522	BCR	C11-C12-C13	-2.22	120.19	126.42
21	f	1852	SQD	O6-C1-C2	2.22	111.76	108.30
17	5	522	BCR	C3-C4-C5	-2.22	110.12	114.08
14	H	1215	CLA	CHB-C1B-NB	2.22	126.60	124.26
17	t	523	BCR	C7-C8-C9	-2.22	122.89	126.23
14	t	503	CLA	C2A-C1A-CHA	2.21	127.73	123.86
14	e	1103	CLA	C3C-C4C-NC	-2.21	108.09	110.57
14	B	1211	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
17	u	522	BCR	C3-C4-C5	-2.21	110.12	114.08
21	q	822	SQD	O6-C1-C2	2.21	111.76	108.30
17	4	522	BCR	C11-C12-C13	-2.21	120.20	126.42
14	G	1130	CLA	C2D-C1D-ND	-2.21	108.47	110.10
14	r	509	CLA	CHB-C1B-NB	2.21	126.60	124.26
14	A	1103	CLA	C3C-C4C-NC	-2.21	108.09	110.57
14	3	516	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
14	r	508	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
17	V	4219	BCR	C4-C5-C6	-2.21	119.52	122.73
14	f	1239	CLA	CHC-C4B-NB	2.21	126.60	124.26
17	B	4009	BCR	C36-C18-C19	2.21	121.56	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	1215	CLA	CHB-C1B-NB	2.21	126.60	124.26
14	A	1104	CLA	CHD-C1D-ND	-2.21	122.42	124.45
14	a	516	CLA	O2A-CGA-O1A	-2.21	117.79	123.30
17	A	4011	BCR	C8-C9-C10	2.21	122.33	118.94
14	A	1119	CLA	C3B-C4B-NB	-2.21	108.47	110.52
14	G	1119	CLA	C3B-C4B-NB	-2.21	108.47	110.52
14	b	508	CLA	C3B-C4B-NB	-2.21	108.47	110.52
14	b	503	CLA	C2A-C1A-CHA	2.21	127.72	123.86
17	3	523	BCR	C11-C12-C13	-2.21	120.21	126.42
14	c	519	CLA	CHC-C4B-NB	2.21	126.59	124.26
14	Z	508	CLA	C3B-C4B-NB	-2.21	108.47	110.52
18	e	5008	LHG	C11-C10-C9	-2.21	103.22	114.42
17	V	4019	BCR	C15-C16-C17	-2.21	118.95	123.47
14	e	1128	CLA	C3B-C2B-C1B	2.21	109.83	107.16
17	b	523	BCR	C7-C8-C9	-2.21	122.90	126.23
14	e	1104	CLA	CHD-C1D-ND	-2.21	122.43	124.45
18	A	5008	LHG	C11-C10-C9	-2.21	103.23	114.42
14	c	509	CLA	C3B-C4B-NB	-2.21	108.47	110.52
14	3	513	CLA	CHC-C4B-NB	2.20	126.59	124.26
14	f	1236	CLA	CHB-C1B-NB	2.20	126.59	124.26
14	v	511	CLA	CHD-C1D-ND	-2.20	122.43	124.45
18	G	5008	LHG	C11-C10-C9	-2.20	103.23	114.42
17	q	523	BCR	C8-C7-C6	-2.20	121.01	127.20
17	4	523	BCR	C7-C8-C9	-2.20	122.91	126.23
14	Z	512	CLA	CHB-C4A-NA	2.20	127.56	124.51
17	b	523	BCR	C36-C18-C19	2.20	121.55	118.08
14	s	516	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
17	3	524	BCR	C38-C26-C27	2.20	117.85	113.62
14	e	1121	CLA	C2D-C1D-ND	-2.20	108.48	110.10
14	B	1221	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	f	1221	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	b	507	CLA	C3B-C4B-NB	-2.20	108.47	110.52
21	1	822	SQD	O6-C1-C2	2.20	111.74	108.30
14	2	503	CLA	C3B-C4B-NB	-2.20	108.47	110.52
14	G	1132	CLA	C2D-C1D-ND	-2.20	108.48	110.10
14	4	503	CLA	C2A-C1A-CHA	2.20	127.71	123.86
14	3	507	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
14	5	512	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	A	1104	CLA	O1D-CGD-CBD	2.20	128.99	124.48
17	d	521	BCR	C2-C1-C6	2.20	113.87	110.48
17	e	4011	BCR	C8-C9-C10	2.20	122.32	118.94
14	Z	503	CLA	C3B-C4B-NB	-2.20	108.47	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1119	CLA	C3B-C4B-NB	-2.20	108.47	110.52
14	B	1236	CLA	CHB-C1B-NB	2.20	126.59	124.26
17	q	522	BCR	C1-C6-C5	-2.20	119.52	122.61
17	4	523	BCR	C36-C18-C19	2.20	121.54	118.08
17	H	4014	BCR	C31-C1-C6	-2.20	106.73	110.30
14	H	1209	CLA	C2A-C1A-CHA	2.20	127.70	123.86
17	G	4011	BCR	C8-C9-C10	2.20	122.32	118.94
17	G	4003	BCR	C8-C7-C6	-2.20	121.03	127.20
17	t	523	BCR	C36-C18-C19	2.20	121.54	118.08
14	B	1226	CLA	C3B-C2B-C1B	2.20	109.82	107.16
14	f	1223	CLA	C1-C2-C3	-2.20	122.24	126.04
17	s	523	BCR	C11-C12-C13	-2.20	120.24	126.42
17	2	521	BCR	C15-C16-C17	-2.20	118.97	123.47
17	l	4012	BCR	C23-C24-C25	-2.20	121.03	127.20
17	W	4021	BCR	C8-C7-C6	-2.20	121.03	127.20
14	v	504	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
21	Y	822	SQD	O6-C1-C2	2.20	111.73	108.30
14	J	1302	CLA	O2D-CGD-CBD	2.20	115.17	111.27
14	A	1011	CLA	CHA-C1A-NA	-2.20	121.36	126.40
17	a	524	BCR	C38-C26-C27	2.20	117.84	113.62
14	6	504	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
21	B	1852	SQD	C44-O6-C1	2.20	118.03	113.74
14	e	1104	CLA	O1D-CGD-CBD	2.20	128.98	124.48
17	4	522	BCR	C3-C4-C5	-2.20	110.15	114.08
14	Z	508	CLA	O2A-CGA-O1A	-2.20	117.82	123.30
17	f	4006	BCR	C29-C30-C25	2.20	113.86	110.48
19	H	1843	LMU	O1'-C1'-C2'	2.20	111.73	108.30
14	H	1236	CLA	CHB-C1B-NB	2.20	126.58	124.26
18	L	5221	LHG	C27-C26-C25	-2.20	103.28	114.42
14	f	1209	CLA	C2A-C1A-CHA	2.20	127.70	123.86
17	J	4012	BCR	C23-C24-C25	-2.20	121.04	127.20
17	e	4003	BCR	C8-C7-C6	-2.20	121.04	127.20
14	r	509	CLA	CMB-C2B-C3B	2.19	131.90	126.59
14	G	1136	CLA	C7-C6-C5	-2.19	107.40	113.36
18	S	5001	LHG	C11-C10-C9	-2.19	103.29	114.42
14	2	509	CLA	CMB-C2B-C3B	2.19	131.90	126.59
18	n	5221	LHG	C27-C26-C25	-2.19	103.29	114.42
19	B	1843	LMU	O1'-C1'-C2'	2.19	111.73	108.30
17	Y	523	BCR	C8-C7-C6	-2.19	121.04	127.20
17	r	521	BCR	C15-C16-C17	-2.19	118.98	123.47
14	A	1120	CLA	CMB-C2B-C3B	2.19	131.90	126.59
17	1	522	BCR	C1-C6-C5	-2.19	119.53	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	522	BCR	C3-C4-C5	-2.19	110.16	114.08
14	5	502	CLA	C3B-C4B-NB	-2.19	108.48	110.52
14	A	1136	CLA	C7-C6-C5	-2.19	107.41	113.36
17	Z	523	BCR	C37-C22-C23	2.19	121.53	118.08
14	G	1118	CLA	C2A-C1A-CHA	2.19	127.69	123.86
14	G	1104	CLA	O1D-CGD-CBD	2.19	128.97	124.48
14	A	1013	CLA	O2D-CGD-CBD	2.19	115.16	111.27
14	T	1302	CLA	O2D-CGD-CBD	2.19	115.16	111.27
17	1	523	BCR	C8-C7-C6	-2.19	121.05	127.20
17	T	4012	BCR	C23-C24-C25	-2.19	121.05	127.20
17	B	4014	BCR	C31-C1-C6	-2.19	106.75	110.30
14	G	1120	CLA	CMB-C2B-C3B	2.19	131.89	126.59
14	2	508	CLA	C3B-C4B-NB	-2.19	108.48	110.52
14	H	1212	CLA	C3B-C4B-NB	-2.19	108.48	110.52
17	l	4013	BCR	C23-C22-C21	2.19	122.30	118.94
14	B	1209	CLA	C2A-C1A-CHA	2.19	127.69	123.86
14	B	1223	CLA	C1-C2-C3	-2.19	122.26	126.04
14	5	511	CLA	CHB-C1B-NB	2.19	126.58	124.26
17	G	4007	BCR	C4-C5-C6	-2.19	119.55	122.73
17	A	4003	BCR	C8-C7-C6	-2.19	121.05	127.20
14	e	1013	CLA	O2D-CGD-CBD	2.19	115.16	111.27
17	B	4004	BCR	C8-C7-C6	-2.19	121.06	127.20
14	J	1303	CLA	CHC-C4B-NB	2.19	126.57	124.26
17	G	4007	BCR	C2-C1-C6	2.19	113.85	110.48
14	B	1226	CLA	C2B-C1B-NB	-2.19	108.77	110.23
14	H	1221	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
17	e	4007	BCR	C33-C5-C4	2.19	117.82	113.62
14	Z	509	CLA	CHB-C1B-NB	2.19	126.57	124.26
17	Z	521	BCR	C15-C16-C17	-2.19	118.99	123.47
14	G	1139	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
17	t	522	BCR	C3-C4-C5	-2.19	110.17	114.08
14	2	508	CLA	O2A-CGA-O1A	-2.19	117.85	123.30
17	L	4219	BCR	C4-C5-C6	-2.19	119.56	122.73
17	d	523	BCR	C16-C15-C14	-2.19	119.00	123.47
17	q	522	BCR	C36-C18-C19	2.19	121.52	118.08
14	e	1104	CLA	CMB-C2B-C3B	2.19	131.88	126.59
17	J	4013	BCR	C23-C22-C21	2.19	122.30	118.94
14	e	1136	CLA	C7-C6-C5	-2.19	107.42	113.36
17	J	4012	BCR	C10-C11-C12	-2.19	116.40	123.22
17	l	4012	BCR	C10-C11-C12	-2.19	116.40	123.22
14	e	1120	CLA	CMB-C2B-C3B	2.19	131.88	126.59
14	c	507	CLA	O2A-CGA-O1A	-2.18	117.85	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	4014	BCR	C31-C1-C6	-2.18	106.75	110.30
14	e	1132	CLA	C2D-C1D-ND	-2.18	108.49	110.10
18	V	5221	LHG	C27-C26-C25	-2.18	103.33	114.42
17	t	523	BCR	C8-C7-C6	-2.18	121.07	127.20
18	I	5001	LHG	C11-C10-C9	-2.18	103.34	114.42
20	f	5002	LMG	O7-C10-O9	-2.18	118.42	123.70
14	G	1112	CLA	CHB-C1B-NB	2.18	126.57	124.26
14	u	502	CLA	C3B-C4B-NB	-2.18	108.49	110.52
14	A	1011	CLA	C2B-C1B-NB	-2.18	108.77	110.23
17	T	4013	BCR	C23-C22-C21	2.18	122.29	118.94
17	6	523	BCR	C16-C15-C14	-2.18	119.00	123.47
14	G	1013	CLA	O2D-CGD-CBD	2.18	115.15	111.27
14	a	507	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
14	a	512	CLA	CHB-C4A-NA	2.18	127.53	124.51
17	V	4219	BCR	C19-C18-C17	-2.18	115.59	118.94
18	G	5004	LHG	C11-C10-C9	-2.18	103.34	114.42
14	r	516	CLA	C3B-C4B-NB	-2.18	108.49	110.52
14	B	1226	CLA	CHA-C4D-ND	2.18	137.06	132.50
14	f	1226	CLA	C3B-C2B-C1B	2.18	109.80	107.16
14	A	1139	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
17	4	523	BCR	C8-C7-C6	-2.18	121.07	127.20
14	H	1213	CLA	CMB-C2B-C3B	2.18	131.87	126.59
14	2	509	CLA	CHB-C1B-NB	2.18	126.57	124.26
14	l	1303	CLA	CHC-C4B-NB	2.18	126.57	124.26
17	6	521	BCR	C2-C1-C6	2.18	113.84	110.48
17	G	4002	BCR	C31-C1-C6	-2.18	106.76	110.30
14	u	507	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
18	k	5001	LHG	C11-C10-C9	-2.18	103.35	114.42
14	2	516	CLA	C3B-C4B-NB	-2.18	108.49	110.52
14	q	502	CLA	C3B-C4B-NB	-2.18	108.49	110.52
14	e	1011	CLA	CHA-C1A-NA	-2.18	121.40	126.40
14	e	1127	CLA	C2A-C1A-CHA	2.18	127.67	123.86
14	A	1104	CLA	CMB-C2B-C3B	2.18	131.87	126.59
14	Z	509	CLA	CMB-C2B-C3B	2.18	131.87	126.59
17	v	522	BCR	C2-C3-C4	-2.18	106.50	111.38
14	5	507	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
14	f	1210	CLA	CHB-C1B-NB	2.18	126.56	124.26
14	A	1118	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
14	u	501	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
14	f	1213	CLA	CMB-C2B-C3B	2.18	131.87	126.59
17	T	4012	BCR	C10-C11-C12	-2.18	116.41	123.22
14	B	1213	CLA	CMB-C2B-C3B	2.18	131.87	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4002	BCR	C31-C1-C6	-2.18	106.76	110.30
14	G	1135	CLA	CHB-C1B-NB	2.18	126.56	124.26
14	H	1204	CLA	C3B-C4B-NB	-2.18	108.49	110.52
14	A	1127	CLA	C2A-C1A-CHA	2.18	127.67	123.86
14	e	1122	CLA	C2A-C1A-CHA	2.18	127.67	123.86
21	f	1852	SQD	C44-O6-C1	2.18	117.99	113.74
17	H	4004	BCR	C8-C7-C6	-2.18	121.08	127.20
14	f	1238	CLA	C2D-C1D-ND	-2.18	108.50	110.10
14	e	1139	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
17	A	4007	BCR	C30-C25-C26	-2.18	119.55	122.61
17	n	4219	BCR	C4-C5-C6	-2.18	119.57	122.73
17	A	4007	BCR	C33-C5-C4	2.18	117.80	113.62
20	B	5002	LMG	O7-C10-O9	-2.18	118.44	123.70
14	G	1137	CLA	C3A-C2A-C1A	2.18	104.60	101.34
17	5	522	BCR	C27-C26-C25	-2.18	119.57	122.73
14	e	1011	CLA	C2B-C1B-NB	-2.18	108.77	110.23
14	G	1104	CLA	CMB-C2B-C3B	2.18	131.86	126.59
14	r	508	CLA	C3B-C4B-NB	-2.18	108.50	110.52
14	A	1117	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	A	1128	CLA	C2D-C1D-ND	-2.18	108.50	110.10
17	b	523	BCR	C8-C7-C6	-2.17	121.09	127.20
14	t	507	CLA	O2D-CGD-CBD	2.17	115.13	111.27
18	A	5004	LHG	C11-C10-C9	-2.17	103.39	114.42
17	n	4219	BCR	C29-C28-C27	-2.17	106.52	111.38
17	q	522	BCR	C15-C16-C17	-2.17	119.02	123.47
18	e	5004	LHG	C11-C10-C9	-2.17	103.39	114.42
17	G	4007	BCR	C16-C15-C14	-2.17	119.02	123.47
17	V	4219	BCR	C29-C28-C27	-2.17	106.52	111.38
14	5	501	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
14	A	1101	CLA	C1-C2-C3	-2.17	122.28	126.04
14	Y	502	CLA	C3B-C4B-NB	-2.17	108.50	110.52
14	e	1101	CLA	C1-C2-C3	-2.17	122.28	126.04
17	u	522	BCR	C27-C26-C25	-2.17	119.58	122.73
17	v	523	BCR	C16-C15-C14	-2.17	119.02	123.47
14	G	1011	CLA	CHA-C1A-NA	-2.17	121.42	126.40
14	f	1226	CLA	CHA-C4D-ND	2.17	137.04	132.50
17	A	4007	BCR	C2-C1-C6	2.17	113.83	110.48
14	A	1121	CLA	CHA-C1A-NA	-2.17	121.42	126.40
14	G	1121	CLA	CHA-C1A-NA	-2.17	121.42	126.40
17	6	522	BCR	C2-C3-C4	-2.17	106.53	111.38
20	H	5002	LMG	O7-C10-O9	-2.17	118.45	123.70
14	H	1223	CLA	C1-C2-C3	-2.17	122.29	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	U	4104	BCR	C30-C25-C24	2.17	121.92	115.78
17	L	4019	BCR	C15-C16-C17	-2.17	119.03	123.47
17	n	4019	BCR	C15-C16-C17	-2.17	119.03	123.47
14	B	1210	CLA	CHB-C1B-NB	2.17	126.56	124.26
14	H	1206	CLA	CHB-C1B-NB	2.17	126.56	124.26
14	f	1206	CLA	CHB-C1B-NB	2.17	126.56	124.26
17	H	4006	BCR	C10-C11-C12	-2.17	116.44	123.22
14	B	1206	CLA	CHB-C1B-NB	2.17	126.55	124.26
17	e	4002	BCR	C31-C1-C6	-2.17	106.78	110.30
17	2	523	BCR	C37-C22-C23	2.17	121.50	118.08
14	A	1122	CLA	C2A-C1A-CHA	2.17	127.65	123.86
14	G	1118	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
14	G	1117	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	e	4007	BCR	C30-C25-C26	-2.17	119.56	122.61
14	H	1226	CLA	CMC-C2C-C1C	-2.17	121.74	125.04
14	c	501	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
14	T	1303	CLA	CHC-C4B-NB	2.17	126.55	124.26
14	c	502	CLA	C3B-C4B-NB	-2.17	108.50	110.52
18	G	5005	LHG	C27-C26-C25	-2.17	103.42	114.42
18	G	5003	LHG	C27-C26-C25	-2.17	103.42	114.42
18	A	5005	LHG	C27-C26-C25	-2.17	103.42	114.42
17	q	522	BCR	C16-C17-C18	-2.17	124.22	127.31
18	e	5003	LHG	C27-C26-C25	-2.17	103.43	114.42
17	A	4007	BCR	C4-C5-C6	-2.17	119.59	122.73
18	n	5221	LHG	C18-C17-C16	-2.17	103.43	114.42
14	A	1115	CLA	CHB-C1B-NB	2.17	126.55	124.26
14	s	509	CLA	CHB-C1B-NB	2.17	126.55	124.26
14	s	513	CLA	CHC-C4B-NB	2.17	126.55	124.26
17	f	4004	BCR	C8-C7-C6	-2.17	121.12	127.20
14	G	1127	CLA	C2A-C1A-CHA	2.17	127.65	123.86
17	v	521	BCR	C2-C1-C6	2.17	113.81	110.48
14	B	1238	CLA	C2D-C1D-ND	-2.17	108.51	110.10
14	d	505	CLA	C2D-C1D-ND	-2.17	108.51	110.10
14	B	1226	CLA	CMC-C2C-C1C	-2.17	121.74	125.04
14	A	1137	CLA	C3A-C2A-C1A	2.16	104.58	101.34
14	A	1130	CLA	C2D-C1D-ND	-2.16	108.51	110.10
18	A	5003	LHG	C27-C26-C25	-2.16	103.44	114.42
17	c	522	BCR	C27-C26-C25	-2.16	119.59	122.73
14	5	519	CLA	CHC-C4B-NB	2.16	126.55	124.26
17	B	4006	BCR	C10-C11-C12	-2.16	116.46	123.22
18	e	5005	LHG	C27-C26-C25	-2.16	103.44	114.42
14	e	1013	CLA	C2C-C1C-NC	-2.16	107.94	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	507	CLA	CHA-C1A-NA	-2.16	121.44	126.40
17	s	522	BCR	C27-C26-C25	-2.16	119.59	122.73
14	Y	513	CLA	CHB-C1B-NB	2.16	126.55	124.26
14	A	1107	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
14	e	1128	CLA	C2D-C1D-ND	-2.16	108.51	110.10
14	q	503	CLA	C2A-C1A-CHA	2.16	127.64	123.86
17	G	4007	BCR	C33-C5-C4	2.16	117.77	113.62
14	r	510	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
14	G	1112	CLA	C2A-C1A-CHA	2.16	127.64	123.86
14	H	1226	CLA	CHA-C4D-ND	2.16	137.02	132.50
17	1	522	BCR	C36-C18-C19	2.16	121.48	118.08
17	m	4104	BCR	C30-C25-C24	2.16	121.89	115.78
14	U	1401	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
14	e	1118	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
14	e	1121	CLA	CHA-C1A-NA	-2.16	121.45	126.40
14	B	1023	CLA	CAC-C3C-C2C	-2.16	123.83	127.53
14	m	1401	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
14	A	1118	CLA	C2A-C1A-CHA	2.16	127.64	123.86
14	K	1401	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
17	d	522	BCR	C2-C3-C4	-2.16	106.55	111.38
17	G	4007	BCR	C30-C25-C26	-2.16	119.57	122.61
17	K	4104	BCR	C30-C25-C24	2.16	121.89	115.78
19	f	1843	LMU	O1'-C1'-C2'	2.16	111.67	108.30
14	H	1023	CLA	CAC-C3C-C2C	-2.16	123.84	127.53
14	4	507	CLA	C3B-C4B-NB	-2.16	108.51	110.52
14	B	1219	CLA	C2D-C1D-ND	-2.16	108.51	110.10
17	e	4007	BCR	C4-C5-C6	-2.16	119.60	122.73
17	e	4007	BCR	C2-C1-C6	2.16	113.80	110.48
17	r	523	BCR	C37-C22-C23	2.16	121.48	118.08
18	L	5221	LHG	C18-C17-C16	-2.16	103.47	114.42
18	V	5221	LHG	C18-C17-C16	-2.16	103.47	114.42
14	H	1215	CLA	C3B-C4B-NB	-2.16	108.51	110.52
14	f	1023	CLA	CAC-C3C-C2C	-2.16	123.84	127.53
14	G	1107	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
14	f	1226	CLA	CMC-C2C-C1C	-2.16	121.75	125.04
14	2	510	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
17	f	4006	BCR	C10-C11-C12	-2.16	116.48	123.22
14	A	1112	CLA	C2A-C1A-CHA	2.16	127.63	123.86
14	s	512	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	Z	517	CLA	C3B-C4B-NB	-2.16	108.51	110.52
14	H	1210	CLA	CHB-C1B-NB	2.16	126.54	124.26
14	m	1103	CLA	O2A-CGA-O1A	-2.16	118.15	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1219	CLA	C2D-C1D-ND	-2.16	108.52	110.10
14	q	507	CLA	CHA-C1A-NA	-2.16	121.46	126.40
14	e	1118	CLA	C2A-C1A-CHA	2.16	127.63	123.86
14	5	508	CLA	CHC-C1C-NC	2.16	127.47	124.20
14	H	1228	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
14	f	1215	CLA	C3B-C4B-NB	-2.16	108.52	110.52
17	J	4013	BCR	C29-C30-C25	2.16	113.80	110.48
14	Z	516	CLA	C3B-C4B-NB	-2.15	108.52	110.52
14	t	507	CLA	C3B-C4B-NB	-2.15	108.52	110.52
14	K	1103	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
17	t	524	BCR	C28-C27-C26	-2.15	110.23	114.08
14	u	508	CLA	CHC-C1C-NC	2.15	127.47	124.20
17	L	4219	BCR	C29-C28-C27	-2.15	106.56	111.38
14	4	507	CLA	O2D-CGD-CBD	2.15	115.09	111.27
14	H	1208	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
17	u	523	BCR	C34-C9-C8	2.15	121.47	118.08
14	G	1011	CLA	C2B-C1B-NB	-2.15	108.79	110.23
17	a	523	BCR	C3-C4-C5	-2.15	110.23	114.08
17	L	4219	BCR	C19-C18-C17	-2.15	115.64	118.94
14	e	1022	CLA	CHB-C1B-NB	2.15	126.53	124.26
17	3	523	BCR	C3-C4-C5	-2.15	110.23	114.08
14	H	1226	CLA	C3D-C2D-C1D	2.15	108.77	105.83
14	G	1022	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	Y	507	CLA	CHA-C1A-NA	-2.15	121.47	126.40
14	G	1013	CLA	C2C-C1C-NC	-2.15	107.96	109.97
14	B	1234	CLA	C2A-C1A-CHA	2.15	127.62	123.86
14	r	512	CLA	CHB-C1B-NB	2.15	126.53	124.26
14	u	519	CLA	CHC-C4B-NB	2.15	126.53	124.26
17	f	4014	BCR	C29-C30-C25	2.15	113.79	110.48
14	e	1117	CLA	CHB-C4A-NA	2.15	127.49	124.51
17	s	523	BCR	C3-C4-C5	-2.15	110.24	114.08
14	Y	507	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
14	f	1208	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
14	G	1122	CLA	C2A-C1A-CHA	2.15	127.62	123.86
14	f	1234	CLA	C2A-C1A-CHA	2.15	127.62	123.86
14	G	1101	CLA	C1-C2-C3	-2.15	122.32	126.04
14	d	501	CLA	O2D-CGD-CBD	2.15	115.09	111.27
14	1	511	CLA	CHB-C1B-NB	2.15	126.53	124.26
14	G	1124	CLA	CMB-C2B-C3B	2.15	131.79	126.59
14	A	1013	CLA	C2C-C1C-NC	-2.15	107.96	109.97
17	Y	522	BCR	C16-C17-C18	-2.15	124.24	127.31
14	d	508	CLA	O2A-CGA-O1A	-2.15	117.94	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4007	BCR	C16-C15-C14	-2.15	119.07	123.47
14	t	509	CLA	CHB-C1B-NB	2.15	126.53	124.26
14	B	1204	CLA	C3B-C4B-NB	-2.15	108.52	110.52
14	H	1216	CLA	C2D-C1D-ND	-2.15	108.52	110.10
14	G	1013	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	H	1218	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	u	503	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	v	507	CLA	CHA-C1A-NA	-2.15	121.48	126.40
17	T	4012	BCR	C2-C1-C6	2.15	113.79	110.48
17	1	522	BCR	C15-C16-C17	-2.15	119.08	123.47
14	r	517	CLA	C3B-C4B-NB	-2.15	108.52	110.52
14	A	1112	CLA	CHB-C1B-NB	2.15	126.53	124.26
14	Z	510	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
14	e	1124	CLA	CMB-C2B-C3B	2.15	131.79	126.59
17	L	4219	BCR	C16-C15-C14	-2.15	119.08	123.47
14	1	513	CLA	CHB-C1B-NB	2.15	126.53	124.26
14	e	1115	CLA	CHB-C1B-NB	2.15	126.53	124.26
14	6	508	CLA	O2A-CGA-O1A	-2.15	117.95	123.30
14	f	1218	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	Z	502	CLA	C2A-C1A-CHA	2.15	127.61	123.86
14	G	1128	CLA	C2D-C1D-ND	-2.15	108.52	110.10
14	a	505	CLA	C2D-C1D-ND	-2.15	108.52	110.10
17	B	4014	BCR	C19-C18-C17	-2.15	115.65	118.94
14	l	1302	CLA	C2A-C1A-CHA	2.15	127.61	123.86
14	B	1215	CLA	C3B-C4B-NB	-2.15	108.53	110.52
14	G	1115	CLA	CHB-C1B-NB	2.14	126.53	124.26
14	f	1226	CLA	C3D-C2D-C1D	2.14	108.76	105.83
17	f	4014	BCR	C19-C18-C17	-2.14	115.65	118.94
14	6	507	CLA	CHA-C1A-NA	-2.14	121.49	126.40
17	Y	522	BCR	C36-C18-C19	2.14	121.45	118.08
14	B	1218	CLA	CHD-C1D-ND	-2.14	122.48	124.45
17	l	4013	BCR	C29-C30-C25	2.14	113.78	110.48
17	V	4219	BCR	C16-C15-C14	-2.14	119.08	123.47
14	A	1022	CLA	CHB-C1B-NB	2.14	126.53	124.26
17	r	524	BCR	C15-C16-C17	-2.14	119.08	123.47
14	v	501	CLA	O2D-CGD-CBD	2.14	115.08	111.27
14	H	1234	CLA	C2A-C1A-CHA	2.14	127.61	123.86
17	H	4014	BCR	C19-C18-C17	-2.14	115.65	118.94
14	d	509	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
17	1	524	BCR	C3-C4-C5	-2.14	110.25	114.08
17	B	4014	BCR	C29-C30-C25	2.14	113.78	110.48
17	e	4007	BCR	C16-C15-C14	-2.14	119.09	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	509	CLA	CHB-C1B-NB	2.14	126.52	124.26
17	Y	524	BCR	C3-C4-C5	-2.14	110.25	114.08
14	U	1103	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
17	n	4019	BCR	C38-C26-C27	2.14	117.73	113.62
17	T	4013	BCR	C29-C30-C25	2.14	113.78	110.48
17	Y	522	BCR	C15-C16-C17	-2.14	119.09	123.47
14	c	508	CLA	CHC-C1C-NC	2.14	127.45	124.20
14	2	512	CLA	CHB-C1B-NB	2.14	126.52	124.26
14	G	1113	CLA	CHB-C1B-NB	2.14	126.52	124.26
14	J	1302	CLA	C2A-C1A-CHA	2.14	127.60	123.86
14	G	1122	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
14	H	1238	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
17	r	522	BCR	C30-C25-C26	-2.14	119.60	122.61
14	q	504	CLA	CAC-C3C-C4C	2.14	127.58	124.81
17	Y	524	BCR	C10-C11-C12	-2.14	116.55	123.22
17	v	524	BCR	C23-C22-C21	-2.14	115.66	118.94
17	L	4019	BCR	C38-C26-C27	2.14	117.72	113.62
17	3	522	BCR	C27-C26-C25	-2.14	119.63	122.73
14	Z	508	CLA	C2D-C1D-ND	-2.14	108.53	110.10
14	c	504	CLA	C2A-C1A-CHA	2.14	127.60	123.86
19	e	1848	LMU	C2'-C3'-C4'	2.14	114.56	109.68
15	B	2002	PQN	C9-C10-C5	2.14	121.64	119.26
17	Z	524	BCR	C15-C16-C17	-2.14	119.10	123.47
14	B	1208	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
17	G	4002	BCR	C27-C26-C25	-2.14	119.63	122.73
17	t	522	BCR	C27-C26-C25	-2.14	119.63	122.73
14	f	1224	CLA	C3B-C4B-NB	-2.14	108.53	110.52
14	v	509	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
14	B	1224	CLA	C2A-C1A-CHA	2.14	127.59	123.86
14	e	1107	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
17	V	4019	BCR	C38-C26-C27	2.14	117.72	113.62
14	5	507	CLA	CHC-C4B-NB	2.14	126.52	124.26
17	L	4019	BCR	C21-C20-C19	-2.14	116.55	123.22
17	T	4012	BCR	C15-C14-C13	-2.14	124.26	127.31
14	6	501	CLA	O2D-CGD-CBD	2.14	115.06	111.27
17	b	523	BCR	C8-C9-C10	-2.14	115.66	118.94
17	n	4219	BCR	C19-C18-C17	-2.14	115.66	118.94
14	e	1112	CLA	C2A-C1A-CHA	2.14	127.59	123.86
14	H	1240	CLA	CHB-C1B-NB	2.13	126.52	124.26
14	a	503	CLA	CHB-C1B-NB	2.13	126.52	124.26
14	q	513	CLA	CHB-C1B-NB	2.13	126.52	124.26
14	u	507	CLA	CHC-C4B-NB	2.13	126.52	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	506	CLA	CMB-C2B-C3B	2.13	131.76	126.59
14	Y	506	CLA	CMB-C2B-C3B	2.13	131.76	126.59
17	Z	522	BCR	C30-C25-C26	-2.13	119.61	122.61
14	3	505	CLA	C2D-C1D-ND	-2.13	108.53	110.10
14	e	1130	CLA	C2D-C1D-ND	-2.13	108.53	110.10
14	2	517	CLA	C3B-C4B-NB	-2.13	108.53	110.52
17	2	524	BCR	C15-C16-C17	-2.13	119.10	123.47
17	Y	524	BCR	C1-C6-C7	2.13	121.82	115.78
14	A	1124	CLA	CMB-C2B-C3B	2.13	131.76	126.59
14	1	504	CLA	CAC-C3C-C4C	2.13	127.58	124.81
14	A	1013	CLA	CHD-C1D-ND	-2.13	122.49	124.45
14	d	513	CLA	CHB-C1B-NB	2.13	126.52	124.26
14	t	512	CLA	CHB-C1B-NB	2.13	126.52	124.26
14	B	1226	CLA	C3D-C2D-C1D	2.13	108.74	105.83
17	4	522	BCR	C27-C26-C25	-2.13	119.63	122.73
14	1	502	CLA	C3B-C4B-NB	-2.13	108.54	110.52
14	c	503	CLA	CHD-C1D-ND	-2.13	122.49	124.45
18	f	1855	LHG	C29-C28-C27	-2.13	103.60	114.42
14	A	1101	CLA	CAC-C3C-C4C	2.13	127.58	124.81
17	n	4019	BCR	C21-C20-C19	-2.13	116.56	123.22
14	1	503	CLA	C2A-C1A-CHA	2.13	127.59	123.86
14	f	1206	CLA	C3C-C4C-NC	-2.13	108.18	110.57
14	e	1101	CLA	CAC-C3C-C4C	2.13	127.58	124.81
14	a	503	CLA	C2D-C1D-ND	-2.13	108.53	110.10
14	H	1219	CLA	O2D-CGD-CBD	2.13	115.06	111.27
17	q	524	BCR	C3-C4-C5	-2.13	110.27	114.08
17	5	523	BCR	C34-C9-C8	2.13	121.43	118.08
14	b	507	CLA	O2D-CGD-CBD	2.13	115.05	111.27
14	B	1228	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
14	1	507	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
17	q	524	BCR	C10-C11-C12	-2.13	116.57	123.22
14	f	1228	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
14	Z	506	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
17	1	524	BCR	C10-C11-C12	-2.13	116.57	123.22
14	G	1108	CLA	C1-C2-C3	-2.13	122.36	126.04
17	V	4019	BCR	C21-C20-C19	-2.13	116.57	123.22
17	q	524	BCR	C1-C6-C7	2.13	121.80	115.78
14	6	509	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
18	B	1855	LHG	C29-C28-C27	-2.13	103.62	114.42
14	3	503	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	3	512	CLA	CHB-C4A-NA	2.13	127.45	124.51
14	e	1116	CLA	CHC-C4B-NB	2.13	126.51	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1110	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
14	A	1126	CLA	C2A-C1A-CHA	2.13	127.58	123.86
14	5	504	CLA	C2A-C1A-CHA	2.13	127.58	123.86
14	Z	507	CLA	CHA-C1A-NA	-2.13	121.53	126.40
17	n	4022	BCR	C28-C27-C26	-2.13	110.28	114.08
14	H	1206	CLA	C3C-C4C-NC	-2.13	108.19	110.57
14	m	1401	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
14	1	516	CLA	CHD-C1D-ND	-2.13	122.50	124.45
14	4	512	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	Y	504	CLA	CAC-C3C-C4C	2.13	127.57	124.81
14	G	1115	CLA	C4-C3-C5	2.13	118.85	115.27
17	1	524	BCR	C1-C6-C7	2.13	121.80	115.78
17	c	523	BCR	C34-C9-C8	2.13	121.43	118.08
17	H	4014	BCR	C29-C30-C25	2.13	113.75	110.48
14	f	1231	CLA	C3B-C4B-NB	-2.13	108.54	110.52
14	A	1140	CLA	O2D-CGD-CBD	2.13	115.05	111.27
14	3	503	CLA	C2D-C1D-ND	-2.13	108.54	110.10
14	Y	511	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	Z	512	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	c	507	CLA	CHC-C4B-NB	2.13	126.51	124.26
14	f	1235	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	f	1238	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
14	e	1121	CLA	C1-C2-C3	-2.13	122.37	126.04
14	v	508	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
17	l	4012	BCR	C15-C14-C13	-2.13	124.28	127.31
17	6	524	BCR	C36-C18-C19	2.13	121.43	118.08
14	q	506	CLA	CMB-C2B-C3B	2.13	131.74	126.59
14	s	503	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	d	507	CLA	CHA-C1A-NA	-2.13	121.53	126.40
19	A	1848	LMU	C2'-C3'-C4'	2.13	114.53	109.68
14	B	1219	CLA	O2D-CGD-CBD	2.12	115.04	111.27
17	d	524	BCR	C36-C18-C19	2.12	121.42	118.08
14	f	1224	CLA	C2A-C1A-CHA	2.12	127.57	123.86
14	A	1122	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
14	G	1110	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
14	q	507	CLA	O2A-CGA-O1A	-2.12	118.00	123.30
14	A	1108	CLA	C1-C2-C3	-2.12	122.37	126.04
14	G	1140	CLA	O2D-CGD-CBD	2.12	115.04	111.27
17	6	524	BCR	C23-C22-C21	-2.12	115.68	118.94
14	A	1110	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
14	f	1219	CLA	C2D-C1D-ND	-2.12	108.54	110.10
14	A	1104	CLA	O2D-CGD-O1D	-2.12	119.69	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	q	505	CLA	CHC-C4B-NB	2.12	126.50	124.26
14	B	1234	CLA	CHA-C1A-NA	-2.12	121.53	126.40
14	e	1122	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
17	t	523	BCR	C8-C9-C10	-2.12	115.68	118.94
14	T	1302	CLA	C2A-C1A-CHA	2.12	127.57	123.86
14	U	1401	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	H	1855	LHG	C29-C28-C27	-2.12	103.65	114.42
15	H	2002	PQN	C9-C10-C5	2.12	121.62	119.26
17	d	524	BCR	C33-C5-C4	2.12	117.69	113.62
14	B	1206	CLA	C3C-C4C-NC	-2.12	108.19	110.57
14	B	1201	CLA	C6-C7-C8	-2.12	109.06	115.92
14	e	1137	CLA	C3A-C2A-C1A	2.12	104.52	101.34
14	H	1224	CLA	C2A-C1A-CHA	2.12	127.57	123.86
14	e	1119	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
14	e	1108	CLA	C1-C2-C3	-2.12	122.37	126.04
14	4	502	CLA	C3B-C4B-NB	-2.12	108.55	110.52
14	r	506	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
14	3	509	CLA	CHB-C1B-NB	2.12	126.50	124.26
14	1	517	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
18	A	5001	LHG	O10-C23-C24	-2.12	115.46	123.73
14	3	502	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
14	2	507	CLA	CHA-C1A-NA	-2.12	121.54	126.40
14	f	1219	CLA	O2D-CGD-CBD	2.12	115.03	111.27
17	v	524	BCR	C36-C18-C19	2.12	121.42	118.08
14	Z	503	CLA	C2D-C1D-ND	-2.12	108.54	110.10
14	f	1201	CLA	C6-C7-C8	-2.12	109.07	115.92
14	K	1401	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
17	b	522	BCR	C27-C26-C25	-2.12	119.65	122.73
18	G	5001	LHG	O10-C23-C24	-2.12	115.46	123.73
17	d	524	BCR	C23-C22-C21	-2.12	115.69	118.94
14	2	506	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
19	G	1848	LMU	C2'-C3'-C4'	2.12	114.52	109.68
17	J	4012	BCR	C2-C1-C6	2.12	113.74	110.48
17	J	4012	BCR	C15-C14-C13	-2.12	124.29	127.31
14	Y	503	CLA	C2A-C1A-CHA	2.12	127.56	123.86
14	6	508	CLA	CHD-C1D-ND	-2.12	122.51	124.45
14	B	1238	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
14	b	502	CLA	C3B-C4B-NB	-2.12	108.55	110.52
14	5	502	CLA	C2A-C1A-CHA	2.12	127.56	123.86
17	e	4002	BCR	C27-C26-C25	-2.12	119.66	122.73
14	c	501	CLA	C2A-C1A-CHA	2.12	127.56	123.86
14	u	504	CLA	C2A-C1A-CHA	2.12	127.56	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	523	BCR	C8-C9-C10	-2.12	115.69	118.94
14	3	502	CLA	C2A-C1A-CHA	2.12	127.56	123.86
17	n	4219	BCR	C16-C15-C14	-2.12	119.14	123.47
14	r	507	CLA	CHA-C1A-NA	-2.12	121.55	126.40
14	s	509	CLA	O1A-CGA-CBA	2.12	129.88	123.08
17	r	522	BCR	C33-C5-C4	2.12	117.68	113.62
17	1	522	BCR	C16-C17-C18	-2.12	124.29	127.31
17	b	524	BCR	C28-C27-C26	-2.12	110.30	114.08
14	f	1231	CLA	CMA-C3A-C2A	-2.12	105.30	113.83
17	6	524	BCR	C33-C5-C4	2.12	117.68	113.62
14	e	1110	CLA	CHB-C1B-NB	2.11	126.50	124.26
14	e	1126	CLA	C2A-C1A-CHA	2.11	127.56	123.86
14	B	1231	CLA	CMA-C3A-C2A	-2.11	105.30	113.83
14	G	1121	CLA	C1-C2-C3	-2.11	122.39	126.04
15	f	2002	PQN	C9-C10-C5	2.11	121.61	119.26
14	a	502	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
14	A	1113	CLA	CHB-C1B-NB	2.11	126.50	124.26
14	A	1129	CLA	CMB-C2B-C3B	2.11	131.71	126.59
14	e	1129	CLA	CMB-C2B-C3B	2.11	131.71	126.59
14	s	502	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
14	H	1234	CLA	CHA-C1A-NA	-2.11	121.56	126.40
14	H	1235	CLA	O2D-CGD-CBD	2.11	115.02	111.27
14	H	1231	CLA	CMA-C3A-C2A	-2.11	105.30	113.83
14	e	1140	CLA	O2D-CGD-CBD	2.11	115.02	111.27
17	A	4002	BCR	C27-C26-C25	-2.11	119.66	122.73
14	G	1116	CLA	CHC-C4B-NB	2.11	126.49	124.26
14	G	1022	CLA	CHB-C1B-NB	2.11	126.49	124.26
14	e	1112	CLA	CHB-C1B-NB	2.11	126.49	124.26
17	4	524	BCR	C28-C27-C26	-2.11	110.30	114.08
14	H	1201	CLA	C6-C7-C8	-2.11	109.09	115.92
14	f	1235	CLA	O2D-CGD-CBD	2.11	115.02	111.27
17	v	524	BCR	C33-C5-C4	2.11	117.67	113.62
14	q	502	CLA	CHC-C4B-NB	2.11	126.49	124.26
14	q	511	CLA	CHB-C1B-NB	2.11	126.49	124.26
14	v	512	CLA	CHC-C4B-NB	2.11	126.49	124.26
14	A	1022	CLA	CHD-C1D-ND	-2.11	122.51	124.45
14	e	1013	CLA	CHD-C1D-ND	-2.11	122.51	124.45
14	r	502	CLA	C2A-C1A-CHA	2.11	127.55	123.86
14	Y	517	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
14	2	507	CLA	C3B-C4B-NB	-2.11	108.56	110.52
14	B	1235	CLA	O2D-CGD-CBD	2.11	115.02	111.27
14	B	1216	CLA	C2D-C1D-ND	-2.11	108.55	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	s	502	CLA	C2A-C1A-CHA	2.11	127.55	123.86
14	e	1104	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
14	K	1401	CLA	CHB-C1B-NB	2.11	126.49	124.26
14	5	503	CLA	CHD-C1D-ND	-2.11	122.51	124.45
14	e	1112	CLA	O2D-CGD-CBD	2.11	115.02	111.27
14	5	501	CLA	C2A-C1A-CHA	2.11	127.55	123.86
14	2	519	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
17	2	522	BCR	C30-C25-C26	-2.11	119.64	122.61
14	b	504	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	Y	513	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
14	q	502	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
14	A	1119	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	B	1224	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	f	1204	CLA	C3B-C4B-NB	-2.11	108.56	110.52
14	G	1022	CLA	C4D-C3D-CAD	-2.11	105.61	108.10
14	G	1101	CLA	CAC-C3C-C4C	2.11	127.55	124.81
14	3	509	CLA	O1A-CGA-CBA	2.11	129.85	123.08
14	q	517	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
14	H	1224	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	f	1234	CLA	CHA-C1A-NA	-2.11	121.57	126.40
14	v	508	CLA	CHD-C1D-ND	-2.11	122.52	124.45
18	e	5001	LHG	O10-C23-C24	-2.11	115.51	123.73
14	u	503	CLA	C2A-C1A-CHA	2.11	127.54	123.86
14	H	1203	CLA	CHB-C1B-NB	2.11	126.49	124.26
14	5	511	CLA	CMB-C2B-C3B	2.11	131.69	126.59
17	G	4001	BCR	C37-C22-C21	-2.11	119.97	122.92
14	f	1012	CLA	C4-C3-C5	2.11	118.82	115.27
14	e	1132	CLA	C3B-C4B-NB	-2.11	108.56	110.52
14	H	1212	CLA	CMB-C2B-C3B	2.11	131.69	126.59
17	2	522	BCR	C33-C5-C4	2.11	117.66	113.62
17	A	4001	BCR	C37-C22-C21	-2.11	119.97	122.92
14	s	511	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
14	Y	512	CLA	CHB-C4A-NA	2.11	127.42	124.51
14	H	1213	CLA	CHC-C4B-NB	2.11	126.49	124.26
14	d	516	CLA	CHC-C4B-NB	2.11	126.49	124.26
14	H	1238	CLA	C2D-C1D-ND	-2.11	108.55	110.10
14	Z	519	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
17	a	523	BCR	C21-C20-C19	-2.11	116.64	123.22
14	a	502	CLA	C2A-C1A-CHA	2.11	127.54	123.86
14	e	1122	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	u	511	CLA	CMB-C2B-C3B	2.11	131.69	126.59
14	G	1104	CLA	O2D-CGD-O1D	-2.11	119.72	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	511	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
14	B	1226	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
14	f	1222	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
14	G	1126	CLA	C2A-C1A-CHA	2.11	127.54	123.86
14	r	502	CLA	O2A-CGA-O1A	-2.10	118.05	123.30
17	3	523	BCR	C21-C20-C19	-2.10	116.65	123.22
18	A	5002	LHG	C27-C26-C25	-2.10	103.74	114.42
14	B	1224	CLA	C3B-C4B-NB	-2.10	108.56	110.52
17	Z	522	BCR	C33-C5-C4	2.10	117.66	113.62
18	e	5002	LHG	C27-C26-C25	-2.10	103.74	114.42
14	r	519	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
14	L	1502	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	n	1502	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	Y	502	CLA	CHC-C4B-NB	2.10	126.48	124.26
14	e	1122	CLA	CHC-C4B-NB	2.10	126.48	124.26
14	f	1226	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
14	f	1203	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	f	1212	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	u	503	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
17	5	523	BCR	C8-C7-C6	-2.10	121.30	127.20
17	L	4022	BCR	C28-C27-C26	-2.10	110.32	114.08
14	5	511	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
14	Z	519	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	a	522	BCR	C27-C26-C25	-2.10	119.68	122.73
17	t	522	BCR	C36-C18-C19	2.10	121.39	118.08
14	B	1231	CLA	C3B-C4B-NB	-2.10	108.56	110.52
14	r	508	CLA	C2D-C1D-ND	-2.10	108.56	110.10
17	b	522	BCR	C30-C25-C26	-2.10	119.65	122.61
19	H	1843	LMU	C3-C2-C1	-2.10	104.17	113.49
17	s	523	BCR	C21-C20-C19	-2.10	116.66	123.22
14	A	1121	CLA	C1-C2-C3	-2.10	122.41	126.04
14	H	1203	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	H	1232	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
14	j	1302	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	T	1303	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	B	1212	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	1	513	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
14	q	516	CLA	CHD-C1D-ND	-2.10	122.52	124.45
14	t	504	CLA	CHD-C1D-ND	-2.10	122.52	124.45
14	H	1226	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
14	2	502	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	c	502	CLA	C2A-C1A-CHA	2.10	127.53	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	517	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	c	511	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
14	e	1113	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	A	1132	CLA	C3B-C4B-NB	-2.10	108.57	110.52
14	G	1129	CLA	CMB-C2B-C3B	2.10	131.67	126.59
14	A	1140	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	G	1119	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
14	a	509	CLA	O1A-CGA-CBA	2.10	129.82	123.08
14	3	501	CLA	CHD-C1D-ND	-2.10	122.53	124.45
17	u	523	BCR	C8-C7-C6	-2.10	121.31	127.20
14	B	1240	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	1	511	CLA	CHC-C4B-NB	2.10	126.48	124.26
14	H	1231	CLA	C3B-C4B-NB	-2.10	108.57	110.52
14	Z	508	CLA	CHC-C1C-NC	2.10	127.39	124.20
17	k	4018	BCR	C31-C1-C6	-2.10	106.89	110.30
17	A	4011	BCR	C16-C15-C14	-2.10	119.17	123.47
17	4	524	BCR	C16-C15-C14	-2.10	119.17	123.47
14	H	1222	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
21	H	1852	SQD	C3-C4-C5	2.10	113.98	110.24
14	A	1115	CLA	C4-C3-C5	2.10	118.80	115.27
14	H	1209	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
14	u	501	CLA	C2A-C1A-CHA	2.10	127.53	123.86
17	t	522	BCR	C30-C25-C26	-2.10	119.66	122.61
14	A	1129	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	f	1224	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	1	502	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
14	V	1501	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	5	503	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	3	511	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
20	f	5002	LMG	C31-C30-C29	-2.10	105.65	113.19
14	1	518	CLA	CHC-C4B-NB	2.10	126.48	124.26
17	4	522	BCR	C30-C25-C26	-2.10	119.66	122.61
19	f	1843	LMU	C3-C2-C1	-2.10	104.20	113.49
20	B	5002	LMG	C31-C30-C29	-2.10	105.65	113.19
14	2	502	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
17	H	4005	BCR	C16-C15-C14	-2.10	119.18	123.47
14	f	1240	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	G	5002	LHG	C27-C26-C25	-2.10	103.78	114.42
14	q	513	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
14	e	1115	CLA	C4-C3-C5	2.10	118.80	115.27
14	4	507	CLA	C2A-C1A-CHA	2.10	127.52	123.86
14	c	503	CLA	C2A-C1A-CHA	2.10	127.52	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1125	CLA	C11-C12-C13	-2.10	109.15	115.92
14	U	1401	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
14	G	1112	CLA	O2D-CGD-CBD	2.10	114.99	111.27
14	A	1116	CLA	CHC-C4B-NB	2.10	126.47	124.26
14	6	513	CLA	CHB-C1B-NB	2.10	126.47	124.26
14	2	507	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
14	B	1203	CLA	CMB-C2B-C3B	2.09	131.66	126.59
14	e	1022	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	B	1222	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
14	Z	507	CLA	C3B-C4B-NB	-2.09	108.57	110.52
14	t	502	CLA	C3B-C4B-NB	-2.09	108.57	110.52
14	1	505	CLA	CHC-C4B-NB	2.09	126.47	124.26
14	v	504	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	c	511	CLA	CMB-C2B-C3B	2.09	131.66	126.59
14	G	1110	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	G	1140	CLA	C2A-C1A-CHA	2.09	127.52	123.86
20	H	5002	LMG	C31-C30-C29	-2.09	105.67	113.19
14	A	1125	CLA	C11-C12-C13	-2.09	109.16	115.92
17	c	523	BCR	C8-C7-C6	-2.09	121.33	127.20
17	B	4005	BCR	C16-C15-C14	-2.09	119.19	123.47
14	f	1206	CLA	O1D-CGD-CBD	2.09	128.76	124.48
14	l	1303	CLA	C2A-C1A-CHA	2.09	127.52	123.86
14	H	1219	CLA	C1-O2A-CGA	2.09	121.93	116.44
19	B	1843	LMU	C3-C2-C1	-2.09	104.22	113.49
14	u	511	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
14	A	1122	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	2	508	CLA	CHC-C1C-NC	2.09	127.38	124.20
14	B	1225	CLA	CHC-C4B-NB	2.09	126.47	124.26
14	q	518	CLA	CHC-C4B-NB	2.09	126.47	124.26
14	e	1120	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	l	4012	BCR	C2-C1-C6	2.09	113.70	110.48
14	B	1216	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
14	H	1210	CLA	CMB-C2B-C3B	2.09	131.65	126.59
14	A	1108	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
14	H	1226	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	f	1216	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
14	A	1112	CLA	O2D-CGD-CBD	2.09	114.98	111.27
14	a	504	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
14	A	1110	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	4	509	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	B	1219	CLA	C1-O2A-CGA	2.09	121.93	116.44
17	f	4017	BCR	C8-C7-C6	-2.09	121.33	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	4	517	CLA	C2A-C1A-CHA	2.09	127.51	123.86
14	b	517	CLA	C2A-C1A-CHA	2.09	127.51	123.86
14	A	1013	CLA	C11-C12-C13	-2.09	109.17	115.92
17	f	4004	BCR	C34-C9-C8	2.09	121.37	118.08
18	n	5220	LHG	C27-C26-C25	-2.09	103.82	114.42
14	G	1122	CLA	CHC-C4B-NB	2.09	126.47	124.26
14	H	1219	CLA	CHB-C1B-NB	2.09	126.47	124.26
17	f	4004	BCR	C11-C12-C13	-2.09	120.55	126.42
14	B	1208	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	H	1216	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
14	t	507	CLA	C2A-C1A-CHA	2.09	127.51	123.86
14	Z	507	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
14	B	1235	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	H	1225	CLA	CHC-C4B-NB	2.09	126.47	124.26
18	L	5220	LHG	C27-C26-C25	-2.09	103.83	114.42
18	V	5220	LHG	C27-C26-C25	-2.09	103.83	114.42
14	1	512	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	6	505	CLA	C2D-C1D-ND	-2.09	108.57	110.10
14	G	1129	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
14	J	1303	CLA	C2A-C1A-CHA	2.09	127.51	123.86
14	f	1219	CLA	C1-O2A-CGA	2.09	121.92	116.44
14	A	1119	CLA	CMB-C2B-C3B	2.09	131.64	126.59
14	Z	502	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
17	B	4017	BCR	C8-C7-C6	-2.09	121.34	127.20
14	e	1119	CLA	CMB-C2B-C3B	2.09	131.64	126.59
14	f	1232	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
17	a	524	BCR	C23-C22-C21	-2.09	115.74	118.94
14	e	1108	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
14	H	1208	CLA	CHD-C1D-ND	-2.09	122.54	124.45
14	d	505	CLA	C3B-C4B-NB	-2.09	108.58	110.52
14	e	1101	CLA	C1-O2A-CGA	-2.09	110.97	116.44
14	Y	502	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
14	4	504	CLA	CHD-C1D-ND	-2.08	122.54	124.45
14	e	1130	CLA	CHD-C1D-ND	-2.08	122.54	124.45
17	3	524	BCR	C23-C22-C21	-2.08	115.74	118.94
18	e	5003	LHG	C18-C17-C16	-2.08	103.84	114.42
14	B	1238	CLA	O2A-C1-C2	-2.08	103.16	108.64
14	B	1012	CLA	C4-C3-C5	2.08	118.78	115.27
14	G	1101	CLA	C1-O2A-CGA	-2.08	110.98	116.44
14	r	503	CLA	CHD-C1D-ND	-2.08	122.54	124.45
14	v	513	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	v	516	CLA	CHC-C4B-NB	2.08	126.46	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1232	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
14	r	505	CLA	C3B-C4B-NB	-2.08	108.58	110.52
14	r	507	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
18	A	5003	LHG	C18-C17-C16	-2.08	103.85	114.42
14	G	1013	CLA	C11-C12-C13	-2.08	109.19	115.92
17	T	4015	BCR	C37-C22-C23	2.08	121.36	118.08
14	B	1203	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	Y	505	CLA	CHC-C4B-NB	2.08	126.46	124.26
17	V	4022	BCR	C28-C27-C26	-2.08	110.36	114.08
17	n	4219	BCR	C32-C1-C6	-2.08	106.92	110.30
14	6	505	CLA	C3B-C4B-NB	-2.08	108.58	110.52
17	b	524	BCR	C16-C15-C14	-2.08	119.21	123.47
17	e	4001	BCR	C37-C22-C21	-2.08	120.01	122.92
14	G	1120	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
14	G	1125	CLA	C11-C12-C13	-2.08	109.19	115.92
14	e	1013	CLA	C11-C12-C13	-2.08	109.19	115.92
14	H	1238	CLA	O2A-C1-C2	-2.08	103.16	108.64
14	G	1108	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
14	B	1021	CLA	O1D-CGD-CBD	2.08	128.74	124.48
14	b	507	CLA	C2A-C1A-CHA	2.08	127.50	123.86
14	f	1238	CLA	O2A-C1-C2	-2.08	103.16	108.64
14	Y	516	CLA	CHD-C1D-ND	-2.08	122.54	124.45
14	2	503	CLA	C2D-C1D-ND	-2.08	108.57	110.10
17	b	522	BCR	C36-C18-C19	2.08	121.36	118.08
14	H	1206	CLA	O1D-CGD-CBD	2.08	128.74	124.48
14	e	1129	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
14	1	502	CLA	CHC-C4B-NB	2.08	126.46	124.26
14	Y	511	CLA	CHC-C4B-NB	2.08	126.46	124.26
14	3	504	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
14	H	1226	CLA	CMC-C2C-C3C	2.08	131.76	126.12
14	u	502	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	H	4004	BCR	C11-C12-C13	-2.08	120.57	126.42
14	c	503	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
14	A	1120	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
14	5	503	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
17	Z	523	BCR	C8-C7-C6	-2.08	121.36	127.20
14	s	504	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
17	T	4012	BCR	C23-C22-C21	2.08	122.13	118.94
17	r	523	BCR	C8-C7-C6	-2.08	121.36	127.20
14	e	1109	CLA	CHC-C4B-NB	2.08	126.46	124.26
14	2	517	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
17	B	4004	BCR	C11-C12-C13	-2.08	120.58	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	q	502	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
14	v	508	CLA	CHC-C1C-NC	2.08	127.36	124.20
14	m	1401	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	t	506	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	G	1119	CLA	CMB-C2B-C3B	2.08	131.62	126.59
14	B	1221	CLA	CHA-C1A-NA	-2.08	121.64	126.40
14	f	1221	CLA	CHA-C1A-NA	-2.08	121.64	126.40
17	f	4005	BCR	C16-C15-C14	-2.08	119.22	123.47
14	G	1132	CLA	C3B-C4B-NB	-2.08	108.59	110.52
17	H	4017	BCR	C8-C7-C6	-2.08	121.37	127.20
14	B	1210	CLA	CMB-C2B-C3B	2.08	131.62	126.59
14	f	1210	CLA	CMB-C2B-C3B	2.08	131.62	126.59
17	d	522	BCR	C30-C25-C26	-2.08	119.69	122.61
14	r	508	CLA	CHC-C1C-NC	2.08	127.35	124.20
14	Y	502	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
14	v	516	CLA	CHB-C1B-NB	2.08	126.45	124.26
14	r	507	CLA	C3B-C4B-NB	-2.08	108.59	110.52
14	G	1104	CLA	C2A-C1A-CHA	2.08	127.49	123.86
18	G	5003	LHG	C18-C17-C16	-2.08	103.89	114.42
17	t	524	BCR	C16-C15-C14	-2.08	119.22	123.47
14	V	1502	CLA	CMB-C2B-C3B	2.08	131.62	126.59
18	e	5008	LHG	C27-C26-C25	-2.08	103.89	114.42
14	t	511	CLA	CHD-C1D-ND	-2.08	122.55	124.45
14	H	1224	CLA	C3B-C4B-NB	-2.08	108.59	110.52
14	v	505	CLA	C3B-C4B-NB	-2.08	108.59	110.52
18	A	5008	LHG	C27-C26-C25	-2.07	103.89	114.42
14	f	1236	CLA	CAA-CBA-CGA	-2.07	107.19	113.25
14	n	1501	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
14	r	517	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
14	B	1219	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	6	504	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	b	509	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	u	513	CLA	CHB-C1B-NB	2.07	126.45	124.26
17	l	4012	BCR	C23-C22-C21	2.07	122.12	118.94
14	e	1140	CLA	C2A-C1A-CHA	2.07	127.49	123.86
17	v	522	BCR	C30-C25-C26	-2.07	119.69	122.61
17	I	4018	BCR	C33-C5-C6	-2.07	122.20	124.53
17	I	4018	BCR	C31-C1-C6	-2.07	106.94	110.30
17	e	4011	BCR	C16-C15-C14	-2.07	119.23	123.47
14	f	1225	CLA	CHC-C4B-NB	2.07	126.45	124.26
14	e	1131	CLA	C7-C6-C5	-2.07	107.73	113.36
14	f	1226	CLA	CHB-C4A-NA	2.07	127.38	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	502	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
14	a	501	CLA	CHD-C1D-ND	-2.07	122.55	124.45
17	4	522	BCR	C36-C18-C19	2.07	121.34	118.08
14	B	1206	CLA	O1D-CGD-CBD	2.07	128.72	124.48
14	Z	518	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
17	2	523	BCR	C34-C9-C8	2.07	121.34	118.08
14	A	1101	CLA	C1-O2A-CGA	-2.07	111.01	116.44
14	c	507	CLA	CHA-C1A-NA	-2.07	121.65	126.40
14	f	1220	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	f	1021	CLA	O1D-CGD-CBD	2.07	128.72	124.48
17	J	4015	BCR	C37-C22-C23	2.07	121.34	118.08
14	B	1023	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	6	516	CLA	CHC-C4B-NB	2.07	126.45	124.26
14	b	512	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	G	5008	LHG	C27-C26-C25	-2.07	103.91	114.42
14	L	1501	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
14	6	508	CLA	CHC-C1C-NC	2.07	127.34	124.20
17	2	523	BCR	C8-C7-C6	-2.07	121.39	127.20
14	2	508	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	A	1119	CLA	C16-C15-C13	-2.07	109.23	115.92
17	G	4011	BCR	C16-C15-C14	-2.07	119.23	123.47
17	d	523	BCR	C15-C16-C17	-2.07	119.23	123.47
17	d	524	BCR	C16-C15-C14	-2.07	119.23	123.47
14	u	518	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
14	f	1208	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	s	503	CLA	C2D-C1D-ND	-2.07	108.58	110.10
21	B	1852	SQD	C3-C4-C5	2.07	113.93	110.24
14	f	1226	CLA	CMC-C2C-C3C	2.07	131.73	126.12
14	H	1221	CLA	CHA-C1A-NA	-2.07	121.66	126.40
14	r	505	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	u	519	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
14	G	1120	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	5	518	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
17	d	523	BCR	C8-C7-C6	-2.07	121.40	127.20
17	v	521	BCR	C10-C11-C12	-2.07	116.77	123.22
14	5	502	CLA	CHC-C4B-NB	2.07	126.44	124.26
14	q	519	CLA	CHB-C1B-NB	2.07	126.44	124.26
17	V	4020	BCR	C33-C5-C4	-2.07	109.65	113.62
17	r	521	BCR	C39-C30-C25	-2.07	106.95	110.30
17	B	4004	BCR	C34-C9-C8	2.07	121.33	118.08
14	j	1302	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
14	2	519	CLA	CHD-C1D-ND	-2.07	122.56	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1226	CLA	CMC-C2C-C3C	2.07	131.73	126.12
14	A	1022	CLA	C4D-C3D-CAD	-2.07	105.66	108.10
14	H	1021	CLA	O1D-CGD-CBD	2.07	128.71	124.48
14	4	506	CLA	CHB-C1B-NB	2.07	126.44	124.26
14	q	511	CLA	CHC-C4B-NB	2.07	126.44	124.26
14	r	519	CLA	CHC-C4B-NB	2.07	126.44	124.26
14	A	1127	CLA	CHA-C1A-NA	-2.07	121.67	126.40
14	G	1114	CLA	CAA-CBA-CGA	-2.07	107.03	112.51
14	2	503	CLA	CHD-C1D-ND	-2.07	122.56	124.45
14	t	501	CLA	CHD-C1D-ND	-2.07	122.56	124.45
14	F	1302	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
14	G	1127	CLA	CHA-C1A-NA	-2.06	121.67	126.40
14	B	1236	CLA	CAA-CBA-CGA	-2.06	107.22	113.25
17	f	4005	BCR	C33-C5-C4	2.06	117.58	113.62
17	J	4012	BCR	C23-C22-C21	2.06	122.11	118.94
17	Y	521	BCR	C29-C30-C25	2.06	113.66	110.48
14	f	1209	CLA	CMB-C2B-C1B	-2.06	122.22	125.37
14	3	506	CLA	C3B-C4B-NB	-2.06	108.60	110.52
14	A	1119	CLA	O2D-CGD-CBD	2.06	114.94	111.27
14	G	1119	CLA	O2D-CGD-CBD	2.06	114.94	111.27
14	Z	508	CLA	O1A-CGA-CBA	2.06	129.71	123.08
19	J	5105	LMU	C6'-C5'-C4'	-2.06	108.17	113.00
14	c	519	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
14	B	1209	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
14	G	1119	CLA	C16-C15-C13	-2.06	109.25	115.92
17	6	524	BCR	C16-C15-C14	-2.06	119.25	123.47
14	H	1203	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
14	5	519	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
14	H	1206	CLA	CHC-C1C-NC	2.06	127.33	124.20
14	q	509	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
14	Y	518	CLA	CHC-C4B-NB	2.06	126.44	124.26
14	G	1107	CLA	C2A-C1A-CHA	2.06	127.47	123.86
18	L	5221	LHG	C15-C14-C13	-2.06	103.95	114.42
14	B	1226	CLA	CHB-C4A-NA	2.06	127.36	124.51
14	2	505	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
14	G	1122	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	H	1226	CLA	CHD-C1D-C2D	2.06	129.81	125.48
14	H	1236	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
14	B	1206	CLA	CHC-C1C-NC	2.06	127.33	124.20
17	L	4219	BCR	C32-C1-C6	-2.06	106.95	110.30
14	f	1216	CLA	C2D-C1D-ND	-2.06	108.58	110.10
14	e	1011	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1213	CLA	CHC-C4B-NB	2.06	126.44	124.26
14	f	1203	CLA	CHB-C1B-NB	2.06	126.44	124.26
14	B	1226	CLA	CHD-C1D-C2D	2.06	129.80	125.48
14	Z	505	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
14	5	507	CLA	CHA-C1A-NA	-2.06	121.68	126.40
14	e	1119	CLA	C16-C15-C13	-2.06	109.26	115.92
14	Y	511	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
14	e	1114	CLA	CAA-CBA-CGA	-2.06	107.04	112.51
14	G	1011	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
14	e	1104	CLA	C2A-C1A-CHA	2.06	127.46	123.86
14	s	511	CLA	C2A-C1A-CHA	2.06	127.46	123.86
17	s	524	BCR	C23-C22-C21	-2.06	115.78	118.94
14	4	511	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	n	4020	BCR	C33-C5-C4	-2.06	109.66	113.62
14	H	1021	CLA	CBA-CAA-C2A	-2.06	107.78	113.86
14	e	1127	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	l	4015	BCR	C37-C22-C23	2.06	121.32	118.08
14	t	516	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
17	d	521	BCR	C10-C11-C12	-2.06	116.79	123.22
14	B	1203	CLA	CAA-C2A-C1A	-2.06	105.23	111.97
14	r	504	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
14	s	504	CLA	O2D-CGD-CBD	2.06	114.93	111.27
14	B	1021	CLA	CBA-CAA-C2A	-2.06	107.78	113.86
18	f	1842	LHG	C27-C26-C25	-2.06	103.97	114.42
14	Z	517	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
14	e	1132	CLA	C3A-C2A-C1A	2.06	104.42	101.34
18	V	5221	LHG	C15-C14-C13	-2.06	103.97	114.42
17	G	4011	BCR	C36-C18-C17	-2.06	120.04	122.92
14	2	504	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
18	B	1842	LHG	C27-C26-C25	-2.06	103.97	114.42
17	v	524	BCR	C16-C15-C14	-2.06	119.26	123.47
14	A	1131	CLA	C7-C6-C5	-2.06	107.77	113.36
17	V	4019	BCR	C29-C30-C25	2.06	113.65	110.48
14	B	1217	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
14	F	1302	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	H	1842	LHG	C27-C26-C25	-2.06	103.98	114.42
17	H	4009	BCR	C19-C18-C17	-2.06	115.78	118.94
17	L	4019	BCR	C29-C30-C25	2.06	113.65	110.48
17	n	4019	BCR	C29-C30-C25	2.06	113.65	110.48
14	f	1206	CLA	CHC-C1C-NC	2.06	127.33	124.20
14	2	505	CLA	C3B-C4B-NB	-2.06	108.61	110.52
14	G	1128	CLA	C3B-C4B-NB	-2.06	108.61	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	v	508	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
14	G	1132	CLA	C3A-C2A-C1A	2.06	104.42	101.34
17	6	523	BCR	C8-C7-C6	-2.06	121.42	127.20
14	2	518	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
14	f	1021	CLA	CBA-CAA-C2A	-2.06	107.79	113.86
14	f	1217	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
18	n	5220	LHG	O8-C23-O10	-2.06	118.40	123.59
14	A	1114	CLA	CAA-CBA-CGA	-2.06	107.05	112.51
14	4	501	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	b	501	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	b	511	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	e	1120	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	b	508	CLA	CMC-C2C-C1C	-2.06	121.91	125.04
14	r	508	CLA	O1A-CGA-CBA	2.06	129.69	123.08
14	G	1109	CLA	CHC-C4B-NB	2.06	126.43	124.26
14	A	1101	CLA	C3A-C2A-C1A	2.06	104.42	101.34
20	f	5002	LMG	C3-C4-C5	-2.06	106.57	110.24
18	L	5218	LHG	C5-O7-C7	-2.06	112.73	117.79
14	H	1240	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
17	V	4219	BCR	C32-C1-C6	-2.06	106.97	110.30
14	r	501	CLA	CHB-C1B-NB	2.06	126.43	124.26
14	v	519	CLA	O2A-CGA-O1A	-2.06	118.18	123.30
14	r	501	CLA	C2A-C1A-CHA	2.06	127.45	123.86
14	A	1011	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
14	B	1240	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
14	s	501	CLA	O2D-CGD-CBD	2.06	114.92	111.27
14	r	505	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
18	n	5221	LHG	C15-C14-C13	-2.06	103.99	114.42
17	s	523	BCR	C1-C6-C5	-2.06	119.72	122.61
14	A	1125	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
14	f	1226	CLA	CHD-C1D-C2D	2.05	129.79	125.48
17	Y	523	BCR	C7-C8-C9	-2.05	123.13	126.23
19	T	5105	LMU	C6'-C5'-C4'	-2.05	108.19	113.00
14	r	504	CLA	C2A-C1A-CHA	2.05	127.45	123.86
17	6	521	BCR	C10-C11-C12	-2.05	116.81	123.22
14	3	502	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
17	v	522	BCR	C27-C26-C25	-2.05	119.75	122.73
17	c	523	BCR	C37-C22-C23	2.05	121.31	118.08
14	e	1022	CLA	C4D-C3D-CAD	-2.05	105.67	108.10
14	H	1012	CLA	C4-C3-C5	2.05	118.73	115.27
17	Z	523	BCR	C34-C9-C8	2.05	121.31	118.08
14	R	1302	CLA	CAA-C2A-C3A	-2.05	107.15	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	5220	LHG	O8-C23-O10	-2.05	118.41	123.59
14	b	506	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	d	517	CLA	CHC-C4B-NB	2.05	126.43	124.26
14	f	1023	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	d	508	CLA	CHC-C1C-NC	2.05	127.32	124.20
14	a	511	CLA	C2A-C1A-CHA	2.05	127.45	123.86
14	a	502	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
20	B	5002	LMG	C3-C4-C5	-2.05	106.58	110.24
17	6	523	BCR	C15-C16-C17	-2.05	119.27	123.47
14	G	1022	CLA	O1D-CGD-CBD	2.05	128.68	124.48
14	c	502	CLA	CHC-C4B-NB	2.05	126.43	124.26
14	q	511	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
17	B	4005	BCR	C33-C5-C4	2.05	117.56	113.62
14	A	1104	CLA	C2A-C1A-CHA	2.05	127.45	123.86
14	5	509	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	2	521	BCR	C39-C30-C25	-2.05	106.97	110.30
14	A	1116	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	u	523	BCR	C37-C22-C23	2.05	121.31	118.08
14	b	516	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
14	u	507	CLA	CHA-C1A-NA	-2.05	121.70	126.40
14	H	1023	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	R	1302	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	d	512	CLA	CHC-C4B-NB	2.05	126.43	124.26
14	d	516	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	A	1132	CLA	C3A-C2A-C1A	2.05	104.41	101.34
14	G	1101	CLA	C3A-C2A-C1A	2.05	104.41	101.34
14	G	1131	CLA	C7-C6-C5	-2.05	107.79	113.36
17	L	4020	BCR	C33-C5-C4	-2.05	109.67	113.62
17	1	521	BCR	C29-C30-C25	2.05	113.64	110.48
17	H	4005	BCR	C33-C5-C4	2.05	117.56	113.62
17	c	522	BCR	C30-C25-C26	-2.05	119.72	122.61
17	G	4003	BCR	C15-C16-C17	-2.05	119.27	123.47
14	6	512	CLA	CHC-C4B-NB	2.05	126.43	124.26
14	c	513	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	1	511	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
14	a	511	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
14	e	1101	CLA	C3A-C2A-C1A	2.05	104.41	101.34
19	l	5105	LMU	C6'-C5'-C4'	-2.05	108.20	113.00
21	f	1852	SQD	C3-C4-C5	2.05	113.90	110.24
17	b	521	BCR	C38-C26-C25	-2.05	122.23	124.53
14	Y	506	CLA	CHB-C1B-NB	2.05	126.43	124.26
17	Z	521	BCR	C39-C30-C25	-2.05	106.97	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	501	CLA	O2D-CGD-CBD	2.05	114.91	111.27
14	e	1119	CLA	O2D-CGD-CBD	2.05	114.91	111.27
14	1	509	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	a	510	CLA	CHB-C1B-NB	2.05	126.43	124.26
14	f	1203	CLA	CAA-C2A-C1A	-2.05	105.26	111.97
14	G	1125	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
14	A	1128	CLA	CHC-C1C-NC	2.05	127.31	124.20
14	q	518	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
14	G	1116	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
14	e	1125	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
17	q	523	BCR	C7-C8-C9	-2.05	123.14	126.23
17	H	4004	BCR	C29-C30-C25	2.05	113.63	110.48
14	Z	505	CLA	C3B-C4B-NB	-2.05	108.61	110.52
14	Z	517	CLA	CHC-C4B-NB	2.05	126.42	124.26
14	b	517	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
14	e	1116	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
14	t	508	CLA	CMC-C2C-C1C	-2.05	121.92	125.04
14	2	508	CLA	O1A-CGA-CBA	2.05	129.66	123.08
18	e	5001	LHG	C18-C17-C16	-2.05	104.03	114.42
14	f	1219	CLA	CHB-C1B-NB	2.05	126.42	124.26
14	e	1132	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
14	f	1240	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
14	3	511	CLA	C2A-C1A-CHA	2.05	127.44	123.86
14	A	1130	CLA	CHB-C1B-C2B	-2.05	121.46	127.24
14	4	516	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
14	6	516	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
14	v	516	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
14	d	507	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
14	H	1217	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
14	t	502	CLA	C2A-C1A-CHA	2.05	127.44	123.86
20	H	5002	LMG	C3-C4-C5	-2.05	106.59	110.24
14	A	1132	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
14	f	1213	CLA	CHC-C4B-NB	2.05	126.42	124.26
14	G	1114	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	d	508	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	v	502	CLA	C2A-C1A-CHA	2.05	127.44	123.86
17	q	522	BCR	C27-C26-C25	-2.05	119.76	122.73
14	j	1302	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
17	e	4011	BCR	C36-C18-C17	-2.05	120.06	122.92
14	s	516	CLA	C2A-C1A-CHA	2.05	127.44	123.86
14	6	516	CLA	CHB-C1B-NB	2.05	126.42	124.26
14	d	516	CLA	CAA-C2A-C3A	-2.04	107.18	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e	1109	CLA	C3B-C4B-NB	-2.04	108.62	110.52
14	s	506	CLA	C3B-C4B-NB	-2.04	108.62	110.52
14	4	508	CLA	CMC-C2C-C1C	-2.04	121.92	125.04
21	2	822	SQD	C45-O47-C7	2.04	122.83	117.79
14	1	509	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
14	f	1202	CLA	O2D-CGD-CBD	2.04	114.90	111.27
14	2	516	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
14	v	507	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
14	A	1122	CLA	CHC-C4B-NB	2.04	126.42	124.26
14	1	519	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	2	501	CLA	CHB-C1B-NB	2.04	126.42	124.26
17	S	4018	BCR	C31-C1-C6	-2.04	106.98	110.30
14	c	518	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
17	6	522	BCR	C30-C25-C26	-2.04	119.73	122.61
17	r	523	BCR	C34-C9-C8	2.04	121.30	118.08
17	q	521	BCR	C29-C30-C25	2.04	113.63	110.48
14	3	516	CLA	C2A-C1A-CHA	2.04	127.43	123.86
14	s	511	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
14	Z	501	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	Z	502	CLA	CHC-C4B-NB	2.04	126.42	124.26
14	a	501	CLA	CHB-C1B-NB	2.04	126.42	124.26
18	V	5220	LHG	O8-C23-O10	-2.04	118.44	123.59
14	v	505	CLA	C2A-C1A-CHA	2.04	127.43	123.86
14	Z	504	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
14	d	508	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
14	v	508	CLA	C3B-C4B-NB	-2.04	108.62	110.52
21	c	822	SQD	O47-C7-O49	-2.04	118.90	122.96
14	2	511	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
14	6	507	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
17	A	4011	BCR	C36-C18-C17	-2.04	120.06	122.92
17	H	4004	BCR	C34-C9-C8	2.04	121.30	118.08
14	H	1202	CLA	O2D-CGD-CBD	2.04	114.90	111.27
14	2	505	CLA	C2D-C1D-ND	-2.04	108.60	110.10
14	u	518	CLA	C2D-C1D-ND	-2.04	108.60	110.10
14	Y	509	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	s	502	CLA	CHC-C4B-NB	2.04	126.42	124.26
14	r	511	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
17	v	523	BCR	C8-C7-C6	-2.04	121.47	127.20
17	U	4104	BCR	C35-C13-C12	2.04	121.29	118.08
20	B	5002	LMG	C23-C22-C21	-2.04	104.06	114.42
14	B	1202	CLA	O2D-CGD-CBD	2.04	114.90	111.27
14	6	508	CLA	C3B-C4B-NB	-2.04	108.62	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	4003	BCR	C15-C16-C17	-2.04	119.29	123.47
18	A	5001	LHG	C18-C17-C16	-2.04	104.06	114.42
14	Y	519	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	r	502	CLA	CHC-C4B-NB	2.04	126.42	124.26
20	H	5002	LMG	C23-C22-C21	-2.04	104.06	114.42
14	4	502	CLA	C2A-C1A-CHA	2.04	127.43	123.86
17	M	4021	BCR	C19-C18-C17	-2.04	115.81	118.94
14	u	503	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
14	q	512	CLA	CHB-C4A-NA	2.04	127.33	124.51
18	V	5218	LHG	C5-O7-C7	-2.04	112.77	117.79
14	a	504	CLA	O2D-CGD-CBD	2.04	114.89	111.27
21	u	822	SQD	O47-C7-O49	-2.04	118.91	122.96
14	H	1235	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	d	503	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	d	504	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	u	502	CLA	CHC-C4B-NB	2.04	126.42	124.26
17	1	523	BCR	C7-C8-C9	-2.04	123.15	126.23
18	e	5006	LHG	C5-O7-C7	-2.04	112.77	117.79
14	5	503	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
14	1	511	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
14	3	504	CLA	O2D-CGD-CBD	2.04	114.89	111.27
14	e	1022	CLA	O1D-CGD-CBD	2.04	128.66	124.48
21	r	822	SQD	C45-O47-C7	2.04	122.81	117.79
14	6	519	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
17	f	4009	BCR	C4-C5-C6	-2.04	119.77	122.73
14	u	509	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
14	d	519	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
14	e	1130	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
14	B	1238	CLA	CAC-C3C-C4C	2.04	127.46	124.81
14	H	1238	CLA	CAC-C3C-C4C	2.04	127.46	124.81
14	H	1238	CLA	CHD-C1D-ND	-2.04	122.58	124.45
14	H	1204	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
14	L	1503	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
14	G	1130	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
14	t	517	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
14	r	506	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	e	1128	CLA	C3B-C4B-NB	-2.04	108.62	110.52
14	d	505	CLA	C2A-C1A-CHA	2.04	127.42	123.86
14	Z	516	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
14	4	517	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
14	6	508	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
14	2	519	CLA	CHC-C4B-NB	2.04	126.41	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	502	CLA	CHC-C4B-NB	2.04	126.41	124.26
14	r	518	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
20	f	5002	LMG	C23-C22-C21	-2.04	104.08	114.42
14	b	502	CLA	C2A-C1A-CHA	2.04	127.42	123.86
14	3	519	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
17	5	523	BCR	C37-C22-C23	2.04	121.29	118.08
17	v	523	BCR	C15-C16-C17	-2.04	119.30	123.47
14	Z	519	CLA	CHC-C4B-NB	2.04	126.41	124.26
14	q	509	CLA	O1D-CGD-CBD	2.04	128.65	124.48
14	2	504	CLA	C2A-C1A-CHA	2.04	127.42	123.86
17	W	4021	BCR	C19-C18-C17	-2.04	115.82	118.94
18	A	5006	LHG	C5-O7-C7	-2.04	112.78	117.79
14	V	1503	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
14	n	1503	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
17	A	4008	BCR	C8-C7-C6	-2.04	121.48	127.20
21	Z	822	SQD	C45-O47-C7	2.04	122.80	117.79
14	e	1131	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
14	c	503	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
17	r	524	BCR	C38-C26-C25	-2.04	122.24	124.53
17	A	4003	BCR	C15-C16-C17	-2.04	119.30	123.47
14	v	505	CLA	C2D-C1D-ND	-2.04	108.60	110.10
14	s	502	CLA	O2A-CGA-O1A	-2.04	118.23	123.30
14	4	511	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
17	e	4008	BCR	C8-C7-C6	-2.03	121.49	127.20
14	u	510	CLA	CHD-C1D-ND	-2.03	122.58	124.45
18	G	5001	LHG	C18-C17-C16	-2.03	104.09	114.42
14	a	519	CLA	CHC-C4B-NB	2.03	126.41	124.26
14	f	1208	CLA	CHC-C4B-NB	2.03	126.41	124.26
14	B	1204	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	B	4005	BCR	C3-C4-C5	-2.03	110.44	114.08
17	H	4005	BCR	C3-C4-C5	-2.03	110.44	114.08
17	B	4009	BCR	C19-C18-C17	-2.03	115.82	118.94
17	o	4021	BCR	C19-C18-C17	-2.03	115.82	118.94
14	A	1131	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
14	a	501	CLA	O2D-CGD-CBD	2.03	114.88	111.27
18	G	5007	LHG	C11-C10-C9	-2.03	104.10	114.42
14	Y	509	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
14	Y	511	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
17	k	4018	BCR	C33-C5-C6	-2.03	122.24	124.53
14	U	1103	CLA	CAC-C3C-C4C	2.03	127.45	124.81
14	s	519	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
14	A	1109	CLA	CHC-C4B-NB	2.03	126.41	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	r	516	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
14	c	509	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	H	4009	BCR	C4-C5-C6	-2.03	119.78	122.73
14	d	506	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
14	5	513	CLA	CHB-C1B-NB	2.03	126.41	124.26
14	H	1208	CLA	CHC-C4B-NB	2.03	126.41	124.26
14	r	506	CLA	CHC-C4B-NB	2.03	126.41	124.26
14	G	1135	CLA	CHA-C1A-NA	-2.03	121.74	126.40
14	1	518	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
14	d	502	CLA	C2A-C1A-CHA	2.03	127.41	123.86
17	Z	523	BCR	C23-C24-C25	-2.03	121.49	127.20
17	4	521	BCR	C38-C26-C25	-2.03	122.25	124.53
14	c	506	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
14	6	502	CLA	C2A-C1A-CHA	2.03	127.41	123.86
17	6	522	BCR	C27-C26-C25	-2.03	119.78	122.73
14	3	502	CLA	CHC-C4B-NB	2.03	126.41	124.26
14	Y	518	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
17	K	4104	BCR	C35-C13-C12	2.03	121.28	118.08
14	A	1130	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	B	1220	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	q	511	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
14	v	506	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
14	F	1302	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
14	s	501	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
17	T	4013	BCR	C35-C13-C12	2.03	121.28	118.08
14	B	1205	CLA	C3A-C2A-C1A	2.03	104.38	101.34
17	3	523	BCR	C1-C6-C5	-2.03	119.75	122.61
18	n	5218	LHG	C5-O7-C7	-2.03	112.79	117.79
14	2	502	CLA	CHC-C4B-NB	2.03	126.41	124.26
14	v	519	CLA	CHB-C1B-NB	2.03	126.41	124.26
17	l	4013	BCR	C39-C30-C25	-2.03	107.00	110.30
14	a	506	CLA	C3B-C4B-NB	-2.03	108.63	110.52
14	H	1239	CLA	C2A-C1A-CHA	2.03	127.41	123.86
21	5	822	SQD	O47-C7-O49	-2.03	118.93	122.96
18	A	5007	LHG	C11-C10-C9	-2.03	104.12	114.42
14	e	1135	CLA	CHA-C1A-NA	-2.03	121.75	126.40
14	G	1131	CLA	CAA-CBA-CGA	-2.03	107.32	113.25
14	G	1132	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
14	B	1206	CLA	CMB-C2B-C3B	2.03	131.50	126.59
14	a	508	CLA	O1A-CGA-CBA	2.03	129.60	123.08
14	v	516	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
17	B	4010	BCR	C10-C11-C12	-2.03	116.88	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1120	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	H	4017	BCR	C16-C15-C14	-2.03	119.32	123.47
14	a	519	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
14	f	1206	CLA	CMB-C2B-C3B	2.03	131.50	126.59
14	a	501	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
14	e	1134	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
17	B	4004	BCR	C29-C30-C25	2.03	113.60	110.48
14	s	507	CLA	CHA-C1A-NA	-2.03	121.75	126.40
14	3	511	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
14	6	504	CLA	C2A-C1A-CHA	2.03	127.41	123.86
14	Z	504	CLA	C2A-C1A-CHA	2.03	127.41	123.86
14	e	1107	CLA	C2A-C1A-CHA	2.03	127.41	123.86
14	A	1128	CLA	CHB-C4A-NA	2.03	127.32	124.51
14	r	519	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	s	501	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	s	506	CLA	CMB-C2B-C3B	2.03	131.50	126.59
14	6	506	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
14	Z	511	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
14	a	516	CLA	C2A-C1A-CHA	2.03	127.40	123.86
17	f	4004	BCR	C29-C30-C25	2.03	113.60	110.48
17	G	4008	BCR	C8-C7-C6	-2.03	121.51	127.20
17	J	4013	BCR	C39-C30-C25	-2.03	107.01	110.30
14	A	1128	CLA	C3B-C4B-NB	-2.03	108.64	110.52
14	G	1109	CLA	C3B-C4B-NB	-2.03	108.64	110.52
14	d	504	CLA	C2A-C1A-CHA	2.03	127.40	123.86
14	2	506	CLA	CHC-C4B-NB	2.03	126.40	124.26
14	3	506	CLA	CMB-C2B-C3B	2.03	131.50	126.59
14	G	1022	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
17	T	4013	BCR	C39-C30-C25	-2.03	107.01	110.30
17	B	4009	BCR	C4-C5-C6	-2.03	119.79	122.73
14	3	501	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
14	R	1302	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
14	c	510	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
18	G	5006	LHG	C5-O7-C7	-2.03	112.81	117.79
14	2	501	CLA	C2A-C1A-CHA	2.03	127.40	123.86
14	G	1123	CLA	O2D-CGD-CBD	2.02	114.87	111.27
14	3	508	CLA	O1A-CGA-CBA	2.02	129.59	123.08
14	A	1127	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
14	v	504	CLA	C2A-C1A-CHA	2.02	127.40	123.86
14	e	1128	CLA	CHB-C4A-NA	2.02	127.31	124.51
14	A	1114	CLA	CHD-C1D-ND	-2.02	122.59	124.45
14	H	1220	CLA	CHD-C1D-ND	-2.02	122.59	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	6	505	CLA	C2A-C1A-CHA	2.02	127.40	123.86
17	G	4003	BCR	C33-C5-C4	2.02	117.50	113.62
17	5	522	BCR	C30-C25-C26	-2.02	119.76	122.61
14	A	1022	CLA	O1D-CGD-CBD	2.02	128.62	124.48
14	a	506	CLA	CMB-C2B-C3B	2.02	131.49	126.59
17	2	523	BCR	C23-C24-C25	-2.02	121.52	127.20
18	e	5007	LHG	C11-C10-C9	-2.02	104.15	114.42
14	A	1107	CLA	C2A-C1A-CHA	2.02	127.40	123.86
14	b	519	CLA	CHB-C1B-NB	2.02	126.40	124.26
14	v	503	CLA	CHB-C1B-NB	2.02	126.40	124.26
14	q	508	CLA	C2D-C1D-ND	-2.02	108.61	110.10
14	H	1205	CLA	C3A-C2A-C1A	2.02	104.37	101.34
17	f	4009	BCR	C19-C18-C17	-2.02	115.84	118.94
14	f	1231	CLA	C1-C2-C3	-2.02	122.55	126.04
17	S	4018	BCR	C33-C5-C6	-2.02	122.26	124.53
14	G	1128	CLA	CHC-C1C-NC	2.02	127.27	124.20
14	A	1111	CLA	C2A-C1A-CHA	2.02	127.39	123.86
14	e	1139	CLA	CHB-C4A-NA	2.02	127.31	124.51
14	r	503	CLA	C2D-C1D-ND	-2.02	108.61	110.10
14	r	518	CLA	CHD-C1D-ND	-2.02	122.60	124.45
14	q	509	CLA	C2A-C1A-CHA	2.02	127.39	123.86
14	4	519	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
14	6	517	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
14	e	1123	CLA	O2D-CGD-CBD	2.02	114.86	111.27
14	f	1238	CLA	CAC-C3C-C4C	2.02	127.43	124.81
17	J	4013	BCR	C35-C13-C12	2.02	121.26	118.08
17	l	4013	BCR	C35-C13-C12	2.02	121.26	118.08
14	6	503	CLA	CHB-C1B-NB	2.02	126.40	124.26
14	1	509	CLA	C2A-C1A-CHA	2.02	127.39	123.86
14	v	517	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
14	H	1240	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
14	A	1139	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	f	4005	BCR	C3-C4-C5	-2.02	110.47	114.08
17	H	4010	BCR	C10-C11-C12	-2.02	116.92	123.22
14	s	504	CLA	C2A-C1A-CHA	2.02	127.39	123.86
14	f	1201	CLA	C11-C10-C8	-2.02	109.39	115.92
14	B	1231	CLA	C1-C2-C3	-2.02	122.55	126.04
18	S	5001	LHG	C27-C26-C25	-2.02	104.18	114.42
14	6	517	CLA	CHC-C4B-NB	2.02	126.39	124.26
14	s	508	CLA	O1A-CGA-CBA	2.02	129.57	123.08
14	f	1239	CLA	CHD-C1D-ND	-2.02	122.60	124.45
14	b	511	CLA	O2A-CGA-O1A	-2.02	118.27	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1214	CLA	C1-C2-C3	2.02	129.53	126.04
18	I	5001	LHG	C27-C26-C25	-2.02	104.18	114.42
18	k	5001	LHG	C27-C26-C25	-2.02	104.18	114.42
17	r	523	BCR	C33-C5-C4	2.02	117.49	113.62
17	c	523	BCR	C23-C24-C25	-2.02	121.53	127.20
17	f	4017	BCR	C16-C15-C14	-2.02	119.34	123.47
14	b	519	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
14	A	1109	CLA	C3B-C4B-NB	-2.02	108.64	110.52
14	1	506	CLA	CHB-C1B-NB	2.02	126.39	124.26
17	A	4003	BCR	C33-C5-C4	2.02	117.49	113.62
14	r	510	CLA	CHD-C1D-ND	-2.02	122.60	124.45
17	r	523	BCR	C23-C24-C25	-2.02	121.54	127.20
17	4	522	BCR	C21-C20-C19	-2.02	116.92	123.22
14	6	508	CLA	O1A-CGA-CBA	2.02	129.56	123.08
21	3	822	SQD	O6-C1-C2	2.02	111.45	108.30
14	A	1123	CLA	O2D-CGD-CBD	2.02	114.85	111.27
14	A	1134	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	4	519	CLA	CHB-C1B-NB	2.02	126.39	124.26
14	q	509	CLA	CHB-C1B-NB	2.02	126.39	124.26
14	A	1103	CLA	CHD-C1D-ND	-2.02	122.60	124.45
14	A	1139	CLA	C11-C10-C8	-2.02	109.40	115.92
17	H	4009	BCR	C29-C28-C27	-2.02	106.87	111.38
14	B	1201	CLA	C11-C10-C8	-2.02	109.40	115.92
17	B	4017	BCR	C16-C15-C14	-2.02	119.35	123.47
14	A	1135	CLA	CHA-C1A-NA	-2.02	121.78	126.40
14	e	1128	CLA	CHC-C1C-NC	2.01	127.26	124.20
14	G	1128	CLA	CHB-C4A-NA	2.01	127.30	124.51
14	A	1022	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
14	5	510	CLA	CHD-C1D-ND	-2.01	122.60	124.45
14	H	1206	CLA	CMB-C2B-C3B	2.01	131.47	126.59
14	Y	519	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
14	t	511	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
17	1	522	BCR	C27-C26-C25	-2.01	119.81	122.73
17	r	523	BCR	C3-C4-C5	-2.01	110.48	114.08
17	G	4007	BCR	C36-C18-C19	2.01	121.25	118.08
17	m	4104	BCR	C35-C13-C12	2.01	121.25	118.08
14	3	507	CLA	CHA-C1A-NA	-2.01	121.79	126.40
14	u	511	CLA	C2A-C1A-CHA	2.01	127.38	123.86
14	f	1205	CLA	C3A-C2A-C1A	2.01	104.36	101.34
14	H	1225	CLA	O2D-CGD-CBD	2.01	114.85	111.27
14	e	1139	CLA	C11-C10-C8	-2.01	109.41	115.92
14	H	1226	CLA	C3C-C4C-NC	-2.01	108.31	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	d	517	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
17	q	524	BCR	C15-C16-C17	-2.01	119.35	123.47
14	Z	503	CLA	CHD-C1D-ND	-2.01	122.60	124.45
14	q	504	CLA	CHD-C1D-ND	-2.01	122.60	124.45
14	Y	509	CLA	O1D-CGD-CBD	2.01	128.60	124.48
17	f	4010	BCR	C10-C11-C12	-2.01	116.94	123.22
14	v	517	CLA	CHC-C4B-NB	2.01	126.39	124.26
18	H	1855	LHG	C27-C26-C25	-2.01	104.21	114.42
14	H	1214	CLA	C1-C2-C3	2.01	129.52	126.04
14	1	509	CLA	O1D-CGD-CBD	2.01	128.60	124.48
14	r	503	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
14	u	506	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
14	G	1127	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
14	5	518	CLA	C2D-C1D-ND	-2.01	108.62	110.10
14	Z	505	CLA	C2D-C1D-ND	-2.01	108.62	110.10
14	t	509	CLA	O1A-CGA-CBA	2.01	129.54	123.08
14	B	1230	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	e	5008	LHG	O8-C23-C24	2.01	118.22	111.91
14	q	519	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
17	H	4009	BCR	C35-C13-C12	2.01	121.25	118.08
18	A	5009	LHG	O8-C23-O10	-2.01	118.52	123.59
14	e	1125	CLA	CMB-C2B-C3B	2.01	131.46	126.59
14	e	1124	CLA	CHB-C4A-NA	2.01	127.29	124.51
14	a	505	CLA	CHC-C4B-NB	2.01	126.39	124.26
14	s	519	CLA	CHC-C4B-NB	2.01	126.39	124.26
14	m	1103	CLA	CAC-C3C-C4C	2.01	127.42	124.81
14	d	508	CLA	O1A-CGA-CBA	2.01	129.54	123.08
17	Z	523	BCR	C33-C5-C4	2.01	117.48	113.62
17	u	522	BCR	C30-C25-C26	-2.01	119.78	122.61
18	f	1855	LHG	C27-C26-C25	-2.01	104.22	114.42
14	v	508	CLA	O1A-CGA-CBA	2.01	129.54	123.08
14	3	501	CLA	CHB-C1B-NB	2.01	126.39	124.26
14	A	1106	CLA	CMB-C2B-C3B	2.01	131.46	126.59
14	G	1103	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	Y	524	BCR	C15-C16-C17	-2.01	119.36	123.47
14	e	1022	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
14	Y	509	CLA	C2A-C1A-CHA	2.01	127.37	123.86
17	Z	523	BCR	C3-C4-C5	-2.01	110.49	114.08
17	I	4018	BCR	C35-C13-C12	2.01	121.24	118.08
14	H	1231	CLA	C1-C2-C3	-2.01	122.57	126.04
14	q	504	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	G	1139	CLA	C11-C10-C8	-2.01	109.42	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	504	CLA	C2A-C1A-CHA	2.01	127.37	123.86
14	G	1130	CLA	CHD-C1D-ND	-2.01	122.61	124.45
14	5	506	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
14	b	502	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
18	B	1855	LHG	C27-C26-C25	-2.01	104.23	114.42
14	4	509	CLA	O1A-CGA-CBA	2.01	129.53	123.08
14	q	501	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	t	519	CLA	CHB-C1B-NB	2.01	126.38	124.26
17	3	522	BCR	C36-C18-C19	2.01	121.24	118.08
14	f	1240	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
17	2	523	BCR	C3-C4-C5	-2.01	110.49	114.08
14	K	1103	CLA	CAC-C3C-C4C	2.01	127.42	124.81
14	t	519	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
14	f	1214	CLA	C1-C2-C3	2.01	129.51	126.04
14	f	1225	CLA	O2D-CGD-CBD	2.01	114.83	111.27
17	V	4020	BCR	C29-C30-C25	2.01	113.57	110.48
14	B	1213	CLA	O2A-C1-C2	-2.01	103.36	108.64
14	H	1213	CLA	O2A-C1-C2	-2.01	103.36	108.64
17	b	522	BCR	C21-C20-C19	-2.01	116.95	123.22
17	2	523	BCR	C33-C5-C4	2.01	117.47	113.62
14	H	1201	CLA	C11-C10-C8	-2.01	109.43	115.92
14	e	1127	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	Y	516	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
14	a	507	CLA	CHA-C1A-NA	-2.01	121.80	126.40
17	d	522	BCR	C27-C26-C25	-2.01	119.82	122.73
17	T	4012	BCR	C38-C26-C25	-2.01	122.28	124.53
14	2	517	CLA	CHC-C4B-NB	2.01	126.38	124.26
14	3	519	CLA	CHC-C4B-NB	2.01	126.38	124.26
14	a	504	CLA	C2A-C1A-CHA	2.01	127.37	123.86
14	d	508	CLA	C3B-C4B-NB	-2.01	108.65	110.52
14	3	508	CLA	CMB-C2B-C3B	2.01	131.45	126.59
14	f	1204	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
17	e	4003	BCR	C33-C5-C4	2.01	117.47	113.62
17	u	522	BCR	C36-C18-C19	2.01	121.24	118.08
14	B	1208	CLA	CHC-C4B-NB	2.01	126.38	124.26
17	t	522	BCR	C21-C20-C19	-2.01	116.96	123.22
17	1	524	BCR	C15-C16-C17	-2.00	119.37	123.47
17	5	524	BCR	C10-C11-C12	-2.00	116.96	123.22
17	a	523	BCR	C1-C6-C5	-2.00	119.79	122.61
14	c	508	CLA	CMB-C2B-C3B	2.00	131.44	126.59
14	e	1111	CLA	C2A-C1A-CHA	2.00	127.36	123.86
14	6	519	CLA	CHB-C1B-NB	2.00	126.38	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	501	CLA	CHB-C1B-NB	2.00	126.38	124.26
14	B	1239	CLA	CHD-C1D-ND	-2.00	122.61	124.45
14	c	518	CLA	C2D-C1D-ND	-2.00	108.63	110.10
18	A	5008	LHG	O8-C23-C24	2.00	118.20	111.91
17	c	524	BCR	C10-C11-C12	-2.00	116.96	123.22
14	B	1240	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
14	B	1239	CLA	C2A-C1A-CHA	2.00	127.36	123.86
17	u	523	BCR	C23-C24-C25	-2.00	121.57	127.20
14	6	516	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
14	G	1108	CLA	CHC-C4B-NB	2.00	126.38	124.26
14	Z	506	CLA	CHC-C4B-NB	2.00	126.38	124.26
17	R	4016	BCR	C15-C16-C17	-2.00	119.37	123.47
14	e	1114	CLA	CHD-C1D-ND	-2.00	122.61	124.45
17	s	522	BCR	C36-C18-C19	2.00	121.23	118.08
14	G	1134	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
14	e	1801	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
14	r	511	CLA	C2D-C1D-ND	-2.00	108.63	110.10
14	d	502	CLA	CHC-C4B-NB	2.00	126.38	124.26
14	5	508	CLA	CMB-C2B-C3B	2.00	131.44	126.59
17	5	523	BCR	C23-C24-C25	-2.00	121.58	127.20
17	Y	522	BCR	C27-C26-C25	-2.00	119.82	122.73
14	H	1214	CLA	CHD-C1D-ND	-2.00	122.61	124.45
14	H	1229	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
14	G	1106	CLA	CMB-C2B-C3B	2.00	131.44	126.59
17	A	4007	BCR	C36-C18-C19	2.00	121.23	118.08
14	A	1111	CLA	CMB-C2B-C3B	2.00	131.44	126.59
14	q	516	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
14	r	517	CLA	CHC-C4B-NB	2.00	126.38	124.26
14	Y	508	CLA	C2D-C1D-ND	-2.00	108.63	110.10
14	q	511	CLA	C2D-C1D-ND	-2.00	108.63	110.10
17	v	523	BCR	C34-C9-C8	2.00	121.23	118.08
14	Y	504	CLA	CED-O2D-CGD	2.00	120.46	115.94
14	c	508	CLA	C3B-C4B-NB	-2.00	108.66	110.52
14	q	504	CLA	CED-O2D-CGD	2.00	120.46	115.94
14	c	511	CLA	C2A-C1A-CHA	2.00	127.36	123.86
17	Y	523	BCR	C11-C10-C9	-2.00	124.45	127.31
14	A	1801	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
17	L	4020	BCR	C29-C30-C25	2.00	113.56	110.48

There are no chirality outliers.

All (7891) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1011	CLA	CHA-CBD-CGD-O1D
14	A	1102	CLA	C3A-C2A-CAA-CBA
14	A	1103	CLA	C1A-C2A-CAA-CBA
14	A	1103	CLA	CHA-CBD-CGD-O1D
14	A	1103	CLA	CHA-CBD-CGD-O2D
14	A	1103	CLA	CAD-CBD-CGD-O1D
14	A	1104	CLA	C1A-C2A-CAA-CBA
14	A	1104	CLA	C4-C3-C5-C6
14	A	1106	CLA	C3A-C2A-CAA-CBA
14	A	1107	CLA	C2B-C3B-CAB-CBB
14	A	1108	CLA	C1A-C2A-CAA-CBA
14	A	1108	CLA	C3A-C2A-CAA-CBA
14	A	1110	CLA	C1A-C2A-CAA-CBA
14	A	1113	CLA	CHA-CBD-CGD-O1D
14	A	1113	CLA	CHA-CBD-CGD-O2D
14	A	1116	CLA	C3A-C2A-CAA-CBA
14	A	1117	CLA	CHA-CBD-CGD-O1D
14	A	1117	CLA	CHA-CBD-CGD-O2D
14	A	1119	CLA	CHA-CBD-CGD-O1D
14	A	1119	CLA	CHA-CBD-CGD-O2D
14	A	1119	CLA	CBD-CGD-O2D-CED
14	A	1120	CLA	CHA-CBD-CGD-O2D
14	A	1121	CLA	C2B-C3B-CAB-CBB
14	A	1121	CLA	C4B-C3B-CAB-CBB
14	A	1122	CLA	C2B-C3B-CAB-CBB
14	A	1122	CLA	C4B-C3B-CAB-CBB
14	A	1122	CLA	C2-C3-C5-C6
14	A	1122	CLA	C4-C3-C5-C6
14	A	1126	CLA	C1A-C2A-CAA-CBA
14	A	1126	CLA	C3A-C2A-CAA-CBA
14	A	1132	CLA	CHA-CBD-CGD-O1D
14	A	1132	CLA	CHA-CBD-CGD-O2D
14	A	1134	CLA	C2-C3-C5-C6
14	A	1134	CLA	C4-C3-C5-C6
14	A	1134	CLA	C11-C10-C8-C7
14	A	1137	CLA	C4-C3-C5-C6
14	A	1138	CLA	CBD-CGD-O2D-CED
14	A	1139	CLA	C1A-C2A-CAA-CBA
14	A	1139	CLA	CHA-CBD-CGD-O1D
14	A	1139	CLA	C2-C3-C5-C6
14	A	1139	CLA	C4-C3-C5-C6
14	A	1139	CLA	C6-C7-C8-C9
14	A	1140	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1140	CLA	C2-C3-C5-C6
14	A	1140	CLA	C4-C3-C5-C6
14	A	1237	CLA	CHA-CBD-CGD-O1D
14	A	1237	CLA	CHA-CBD-CGD-O2D
14	A	1237	CLA	C4-C3-C5-C6
14	A	1801	CLA	CHA-CBD-CGD-O1D
14	A	1801	CLA	CHA-CBD-CGD-O2D
14	A	1101	CLA	CHA-CBD-CGD-O1D
14	A	1101	CLA	CHA-CBD-CGD-O2D
14	B	1012	CLA	CHA-CBD-CGD-O1D
14	B	1012	CLA	CHA-CBD-CGD-O2D
14	B	1012	CLA	C2-C3-C5-C6
14	B	1012	CLA	C4-C3-C5-C6
14	B	1021	CLA	CHA-CBD-CGD-O1D
14	B	1021	CLA	CHA-CBD-CGD-O2D
14	B	1202	CLA	C1A-C2A-CAA-CBA
14	B	1202	CLA	C3A-C2A-CAA-CBA
14	B	1202	CLA	CHA-CBD-CGD-O1D
14	B	1202	CLA	CHA-CBD-CGD-O2D
14	B	1202	CLA	CAD-CBD-CGD-O1D
14	B	1205	CLA	CHA-CBD-CGD-O1D
14	B	1205	CLA	CHA-CBD-CGD-O2D
14	B	1206	CLA	CBD-CGD-O2D-CED
14	B	1209	CLA	C1A-C2A-CAA-CBA
14	B	1209	CLA	C3A-C2A-CAA-CBA
14	B	1209	CLA	CHA-CBD-CGD-O2D
14	B	1210	CLA	C1A-C2A-CAA-CBA
14	B	1211	CLA	CHA-CBD-CGD-O1D
14	B	1211	CLA	CHA-CBD-CGD-O2D
14	B	1212	CLA	C2-C3-C5-C6
14	B	1212	CLA	C4-C3-C5-C6
14	B	1214	CLA	C2A-CAA-CBA-CGA
14	B	1214	CLA	C2B-C3B-CAB-CBB
14	B	1214	CLA	C4B-C3B-CAB-CBB
14	B	1214	CLA	O2A-C1-C2-C3
14	B	1215	CLA	C1A-C2A-CAA-CBA
14	B	1215	CLA	C3A-C2A-CAA-CBA
14	B	1216	CLA	CBA-CGA-O2A-C1
14	B	1216	CLA	O1A-CGA-O2A-C1
14	B	1216	CLA	C2B-C3B-CAB-CBB
14	B	1216	CLA	C4B-C3B-CAB-CBB
14	B	1217	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1217	CLA	C3A-C2A-CAA-CBA
14	B	1217	CLA	C2A-CAA-CBA-CGA
14	B	1217	CLA	C2B-C3B-CAB-CBB
14	B	1217	CLA	C4B-C3B-CAB-CBB
14	B	1219	CLA	CBA-CGA-O2A-C1
14	B	1219	CLA	O1A-CGA-O2A-C1
14	B	1220	CLA	C2B-C3B-CAB-CBB
14	B	1220	CLA	C4B-C3B-CAB-CBB
14	B	1220	CLA	CHA-CBD-CGD-O1D
14	B	1220	CLA	CHA-CBD-CGD-O2D
14	B	1224	CLA	C1A-C2A-CAA-CBA
14	B	1224	CLA	C3A-C2A-CAA-CBA
14	B	1227	CLA	CBA-CGA-O2A-C1
14	B	1234	CLA	CHA-CBD-CGD-O1D
14	B	1239	CLA	C4B-C3B-CAB-CBB
14	B	1240	CLA	C1A-C2A-CAA-CBA
14	B	1240	CLA	CHA-CBD-CGD-O1D
14	B	1240	CLA	CHA-CBD-CGD-O2D
14	B	1230	CLA	C1A-C2A-CAA-CBA
14	B	1230	CLA	C3A-C2A-CAA-CBA
14	B	1230	CLA	C2B-C3B-CAB-CBB
14	B	1230	CLA	C4B-C3B-CAB-CBB
14	J	1302	CLA	C2B-C3B-CAB-CBB
14	J	1302	CLA	C4B-C3B-CAB-CBB
14	J	1302	CLA	CHA-CBD-CGD-O1D
14	J	1302	CLA	CHA-CBD-CGD-O2D
14	J	1302	CLA	CAD-CBD-CGD-O1D
14	J	1302	CLA	CAD-CBD-CGD-O2D
14	J	1302	CLA	CBD-CGD-O2D-CED
14	K	1401	CLA	C1A-C2A-CAA-CBA
14	K	1401	CLA	CHA-CBD-CGD-O1D
14	K	1401	CLA	CHA-CBD-CGD-O2D
14	K	1103	CLA	C2B-C3B-CAB-CBB
14	K	1103	CLA	C4B-C3B-CAB-CBB
14	K	1105	CLA	C2B-C3B-CAB-CBB
14	K	1105	CLA	C4B-C3B-CAB-CBB
14	K	1105	CLA	CBD-CGD-O2D-CED
14	L	1501	CLA	C2B-C3B-CAB-CBB
14	L	1501	CLA	C4B-C3B-CAB-CBB
14	1	501	CLA	CHA-CBD-CGD-O1D
14	1	501	CLA	CBD-CGD-O2D-CED
14	1	503	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	1	503	CLA	C4B-C3B-CAB-CBB
14	1	503	CLA	CBD-CGD-O2D-CED
14	1	504	CLA	C4B-C3B-CAB-CBB
14	1	504	CLA	CHA-CBD-CGD-O1D
14	1	504	CLA	CHA-CBD-CGD-O2D
14	1	504	CLA	CAD-CBD-CGD-O1D
14	1	506	CLA	CHA-CBD-CGD-O1D
14	1	506	CLA	CHA-CBD-CGD-O2D
14	1	510	CLA	C4B-C3B-CAB-CBB
14	1	510	CLA	CBD-CGD-O2D-CED
14	1	512	CLA	C4B-C3B-CAB-CBB
14	1	516	CLA	C3A-C2A-CAA-CBA
14	1	516	CLA	C2B-C3B-CAB-CBB
14	1	516	CLA	C4B-C3B-CAB-CBB
14	1	516	CLA	CHA-CBD-CGD-O1D
14	1	516	CLA	CHA-CBD-CGD-O2D
14	1	516	CLA	CAD-CBD-CGD-O1D
14	1	516	CLA	CBD-CGD-O2D-CED
14	1	517	CLA	C2B-C3B-CAB-CBB
14	1	517	CLA	C4B-C3B-CAB-CBB
14	1	519	CLA	C2B-C3B-CAB-CBB
14	1	519	CLA	C4B-C3B-CAB-CBB
14	2	501	CLA	C4B-C3B-CAB-CBB
14	2	501	CLA	CBD-CGD-O2D-CED
14	2	501	CLA	C2-C3-C5-C6
14	2	501	CLA	C4-C3-C5-C6
14	2	506	CLA	CBD-CGD-O2D-CED
14	2	510	CLA	CHA-CBD-CGD-O1D
14	2	510	CLA	CHA-CBD-CGD-O2D
14	2	513	CLA	CBD-CGD-O2D-CED
14	2	516	CLA	C3A-C2A-CAA-CBA
14	2	516	CLA	C2B-C3B-CAB-CBB
14	2	516	CLA	C4B-C3B-CAB-CBB
14	2	517	CLA	CAD-CBD-CGD-O1D
14	2	517	CLA	CAD-CBD-CGD-O2D
14	2	517	CLA	CBD-CGD-O2D-CED
14	2	518	CLA	CHA-CBD-CGD-O1D
14	2	518	CLA	CHA-CBD-CGD-O2D
14	2	518	CLA	C2-C3-C5-C6
14	2	518	CLA	C4-C3-C5-C6
14	2	519	CLA	C2B-C3B-CAB-CBB
14	2	519	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	3	503	CLA	C2B-C3B-CAB-CBB
14	3	503	CLA	C4B-C3B-CAB-CBB
14	3	504	CLA	CHA-CBD-CGD-O1D
14	3	504	CLA	CHA-CBD-CGD-O2D
14	3	507	CLA	CHA-CBD-CGD-O1D
14	3	507	CLA	CHA-CBD-CGD-O2D
14	3	507	CLA	CAD-CBD-CGD-O1D
14	3	511	CLA	CBD-CGD-O2D-CED
14	3	513	CLA	C2B-C3B-CAB-CBB
14	3	513	CLA	C4B-C3B-CAB-CBB
14	3	516	CLA	C2A-CAA-CBA-CGA
14	3	516	CLA	CHA-CBD-CGD-O1D
14	3	516	CLA	CHA-CBD-CGD-O2D
14	3	517	CLA	C2B-C3B-CAB-CBB
14	3	517	CLA	C4B-C3B-CAB-CBB
14	3	517	CLA	CAD-CBD-CGD-O1D
14	3	517	CLA	CAD-CBD-CGD-O2D
14	3	517	CLA	CBD-CGD-O2D-CED
14	3	518	CLA	C2B-C3B-CAB-CBB
14	3	518	CLA	C4B-C3B-CAB-CBB
14	4	501	CLA	C2B-C3B-CAB-CBB
14	4	501	CLA	C4B-C3B-CAB-CBB
14	4	501	CLA	CBD-CGD-O2D-CED
14	4	503	CLA	C2B-C3B-CAB-CBB
14	4	503	CLA	C4B-C3B-CAB-CBB
14	4	516	CLA	CHA-CBD-CGD-O1D
14	4	516	CLA	CHA-CBD-CGD-O2D
14	4	519	CLA	CHA-CBD-CGD-O1D
14	4	519	CLA	CHA-CBD-CGD-O2D
14	4	519	CLA	CAD-CBD-CGD-O1D
14	4	519	CLA	CAD-CBD-CGD-O2D
14	4	519	CLA	CBD-CGD-O2D-CED
14	5	501	CLA	CBD-CGD-O2D-CED
14	5	502	CLA	CBD-CGD-O2D-CED
14	5	503	CLA	C2B-C3B-CAB-CBB
14	5	503	CLA	C4B-C3B-CAB-CBB
14	5	506	CLA	CHA-CBD-CGD-O1D
14	5	506	CLA	CHA-CBD-CGD-O2D
14	5	507	CLA	CBD-CGD-O2D-CED
14	5	510	CLA	CHA-CBD-CGD-O1D
14	5	510	CLA	CHA-CBD-CGD-O2D
14	5	511	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	5	512	CLA	C4B-C3B-CAB-CBB
14	5	513	CLA	C2B-C3B-CAB-CBB
14	5	513	CLA	C4B-C3B-CAB-CBB
14	5	513	CLA	CBD-CGD-O2D-CED
14	5	516	CLA	C4B-C3B-CAB-CBB
14	5	517	CLA	C4B-C3B-CAB-CBB
14	5	517	CLA	CHA-CBD-CGD-O1D
14	5	517	CLA	CHA-CBD-CGD-O2D
14	5	517	CLA	CAD-CBD-CGD-O1D
14	5	517	CLA	CBD-CGD-O2D-CED
14	5	518	CLA	C1A-C2A-CAA-CBA
14	5	518	CLA	C2B-C3B-CAB-CBB
14	5	518	CLA	C4B-C3B-CAB-CBB
14	5	519	CLA	CBD-CGD-O2D-CED
14	6	502	CLA	C2B-C3B-CAB-CBB
14	6	502	CLA	C4B-C3B-CAB-CBB
14	6	503	CLA	C2B-C3B-CAB-CBB
14	6	503	CLA	C4B-C3B-CAB-CBB
14	6	506	CLA	CHA-CBD-CGD-O1D
14	6	506	CLA	CHA-CBD-CGD-O2D
14	6	506	CLA	CAD-CBD-CGD-O1D
14	6	507	CLA	CBD-CGD-O2D-CED
14	6	508	CLA	CHA-CBD-CGD-O1D
14	6	508	CLA	CHA-CBD-CGD-O2D
14	6	510	CLA	CHA-CBD-CGD-O1D
14	6	510	CLA	CHA-CBD-CGD-O2D
14	6	510	CLA	CAD-CBD-CGD-O1D
14	6	510	CLA	CAD-CBD-CGD-O2D
14	6	512	CLA	C4B-C3B-CAB-CBB
14	6	513	CLA	CBD-CGD-O2D-CED
14	6	516	CLA	CBD-CGD-O2D-CED
14	6	517	CLA	CHA-CBD-CGD-O1D
14	6	517	CLA	CHA-CBD-CGD-O2D
14	6	517	CLA	CAD-CBD-CGD-O1D
14	6	518	CLA	CHA-CBD-CGD-O1D
14	6	518	CLA	CHA-CBD-CGD-O2D
14	6	518	CLA	CAD-CBD-CGD-O1D
14	6	519	CLA	C2B-C3B-CAB-CBB
14	6	519	CLA	C4B-C3B-CAB-CBB
14	G	1011	CLA	CHA-CBD-CGD-O1D
14	G	1102	CLA	C3A-C2A-CAA-CBA
14	G	1103	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1103	CLA	CHA-CBD-CGD-O1D
14	G	1103	CLA	CHA-CBD-CGD-O2D
14	G	1103	CLA	CAD-CBD-CGD-O1D
14	G	1104	CLA	C1A-C2A-CAA-CBA
14	G	1104	CLA	C4-C3-C5-C6
14	G	1106	CLA	C3A-C2A-CAA-CBA
14	G	1107	CLA	C2B-C3B-CAB-CBB
14	G	1108	CLA	C1A-C2A-CAA-CBA
14	G	1108	CLA	C3A-C2A-CAA-CBA
14	G	1110	CLA	C1A-C2A-CAA-CBA
14	G	1113	CLA	CHA-CBD-CGD-O1D
14	G	1113	CLA	CHA-CBD-CGD-O2D
14	G	1116	CLA	C3A-C2A-CAA-CBA
14	G	1117	CLA	CHA-CBD-CGD-O1D
14	G	1117	CLA	CHA-CBD-CGD-O2D
14	G	1119	CLA	CHA-CBD-CGD-O1D
14	G	1119	CLA	CHA-CBD-CGD-O2D
14	G	1119	CLA	CBD-CGD-O2D-CED
14	G	1120	CLA	CHA-CBD-CGD-O2D
14	G	1121	CLA	C2B-C3B-CAB-CBB
14	G	1121	CLA	C4B-C3B-CAB-CBB
14	G	1122	CLA	C2B-C3B-CAB-CBB
14	G	1122	CLA	C4B-C3B-CAB-CBB
14	G	1122	CLA	C2-C3-C5-C6
14	G	1122	CLA	C4-C3-C5-C6
14	G	1126	CLA	C1A-C2A-CAA-CBA
14	G	1126	CLA	C3A-C2A-CAA-CBA
14	G	1132	CLA	CHA-CBD-CGD-O1D
14	G	1132	CLA	CHA-CBD-CGD-O2D
14	G	1134	CLA	C2-C3-C5-C6
14	G	1134	CLA	C4-C3-C5-C6
14	G	1134	CLA	C11-C10-C8-C7
14	G	1137	CLA	C4-C3-C5-C6
14	G	1138	CLA	CBD-CGD-O2D-CED
14	G	1139	CLA	C1A-C2A-CAA-CBA
14	G	1139	CLA	CHA-CBD-CGD-O1D
14	G	1139	CLA	C2-C3-C5-C6
14	G	1139	CLA	C4-C3-C5-C6
14	G	1139	CLA	C6-C7-C8-C9
14	G	1140	CLA	C1A-C2A-CAA-CBA
14	G	1140	CLA	C2-C3-C5-C6
14	G	1140	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1237	CLA	CHA-CBD-CGD-O1D
14	G	1237	CLA	CHA-CBD-CGD-O2D
14	G	1237	CLA	C4-C3-C5-C6
14	G	1801	CLA	CHA-CBD-CGD-O1D
14	G	1801	CLA	CHA-CBD-CGD-O2D
14	G	1101	CLA	CHA-CBD-CGD-O1D
14	G	1101	CLA	CHA-CBD-CGD-O2D
14	H	1012	CLA	CHA-CBD-CGD-O1D
14	H	1012	CLA	CHA-CBD-CGD-O2D
14	H	1012	CLA	C2-C3-C5-C6
14	H	1012	CLA	C4-C3-C5-C6
14	H	1021	CLA	CHA-CBD-CGD-O1D
14	H	1021	CLA	CHA-CBD-CGD-O2D
14	H	1202	CLA	C1A-C2A-CAA-CBA
14	H	1202	CLA	C3A-C2A-CAA-CBA
14	H	1202	CLA	CHA-CBD-CGD-O1D
14	H	1202	CLA	CHA-CBD-CGD-O2D
14	H	1202	CLA	CAD-CBD-CGD-O1D
14	H	1205	CLA	CHA-CBD-CGD-O1D
14	H	1205	CLA	CHA-CBD-CGD-O2D
14	H	1206	CLA	CBD-CGD-O2D-CED
14	H	1209	CLA	C1A-C2A-CAA-CBA
14	H	1209	CLA	C3A-C2A-CAA-CBA
14	H	1209	CLA	CHA-CBD-CGD-O2D
14	H	1210	CLA	C1A-C2A-CAA-CBA
14	H	1211	CLA	CHA-CBD-CGD-O1D
14	H	1211	CLA	CHA-CBD-CGD-O2D
14	H	1212	CLA	C2-C3-C5-C6
14	H	1212	CLA	C4-C3-C5-C6
14	H	1214	CLA	C2A-CAA-CBA-CGA
14	H	1214	CLA	C2B-C3B-CAB-CBB
14	H	1214	CLA	C4B-C3B-CAB-CBB
14	H	1214	CLA	O2A-C1-C2-C3
14	H	1215	CLA	C1A-C2A-CAA-CBA
14	H	1215	CLA	C3A-C2A-CAA-CBA
14	H	1216	CLA	CBA-CGA-O2A-C1
14	H	1216	CLA	O1A-CGA-O2A-C1
14	H	1216	CLA	C2B-C3B-CAB-CBB
14	H	1216	CLA	C4B-C3B-CAB-CBB
14	H	1217	CLA	C1A-C2A-CAA-CBA
14	H	1217	CLA	C3A-C2A-CAA-CBA
14	H	1217	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1217	CLA	C2B-C3B-CAB-CBB
14	H	1217	CLA	C4B-C3B-CAB-CBB
14	H	1219	CLA	CBA-CGA-O2A-C1
14	H	1219	CLA	O1A-CGA-O2A-C1
14	H	1220	CLA	C2B-C3B-CAB-CBB
14	H	1220	CLA	C4B-C3B-CAB-CBB
14	H	1220	CLA	CHA-CBD-CGD-O1D
14	H	1220	CLA	CHA-CBD-CGD-O2D
14	H	1224	CLA	C1A-C2A-CAA-CBA
14	H	1224	CLA	C3A-C2A-CAA-CBA
14	H	1227	CLA	CBA-CGA-O2A-C1
14	H	1234	CLA	CHA-CBD-CGD-O1D
14	H	1239	CLA	C4B-C3B-CAB-CBB
14	H	1239	CLA	CBD-CGD-O2D-CED
14	H	1240	CLA	C1A-C2A-CAA-CBA
14	H	1240	CLA	CHA-CBD-CGD-O1D
14	H	1240	CLA	CHA-CBD-CGD-O2D
14	H	1230	CLA	C1A-C2A-CAA-CBA
14	H	1230	CLA	C3A-C2A-CAA-CBA
14	H	1230	CLA	C2B-C3B-CAB-CBB
14	H	1230	CLA	C4B-C3B-CAB-CBB
14	T	1302	CLA	C2B-C3B-CAB-CBB
14	T	1302	CLA	C4B-C3B-CAB-CBB
14	T	1302	CLA	CHA-CBD-CGD-O1D
14	T	1302	CLA	CHA-CBD-CGD-O2D
14	T	1302	CLA	CAD-CBD-CGD-O1D
14	T	1302	CLA	CAD-CBD-CGD-O2D
14	T	1302	CLA	CBD-CGD-O2D-CED
14	U	1401	CLA	C1A-C2A-CAA-CBA
14	U	1401	CLA	CHA-CBD-CGD-O1D
14	U	1401	CLA	CHA-CBD-CGD-O2D
14	U	1103	CLA	C2B-C3B-CAB-CBB
14	U	1103	CLA	C4B-C3B-CAB-CBB
14	U	1105	CLA	C2B-C3B-CAB-CBB
14	U	1105	CLA	C4B-C3B-CAB-CBB
14	U	1105	CLA	CBD-CGD-O2D-CED
14	V	1501	CLA	C2B-C3B-CAB-CBB
14	V	1501	CLA	C4B-C3B-CAB-CBB
14	Y	501	CLA	CHA-CBD-CGD-O1D
14	Y	501	CLA	CBD-CGD-O2D-CED
14	Y	503	CLA	C2B-C3B-CAB-CBB
14	Y	503	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Y	503	CLA	CBD-CGD-O2D-CED
14	Y	504	CLA	C4B-C3B-CAB-CBB
14	Y	504	CLA	CHA-CBD-CGD-O1D
14	Y	504	CLA	CHA-CBD-CGD-O2D
14	Y	504	CLA	CAD-CBD-CGD-O1D
14	Y	506	CLA	CHA-CBD-CGD-O1D
14	Y	506	CLA	CHA-CBD-CGD-O2D
14	Y	510	CLA	C4B-C3B-CAB-CBB
14	Y	510	CLA	CBD-CGD-O2D-CED
14	Y	512	CLA	C4B-C3B-CAB-CBB
14	Y	516	CLA	C3A-C2A-CAA-CBA
14	Y	516	CLA	C2B-C3B-CAB-CBB
14	Y	516	CLA	C4B-C3B-CAB-CBB
14	Y	516	CLA	CHA-CBD-CGD-O1D
14	Y	516	CLA	CHA-CBD-CGD-O2D
14	Y	516	CLA	CAD-CBD-CGD-O1D
14	Y	516	CLA	CBD-CGD-O2D-CED
14	Y	517	CLA	C2B-C3B-CAB-CBB
14	Y	517	CLA	C4B-C3B-CAB-CBB
14	Y	519	CLA	C2B-C3B-CAB-CBB
14	Y	519	CLA	C4B-C3B-CAB-CBB
14	Z	501	CLA	C4B-C3B-CAB-CBB
14	Z	501	CLA	CBD-CGD-O2D-CED
14	Z	501	CLA	C2-C3-C5-C6
14	Z	501	CLA	C4-C3-C5-C6
14	Z	506	CLA	CBD-CGD-O2D-CED
14	Z	510	CLA	CHA-CBD-CGD-O1D
14	Z	510	CLA	CHA-CBD-CGD-O2D
14	Z	513	CLA	CBD-CGD-O2D-CED
14	Z	516	CLA	C3A-C2A-CAA-CBA
14	Z	516	CLA	C2B-C3B-CAB-CBB
14	Z	516	CLA	C4B-C3B-CAB-CBB
14	Z	517	CLA	CAD-CBD-CGD-O1D
14	Z	517	CLA	CAD-CBD-CGD-O2D
14	Z	517	CLA	CBD-CGD-O2D-CED
14	Z	518	CLA	CHA-CBD-CGD-O1D
14	Z	518	CLA	CHA-CBD-CGD-O2D
14	Z	518	CLA	C2-C3-C5-C6
14	Z	518	CLA	C4-C3-C5-C6
14	Z	519	CLA	C2B-C3B-CAB-CBB
14	Z	519	CLA	C4B-C3B-CAB-CBB
14	a	503	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	503	CLA	C4B-C3B-CAB-CBB
14	a	504	CLA	CHA-CBD-CGD-O1D
14	a	504	CLA	CHA-CBD-CGD-O2D
14	a	507	CLA	CHA-CBD-CGD-O1D
14	a	507	CLA	CHA-CBD-CGD-O2D
14	a	507	CLA	CAD-CBD-CGD-O1D
14	a	511	CLA	CBD-CGD-O2D-CED
14	a	513	CLA	C2B-C3B-CAB-CBB
14	a	513	CLA	C4B-C3B-CAB-CBB
14	a	516	CLA	C2A-CAA-CBA-CGA
14	a	516	CLA	CHA-CBD-CGD-O1D
14	a	516	CLA	CHA-CBD-CGD-O2D
14	a	517	CLA	C2B-C3B-CAB-CBB
14	a	517	CLA	C4B-C3B-CAB-CBB
14	a	517	CLA	CAD-CBD-CGD-O1D
14	a	517	CLA	CAD-CBD-CGD-O2D
14	a	517	CLA	CBD-CGD-O2D-CED
14	a	518	CLA	C2B-C3B-CAB-CBB
14	a	518	CLA	C4B-C3B-CAB-CBB
14	b	501	CLA	C2B-C3B-CAB-CBB
14	b	501	CLA	C4B-C3B-CAB-CBB
14	b	501	CLA	CBD-CGD-O2D-CED
14	b	503	CLA	C2B-C3B-CAB-CBB
14	b	503	CLA	C4B-C3B-CAB-CBB
14	b	516	CLA	CHA-CBD-CGD-O1D
14	b	516	CLA	CHA-CBD-CGD-O2D
14	b	519	CLA	CHA-CBD-CGD-O1D
14	b	519	CLA	CHA-CBD-CGD-O2D
14	b	519	CLA	CAD-CBD-CGD-O1D
14	b	519	CLA	CAD-CBD-CGD-O2D
14	b	519	CLA	CBD-CGD-O2D-CED
14	c	501	CLA	CBD-CGD-O2D-CED
14	c	502	CLA	CBD-CGD-O2D-CED
14	c	503	CLA	C2B-C3B-CAB-CBB
14	c	503	CLA	C4B-C3B-CAB-CBB
14	c	506	CLA	CHA-CBD-CGD-O1D
14	c	506	CLA	CHA-CBD-CGD-O2D
14	c	507	CLA	CBD-CGD-O2D-CED
14	c	510	CLA	CHA-CBD-CGD-O1D
14	c	510	CLA	CHA-CBD-CGD-O2D
14	c	511	CLA	CBD-CGD-O2D-CED
14	c	512	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	c	513	CLA	C2B-C3B-CAB-CBB
14	c	513	CLA	C4B-C3B-CAB-CBB
14	c	513	CLA	CBD-CGD-O2D-CED
14	c	516	CLA	C4B-C3B-CAB-CBB
14	c	517	CLA	C4B-C3B-CAB-CBB
14	c	517	CLA	CHA-CBD-CGD-O1D
14	c	517	CLA	CHA-CBD-CGD-O2D
14	c	517	CLA	CAD-CBD-CGD-O1D
14	c	517	CLA	CBD-CGD-O2D-CED
14	c	518	CLA	C1A-C2A-CAA-CBA
14	c	518	CLA	C2B-C3B-CAB-CBB
14	c	518	CLA	C4B-C3B-CAB-CBB
14	c	519	CLA	CBD-CGD-O2D-CED
14	d	502	CLA	C2B-C3B-CAB-CBB
14	d	502	CLA	C4B-C3B-CAB-CBB
14	d	503	CLA	C2B-C3B-CAB-CBB
14	d	503	CLA	C4B-C3B-CAB-CBB
14	d	506	CLA	CHA-CBD-CGD-O1D
14	d	506	CLA	CHA-CBD-CGD-O2D
14	d	506	CLA	CAD-CBD-CGD-O1D
14	d	507	CLA	CBD-CGD-O2D-CED
14	d	508	CLA	CHA-CBD-CGD-O1D
14	d	508	CLA	CHA-CBD-CGD-O2D
14	d	510	CLA	CHA-CBD-CGD-O1D
14	d	510	CLA	CHA-CBD-CGD-O2D
14	d	510	CLA	CAD-CBD-CGD-O1D
14	d	510	CLA	CAD-CBD-CGD-O2D
14	d	512	CLA	C4B-C3B-CAB-CBB
14	d	513	CLA	CBD-CGD-O2D-CED
14	d	516	CLA	CBD-CGD-O2D-CED
14	d	517	CLA	CHA-CBD-CGD-O1D
14	d	517	CLA	CHA-CBD-CGD-O2D
14	d	517	CLA	CAD-CBD-CGD-O1D
14	d	518	CLA	CHA-CBD-CGD-O1D
14	d	518	CLA	CHA-CBD-CGD-O2D
14	d	518	CLA	CAD-CBD-CGD-O1D
14	d	519	CLA	C2B-C3B-CAB-CBB
14	d	519	CLA	C4B-C3B-CAB-CBB
14	e	1011	CLA	CHA-CBD-CGD-O1D
14	e	1102	CLA	C3A-C2A-CAA-CBA
14	e	1103	CLA	C1A-C2A-CAA-CBA
14	e	1103	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1103	CLA	CHA-CBD-CGD-O2D
14	e	1103	CLA	CAD-CBD-CGD-O1D
14	e	1104	CLA	C1A-C2A-CAA-CBA
14	e	1104	CLA	C4-C3-C5-C6
14	e	1106	CLA	C3A-C2A-CAA-CBA
14	e	1107	CLA	C2B-C3B-CAB-CBB
14	e	1108	CLA	C1A-C2A-CAA-CBA
14	e	1108	CLA	C3A-C2A-CAA-CBA
14	e	1110	CLA	C1A-C2A-CAA-CBA
14	e	1113	CLA	CHA-CBD-CGD-O1D
14	e	1113	CLA	CHA-CBD-CGD-O2D
14	e	1116	CLA	C3A-C2A-CAA-CBA
14	e	1117	CLA	CHA-CBD-CGD-O1D
14	e	1117	CLA	CHA-CBD-CGD-O2D
14	e	1119	CLA	CHA-CBD-CGD-O1D
14	e	1119	CLA	CHA-CBD-CGD-O2D
14	e	1119	CLA	CBD-CGD-O2D-CED
14	e	1120	CLA	CHA-CBD-CGD-O2D
14	e	1121	CLA	C2B-C3B-CAB-CBB
14	e	1121	CLA	C4B-C3B-CAB-CBB
14	e	1122	CLA	C2B-C3B-CAB-CBB
14	e	1122	CLA	C4B-C3B-CAB-CBB
14	e	1122	CLA	C2-C3-C5-C6
14	e	1122	CLA	C4-C3-C5-C6
14	e	1126	CLA	C1A-C2A-CAA-CBA
14	e	1126	CLA	C3A-C2A-CAA-CBA
14	e	1132	CLA	CHA-CBD-CGD-O1D
14	e	1132	CLA	CHA-CBD-CGD-O2D
14	e	1134	CLA	C2-C3-C5-C6
14	e	1134	CLA	C4-C3-C5-C6
14	e	1134	CLA	C11-C10-C8-C7
14	e	1137	CLA	C4-C3-C5-C6
14	e	1138	CLA	CBD-CGD-O2D-CED
14	e	1139	CLA	C1A-C2A-CAA-CBA
14	e	1139	CLA	CHA-CBD-CGD-O1D
14	e	1139	CLA	C2-C3-C5-C6
14	e	1139	CLA	C4-C3-C5-C6
14	e	1139	CLA	C6-C7-C8-C9
14	e	1140	CLA	C1A-C2A-CAA-CBA
14	e	1140	CLA	C2-C3-C5-C6
14	e	1140	CLA	C4-C3-C5-C6
14	e	1237	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1237	CLA	CHA-CBD-CGD-O2D
14	e	1237	CLA	C4-C3-C5-C6
14	e	1801	CLA	CHA-CBD-CGD-O1D
14	e	1801	CLA	CHA-CBD-CGD-O2D
14	e	1101	CLA	CHA-CBD-CGD-O1D
14	e	1101	CLA	CHA-CBD-CGD-O2D
14	f	1012	CLA	CHA-CBD-CGD-O1D
14	f	1012	CLA	CHA-CBD-CGD-O2D
14	f	1012	CLA	C2-C3-C5-C6
14	f	1012	CLA	C4-C3-C5-C6
14	f	1021	CLA	CHA-CBD-CGD-O1D
14	f	1021	CLA	CHA-CBD-CGD-O2D
14	f	1202	CLA	C1A-C2A-CAA-CBA
14	f	1202	CLA	C3A-C2A-CAA-CBA
14	f	1202	CLA	CHA-CBD-CGD-O1D
14	f	1202	CLA	CHA-CBD-CGD-O2D
14	f	1202	CLA	CAD-CBD-CGD-O1D
14	f	1205	CLA	CHA-CBD-CGD-O1D
14	f	1205	CLA	CHA-CBD-CGD-O2D
14	f	1206	CLA	CBD-CGD-O2D-CED
14	f	1209	CLA	C1A-C2A-CAA-CBA
14	f	1209	CLA	C3A-C2A-CAA-CBA
14	f	1209	CLA	CHA-CBD-CGD-O2D
14	f	1210	CLA	C1A-C2A-CAA-CBA
14	f	1211	CLA	CHA-CBD-CGD-O1D
14	f	1211	CLA	CHA-CBD-CGD-O2D
14	f	1212	CLA	C2-C3-C5-C6
14	f	1212	CLA	C4-C3-C5-C6
14	f	1214	CLA	C2A-CAA-CBA-CGA
14	f	1214	CLA	C2B-C3B-CAB-CBB
14	f	1214	CLA	C4B-C3B-CAB-CBB
14	f	1214	CLA	O2A-C1-C2-C3
14	f	1215	CLA	C1A-C2A-CAA-CBA
14	f	1215	CLA	C3A-C2A-CAA-CBA
14	f	1216	CLA	CBA-CGA-O2A-C1
14	f	1216	CLA	O1A-CGA-O2A-C1
14	f	1216	CLA	C2B-C3B-CAB-CBB
14	f	1216	CLA	C4B-C3B-CAB-CBB
14	f	1217	CLA	C1A-C2A-CAA-CBA
14	f	1217	CLA	C3A-C2A-CAA-CBA
14	f	1217	CLA	C2A-CAA-CBA-CGA
14	f	1217	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1217	CLA	C4B-C3B-CAB-CBB
14	f	1219	CLA	CBA-CGA-O2A-C1
14	f	1219	CLA	O1A-CGA-O2A-C1
14	f	1220	CLA	C2B-C3B-CAB-CBB
14	f	1220	CLA	C4B-C3B-CAB-CBB
14	f	1220	CLA	CHA-CBD-CGD-O1D
14	f	1220	CLA	CHA-CBD-CGD-O2D
14	f	1224	CLA	C1A-C2A-CAA-CBA
14	f	1224	CLA	C3A-C2A-CAA-CBA
14	f	1227	CLA	CBA-CGA-O2A-C1
14	f	1234	CLA	CHA-CBD-CGD-O1D
14	f	1239	CLA	C4B-C3B-CAB-CBB
14	f	1240	CLA	C1A-C2A-CAA-CBA
14	f	1240	CLA	CHA-CBD-CGD-O1D
14	f	1240	CLA	CHA-CBD-CGD-O2D
14	f	1230	CLA	C1A-C2A-CAA-CBA
14	f	1230	CLA	C3A-C2A-CAA-CBA
14	f	1230	CLA	C2B-C3B-CAB-CBB
14	f	1230	CLA	C4B-C3B-CAB-CBB
14	l	1302	CLA	C2B-C3B-CAB-CBB
14	l	1302	CLA	C4B-C3B-CAB-CBB
14	l	1302	CLA	CHA-CBD-CGD-O1D
14	l	1302	CLA	CHA-CBD-CGD-O2D
14	l	1302	CLA	CAD-CBD-CGD-O1D
14	l	1302	CLA	CAD-CBD-CGD-O2D
14	l	1302	CLA	CBD-CGD-O2D-CED
14	m	1401	CLA	C1A-C2A-CAA-CBA
14	m	1401	CLA	CHA-CBD-CGD-O1D
14	m	1401	CLA	CHA-CBD-CGD-O2D
14	m	1103	CLA	C2B-C3B-CAB-CBB
14	m	1103	CLA	C4B-C3B-CAB-CBB
14	m	1105	CLA	C2B-C3B-CAB-CBB
14	m	1105	CLA	C4B-C3B-CAB-CBB
14	m	1105	CLA	CBD-CGD-O2D-CED
14	n	1501	CLA	C2B-C3B-CAB-CBB
14	n	1501	CLA	C4B-C3B-CAB-CBB
14	q	501	CLA	CHA-CBD-CGD-O1D
14	q	501	CLA	CBD-CGD-O2D-CED
14	q	503	CLA	C2B-C3B-CAB-CBB
14	q	503	CLA	C4B-C3B-CAB-CBB
14	q	503	CLA	CBD-CGD-O2D-CED
14	q	504	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	q	504	CLA	CHA-CBD-CGD-O1D
14	q	504	CLA	CHA-CBD-CGD-O2D
14	q	504	CLA	CAD-CBD-CGD-O1D
14	q	506	CLA	CHA-CBD-CGD-O1D
14	q	506	CLA	CHA-CBD-CGD-O2D
14	q	510	CLA	C4B-C3B-CAB-CBB
14	q	510	CLA	CBD-CGD-O2D-CED
14	q	512	CLA	C4B-C3B-CAB-CBB
14	q	516	CLA	C3A-C2A-CAA-CBA
14	q	516	CLA	C2B-C3B-CAB-CBB
14	q	516	CLA	C4B-C3B-CAB-CBB
14	q	516	CLA	CHA-CBD-CGD-O1D
14	q	516	CLA	CHA-CBD-CGD-O2D
14	q	516	CLA	CAD-CBD-CGD-O1D
14	q	516	CLA	CBD-CGD-O2D-CED
14	q	517	CLA	C2B-C3B-CAB-CBB
14	q	517	CLA	C4B-C3B-CAB-CBB
14	q	519	CLA	C2B-C3B-CAB-CBB
14	q	519	CLA	C4B-C3B-CAB-CBB
14	r	501	CLA	C4B-C3B-CAB-CBB
14	r	501	CLA	CBD-CGD-O2D-CED
14	r	501	CLA	C2-C3-C5-C6
14	r	501	CLA	C4-C3-C5-C6
14	r	506	CLA	CBD-CGD-O2D-CED
14	r	510	CLA	CHA-CBD-CGD-O1D
14	r	510	CLA	CHA-CBD-CGD-O2D
14	r	513	CLA	CBD-CGD-O2D-CED
14	r	516	CLA	C3A-C2A-CAA-CBA
14	r	516	CLA	C2B-C3B-CAB-CBB
14	r	516	CLA	C4B-C3B-CAB-CBB
14	r	517	CLA	CAD-CBD-CGD-O1D
14	r	517	CLA	CAD-CBD-CGD-O2D
14	r	517	CLA	CBD-CGD-O2D-CED
14	r	518	CLA	CHA-CBD-CGD-O1D
14	r	518	CLA	CHA-CBD-CGD-O2D
14	r	518	CLA	C2-C3-C5-C6
14	r	518	CLA	C4-C3-C5-C6
14	r	519	CLA	C2B-C3B-CAB-CBB
14	r	519	CLA	C4B-C3B-CAB-CBB
14	s	503	CLA	C2B-C3B-CAB-CBB
14	s	503	CLA	C4B-C3B-CAB-CBB
14	s	504	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	s	504	CLA	CHA-CBD-CGD-O2D
14	s	507	CLA	CHA-CBD-CGD-O1D
14	s	507	CLA	CHA-CBD-CGD-O2D
14	s	507	CLA	CAD-CBD-CGD-O1D
14	s	511	CLA	CBD-CGD-O2D-CED
14	s	513	CLA	C2B-C3B-CAB-CBB
14	s	513	CLA	C4B-C3B-CAB-CBB
14	s	516	CLA	C2A-CAA-CBA-CGA
14	s	516	CLA	CHA-CBD-CGD-O1D
14	s	516	CLA	CHA-CBD-CGD-O2D
14	s	517	CLA	C2B-C3B-CAB-CBB
14	s	517	CLA	C4B-C3B-CAB-CBB
14	s	517	CLA	CAD-CBD-CGD-O1D
14	s	517	CLA	CAD-CBD-CGD-O2D
14	s	517	CLA	CBD-CGD-O2D-CED
14	s	518	CLA	C2B-C3B-CAB-CBB
14	s	518	CLA	C4B-C3B-CAB-CBB
14	t	501	CLA	C2B-C3B-CAB-CBB
14	t	501	CLA	C4B-C3B-CAB-CBB
14	t	501	CLA	CBD-CGD-O2D-CED
14	t	503	CLA	C2B-C3B-CAB-CBB
14	t	503	CLA	C4B-C3B-CAB-CBB
14	t	516	CLA	CHA-CBD-CGD-O1D
14	t	516	CLA	CHA-CBD-CGD-O2D
14	t	519	CLA	CHA-CBD-CGD-O1D
14	t	519	CLA	CHA-CBD-CGD-O2D
14	t	519	CLA	CAD-CBD-CGD-O1D
14	t	519	CLA	CAD-CBD-CGD-O2D
14	t	519	CLA	CBD-CGD-O2D-CED
14	u	501	CLA	CBD-CGD-O2D-CED
14	u	502	CLA	CBD-CGD-O2D-CED
14	u	503	CLA	C2B-C3B-CAB-CBB
14	u	503	CLA	C4B-C3B-CAB-CBB
14	u	506	CLA	CHA-CBD-CGD-O1D
14	u	506	CLA	CHA-CBD-CGD-O2D
14	u	507	CLA	CBD-CGD-O2D-CED
14	u	510	CLA	CHA-CBD-CGD-O1D
14	u	510	CLA	CHA-CBD-CGD-O2D
14	u	511	CLA	CBD-CGD-O2D-CED
14	u	512	CLA	C4B-C3B-CAB-CBB
14	u	513	CLA	C2B-C3B-CAB-CBB
14	u	513	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	513	CLA	CBD-CGD-O2D-CED
14	u	516	CLA	C4B-C3B-CAB-CBB
14	u	517	CLA	C4B-C3B-CAB-CBB
14	u	517	CLA	CHA-CBD-CGD-O1D
14	u	517	CLA	CHA-CBD-CGD-O2D
14	u	517	CLA	CAD-CBD-CGD-O1D
14	u	517	CLA	CBD-CGD-O2D-CED
14	u	518	CLA	C1A-C2A-CAA-CBA
14	u	518	CLA	C2B-C3B-CAB-CBB
14	u	518	CLA	C4B-C3B-CAB-CBB
14	u	519	CLA	CBD-CGD-O2D-CED
14	v	502	CLA	C2B-C3B-CAB-CBB
14	v	502	CLA	C4B-C3B-CAB-CBB
14	v	503	CLA	C2B-C3B-CAB-CBB
14	v	503	CLA	C4B-C3B-CAB-CBB
14	v	506	CLA	CHA-CBD-CGD-O1D
14	v	506	CLA	CHA-CBD-CGD-O2D
14	v	506	CLA	CAD-CBD-CGD-O1D
14	v	507	CLA	CBD-CGD-O2D-CED
14	v	508	CLA	CHA-CBD-CGD-O1D
14	v	508	CLA	CHA-CBD-CGD-O2D
14	v	510	CLA	CHA-CBD-CGD-O1D
14	v	510	CLA	CHA-CBD-CGD-O2D
14	v	510	CLA	CAD-CBD-CGD-O1D
14	v	510	CLA	CAD-CBD-CGD-O2D
14	v	512	CLA	C4B-C3B-CAB-CBB
14	v	513	CLA	CBD-CGD-O2D-CED
14	v	516	CLA	CBD-CGD-O2D-CED
14	v	517	CLA	CHA-CBD-CGD-O1D
14	v	517	CLA	CHA-CBD-CGD-O2D
14	v	517	CLA	CAD-CBD-CGD-O1D
14	v	518	CLA	CHA-CBD-CGD-O1D
14	v	518	CLA	CHA-CBD-CGD-O2D
14	v	518	CLA	CAD-CBD-CGD-O1D
14	v	519	CLA	C2B-C3B-CAB-CBB
14	v	519	CLA	C4B-C3B-CAB-CBB
17	A	4001	BCR	C11-C12-C13-C14
17	A	4001	BCR	C37-C22-C23-C24
17	A	4008	BCR	C21-C22-C23-C24
17	A	4008	BCR	C37-C22-C23-C24
17	A	4008	BCR	C23-C24-C25-C26
17	A	4011	BCR	C36-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	4004	BCR	C7-C8-C9-C10
17	B	4004	BCR	C7-C8-C9-C34
17	B	4004	BCR	C21-C22-C23-C24
17	B	4004	BCR	C37-C22-C23-C24
17	B	4004	BCR	C23-C24-C25-C30
17	B	4005	BCR	C7-C8-C9-C10
17	B	4005	BCR	C7-C8-C9-C34
17	B	4005	BCR	C21-C22-C23-C24
17	B	4005	BCR	C37-C22-C23-C24
17	B	4005	BCR	C23-C24-C25-C30
17	B	4010	BCR	C23-C24-C25-C26
17	B	4017	BCR	C1-C6-C7-C8
17	B	4014	BCR	C17-C18-C19-C20
17	B	4014	BCR	C36-C18-C19-C20
17	J	4013	BCR	C17-C18-C19-C20
17	J	4013	BCR	C36-C18-C19-C20
17	J	4015	BCR	C23-C24-C25-C30
17	J	4012	BCR	C5-C6-C7-C8
17	J	4012	BCR	C11-C12-C13-C14
17	J	4012	BCR	C11-C12-C13-C35
17	K	4104	BCR	C21-C22-C23-C24
17	K	4104	BCR	C37-C22-C23-C24
17	L	4019	BCR	C7-C8-C9-C10
17	L	4019	BCR	C7-C8-C9-C34
17	L	4219	BCR	C7-C8-C9-C10
17	M	4021	BCR	C5-C6-C7-C8
17	M	4021	BCR	C11-C12-C13-C35
17	M	4021	BCR	C17-C18-C19-C20
17	M	4021	BCR	C36-C18-C19-C20
17	1	521	BCR	C7-C8-C9-C10
17	1	521	BCR	C7-C8-C9-C34
17	1	522	BCR	C1-C6-C7-C8
17	1	522	BCR	C5-C6-C7-C8
17	1	522	BCR	C7-C8-C9-C10
17	1	522	BCR	C7-C8-C9-C34
17	1	523	BCR	C21-C22-C23-C24
17	1	523	BCR	C37-C22-C23-C24
17	2	521	BCR	C7-C8-C9-C10
17	2	521	BCR	C7-C8-C9-C34
17	2	522	BCR	C5-C6-C7-C8
17	2	522	BCR	C7-C8-C9-C10
17	2	522	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	2	523	BCR	C21-C22-C23-C24
17	2	523	BCR	C37-C22-C23-C24
17	3	521	BCR	C7-C8-C9-C34
17	3	522	BCR	C7-C8-C9-C10
17	3	522	BCR	C7-C8-C9-C34
17	3	523	BCR	C37-C22-C23-C24
17	4	521	BCR	C7-C8-C9-C10
17	4	521	BCR	C7-C8-C9-C34
17	4	523	BCR	C37-C22-C23-C24
17	5	521	BCR	C7-C8-C9-C10
17	5	521	BCR	C7-C8-C9-C34
17	5	521	BCR	C17-C18-C19-C20
17	5	521	BCR	C36-C18-C19-C20
17	5	522	BCR	C5-C6-C7-C8
17	5	522	BCR	C7-C8-C9-C10
17	5	522	BCR	C7-C8-C9-C34
17	5	523	BCR	C21-C22-C23-C24
17	5	523	BCR	C37-C22-C23-C24
17	6	522	BCR	C5-C6-C7-C8
17	6	523	BCR	C21-C22-C23-C24
17	6	523	BCR	C37-C22-C23-C24
17	6	524	BCR	C7-C8-C9-C10
17	6	524	BCR	C7-C8-C9-C34
17	G	4001	BCR	C11-C12-C13-C14
17	G	4001	BCR	C37-C22-C23-C24
17	G	4008	BCR	C21-C22-C23-C24
17	G	4008	BCR	C37-C22-C23-C24
17	G	4008	BCR	C23-C24-C25-C26
17	G	4011	BCR	C36-C18-C19-C20
17	H	4004	BCR	C7-C8-C9-C10
17	H	4004	BCR	C7-C8-C9-C34
17	H	4004	BCR	C21-C22-C23-C24
17	H	4004	BCR	C37-C22-C23-C24
17	H	4004	BCR	C23-C24-C25-C30
17	H	4005	BCR	C7-C8-C9-C10
17	H	4005	BCR	C7-C8-C9-C34
17	H	4005	BCR	C21-C22-C23-C24
17	H	4005	BCR	C37-C22-C23-C24
17	H	4005	BCR	C23-C24-C25-C30
17	H	4010	BCR	C23-C24-C25-C26
17	H	4017	BCR	C1-C6-C7-C8
17	H	4014	BCR	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	4014	BCR	C36-C18-C19-C20
17	T	4013	BCR	C17-C18-C19-C20
17	T	4013	BCR	C36-C18-C19-C20
17	T	4015	BCR	C23-C24-C25-C30
17	T	4012	BCR	C5-C6-C7-C8
17	T	4012	BCR	C11-C12-C13-C14
17	T	4012	BCR	C11-C12-C13-C35
17	U	4104	BCR	C21-C22-C23-C24
17	U	4104	BCR	C37-C22-C23-C24
17	V	4019	BCR	C7-C8-C9-C10
17	V	4019	BCR	C7-C8-C9-C34
17	V	4219	BCR	C7-C8-C9-C10
17	W	4021	BCR	C5-C6-C7-C8
17	W	4021	BCR	C11-C12-C13-C35
17	W	4021	BCR	C17-C18-C19-C20
17	W	4021	BCR	C36-C18-C19-C20
17	Y	521	BCR	C7-C8-C9-C10
17	Y	521	BCR	C7-C8-C9-C34
17	Y	522	BCR	C1-C6-C7-C8
17	Y	522	BCR	C5-C6-C7-C8
17	Y	522	BCR	C7-C8-C9-C10
17	Y	522	BCR	C7-C8-C9-C34
17	Y	523	BCR	C21-C22-C23-C24
17	Y	523	BCR	C37-C22-C23-C24
17	Z	521	BCR	C7-C8-C9-C10
17	Z	521	BCR	C7-C8-C9-C34
17	Z	522	BCR	C5-C6-C7-C8
17	Z	522	BCR	C7-C8-C9-C10
17	Z	522	BCR	C7-C8-C9-C34
17	Z	523	BCR	C21-C22-C23-C24
17	Z	523	BCR	C37-C22-C23-C24
17	a	521	BCR	C7-C8-C9-C34
17	a	522	BCR	C7-C8-C9-C10
17	a	522	BCR	C7-C8-C9-C34
17	a	523	BCR	C37-C22-C23-C24
17	b	521	BCR	C7-C8-C9-C10
17	b	521	BCR	C7-C8-C9-C34
17	b	523	BCR	C37-C22-C23-C24
17	c	521	BCR	C7-C8-C9-C10
17	c	521	BCR	C7-C8-C9-C34
17	c	521	BCR	C17-C18-C19-C20
17	c	521	BCR	C36-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	c	522	BCR	C5-C6-C7-C8
17	c	522	BCR	C7-C8-C9-C10
17	c	522	BCR	C7-C8-C9-C34
17	c	523	BCR	C21-C22-C23-C24
17	c	523	BCR	C37-C22-C23-C24
17	d	522	BCR	C5-C6-C7-C8
17	d	523	BCR	C21-C22-C23-C24
17	d	523	BCR	C37-C22-C23-C24
17	d	524	BCR	C7-C8-C9-C10
17	d	524	BCR	C7-C8-C9-C34
17	e	4001	BCR	C11-C12-C13-C14
17	e	4001	BCR	C37-C22-C23-C24
17	e	4008	BCR	C21-C22-C23-C24
17	e	4008	BCR	C37-C22-C23-C24
17	e	4008	BCR	C23-C24-C25-C26
17	e	4011	BCR	C36-C18-C19-C20
17	f	4004	BCR	C7-C8-C9-C10
17	f	4004	BCR	C7-C8-C9-C34
17	f	4004	BCR	C21-C22-C23-C24
17	f	4004	BCR	C37-C22-C23-C24
17	f	4004	BCR	C23-C24-C25-C30
17	f	4005	BCR	C7-C8-C9-C10
17	f	4005	BCR	C7-C8-C9-C34
17	f	4005	BCR	C21-C22-C23-C24
17	f	4005	BCR	C37-C22-C23-C24
17	f	4005	BCR	C23-C24-C25-C30
17	f	4010	BCR	C23-C24-C25-C26
17	f	4017	BCR	C1-C6-C7-C8
17	f	4014	BCR	C17-C18-C19-C20
17	f	4014	BCR	C36-C18-C19-C20
17	l	4013	BCR	C17-C18-C19-C20
17	l	4013	BCR	C36-C18-C19-C20
17	l	4015	BCR	C23-C24-C25-C30
17	l	4012	BCR	C5-C6-C7-C8
17	l	4012	BCR	C11-C12-C13-C14
17	l	4012	BCR	C11-C12-C13-C35
17	m	4104	BCR	C21-C22-C23-C24
17	m	4104	BCR	C37-C22-C23-C24
17	n	4019	BCR	C7-C8-C9-C10
17	n	4019	BCR	C7-C8-C9-C34
17	n	4219	BCR	C7-C8-C9-C10
17	o	4021	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	o	4021	BCR	C11-C12-C13-C35
17	o	4021	BCR	C17-C18-C19-C20
17	o	4021	BCR	C36-C18-C19-C20
17	q	521	BCR	C7-C8-C9-C10
17	q	521	BCR	C7-C8-C9-C34
17	q	522	BCR	C1-C6-C7-C8
17	q	522	BCR	C5-C6-C7-C8
17	q	522	BCR	C7-C8-C9-C10
17	q	522	BCR	C7-C8-C9-C34
17	q	523	BCR	C21-C22-C23-C24
17	q	523	BCR	C37-C22-C23-C24
17	r	521	BCR	C7-C8-C9-C10
17	r	521	BCR	C7-C8-C9-C34
17	r	522	BCR	C5-C6-C7-C8
17	r	522	BCR	C7-C8-C9-C10
17	r	522	BCR	C7-C8-C9-C34
17	r	523	BCR	C21-C22-C23-C24
17	r	523	BCR	C37-C22-C23-C24
17	s	521	BCR	C7-C8-C9-C34
17	s	522	BCR	C7-C8-C9-C10
17	s	522	BCR	C7-C8-C9-C34
17	s	523	BCR	C37-C22-C23-C24
17	t	521	BCR	C7-C8-C9-C10
17	t	521	BCR	C7-C8-C9-C34
17	t	523	BCR	C37-C22-C23-C24
17	u	521	BCR	C7-C8-C9-C10
17	u	521	BCR	C7-C8-C9-C34
17	u	521	BCR	C17-C18-C19-C20
17	u	521	BCR	C36-C18-C19-C20
17	u	522	BCR	C5-C6-C7-C8
17	u	522	BCR	C7-C8-C9-C10
17	u	522	BCR	C7-C8-C9-C34
17	u	523	BCR	C21-C22-C23-C24
17	u	523	BCR	C37-C22-C23-C24
17	v	522	BCR	C5-C6-C7-C8
17	v	523	BCR	C21-C22-C23-C24
17	v	523	BCR	C37-C22-C23-C24
17	v	524	BCR	C7-C8-C9-C10
17	v	524	BCR	C7-C8-C9-C34
18	A	5002	LHG	O2-C2-C3-O3
18	A	5002	LHG	O9-C7-O7-C5
18	A	5002	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	5004	LHG	O1-C1-C2-C3
18	A	5004	LHG	C3-O3-P-O4
18	A	5004	LHG	C3-O3-P-O6
18	A	5004	LHG	C8-C7-O7-C5
18	A	5005	LHG	C3-O3-P-O4
18	A	5006	LHG	C4-O6-P-O4
18	A	5008	LHG	C4-O6-P-O3
18	A	5008	LHG	O7-C5-C6-O8
18	A	5008	LHG	C8-C7-O7-C5
18	A	5009	LHG	C3-O3-P-O4
18	A	5009	LHG	C3-O3-P-O5
18	A	5009	LHG	C3-O3-P-O6
18	A	5009	LHG	C4-O6-P-O4
18	A	5009	LHG	O9-C7-O7-C5
18	B	1842	LHG	C3-O3-P-O5
18	B	1842	LHG	O9-C7-O7-C5
18	B	1842	LHG	C8-C7-O7-C5
18	B	1855	LHG	C3-O3-P-O4
18	B	1855	LHG	C4-O6-P-O5
18	I	5001	LHG	O1-C1-C2-C3
18	I	5001	LHG	C3-O3-P-O4
18	I	5001	LHG	O9-C7-O7-C5
18	I	5001	LHG	C8-C7-O7-C5
18	I	5001	LHG	C24-C23-O8-C6
18	L	5218	LHG	C3-O3-P-O4
18	L	5218	LHG	C3-O3-P-O5
18	L	5218	LHG	O7-C5-C6-O8
18	L	5218	LHG	C8-C7-O7-C5
18	L	5220	LHG	C4-O6-P-O5
18	L	5220	LHG	C8-C7-O7-C5
18	L	5221	LHG	O1-C1-C2-C3
18	L	5221	LHG	C3-O3-P-O5
18	L	5221	LHG	C4-O6-P-O3
18	L	5221	LHG	C4-O6-P-O5
18	G	5002	LHG	O2-C2-C3-O3
18	G	5002	LHG	O9-C7-O7-C5
18	G	5002	LHG	C8-C7-O7-C5
18	G	5004	LHG	O1-C1-C2-C3
18	G	5004	LHG	C3-O3-P-O4
18	G	5004	LHG	C3-O3-P-O6
18	G	5004	LHG	C8-C7-O7-C5
18	G	5005	LHG	C3-O3-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	5006	LHG	C4-O6-P-O4
18	G	5008	LHG	C4-O6-P-O3
18	G	5008	LHG	O7-C5-C6-O8
18	G	5008	LHG	C8-C7-O7-C5
18	G	5009	LHG	C3-O3-P-O4
18	G	5009	LHG	C3-O3-P-O5
18	G	5009	LHG	C3-O3-P-O6
18	G	5009	LHG	C4-O6-P-O4
18	G	5009	LHG	O9-C7-O7-C5
18	H	1842	LHG	C3-O3-P-O5
18	H	1842	LHG	O9-C7-O7-C5
18	H	1842	LHG	C8-C7-O7-C5
18	H	1855	LHG	C3-O3-P-O4
18	H	1855	LHG	C4-O6-P-O5
18	S	5001	LHG	O1-C1-C2-C3
18	S	5001	LHG	C3-O3-P-O4
18	S	5001	LHG	O9-C7-O7-C5
18	S	5001	LHG	C8-C7-O7-C5
18	S	5001	LHG	C24-C23-O8-C6
18	V	5218	LHG	C3-O3-P-O4
18	V	5218	LHG	C3-O3-P-O5
18	V	5218	LHG	O7-C5-C6-O8
18	V	5218	LHG	C8-C7-O7-C5
18	V	5220	LHG	C4-O6-P-O5
18	V	5220	LHG	C8-C7-O7-C5
18	V	5221	LHG	O1-C1-C2-C3
18	V	5221	LHG	C3-O3-P-O5
18	V	5221	LHG	C4-O6-P-O3
18	V	5221	LHG	C4-O6-P-O5
18	e	5002	LHG	O2-C2-C3-O3
18	e	5002	LHG	O9-C7-O7-C5
18	e	5002	LHG	C8-C7-O7-C5
18	e	5004	LHG	O1-C1-C2-C3
18	e	5004	LHG	C3-O3-P-O4
18	e	5004	LHG	C3-O3-P-O6
18	e	5004	LHG	C8-C7-O7-C5
18	e	5005	LHG	C3-O3-P-O4
18	e	5006	LHG	C4-O6-P-O4
18	e	5008	LHG	C4-O6-P-O3
18	e	5008	LHG	O7-C5-C6-O8
18	e	5008	LHG	C8-C7-O7-C5
18	e	5009	LHG	C3-O3-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	5009	LHG	C3-O3-P-O5
18	e	5009	LHG	C3-O3-P-O6
18	e	5009	LHG	C4-O6-P-O4
18	e	5009	LHG	O9-C7-O7-C5
18	f	1842	LHG	C3-O3-P-O5
18	f	1842	LHG	O9-C7-O7-C5
18	f	1842	LHG	C8-C7-O7-C5
18	f	1855	LHG	C3-O3-P-O4
18	f	1855	LHG	C4-O6-P-O5
18	k	5001	LHG	O1-C1-C2-C3
18	k	5001	LHG	C3-O3-P-O4
18	k	5001	LHG	O9-C7-O7-C5
18	k	5001	LHG	C8-C7-O7-C5
18	k	5001	LHG	C24-C23-O8-C6
18	n	5218	LHG	C3-O3-P-O4
18	n	5218	LHG	C3-O3-P-O5
18	n	5218	LHG	O7-C5-C6-O8
18	n	5218	LHG	C8-C7-O7-C5
18	n	5220	LHG	C4-O6-P-O5
18	n	5220	LHG	C8-C7-O7-C5
18	n	5221	LHG	O1-C1-C2-C3
18	n	5221	LHG	C3-O3-P-O5
18	n	5221	LHG	C4-O6-P-O3
18	n	5221	LHG	C4-O6-P-O5
19	B	1843	LMU	C2'-C1'-O1'-C1
19	B	1843	LMU	O5'-C1'-O1'-C1
19	J	5105	LMU	C2'-C1'-O1'-C1
19	J	5105	LMU	O5'-C1'-O1'-C1
19	H	1843	LMU	C2'-C1'-O1'-C1
19	H	1843	LMU	O5'-C1'-O1'-C1
19	T	5105	LMU	C2'-C1'-O1'-C1
19	T	5105	LMU	O5'-C1'-O1'-C1
19	f	1843	LMU	C2'-C1'-O1'-C1
19	f	1843	LMU	O5'-C1'-O1'-C1
19	l	5105	LMU	C2'-C1'-O1'-C1
19	l	5105	LMU	O5'-C1'-O1'-C1
21	L	5216	SQD	C5-C6-S-O7
21	L	5216	SQD	C5-C6-S-O8
21	L	5216	SQD	C5-C6-S-O9
21	1	822	SQD	O47-C45-C46-O48
21	1	822	SQD	O49-C7-O47-C45
21	1	822	SQD	C8-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	822	SQD	O49-C7-O47-C45
21	2	822	SQD	C8-C7-O47-C45
21	3	822	SQD	O47-C45-C46-O48
21	3	822	SQD	O49-C7-O47-C45
21	3	822	SQD	C8-C7-O47-C45
21	4	822	SQD	C8-C7-O47-C45
21	6	822	SQD	C46-C45-O47-C7
21	V	5216	SQD	C5-C6-S-O7
21	V	5216	SQD	C5-C6-S-O8
21	V	5216	SQD	C5-C6-S-O9
21	Y	822	SQD	O47-C45-C46-O48
21	Y	822	SQD	O49-C7-O47-C45
21	Y	822	SQD	C8-C7-O47-C45
21	Z	822	SQD	O49-C7-O47-C45
21	Z	822	SQD	C8-C7-O47-C45
21	a	822	SQD	O47-C45-C46-O48
21	a	822	SQD	O49-C7-O47-C45
21	a	822	SQD	C8-C7-O47-C45
21	b	822	SQD	C8-C7-O47-C45
21	d	822	SQD	C46-C45-O47-C7
21	n	5216	SQD	C5-C6-S-O7
21	n	5216	SQD	C5-C6-S-O8
21	n	5216	SQD	C5-C6-S-O9
21	q	822	SQD	O47-C45-C46-O48
21	q	822	SQD	O49-C7-O47-C45
21	q	822	SQD	C8-C7-O47-C45
21	r	822	SQD	O49-C7-O47-C45
21	r	822	SQD	C8-C7-O47-C45
21	s	822	SQD	O47-C45-C46-O48
21	s	822	SQD	O49-C7-O47-C45
21	s	822	SQD	C8-C7-O47-C45
21	t	822	SQD	C8-C7-O47-C45
21	v	822	SQD	C46-C45-O47-C7
21	4	822	SQD	O49-C7-O47-C45
21	5	822	SQD	O49-C7-O47-C45
21	5	822	SQD	C8-C7-O47-C45
21	6	822	SQD	C8-C7-O47-C45
21	b	822	SQD	O49-C7-O47-C45
21	c	822	SQD	O49-C7-O47-C45
21	c	822	SQD	C8-C7-O47-C45
21	d	822	SQD	C8-C7-O47-C45
21	t	822	SQD	O49-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	u	822	SQD	O49-C7-O47-C45
21	u	822	SQD	C8-C7-O47-C45
21	v	822	SQD	C8-C7-O47-C45
14	A	1139	CLA	O1D-CGD-O2D-CED
14	B	1023	CLA	O1D-CGD-O2D-CED
14	2	513	CLA	O1D-CGD-O2D-CED
14	3	511	CLA	O1D-CGD-O2D-CED
14	4	501	CLA	O1D-CGD-O2D-CED
14	4	506	CLA	O1D-CGD-O2D-CED
14	5	506	CLA	O1D-CGD-O2D-CED
14	5	513	CLA	O1D-CGD-O2D-CED
14	6	503	CLA	O1D-CGD-O2D-CED
14	6	511	CLA	O1D-CGD-O2D-CED
14	6	518	CLA	O1D-CGD-O2D-CED
14	G	1139	CLA	O1D-CGD-O2D-CED
14	H	1023	CLA	O1D-CGD-O2D-CED
14	Z	513	CLA	O1D-CGD-O2D-CED
14	a	511	CLA	O1D-CGD-O2D-CED
14	b	501	CLA	O1D-CGD-O2D-CED
14	b	506	CLA	O1D-CGD-O2D-CED
14	c	506	CLA	O1D-CGD-O2D-CED
14	c	513	CLA	O1D-CGD-O2D-CED
14	d	503	CLA	O1D-CGD-O2D-CED
14	d	511	CLA	O1D-CGD-O2D-CED
14	d	518	CLA	O1D-CGD-O2D-CED
14	e	1139	CLA	O1D-CGD-O2D-CED
14	f	1023	CLA	O1D-CGD-O2D-CED
14	r	513	CLA	O1D-CGD-O2D-CED
14	s	511	CLA	O1D-CGD-O2D-CED
14	t	501	CLA	O1D-CGD-O2D-CED
14	t	506	CLA	O1D-CGD-O2D-CED
14	u	506	CLA	O1D-CGD-O2D-CED
14	u	513	CLA	O1D-CGD-O2D-CED
14	v	503	CLA	O1D-CGD-O2D-CED
14	v	511	CLA	O1D-CGD-O2D-CED
14	v	518	CLA	O1D-CGD-O2D-CED
21	6	822	SQD	O49-C7-O47-C45
21	d	822	SQD	O49-C7-O47-C45
21	v	822	SQD	O49-C7-O47-C45
14	B	1219	CLA	O1D-CGD-O2D-CED
14	1	506	CLA	O1D-CGD-O2D-CED
14	2	503	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	3	503	CLA	O1D-CGD-O2D-CED
14	5	503	CLA	O1D-CGD-O2D-CED
14	5	519	CLA	O1D-CGD-O2D-CED
14	6	506	CLA	O1D-CGD-O2D-CED
14	H	1219	CLA	O1D-CGD-O2D-CED
14	Y	506	CLA	O1D-CGD-O2D-CED
14	Z	503	CLA	O1D-CGD-O2D-CED
14	a	503	CLA	O1D-CGD-O2D-CED
14	c	503	CLA	O1D-CGD-O2D-CED
14	c	519	CLA	O1D-CGD-O2D-CED
14	d	506	CLA	O1D-CGD-O2D-CED
14	f	1219	CLA	O1D-CGD-O2D-CED
14	q	506	CLA	O1D-CGD-O2D-CED
14	r	503	CLA	O1D-CGD-O2D-CED
14	s	503	CLA	O1D-CGD-O2D-CED
14	u	503	CLA	O1D-CGD-O2D-CED
14	u	519	CLA	O1D-CGD-O2D-CED
14	v	506	CLA	O1D-CGD-O2D-CED
21	4	822	SQD	C24-C23-O48-C46
21	b	822	SQD	C24-C23-O48-C46
21	t	822	SQD	C24-C23-O48-C46
14	A	1108	CLA	CBD-CGD-O2D-CED
14	A	1123	CLA	CBD-CGD-O2D-CED
14	A	1132	CLA	CBD-CGD-O2D-CED
14	A	1139	CLA	CBD-CGD-O2D-CED
14	A	1801	CLA	CBD-CGD-O2D-CED
14	B	1021	CLA	CBD-CGD-O2D-CED
14	B	1023	CLA	CBD-CGD-O2D-CED
14	B	1203	CLA	CBD-CGD-O2D-CED
14	B	1216	CLA	CBD-CGD-O2D-CED
14	B	1219	CLA	CBD-CGD-O2D-CED
14	B	1239	CLA	CBD-CGD-O2D-CED
14	B	1207	CLA	CBD-CGD-O2D-CED
14	F	1301	CLA	CBD-CGD-O2D-CED
14	1	506	CLA	CBD-CGD-O2D-CED
14	1	508	CLA	CBD-CGD-O2D-CED
14	1	518	CLA	CBD-CGD-O2D-CED
14	2	503	CLA	CBD-CGD-O2D-CED
14	2	510	CLA	CBD-CGD-O2D-CED
14	2	516	CLA	CBD-CGD-O2D-CED
14	2	519	CLA	CBD-CGD-O2D-CED
14	3	503	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	3	506	CLA	CBD-CGD-O2D-CED
14	3	513	CLA	CBD-CGD-O2D-CED
14	4	504	CLA	CBD-CGD-O2D-CED
14	4	506	CLA	CBD-CGD-O2D-CED
14	4	510	CLA	CBD-CGD-O2D-CED
14	4	511	CLA	CBD-CGD-O2D-CED
14	4	517	CLA	CBD-CGD-O2D-CED
14	4	518	CLA	CBD-CGD-O2D-CED
14	5	503	CLA	CBD-CGD-O2D-CED
14	5	504	CLA	CBD-CGD-O2D-CED
14	5	506	CLA	CBD-CGD-O2D-CED
14	6	501	CLA	CBD-CGD-O2D-CED
14	6	503	CLA	CBD-CGD-O2D-CED
14	6	506	CLA	CBD-CGD-O2D-CED
14	6	511	CLA	CBD-CGD-O2D-CED
14	6	517	CLA	CBD-CGD-O2D-CED
14	6	518	CLA	CBD-CGD-O2D-CED
14	6	519	CLA	CBD-CGD-O2D-CED
14	G	1108	CLA	CBD-CGD-O2D-CED
14	G	1123	CLA	CBD-CGD-O2D-CED
14	G	1132	CLA	CBD-CGD-O2D-CED
14	G	1139	CLA	CBD-CGD-O2D-CED
14	G	1801	CLA	CBD-CGD-O2D-CED
14	H	1021	CLA	CBD-CGD-O2D-CED
14	H	1023	CLA	CBD-CGD-O2D-CED
14	H	1203	CLA	CBD-CGD-O2D-CED
14	H	1216	CLA	CBD-CGD-O2D-CED
14	H	1219	CLA	CBD-CGD-O2D-CED
14	H	1207	CLA	CBD-CGD-O2D-CED
14	R	1301	CLA	CBD-CGD-O2D-CED
14	Y	506	CLA	CBD-CGD-O2D-CED
14	Y	508	CLA	CBD-CGD-O2D-CED
14	Y	518	CLA	CBD-CGD-O2D-CED
14	Z	503	CLA	CBD-CGD-O2D-CED
14	Z	510	CLA	CBD-CGD-O2D-CED
14	Z	516	CLA	CBD-CGD-O2D-CED
14	Z	519	CLA	CBD-CGD-O2D-CED
14	a	503	CLA	CBD-CGD-O2D-CED
14	a	506	CLA	CBD-CGD-O2D-CED
14	a	513	CLA	CBD-CGD-O2D-CED
14	b	504	CLA	CBD-CGD-O2D-CED
14	b	506	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	510	CLA	CBD-CGD-O2D-CED
14	b	511	CLA	CBD-CGD-O2D-CED
14	b	517	CLA	CBD-CGD-O2D-CED
14	b	518	CLA	CBD-CGD-O2D-CED
14	c	503	CLA	CBD-CGD-O2D-CED
14	c	504	CLA	CBD-CGD-O2D-CED
14	c	506	CLA	CBD-CGD-O2D-CED
14	d	501	CLA	CBD-CGD-O2D-CED
14	d	503	CLA	CBD-CGD-O2D-CED
14	d	506	CLA	CBD-CGD-O2D-CED
14	d	511	CLA	CBD-CGD-O2D-CED
14	d	517	CLA	CBD-CGD-O2D-CED
14	d	518	CLA	CBD-CGD-O2D-CED
14	d	519	CLA	CBD-CGD-O2D-CED
14	e	1108	CLA	CBD-CGD-O2D-CED
14	e	1123	CLA	CBD-CGD-O2D-CED
14	e	1132	CLA	CBD-CGD-O2D-CED
14	e	1139	CLA	CBD-CGD-O2D-CED
14	e	1801	CLA	CBD-CGD-O2D-CED
14	f	1021	CLA	CBD-CGD-O2D-CED
14	f	1023	CLA	CBD-CGD-O2D-CED
14	f	1203	CLA	CBD-CGD-O2D-CED
14	f	1216	CLA	CBD-CGD-O2D-CED
14	f	1219	CLA	CBD-CGD-O2D-CED
14	f	1239	CLA	CBD-CGD-O2D-CED
14	f	1207	CLA	CBD-CGD-O2D-CED
14	j	1301	CLA	CBD-CGD-O2D-CED
14	q	506	CLA	CBD-CGD-O2D-CED
14	q	508	CLA	CBD-CGD-O2D-CED
14	q	518	CLA	CBD-CGD-O2D-CED
14	r	503	CLA	CBD-CGD-O2D-CED
14	r	510	CLA	CBD-CGD-O2D-CED
14	r	516	CLA	CBD-CGD-O2D-CED
14	r	519	CLA	CBD-CGD-O2D-CED
14	s	503	CLA	CBD-CGD-O2D-CED
14	s	506	CLA	CBD-CGD-O2D-CED
14	s	513	CLA	CBD-CGD-O2D-CED
14	t	504	CLA	CBD-CGD-O2D-CED
14	t	506	CLA	CBD-CGD-O2D-CED
14	t	510	CLA	CBD-CGD-O2D-CED
14	t	511	CLA	CBD-CGD-O2D-CED
14	t	517	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	t	518	CLA	CBD-CGD-O2D-CED
14	u	503	CLA	CBD-CGD-O2D-CED
14	u	504	CLA	CBD-CGD-O2D-CED
14	u	506	CLA	CBD-CGD-O2D-CED
14	v	501	CLA	CBD-CGD-O2D-CED
14	v	503	CLA	CBD-CGD-O2D-CED
14	v	506	CLA	CBD-CGD-O2D-CED
14	v	511	CLA	CBD-CGD-O2D-CED
14	v	517	CLA	CBD-CGD-O2D-CED
14	v	518	CLA	CBD-CGD-O2D-CED
14	v	519	CLA	CBD-CGD-O2D-CED
14	A	1109	CLA	O1A-CGA-O2A-C1
14	B	1209	CLA	O1A-CGA-O2A-C1
14	B	1227	CLA	O1A-CGA-O2A-C1
14	3	505	CLA	O1A-CGA-O2A-C1
14	6	505	CLA	O1A-CGA-O2A-C1
14	G	1109	CLA	O1A-CGA-O2A-C1
14	H	1209	CLA	O1A-CGA-O2A-C1
14	H	1227	CLA	O1A-CGA-O2A-C1
14	a	505	CLA	O1A-CGA-O2A-C1
14	d	505	CLA	O1A-CGA-O2A-C1
14	e	1109	CLA	O1A-CGA-O2A-C1
14	f	1209	CLA	O1A-CGA-O2A-C1
14	f	1227	CLA	O1A-CGA-O2A-C1
14	s	505	CLA	O1A-CGA-O2A-C1
14	v	505	CLA	O1A-CGA-O2A-C1
18	I	5001	LHG	O10-C23-O8-C6
18	L	5221	LHG	O10-C23-O8-C6
18	S	5001	LHG	O10-C23-O8-C6
18	V	5221	LHG	O10-C23-O8-C6
18	k	5001	LHG	O10-C23-O8-C6
18	n	5221	LHG	O10-C23-O8-C6
14	A	1108	CLA	O1D-CGD-O2D-CED
14	1	516	CLA	O1D-CGD-O2D-CED
14	2	516	CLA	O1D-CGD-O2D-CED
14	3	506	CLA	O1D-CGD-O2D-CED
14	4	504	CLA	O1D-CGD-O2D-CED
14	6	513	CLA	O1D-CGD-O2D-CED
14	G	1108	CLA	O1D-CGD-O2D-CED
14	Z	516	CLA	O1D-CGD-O2D-CED
14	a	506	CLA	O1D-CGD-O2D-CED
14	b	504	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	d	513	CLA	O1D-CGD-O2D-CED
14	e	1108	CLA	O1D-CGD-O2D-CED
14	q	516	CLA	O1D-CGD-O2D-CED
14	r	516	CLA	O1D-CGD-O2D-CED
14	s	506	CLA	O1D-CGD-O2D-CED
14	t	504	CLA	O1D-CGD-O2D-CED
14	v	513	CLA	O1D-CGD-O2D-CED
14	v	516	CLA	O1D-CGD-O2D-CED
14	K	1105	CLA	C4C-C3C-CAC-CBC
14	U	1105	CLA	C4C-C3C-CAC-CBC
14	m	1105	CLA	C4C-C3C-CAC-CBC
14	B	1021	CLA	O1D-CGD-O2D-CED
14	K	1105	CLA	O1D-CGD-O2D-CED
14	1	510	CLA	O1D-CGD-O2D-CED
14	2	501	CLA	O1D-CGD-O2D-CED
14	2	517	CLA	O1D-CGD-O2D-CED
14	3	517	CLA	O1D-CGD-O2D-CED
14	5	501	CLA	O1D-CGD-O2D-CED
14	5	502	CLA	O1D-CGD-O2D-CED
14	5	511	CLA	O1D-CGD-O2D-CED
14	5	517	CLA	O1D-CGD-O2D-CED
14	6	507	CLA	O1D-CGD-O2D-CED
14	6	516	CLA	O1D-CGD-O2D-CED
14	H	1021	CLA	O1D-CGD-O2D-CED
14	U	1105	CLA	O1D-CGD-O2D-CED
14	Y	510	CLA	O1D-CGD-O2D-CED
14	Y	516	CLA	O1D-CGD-O2D-CED
14	Z	501	CLA	O1D-CGD-O2D-CED
14	Z	517	CLA	O1D-CGD-O2D-CED
14	a	517	CLA	O1D-CGD-O2D-CED
14	c	501	CLA	O1D-CGD-O2D-CED
14	c	502	CLA	O1D-CGD-O2D-CED
14	c	511	CLA	O1D-CGD-O2D-CED
14	c	517	CLA	O1D-CGD-O2D-CED
14	d	507	CLA	O1D-CGD-O2D-CED
14	d	516	CLA	O1D-CGD-O2D-CED
14	f	1021	CLA	O1D-CGD-O2D-CED
14	m	1105	CLA	O1D-CGD-O2D-CED
14	q	510	CLA	O1D-CGD-O2D-CED
14	r	501	CLA	O1D-CGD-O2D-CED
14	r	517	CLA	O1D-CGD-O2D-CED
14	s	517	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	501	CLA	O1D-CGD-O2D-CED
14	u	502	CLA	O1D-CGD-O2D-CED
14	u	511	CLA	O1D-CGD-O2D-CED
14	u	517	CLA	O1D-CGD-O2D-CED
14	v	507	CLA	O1D-CGD-O2D-CED
14	A	1109	CLA	CBA-CGA-O2A-C1
14	B	1206	CLA	CBA-CGA-O2A-C1
14	B	1209	CLA	CBA-CGA-O2A-C1
14	6	505	CLA	CBA-CGA-O2A-C1
14	G	1109	CLA	CBA-CGA-O2A-C1
14	H	1206	CLA	CBA-CGA-O2A-C1
14	H	1209	CLA	CBA-CGA-O2A-C1
14	d	505	CLA	CBA-CGA-O2A-C1
14	e	1109	CLA	CBA-CGA-O2A-C1
14	f	1206	CLA	CBA-CGA-O2A-C1
14	f	1209	CLA	CBA-CGA-O2A-C1
14	v	505	CLA	CBA-CGA-O2A-C1
14	A	1106	CLA	CBD-CGD-O2D-CED
14	A	1111	CLA	CBD-CGD-O2D-CED
14	A	1115	CLA	CBD-CGD-O2D-CED
14	A	1126	CLA	CBD-CGD-O2D-CED
14	A	1131	CLA	CBD-CGD-O2D-CED
14	A	1022	CLA	CBD-CGD-O2D-CED
14	B	1204	CLA	CBD-CGD-O2D-CED
14	B	1209	CLA	CBD-CGD-O2D-CED
14	B	1229	CLA	CBD-CGD-O2D-CED
14	K	1103	CLA	CBD-CGD-O2D-CED
14	L	1503	CLA	CBD-CGD-O2D-CED
14	1	507	CLA	CBD-CGD-O2D-CED
14	1	512	CLA	CBD-CGD-O2D-CED
14	3	518	CLA	CBD-CGD-O2D-CED
14	3	519	CLA	CBD-CGD-O2D-CED
14	4	507	CLA	CBD-CGD-O2D-CED
14	4	509	CLA	CBD-CGD-O2D-CED
14	4	513	CLA	CBD-CGD-O2D-CED
14	G	1106	CLA	CBD-CGD-O2D-CED
14	G	1111	CLA	CBD-CGD-O2D-CED
14	G	1115	CLA	CBD-CGD-O2D-CED
14	G	1126	CLA	CBD-CGD-O2D-CED
14	G	1131	CLA	CBD-CGD-O2D-CED
14	G	1022	CLA	CBD-CGD-O2D-CED
14	H	1204	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1209	CLA	CBD-CGD-O2D-CED
14	H	1229	CLA	CBD-CGD-O2D-CED
14	U	1103	CLA	CBD-CGD-O2D-CED
14	V	1503	CLA	CBD-CGD-O2D-CED
14	Y	507	CLA	CBD-CGD-O2D-CED
14	Y	512	CLA	CBD-CGD-O2D-CED
14	a	518	CLA	CBD-CGD-O2D-CED
14	a	519	CLA	CBD-CGD-O2D-CED
14	b	507	CLA	CBD-CGD-O2D-CED
14	b	509	CLA	CBD-CGD-O2D-CED
14	b	513	CLA	CBD-CGD-O2D-CED
14	e	1106	CLA	CBD-CGD-O2D-CED
14	e	1111	CLA	CBD-CGD-O2D-CED
14	e	1115	CLA	CBD-CGD-O2D-CED
14	e	1126	CLA	CBD-CGD-O2D-CED
14	e	1131	CLA	CBD-CGD-O2D-CED
14	e	1022	CLA	CBD-CGD-O2D-CED
14	f	1204	CLA	CBD-CGD-O2D-CED
14	f	1209	CLA	CBD-CGD-O2D-CED
14	f	1229	CLA	CBD-CGD-O2D-CED
14	m	1103	CLA	CBD-CGD-O2D-CED
14	n	1503	CLA	CBD-CGD-O2D-CED
14	q	507	CLA	CBD-CGD-O2D-CED
14	q	512	CLA	CBD-CGD-O2D-CED
14	s	518	CLA	CBD-CGD-O2D-CED
14	s	519	CLA	CBD-CGD-O2D-CED
14	t	507	CLA	CBD-CGD-O2D-CED
14	t	509	CLA	CBD-CGD-O2D-CED
14	t	513	CLA	CBD-CGD-O2D-CED
14	A	1110	CLA	O1A-CGA-O2A-C1
14	A	1119	CLA	O1A-CGA-O2A-C1
14	A	1140	CLA	O1A-CGA-O2A-C1
14	B	1206	CLA	O1A-CGA-O2A-C1
14	B	1217	CLA	O1A-CGA-O2A-C1
14	B	1240	CLA	O1A-CGA-O2A-C1
14	B	1207	CLA	O1A-CGA-O2A-C1
14	2	505	CLA	O1A-CGA-O2A-C1
14	G	1110	CLA	O1A-CGA-O2A-C1
14	G	1119	CLA	O1A-CGA-O2A-C1
14	G	1140	CLA	O1A-CGA-O2A-C1
14	H	1206	CLA	O1A-CGA-O2A-C1
14	H	1217	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1240	CLA	O1A-CGA-O2A-C1
14	H	1207	CLA	O1A-CGA-O2A-C1
14	Z	505	CLA	O1A-CGA-O2A-C1
14	e	1110	CLA	O1A-CGA-O2A-C1
14	e	1119	CLA	O1A-CGA-O2A-C1
14	e	1140	CLA	O1A-CGA-O2A-C1
14	f	1206	CLA	O1A-CGA-O2A-C1
14	f	1217	CLA	O1A-CGA-O2A-C1
14	f	1240	CLA	O1A-CGA-O2A-C1
14	f	1207	CLA	O1A-CGA-O2A-C1
14	r	505	CLA	O1A-CGA-O2A-C1
18	A	5006	LHG	O10-C23-O8-C6
18	A	5009	LHG	O10-C23-O8-C6
18	L	5220	LHG	O10-C23-O8-C6
18	G	5006	LHG	O10-C23-O8-C6
18	G	5009	LHG	O10-C23-O8-C6
18	V	5220	LHG	O10-C23-O8-C6
18	e	5006	LHG	O10-C23-O8-C6
18	e	5009	LHG	O10-C23-O8-C6
18	n	5220	LHG	O10-C23-O8-C6
21	1	822	SQD	O10-C23-O48-C46
21	Y	822	SQD	O10-C23-O48-C46
21	q	822	SQD	O10-C23-O48-C46
14	A	1119	CLA	O1D-CGD-O2D-CED
14	A	1138	CLA	O1D-CGD-O2D-CED
14	1	501	CLA	O1D-CGD-O2D-CED
14	G	1119	CLA	O1D-CGD-O2D-CED
14	G	1138	CLA	O1D-CGD-O2D-CED
14	Y	501	CLA	O1D-CGD-O2D-CED
14	e	1119	CLA	O1D-CGD-O2D-CED
14	e	1138	CLA	O1D-CGD-O2D-CED
14	q	501	CLA	O1D-CGD-O2D-CED
14	J	1302	CLA	O1D-CGD-O2D-CED
14	1	503	CLA	O1D-CGD-O2D-CED
14	2	506	CLA	O1D-CGD-O2D-CED
14	4	518	CLA	O1D-CGD-O2D-CED
14	5	507	CLA	O1D-CGD-O2D-CED
14	T	1302	CLA	O1D-CGD-O2D-CED
14	Y	503	CLA	O1D-CGD-O2D-CED
14	Z	506	CLA	O1D-CGD-O2D-CED
14	b	518	CLA	O1D-CGD-O2D-CED
14	c	507	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	l	1302	CLA	O1D-CGD-O2D-CED
14	q	503	CLA	O1D-CGD-O2D-CED
14	r	506	CLA	O1D-CGD-O2D-CED
14	t	518	CLA	O1D-CGD-O2D-CED
14	u	507	CLA	O1D-CGD-O2D-CED
14	A	1013	CLA	CBD-CGD-O2D-CED
14	A	1121	CLA	CBD-CGD-O2D-CED
14	A	1237	CLA	CBD-CGD-O2D-CED
14	B	1201	CLA	CBD-CGD-O2D-CED
14	B	1231	CLA	CBD-CGD-O2D-CED
14	B	1234	CLA	CBD-CGD-O2D-CED
14	2	507	CLA	CBD-CGD-O2D-CED
14	3	505	CLA	CBD-CGD-O2D-CED
14	4	508	CLA	CBD-CGD-O2D-CED
14	G	1013	CLA	CBD-CGD-O2D-CED
14	G	1121	CLA	CBD-CGD-O2D-CED
14	G	1237	CLA	CBD-CGD-O2D-CED
14	H	1201	CLA	CBD-CGD-O2D-CED
14	H	1231	CLA	CBD-CGD-O2D-CED
14	H	1234	CLA	CBD-CGD-O2D-CED
14	Z	507	CLA	CBD-CGD-O2D-CED
14	a	505	CLA	CBD-CGD-O2D-CED
14	b	508	CLA	CBD-CGD-O2D-CED
14	e	1013	CLA	CBD-CGD-O2D-CED
14	e	1121	CLA	CBD-CGD-O2D-CED
14	e	1237	CLA	CBD-CGD-O2D-CED
14	f	1201	CLA	CBD-CGD-O2D-CED
14	f	1231	CLA	CBD-CGD-O2D-CED
14	f	1234	CLA	CBD-CGD-O2D-CED
14	r	507	CLA	CBD-CGD-O2D-CED
14	s	505	CLA	CBD-CGD-O2D-CED
14	t	508	CLA	CBD-CGD-O2D-CED
14	B	1206	CLA	O1D-CGD-O2D-CED
14	B	1239	CLA	O1D-CGD-O2D-CED
14	4	519	CLA	O1D-CGD-O2D-CED
14	H	1206	CLA	O1D-CGD-O2D-CED
14	H	1239	CLA	O1D-CGD-O2D-CED
14	b	519	CLA	O1D-CGD-O2D-CED
14	f	1206	CLA	O1D-CGD-O2D-CED
14	f	1239	CLA	O1D-CGD-O2D-CED
14	t	519	CLA	O1D-CGD-O2D-CED
18	A	5004	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	5007	LHG	O9-C7-O7-C5
18	A	5008	LHG	O9-C7-O7-C5
18	B	1855	LHG	O9-C7-O7-C5
18	L	5218	LHG	O9-C7-O7-C5
18	L	5220	LHG	O9-C7-O7-C5
18	G	5004	LHG	O9-C7-O7-C5
18	G	5007	LHG	O9-C7-O7-C5
18	G	5008	LHG	O9-C7-O7-C5
18	H	1855	LHG	O9-C7-O7-C5
18	V	5218	LHG	O9-C7-O7-C5
18	V	5220	LHG	O9-C7-O7-C5
18	e	5004	LHG	O9-C7-O7-C5
18	e	5007	LHG	O9-C7-O7-C5
18	e	5008	LHG	O9-C7-O7-C5
18	f	1855	LHG	O9-C7-O7-C5
18	n	5218	LHG	O9-C7-O7-C5
18	n	5220	LHG	O9-C7-O7-C5
18	L	5218	LHG	O10-C23-O8-C6
18	V	5218	LHG	O10-C23-O8-C6
18	n	5218	LHG	O10-C23-O8-C6
14	K	1105	CLA	C2C-C3C-CAC-CBC
14	U	1105	CLA	C2C-C3C-CAC-CBC
14	m	1105	CLA	C2C-C3C-CAC-CBC
14	A	1116	CLA	C3-C5-C6-C7
14	A	1118	CLA	C3-C5-C6-C7
14	A	1119	CLA	C3-C5-C6-C7
14	A	1121	CLA	C3-C5-C6-C7
14	A	1122	CLA	C3-C5-C6-C7
14	A	1133	CLA	C3-C5-C6-C7
14	A	1136	CLA	C3-C5-C6-C7
14	A	1139	CLA	C3-C5-C6-C7
14	B	1211	CLA	C3-C5-C6-C7
14	B	1231	CLA	C3-C5-C6-C7
14	B	1239	CLA	C3-C5-C6-C7
14	L	1503	CLA	C3-C5-C6-C7
14	2	501	CLA	C3-C5-C6-C7
14	2	505	CLA	C3-C5-C6-C7
14	2	518	CLA	C3-C5-C6-C7
14	6	505	CLA	C3-C5-C6-C7
14	G	1116	CLA	C3-C5-C6-C7
14	G	1118	CLA	C3-C5-C6-C7
14	G	1119	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1121	CLA	C3-C5-C6-C7
14	G	1122	CLA	C3-C5-C6-C7
14	G	1133	CLA	C3-C5-C6-C7
14	G	1136	CLA	C3-C5-C6-C7
14	G	1139	CLA	C3-C5-C6-C7
14	H	1211	CLA	C3-C5-C6-C7
14	H	1231	CLA	C3-C5-C6-C7
14	H	1239	CLA	C3-C5-C6-C7
14	V	1503	CLA	C3-C5-C6-C7
14	Z	501	CLA	C3-C5-C6-C7
14	Z	505	CLA	C3-C5-C6-C7
14	Z	518	CLA	C3-C5-C6-C7
14	d	505	CLA	C3-C5-C6-C7
14	e	1116	CLA	C3-C5-C6-C7
14	e	1118	CLA	C3-C5-C6-C7
14	e	1119	CLA	C3-C5-C6-C7
14	e	1121	CLA	C3-C5-C6-C7
14	e	1122	CLA	C3-C5-C6-C7
14	e	1133	CLA	C3-C5-C6-C7
14	e	1136	CLA	C3-C5-C6-C7
14	e	1139	CLA	C3-C5-C6-C7
14	f	1211	CLA	C3-C5-C6-C7
14	f	1231	CLA	C3-C5-C6-C7
14	f	1239	CLA	C3-C5-C6-C7
14	n	1503	CLA	C3-C5-C6-C7
14	r	501	CLA	C3-C5-C6-C7
14	r	505	CLA	C3-C5-C6-C7
14	r	518	CLA	C3-C5-C6-C7
14	v	505	CLA	C3-C5-C6-C7
14	A	1110	CLA	CBA-CGA-O2A-C1
14	B	1217	CLA	CBA-CGA-O2A-C1
14	2	505	CLA	CBA-CGA-O2A-C1
14	3	505	CLA	CBA-CGA-O2A-C1
14	G	1110	CLA	CBA-CGA-O2A-C1
14	H	1217	CLA	CBA-CGA-O2A-C1
14	Z	505	CLA	CBA-CGA-O2A-C1
14	a	505	CLA	CBA-CGA-O2A-C1
14	e	1110	CLA	CBA-CGA-O2A-C1
14	f	1217	CLA	CBA-CGA-O2A-C1
14	r	505	CLA	CBA-CGA-O2A-C1
14	s	505	CLA	CBA-CGA-O2A-C1
18	A	5006	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	L	5218	LHG	C24-C23-O8-C6
18	L	5220	LHG	C24-C23-O8-C6
18	G	5006	LHG	C24-C23-O8-C6
18	V	5218	LHG	C24-C23-O8-C6
18	V	5220	LHG	C24-C23-O8-C6
18	e	5006	LHG	C24-C23-O8-C6
18	n	5218	LHG	C24-C23-O8-C6
18	n	5220	LHG	C24-C23-O8-C6
21	4	822	SQD	O10-C23-O48-C46
21	b	822	SQD	O10-C23-O48-C46
21	t	822	SQD	O10-C23-O48-C46
18	A	5009	LHG	C8-C7-O7-C5
18	G	5009	LHG	C8-C7-O7-C5
18	e	5009	LHG	C8-C7-O7-C5
14	3	513	CLA	O1D-CGD-O2D-CED
14	a	513	CLA	O1D-CGD-O2D-CED
14	s	513	CLA	O1D-CGD-O2D-CED
14	A	1011	CLA	CBD-CGD-O2D-CED
14	G	1011	CLA	CBD-CGD-O2D-CED
14	e	1011	CLA	CBD-CGD-O2D-CED
14	3	516	CLA	C2C-C3C-CAC-CBC
14	a	516	CLA	C2C-C3C-CAC-CBC
14	s	516	CLA	C2C-C3C-CAC-CBC
19	J	5105	LMU	O5'-C5'-C6'-O6'
19	T	5105	LMU	O5'-C5'-C6'-O6'
19	l	5105	LMU	O5'-C5'-C6'-O6'
14	A	1133	CLA	C4-C3-C5-C6
14	A	1130	CLA	C4-C3-C5-C6
14	L	1503	CLA	C4-C3-C5-C6
14	G	1133	CLA	C4-C3-C5-C6
14	G	1130	CLA	C4-C3-C5-C6
14	V	1503	CLA	C4-C3-C5-C6
14	e	1133	CLA	C4-C3-C5-C6
14	e	1130	CLA	C4-C3-C5-C6
14	n	1503	CLA	C4-C3-C5-C6
14	A	1104	CLA	C2-C3-C5-C6
14	A	1237	CLA	C2-C3-C5-C6
14	A	1130	CLA	C2-C3-C5-C6
14	G	1104	CLA	C2-C3-C5-C6
14	G	1237	CLA	C2-C3-C5-C6
14	G	1130	CLA	C2-C3-C5-C6
14	e	1104	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1237	CLA	C2-C3-C5-C6
14	e	1130	CLA	C2-C3-C5-C6
14	A	1133	CLA	CBD-CGD-O2D-CED
14	B	1220	CLA	CBD-CGD-O2D-CED
14	2	504	CLA	CBD-CGD-O2D-CED
14	5	512	CLA	CBD-CGD-O2D-CED
14	6	512	CLA	CBD-CGD-O2D-CED
14	G	1133	CLA	CBD-CGD-O2D-CED
14	H	1220	CLA	CBD-CGD-O2D-CED
14	Z	504	CLA	CBD-CGD-O2D-CED
14	c	512	CLA	CBD-CGD-O2D-CED
14	d	512	CLA	CBD-CGD-O2D-CED
14	e	1133	CLA	CBD-CGD-O2D-CED
14	f	1220	CLA	CBD-CGD-O2D-CED
14	r	504	CLA	CBD-CGD-O2D-CED
14	u	512	CLA	CBD-CGD-O2D-CED
14	v	512	CLA	CBD-CGD-O2D-CED
14	A	1108	CLA	C2A-CAA-CBA-CGA
14	A	1119	CLA	C2A-CAA-CBA-CGA
14	A	1127	CLA	C2A-CAA-CBA-CGA
14	B	1012	CLA	C2A-CAA-CBA-CGA
14	B	1206	CLA	C2A-CAA-CBA-CGA
14	B	1221	CLA	C2A-CAA-CBA-CGA
14	B	1228	CLA	C2A-CAA-CBA-CGA
14	B	1232	CLA	C2A-CAA-CBA-CGA
14	B	1238	CLA	C2A-CAA-CBA-CGA
14	1	507	CLA	C2A-CAA-CBA-CGA
14	1	513	CLA	C2A-CAA-CBA-CGA
14	2	505	CLA	C2A-CAA-CBA-CGA
14	2	507	CLA	C2A-CAA-CBA-CGA
14	5	507	CLA	C2A-CAA-CBA-CGA
14	6	505	CLA	C2A-CAA-CBA-CGA
14	6	513	CLA	C2A-CAA-CBA-CGA
14	G	1108	CLA	C2A-CAA-CBA-CGA
14	G	1119	CLA	C2A-CAA-CBA-CGA
14	G	1127	CLA	C2A-CAA-CBA-CGA
14	H	1012	CLA	C2A-CAA-CBA-CGA
14	H	1206	CLA	C2A-CAA-CBA-CGA
14	H	1221	CLA	C2A-CAA-CBA-CGA
14	H	1228	CLA	C2A-CAA-CBA-CGA
14	H	1232	CLA	C2A-CAA-CBA-CGA
14	H	1238	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Y	507	CLA	C2A-CAA-CBA-CGA
14	Y	513	CLA	C2A-CAA-CBA-CGA
14	Z	505	CLA	C2A-CAA-CBA-CGA
14	Z	507	CLA	C2A-CAA-CBA-CGA
14	c	507	CLA	C2A-CAA-CBA-CGA
14	d	505	CLA	C2A-CAA-CBA-CGA
14	d	513	CLA	C2A-CAA-CBA-CGA
14	e	1108	CLA	C2A-CAA-CBA-CGA
14	e	1119	CLA	C2A-CAA-CBA-CGA
14	e	1127	CLA	C2A-CAA-CBA-CGA
14	f	1012	CLA	C2A-CAA-CBA-CGA
14	f	1206	CLA	C2A-CAA-CBA-CGA
14	f	1221	CLA	C2A-CAA-CBA-CGA
14	f	1228	CLA	C2A-CAA-CBA-CGA
14	f	1232	CLA	C2A-CAA-CBA-CGA
14	f	1238	CLA	C2A-CAA-CBA-CGA
14	q	507	CLA	C2A-CAA-CBA-CGA
14	q	513	CLA	C2A-CAA-CBA-CGA
14	r	505	CLA	C2A-CAA-CBA-CGA
14	r	507	CLA	C2A-CAA-CBA-CGA
14	u	507	CLA	C2A-CAA-CBA-CGA
14	v	505	CLA	C2A-CAA-CBA-CGA
14	v	513	CLA	C2A-CAA-CBA-CGA
14	A	1801	CLA	O1D-CGD-O2D-CED
14	B	1216	CLA	O1D-CGD-O2D-CED
14	G	1801	CLA	O1D-CGD-O2D-CED
14	H	1216	CLA	O1D-CGD-O2D-CED
14	e	1801	CLA	O1D-CGD-O2D-CED
14	f	1216	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	C3-C5-C6-C7
14	B	1206	CLA	C3-C5-C6-C7
14	B	1232	CLA	C3-C5-C6-C7
14	G	1102	CLA	C3-C5-C6-C7
14	H	1206	CLA	C3-C5-C6-C7
14	H	1232	CLA	C3-C5-C6-C7
14	e	1102	CLA	C3-C5-C6-C7
14	f	1206	CLA	C3-C5-C6-C7
14	f	1232	CLA	C3-C5-C6-C7
14	A	1119	CLA	CBA-CGA-O2A-C1
14	A	1122	CLA	CBA-CGA-O2A-C1
14	A	1140	CLA	CBA-CGA-O2A-C1
14	B	1240	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1207	CLA	CBA-CGA-O2A-C1
14	B	1230	CLA	CBA-CGA-O2A-C1
14	K	1401	CLA	CBA-CGA-O2A-C1
14	G	1119	CLA	CBA-CGA-O2A-C1
14	G	1122	CLA	CBA-CGA-O2A-C1
14	G	1140	CLA	CBA-CGA-O2A-C1
14	H	1240	CLA	CBA-CGA-O2A-C1
14	H	1207	CLA	CBA-CGA-O2A-C1
14	H	1230	CLA	CBA-CGA-O2A-C1
14	U	1401	CLA	CBA-CGA-O2A-C1
14	e	1119	CLA	CBA-CGA-O2A-C1
14	e	1122	CLA	CBA-CGA-O2A-C1
14	e	1140	CLA	CBA-CGA-O2A-C1
14	f	1240	CLA	CBA-CGA-O2A-C1
14	f	1207	CLA	CBA-CGA-O2A-C1
14	f	1230	CLA	CBA-CGA-O2A-C1
14	m	1401	CLA	CBA-CGA-O2A-C1
18	A	5009	LHG	C24-C23-O8-C6
18	G	5009	LHG	C24-C23-O8-C6
18	e	5009	LHG	C24-C23-O8-C6
21	3	822	SQD	C24-C23-O48-C46
21	a	822	SQD	C24-C23-O48-C46
21	s	822	SQD	C24-C23-O48-C46
21	2	822	SQD	C24-C23-O48-C46
21	Z	822	SQD	C24-C23-O48-C46
21	r	822	SQD	C24-C23-O48-C46
14	F	1301	CLA	O1D-CGD-O2D-CED
14	6	517	CLA	O1D-CGD-O2D-CED
14	R	1301	CLA	O1D-CGD-O2D-CED
14	d	517	CLA	O1D-CGD-O2D-CED
14	j	1301	CLA	O1D-CGD-O2D-CED
14	v	517	CLA	O1D-CGD-O2D-CED
15	A	2001	PQN	C11-C12-C13-C14
15	B	2002	PQN	C11-C12-C13-C14
15	G	2001	PQN	C11-C12-C13-C14
15	H	2002	PQN	C11-C12-C13-C14
15	e	2001	PQN	C11-C12-C13-C14
15	f	2002	PQN	C11-C12-C13-C14
14	A	1113	CLA	CBD-CGD-O2D-CED
14	B	1012	CLA	CBD-CGD-O2D-CED
14	J	1303	CLA	CBD-CGD-O2D-CED
14	G	1113	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1012	CLA	CBD-CGD-O2D-CED
14	T	1303	CLA	CBD-CGD-O2D-CED
14	e	1113	CLA	CBD-CGD-O2D-CED
14	f	1012	CLA	CBD-CGD-O2D-CED
14	l	1303	CLA	CBD-CGD-O2D-CED
14	A	1123	CLA	O1D-CGD-O2D-CED
14	B	1203	CLA	O1D-CGD-O2D-CED
14	B	1207	CLA	O1D-CGD-O2D-CED
14	1	508	CLA	O1D-CGD-O2D-CED
14	6	519	CLA	O1D-CGD-O2D-CED
14	G	1123	CLA	O1D-CGD-O2D-CED
14	H	1203	CLA	O1D-CGD-O2D-CED
14	H	1207	CLA	O1D-CGD-O2D-CED
14	Y	508	CLA	O1D-CGD-O2D-CED
14	d	519	CLA	O1D-CGD-O2D-CED
14	e	1123	CLA	O1D-CGD-O2D-CED
14	f	1203	CLA	O1D-CGD-O2D-CED
14	f	1207	CLA	O1D-CGD-O2D-CED
14	q	508	CLA	O1D-CGD-O2D-CED
14	v	519	CLA	O1D-CGD-O2D-CED
21	B	1852	SQD	O49-C7-O47-C45
21	H	1852	SQD	O49-C7-O47-C45
21	f	1852	SQD	O49-C7-O47-C45
14	A	1130	CLA	O1A-CGA-O2A-C1
14	B	1230	CLA	O1A-CGA-O2A-C1
14	G	1130	CLA	O1A-CGA-O2A-C1
14	H	1230	CLA	O1A-CGA-O2A-C1
14	e	1130	CLA	O1A-CGA-O2A-C1
14	f	1230	CLA	O1A-CGA-O2A-C1
18	A	5001	LHG	O10-C23-O8-C6
18	G	5001	LHG	O10-C23-O8-C6
18	e	5001	LHG	O10-C23-O8-C6
21	3	822	SQD	O10-C23-O48-C46
21	a	822	SQD	O10-C23-O48-C46
21	s	822	SQD	O10-C23-O48-C46
21	2	822	SQD	O10-C23-O48-C46
21	Z	822	SQD	O10-C23-O48-C46
21	r	822	SQD	O10-C23-O48-C46
14	6	501	CLA	O1D-CGD-O2D-CED
14	d	501	CLA	O1D-CGD-O2D-CED
14	v	501	CLA	O1D-CGD-O2D-CED
19	A	1848	LMU	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	1843	LMU	O5B-C5B-C6B-O6B
19	G	1848	LMU	O5'-C5'-C6'-O6'
19	H	1843	LMU	O5B-C5B-C6B-O6B
19	e	1848	LMU	O5'-C5'-C6'-O6'
19	f	1843	LMU	O5B-C5B-C6B-O6B
14	A	1120	CLA	CBD-CGD-O2D-CED
14	A	1122	CLA	CBD-CGD-O2D-CED
14	B	1221	CLA	CBD-CGD-O2D-CED
14	B	1235	CLA	CBD-CGD-O2D-CED
14	B	1230	CLA	CBD-CGD-O2D-CED
14	1	511	CLA	CBD-CGD-O2D-CED
14	1	517	CLA	CBD-CGD-O2D-CED
14	5	510	CLA	CBD-CGD-O2D-CED
14	6	509	CLA	CBD-CGD-O2D-CED
14	G	1120	CLA	CBD-CGD-O2D-CED
14	G	1122	CLA	CBD-CGD-O2D-CED
14	H	1221	CLA	CBD-CGD-O2D-CED
14	H	1235	CLA	CBD-CGD-O2D-CED
14	H	1230	CLA	CBD-CGD-O2D-CED
14	Y	511	CLA	CBD-CGD-O2D-CED
14	Y	517	CLA	CBD-CGD-O2D-CED
14	c	510	CLA	CBD-CGD-O2D-CED
14	d	509	CLA	CBD-CGD-O2D-CED
14	e	1120	CLA	CBD-CGD-O2D-CED
14	e	1122	CLA	CBD-CGD-O2D-CED
14	f	1221	CLA	CBD-CGD-O2D-CED
14	f	1235	CLA	CBD-CGD-O2D-CED
14	f	1230	CLA	CBD-CGD-O2D-CED
14	q	511	CLA	CBD-CGD-O2D-CED
14	q	517	CLA	CBD-CGD-O2D-CED
14	u	510	CLA	CBD-CGD-O2D-CED
14	v	509	CLA	CBD-CGD-O2D-CED
14	2	519	CLA	O1D-CGD-O2D-CED
14	4	517	CLA	O1D-CGD-O2D-CED
14	Z	519	CLA	O1D-CGD-O2D-CED
14	b	517	CLA	O1D-CGD-O2D-CED
14	r	519	CLA	O1D-CGD-O2D-CED
14	t	517	CLA	O1D-CGD-O2D-CED
18	A	5005	LHG	O2-C2-C3-O3
18	L	5220	LHG	O2-C2-C3-O3
18	G	5005	LHG	O2-C2-C3-O3
18	V	5220	LHG	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	5005	LHG	O2-C2-C3-O3
18	n	5220	LHG	O2-C2-C3-O3
14	A	1107	CLA	C3-C5-C6-C7
14	A	1108	CLA	C3-C5-C6-C7
14	A	1129	CLA	C3-C5-C6-C7
14	B	1205	CLA	C3-C5-C6-C7
14	G	1107	CLA	C3-C5-C6-C7
14	G	1108	CLA	C3-C5-C6-C7
14	G	1129	CLA	C3-C5-C6-C7
14	H	1205	CLA	C3-C5-C6-C7
14	e	1107	CLA	C3-C5-C6-C7
14	e	1108	CLA	C3-C5-C6-C7
14	e	1129	CLA	C3-C5-C6-C7
14	f	1205	CLA	C3-C5-C6-C7
14	A	1108	CLA	CBA-CGA-O2A-C1
14	A	1129	CLA	CBA-CGA-O2A-C1
14	A	1130	CLA	CBA-CGA-O2A-C1
14	B	1234	CLA	CBA-CGA-O2A-C1
14	G	1108	CLA	CBA-CGA-O2A-C1
14	G	1129	CLA	CBA-CGA-O2A-C1
14	G	1130	CLA	CBA-CGA-O2A-C1
14	H	1234	CLA	CBA-CGA-O2A-C1
14	e	1108	CLA	CBA-CGA-O2A-C1
14	e	1129	CLA	CBA-CGA-O2A-C1
14	e	1130	CLA	CBA-CGA-O2A-C1
14	f	1234	CLA	CBA-CGA-O2A-C1
18	L	5221	LHG	C24-C23-O8-C6
18	V	5221	LHG	C24-C23-O8-C6
18	n	5221	LHG	C24-C23-O8-C6
21	1	822	SQD	C24-C23-O48-C46
21	Y	822	SQD	C24-C23-O48-C46
21	q	822	SQD	C24-C23-O48-C46
19	B	1843	LMU	O5'-C5'-C6'-O6'
19	H	1843	LMU	O5'-C5'-C6'-O6'
19	f	1843	LMU	O5'-C5'-C6'-O6'
20	J	5104	LMG	O6-C5-C6-O5
20	T	5104	LMG	O6-C5-C6-O5
20	l	5104	LMG	O6-C5-C6-O5
19	B	1843	LMU	C4'-C5'-C6'-O6'
19	H	1843	LMU	C4'-C5'-C6'-O6'
19	f	1843	LMU	C4'-C5'-C6'-O6'
14	A	1132	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	1	518	CLA	O1D-CGD-O2D-CED
14	4	510	CLA	O1D-CGD-O2D-CED
14	4	511	CLA	O1D-CGD-O2D-CED
14	5	504	CLA	O1D-CGD-O2D-CED
14	G	1132	CLA	O1D-CGD-O2D-CED
14	Y	518	CLA	O1D-CGD-O2D-CED
14	b	510	CLA	O1D-CGD-O2D-CED
14	b	511	CLA	O1D-CGD-O2D-CED
14	c	504	CLA	O1D-CGD-O2D-CED
14	e	1132	CLA	O1D-CGD-O2D-CED
14	q	518	CLA	O1D-CGD-O2D-CED
14	t	510	CLA	O1D-CGD-O2D-CED
14	t	511	CLA	O1D-CGD-O2D-CED
14	u	504	CLA	O1D-CGD-O2D-CED
14	A	1103	CLA	CBD-CGD-O2D-CED
14	G	1103	CLA	CBD-CGD-O2D-CED
14	e	1103	CLA	CBD-CGD-O2D-CED
18	B	1855	LHG	C5-C6-O8-C23
18	H	1855	LHG	C5-C6-O8-C23
18	f	1855	LHG	C5-C6-O8-C23
20	B	5002	LMG	O6-C5-C6-O5
20	H	5002	LMG	O6-C5-C6-O5
20	f	5002	LMG	O6-C5-C6-O5
14	A	1013	CLA	C3-C5-C6-C7
14	B	1215	CLA	C3-C5-C6-C7
14	G	1013	CLA	C3-C5-C6-C7
14	H	1215	CLA	C3-C5-C6-C7
14	e	1013	CLA	C3-C5-C6-C7
14	f	1215	CLA	C3-C5-C6-C7
19	B	1843	LMU	C4B-C5B-C6B-O6B
19	H	1843	LMU	C4B-C5B-C6B-O6B
19	f	1843	LMU	C4B-C5B-C6B-O6B
14	A	1122	CLA	O1A-CGA-O2A-C1
14	A	1129	CLA	O1A-CGA-O2A-C1
14	K	1401	CLA	O1A-CGA-O2A-C1
14	G	1108	CLA	O1A-CGA-O2A-C1
14	G	1122	CLA	O1A-CGA-O2A-C1
14	G	1129	CLA	O1A-CGA-O2A-C1
14	U	1401	CLA	O1A-CGA-O2A-C1
14	e	1122	CLA	O1A-CGA-O2A-C1
14	e	1129	CLA	O1A-CGA-O2A-C1
14	m	1401	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1115	CLA	C4-C3-C5-C6
14	G	1115	CLA	C4-C3-C5-C6
14	e	1115	CLA	C4-C3-C5-C6
14	A	1115	CLA	C2-C3-C5-C6
14	A	1137	CLA	C2-C3-C5-C6
14	G	1115	CLA	C2-C3-C5-C6
14	G	1137	CLA	C2-C3-C5-C6
14	e	1115	CLA	C2-C3-C5-C6
14	e	1137	CLA	C2-C3-C5-C6
14	A	1134	CLA	C2A-CAA-CBA-CGA
14	B	1218	CLA	C2A-CAA-CBA-CGA
14	1	517	CLA	C2A-CAA-CBA-CGA
14	3	505	CLA	C2A-CAA-CBA-CGA
14	5	505	CLA	C2A-CAA-CBA-CGA
14	G	1134	CLA	C2A-CAA-CBA-CGA
14	H	1218	CLA	C2A-CAA-CBA-CGA
14	Y	517	CLA	C2A-CAA-CBA-CGA
14	a	505	CLA	C2A-CAA-CBA-CGA
14	c	505	CLA	C2A-CAA-CBA-CGA
14	e	1134	CLA	C2A-CAA-CBA-CGA
14	f	1218	CLA	C2A-CAA-CBA-CGA
14	q	517	CLA	C2A-CAA-CBA-CGA
14	s	505	CLA	C2A-CAA-CBA-CGA
14	u	505	CLA	C2A-CAA-CBA-CGA
14	2	510	CLA	O1D-CGD-O2D-CED
14	Z	510	CLA	O1D-CGD-O2D-CED
14	r	510	CLA	O1D-CGD-O2D-CED
14	A	1108	CLA	O1A-CGA-O2A-C1
14	e	1108	CLA	O1A-CGA-O2A-C1
19	A	1848	LMU	O5'-C1'-O1'-C1
19	G	1848	LMU	O5'-C1'-O1'-C1
19	e	1848	LMU	O5'-C1'-O1'-C1
14	A	1133	CLA	CBA-CGA-O2A-C1
14	A	1135	CLA	CBA-CGA-O2A-C1
14	A	1237	CLA	CBA-CGA-O2A-C1
14	B	1211	CLA	CBA-CGA-O2A-C1
14	3	518	CLA	CBA-CGA-O2A-C1
14	G	1133	CLA	CBA-CGA-O2A-C1
14	G	1135	CLA	CBA-CGA-O2A-C1
14	G	1237	CLA	CBA-CGA-O2A-C1
14	H	1211	CLA	CBA-CGA-O2A-C1
14	a	518	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1133	CLA	CBA-CGA-O2A-C1
14	e	1135	CLA	CBA-CGA-O2A-C1
14	e	1237	CLA	CBA-CGA-O2A-C1
14	f	1211	CLA	CBA-CGA-O2A-C1
14	s	518	CLA	CBA-CGA-O2A-C1
18	A	5001	LHG	C24-C23-O8-C6
18	G	5001	LHG	C24-C23-O8-C6
14	B	1204	CLA	O1D-CGD-O2D-CED
14	4	507	CLA	O1D-CGD-O2D-CED
14	H	1204	CLA	O1D-CGD-O2D-CED
14	b	507	CLA	O1D-CGD-O2D-CED
14	f	1204	CLA	O1D-CGD-O2D-CED
14	t	507	CLA	O1D-CGD-O2D-CED
14	B	1234	CLA	O1A-CGA-O2A-C1
14	H	1234	CLA	O1A-CGA-O2A-C1
14	f	1234	CLA	O1A-CGA-O2A-C1
14	A	1022	CLA	O1D-CGD-O2D-CED
14	G	1022	CLA	O1D-CGD-O2D-CED
14	e	1022	CLA	O1D-CGD-O2D-CED
18	A	5002	LHG	C1-C2-C3-O3
18	G	5002	LHG	C1-C2-C3-O3
18	e	5002	LHG	C1-C2-C3-O3
20	B	5002	LMG	C4-C5-C6-O5
20	H	5002	LMG	C4-C5-C6-O5
20	f	5002	LMG	C4-C5-C6-O5
14	A	1135	CLA	O1A-CGA-O2A-C1
14	B	1211	CLA	O1A-CGA-O2A-C1
14	3	518	CLA	O1A-CGA-O2A-C1
14	G	1135	CLA	O1A-CGA-O2A-C1
14	H	1211	CLA	O1A-CGA-O2A-C1
14	a	518	CLA	O1A-CGA-O2A-C1
14	e	1135	CLA	O1A-CGA-O2A-C1
14	f	1211	CLA	O1A-CGA-O2A-C1
14	s	518	CLA	O1A-CGA-O2A-C1
14	B	1204	CLA	C3-C5-C6-C7
14	H	1204	CLA	C3-C5-C6-C7
14	f	1204	CLA	C3-C5-C6-C7
14	1	507	CLA	O1D-CGD-O2D-CED
14	Y	507	CLA	O1D-CGD-O2D-CED
14	q	507	CLA	O1D-CGD-O2D-CED
14	A	1104	CLA	CBA-CGA-O2A-C1
14	A	1106	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1118	CLA	CBA-CGA-O2A-C1
14	B	1214	CLA	CBA-CGA-O2A-C1
14	B	1225	CLA	CBA-CGA-O2A-C1
14	B	1239	CLA	CBA-CGA-O2A-C1
14	J	1302	CLA	CBA-CGA-O2A-C1
14	G	1104	CLA	CBA-CGA-O2A-C1
14	G	1106	CLA	CBA-CGA-O2A-C1
14	G	1118	CLA	CBA-CGA-O2A-C1
14	H	1214	CLA	CBA-CGA-O2A-C1
14	H	1225	CLA	CBA-CGA-O2A-C1
14	H	1239	CLA	CBA-CGA-O2A-C1
14	T	1302	CLA	CBA-CGA-O2A-C1
14	e	1104	CLA	CBA-CGA-O2A-C1
14	e	1106	CLA	CBA-CGA-O2A-C1
14	e	1118	CLA	CBA-CGA-O2A-C1
14	f	1214	CLA	CBA-CGA-O2A-C1
14	f	1225	CLA	CBA-CGA-O2A-C1
14	f	1239	CLA	CBA-CGA-O2A-C1
14	l	1302	CLA	CBA-CGA-O2A-C1
18	e	5001	LHG	C24-C23-O8-C6
19	J	5105	LMU	C4'-C5'-C6'-O6'
19	T	5105	LMU	C4'-C5'-C6'-O6'
19	l	5105	LMU	C4'-C5'-C6'-O6'
14	A	1115	CLA	C10-C11-C12-C13
14	G	1115	CLA	C10-C11-C12-C13
14	B	1211	CLA	C5-C6-C7-C8
14	B	1215	CLA	C10-C11-C12-C13
14	B	1220	CLA	C5-C6-C7-C8
14	B	1223	CLA	C8-C10-C11-C12
14	B	1225	CLA	C15-C16-C17-C18
14	L	1503	CLA	C5-C6-C7-C8
14	L	1503	CLA	C8-C10-C11-C12
14	H	1211	CLA	C5-C6-C7-C8
14	H	1215	CLA	C10-C11-C12-C13
14	H	1220	CLA	C5-C6-C7-C8
14	H	1223	CLA	C8-C10-C11-C12
14	H	1225	CLA	C15-C16-C17-C18
14	V	1503	CLA	C5-C6-C7-C8
14	V	1503	CLA	C8-C10-C11-C12
14	e	1115	CLA	C10-C11-C12-C13
14	f	1211	CLA	C5-C6-C7-C8
14	f	1215	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1220	CLA	C5-C6-C7-C8
14	f	1223	CLA	C8-C10-C11-C12
14	f	1225	CLA	C15-C16-C17-C18
14	n	1503	CLA	C5-C6-C7-C8
14	n	1503	CLA	C8-C10-C11-C12
18	A	5003	LHG	O2-C2-C3-O3
18	G	5003	LHG	O2-C2-C3-O3
18	e	5003	LHG	O2-C2-C3-O3
14	K	1103	CLA	O2A-C1-C2-C3
14	U	1103	CLA	O2A-C1-C2-C3
14	m	1103	CLA	O2A-C1-C2-C3
21	L	5216	SQD	O47-C45-C46-O48
21	V	5216	SQD	O47-C45-C46-O48
21	n	5216	SQD	O47-C45-C46-O48
14	A	1118	CLA	O1A-CGA-O2A-C1
14	G	1118	CLA	O1A-CGA-O2A-C1
14	e	1118	CLA	O1A-CGA-O2A-C1
14	A	1133	CLA	C2-C3-C5-C6
14	G	1133	CLA	C2-C3-C5-C6
14	e	1133	CLA	C2-C3-C5-C6
14	A	1109	CLA	C14-C13-C15-C16
14	A	1116	CLA	C6-C7-C8-C9
14	A	1137	CLA	C6-C7-C8-C9
14	A	1137	CLA	C11-C10-C8-C9
14	B	1213	CLA	C11-C12-C13-C14
14	B	1215	CLA	C6-C7-C8-C9
14	B	1215	CLA	C11-C12-C13-C14
14	B	1219	CLA	C6-C7-C8-C9
14	B	1234	CLA	C11-C12-C13-C14
14	L	1503	CLA	C6-C7-C8-C9
14	6	505	CLA	C6-C7-C8-C9
14	G	1109	CLA	C14-C13-C15-C16
14	G	1116	CLA	C6-C7-C8-C9
14	G	1137	CLA	C6-C7-C8-C9
14	G	1137	CLA	C11-C10-C8-C9
14	H	1213	CLA	C11-C12-C13-C14
14	H	1215	CLA	C6-C7-C8-C9
14	H	1215	CLA	C11-C12-C13-C14
14	H	1219	CLA	C6-C7-C8-C9
14	H	1234	CLA	C11-C12-C13-C14
14	V	1503	CLA	C6-C7-C8-C9
14	d	505	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1109	CLA	C14-C13-C15-C16
14	e	1116	CLA	C6-C7-C8-C9
14	e	1137	CLA	C6-C7-C8-C9
14	e	1137	CLA	C11-C10-C8-C9
14	f	1213	CLA	C11-C12-C13-C14
14	f	1215	CLA	C6-C7-C8-C9
14	f	1215	CLA	C11-C12-C13-C14
14	f	1219	CLA	C6-C7-C8-C9
14	f	1234	CLA	C11-C12-C13-C14
14	n	1503	CLA	C6-C7-C8-C9
14	v	505	CLA	C6-C7-C8-C9
15	A	2001	PQN	C21-C22-C23-C24
15	G	2001	PQN	C21-C22-C23-C24
15	e	2001	PQN	C21-C22-C23-C24
14	A	1111	CLA	O1D-CGD-O2D-CED
14	B	1209	CLA	O1D-CGD-O2D-CED
14	B	1229	CLA	O1D-CGD-O2D-CED
14	K	1103	CLA	O1D-CGD-O2D-CED
14	G	1111	CLA	O1D-CGD-O2D-CED
14	H	1209	CLA	O1D-CGD-O2D-CED
14	H	1229	CLA	O1D-CGD-O2D-CED
14	U	1103	CLA	O1D-CGD-O2D-CED
14	e	1111	CLA	O1D-CGD-O2D-CED
14	e	1115	CLA	O1D-CGD-O2D-CED
14	f	1209	CLA	O1D-CGD-O2D-CED
14	f	1229	CLA	O1D-CGD-O2D-CED
14	m	1103	CLA	O1D-CGD-O2D-CED
14	A	1106	CLA	C8-C10-C11-C12
14	A	1133	CLA	C8-C10-C11-C12
14	A	1101	CLA	C10-C11-C12-C13
14	G	1106	CLA	C8-C10-C11-C12
14	G	1133	CLA	C8-C10-C11-C12
14	G	1101	CLA	C10-C11-C12-C13
14	e	1106	CLA	C8-C10-C11-C12
14	e	1133	CLA	C8-C10-C11-C12
14	e	1101	CLA	C10-C11-C12-C13
14	B	1207	CLA	C2A-CAA-CBA-CGA
14	H	1207	CLA	C2A-CAA-CBA-CGA
14	f	1207	CLA	C2A-CAA-CBA-CGA
14	u	502	CLA	C2A-CAA-CBA-CGA
17	A	4001	BCR	C7-C8-C9-C34
17	A	4011	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	4014	BCR	C7-C8-C9-C34
17	J	4013	BCR	C37-C22-C23-C24
17	J	4012	BCR	C37-C22-C23-C24
17	L	4219	BCR	C7-C8-C9-C34
17	L	4020	BCR	C37-C22-C23-C24
17	3	524	BCR	C7-C8-C9-C34
17	3	524	BCR	C37-C22-C23-C24
17	4	521	BCR	C36-C18-C19-C20
17	4	524	BCR	C7-C8-C9-C34
17	6	522	BCR	C7-C8-C9-C34
17	G	4001	BCR	C7-C8-C9-C34
17	G	4011	BCR	C37-C22-C23-C24
17	H	4014	BCR	C7-C8-C9-C34
17	T	4013	BCR	C37-C22-C23-C24
17	T	4012	BCR	C37-C22-C23-C24
17	V	4219	BCR	C7-C8-C9-C34
17	V	4020	BCR	C37-C22-C23-C24
17	a	524	BCR	C7-C8-C9-C34
17	a	524	BCR	C37-C22-C23-C24
17	b	524	BCR	C7-C8-C9-C34
17	d	522	BCR	C7-C8-C9-C34
17	e	4001	BCR	C7-C8-C9-C34
17	e	4011	BCR	C37-C22-C23-C24
17	f	4014	BCR	C7-C8-C9-C34
17	l	4013	BCR	C37-C22-C23-C24
17	l	4012	BCR	C37-C22-C23-C24
17	n	4219	BCR	C7-C8-C9-C34
17	n	4020	BCR	C37-C22-C23-C24
17	s	524	BCR	C7-C8-C9-C34
17	s	524	BCR	C37-C22-C23-C24
17	t	524	BCR	C7-C8-C9-C34
17	v	522	BCR	C7-C8-C9-C34
17	A	4011	BCR	C21-C22-C23-C24
17	J	4013	BCR	C21-C22-C23-C24
17	J	4012	BCR	C21-C22-C23-C24
17	L	4022	BCR	C7-C8-C9-C10
17	3	521	BCR	C7-C8-C9-C10
17	G	4011	BCR	C21-C22-C23-C24
17	T	4013	BCR	C21-C22-C23-C24
17	T	4012	BCR	C21-C22-C23-C24
17	V	4022	BCR	C7-C8-C9-C10
17	a	521	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	4011	BCR	C21-C22-C23-C24
17	l	4013	BCR	C21-C22-C23-C24
17	l	4012	BCR	C21-C22-C23-C24
17	n	4022	BCR	C7-C8-C9-C10
17	s	521	BCR	C7-C8-C9-C10
14	A	1115	CLA	O1D-CGD-O2D-CED
21	B	1852	SQD	C8-C7-O47-C45
21	H	1852	SQD	C8-C7-O47-C45
21	f	1852	SQD	C8-C7-O47-C45
14	B	1023	CLA	C2C-C3C-CAC-CBC
14	H	1023	CLA	C2C-C3C-CAC-CBC
14	f	1023	CLA	C2C-C3C-CAC-CBC
20	J	5104	LMG	C4-C5-C6-O5
20	T	5104	LMG	C4-C5-C6-O5
20	l	5104	LMG	C4-C5-C6-O5
14	A	1106	CLA	O1A-CGA-O2A-C1
14	B	1239	CLA	O1A-CGA-O2A-C1
14	G	1106	CLA	O1A-CGA-O2A-C1
14	H	1239	CLA	O1A-CGA-O2A-C1
14	e	1106	CLA	O1A-CGA-O2A-C1
14	f	1239	CLA	O1A-CGA-O2A-C1
14	A	1013	CLA	C13-C15-C16-C17
14	A	1126	CLA	C15-C16-C17-C18
14	B	1214	CLA	C13-C15-C16-C17
14	G	1013	CLA	C13-C15-C16-C17
14	G	1126	CLA	C15-C16-C17-C18
14	H	1214	CLA	C13-C15-C16-C17
14	e	1013	CLA	C13-C15-C16-C17
14	f	1214	CLA	C13-C15-C16-C17
14	G	1115	CLA	O1D-CGD-O2D-CED
14	A	1101	CLA	C3-C5-C6-C7
14	G	1101	CLA	C3-C5-C6-C7
14	H	1210	CLA	C3-C5-C6-C7
14	e	1101	CLA	C3-C5-C6-C7
14	A	1137	CLA	CBA-CGA-O2A-C1
14	G	1137	CLA	CBA-CGA-O2A-C1
14	e	1137	CLA	CBA-CGA-O2A-C1
18	B	1842	LHG	C24-C23-O8-C6
18	H	1842	LHG	C24-C23-O8-C6
14	A	1115	CLA	C5-C6-C7-C8
14	A	1125	CLA	C5-C6-C7-C8
14	A	1137	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1203	CLA	C8-C10-C11-C12
14	B	1240	CLA	C10-C11-C12-C13
14	G	1115	CLA	C5-C6-C7-C8
14	G	1125	CLA	C5-C6-C7-C8
14	G	1137	CLA	C10-C11-C12-C13
14	H	1203	CLA	C8-C10-C11-C12
14	H	1240	CLA	C10-C11-C12-C13
14	e	1115	CLA	C5-C6-C7-C8
14	e	1125	CLA	C5-C6-C7-C8
14	e	1126	CLA	C15-C16-C17-C18
14	e	1137	CLA	C10-C11-C12-C13
14	f	1203	CLA	C8-C10-C11-C12
14	f	1240	CLA	C10-C11-C12-C13
18	L	5220	LHG	C23-C24-C25-C26
18	V	5220	LHG	C23-C24-C25-C26
18	n	5220	LHG	C23-C24-C25-C26
14	2	518	CLA	CBD-CGD-O2D-CED
14	Z	518	CLA	CBD-CGD-O2D-CED
14	r	518	CLA	CBD-CGD-O2D-CED
14	A	1106	CLA	C5-C6-C7-C8
14	A	1116	CLA	C5-C6-C7-C8
14	B	1012	CLA	C5-C6-C7-C8
14	B	1204	CLA	C5-C6-C7-C8
14	B	1213	CLA	C5-C6-C7-C8
14	B	1219	CLA	C5-C6-C7-C8
14	B	1223	CLA	C13-C15-C16-C17
14	B	1239	CLA	C15-C16-C17-C18
14	L	1503	CLA	C10-C11-C12-C13
14	G	1106	CLA	C5-C6-C7-C8
14	G	1116	CLA	C5-C6-C7-C8
14	H	1012	CLA	C5-C6-C7-C8
14	H	1204	CLA	C5-C6-C7-C8
14	H	1213	CLA	C5-C6-C7-C8
14	H	1219	CLA	C5-C6-C7-C8
14	H	1223	CLA	C13-C15-C16-C17
14	H	1239	CLA	C15-C16-C17-C18
14	V	1503	CLA	C10-C11-C12-C13
14	e	1106	CLA	C5-C6-C7-C8
14	e	1116	CLA	C5-C6-C7-C8
14	f	1012	CLA	C5-C6-C7-C8
14	f	1204	CLA	C5-C6-C7-C8
14	f	1213	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1219	CLA	C5-C6-C7-C8
14	f	1223	CLA	C13-C15-C16-C17
14	f	1239	CLA	C15-C16-C17-C18
14	n	1503	CLA	C10-C11-C12-C13
14	A	1013	CLA	O1D-CGD-O2D-CED
14	A	1126	CLA	O1D-CGD-O2D-CED
14	3	519	CLA	O1D-CGD-O2D-CED
14	4	509	CLA	O1D-CGD-O2D-CED
14	G	1013	CLA	O1D-CGD-O2D-CED
14	G	1126	CLA	O1D-CGD-O2D-CED
14	a	519	CLA	O1D-CGD-O2D-CED
14	b	509	CLA	O1D-CGD-O2D-CED
14	e	1013	CLA	O1D-CGD-O2D-CED
14	e	1126	CLA	O1D-CGD-O2D-CED
14	s	519	CLA	O1D-CGD-O2D-CED
14	t	509	CLA	O1D-CGD-O2D-CED
18	L	5218	LHG	O1-C1-C2-O2
18	V	5218	LHG	O1-C1-C2-O2
18	n	5218	LHG	O1-C1-C2-O2
18	A	5002	LHG	C7-C8-C9-C10
18	A	5008	LHG	C23-C24-C25-C26
18	A	5009	LHG	C23-C24-C25-C26
18	A	5001	LHG	C23-C24-C25-C26
18	I	5001	LHG	C23-C24-C25-C26
18	L	5220	LHG	C7-C8-C9-C10
18	G	5002	LHG	C7-C8-C9-C10
18	G	5008	LHG	C23-C24-C25-C26
18	G	5009	LHG	C23-C24-C25-C26
18	G	5001	LHG	C23-C24-C25-C26
18	S	5001	LHG	C23-C24-C25-C26
18	V	5220	LHG	C7-C8-C9-C10
18	e	5002	LHG	C7-C8-C9-C10
18	e	5008	LHG	C23-C24-C25-C26
18	e	5009	LHG	C23-C24-C25-C26
18	e	5001	LHG	C23-C24-C25-C26
18	k	5001	LHG	C23-C24-C25-C26
18	n	5220	LHG	C7-C8-C9-C10
14	2	511	CLA	CBD-CGD-O2D-CED
14	6	510	CLA	CBD-CGD-O2D-CED
14	Z	511	CLA	CBD-CGD-O2D-CED
14	d	510	CLA	CBD-CGD-O2D-CED
14	r	511	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	v	510	CLA	CBD-CGD-O2D-CED
14	A	1124	CLA	C10-C11-C12-C13
14	B	1205	CLA	C13-C15-C16-C17
14	B	1210	CLA	C8-C10-C11-C12
14	B	1207	CLA	C13-C15-C16-C17
14	2	505	CLA	C8-C10-C11-C12
14	5	509	CLA	C8-C10-C11-C12
14	H	1205	CLA	C13-C15-C16-C17
14	H	1210	CLA	C8-C10-C11-C12
14	H	1207	CLA	C13-C15-C16-C17
14	Z	505	CLA	C8-C10-C11-C12
14	c	509	CLA	C8-C10-C11-C12
14	e	1124	CLA	C10-C11-C12-C13
14	f	1205	CLA	C13-C15-C16-C17
14	f	1210	CLA	C8-C10-C11-C12
14	f	1207	CLA	C13-C15-C16-C17
14	r	505	CLA	C8-C10-C11-C12
14	u	509	CLA	C8-C10-C11-C12
15	A	2001	PQN	C15-C16-C17-C18
15	G	2001	PQN	C15-C16-C17-C18
15	e	2001	PQN	C15-C16-C17-C18
14	A	1125	CLA	C3-C5-C6-C7
14	B	1210	CLA	C3-C5-C6-C7
14	G	1125	CLA	C3-C5-C6-C7
14	e	1125	CLA	C3-C5-C6-C7
14	f	1210	CLA	C3-C5-C6-C7
18	f	1842	LHG	C24-C23-O8-C6
19	A	1849	LMU	O1'-C1-C2-C3
19	G	1849	LMU	O1'-C1-C2-C3
19	e	1849	LMU	O1'-C1-C2-C3
21	L	5216	SQD	C17-C18-C19-C20
21	V	5216	SQD	C17-C18-C19-C20
21	n	5216	SQD	C17-C18-C19-C20
14	A	1131	CLA	O1D-CGD-O2D-CED
14	G	1131	CLA	O1D-CGD-O2D-CED
14	a	518	CLA	O1D-CGD-O2D-CED
14	e	1131	CLA	O1D-CGD-O2D-CED
14	A	1104	CLA	C15-C16-C17-C18
14	B	1023	CLA	C10-C11-C12-C13
14	G	1104	CLA	C15-C16-C17-C18
14	G	1124	CLA	C10-C11-C12-C13
14	H	1023	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1104	CLA	C15-C16-C17-C18
14	f	1023	CLA	C10-C11-C12-C13
14	s	518	CLA	O1D-CGD-O2D-CED
18	A	5005	LHG	C23-C24-C25-C26
18	A	5006	LHG	C23-C24-C25-C26
18	A	5008	LHG	C7-C8-C9-C10
18	G	5005	LHG	C23-C24-C25-C26
18	G	5006	LHG	C23-C24-C25-C26
18	G	5008	LHG	C7-C8-C9-C10
18	e	5005	LHG	C23-C24-C25-C26
18	e	5006	LHG	C23-C24-C25-C26
18	e	5008	LHG	C7-C8-C9-C10
21	B	1852	SQD	C23-C24-C25-C26
21	1	822	SQD	C23-C24-C25-C26
21	H	1852	SQD	C23-C24-C25-C26
21	Y	822	SQD	C23-C24-C25-C26
21	f	1852	SQD	C23-C24-C25-C26
21	q	822	SQD	C23-C24-C25-C26
14	A	1109	CLA	CBD-CGD-O2D-CED
14	1	505	CLA	CBD-CGD-O2D-CED
14	G	1109	CLA	CBD-CGD-O2D-CED
14	Y	505	CLA	CBD-CGD-O2D-CED
14	e	1109	CLA	CBD-CGD-O2D-CED
14	q	505	CLA	CBD-CGD-O2D-CED
14	A	1126	CLA	C10-C11-C12-C13
14	B	1214	CLA	C5-C6-C7-C8
14	6	505	CLA	C8-C10-C11-C12
14	G	1126	CLA	C10-C11-C12-C13
14	H	1214	CLA	C5-C6-C7-C8
14	d	505	CLA	C8-C10-C11-C12
14	e	1126	CLA	C10-C11-C12-C13
14	f	1214	CLA	C5-C6-C7-C8
14	v	505	CLA	C8-C10-C11-C12
14	A	1237	CLA	O1D-CGD-O2D-CED
14	L	1503	CLA	O1D-CGD-O2D-CED
14	3	505	CLA	O1D-CGD-O2D-CED
14	3	518	CLA	O1D-CGD-O2D-CED
14	V	1503	CLA	O1D-CGD-O2D-CED
14	a	505	CLA	O1D-CGD-O2D-CED
14	n	1503	CLA	O1D-CGD-O2D-CED
14	r	507	CLA	O1D-CGD-O2D-CED
14	s	505	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1106	CLA	C12-C13-C15-C16
14	A	1107	CLA	C11-C10-C8-C7
14	A	1109	CLA	C11-C12-C13-C15
14	A	1119	CLA	C6-C7-C8-C10
14	A	1139	CLA	C11-C10-C8-C7
14	B	1210	CLA	C11-C12-C13-C15
14	B	1216	CLA	C6-C7-C8-C10
14	B	1221	CLA	C11-C10-C8-C7
14	B	1230	CLA	C6-C7-C8-C10
14	G	1106	CLA	C12-C13-C15-C16
14	G	1107	CLA	C11-C10-C8-C7
14	G	1109	CLA	C11-C12-C13-C15
14	G	1119	CLA	C6-C7-C8-C10
14	G	1139	CLA	C11-C10-C8-C7
14	H	1210	CLA	C11-C12-C13-C15
14	H	1216	CLA	C6-C7-C8-C10
14	H	1221	CLA	C11-C10-C8-C7
14	H	1230	CLA	C6-C7-C8-C10
14	e	1106	CLA	C12-C13-C15-C16
14	e	1107	CLA	C11-C10-C8-C7
14	e	1109	CLA	C11-C12-C13-C15
14	e	1119	CLA	C6-C7-C8-C10
14	e	1139	CLA	C11-C10-C8-C7
14	f	1210	CLA	C11-C12-C13-C15
14	f	1216	CLA	C6-C7-C8-C10
14	f	1221	CLA	C11-C10-C8-C7
14	f	1230	CLA	C6-C7-C8-C10
15	A	2001	PQN	C21-C22-C23-C25
15	G	2001	PQN	C21-C22-C23-C25
15	e	2001	PQN	C21-C22-C23-C25
14	A	1115	CLA	C3-C5-C6-C7
14	G	1115	CLA	C3-C5-C6-C7
14	e	1115	CLA	C3-C5-C6-C7
14	A	1133	CLA	O1A-CGA-O2A-C1
14	A	1137	CLA	O1A-CGA-O2A-C1
14	B	1225	CLA	O1A-CGA-O2A-C1
14	G	1133	CLA	O1A-CGA-O2A-C1
14	G	1137	CLA	O1A-CGA-O2A-C1
14	H	1225	CLA	O1A-CGA-O2A-C1
14	e	1133	CLA	O1A-CGA-O2A-C1
14	e	1137	CLA	O1A-CGA-O2A-C1
14	f	1225	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	1855	LHG	O10-C23-O8-C6
18	H	1855	LHG	O10-C23-O8-C6
18	f	1855	LHG	O10-C23-O8-C6
14	3	516	CLA	C4C-C3C-CAC-CBC
17	4	522	BCR	C9-C10-C11-C12
17	6	522	BCR	C9-C10-C11-C12
17	b	522	BCR	C9-C10-C11-C12
17	d	522	BCR	C9-C10-C11-C12
17	t	522	BCR	C9-C10-C11-C12
17	v	522	BCR	C9-C10-C11-C12
14	A	1107	CLA	C2A-CAA-CBA-CGA
14	B	1201	CLA	C2A-CAA-CBA-CGA
14	1	505	CLA	C2A-CAA-CBA-CGA
14	1	516	CLA	C2A-CAA-CBA-CGA
14	5	502	CLA	C2A-CAA-CBA-CGA
14	6	503	CLA	C2A-CAA-CBA-CGA
14	G	1107	CLA	C2A-CAA-CBA-CGA
14	H	1201	CLA	C2A-CAA-CBA-CGA
14	Y	505	CLA	C2A-CAA-CBA-CGA
14	Y	516	CLA	C2A-CAA-CBA-CGA
14	c	502	CLA	C2A-CAA-CBA-CGA
14	d	503	CLA	C2A-CAA-CBA-CGA
14	e	1107	CLA	C2A-CAA-CBA-CGA
14	f	1201	CLA	C2A-CAA-CBA-CGA
14	q	505	CLA	C2A-CAA-CBA-CGA
14	q	516	CLA	C2A-CAA-CBA-CGA
14	v	503	CLA	C2A-CAA-CBA-CGA
14	v	516	CLA	C2A-CAA-CBA-CGA
14	A	1106	CLA	O1D-CGD-O2D-CED
14	1	512	CLA	O1D-CGD-O2D-CED
14	2	507	CLA	O1D-CGD-O2D-CED
14	4	508	CLA	O1D-CGD-O2D-CED
14	4	513	CLA	O1D-CGD-O2D-CED
14	G	1106	CLA	O1D-CGD-O2D-CED
14	G	1237	CLA	O1D-CGD-O2D-CED
14	Y	512	CLA	O1D-CGD-O2D-CED
14	Z	507	CLA	O1D-CGD-O2D-CED
14	b	508	CLA	O1D-CGD-O2D-CED
14	b	513	CLA	O1D-CGD-O2D-CED
14	e	1106	CLA	O1D-CGD-O2D-CED
14	e	1237	CLA	O1D-CGD-O2D-CED
14	q	512	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	t	508	CLA	O1D-CGD-O2D-CED
14	t	513	CLA	O1D-CGD-O2D-CED
14	A	1126	CLA	C8-C10-C11-C12
14	B	1216	CLA	C5-C6-C7-C8
14	2	509	CLA	C15-C16-C17-C18
14	6	505	CLA	C5-C6-C7-C8
14	G	1126	CLA	C8-C10-C11-C12
14	H	1216	CLA	C5-C6-C7-C8
14	Z	509	CLA	C15-C16-C17-C18
14	d	505	CLA	C5-C6-C7-C8
14	e	1126	CLA	C8-C10-C11-C12
14	f	1216	CLA	C5-C6-C7-C8
14	r	509	CLA	C15-C16-C17-C18
14	v	505	CLA	C5-C6-C7-C8
15	A	2001	PQN	C18-C20-C21-C22
15	G	2001	PQN	C18-C20-C21-C22
15	e	2001	PQN	C18-C20-C21-C22
14	a	516	CLA	C4C-C3C-CAC-CBC
14	s	516	CLA	C4C-C3C-CAC-CBC
14	B	1239	CLA	C4C-C3C-CAC-CBC
14	H	1239	CLA	C4C-C3C-CAC-CBC
14	f	1239	CLA	C4C-C3C-CAC-CBC
14	A	1104	CLA	O1A-CGA-O2A-C1
14	A	1237	CLA	O1A-CGA-O2A-C1
14	J	1302	CLA	O1A-CGA-O2A-C1
14	G	1104	CLA	O1A-CGA-O2A-C1
14	G	1237	CLA	O1A-CGA-O2A-C1
14	T	1302	CLA	O1A-CGA-O2A-C1
14	e	1104	CLA	O1A-CGA-O2A-C1
14	e	1237	CLA	O1A-CGA-O2A-C1
14	l	1302	CLA	O1A-CGA-O2A-C1
14	A	1136	CLA	C8-C10-C11-C12
14	B	1208	CLA	C10-C11-C12-C13
14	B	1210	CLA	C10-C11-C12-C13
14	G	1136	CLA	C8-C10-C11-C12
14	H	1208	CLA	C10-C11-C12-C13
14	H	1210	CLA	C10-C11-C12-C13
14	e	1136	CLA	C8-C10-C11-C12
14	f	1208	CLA	C10-C11-C12-C13
14	B	1231	CLA	O1D-CGD-O2D-CED
14	H	1231	CLA	O1D-CGD-O2D-CED
14	f	1231	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1013	CLA	C15-C16-C17-C18
14	A	1122	CLA	C8-C10-C11-C12
14	B	1203	CLA	C5-C6-C7-C8
14	B	1219	CLA	C8-C10-C11-C12
14	B	1234	CLA	C10-C11-C12-C13
14	G	1013	CLA	C15-C16-C17-C18
14	G	1122	CLA	C8-C10-C11-C12
14	H	1203	CLA	C5-C6-C7-C8
14	H	1219	CLA	C8-C10-C11-C12
14	H	1234	CLA	C10-C11-C12-C13
14	e	1013	CLA	C15-C16-C17-C18
14	e	1122	CLA	C8-C10-C11-C12
14	f	1203	CLA	C5-C6-C7-C8
14	f	1210	CLA	C10-C11-C12-C13
14	f	1219	CLA	C8-C10-C11-C12
14	f	1234	CLA	C10-C11-C12-C13
14	B	1232	CLA	CBA-CGA-O2A-C1
14	H	1232	CLA	CBA-CGA-O2A-C1
14	f	1232	CLA	CBA-CGA-O2A-C1
18	A	5002	LHG	C28-C29-C30-C31
18	G	5002	LHG	C28-C29-C30-C31
18	e	5002	LHG	C28-C29-C30-C31
14	B	1214	CLA	O1A-CGA-O2A-C1
14	H	1214	CLA	O1A-CGA-O2A-C1
14	f	1214	CLA	O1A-CGA-O2A-C1
19	e	1848	LMU	C4'-C5'-C6'-O6'
18	A	5005	LHG	C28-C29-C30-C31
18	G	5005	LHG	C28-C29-C30-C31
18	e	5005	LHG	C28-C29-C30-C31
14	B	1221	CLA	C8-C10-C11-C12
14	B	1225	CLA	C13-C15-C16-C17
14	H	1217	CLA	C8-C10-C11-C12
14	H	1221	CLA	C8-C10-C11-C12
14	H	1225	CLA	C13-C15-C16-C17
14	f	1221	CLA	C8-C10-C11-C12
14	f	1225	CLA	C13-C15-C16-C17
14	r	501	CLA	C8-C10-C11-C12
14	A	1121	CLA	O1D-CGD-O2D-CED
14	B	1201	CLA	O1D-CGD-O2D-CED
14	G	1121	CLA	O1D-CGD-O2D-CED
14	H	1201	CLA	O1D-CGD-O2D-CED
14	e	1121	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1201	CLA	O1D-CGD-O2D-CED
19	A	1848	LMU	C4'-C5'-C6'-O6'
19	G	1848	LMU	C4'-C5'-C6'-O6'
14	A	1109	CLA	C13-C15-C16-C17
14	A	1126	CLA	C5-C6-C7-C8
14	A	1133	CLA	C10-C11-C12-C13
14	A	1139	CLA	C13-C15-C16-C17
14	B	1214	CLA	C10-C11-C12-C13
14	B	1217	CLA	C8-C10-C11-C12
14	B	1235	CLA	C8-C10-C11-C12
14	2	501	CLA	C8-C10-C11-C12
14	G	1109	CLA	C13-C15-C16-C17
14	G	1126	CLA	C5-C6-C7-C8
14	G	1133	CLA	C10-C11-C12-C13
14	G	1139	CLA	C13-C15-C16-C17
14	H	1214	CLA	C10-C11-C12-C13
14	H	1235	CLA	C8-C10-C11-C12
14	Z	501	CLA	C8-C10-C11-C12
14	e	1109	CLA	C13-C15-C16-C17
14	e	1126	CLA	C5-C6-C7-C8
14	e	1133	CLA	C10-C11-C12-C13
14	e	1139	CLA	C13-C15-C16-C17
14	f	1214	CLA	C10-C11-C12-C13
14	f	1217	CLA	C8-C10-C11-C12
14	f	1235	CLA	C8-C10-C11-C12
18	A	5005	LHG	C3-O3-P-O6
18	A	5006	LHG	C4-O6-P-O3
18	A	5009	LHG	C4-O6-P-O3
18	B	1842	LHG	C3-O3-P-O6
18	B	1855	LHG	C3-O3-P-O6
18	B	1855	LHG	C4-O6-P-O3
18	L	5218	LHG	C3-O3-P-O6
18	L	5220	LHG	C4-O6-P-O3
18	L	5221	LHG	C3-O3-P-O6
18	G	5005	LHG	C3-O3-P-O6
18	G	5006	LHG	C4-O6-P-O3
18	G	5009	LHG	C4-O6-P-O3
18	H	1842	LHG	C3-O3-P-O6
18	H	1855	LHG	C3-O3-P-O6
18	H	1855	LHG	C4-O6-P-O3
18	V	5218	LHG	C3-O3-P-O6
18	V	5220	LHG	C4-O6-P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5221	LHG	C3-O3-P-O6
18	e	5005	LHG	C3-O3-P-O6
18	e	5006	LHG	C4-O6-P-O3
18	e	5009	LHG	C4-O6-P-O3
18	f	1842	LHG	C3-O3-P-O6
18	f	1855	LHG	C3-O3-P-O6
18	f	1855	LHG	C4-O6-P-O3
18	n	5218	LHG	C3-O3-P-O6
18	n	5220	LHG	C4-O6-P-O3
18	n	5221	LHG	C3-O3-P-O6
18	A	5009	LHG	C7-C8-C9-C10
18	e	5009	LHG	C7-C8-C9-C10
21	B	1852	SQD	C7-C8-C9-C10
21	H	1852	SQD	C7-C8-C9-C10
21	f	1852	SQD	C7-C8-C9-C10
14	A	1128	CLA	C3-C5-C6-C7
14	G	1128	CLA	C3-C5-C6-C7
14	e	1128	CLA	C3-C5-C6-C7
14	B	1239	CLA	C2C-C3C-CAC-CBC
14	f	1239	CLA	C2C-C3C-CAC-CBC
14	H	1239	CLA	C2C-C3C-CAC-CBC
15	B	2002	PQN	C15-C16-C17-C18
15	H	2002	PQN	C15-C16-C17-C18
15	f	2002	PQN	C15-C16-C17-C18
18	G	5009	LHG	C7-C8-C9-C10
14	B	1234	CLA	O1D-CGD-O2D-CED
14	H	1234	CLA	O1D-CGD-O2D-CED
14	f	1234	CLA	O1D-CGD-O2D-CED
18	A	5003	LHG	C1-C2-C3-O3
18	G	5003	LHG	C1-C2-C3-O3
18	e	5003	LHG	C1-C2-C3-O3
18	A	5001	LHG	O9-C7-O7-C5
18	G	5001	LHG	O9-C7-O7-C5
18	e	5001	LHG	O9-C7-O7-C5
14	A	1132	CLA	C4-C3-C5-C6
14	G	1132	CLA	C4-C3-C5-C6
14	e	1132	CLA	C4-C3-C5-C6
19	J	5105	LMU	O1'-C1-C2-C3
14	5	509	CLA	C15-C16-C17-C18
14	c	509	CLA	C15-C16-C17-C18
14	u	509	CLA	C15-C16-C17-C18
14	6	512	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	T	5105	LMU	O1'-C1-C2-C3
19	l	5105	LMU	O1'-C1-C2-C3
14	A	1125	CLA	C2A-CAA-CBA-CGA
14	A	1022	CLA	C2A-CAA-CBA-CGA
14	B	1203	CLA	C2A-CAA-CBA-CGA
14	B	1224	CLA	C2A-CAA-CBA-CGA
14	K	1103	CLA	C2A-CAA-CBA-CGA
14	1	518	CLA	C2A-CAA-CBA-CGA
14	3	501	CLA	C2A-CAA-CBA-CGA
14	4	501	CLA	C2A-CAA-CBA-CGA
14	6	516	CLA	C2A-CAA-CBA-CGA
14	G	1125	CLA	C2A-CAA-CBA-CGA
14	G	1022	CLA	C2A-CAA-CBA-CGA
14	H	1203	CLA	C2A-CAA-CBA-CGA
14	H	1224	CLA	C2A-CAA-CBA-CGA
14	U	1103	CLA	C2A-CAA-CBA-CGA
14	Y	518	CLA	C2A-CAA-CBA-CGA
14	a	501	CLA	C2A-CAA-CBA-CGA
14	b	501	CLA	C2A-CAA-CBA-CGA
14	d	516	CLA	C2A-CAA-CBA-CGA
14	e	1125	CLA	C2A-CAA-CBA-CGA
14	e	1022	CLA	C2A-CAA-CBA-CGA
14	f	1203	CLA	C2A-CAA-CBA-CGA
14	f	1224	CLA	C2A-CAA-CBA-CGA
14	m	1103	CLA	C2A-CAA-CBA-CGA
14	q	518	CLA	C2A-CAA-CBA-CGA
14	s	501	CLA	C2A-CAA-CBA-CGA
14	t	501	CLA	C2A-CAA-CBA-CGA
14	B	1211	CLA	C6-C7-C8-C9
14	H	1211	CLA	C6-C7-C8-C9
14	f	1211	CLA	C6-C7-C8-C9
15	B	2002	PQN	C26-C27-C28-C30
15	H	2002	PQN	C26-C27-C28-C30
15	f	2002	PQN	C26-C27-C28-C30
14	A	1011	CLA	C3-C5-C6-C7
14	G	1011	CLA	C3-C5-C6-C7
14	e	1011	CLA	C3-C5-C6-C7
14	Z	504	CLA	O1D-CGD-O2D-CED
14	d	512	CLA	O1D-CGD-O2D-CED
14	r	504	CLA	O1D-CGD-O2D-CED
14	v	512	CLA	O1D-CGD-O2D-CED
14	L	1502	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	V	1502	CLA	CBA-CGA-O2A-C1
14	n	1502	CLA	CBA-CGA-O2A-C1
20	B	5002	LMG	C29-C28-O8-C9
20	H	5002	LMG	C29-C28-O8-C9
20	f	5002	LMG	C29-C28-O8-C9
14	2	504	CLA	O1D-CGD-O2D-CED
17	4	522	BCR	C13-C14-C15-C16
17	b	522	BCR	C13-C14-C15-C16
17	t	522	BCR	C13-C14-C15-C16
18	G	5001	LHG	C15-C16-C17-C18
18	e	5001	LHG	C15-C16-C17-C18
14	A	1133	CLA	O1D-CGD-O2D-CED
18	B	1855	LHG	C8-C7-O7-C5
18	H	1855	LHG	C8-C7-O7-C5
18	f	1855	LHG	C8-C7-O7-C5
14	5	509	CLA	C13-C15-C16-C17
14	c	509	CLA	C13-C15-C16-C17
14	u	509	CLA	C13-C15-C16-C17
18	A	5005	LHG	C12-C13-C14-C15
18	A	5005	LHG	C24-C25-C26-C27
18	A	5007	LHG	C31-C32-C33-C34
18	A	5009	LHG	C9-C10-C11-C12
18	A	5001	LHG	C15-C16-C17-C18
18	A	5001	LHG	C25-C26-C27-C28
18	A	5003	LHG	C11-C10-C9-C8
18	A	5003	LHG	C10-C11-C12-C13
18	L	5221	LHG	C30-C31-C32-C33
18	G	5005	LHG	C12-C13-C14-C15
18	G	5005	LHG	C24-C25-C26-C27
18	G	5007	LHG	C31-C32-C33-C34
18	G	5009	LHG	C9-C10-C11-C12
18	G	5001	LHG	C25-C26-C27-C28
18	G	5003	LHG	C11-C10-C9-C8
18	G	5003	LHG	C10-C11-C12-C13
18	V	5221	LHG	C30-C31-C32-C33
18	e	5005	LHG	C10-C11-C12-C13
18	e	5005	LHG	C12-C13-C14-C15
18	e	5005	LHG	C24-C25-C26-C27
18	e	5007	LHG	C31-C32-C33-C34
18	e	5009	LHG	C9-C10-C11-C12
18	e	5001	LHG	C25-C26-C27-C28
18	e	5003	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	5003	LHG	C10-C11-C12-C13
18	n	5221	LHG	C30-C31-C32-C33
20	B	5002	LMG	C29-C30-C31-C32
20	H	5002	LMG	C29-C30-C31-C32
20	f	5002	LMG	C29-C30-C31-C32
14	B	1220	CLA	O1D-CGD-O2D-CED
14	5	512	CLA	O1D-CGD-O2D-CED
14	G	1133	CLA	O1D-CGD-O2D-CED
14	H	1220	CLA	O1D-CGD-O2D-CED
14	c	512	CLA	O1D-CGD-O2D-CED
14	e	1133	CLA	O1D-CGD-O2D-CED
14	f	1220	CLA	O1D-CGD-O2D-CED
14	u	512	CLA	O1D-CGD-O2D-CED
14	3	505	CLA	C6-C7-C8-C9
14	a	505	CLA	C6-C7-C8-C9
14	s	505	CLA	C6-C7-C8-C9
18	A	5005	LHG	C10-C11-C12-C13
18	A	5005	LHG	C14-C15-C16-C17
18	B	1855	LHG	C12-C13-C14-C15
18	G	5005	LHG	C10-C11-C12-C13
18	G	5005	LHG	C14-C15-C16-C17
18	H	1855	LHG	C12-C13-C14-C15
18	V	5221	LHG	C31-C32-C33-C34
18	e	5005	LHG	C14-C15-C16-C17
18	f	1855	LHG	C12-C13-C14-C15
21	2	822	SQD	C46-C45-O47-C7
21	Z	822	SQD	C46-C45-O47-C7
21	r	822	SQD	C46-C45-O47-C7
18	L	5221	LHG	C31-C32-C33-C34
18	n	5221	LHG	C31-C32-C33-C34
14	J	1303	CLA	O1D-CGD-O2D-CED
14	T	1303	CLA	O1D-CGD-O2D-CED
14	l	1303	CLA	O1D-CGD-O2D-CED
18	A	5004	LHG	C27-C28-C29-C30
18	L	5220	LHG	C27-C28-C29-C30
18	G	5004	LHG	C27-C28-C29-C30
18	V	5220	LHG	C27-C28-C29-C30
18	e	5004	LHG	C27-C28-C29-C30
18	n	5220	LHG	C27-C28-C29-C30
21	f	1852	SQD	C11-C10-C9-C8
14	f	1235	CLA	O1D-CGD-O2D-CED
18	H	1855	LHG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1852	SQD	C11-C10-C9-C8
21	H	1852	SQD	C11-C10-C9-C8
20	J	5104	LMG	C10-C11-C12-C13
20	T	5104	LMG	C10-C11-C12-C13
20	l	5104	LMG	C10-C11-C12-C13
14	B	1235	CLA	O1D-CGD-O2D-CED
19	A	1849	LMU	C2'-C1'-O1'-C1
19	G	1849	LMU	C2'-C1'-O1'-C1
19	e	1849	LMU	C2'-C1'-O1'-C1
21	B	1852	SQD	C2-C1-O6-C44
21	H	1852	SQD	C2-C1-O6-C44
21	f	1852	SQD	C2-C1-O6-C44
18	A	5005	LHG	C11-C10-C9-C8
18	A	5003	LHG	C12-C13-C14-C15
18	B	1855	LHG	C11-C12-C13-C14
18	G	5005	LHG	C11-C10-C9-C8
18	G	5003	LHG	C12-C13-C14-C15
18	e	5005	LHG	C11-C10-C9-C8
18	e	5003	LHG	C12-C13-C14-C15
18	f	1855	LHG	C11-C12-C13-C14
19	A	1849	LMU	C4-C5-C6-C7
19	B	1843	LMU	C5-C6-C7-C8
19	G	1849	LMU	C4-C5-C6-C7
19	H	1843	LMU	C5-C6-C7-C8
19	e	1849	LMU	C4-C5-C6-C7
19	f	1843	LMU	C5-C6-C7-C8
14	A	1103	CLA	C10-C11-C12-C13
14	A	1103	CLA	C15-C16-C17-C18
14	B	1218	CLA	C8-C10-C11-C12
14	G	1103	CLA	C10-C11-C12-C13
14	G	1103	CLA	C15-C16-C17-C18
14	H	1218	CLA	C8-C10-C11-C12
14	e	1103	CLA	C10-C11-C12-C13
14	e	1103	CLA	C15-C16-C17-C18
14	f	1218	CLA	C8-C10-C11-C12
14	A	1121	CLA	C6-C7-C8-C9
14	A	1140	CLA	C16-C17-C18-C20
14	B	1217	CLA	C11-C12-C13-C14
14	B	1207	CLA	C16-C17-C18-C19
14	6	505	CLA	C16-C17-C18-C20
14	G	1121	CLA	C6-C7-C8-C9
14	G	1140	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1217	CLA	C11-C12-C13-C14
14	H	1207	CLA	C16-C17-C18-C19
14	d	505	CLA	C16-C17-C18-C20
14	e	1121	CLA	C6-C7-C8-C9
14	e	1140	CLA	C16-C17-C18-C20
14	f	1217	CLA	C11-C12-C13-C14
14	f	1207	CLA	C16-C17-C18-C19
14	v	505	CLA	C16-C17-C18-C20
14	B	1012	CLA	O1D-CGD-O2D-CED
14	H	1012	CLA	O1D-CGD-O2D-CED
14	H	1235	CLA	O1D-CGD-O2D-CED
14	f	1012	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	C4-C3-C5-C6
14	B	1229	CLA	C4-C3-C5-C6
14	G	1102	CLA	C4-C3-C5-C6
14	H	1229	CLA	C4-C3-C5-C6
14	e	1102	CLA	C4-C3-C5-C6
14	f	1229	CLA	C4-C3-C5-C6
18	A	5004	LHG	C24-C25-C26-C27
18	G	5004	LHG	C24-C25-C26-C27
18	e	5004	LHG	C24-C25-C26-C27
18	n	5220	LHG	C10-C11-C12-C13
19	A	1848	LMU	C2-C3-C4-C5
19	G	1848	LMU	C2-C3-C4-C5
19	e	1848	LMU	C2-C3-C4-C5
14	B	1229	CLA	C2-C3-C5-C6
14	H	1229	CLA	C2-C3-C5-C6
14	f	1229	CLA	C2-C3-C5-C6
14	A	1133	CLA	C11-C12-C13-C14
14	B	1223	CLA	C14-C13-C15-C16
14	G	1133	CLA	C11-C12-C13-C14
14	H	1223	CLA	C14-C13-C15-C16
14	e	1133	CLA	C11-C12-C13-C14
14	f	1223	CLA	C14-C13-C15-C16
14	A	1113	CLA	O1D-CGD-O2D-CED
14	G	1113	CLA	O1D-CGD-O2D-CED
14	e	1113	CLA	O1D-CGD-O2D-CED
18	A	5007	LHG	C11-C10-C9-C8
18	L	5220	LHG	C10-C11-C12-C13
18	L	5221	LHG	C25-C26-C27-C28
18	G	5007	LHG	C11-C10-C9-C8
18	V	5220	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5221	LHG	C25-C26-C27-C28
18	e	5007	LHG	C11-C10-C9-C8
20	B	5002	LMG	C22-C23-C24-C25
20	B	5002	LMG	C32-C33-C34-C35
20	H	5002	LMG	C22-C23-C24-C25
20	f	5002	LMG	C22-C23-C24-C25
20	f	5002	LMG	C32-C33-C34-C35
14	5	509	CLA	C10-C11-C12-C13
14	c	509	CLA	C10-C11-C12-C13
14	u	509	CLA	C10-C11-C12-C13
14	A	1116	CLA	C2A-CAA-CBA-CGA
14	4	518	CLA	C2A-CAA-CBA-CGA
14	5	518	CLA	C2A-CAA-CBA-CGA
14	G	1116	CLA	C2A-CAA-CBA-CGA
14	b	518	CLA	C2A-CAA-CBA-CGA
14	c	518	CLA	C2A-CAA-CBA-CGA
14	e	1116	CLA	C2A-CAA-CBA-CGA
14	t	518	CLA	C2A-CAA-CBA-CGA
14	u	518	CLA	C2A-CAA-CBA-CGA
17	A	4001	BCR	C11-C12-C13-C35
17	L	4019	BCR	C37-C22-C23-C24
17	L	4022	BCR	C7-C8-C9-C34
17	G	4001	BCR	C11-C12-C13-C35
17	V	4019	BCR	C37-C22-C23-C24
17	V	4022	BCR	C7-C8-C9-C34
17	b	521	BCR	C36-C18-C19-C20
17	n	4019	BCR	C37-C22-C23-C24
17	n	4022	BCR	C7-C8-C9-C34
17	t	521	BCR	C36-C18-C19-C20
18	n	5221	LHG	C25-C26-C27-C28
20	H	5002	LMG	C32-C33-C34-C35
18	A	5008	LHG	O1-C1-C2-C3
18	L	5218	LHG	O1-C1-C2-C3
18	L	5220	LHG	O1-C1-C2-C3
18	G	5008	LHG	O1-C1-C2-C3
18	V	5218	LHG	O1-C1-C2-C3
18	V	5220	LHG	O1-C1-C2-C3
18	e	5008	LHG	O1-C1-C2-C3
18	n	5218	LHG	O1-C1-C2-C3
18	n	5220	LHG	O1-C1-C2-C3
17	L	4019	BCR	C21-C22-C23-C24
17	4	523	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	V	4019	BCR	C21-C22-C23-C24
17	b	523	BCR	C21-C22-C23-C24
17	n	4019	BCR	C21-C22-C23-C24
17	t	523	BCR	C21-C22-C23-C24
14	B	1203	CLA	C3-C5-C6-C7
14	B	1218	CLA	C3-C5-C6-C7
14	H	1203	CLA	C3-C5-C6-C7
14	H	1218	CLA	C3-C5-C6-C7
14	f	1203	CLA	C3-C5-C6-C7
14	f	1218	CLA	C3-C5-C6-C7
14	B	1208	CLA	C8-C10-C11-C12
14	H	1208	CLA	C8-C10-C11-C12
14	f	1208	CLA	C8-C10-C11-C12
18	A	5005	LHG	C8-C7-O7-C5
18	A	5007	LHG	C8-C7-O7-C5
18	G	5005	LHG	C8-C7-O7-C5
18	G	5007	LHG	C8-C7-O7-C5
18	e	5005	LHG	C8-C7-O7-C5
18	e	5007	LHG	C8-C7-O7-C5
18	A	5006	LHG	C24-C25-C26-C27
18	I	5001	LHG	C10-C11-C12-C13
18	G	5006	LHG	C24-C25-C26-C27
18	S	5001	LHG	C10-C11-C12-C13
18	e	5006	LHG	C24-C25-C26-C27
18	k	5001	LHG	C10-C11-C12-C13
14	B	1230	CLA	O1D-CGD-O2D-CED
14	1	511	CLA	O1D-CGD-O2D-CED
14	H	1230	CLA	O1D-CGD-O2D-CED
14	Y	511	CLA	O1D-CGD-O2D-CED
14	f	1230	CLA	O1D-CGD-O2D-CED
14	q	511	CLA	O1D-CGD-O2D-CED
18	A	5006	LHG	C30-C31-C32-C33
18	A	5008	LHG	C10-C11-C12-C13
18	A	5001	LHG	C27-C28-C29-C30
18	L	5220	LHG	C9-C10-C11-C12
18	L	5220	LHG	C13-C14-C15-C16
18	L	5221	LHG	C11-C12-C13-C14
18	G	5006	LHG	C30-C31-C32-C33
18	G	5008	LHG	C10-C11-C12-C13
18	G	5001	LHG	C27-C28-C29-C30
18	V	5220	LHG	C9-C10-C11-C12
18	V	5220	LHG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5221	LHG	C11-C12-C13-C14
18	e	5006	LHG	C30-C31-C32-C33
18	e	5001	LHG	C27-C28-C29-C30
18	n	5220	LHG	C9-C10-C11-C12
18	n	5220	LHG	C13-C14-C15-C16
18	n	5221	LHG	C11-C12-C13-C14
19	B	1843	LMU	C4-C5-C6-C7
19	H	1843	LMU	C4-C5-C6-C7
19	f	1843	LMU	C4-C5-C6-C7
14	A	1107	CLA	C4B-C3B-CAB-CBB
14	A	1118	CLA	C4B-C3B-CAB-CBB
14	A	1129	CLA	C4B-C3B-CAB-CBB
14	A	1131	CLA	C4B-C3B-CAB-CBB
14	A	1132	CLA	C4B-C3B-CAB-CBB
14	A	1134	CLA	C4B-C3B-CAB-CBB
14	A	1138	CLA	C4B-C3B-CAB-CBB
14	A	1139	CLA	C4B-C3B-CAB-CBB
14	A	1237	CLA	C4B-C3B-CAB-CBB
14	B	1021	CLA	C4B-C3B-CAB-CBB
14	B	1218	CLA	C4B-C3B-CAB-CBB
14	B	1227	CLA	C4B-C3B-CAB-CBB
14	B	1235	CLA	C4B-C3B-CAB-CBB
14	B	1207	CLA	C4B-C3B-CAB-CBB
14	F	1302	CLA	C4B-C3B-CAB-CBB
14	1	502	CLA	C4B-C3B-CAB-CBB
14	1	518	CLA	C4B-C3B-CAB-CBB
14	2	502	CLA	C4B-C3B-CAB-CBB
14	2	504	CLA	C4B-C3B-CAB-CBB
14	2	506	CLA	C4B-C3B-CAB-CBB
14	2	513	CLA	C4B-C3B-CAB-CBB
14	3	502	CLA	C4B-C3B-CAB-CBB
14	3	519	CLA	C4B-C3B-CAB-CBB
14	4	502	CLA	C4B-C3B-CAB-CBB
14	4	505	CLA	C4B-C3B-CAB-CBB
14	4	508	CLA	C4B-C3B-CAB-CBB
14	4	512	CLA	C4B-C3B-CAB-CBB
14	4	518	CLA	C4B-C3B-CAB-CBB
14	5	502	CLA	C4B-C3B-CAB-CBB
14	5	504	CLA	C4B-C3B-CAB-CBB
14	5	519	CLA	C4B-C3B-CAB-CBB
14	6	501	CLA	C4B-C3B-CAB-CBB
14	6	507	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	6	516	CLA	C4B-C3B-CAB-CBB
14	6	518	CLA	C4B-C3B-CAB-CBB
14	G	1107	CLA	C4B-C3B-CAB-CBB
14	G	1118	CLA	C4B-C3B-CAB-CBB
14	G	1129	CLA	C4B-C3B-CAB-CBB
14	G	1131	CLA	C4B-C3B-CAB-CBB
14	G	1132	CLA	C4B-C3B-CAB-CBB
14	G	1134	CLA	C4B-C3B-CAB-CBB
14	G	1138	CLA	C4B-C3B-CAB-CBB
14	G	1139	CLA	C4B-C3B-CAB-CBB
14	G	1237	CLA	C4B-C3B-CAB-CBB
14	H	1021	CLA	C4B-C3B-CAB-CBB
14	H	1218	CLA	C4B-C3B-CAB-CBB
14	H	1227	CLA	C4B-C3B-CAB-CBB
14	H	1235	CLA	C4B-C3B-CAB-CBB
14	H	1207	CLA	C4B-C3B-CAB-CBB
14	R	1302	CLA	C4B-C3B-CAB-CBB
14	Y	502	CLA	C4B-C3B-CAB-CBB
14	Y	518	CLA	C4B-C3B-CAB-CBB
14	Z	502	CLA	C4B-C3B-CAB-CBB
14	Z	504	CLA	C4B-C3B-CAB-CBB
14	Z	506	CLA	C4B-C3B-CAB-CBB
14	Z	513	CLA	C4B-C3B-CAB-CBB
14	a	502	CLA	C4B-C3B-CAB-CBB
14	a	519	CLA	C4B-C3B-CAB-CBB
14	b	502	CLA	C4B-C3B-CAB-CBB
14	b	505	CLA	C4B-C3B-CAB-CBB
14	b	508	CLA	C4B-C3B-CAB-CBB
14	b	512	CLA	C4B-C3B-CAB-CBB
14	b	518	CLA	C4B-C3B-CAB-CBB
14	c	502	CLA	C4B-C3B-CAB-CBB
14	c	504	CLA	C4B-C3B-CAB-CBB
14	c	519	CLA	C4B-C3B-CAB-CBB
14	d	501	CLA	C4B-C3B-CAB-CBB
14	d	507	CLA	C4B-C3B-CAB-CBB
14	d	516	CLA	C4B-C3B-CAB-CBB
14	d	518	CLA	C4B-C3B-CAB-CBB
14	e	1107	CLA	C4B-C3B-CAB-CBB
14	e	1118	CLA	C4B-C3B-CAB-CBB
14	e	1129	CLA	C4B-C3B-CAB-CBB
14	e	1131	CLA	C4B-C3B-CAB-CBB
14	e	1132	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1134	CLA	C4B-C3B-CAB-CBB
14	e	1138	CLA	C4B-C3B-CAB-CBB
14	e	1139	CLA	C4B-C3B-CAB-CBB
14	e	1237	CLA	C4B-C3B-CAB-CBB
14	f	1021	CLA	C4B-C3B-CAB-CBB
14	f	1218	CLA	C4B-C3B-CAB-CBB
14	f	1227	CLA	C4B-C3B-CAB-CBB
14	f	1235	CLA	C4B-C3B-CAB-CBB
14	f	1207	CLA	C4B-C3B-CAB-CBB
14	j	1302	CLA	C4B-C3B-CAB-CBB
14	q	502	CLA	C4B-C3B-CAB-CBB
14	q	518	CLA	C4B-C3B-CAB-CBB
14	r	502	CLA	C4B-C3B-CAB-CBB
14	r	504	CLA	C4B-C3B-CAB-CBB
14	r	506	CLA	C4B-C3B-CAB-CBB
14	r	513	CLA	C4B-C3B-CAB-CBB
14	s	502	CLA	C4B-C3B-CAB-CBB
14	s	519	CLA	C4B-C3B-CAB-CBB
14	t	502	CLA	C4B-C3B-CAB-CBB
14	t	505	CLA	C4B-C3B-CAB-CBB
14	t	508	CLA	C4B-C3B-CAB-CBB
14	t	512	CLA	C4B-C3B-CAB-CBB
14	t	518	CLA	C4B-C3B-CAB-CBB
14	u	502	CLA	C4B-C3B-CAB-CBB
14	u	504	CLA	C4B-C3B-CAB-CBB
14	u	519	CLA	C4B-C3B-CAB-CBB
14	v	501	CLA	C4B-C3B-CAB-CBB
14	v	507	CLA	C4B-C3B-CAB-CBB
14	v	516	CLA	C4B-C3B-CAB-CBB
14	v	518	CLA	C4B-C3B-CAB-CBB
14	A	1105	CLA	C6-C7-C8-C10
14	A	1126	CLA	C16-C17-C18-C20
14	A	1101	CLA	C16-C17-C18-C19
14	A	1101	CLA	C16-C17-C18-C20
14	B	1218	CLA	C11-C12-C13-C14
14	B	1238	CLA	C16-C17-C18-C19
14	3	505	CLA	C6-C7-C8-C10
14	G	1105	CLA	C6-C7-C8-C10
14	G	1126	CLA	C16-C17-C18-C20
14	G	1101	CLA	C16-C17-C18-C19
14	G	1101	CLA	C16-C17-C18-C20
14	H	1208	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1218	CLA	C11-C12-C13-C14
14	H	1238	CLA	C16-C17-C18-C19
14	a	505	CLA	C6-C7-C8-C10
14	e	1105	CLA	C6-C7-C8-C10
14	e	1126	CLA	C16-C17-C18-C20
14	e	1101	CLA	C16-C17-C18-C19
14	e	1101	CLA	C16-C17-C18-C20
14	f	1208	CLA	C16-C17-C18-C19
14	f	1218	CLA	C11-C12-C13-C14
14	f	1238	CLA	C16-C17-C18-C19
14	s	505	CLA	C6-C7-C8-C10
15	A	2001	PQN	C26-C27-C28-C29
15	G	2001	PQN	C26-C27-C28-C29
15	e	2001	PQN	C26-C27-C28-C29
21	B	1852	SQD	O5-C1-O6-C44
21	H	1852	SQD	O5-C1-O6-C44
21	f	1852	SQD	O5-C1-O6-C44
14	A	1127	CLA	C15-C16-C17-C18
14	B	1229	CLA	C15-C16-C17-C18
14	G	1127	CLA	C15-C16-C17-C18
14	e	1127	CLA	C15-C16-C17-C18
18	A	5002	LHG	C11-C10-C9-C8
18	B	1855	LHG	C26-C27-C28-C29
18	I	5001	LHG	C29-C30-C31-C32
18	G	5002	LHG	C11-C10-C9-C8
18	H	1855	LHG	C26-C27-C28-C29
18	S	5001	LHG	C29-C30-C31-C32
18	e	5002	LHG	C11-C10-C9-C8
18	e	5008	LHG	C10-C11-C12-C13
18	f	1855	LHG	C26-C27-C28-C29
18	k	5001	LHG	C29-C30-C31-C32
21	B	1852	SQD	C27-C28-C29-C30
21	H	1852	SQD	C27-C28-C29-C30
21	f	1852	SQD	C27-C28-C29-C30
14	B	1221	CLA	O1D-CGD-O2D-CED
14	6	509	CLA	O1D-CGD-O2D-CED
14	H	1221	CLA	O1D-CGD-O2D-CED
14	f	1221	CLA	O1D-CGD-O2D-CED
14	v	509	CLA	O1D-CGD-O2D-CED
18	A	5002	LHG	C31-C32-C33-C34
18	A	5007	LHG	C32-C33-C34-C35
18	L	5218	LHG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	5002	LHG	C31-C32-C33-C34
18	G	5007	LHG	C32-C33-C34-C35
18	V	5218	LHG	C32-C33-C34-C35
18	e	5002	LHG	C31-C32-C33-C34
18	e	5007	LHG	C32-C33-C34-C35
18	n	5218	LHG	C32-C33-C34-C35
14	H	1229	CLA	C15-C16-C17-C18
14	f	1229	CLA	C15-C16-C17-C18
18	A	5005	LHG	C13-C14-C15-C16
18	G	5005	LHG	C13-C14-C15-C16
18	e	5005	LHG	C13-C14-C15-C16
21	L	5216	SQD	C24-C23-O48-C46
21	V	5216	SQD	C24-C23-O48-C46
21	n	5216	SQD	C24-C23-O48-C46
18	A	5001	LHG	C32-C33-C34-C35
18	G	5001	LHG	C32-C33-C34-C35
18	e	5001	LHG	C32-C33-C34-C35
14	5	510	CLA	O1D-CGD-O2D-CED
14	c	510	CLA	O1D-CGD-O2D-CED
14	d	509	CLA	O1D-CGD-O2D-CED
14	u	510	CLA	O1D-CGD-O2D-CED
14	A	1103	CLA	C3A-C2A-CAA-CBA
14	A	1110	CLA	C3A-C2A-CAA-CBA
14	A	1125	CLA	C3A-C2A-CAA-CBA
14	A	1134	CLA	C3A-C2A-CAA-CBA
14	A	1135	CLA	C3A-C2A-CAA-CBA
14	A	1139	CLA	C3A-C2A-CAA-CBA
14	A	1140	CLA	C3A-C2A-CAA-CBA
14	A	1022	CLA	C3A-C2A-CAA-CBA
14	A	1101	CLA	C3A-C2A-CAA-CBA
14	B	1210	CLA	C3A-C2A-CAA-CBA
14	B	1219	CLA	C3A-C2A-CAA-CBA
14	B	1221	CLA	C3A-C2A-CAA-CBA
14	F	1302	CLA	C3A-C2A-CAA-CBA
14	K	1105	CLA	C3A-C2A-CAA-CBA
14	5	516	CLA	C3A-C2A-CAA-CBA
14	6	512	CLA	C3A-C2A-CAA-CBA
14	6	516	CLA	C3A-C2A-CAA-CBA
14	G	1103	CLA	C3A-C2A-CAA-CBA
14	G	1110	CLA	C3A-C2A-CAA-CBA
14	G	1125	CLA	C3A-C2A-CAA-CBA
14	G	1134	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1135	CLA	C3A-C2A-CAA-CBA
14	G	1139	CLA	C3A-C2A-CAA-CBA
14	G	1140	CLA	C3A-C2A-CAA-CBA
14	G	1022	CLA	C3A-C2A-CAA-CBA
14	G	1101	CLA	C3A-C2A-CAA-CBA
14	H	1210	CLA	C3A-C2A-CAA-CBA
14	H	1219	CLA	C3A-C2A-CAA-CBA
14	H	1221	CLA	C3A-C2A-CAA-CBA
14	R	1302	CLA	C3A-C2A-CAA-CBA
14	U	1105	CLA	C3A-C2A-CAA-CBA
14	c	516	CLA	C3A-C2A-CAA-CBA
14	d	512	CLA	C3A-C2A-CAA-CBA
14	d	516	CLA	C3A-C2A-CAA-CBA
14	e	1103	CLA	C3A-C2A-CAA-CBA
14	e	1110	CLA	C3A-C2A-CAA-CBA
14	e	1125	CLA	C3A-C2A-CAA-CBA
14	e	1134	CLA	C3A-C2A-CAA-CBA
14	e	1135	CLA	C3A-C2A-CAA-CBA
14	e	1139	CLA	C3A-C2A-CAA-CBA
14	e	1140	CLA	C3A-C2A-CAA-CBA
14	e	1022	CLA	C3A-C2A-CAA-CBA
14	e	1101	CLA	C3A-C2A-CAA-CBA
14	f	1210	CLA	C3A-C2A-CAA-CBA
14	f	1219	CLA	C3A-C2A-CAA-CBA
14	f	1221	CLA	C3A-C2A-CAA-CBA
14	j	1302	CLA	C3A-C2A-CAA-CBA
14	m	1105	CLA	C3A-C2A-CAA-CBA
14	u	516	CLA	C3A-C2A-CAA-CBA
14	v	512	CLA	C3A-C2A-CAA-CBA
14	v	516	CLA	C3A-C2A-CAA-CBA
14	B	1208	CLA	C13-C15-C16-C17
14	B	1210	CLA	C5-C6-C7-C8
14	H	1208	CLA	C13-C15-C16-C17
14	f	1208	CLA	C13-C15-C16-C17
19	B	1843	LMU	C2-C1-O1'-C1'
19	J	5105	LMU	C2-C1-O1'-C1'
19	H	1843	LMU	C2-C1-O1'-C1'
19	T	5105	LMU	C2-C1-O1'-C1'
19	f	1843	LMU	C2-C1-O1'-C1'
19	l	5105	LMU	C2-C1-O1'-C1'
18	A	5001	LHG	C29-C30-C31-C32
18	G	5001	LHG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	5001	LHG	C29-C30-C31-C32
14	A	1105	CLA	C6-C7-C8-C9
14	A	1140	CLA	C16-C17-C18-C19
14	B	1208	CLA	C16-C17-C18-C19
14	B	1210	CLA	C16-C17-C18-C19
14	B	1238	CLA	C16-C17-C18-C20
14	6	505	CLA	C16-C17-C18-C19
14	G	1105	CLA	C6-C7-C8-C9
14	G	1140	CLA	C16-C17-C18-C19
14	H	1210	CLA	C16-C17-C18-C19
14	H	1238	CLA	C16-C17-C18-C20
14	d	505	CLA	C16-C17-C18-C19
14	e	1105	CLA	C6-C7-C8-C9
14	e	1140	CLA	C16-C17-C18-C19
14	f	1210	CLA	C16-C17-C18-C19
14	f	1238	CLA	C16-C17-C18-C20
14	v	505	CLA	C16-C17-C18-C19
20	B	5002	LMG	C21-C22-C23-C24
20	H	5002	LMG	C21-C22-C23-C24
20	f	5002	LMG	C21-C22-C23-C24
14	H	1210	CLA	C5-C6-C7-C8
18	A	5001	LHG	C4-C5-C6-O8
18	G	5001	LHG	C4-C5-C6-O8
18	e	5001	LHG	C4-C5-C6-O8
14	A	1110	CLA	CBD-CGD-O2D-CED
14	1	519	CLA	CBD-CGD-O2D-CED
14	G	1110	CLA	CBD-CGD-O2D-CED
14	e	1110	CLA	CBD-CGD-O2D-CED
14	q	519	CLA	CBD-CGD-O2D-CED
18	I	5001	LHG	C33-C34-C35-C36
18	S	5001	LHG	C33-C34-C35-C36
18	k	5001	LHG	C33-C34-C35-C36
14	q	517	CLA	O1D-CGD-O2D-CED
18	L	5221	LHG	C28-C29-C30-C31
18	V	5221	LHG	C28-C29-C30-C31
18	f	1842	LHG	C31-C32-C33-C34
18	n	5221	LHG	C28-C29-C30-C31
14	L	1502	CLA	O1A-CGA-O2A-C1
14	V	1502	CLA	O1A-CGA-O2A-C1
14	n	1502	CLA	O1A-CGA-O2A-C1
14	f	1210	CLA	C5-C6-C7-C8
14	A	1124	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1208	CLA	C4-C3-C5-C6
14	G	1124	CLA	C4-C3-C5-C6
14	H	1208	CLA	C4-C3-C5-C6
14	e	1124	CLA	C4-C3-C5-C6
14	f	1208	CLA	C4-C3-C5-C6
15	B	2002	PQN	C14-C13-C15-C16
15	H	2002	PQN	C14-C13-C15-C16
15	f	2002	PQN	C14-C13-C15-C16
14	A	1120	CLA	CBA-CGA-O2A-C1
14	G	1120	CLA	CBA-CGA-O2A-C1
14	e	1120	CLA	CBA-CGA-O2A-C1
14	A	1102	CLA	C2-C3-C5-C6
14	A	1124	CLA	C2-C3-C5-C6
14	B	1227	CLA	C2-C3-C5-C6
14	L	1503	CLA	C2-C3-C5-C6
14	G	1102	CLA	C2-C3-C5-C6
14	G	1124	CLA	C2-C3-C5-C6
14	H	1227	CLA	C2-C3-C5-C6
14	V	1503	CLA	C2-C3-C5-C6
14	e	1102	CLA	C2-C3-C5-C6
14	e	1124	CLA	C2-C3-C5-C6
14	f	1227	CLA	C2-C3-C5-C6
14	n	1503	CLA	C2-C3-C5-C6
14	A	1011	CLA	O1D-CGD-O2D-CED
14	A	1122	CLA	O1D-CGD-O2D-CED
14	1	517	CLA	O1D-CGD-O2D-CED
14	G	1011	CLA	O1D-CGD-O2D-CED
14	G	1122	CLA	O1D-CGD-O2D-CED
14	e	1011	CLA	O1D-CGD-O2D-CED
14	e	1122	CLA	O1D-CGD-O2D-CED
14	Y	519	CLA	CBD-CGD-O2D-CED
18	A	5009	LHG	C24-C25-C26-C27
18	B	1842	LHG	C31-C32-C33-C34
18	G	5009	LHG	C24-C25-C26-C27
18	H	1842	LHG	C31-C32-C33-C34
18	e	5009	LHG	C24-C25-C26-C27
14	Y	517	CLA	O1D-CGD-O2D-CED
18	I	5001	LHG	O1-C1-C2-O2
18	L	5221	LHG	O1-C1-C2-O2
18	S	5001	LHG	O1-C1-C2-O2
18	V	5221	LHG	O1-C1-C2-O2
18	k	5001	LHG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	n	5221	LHG	O1-C1-C2-O2
14	A	1121	CLA	C6-C7-C8-C10
14	B	1207	CLA	C16-C17-C18-C20
14	G	1121	CLA	C6-C7-C8-C10
14	H	1207	CLA	C16-C17-C18-C20
14	e	1121	CLA	C6-C7-C8-C10
14	f	1207	CLA	C16-C17-C18-C20
18	A	5008	LHG	C13-C14-C15-C16
18	G	5008	LHG	C13-C14-C15-C16
18	e	5008	LHG	C13-C14-C15-C16
14	A	1118	CLA	C2B-C3B-CAB-CBB
14	A	1131	CLA	C2B-C3B-CAB-CBB
14	A	1132	CLA	C2B-C3B-CAB-CBB
14	A	1134	CLA	C2B-C3B-CAB-CBB
14	A	1138	CLA	C2B-C3B-CAB-CBB
14	A	1139	CLA	C2B-C3B-CAB-CBB
14	A	1237	CLA	C2B-C3B-CAB-CBB
14	B	1218	CLA	C2B-C3B-CAB-CBB
14	B	1219	CLA	C2B-C3B-CAB-CBB
14	B	1227	CLA	C2B-C3B-CAB-CBB
14	B	1235	CLA	C2B-C3B-CAB-CBB
14	B	1239	CLA	C2B-C3B-CAB-CBB
14	B	1207	CLA	C2B-C3B-CAB-CBB
14	F	1302	CLA	C2B-C3B-CAB-CBB
14	J	1303	CLA	C2B-C3B-CAB-CBB
14	1	502	CLA	C2B-C3B-CAB-CBB
14	1	504	CLA	C2B-C3B-CAB-CBB
14	1	510	CLA	C2B-C3B-CAB-CBB
14	1	512	CLA	C2B-C3B-CAB-CBB
14	1	518	CLA	C2B-C3B-CAB-CBB
14	2	501	CLA	C2B-C3B-CAB-CBB
14	2	502	CLA	C2B-C3B-CAB-CBB
14	2	504	CLA	C2B-C3B-CAB-CBB
14	2	506	CLA	C2B-C3B-CAB-CBB
14	2	513	CLA	C2B-C3B-CAB-CBB
14	3	502	CLA	C2B-C3B-CAB-CBB
14	3	510	CLA	C2B-C3B-CAB-CBB
14	3	519	CLA	C2B-C3B-CAB-CBB
14	4	502	CLA	C2B-C3B-CAB-CBB
14	4	505	CLA	C2B-C3B-CAB-CBB
14	4	508	CLA	C2B-C3B-CAB-CBB
14	4	518	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	4	519	CLA	C2B-C3B-CAB-CBB
14	5	502	CLA	C2B-C3B-CAB-CBB
14	5	512	CLA	C2B-C3B-CAB-CBB
14	5	516	CLA	C2B-C3B-CAB-CBB
14	5	517	CLA	C2B-C3B-CAB-CBB
14	5	519	CLA	C2B-C3B-CAB-CBB
14	6	501	CLA	C2B-C3B-CAB-CBB
14	6	512	CLA	C2B-C3B-CAB-CBB
14	6	518	CLA	C2B-C3B-CAB-CBB
14	G	1118	CLA	C2B-C3B-CAB-CBB
14	G	1131	CLA	C2B-C3B-CAB-CBB
14	G	1132	CLA	C2B-C3B-CAB-CBB
14	G	1134	CLA	C2B-C3B-CAB-CBB
14	G	1138	CLA	C2B-C3B-CAB-CBB
14	G	1139	CLA	C2B-C3B-CAB-CBB
14	G	1237	CLA	C2B-C3B-CAB-CBB
14	H	1218	CLA	C2B-C3B-CAB-CBB
14	H	1219	CLA	C2B-C3B-CAB-CBB
14	H	1227	CLA	C2B-C3B-CAB-CBB
14	H	1235	CLA	C2B-C3B-CAB-CBB
14	H	1239	CLA	C2B-C3B-CAB-CBB
14	H	1207	CLA	C2B-C3B-CAB-CBB
14	R	1302	CLA	C2B-C3B-CAB-CBB
14	T	1303	CLA	C2B-C3B-CAB-CBB
14	Y	502	CLA	C2B-C3B-CAB-CBB
14	Y	504	CLA	C2B-C3B-CAB-CBB
14	Y	510	CLA	C2B-C3B-CAB-CBB
14	Y	512	CLA	C2B-C3B-CAB-CBB
14	Y	518	CLA	C2B-C3B-CAB-CBB
14	Z	501	CLA	C2B-C3B-CAB-CBB
14	Z	502	CLA	C2B-C3B-CAB-CBB
14	Z	504	CLA	C2B-C3B-CAB-CBB
14	Z	506	CLA	C2B-C3B-CAB-CBB
14	Z	513	CLA	C2B-C3B-CAB-CBB
14	a	502	CLA	C2B-C3B-CAB-CBB
14	a	510	CLA	C2B-C3B-CAB-CBB
14	a	519	CLA	C2B-C3B-CAB-CBB
14	b	502	CLA	C2B-C3B-CAB-CBB
14	b	505	CLA	C2B-C3B-CAB-CBB
14	b	508	CLA	C2B-C3B-CAB-CBB
14	b	518	CLA	C2B-C3B-CAB-CBB
14	b	519	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	c	502	CLA	C2B-C3B-CAB-CBB
14	c	512	CLA	C2B-C3B-CAB-CBB
14	c	516	CLA	C2B-C3B-CAB-CBB
14	c	517	CLA	C2B-C3B-CAB-CBB
14	c	519	CLA	C2B-C3B-CAB-CBB
14	d	501	CLA	C2B-C3B-CAB-CBB
14	d	512	CLA	C2B-C3B-CAB-CBB
14	d	517	CLA	C2B-C3B-CAB-CBB
14	d	518	CLA	C2B-C3B-CAB-CBB
14	e	1118	CLA	C2B-C3B-CAB-CBB
14	e	1131	CLA	C2B-C3B-CAB-CBB
14	e	1132	CLA	C2B-C3B-CAB-CBB
14	e	1134	CLA	C2B-C3B-CAB-CBB
14	e	1138	CLA	C2B-C3B-CAB-CBB
14	e	1139	CLA	C2B-C3B-CAB-CBB
14	e	1237	CLA	C2B-C3B-CAB-CBB
14	f	1218	CLA	C2B-C3B-CAB-CBB
14	f	1219	CLA	C2B-C3B-CAB-CBB
14	f	1227	CLA	C2B-C3B-CAB-CBB
14	f	1235	CLA	C2B-C3B-CAB-CBB
14	f	1239	CLA	C2B-C3B-CAB-CBB
14	f	1207	CLA	C2B-C3B-CAB-CBB
14	j	1302	CLA	C2B-C3B-CAB-CBB
14	l	1303	CLA	C2B-C3B-CAB-CBB
14	q	502	CLA	C2B-C3B-CAB-CBB
14	q	504	CLA	C2B-C3B-CAB-CBB
14	q	510	CLA	C2B-C3B-CAB-CBB
14	q	512	CLA	C2B-C3B-CAB-CBB
14	q	518	CLA	C2B-C3B-CAB-CBB
14	r	501	CLA	C2B-C3B-CAB-CBB
14	r	502	CLA	C2B-C3B-CAB-CBB
14	r	504	CLA	C2B-C3B-CAB-CBB
14	r	506	CLA	C2B-C3B-CAB-CBB
14	r	513	CLA	C2B-C3B-CAB-CBB
14	s	502	CLA	C2B-C3B-CAB-CBB
14	s	510	CLA	C2B-C3B-CAB-CBB
14	s	519	CLA	C2B-C3B-CAB-CBB
14	t	502	CLA	C2B-C3B-CAB-CBB
14	t	505	CLA	C2B-C3B-CAB-CBB
14	t	508	CLA	C2B-C3B-CAB-CBB
14	t	518	CLA	C2B-C3B-CAB-CBB
14	t	519	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	502	CLA	C2B-C3B-CAB-CBB
14	u	512	CLA	C2B-C3B-CAB-CBB
14	u	516	CLA	C2B-C3B-CAB-CBB
14	u	517	CLA	C2B-C3B-CAB-CBB
14	u	519	CLA	C2B-C3B-CAB-CBB
14	v	501	CLA	C2B-C3B-CAB-CBB
14	v	512	CLA	C2B-C3B-CAB-CBB
14	v	518	CLA	C2B-C3B-CAB-CBB
14	A	1127	CLA	C8-C10-C11-C12
14	B	1235	CLA	C5-C6-C7-C8
14	2	503	CLA	C8-C10-C11-C12
14	G	1127	CLA	C8-C10-C11-C12
14	H	1235	CLA	C5-C6-C7-C8
14	Z	503	CLA	C8-C10-C11-C12
14	e	1127	CLA	C8-C10-C11-C12
14	f	1235	CLA	C5-C6-C7-C8
14	r	503	CLA	C8-C10-C11-C12
18	A	5006	LHG	C26-C27-C28-C29
18	G	5006	LHG	C26-C27-C28-C29
18	e	5006	LHG	C26-C27-C28-C29
14	B	1232	CLA	O1A-CGA-O2A-C1
14	H	1232	CLA	O1A-CGA-O2A-C1
14	f	1232	CLA	O1A-CGA-O2A-C1
18	A	5005	LHG	O10-C23-O8-C6
18	G	5005	LHG	O10-C23-O8-C6
18	e	5005	LHG	O10-C23-O8-C6
15	B	2002	PQN	C25-C26-C27-C28
15	H	2002	PQN	C25-C26-C27-C28
15	f	2002	PQN	C25-C26-C27-C28
18	G	5009	LHG	C10-C11-C12-C13
18	e	5009	LHG	C10-C11-C12-C13
20	B	5002	LMG	C16-C17-C18-C19
20	H	5002	LMG	C16-C17-C18-C19
20	f	5002	LMG	C16-C17-C18-C19
21	L	5216	SQD	C13-C14-C15-C16
21	V	5216	SQD	C13-C14-C15-C16
21	n	5216	SQD	C13-C14-C15-C16
14	A	1118	CLA	C2-C1-O2A-CGA
14	G	1118	CLA	C2-C1-O2A-CGA
14	e	1118	CLA	C2-C1-O2A-CGA
18	A	5009	LHG	C10-C11-C12-C13
14	A	1117	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1117	CLA	C13-C15-C16-C17
14	e	1117	CLA	C13-C15-C16-C17
14	A	1137	CLA	C3-C5-C6-C7
14	G	1137	CLA	C3-C5-C6-C7
14	e	1137	CLA	C3-C5-C6-C7
17	A	4008	BCR	C23-C24-C25-C30
17	A	4011	BCR	C23-C24-C25-C26
17	A	4011	BCR	C23-C24-C25-C30
17	B	4004	BCR	C1-C6-C7-C8
17	B	4004	BCR	C5-C6-C7-C8
17	B	4004	BCR	C23-C24-C25-C26
17	B	4005	BCR	C23-C24-C25-C26
17	B	4010	BCR	C23-C24-C25-C30
17	B	4017	BCR	C5-C6-C7-C8
17	B	4014	BCR	C23-C24-C25-C26
17	J	4015	BCR	C23-C24-C25-C26
17	J	4012	BCR	C1-C6-C7-C8
17	J	4012	BCR	C23-C24-C25-C26
17	J	4012	BCR	C23-C24-C25-C30
17	L	4019	BCR	C23-C24-C25-C26
17	L	4019	BCR	C23-C24-C25-C30
17	M	4021	BCR	C1-C6-C7-C8
17	1	521	BCR	C1-C6-C7-C8
17	1	521	BCR	C5-C6-C7-C8
17	1	521	BCR	C23-C24-C25-C26
17	1	521	BCR	C23-C24-C25-C30
17	1	523	BCR	C1-C6-C7-C8
17	1	523	BCR	C5-C6-C7-C8
17	1	523	BCR	C23-C24-C25-C26
17	1	523	BCR	C23-C24-C25-C30
17	2	521	BCR	C1-C6-C7-C8
17	2	521	BCR	C5-C6-C7-C8
17	2	522	BCR	C1-C6-C7-C8
17	2	523	BCR	C23-C24-C25-C26
17	2	523	BCR	C23-C24-C25-C30
17	2	524	BCR	C23-C24-C25-C26
17	2	524	BCR	C23-C24-C25-C30
17	3	521	BCR	C1-C6-C7-C8
17	3	521	BCR	C5-C6-C7-C8
17	3	523	BCR	C23-C24-C25-C26
17	3	523	BCR	C23-C24-C25-C30
17	4	521	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	4	521	BCR	C5-C6-C7-C8
17	4	521	BCR	C23-C24-C25-C26
17	4	521	BCR	C23-C24-C25-C30
17	4	522	BCR	C1-C6-C7-C8
17	4	522	BCR	C5-C6-C7-C8
17	4	523	BCR	C23-C24-C25-C26
17	4	523	BCR	C23-C24-C25-C30
17	4	524	BCR	C23-C24-C25-C26
17	4	524	BCR	C23-C24-C25-C30
17	5	522	BCR	C1-C6-C7-C8
17	5	523	BCR	C23-C24-C25-C26
17	5	523	BCR	C23-C24-C25-C30
17	5	524	BCR	C23-C24-C25-C26
17	5	524	BCR	C23-C24-C25-C30
17	6	521	BCR	C1-C6-C7-C8
17	6	521	BCR	C5-C6-C7-C8
17	6	522	BCR	C1-C6-C7-C8
17	6	523	BCR	C23-C24-C25-C26
17	6	523	BCR	C23-C24-C25-C30
17	G	4008	BCR	C23-C24-C25-C30
17	G	4011	BCR	C23-C24-C25-C26
17	G	4011	BCR	C23-C24-C25-C30
17	H	4004	BCR	C1-C6-C7-C8
17	H	4004	BCR	C5-C6-C7-C8
17	H	4004	BCR	C23-C24-C25-C26
17	H	4005	BCR	C23-C24-C25-C26
17	H	4010	BCR	C23-C24-C25-C30
17	H	4017	BCR	C5-C6-C7-C8
17	H	4014	BCR	C23-C24-C25-C26
17	T	4015	BCR	C23-C24-C25-C26
17	T	4012	BCR	C1-C6-C7-C8
17	T	4012	BCR	C23-C24-C25-C26
17	T	4012	BCR	C23-C24-C25-C30
17	V	4019	BCR	C23-C24-C25-C26
17	V	4019	BCR	C23-C24-C25-C30
17	W	4021	BCR	C1-C6-C7-C8
17	Y	521	BCR	C1-C6-C7-C8
17	Y	521	BCR	C5-C6-C7-C8
17	Y	521	BCR	C23-C24-C25-C26
17	Y	521	BCR	C23-C24-C25-C30
17	Y	523	BCR	C1-C6-C7-C8
17	Y	523	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	Y	523	BCR	C23-C24-C25-C26
17	Y	523	BCR	C23-C24-C25-C30
17	Z	521	BCR	C1-C6-C7-C8
17	Z	521	BCR	C5-C6-C7-C8
17	Z	522	BCR	C1-C6-C7-C8
17	Z	523	BCR	C23-C24-C25-C26
17	Z	523	BCR	C23-C24-C25-C30
17	Z	524	BCR	C23-C24-C25-C26
17	Z	524	BCR	C23-C24-C25-C30
17	a	521	BCR	C1-C6-C7-C8
17	a	521	BCR	C5-C6-C7-C8
17	a	523	BCR	C23-C24-C25-C26
17	a	523	BCR	C23-C24-C25-C30
17	b	521	BCR	C1-C6-C7-C8
17	b	521	BCR	C5-C6-C7-C8
17	b	521	BCR	C23-C24-C25-C26
17	b	521	BCR	C23-C24-C25-C30
17	b	522	BCR	C1-C6-C7-C8
17	b	522	BCR	C5-C6-C7-C8
17	b	523	BCR	C23-C24-C25-C26
17	b	523	BCR	C23-C24-C25-C30
17	b	524	BCR	C23-C24-C25-C26
17	b	524	BCR	C23-C24-C25-C30
17	c	522	BCR	C1-C6-C7-C8
17	c	523	BCR	C23-C24-C25-C26
17	c	523	BCR	C23-C24-C25-C30
17	c	524	BCR	C23-C24-C25-C26
17	c	524	BCR	C23-C24-C25-C30
17	d	521	BCR	C1-C6-C7-C8
17	d	521	BCR	C5-C6-C7-C8
17	d	522	BCR	C1-C6-C7-C8
17	d	523	BCR	C23-C24-C25-C26
17	d	523	BCR	C23-C24-C25-C30
17	e	4008	BCR	C23-C24-C25-C30
17	e	4011	BCR	C23-C24-C25-C26
17	e	4011	BCR	C23-C24-C25-C30
17	f	4004	BCR	C1-C6-C7-C8
17	f	4004	BCR	C5-C6-C7-C8
17	f	4004	BCR	C23-C24-C25-C26
17	f	4005	BCR	C23-C24-C25-C26
17	f	4010	BCR	C23-C24-C25-C30
17	f	4017	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	f	4014	BCR	C23-C24-C25-C26
17	l	4015	BCR	C23-C24-C25-C26
17	l	4012	BCR	C1-C6-C7-C8
17	l	4012	BCR	C23-C24-C25-C26
17	l	4012	BCR	C23-C24-C25-C30
17	n	4019	BCR	C23-C24-C25-C26
17	n	4019	BCR	C23-C24-C25-C30
17	o	4021	BCR	C1-C6-C7-C8
17	q	521	BCR	C1-C6-C7-C8
17	q	521	BCR	C5-C6-C7-C8
17	q	521	BCR	C23-C24-C25-C26
17	q	521	BCR	C23-C24-C25-C30
17	q	523	BCR	C1-C6-C7-C8
17	q	523	BCR	C5-C6-C7-C8
17	q	523	BCR	C23-C24-C25-C26
17	q	523	BCR	C23-C24-C25-C30
17	r	521	BCR	C1-C6-C7-C8
17	r	521	BCR	C5-C6-C7-C8
17	r	522	BCR	C1-C6-C7-C8
17	r	523	BCR	C23-C24-C25-C26
17	r	523	BCR	C23-C24-C25-C30
17	r	524	BCR	C23-C24-C25-C26
17	r	524	BCR	C23-C24-C25-C30
17	s	521	BCR	C1-C6-C7-C8
17	s	521	BCR	C5-C6-C7-C8
17	s	523	BCR	C23-C24-C25-C26
17	s	523	BCR	C23-C24-C25-C30
17	t	521	BCR	C1-C6-C7-C8
17	t	521	BCR	C5-C6-C7-C8
17	t	521	BCR	C23-C24-C25-C26
17	t	521	BCR	C23-C24-C25-C30
17	t	522	BCR	C1-C6-C7-C8
17	t	522	BCR	C5-C6-C7-C8
17	t	523	BCR	C23-C24-C25-C26
17	t	523	BCR	C23-C24-C25-C30
17	t	524	BCR	C23-C24-C25-C26
17	t	524	BCR	C23-C24-C25-C30
17	u	522	BCR	C1-C6-C7-C8
17	u	523	BCR	C23-C24-C25-C26
17	u	523	BCR	C23-C24-C25-C30
17	u	524	BCR	C23-C24-C25-C26
17	u	524	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	v	521	BCR	C1-C6-C7-C8
17	v	521	BCR	C5-C6-C7-C8
17	v	522	BCR	C1-C6-C7-C8
17	v	523	BCR	C23-C24-C25-C26
17	v	523	BCR	C23-C24-C25-C30
18	L	5221	LHG	C32-C33-C34-C35
14	B	1215	CLA	CBA-CGA-O2A-C1
14	H	1215	CLA	CBA-CGA-O2A-C1
14	f	1215	CLA	CBA-CGA-O2A-C1
20	J	5104	LMG	C29-C28-O8-C9
20	T	5104	LMG	C29-C28-O8-C9
20	l	5104	LMG	C29-C28-O8-C9
14	A	1133	CLA	C13-C15-C16-C17
14	A	1136	CLA	C13-C15-C16-C17
14	2	501	CLA	C10-C11-C12-C13
14	G	1133	CLA	C13-C15-C16-C17
14	G	1136	CLA	C13-C15-C16-C17
14	Z	501	CLA	C10-C11-C12-C13
14	e	1133	CLA	C13-C15-C16-C17
14	e	1136	CLA	C13-C15-C16-C17
14	r	501	CLA	C10-C11-C12-C13
18	L	5221	LHG	C27-C28-C29-C30
18	V	5221	LHG	C27-C28-C29-C30
18	V	5221	LHG	C32-C33-C34-C35
18	n	5221	LHG	C27-C28-C29-C30
18	n	5221	LHG	C32-C33-C34-C35
14	A	1120	CLA	O1D-CGD-O2D-CED
14	e	1120	CLA	O1D-CGD-O2D-CED
14	j	1302	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	C15-C16-C17-C18
14	B	1218	CLA	C5-C6-C7-C8
14	H	1218	CLA	C5-C6-C7-C8
14	e	1133	CLA	C15-C16-C17-C18
14	f	1218	CLA	C5-C6-C7-C8
14	G	1120	CLA	O1D-CGD-O2D-CED
21	6	822	SQD	C24-C23-O48-C46
21	d	822	SQD	C24-C23-O48-C46
21	v	822	SQD	C24-C23-O48-C46
18	A	5009	LHG	C27-C28-C29-C30
18	G	5009	LHG	C27-C28-C29-C30
18	e	5009	LHG	C27-C28-C29-C30
20	B	5002	LMG	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	H	5002	LMG	C37-C38-C39-C40
20	f	5002	LMG	C37-C38-C39-C40
14	A	1117	CLA	C4-C3-C5-C6
14	B	1227	CLA	C4-C3-C5-C6
14	G	1117	CLA	C4-C3-C5-C6
14	H	1227	CLA	C4-C3-C5-C6
14	e	1117	CLA	C4-C3-C5-C6
14	f	1227	CLA	C4-C3-C5-C6
14	A	1103	CLA	C11-C10-C8-C7
14	A	1110	CLA	C2-C3-C5-C6
14	A	1117	CLA	C2-C3-C5-C6
14	A	1132	CLA	C2-C3-C5-C6
14	A	1133	CLA	C11-C12-C13-C15
14	B	1208	CLA	C2-C3-C5-C6
14	B	1214	CLA	C12-C13-C15-C16
14	B	1223	CLA	C12-C13-C15-C16
14	B	1231	CLA	C2-C3-C5-C6
14	B	1234	CLA	C11-C12-C13-C15
14	B	1239	CLA	C6-C7-C8-C10
14	L	1503	CLA	C6-C7-C8-C10
14	G	1103	CLA	C11-C10-C8-C7
14	G	1110	CLA	C2-C3-C5-C6
14	G	1117	CLA	C2-C3-C5-C6
14	G	1132	CLA	C2-C3-C5-C6
14	G	1133	CLA	C11-C12-C13-C15
14	H	1208	CLA	C2-C3-C5-C6
14	H	1214	CLA	C12-C13-C15-C16
14	H	1223	CLA	C12-C13-C15-C16
14	H	1231	CLA	C2-C3-C5-C6
14	H	1234	CLA	C11-C12-C13-C15
14	H	1239	CLA	C6-C7-C8-C10
14	V	1503	CLA	C6-C7-C8-C10
14	e	1103	CLA	C11-C10-C8-C7
14	e	1110	CLA	C2-C3-C5-C6
14	e	1132	CLA	C2-C3-C5-C6
14	e	1133	CLA	C11-C12-C13-C15
14	f	1208	CLA	C2-C3-C5-C6
14	f	1214	CLA	C12-C13-C15-C16
14	f	1223	CLA	C12-C13-C15-C16
14	f	1231	CLA	C2-C3-C5-C6
14	f	1234	CLA	C11-C12-C13-C15
14	f	1239	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	n	1503	CLA	C6-C7-C8-C10
14	A	1124	CLA	C3-C5-C6-C7
14	G	1124	CLA	C3-C5-C6-C7
14	e	1124	CLA	C3-C5-C6-C7
14	A	1120	CLA	O1A-CGA-O2A-C1
14	G	1120	CLA	O1A-CGA-O2A-C1
14	e	1120	CLA	O1A-CGA-O2A-C1
18	A	5009	LHG	C11-C12-C13-C14
18	G	5009	LHG	C11-C12-C13-C14
18	e	5009	LHG	C11-C12-C13-C14
14	A	1117	CLA	C8-C10-C11-C12
14	A	1136	CLA	C10-C11-C12-C13
14	A	1138	CLA	C8-C10-C11-C12
14	B	1202	CLA	C13-C15-C16-C17
14	B	1221	CLA	C5-C6-C7-C8
14	G	1117	CLA	C8-C10-C11-C12
14	G	1133	CLA	C15-C16-C17-C18
14	G	1138	CLA	C8-C10-C11-C12
14	H	1202	CLA	C13-C15-C16-C17
14	e	1136	CLA	C10-C11-C12-C13
14	e	1138	CLA	C8-C10-C11-C12
14	f	1202	CLA	C13-C15-C16-C17
14	f	1221	CLA	C5-C6-C7-C8
17	B	4010	BCR	C9-C10-C11-C12
17	2	522	BCR	C9-C10-C11-C12
17	H	4010	BCR	C9-C10-C11-C12
17	Z	522	BCR	C9-C10-C11-C12
17	f	4010	BCR	C9-C10-C11-C12
17	r	522	BCR	C9-C10-C11-C12
14	F	1302	CLA	CBD-CGD-O2D-CED
14	R	1302	CLA	CBD-CGD-O2D-CED
14	A	1111	CLA	C16-C17-C18-C20
14	B	1226	CLA	C6-C7-C8-C10
14	G	1111	CLA	C16-C17-C18-C20
14	H	1226	CLA	C6-C7-C8-C10
14	e	1111	CLA	C16-C17-C18-C20
14	f	1226	CLA	C6-C7-C8-C10
14	A	1132	CLA	CBA-CGA-O2A-C1
14	B	1201	CLA	CBA-CGA-O2A-C1
14	G	1132	CLA	CBA-CGA-O2A-C1
14	H	1201	CLA	CBA-CGA-O2A-C1
14	e	1132	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1201	CLA	CBA-CGA-O2A-C1
14	A	1135	CLA	C2A-CAA-CBA-CGA
14	B	1023	CLA	C2A-CAA-CBA-CGA
14	L	1501	CLA	C2A-CAA-CBA-CGA
14	1	501	CLA	C2A-CAA-CBA-CGA
14	4	505	CLA	C2A-CAA-CBA-CGA
14	G	1135	CLA	C2A-CAA-CBA-CGA
14	H	1023	CLA	C2A-CAA-CBA-CGA
14	V	1501	CLA	C2A-CAA-CBA-CGA
14	Y	501	CLA	C2A-CAA-CBA-CGA
14	b	505	CLA	C2A-CAA-CBA-CGA
14	e	1135	CLA	C2A-CAA-CBA-CGA
14	f	1023	CLA	C2A-CAA-CBA-CGA
14	n	1501	CLA	C2A-CAA-CBA-CGA
14	q	501	CLA	C2A-CAA-CBA-CGA
14	t	505	CLA	C2A-CAA-CBA-CGA
14	B	1210	CLA	C13-C15-C16-C17
14	B	1207	CLA	C10-C11-C12-C13
14	G	1136	CLA	C10-C11-C12-C13
14	H	1210	CLA	C13-C15-C16-C17
14	H	1221	CLA	C5-C6-C7-C8
14	H	1207	CLA	C10-C11-C12-C13
14	e	1117	CLA	C8-C10-C11-C12
14	f	1210	CLA	C13-C15-C16-C17
14	f	1207	CLA	C10-C11-C12-C13
18	I	5001	LHG	C27-C28-C29-C30
18	L	5220	LHG	C29-C30-C31-C32
18	S	5001	LHG	C27-C28-C29-C30
18	k	5001	LHG	C27-C28-C29-C30
14	G	1103	CLA	O1D-CGD-O2D-CED
14	B	1240	CLA	CBD-CGD-O2D-CED
14	f	1240	CLA	CBD-CGD-O2D-CED
18	V	5220	LHG	C29-C30-C31-C32
18	n	5220	LHG	C29-C30-C31-C32
14	A	1103	CLA	O1D-CGD-O2D-CED
14	e	1103	CLA	O1D-CGD-O2D-CED
20	T	5104	LMG	C31-C32-C33-C34
20	l	5104	LMG	C31-C32-C33-C34
19	A	1848	LMU	O5B-C5B-C6B-O6B
19	G	1848	LMU	O5B-C5B-C6B-O6B
19	e	1848	LMU	O5B-C5B-C6B-O6B
14	H	1240	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1227	CLA	CBD-CGD-O2D-CED
14	A	1105	CLA	CBA-CGA-O2A-C1
14	G	1105	CLA	CBA-CGA-O2A-C1
14	e	1105	CLA	CBA-CGA-O2A-C1
19	A	1849	LMU	O5'-C1'-O1'-C1
19	G	1849	LMU	O5'-C1'-O1'-C1
19	e	1849	LMU	O5'-C1'-O1'-C1
18	A	5009	LHG	C11-C10-C9-C8
18	G	5009	LHG	C11-C10-C9-C8
18	e	5009	LHG	C11-C10-C9-C8
20	J	5104	LMG	C31-C32-C33-C34
20	B	5002	LMG	C28-C29-C30-C31
20	H	5002	LMG	C28-C29-C30-C31
20	f	5002	LMG	C28-C29-C30-C31
18	A	5001	LHG	C8-C7-O7-C5
18	G	5001	LHG	C8-C7-O7-C5
18	e	5001	LHG	C8-C7-O7-C5
20	J	5104	LMG	C11-C10-O7-C8
20	T	5104	LMG	C11-C10-O7-C8
20	l	5104	LMG	C11-C10-O7-C8
14	2	509	CLA	C5-C6-C7-C8
14	B	1227	CLA	CBD-CGD-O2D-CED
14	H	1227	CLA	CBD-CGD-O2D-CED
18	A	5005	LHG	O9-C7-O7-C5
18	G	5005	LHG	O9-C7-O7-C5
18	e	5005	LHG	O9-C7-O7-C5
14	B	1213	CLA	C3-C5-C6-C7
14	H	1213	CLA	C3-C5-C6-C7
14	f	1213	CLA	C3-C5-C6-C7
18	A	5002	LHG	C25-C26-C27-C28
18	G	5002	LHG	C25-C26-C27-C28
18	e	5002	LHG	C25-C26-C27-C28
14	Z	509	CLA	C5-C6-C7-C8
14	r	509	CLA	C5-C6-C7-C8
18	I	5001	LHG	O7-C5-C6-O8
18	S	5001	LHG	O7-C5-C6-O8
18	k	5001	LHG	O7-C5-C6-O8
20	B	5002	LMG	O7-C8-C9-O8
20	H	5002	LMG	O7-C8-C9-O8
20	f	5002	LMG	O7-C8-C9-O8
18	k	5001	LHG	C28-C29-C30-C31
14	A	1125	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1125	CLA	C13-C15-C16-C17
14	e	1125	CLA	C13-C15-C16-C17
14	A	1110	CLA	C4-C3-C5-C6
14	A	1101	CLA	C4-C3-C5-C6
14	B	1231	CLA	C4-C3-C5-C6
14	G	1110	CLA	C4-C3-C5-C6
14	G	1101	CLA	C4-C3-C5-C6
14	H	1231	CLA	C4-C3-C5-C6
14	e	1110	CLA	C4-C3-C5-C6
14	e	1101	CLA	C4-C3-C5-C6
14	f	1231	CLA	C4-C3-C5-C6
14	e	1117	CLA	C2-C3-C5-C6
18	A	5009	LHG	C28-C29-C30-C31
18	I	5001	LHG	C28-C29-C30-C31
18	G	5009	LHG	C28-C29-C30-C31
18	S	5001	LHG	C28-C29-C30-C31
18	e	5009	LHG	C28-C29-C30-C31
14	A	1103	CLA	C11-C10-C8-C9
14	A	1109	CLA	C11-C12-C13-C14
14	A	1123	CLA	C11-C10-C8-C9
14	A	1127	CLA	C14-C13-C15-C16
14	A	1138	CLA	C11-C10-C8-C9
14	A	1139	CLA	C11-C10-C8-C9
14	B	1216	CLA	C6-C7-C8-C9
14	B	1221	CLA	C11-C10-C8-C9
14	B	1223	CLA	C11-C12-C13-C14
14	5	509	CLA	C11-C10-C8-C9
14	G	1103	CLA	C11-C10-C8-C9
14	G	1109	CLA	C11-C12-C13-C14
14	G	1119	CLA	C6-C7-C8-C9
14	G	1123	CLA	C11-C10-C8-C9
14	G	1127	CLA	C14-C13-C15-C16
14	G	1138	CLA	C11-C10-C8-C9
14	G	1139	CLA	C11-C10-C8-C9
14	H	1216	CLA	C6-C7-C8-C9
14	H	1221	CLA	C11-C10-C8-C9
14	H	1223	CLA	C11-C12-C13-C14
14	c	509	CLA	C11-C10-C8-C9
14	e	1103	CLA	C11-C10-C8-C9
14	e	1109	CLA	C11-C12-C13-C14
14	e	1123	CLA	C11-C10-C8-C9
14	e	1127	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1138	CLA	C11-C10-C8-C9
14	e	1139	CLA	C11-C10-C8-C9
14	f	1221	CLA	C11-C10-C8-C9
14	f	1223	CLA	C11-C12-C13-C14
14	u	509	CLA	C11-C10-C8-C9
18	A	5001	LHG	C10-C11-C12-C13
18	G	5001	LHG	C10-C11-C12-C13
18	e	5001	LHG	C10-C11-C12-C13
14	A	1118	CLA	C2A-CAA-CBA-CGA
14	A	1120	CLA	C2A-CAA-CBA-CGA
14	A	1121	CLA	C2A-CAA-CBA-CGA
14	3	512	CLA	C2A-CAA-CBA-CGA
14	5	517	CLA	C2A-CAA-CBA-CGA
14	G	1118	CLA	C2A-CAA-CBA-CGA
14	G	1120	CLA	C2A-CAA-CBA-CGA
14	G	1121	CLA	C2A-CAA-CBA-CGA
14	a	512	CLA	C2A-CAA-CBA-CGA
14	c	517	CLA	C2A-CAA-CBA-CGA
14	e	1118	CLA	C2A-CAA-CBA-CGA
14	e	1120	CLA	C2A-CAA-CBA-CGA
14	e	1121	CLA	C2A-CAA-CBA-CGA
14	s	512	CLA	C2A-CAA-CBA-CGA
14	u	517	CLA	C2A-CAA-CBA-CGA
19	B	1843	LMU	C7-C8-C9-C10
19	f	1843	LMU	C7-C8-C9-C10
17	e	4001	BCR	C11-C12-C13-C35
14	G	1131	CLA	C13-C15-C16-C17
19	H	1843	LMU	C7-C8-C9-C10
17	3	523	BCR	C21-C22-C23-C24
17	a	523	BCR	C21-C22-C23-C24
17	s	523	BCR	C21-C22-C23-C24
14	A	1102	CLA	C1A-C2A-CAA-CBA
14	A	1106	CLA	C1A-C2A-CAA-CBA
14	A	1107	CLA	C1A-C2A-CAA-CBA
14	A	1109	CLA	C1A-C2A-CAA-CBA
14	A	1116	CLA	C1A-C2A-CAA-CBA
14	A	1118	CLA	C1A-C2A-CAA-CBA
14	A	1120	CLA	C1A-C2A-CAA-CBA
14	A	1122	CLA	C1A-C2A-CAA-CBA
14	A	1125	CLA	C1A-C2A-CAA-CBA
14	A	1129	CLA	C1A-C2A-CAA-CBA
14	A	1132	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1134	CLA	C1A-C2A-CAA-CBA
14	A	1135	CLA	C1A-C2A-CAA-CBA
14	A	1022	CLA	C1A-C2A-CAA-CBA
14	A	1130	CLA	C1A-C2A-CAA-CBA
14	A	1101	CLA	C1A-C2A-CAA-CBA
14	B	1219	CLA	C1A-C2A-CAA-CBA
14	B	1221	CLA	C1A-C2A-CAA-CBA
14	B	1225	CLA	C1A-C2A-CAA-CBA
14	B	1226	CLA	C1A-C2A-CAA-CBA
14	B	1227	CLA	C1A-C2A-CAA-CBA
14	F	1302	CLA	C1A-C2A-CAA-CBA
14	J	1302	CLA	C1A-C2A-CAA-CBA
14	J	1303	CLA	C1A-C2A-CAA-CBA
14	K	1103	CLA	C1A-C2A-CAA-CBA
14	K	1105	CLA	C1A-C2A-CAA-CBA
14	L	1501	CLA	C1A-C2A-CAA-CBA
14	1	503	CLA	C1A-C2A-CAA-CBA
14	1	505	CLA	C1A-C2A-CAA-CBA
14	1	516	CLA	C1A-C2A-CAA-CBA
14	1	519	CLA	C1A-C2A-CAA-CBA
14	2	501	CLA	C1A-C2A-CAA-CBA
14	2	505	CLA	C1A-C2A-CAA-CBA
14	2	516	CLA	C1A-C2A-CAA-CBA
14	2	518	CLA	C1A-C2A-CAA-CBA
14	3	501	CLA	C1A-C2A-CAA-CBA
14	3	503	CLA	C1A-C2A-CAA-CBA
14	3	505	CLA	C1A-C2A-CAA-CBA
14	3	518	CLA	C1A-C2A-CAA-CBA
14	4	501	CLA	C1A-C2A-CAA-CBA
14	4	504	CLA	C1A-C2A-CAA-CBA
14	4	511	CLA	C1A-C2A-CAA-CBA
14	5	501	CLA	C1A-C2A-CAA-CBA
14	5	502	CLA	C1A-C2A-CAA-CBA
14	5	504	CLA	C1A-C2A-CAA-CBA
14	5	505	CLA	C1A-C2A-CAA-CBA
14	5	513	CLA	C1A-C2A-CAA-CBA
14	5	516	CLA	C1A-C2A-CAA-CBA
14	6	501	CLA	C1A-C2A-CAA-CBA
14	6	505	CLA	C1A-C2A-CAA-CBA
14	6	508	CLA	C1A-C2A-CAA-CBA
14	6	512	CLA	C1A-C2A-CAA-CBA
14	6	516	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	6	518	CLA	C1A-C2A-CAA-CBA
14	G	1102	CLA	C1A-C2A-CAA-CBA
14	G	1106	CLA	C1A-C2A-CAA-CBA
14	G	1107	CLA	C1A-C2A-CAA-CBA
14	G	1109	CLA	C1A-C2A-CAA-CBA
14	G	1116	CLA	C1A-C2A-CAA-CBA
14	G	1118	CLA	C1A-C2A-CAA-CBA
14	G	1120	CLA	C1A-C2A-CAA-CBA
14	G	1122	CLA	C1A-C2A-CAA-CBA
14	G	1125	CLA	C1A-C2A-CAA-CBA
14	G	1129	CLA	C1A-C2A-CAA-CBA
14	G	1132	CLA	C1A-C2A-CAA-CBA
14	G	1134	CLA	C1A-C2A-CAA-CBA
14	G	1135	CLA	C1A-C2A-CAA-CBA
14	G	1022	CLA	C1A-C2A-CAA-CBA
14	G	1130	CLA	C1A-C2A-CAA-CBA
14	G	1101	CLA	C1A-C2A-CAA-CBA
14	H	1219	CLA	C1A-C2A-CAA-CBA
14	H	1221	CLA	C1A-C2A-CAA-CBA
14	H	1225	CLA	C1A-C2A-CAA-CBA
14	H	1226	CLA	C1A-C2A-CAA-CBA
14	H	1227	CLA	C1A-C2A-CAA-CBA
14	R	1302	CLA	C1A-C2A-CAA-CBA
14	T	1302	CLA	C1A-C2A-CAA-CBA
14	T	1303	CLA	C1A-C2A-CAA-CBA
14	U	1103	CLA	C1A-C2A-CAA-CBA
14	U	1105	CLA	C1A-C2A-CAA-CBA
14	V	1501	CLA	C1A-C2A-CAA-CBA
14	Y	503	CLA	C1A-C2A-CAA-CBA
14	Y	505	CLA	C1A-C2A-CAA-CBA
14	Y	516	CLA	C1A-C2A-CAA-CBA
14	Y	519	CLA	C1A-C2A-CAA-CBA
14	Z	501	CLA	C1A-C2A-CAA-CBA
14	Z	505	CLA	C1A-C2A-CAA-CBA
14	Z	516	CLA	C1A-C2A-CAA-CBA
14	Z	518	CLA	C1A-C2A-CAA-CBA
14	a	501	CLA	C1A-C2A-CAA-CBA
14	a	503	CLA	C1A-C2A-CAA-CBA
14	a	505	CLA	C1A-C2A-CAA-CBA
14	a	518	CLA	C1A-C2A-CAA-CBA
14	b	501	CLA	C1A-C2A-CAA-CBA
14	b	504	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	511	CLA	C1A-C2A-CAA-CBA
14	c	501	CLA	C1A-C2A-CAA-CBA
14	c	502	CLA	C1A-C2A-CAA-CBA
14	c	504	CLA	C1A-C2A-CAA-CBA
14	c	505	CLA	C1A-C2A-CAA-CBA
14	c	513	CLA	C1A-C2A-CAA-CBA
14	c	516	CLA	C1A-C2A-CAA-CBA
14	d	501	CLA	C1A-C2A-CAA-CBA
14	d	505	CLA	C1A-C2A-CAA-CBA
14	d	508	CLA	C1A-C2A-CAA-CBA
14	d	512	CLA	C1A-C2A-CAA-CBA
14	d	516	CLA	C1A-C2A-CAA-CBA
14	d	518	CLA	C1A-C2A-CAA-CBA
14	e	1102	CLA	C1A-C2A-CAA-CBA
14	e	1106	CLA	C1A-C2A-CAA-CBA
14	e	1107	CLA	C1A-C2A-CAA-CBA
14	e	1109	CLA	C1A-C2A-CAA-CBA
14	e	1116	CLA	C1A-C2A-CAA-CBA
14	e	1118	CLA	C1A-C2A-CAA-CBA
14	e	1120	CLA	C1A-C2A-CAA-CBA
14	e	1122	CLA	C1A-C2A-CAA-CBA
14	e	1125	CLA	C1A-C2A-CAA-CBA
14	e	1129	CLA	C1A-C2A-CAA-CBA
14	e	1132	CLA	C1A-C2A-CAA-CBA
14	e	1134	CLA	C1A-C2A-CAA-CBA
14	e	1135	CLA	C1A-C2A-CAA-CBA
14	e	1022	CLA	C1A-C2A-CAA-CBA
14	e	1130	CLA	C1A-C2A-CAA-CBA
14	e	1101	CLA	C1A-C2A-CAA-CBA
14	f	1219	CLA	C1A-C2A-CAA-CBA
14	f	1221	CLA	C1A-C2A-CAA-CBA
14	f	1225	CLA	C1A-C2A-CAA-CBA
14	f	1226	CLA	C1A-C2A-CAA-CBA
14	f	1227	CLA	C1A-C2A-CAA-CBA
14	j	1302	CLA	C1A-C2A-CAA-CBA
14	l	1302	CLA	C1A-C2A-CAA-CBA
14	l	1303	CLA	C1A-C2A-CAA-CBA
14	m	1103	CLA	C1A-C2A-CAA-CBA
14	m	1105	CLA	C1A-C2A-CAA-CBA
14	n	1501	CLA	C1A-C2A-CAA-CBA
14	q	503	CLA	C1A-C2A-CAA-CBA
14	q	505	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	q	516	CLA	C1A-C2A-CAA-CBA
14	q	519	CLA	C1A-C2A-CAA-CBA
14	r	501	CLA	C1A-C2A-CAA-CBA
14	r	505	CLA	C1A-C2A-CAA-CBA
14	r	516	CLA	C1A-C2A-CAA-CBA
14	r	518	CLA	C1A-C2A-CAA-CBA
14	s	501	CLA	C1A-C2A-CAA-CBA
14	s	503	CLA	C1A-C2A-CAA-CBA
14	s	505	CLA	C1A-C2A-CAA-CBA
14	s	518	CLA	C1A-C2A-CAA-CBA
14	t	501	CLA	C1A-C2A-CAA-CBA
14	t	504	CLA	C1A-C2A-CAA-CBA
14	t	511	CLA	C1A-C2A-CAA-CBA
14	u	501	CLA	C1A-C2A-CAA-CBA
14	u	502	CLA	C1A-C2A-CAA-CBA
14	u	504	CLA	C1A-C2A-CAA-CBA
14	u	505	CLA	C1A-C2A-CAA-CBA
14	u	513	CLA	C1A-C2A-CAA-CBA
14	u	516	CLA	C1A-C2A-CAA-CBA
14	v	501	CLA	C1A-C2A-CAA-CBA
14	v	505	CLA	C1A-C2A-CAA-CBA
14	v	508	CLA	C1A-C2A-CAA-CBA
14	v	512	CLA	C1A-C2A-CAA-CBA
14	v	516	CLA	C1A-C2A-CAA-CBA
14	v	518	CLA	C1A-C2A-CAA-CBA
14	B	1208	CLA	C16-C17-C18-C20
14	B	1218	CLA	C11-C12-C13-C15
14	B	1239	CLA	C16-C17-C18-C19
14	B	1239	CLA	C16-C17-C18-C20
14	H	1208	CLA	C16-C17-C18-C20
14	H	1218	CLA	C11-C12-C13-C15
14	H	1239	CLA	C16-C17-C18-C19
14	H	1239	CLA	C16-C17-C18-C20
14	f	1208	CLA	C16-C17-C18-C20
14	f	1218	CLA	C11-C12-C13-C15
14	f	1239	CLA	C16-C17-C18-C19
14	f	1239	CLA	C16-C17-C18-C20
15	B	2002	PQN	C26-C27-C28-C29
15	H	2002	PQN	C26-C27-C28-C29
15	f	2002	PQN	C26-C27-C28-C29
18	L	5221	LHG	C8-C7-O7-C5
18	V	5221	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	n	5221	LHG	C8-C7-O7-C5
18	A	5006	LHG	C27-C28-C29-C30
18	G	5006	LHG	C27-C28-C29-C30
18	e	5006	LHG	C27-C28-C29-C30
14	A	1131	CLA	C13-C15-C16-C17
14	B	1223	CLA	C10-C11-C12-C13
14	H	1224	CLA	C5-C6-C7-C8
14	e	1131	CLA	C13-C15-C16-C17
14	f	1223	CLA	C10-C11-C12-C13
18	A	5002	LHG	C4-O6-P-O3
18	I	5001	LHG	C3-O3-P-O6
18	G	5002	LHG	C4-O6-P-O3
18	S	5001	LHG	C3-O3-P-O6
18	e	5002	LHG	C4-O6-P-O3
18	k	5001	LHG	C3-O3-P-O6
18	A	5008	LHG	C25-C26-C27-C28
18	G	5008	LHG	C25-C26-C27-C28
18	e	5008	LHG	C25-C26-C27-C28
14	A	1132	CLA	O1A-CGA-O2A-C1
14	G	1132	CLA	O1A-CGA-O2A-C1
14	e	1132	CLA	O1A-CGA-O2A-C1
14	B	1203	CLA	C13-C15-C16-C17
14	B	1224	CLA	C5-C6-C7-C8
14	H	1203	CLA	C13-C15-C16-C17
14	H	1223	CLA	C10-C11-C12-C13
14	f	1203	CLA	C13-C15-C16-C17
14	f	1224	CLA	C5-C6-C7-C8
18	A	5007	LHG	O6-C4-C5-C6
18	G	5007	LHG	O6-C4-C5-C6
18	e	5007	LHG	O6-C4-C5-C6
18	L	5218	LHG	C11-C10-C9-C8
18	V	5218	LHG	C11-C10-C9-C8
18	n	5218	LHG	C11-C10-C9-C8
18	A	5002	LHG	C30-C31-C32-C33
18	A	5008	LHG	C12-C13-C14-C15
18	G	5002	LHG	C30-C31-C32-C33
18	G	5008	LHG	C12-C13-C14-C15
18	e	5002	LHG	C30-C31-C32-C33
18	e	5008	LHG	C12-C13-C14-C15
15	A	2001	PQN	C25-C26-C27-C28
15	G	2001	PQN	C25-C26-C27-C28
15	e	2001	PQN	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1217	CLA	C11-C12-C13-C15
14	H	1217	CLA	C11-C12-C13-C15
14	f	1217	CLA	C11-C12-C13-C15
18	A	5002	LHG	C23-C24-C25-C26
18	G	5002	LHG	C23-C24-C25-C26
18	e	5002	LHG	C23-C24-C25-C26
18	B	1842	LHG	C25-C26-C27-C28
18	H	1842	LHG	C25-C26-C27-C28
18	f	1842	LHG	C25-C26-C27-C28
20	J	5104	LMG	C30-C31-C32-C33
14	A	1108	CLA	C4-C3-C5-C6
14	B	1210	CLA	C4-C3-C5-C6
14	G	1108	CLA	C4-C3-C5-C6
14	H	1210	CLA	C4-C3-C5-C6
14	e	1108	CLA	C4-C3-C5-C6
14	f	1210	CLA	C4-C3-C5-C6
15	A	2001	PQN	C14-C13-C15-C16
15	G	2001	PQN	C14-C13-C15-C16
15	e	2001	PQN	C14-C13-C15-C16
20	T	5104	LMG	C30-C31-C32-C33
20	l	5104	LMG	C30-C31-C32-C33
18	G	5003	LHG	C9-C10-C11-C12
14	A	1105	CLA	O1A-CGA-O2A-C1
14	G	1105	CLA	O1A-CGA-O2A-C1
14	e	1105	CLA	O1A-CGA-O2A-C1
20	B	5002	LMG	O10-C28-O8-C9
20	H	5002	LMG	O10-C28-O8-C9
20	f	5002	LMG	O10-C28-O8-C9
18	A	5003	LHG	C9-C10-C11-C12
18	B	1855	LHG	C27-C28-C29-C30
18	H	1855	LHG	C27-C28-C29-C30
18	e	5003	LHG	C9-C10-C11-C12
18	f	1855	LHG	C27-C28-C29-C30
14	A	1103	CLA	C16-C17-C18-C20
14	L	1502	CLA	C16-C17-C18-C19
14	2	505	CLA	C16-C17-C18-C20
14	G	1103	CLA	C16-C17-C18-C20
14	V	1502	CLA	C16-C17-C18-C19
14	Z	505	CLA	C16-C17-C18-C20
14	e	1103	CLA	C16-C17-C18-C20
14	n	1502	CLA	C16-C17-C18-C19
14	r	505	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	5002	LHG	C4-C5-C6-O8
18	A	5004	LHG	C4-C5-C6-O8
18	A	5008	LHG	C4-C5-C6-O8
18	L	5218	LHG	C4-C5-C6-O8
18	L	5221	LHG	C4-C5-C6-O8
18	G	5002	LHG	C4-C5-C6-O8
18	G	5004	LHG	C4-C5-C6-O8
18	G	5008	LHG	C4-C5-C6-O8
18	S	5001	LHG	C31-C32-C33-C34
18	V	5218	LHG	C4-C5-C6-O8
18	V	5221	LHG	C4-C5-C6-O8
18	e	5002	LHG	C4-C5-C6-O8
18	e	5004	LHG	C4-C5-C6-O8
18	e	5008	LHG	C4-C5-C6-O8
18	n	5218	LHG	C4-C5-C6-O8
18	n	5221	LHG	C4-C5-C6-O8
21	3	822	SQD	C44-C45-C46-O48
21	6	822	SQD	C44-C45-C46-O48
21	a	822	SQD	C44-C45-C46-O48
21	d	822	SQD	C44-C45-C46-O48
21	s	822	SQD	C44-C45-C46-O48
21	v	822	SQD	C44-C45-C46-O48
18	I	5001	LHG	C31-C32-C33-C34
18	G	5007	LHG	C25-C26-C27-C28
18	e	5005	LHG	C31-C32-C33-C34
18	k	5001	LHG	C31-C32-C33-C34
14	B	1215	CLA	O1A-CGA-O2A-C1
14	H	1215	CLA	O1A-CGA-O2A-C1
14	f	1215	CLA	O1A-CGA-O2A-C1
18	A	5005	LHG	C31-C32-C33-C34
18	A	5007	LHG	C25-C26-C27-C28
18	G	5005	LHG	C31-C32-C33-C34
18	e	5007	LHG	C25-C26-C27-C28
14	A	1137	CLA	C5-C6-C7-C8
14	G	1137	CLA	C5-C6-C7-C8
14	e	1137	CLA	C5-C6-C7-C8
14	A	1108	CLA	C5-C6-C7-C8
14	G	1108	CLA	C5-C6-C7-C8
14	e	1108	CLA	C5-C6-C7-C8
14	A	1135	CLA	C3-C5-C6-C7
14	G	1135	CLA	C3-C5-C6-C7
14	e	1135	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1127	CLA	C16-C17-C18-C19
14	G	1127	CLA	C16-C17-C18-C19
14	e	1127	CLA	C16-C17-C18-C19
19	A	1849	LMU	O5'-C5'-C6'-O6'
19	G	1849	LMU	O5'-C5'-C6'-O6'
19	e	1849	LMU	O5'-C5'-C6'-O6'
18	L	5220	LHG	O1-C1-C2-O2
18	V	5220	LHG	O1-C1-C2-O2
18	n	5220	LHG	O1-C1-C2-O2
18	G	5001	LHG	C9-C10-C11-C12
18	A	5001	LHG	C9-C10-C11-C12
18	e	5001	LHG	C9-C10-C11-C12
21	H	1852	SQD	C28-C29-C30-C31
14	2	518	CLA	O1D-CGD-O2D-CED
14	Z	518	CLA	O1D-CGD-O2D-CED
14	B	1204	CLA	C13-C15-C16-C17
14	B	1215	CLA	C13-C15-C16-C17
14	6	505	CLA	C13-C15-C16-C17
14	H	1215	CLA	C13-C15-C16-C17
14	d	505	CLA	C13-C15-C16-C17
14	f	1215	CLA	C13-C15-C16-C17
14	v	505	CLA	C13-C15-C16-C17
14	A	1119	CLA	C4-C3-C5-C6
14	G	1119	CLA	C4-C3-C5-C6
14	e	1119	CLA	C4-C3-C5-C6
21	B	1852	SQD	C28-C29-C30-C31
21	f	1852	SQD	C28-C29-C30-C31
14	r	518	CLA	O1D-CGD-O2D-CED
14	A	1127	CLA	C16-C17-C18-C20
14	B	1215	CLA	C16-C17-C18-C20
14	G	1127	CLA	C16-C17-C18-C20
14	H	1215	CLA	C16-C17-C18-C20
14	e	1127	CLA	C16-C17-C18-C20
14	f	1215	CLA	C16-C17-C18-C20
14	A	1111	CLA	CBA-CGA-O2A-C1
14	G	1111	CLA	CBA-CGA-O2A-C1
14	e	1111	CLA	CBA-CGA-O2A-C1
19	B	1843	LMU	C11-C10-C9-C8
19	H	1843	LMU	C11-C10-C9-C8
19	f	1843	LMU	C11-C10-C9-C8
14	B	1226	CLA	CBD-CGD-O2D-CED
14	5	508	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1226	CLA	CBD-CGD-O2D-CED
14	c	508	CLA	CBD-CGD-O2D-CED
14	f	1226	CLA	CBD-CGD-O2D-CED
14	u	508	CLA	CBD-CGD-O2D-CED
14	A	1126	CLA	C13-C15-C16-C17
14	G	1121	CLA	C5-C6-C7-C8
14	G	1126	CLA	C13-C15-C16-C17
14	e	1121	CLA	C5-C6-C7-C8
14	e	1126	CLA	C13-C15-C16-C17
14	f	1204	CLA	C13-C15-C16-C17
18	A	5004	LHG	C9-C10-C11-C12
18	G	5004	LHG	C9-C10-C11-C12
21	B	1852	SQD	C9-C10-C11-C12
21	H	1852	SQD	C9-C10-C11-C12
21	f	1852	SQD	C9-C10-C11-C12
21	4	822	SQD	C46-C45-O47-C7
21	b	822	SQD	C46-C45-O47-C7
21	t	822	SQD	C46-C45-O47-C7
14	A	1129	CLA	C2A-CAA-CBA-CGA
14	3	504	CLA	C2A-CAA-CBA-CGA
14	G	1129	CLA	C2A-CAA-CBA-CGA
14	a	504	CLA	C2A-CAA-CBA-CGA
14	e	1129	CLA	C2A-CAA-CBA-CGA
14	s	504	CLA	C2A-CAA-CBA-CGA
14	A	1106	CLA	C13-C15-C16-C17
14	A	1121	CLA	C5-C6-C7-C8
14	A	1132	CLA	C5-C6-C7-C8
14	A	1138	CLA	C13-C15-C16-C17
14	G	1106	CLA	C13-C15-C16-C17
14	G	1132	CLA	C5-C6-C7-C8
14	G	1138	CLA	C13-C15-C16-C17
14	H	1204	CLA	C13-C15-C16-C17
14	e	1106	CLA	C13-C15-C16-C17
14	e	1132	CLA	C5-C6-C7-C8
14	e	1138	CLA	C13-C15-C16-C17
14	A	1105	CLA	C2-C1-O2A-CGA
14	A	1120	CLA	C2-C1-O2A-CGA
14	G	1105	CLA	C2-C1-O2A-CGA
14	G	1120	CLA	C2-C1-O2A-CGA
14	e	1105	CLA	C2-C1-O2A-CGA
14	e	1120	CLA	C2-C1-O2A-CGA
18	V	5218	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	5004	LHG	C9-C10-C11-C12
14	r	511	CLA	O1D-CGD-O2D-CED
18	B	1842	LHG	C30-C31-C32-C33
18	L	5218	LHG	C28-C29-C30-C31
18	H	1842	LHG	C30-C31-C32-C33
18	f	1842	LHG	C30-C31-C32-C33
18	n	5218	LHG	C28-C29-C30-C31
14	A	1109	CLA	O1D-CGD-O2D-CED
14	1	505	CLA	O1D-CGD-O2D-CED
14	2	511	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	O1D-CGD-O2D-CED
14	Y	505	CLA	O1D-CGD-O2D-CED
14	Z	511	CLA	O1D-CGD-O2D-CED
14	e	1109	CLA	O1D-CGD-O2D-CED
14	q	505	CLA	O1D-CGD-O2D-CED
18	A	5006	LHG	C32-C33-C34-C35
20	B	5002	LMG	C41-C42-C43-C44
20	H	5002	LMG	C41-C42-C43-C44
20	f	5002	LMG	C41-C42-C43-C44
14	A	1103	CLA	CBA-CGA-O2A-C1
14	G	1103	CLA	CBA-CGA-O2A-C1
14	e	1103	CLA	CBA-CGA-O2A-C1
14	6	510	CLA	O1D-CGD-O2D-CED
14	d	510	CLA	O1D-CGD-O2D-CED
14	v	510	CLA	O1D-CGD-O2D-CED
14	2	505	CLA	C16-C17-C18-C19
14	Z	505	CLA	C16-C17-C18-C19
14	r	505	CLA	C16-C17-C18-C19
18	G	5006	LHG	C32-C33-C34-C35
18	e	5006	LHG	C32-C33-C34-C35
14	B	1240	CLA	C8-C10-C11-C12
18	H	1842	LHG	C32-C33-C34-C35
18	f	1842	LHG	C32-C33-C34-C35
14	A	1103	CLA	C13-C15-C16-C17
14	A	1140	CLA	C15-C16-C17-C18
14	G	1103	CLA	C13-C15-C16-C17
14	G	1140	CLA	C15-C16-C17-C18
14	H	1240	CLA	C8-C10-C11-C12
14	e	1140	CLA	C15-C16-C17-C18
14	f	1240	CLA	C8-C10-C11-C12
18	B	1842	LHG	C32-C33-C34-C35
18	A	5001	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	5001	LHG	O7-C5-C6-O8
18	e	5001	LHG	O7-C5-C6-O8
21	2	822	SQD	O47-C45-C46-O48
21	Z	822	SQD	O47-C45-C46-O48
21	r	822	SQD	O47-C45-C46-O48
18	e	5008	LHG	C26-C27-C28-C29
14	e	1103	CLA	C13-C15-C16-C17
14	G	1111	CLA	O1A-CGA-O2A-C1
18	A	5008	LHG	C26-C27-C28-C29
18	G	5008	LHG	C26-C27-C28-C29
20	B	5002	LMG	C35-C36-C37-C38
20	H	5002	LMG	C35-C36-C37-C38
20	f	5002	LMG	C35-C36-C37-C38
21	f	1852	SQD	C24-C25-C26-C27
21	B	1852	SQD	C24-C25-C26-C27
21	H	1852	SQD	C24-C25-C26-C27
14	A	1106	CLA	C11-C12-C13-C15
14	A	1116	CLA	C6-C7-C8-C10
14	A	1119	CLA	C2-C3-C5-C6
14	A	1123	CLA	C11-C10-C8-C7
14	A	1127	CLA	C11-C12-C13-C15
14	A	1127	CLA	C12-C13-C15-C16
14	A	1138	CLA	C11-C10-C8-C7
14	A	1139	CLA	C12-C13-C15-C16
14	A	1237	CLA	C11-C10-C8-C7
14	A	1237	CLA	C12-C13-C15-C16
14	A	1101	CLA	C11-C12-C13-C15
14	B	1012	CLA	C11-C10-C8-C7
14	B	1225	CLA	C12-C13-C15-C16
14	B	1231	CLA	C6-C7-C8-C10
14	L	1502	CLA	C11-C10-C8-C7
14	2	503	CLA	C12-C13-C15-C16
14	5	509	CLA	C11-C10-C8-C7
14	5	509	CLA	C12-C13-C15-C16
14	G	1106	CLA	C11-C12-C13-C15
14	G	1116	CLA	C6-C7-C8-C10
14	G	1119	CLA	C2-C3-C5-C6
14	G	1123	CLA	C11-C10-C8-C7
14	G	1127	CLA	C11-C12-C13-C15
14	G	1127	CLA	C12-C13-C15-C16
14	G	1138	CLA	C11-C10-C8-C7
14	G	1139	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1237	CLA	C11-C10-C8-C7
14	G	1237	CLA	C12-C13-C15-C16
14	G	1101	CLA	C11-C12-C13-C15
14	H	1012	CLA	C11-C10-C8-C7
14	H	1225	CLA	C12-C13-C15-C16
14	H	1231	CLA	C6-C7-C8-C10
14	V	1502	CLA	C11-C10-C8-C7
14	Z	503	CLA	C12-C13-C15-C16
14	c	509	CLA	C11-C10-C8-C7
14	c	509	CLA	C12-C13-C15-C16
14	e	1106	CLA	C11-C12-C13-C15
14	e	1116	CLA	C6-C7-C8-C10
14	e	1119	CLA	C2-C3-C5-C6
14	e	1123	CLA	C11-C10-C8-C7
14	e	1127	CLA	C11-C12-C13-C15
14	e	1127	CLA	C12-C13-C15-C16
14	e	1138	CLA	C11-C10-C8-C7
14	e	1139	CLA	C12-C13-C15-C16
14	e	1237	CLA	C11-C10-C8-C7
14	e	1237	CLA	C12-C13-C15-C16
14	e	1101	CLA	C11-C12-C13-C15
14	f	1012	CLA	C11-C10-C8-C7
14	f	1225	CLA	C12-C13-C15-C16
14	f	1231	CLA	C6-C7-C8-C10
14	n	1502	CLA	C11-C10-C8-C7
14	r	503	CLA	C12-C13-C15-C16
14	u	509	CLA	C11-C10-C8-C7
14	u	509	CLA	C12-C13-C15-C16
15	A	2001	PQN	C17-C18-C20-C21
15	A	2001	PQN	C22-C23-C25-C26
15	G	2001	PQN	C17-C18-C20-C21
15	G	2001	PQN	C22-C23-C25-C26
15	e	2001	PQN	C17-C18-C20-C21
15	e	2001	PQN	C22-C23-C25-C26
14	e	1111	CLA	O1A-CGA-O2A-C1
14	A	1106	CLA	C11-C12-C13-C14
14	A	1107	CLA	C11-C12-C13-C14
14	A	1111	CLA	C11-C12-C13-C14
14	A	1119	CLA	C6-C7-C8-C9
14	A	1124	CLA	C11-C10-C8-C9
14	A	1127	CLA	C11-C12-C13-C14
14	A	1128	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1132	CLA	C14-C13-C15-C16
14	A	1136	CLA	C11-C12-C13-C14
14	A	1138	CLA	C14-C13-C15-C16
14	A	1237	CLA	C11-C10-C8-C9
14	B	1012	CLA	C14-C13-C15-C16
14	B	1206	CLA	C6-C7-C8-C9
14	B	1210	CLA	C6-C7-C8-C9
14	B	1214	CLA	C11-C10-C8-C9
14	B	1214	CLA	C14-C13-C15-C16
14	B	1219	CLA	C11-C12-C13-C14
14	B	1231	CLA	C6-C7-C8-C9
14	B	1234	CLA	C11-C10-C8-C9
14	B	1239	CLA	C6-C7-C8-C9
14	5	509	CLA	C14-C13-C15-C16
14	G	1106	CLA	C11-C12-C13-C14
14	G	1107	CLA	C11-C12-C13-C14
14	G	1111	CLA	C11-C12-C13-C14
14	G	1124	CLA	C11-C10-C8-C9
14	G	1127	CLA	C11-C12-C13-C14
14	G	1128	CLA	C6-C7-C8-C9
14	G	1132	CLA	C14-C13-C15-C16
14	G	1136	CLA	C11-C12-C13-C14
14	G	1138	CLA	C14-C13-C15-C16
14	G	1237	CLA	C11-C10-C8-C9
14	H	1012	CLA	C14-C13-C15-C16
14	H	1206	CLA	C6-C7-C8-C9
14	H	1210	CLA	C6-C7-C8-C9
14	H	1214	CLA	C11-C10-C8-C9
14	H	1214	CLA	C14-C13-C15-C16
14	H	1219	CLA	C11-C12-C13-C14
14	H	1231	CLA	C6-C7-C8-C9
14	H	1234	CLA	C11-C10-C8-C9
14	H	1239	CLA	C6-C7-C8-C9
14	c	509	CLA	C14-C13-C15-C16
14	e	1106	CLA	C11-C12-C13-C14
14	e	1107	CLA	C11-C12-C13-C14
14	e	1111	CLA	C11-C12-C13-C14
14	e	1119	CLA	C6-C7-C8-C9
14	e	1124	CLA	C11-C10-C8-C9
14	e	1127	CLA	C11-C12-C13-C14
14	e	1128	CLA	C6-C7-C8-C9
14	e	1132	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1136	CLA	C11-C12-C13-C14
14	e	1138	CLA	C14-C13-C15-C16
14	e	1237	CLA	C11-C10-C8-C9
14	f	1012	CLA	C14-C13-C15-C16
14	f	1206	CLA	C6-C7-C8-C9
14	f	1210	CLA	C6-C7-C8-C9
14	f	1214	CLA	C11-C10-C8-C9
14	f	1214	CLA	C14-C13-C15-C16
14	f	1216	CLA	C6-C7-C8-C9
14	f	1219	CLA	C11-C12-C13-C14
14	f	1231	CLA	C6-C7-C8-C9
14	f	1234	CLA	C11-C10-C8-C9
14	f	1239	CLA	C6-C7-C8-C9
14	u	509	CLA	C14-C13-C15-C16
15	A	2001	PQN	C19-C18-C20-C21
15	A	2001	PQN	C24-C23-C25-C26
15	G	2001	PQN	C19-C18-C20-C21
15	G	2001	PQN	C24-C23-C25-C26
15	e	2001	PQN	C19-C18-C20-C21
15	e	2001	PQN	C24-C23-C25-C26
17	1	522	BCR	C9-C10-C11-C12
17	Y	522	BCR	C9-C10-C11-C12
17	q	522	BCR	C9-C10-C11-C12
18	G	5006	LHG	C7-C8-C9-C10
18	G	5003	LHG	C15-C16-C17-C18
18	e	5003	LHG	C15-C16-C17-C18
14	e	1111	CLA	C2A-CAA-CBA-CGA
18	A	5003	LHG	C15-C16-C17-C18
14	A	1111	CLA	O1A-CGA-O2A-C1
17	2	523	BCR	C7-C8-C9-C34
17	Z	523	BCR	C7-C8-C9-C34
17	r	523	BCR	C7-C8-C9-C34
14	A	1126	CLA	C16-C17-C18-C19
14	A	1133	CLA	C16-C17-C18-C20
14	G	1126	CLA	C16-C17-C18-C19
14	G	1133	CLA	C16-C17-C18-C20
14	e	1126	CLA	C16-C17-C18-C19
14	e	1133	CLA	C16-C17-C18-C20
18	n	5221	LHG	C15-C16-C17-C18
17	A	4001	BCR	C21-C22-C23-C24
17	G	4001	BCR	C21-C22-C23-C24
17	e	4001	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	1855	LHG	C13-C14-C15-C16
18	L	5221	LHG	C15-C16-C17-C18
18	H	1855	LHG	C13-C14-C15-C16
18	V	5221	LHG	C15-C16-C17-C18
18	f	1855	LHG	C13-C14-C15-C16
20	B	5002	LMG	C30-C31-C32-C33
20	f	5002	LMG	C30-C31-C32-C33
14	A	1117	CLA	C15-C16-C17-C18
14	A	1136	CLA	C15-C16-C17-C18
14	B	1231	CLA	C5-C6-C7-C8
14	G	1117	CLA	C15-C16-C17-C18
14	G	1136	CLA	C15-C16-C17-C18
14	H	1231	CLA	C5-C6-C7-C8
14	e	1117	CLA	C15-C16-C17-C18
14	e	1136	CLA	C15-C16-C17-C18
20	H	5002	LMG	C30-C31-C32-C33
14	2	518	CLA	CBA-CGA-O2A-C1
14	Z	518	CLA	CBA-CGA-O2A-C1
14	r	518	CLA	CBA-CGA-O2A-C1
14	H	1023	CLA	C4C-C3C-CAC-CBC
14	f	1023	CLA	C4C-C3C-CAC-CBC
18	A	5006	LHG	C7-C8-C9-C10
18	e	5006	LHG	C7-C8-C9-C10
14	B	1230	CLA	C5-C6-C7-C8
14	H	1230	CLA	C5-C6-C7-C8
14	f	1231	CLA	C5-C6-C7-C8
14	f	1230	CLA	C5-C6-C7-C8
14	B	1023	CLA	C4C-C3C-CAC-CBC
18	B	1842	LHG	C28-C29-C30-C31
18	H	1842	LHG	C28-C29-C30-C31
18	f	1842	LHG	C28-C29-C30-C31
14	A	1011	CLA	C4B-C3B-CAB-CBB
14	A	1110	CLA	C4B-C3B-CAB-CBB
14	A	1112	CLA	C4B-C3B-CAB-CBB
14	B	1208	CLA	C4B-C3B-CAB-CBB
14	B	1219	CLA	C4B-C3B-CAB-CBB
14	B	1240	CLA	C4B-C3B-CAB-CBB
14	J	1303	CLA	C4B-C3B-CAB-CBB
14	K	1401	CLA	C4B-C3B-CAB-CBB
14	L	1502	CLA	C4B-C3B-CAB-CBB
14	1	501	CLA	C4B-C3B-CAB-CBB
14	1	507	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	1	509	CLA	C4B-C3B-CAB-CBB
14	1	513	CLA	C4B-C3B-CAB-CBB
14	2	517	CLA	C4B-C3B-CAB-CBB
14	3	507	CLA	C4B-C3B-CAB-CBB
14	3	508	CLA	C4B-C3B-CAB-CBB
14	3	510	CLA	C4B-C3B-CAB-CBB
14	3	516	CLA	C4B-C3B-CAB-CBB
14	4	506	CLA	C4B-C3B-CAB-CBB
14	4	507	CLA	C4B-C3B-CAB-CBB
14	4	513	CLA	C4B-C3B-CAB-CBB
14	4	516	CLA	C4B-C3B-CAB-CBB
14	4	517	CLA	C4B-C3B-CAB-CBB
14	4	519	CLA	C4B-C3B-CAB-CBB
14	5	501	CLA	C4B-C3B-CAB-CBB
14	5	507	CLA	C4B-C3B-CAB-CBB
14	5	510	CLA	C4B-C3B-CAB-CBB
14	6	510	CLA	C4B-C3B-CAB-CBB
14	6	511	CLA	C4B-C3B-CAB-CBB
14	6	517	CLA	C4B-C3B-CAB-CBB
14	G	1011	CLA	C4B-C3B-CAB-CBB
14	G	1110	CLA	C4B-C3B-CAB-CBB
14	G	1112	CLA	C4B-C3B-CAB-CBB
14	H	1208	CLA	C4B-C3B-CAB-CBB
14	H	1219	CLA	C4B-C3B-CAB-CBB
14	H	1240	CLA	C4B-C3B-CAB-CBB
14	T	1303	CLA	C4B-C3B-CAB-CBB
14	U	1401	CLA	C4B-C3B-CAB-CBB
14	V	1502	CLA	C4B-C3B-CAB-CBB
14	Y	501	CLA	C4B-C3B-CAB-CBB
14	Y	507	CLA	C4B-C3B-CAB-CBB
14	Y	509	CLA	C4B-C3B-CAB-CBB
14	Y	513	CLA	C4B-C3B-CAB-CBB
14	Z	517	CLA	C4B-C3B-CAB-CBB
14	a	507	CLA	C4B-C3B-CAB-CBB
14	a	508	CLA	C4B-C3B-CAB-CBB
14	a	510	CLA	C4B-C3B-CAB-CBB
14	a	516	CLA	C4B-C3B-CAB-CBB
14	b	506	CLA	C4B-C3B-CAB-CBB
14	b	507	CLA	C4B-C3B-CAB-CBB
14	b	513	CLA	C4B-C3B-CAB-CBB
14	b	516	CLA	C4B-C3B-CAB-CBB
14	b	517	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	519	CLA	C4B-C3B-CAB-CBB
14	c	501	CLA	C4B-C3B-CAB-CBB
14	c	507	CLA	C4B-C3B-CAB-CBB
14	c	510	CLA	C4B-C3B-CAB-CBB
14	d	510	CLA	C4B-C3B-CAB-CBB
14	d	511	CLA	C4B-C3B-CAB-CBB
14	d	517	CLA	C4B-C3B-CAB-CBB
14	e	1011	CLA	C4B-C3B-CAB-CBB
14	e	1110	CLA	C4B-C3B-CAB-CBB
14	e	1112	CLA	C4B-C3B-CAB-CBB
14	e	1115	CLA	C4B-C3B-CAB-CBB
14	f	1208	CLA	C4B-C3B-CAB-CBB
14	f	1219	CLA	C4B-C3B-CAB-CBB
14	f	1240	CLA	C4B-C3B-CAB-CBB
14	l	1303	CLA	C4B-C3B-CAB-CBB
14	m	1401	CLA	C4B-C3B-CAB-CBB
14	n	1502	CLA	C4B-C3B-CAB-CBB
14	q	501	CLA	C4B-C3B-CAB-CBB
14	q	507	CLA	C4B-C3B-CAB-CBB
14	q	509	CLA	C4B-C3B-CAB-CBB
14	q	513	CLA	C4B-C3B-CAB-CBB
14	r	517	CLA	C4B-C3B-CAB-CBB
14	s	507	CLA	C4B-C3B-CAB-CBB
14	s	508	CLA	C4B-C3B-CAB-CBB
14	s	510	CLA	C4B-C3B-CAB-CBB
14	s	516	CLA	C4B-C3B-CAB-CBB
14	t	506	CLA	C4B-C3B-CAB-CBB
14	t	507	CLA	C4B-C3B-CAB-CBB
14	t	513	CLA	C4B-C3B-CAB-CBB
14	t	516	CLA	C4B-C3B-CAB-CBB
14	t	517	CLA	C4B-C3B-CAB-CBB
14	t	519	CLA	C4B-C3B-CAB-CBB
14	u	501	CLA	C4B-C3B-CAB-CBB
14	u	507	CLA	C4B-C3B-CAB-CBB
14	u	510	CLA	C4B-C3B-CAB-CBB
14	v	510	CLA	C4B-C3B-CAB-CBB
14	v	511	CLA	C4B-C3B-CAB-CBB
14	v	517	CLA	C4B-C3B-CAB-CBB
18	A	5005	LHG	O6-C4-C5-C6
18	G	5005	LHG	O6-C4-C5-C6
18	e	5005	LHG	O6-C4-C5-C6
18	L	5220	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	l	5105	LMU	C3-C4-C5-C6
18	G	5004	LHG	C11-C10-C9-C8
18	V	5220	LHG	C28-C29-C30-C31
18	n	5220	LHG	C28-C29-C30-C31
19	J	5105	LMU	C3-C4-C5-C6
19	T	5105	LMU	C3-C4-C5-C6
14	A	1125	CLA	CBA-CGA-O2A-C1
14	G	1125	CLA	CBA-CGA-O2A-C1
14	e	1125	CLA	CBA-CGA-O2A-C1
18	A	5004	LHG	C11-C10-C9-C8
18	e	5004	LHG	C11-C10-C9-C8
18	A	5009	LHG	O2-C2-C3-O3
18	G	5009	LHG	O2-C2-C3-O3
18	e	5009	LHG	O2-C2-C3-O3
14	A	1134	CLA	C11-C10-C8-C9
14	B	1213	CLA	C14-C13-C15-C16
14	G	1134	CLA	C11-C10-C8-C9
14	H	1213	CLA	C14-C13-C15-C16
14	e	1134	CLA	C11-C10-C8-C9
14	f	1213	CLA	C14-C13-C15-C16
20	H	5002	LMG	C23-C24-C25-C26
21	L	5216	SQD	C14-C15-C16-C17
21	n	5216	SQD	C14-C15-C16-C17
18	A	5003	LHG	C25-C26-C27-C28
18	G	5003	LHG	C25-C26-C27-C28
18	e	5003	LHG	C25-C26-C27-C28
21	V	5216	SQD	C14-C15-C16-C17
14	q	519	CLA	O1D-CGD-O2D-CED
18	A	5006	LHG	C8-C7-O7-C5
18	G	5006	LHG	C8-C7-O7-C5
18	e	5006	LHG	C8-C7-O7-C5
18	G	5001	LHG	C31-C32-C33-C34
18	V	5221	LHG	C13-C14-C15-C16
18	e	5001	LHG	C31-C32-C33-C34
20	B	5002	LMG	C23-C24-C25-C26
20	f	5002	LMG	C23-C24-C25-C26
21	L	5216	SQD	C25-C26-C27-C28
21	V	5216	SQD	C25-C26-C27-C28
18	L	5221	LHG	C5-C4-O6-P
18	V	5221	LHG	C5-C4-O6-P
18	n	5221	LHG	C5-C4-O6-P
14	1	519	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Y	519	CLA	O1D-CGD-O2D-CED
14	B	1227	CLA	C3A-C2A-CAA-CBA
14	B	1240	CLA	C3A-C2A-CAA-CBA
14	K	1401	CLA	C3A-C2A-CAA-CBA
14	6	517	CLA	C3A-C2A-CAA-CBA
14	H	1227	CLA	C3A-C2A-CAA-CBA
14	H	1240	CLA	C3A-C2A-CAA-CBA
14	U	1401	CLA	C3A-C2A-CAA-CBA
14	d	517	CLA	C3A-C2A-CAA-CBA
14	f	1227	CLA	C3A-C2A-CAA-CBA
14	f	1240	CLA	C3A-C2A-CAA-CBA
14	m	1401	CLA	C3A-C2A-CAA-CBA
14	v	517	CLA	C3A-C2A-CAA-CBA
18	A	5005	LHG	C29-C30-C31-C32
18	A	5001	LHG	C31-C32-C33-C34
18	L	5221	LHG	C13-C14-C15-C16
18	G	5005	LHG	C29-C30-C31-C32
18	e	5005	LHG	C29-C30-C31-C32
18	n	5221	LHG	C13-C14-C15-C16
21	n	5216	SQD	C25-C26-C27-C28
14	A	1108	CLA	C6-C7-C8-C9
14	G	1108	CLA	C6-C7-C8-C9
14	e	1108	CLA	C6-C7-C8-C9
18	G	5007	LHG	C34-C35-C36-C37
18	e	5007	LHG	C34-C35-C36-C37
18	A	5007	LHG	C34-C35-C36-C37
18	A	5006	LHG	C12-C13-C14-C15
18	G	5006	LHG	C12-C13-C14-C15
18	e	5006	LHG	C12-C13-C14-C15
14	A	1139	CLA	C10-C11-C12-C13
14	B	1206	CLA	C13-C15-C16-C17
14	G	1139	CLA	C10-C11-C12-C13
14	H	1206	CLA	C13-C15-C16-C17
14	e	1139	CLA	C10-C11-C12-C13
14	f	1206	CLA	C13-C15-C16-C17
18	A	5005	LHG	C4-C5-C6-O8
18	A	5006	LHG	C4-C5-C6-O8
18	A	5007	LHG	C4-C5-C6-O8
18	L	5220	LHG	C4-C5-C6-O8
18	G	5005	LHG	C4-C5-C6-O8
18	G	5006	LHG	C4-C5-C6-O8
18	G	5007	LHG	C4-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5220	LHG	C4-C5-C6-O8
18	e	5005	LHG	C4-C5-C6-O8
18	e	5006	LHG	C4-C5-C6-O8
18	e	5007	LHG	C4-C5-C6-O8
18	n	5220	LHG	C4-C5-C6-O8
21	L	5216	SQD	C44-C45-C46-O48
21	1	822	SQD	C44-C45-C46-O48
21	V	5216	SQD	C44-C45-C46-O48
21	Y	822	SQD	C44-C45-C46-O48
21	n	5216	SQD	C44-C45-C46-O48
21	q	822	SQD	C44-C45-C46-O48
18	G	5009	LHG	C32-C33-C34-C35
20	f	5002	LMG	C34-C35-C36-C37
14	H	1209	CLA	C5-C6-C7-C8
14	f	1209	CLA	C5-C6-C7-C8
18	A	5009	LHG	C32-C33-C34-C35
18	G	5004	LHG	C25-C26-C27-C28
18	e	5004	LHG	C25-C26-C27-C28
18	e	5009	LHG	C32-C33-C34-C35
20	B	5002	LMG	C34-C35-C36-C37
20	H	5002	LMG	C34-C35-C36-C37
14	B	1209	CLA	C5-C6-C7-C8
18	A	5004	LHG	C25-C26-C27-C28
18	G	5007	LHG	C15-C16-C17-C18
18	e	5007	LHG	C15-C16-C17-C18
18	A	5007	LHG	C15-C16-C17-C18
14	A	1110	CLA	O1D-CGD-O2D-CED
18	L	5220	LHG	C11-C10-C9-C8
18	V	5220	LHG	C11-C10-C9-C8
18	n	5220	LHG	C11-C10-C9-C8
14	G	1110	CLA	O1D-CGD-O2D-CED
14	e	1110	CLA	O1D-CGD-O2D-CED
18	A	5006	LHG	C3-O3-P-O6
18	G	5006	LHG	C3-O3-P-O6
18	e	5006	LHG	C3-O3-P-O6
14	B	1201	CLA	O1A-CGA-O2A-C1
14	H	1201	CLA	O1A-CGA-O2A-C1
14	f	1201	CLA	O1A-CGA-O2A-C1
18	L	5221	LHG	C17-C18-C19-C20
14	A	1104	CLA	C3-C5-C6-C7
14	B	1012	CLA	C3-C5-C6-C7
14	B	1227	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1104	CLA	C3-C5-C6-C7
14	H	1012	CLA	C3-C5-C6-C7
14	H	1227	CLA	C3-C5-C6-C7
14	e	1104	CLA	C3-C5-C6-C7
14	f	1227	CLA	C3-C5-C6-C7
14	A	1111	CLA	C2A-CAA-CBA-CGA
14	G	1111	CLA	C2A-CAA-CBA-CGA
18	A	5007	LHG	O1-C1-C2-O2
18	A	5008	LHG	O1-C1-C2-O2
18	G	5007	LHG	O1-C1-C2-O2
18	G	5008	LHG	O1-C1-C2-O2
18	e	5007	LHG	O1-C1-C2-O2
18	e	5008	LHG	O1-C1-C2-O2
18	V	5221	LHG	C17-C18-C19-C20
18	n	5221	LHG	C17-C18-C19-C20
21	L	5216	SQD	C9-C10-C11-C12
21	V	5216	SQD	C9-C10-C11-C12
14	H	1221	CLA	C13-C15-C16-C17
18	B	1855	LHG	O6-C4-C5-O7
18	H	1855	LHG	O6-C4-C5-O7
18	f	1855	LHG	O6-C4-C5-O7
14	B	1021	CLA	CBA-CGA-O2A-C1
14	H	1021	CLA	CBA-CGA-O2A-C1
14	f	1021	CLA	CBA-CGA-O2A-C1
21	n	5216	SQD	C9-C10-C11-C12
18	I	5001	LHG	C7-C8-C9-C10
18	S	5001	LHG	C7-C8-C9-C10
18	k	5001	LHG	C7-C8-C9-C10
14	B	1226	CLA	C6-C7-C8-C9
14	H	1226	CLA	C6-C7-C8-C9
14	f	1226	CLA	C6-C7-C8-C9
18	f	1855	LHG	C24-C25-C26-C27
14	A	1112	CLA	C2B-C3B-CAB-CBB
14	A	1129	CLA	C2B-C3B-CAB-CBB
14	B	1021	CLA	C2B-C3B-CAB-CBB
14	1	501	CLA	C2B-C3B-CAB-CBB
14	1	509	CLA	C2B-C3B-CAB-CBB
14	2	517	CLA	C2B-C3B-CAB-CBB
14	4	507	CLA	C2B-C3B-CAB-CBB
14	4	516	CLA	C2B-C3B-CAB-CBB
14	4	517	CLA	C2B-C3B-CAB-CBB
14	5	501	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	5	504	CLA	C2B-C3B-CAB-CBB
14	5	507	CLA	C2B-C3B-CAB-CBB
14	5	510	CLA	C2B-C3B-CAB-CBB
14	6	507	CLA	C2B-C3B-CAB-CBB
14	6	510	CLA	C2B-C3B-CAB-CBB
14	6	516	CLA	C2B-C3B-CAB-CBB
14	6	517	CLA	C2B-C3B-CAB-CBB
14	G	1112	CLA	C2B-C3B-CAB-CBB
14	G	1129	CLA	C2B-C3B-CAB-CBB
14	H	1021	CLA	C2B-C3B-CAB-CBB
14	Y	501	CLA	C2B-C3B-CAB-CBB
14	Y	509	CLA	C2B-C3B-CAB-CBB
14	Z	517	CLA	C2B-C3B-CAB-CBB
14	b	507	CLA	C2B-C3B-CAB-CBB
14	b	516	CLA	C2B-C3B-CAB-CBB
14	b	517	CLA	C2B-C3B-CAB-CBB
14	c	501	CLA	C2B-C3B-CAB-CBB
14	c	504	CLA	C2B-C3B-CAB-CBB
14	c	507	CLA	C2B-C3B-CAB-CBB
14	c	510	CLA	C2B-C3B-CAB-CBB
14	d	507	CLA	C2B-C3B-CAB-CBB
14	d	510	CLA	C2B-C3B-CAB-CBB
14	d	516	CLA	C2B-C3B-CAB-CBB
14	e	1112	CLA	C2B-C3B-CAB-CBB
14	e	1129	CLA	C2B-C3B-CAB-CBB
14	f	1021	CLA	C2B-C3B-CAB-CBB
14	q	501	CLA	C2B-C3B-CAB-CBB
14	q	509	CLA	C2B-C3B-CAB-CBB
14	r	517	CLA	C2B-C3B-CAB-CBB
14	t	507	CLA	C2B-C3B-CAB-CBB
14	t	516	CLA	C2B-C3B-CAB-CBB
14	t	517	CLA	C2B-C3B-CAB-CBB
14	u	501	CLA	C2B-C3B-CAB-CBB
14	u	504	CLA	C2B-C3B-CAB-CBB
14	u	507	CLA	C2B-C3B-CAB-CBB
14	u	510	CLA	C2B-C3B-CAB-CBB
14	v	507	CLA	C2B-C3B-CAB-CBB
14	v	510	CLA	C2B-C3B-CAB-CBB
14	v	516	CLA	C2B-C3B-CAB-CBB
14	v	517	CLA	C2B-C3B-CAB-CBB
18	A	5002	LHG	C29-C30-C31-C32
18	B	1855	LHG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	5002	LHG	C29-C30-C31-C32
14	A	1125	CLA	O1A-CGA-O2A-C1
14	G	1125	CLA	O1A-CGA-O2A-C1
14	e	1125	CLA	O1A-CGA-O2A-C1
18	H	1855	LHG	C24-C25-C26-C27
18	e	5002	LHG	C29-C30-C31-C32
14	f	1012	CLA	C3-C5-C6-C7
18	A	5006	LHG	O7-C5-C6-O8
18	B	1842	LHG	O7-C5-C6-O8
18	G	5006	LHG	O7-C5-C6-O8
18	H	1842	LHG	O7-C5-C6-O8
18	e	5006	LHG	O7-C5-C6-O8
18	f	1842	LHG	O7-C5-C6-O8
21	1	822	SQD	O6-C44-C45-O47
21	Y	822	SQD	O6-C44-C45-O47
21	f	1852	SQD	O6-C44-C45-O47
21	q	822	SQD	O6-C44-C45-O47
14	G	1122	CLA	C10-C11-C12-C13
14	G	1132	CLA	C13-C15-C16-C17
14	B	1226	CLA	O1D-CGD-O2D-CED
14	f	1226	CLA	O1D-CGD-O2D-CED
14	B	1221	CLA	C13-C15-C16-C17
14	f	1221	CLA	C13-C15-C16-C17
14	L	1502	CLA	C16-C17-C18-C20
14	V	1502	CLA	C16-C17-C18-C20
14	n	1502	CLA	C16-C17-C18-C20
15	A	2001	PQN	C26-C27-C28-C30
15	G	2001	PQN	C26-C27-C28-C30
15	e	2001	PQN	C26-C27-C28-C30
14	A	1122	CLA	C10-C11-C12-C13
14	A	1128	CLA	C5-C6-C7-C8
14	A	1132	CLA	C13-C15-C16-C17
14	A	1237	CLA	C10-C11-C12-C13
14	G	1128	CLA	C5-C6-C7-C8
14	G	1237	CLA	C10-C11-C12-C13
14	e	1122	CLA	C10-C11-C12-C13
14	e	1128	CLA	C5-C6-C7-C8
14	e	1132	CLA	C13-C15-C16-C17
18	A	5004	LHG	C1-C2-C3-O3
18	G	5004	LHG	C1-C2-C3-O3
18	e	5004	LHG	C1-C2-C3-O3
14	B	1223	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	L	1501	CLA	C2-C1-O2A-CGA
14	H	1223	CLA	C2-C1-O2A-CGA
14	V	1501	CLA	C2-C1-O2A-CGA
14	f	1223	CLA	C2-C1-O2A-CGA
14	n	1501	CLA	C2-C1-O2A-CGA
18	B	1855	LHG	C14-C15-C16-C17
18	H	1855	LHG	C14-C15-C16-C17
18	V	5220	LHG	C30-C31-C32-C33
14	e	1237	CLA	C10-C11-C12-C13
14	A	1117	CLA	C11-C12-C13-C14
14	A	1140	CLA	C6-C7-C8-C9
14	A	1237	CLA	C6-C7-C8-C9
14	A	1130	CLA	C6-C7-C8-C9
14	A	1101	CLA	C11-C12-C13-C14
14	B	1203	CLA	C11-C12-C13-C14
14	B	1205	CLA	C14-C13-C15-C16
14	B	1215	CLA	C11-C10-C8-C9
14	B	1217	CLA	C11-C10-C8-C9
14	B	1219	CLA	C14-C13-C15-C16
14	L	1501	CLA	C11-C10-C8-C9
14	G	1117	CLA	C11-C12-C13-C14
14	G	1140	CLA	C6-C7-C8-C9
14	G	1237	CLA	C6-C7-C8-C9
14	G	1130	CLA	C6-C7-C8-C9
14	G	1101	CLA	C11-C12-C13-C14
14	H	1203	CLA	C11-C12-C13-C14
14	H	1205	CLA	C14-C13-C15-C16
14	H	1215	CLA	C11-C10-C8-C9
14	H	1217	CLA	C11-C10-C8-C9
14	H	1219	CLA	C14-C13-C15-C16
14	V	1501	CLA	C11-C10-C8-C9
14	e	1117	CLA	C11-C12-C13-C14
14	e	1140	CLA	C6-C7-C8-C9
14	e	1237	CLA	C6-C7-C8-C9
14	e	1130	CLA	C6-C7-C8-C9
14	e	1101	CLA	C11-C12-C13-C14
14	f	1203	CLA	C11-C12-C13-C14
14	f	1205	CLA	C14-C13-C15-C16
14	f	1215	CLA	C11-C10-C8-C9
14	f	1217	CLA	C11-C10-C8-C9
14	n	1501	CLA	C11-C10-C8-C9
18	L	5220	LHG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	f	1855	LHG	C14-C15-C16-C17
18	n	5220	LHG	C30-C31-C32-C33
18	A	5004	LHG	C2-C3-O3-P
18	A	5005	LHG	C2-C3-O3-P
18	L	5218	LHG	C2-C3-O3-P
18	L	5221	LHG	C2-C3-O3-P
18	G	5004	LHG	C2-C3-O3-P
18	G	5005	LHG	C2-C3-O3-P
18	V	5218	LHG	C2-C3-O3-P
18	V	5221	LHG	C2-C3-O3-P
18	e	5004	LHG	C2-C3-O3-P
18	e	5005	LHG	C2-C3-O3-P
18	n	5218	LHG	C2-C3-O3-P
18	n	5221	LHG	C2-C3-O3-P
20	J	5104	LMG	C32-C33-C34-C35
20	T	5104	LMG	C32-C33-C34-C35
20	l	5104	LMG	C32-C33-C34-C35
14	A	1106	CLA	C2A-CAA-CBA-CGA
14	A	1115	CLA	C2A-CAA-CBA-CGA
14	G	1106	CLA	C2A-CAA-CBA-CGA
14	G	1115	CLA	C2A-CAA-CBA-CGA
14	e	1106	CLA	C2A-CAA-CBA-CGA
14	e	1115	CLA	C2A-CAA-CBA-CGA
14	H	1226	CLA	O1D-CGD-O2D-CED
14	A	1103	CLA	C16-C17-C18-C19
14	B	1210	CLA	C16-C17-C18-C20
14	B	1211	CLA	C6-C7-C8-C10
14	B	1215	CLA	C16-C17-C18-C19
14	G	1103	CLA	C16-C17-C18-C19
14	H	1210	CLA	C16-C17-C18-C20
14	H	1211	CLA	C6-C7-C8-C10
14	H	1215	CLA	C16-C17-C18-C19
14	e	1103	CLA	C16-C17-C18-C19
14	f	1210	CLA	C16-C17-C18-C20
14	f	1211	CLA	C6-C7-C8-C10
14	f	1215	CLA	C16-C17-C18-C19
14	A	1237	CLA	C3-C5-C6-C7
14	G	1237	CLA	C3-C5-C6-C7
14	e	1237	CLA	C3-C5-C6-C7
17	3	521	BCR	C23-C24-C25-C26
17	3	521	BCR	C23-C24-C25-C30
17	3	522	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	5	521	BCR	C5-C6-C7-C8
17	6	524	BCR	C5-C6-C7-C8
17	a	521	BCR	C23-C24-C25-C26
17	a	521	BCR	C23-C24-C25-C30
17	a	522	BCR	C5-C6-C7-C8
17	c	521	BCR	C5-C6-C7-C8
17	d	524	BCR	C5-C6-C7-C8
17	s	521	BCR	C23-C24-C25-C26
17	s	521	BCR	C23-C24-C25-C30
17	s	522	BCR	C5-C6-C7-C8
17	u	521	BCR	C5-C6-C7-C8
17	v	524	BCR	C5-C6-C7-C8
18	A	5005	LHG	C33-C34-C35-C36
18	e	5005	LHG	C33-C34-C35-C36
14	j	1302	CLA	O1D-CGD-O2D-CED
17	B	4010	BCR	C37-C22-C23-C24
17	J	4015	BCR	C7-C8-C9-C34
17	T	4015	BCR	C7-C8-C9-C34
17	f	4010	BCR	C37-C22-C23-C24
17	l	4015	BCR	C7-C8-C9-C34
18	A	5004	LHG	C30-C31-C32-C33
18	L	5221	LHG	C18-C19-C20-C21
18	G	5004	LHG	C30-C31-C32-C33
18	G	5005	LHG	C33-C34-C35-C36
18	V	5221	LHG	C18-C19-C20-C21
18	e	5004	LHG	C30-C31-C32-C33
14	F	1302	CLA	O1D-CGD-O2D-CED
14	R	1302	CLA	O1D-CGD-O2D-CED
17	A	4001	BCR	C7-C8-C9-C10
17	A	4011	BCR	C17-C18-C19-C20
17	M	4021	BCR	C11-C12-C13-C14
17	3	524	BCR	C7-C8-C9-C10
17	4	524	BCR	C7-C8-C9-C10
17	6	522	BCR	C7-C8-C9-C10
17	G	4001	BCR	C7-C8-C9-C10
17	G	4011	BCR	C17-C18-C19-C20
17	W	4021	BCR	C11-C12-C13-C14
17	a	524	BCR	C7-C8-C9-C10
17	a	524	BCR	C21-C22-C23-C24
17	b	524	BCR	C7-C8-C9-C10
17	d	522	BCR	C7-C8-C9-C10
17	e	4001	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	4011	BCR	C17-C18-C19-C20
17	o	4021	BCR	C11-C12-C13-C14
17	s	524	BCR	C7-C8-C9-C10
17	s	524	BCR	C21-C22-C23-C24
17	t	524	BCR	C7-C8-C9-C10
17	v	522	BCR	C7-C8-C9-C10
18	n	5221	LHG	C18-C19-C20-C21
18	A	5002	LHG	C13-C14-C15-C16
18	G	5002	LHG	C13-C14-C15-C16
18	e	5002	LHG	C13-C14-C15-C16
14	A	1111	CLA	C16-C17-C18-C19
14	G	1111	CLA	C16-C17-C18-C19
14	e	1111	CLA	C16-C17-C18-C19
18	f	1842	LHG	C26-C27-C28-C29
18	B	1842	LHG	C26-C27-C28-C29
18	H	1842	LHG	C26-C27-C28-C29
14	A	1013	CLA	C11-C12-C13-C15
14	A	1104	CLA	C12-C13-C15-C16
14	A	1107	CLA	C11-C12-C13-C15
14	A	1109	CLA	C12-C13-C15-C16
14	A	1111	CLA	C11-C12-C13-C15
14	A	1124	CLA	C11-C10-C8-C7
14	A	1128	CLA	C6-C7-C8-C10
14	A	1131	CLA	C12-C13-C15-C16
14	A	1132	CLA	C12-C13-C15-C16
14	A	1136	CLA	C11-C12-C13-C15
14	A	1138	CLA	C12-C13-C15-C16
14	A	1139	CLA	C6-C7-C8-C10
14	B	1012	CLA	C12-C13-C15-C16
14	B	1203	CLA	C6-C7-C8-C10
14	B	1206	CLA	C6-C7-C8-C10
14	B	1215	CLA	C11-C10-C8-C7
14	B	1217	CLA	C11-C10-C8-C7
14	B	1219	CLA	C11-C10-C8-C7
14	B	1219	CLA	C11-C12-C13-C15
14	B	1219	CLA	C12-C13-C15-C16
14	B	1234	CLA	C11-C10-C8-C7
14	B	1239	CLA	C12-C13-C15-C16
14	B	1240	CLA	C11-C12-C13-C15
14	5	509	CLA	C11-C12-C13-C15
14	6	505	CLA	C6-C7-C8-C10
14	G	1013	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1104	CLA	C12-C13-C15-C16
14	G	1107	CLA	C11-C12-C13-C15
14	G	1109	CLA	C12-C13-C15-C16
14	G	1111	CLA	C11-C12-C13-C15
14	G	1124	CLA	C11-C10-C8-C7
14	G	1128	CLA	C6-C7-C8-C10
14	G	1131	CLA	C12-C13-C15-C16
14	G	1132	CLA	C12-C13-C15-C16
14	G	1136	CLA	C11-C12-C13-C15
14	G	1138	CLA	C12-C13-C15-C16
14	G	1139	CLA	C6-C7-C8-C10
14	H	1012	CLA	C12-C13-C15-C16
14	H	1203	CLA	C6-C7-C8-C10
14	H	1206	CLA	C6-C7-C8-C10
14	H	1215	CLA	C11-C10-C8-C7
14	H	1217	CLA	C11-C10-C8-C7
14	H	1219	CLA	C11-C10-C8-C7
14	H	1219	CLA	C11-C12-C13-C15
14	H	1219	CLA	C12-C13-C15-C16
14	H	1234	CLA	C11-C10-C8-C7
14	H	1239	CLA	C12-C13-C15-C16
14	H	1240	CLA	C11-C12-C13-C15
14	c	509	CLA	C11-C12-C13-C15
14	d	505	CLA	C6-C7-C8-C10
14	e	1013	CLA	C11-C12-C13-C15
14	e	1104	CLA	C12-C13-C15-C16
14	e	1107	CLA	C11-C12-C13-C15
14	e	1109	CLA	C12-C13-C15-C16
14	e	1111	CLA	C11-C12-C13-C15
14	e	1124	CLA	C11-C10-C8-C7
14	e	1128	CLA	C6-C7-C8-C10
14	e	1131	CLA	C12-C13-C15-C16
14	e	1132	CLA	C12-C13-C15-C16
14	e	1136	CLA	C11-C12-C13-C15
14	e	1138	CLA	C12-C13-C15-C16
14	e	1139	CLA	C6-C7-C8-C10
14	f	1012	CLA	C12-C13-C15-C16
14	f	1203	CLA	C6-C7-C8-C10
14	f	1206	CLA	C6-C7-C8-C10
14	f	1215	CLA	C11-C10-C8-C7
14	f	1217	CLA	C11-C10-C8-C7
14	f	1219	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1219	CLA	C11-C12-C13-C15
14	f	1219	CLA	C12-C13-C15-C16
14	f	1234	CLA	C11-C10-C8-C7
14	f	1239	CLA	C12-C13-C15-C16
14	f	1240	CLA	C11-C12-C13-C15
14	u	509	CLA	C11-C12-C13-C15
14	v	505	CLA	C6-C7-C8-C10
14	G	1103	CLA	C3-C5-C6-C7
18	A	5002	LHG	C12-C13-C14-C15
18	A	5007	LHG	C10-C11-C12-C13
18	G	5002	LHG	C12-C13-C14-C15
18	G	5007	LHG	C10-C11-C12-C13
18	e	5002	LHG	C12-C13-C14-C15
18	e	5007	LHG	C10-C11-C12-C13
17	5	522	BCR	C9-C10-C11-C12
17	c	522	BCR	C9-C10-C11-C12
17	u	522	BCR	C9-C10-C11-C12
14	B	1208	CLA	CBA-CGA-O2A-C1
14	H	1208	CLA	CBA-CGA-O2A-C1
14	f	1208	CLA	CBA-CGA-O2A-C1
18	B	1855	LHG	C24-C23-O8-C6
18	H	1855	LHG	C24-C23-O8-C6
18	f	1855	LHG	C24-C23-O8-C6
14	G	1121	CLA	CAA-CBA-CGA-O2A
14	e	1121	CLA	CAA-CBA-CGA-O2A
14	2	518	CLA	O1A-CGA-O2A-C1
14	Z	518	CLA	O1A-CGA-O2A-C1
14	r	518	CLA	O1A-CGA-O2A-C1
14	1	503	CLA	C2A-CAA-CBA-CGA
14	Y	503	CLA	C2A-CAA-CBA-CGA
14	q	503	CLA	C2A-CAA-CBA-CGA
18	A	5008	LHG	C11-C12-C13-C14
18	G	5008	LHG	C11-C12-C13-C14
18	e	5008	LHG	C11-C12-C13-C14
18	e	5003	LHG	C23-C24-C25-C26
14	A	1103	CLA	C3-C5-C6-C7
14	e	1103	CLA	C3-C5-C6-C7
14	e	1140	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	C16-C17-C18-C19
14	G	1133	CLA	C16-C17-C18-C19
14	e	1133	CLA	C16-C17-C18-C19
14	A	1121	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	e	5003	LHG	C13-C14-C15-C16
18	A	5003	LHG	C23-C24-C25-C26
18	G	5003	LHG	C23-C24-C25-C26
18	A	5003	LHG	C13-C14-C15-C16
18	G	5003	LHG	C13-C14-C15-C16
14	A	1101	CLA	C5-C6-C7-C8
14	A	1140	CLA	CBD-CGD-O2D-CED
14	G	1140	CLA	CBD-CGD-O2D-CED
14	H	1212	CLA	CBD-CGD-O2D-CED
14	A	1103	CLA	CAD-CBD-CGD-O2D
14	A	1105	CLA	CAD-CBD-CGD-O2D
14	A	1107	CLA	CAD-CBD-CGD-O2D
14	A	1118	CLA	CAD-CBD-CGD-O2D
14	A	1124	CLA	CAD-CBD-CGD-O2D
14	B	1202	CLA	CAD-CBD-CGD-O2D
14	B	1208	CLA	CAD-CBD-CGD-O2D
14	B	1216	CLA	CAD-CBD-CGD-O2D
14	B	1218	CLA	CAD-CBD-CGD-O2D
14	B	1238	CLA	CAD-CBD-CGD-O2D
14	J	1303	CLA	CAD-CBD-CGD-O2D
14	1	502	CLA	CAD-CBD-CGD-O2D
14	1	512	CLA	CAD-CBD-CGD-O2D
14	1	513	CLA	CAD-CBD-CGD-O2D
14	1	516	CLA	CAD-CBD-CGD-O2D
14	2	505	CLA	CAD-CBD-CGD-O2D
14	2	511	CLA	CAD-CBD-CGD-O2D
14	3	508	CLA	CAD-CBD-CGD-O2D
14	4	518	CLA	CAD-CBD-CGD-O2D
14	5	517	CLA	CAD-CBD-CGD-O2D
14	6	506	CLA	CAD-CBD-CGD-O2D
14	6	517	CLA	CAD-CBD-CGD-O2D
14	G	1103	CLA	CAD-CBD-CGD-O2D
14	G	1105	CLA	CAD-CBD-CGD-O2D
14	G	1107	CLA	CAD-CBD-CGD-O2D
14	G	1118	CLA	CAD-CBD-CGD-O2D
14	G	1124	CLA	CAD-CBD-CGD-O2D
14	H	1202	CLA	CAD-CBD-CGD-O2D
14	H	1208	CLA	CAD-CBD-CGD-O2D
14	H	1216	CLA	CAD-CBD-CGD-O2D
14	H	1218	CLA	CAD-CBD-CGD-O2D
14	H	1238	CLA	CAD-CBD-CGD-O2D
14	T	1303	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Y	502	CLA	CAD-CBD-CGD-O2D
14	Y	512	CLA	CAD-CBD-CGD-O2D
14	Y	513	CLA	CAD-CBD-CGD-O2D
14	Y	516	CLA	CAD-CBD-CGD-O2D
14	Z	505	CLA	CAD-CBD-CGD-O2D
14	Z	511	CLA	CAD-CBD-CGD-O2D
14	a	508	CLA	CAD-CBD-CGD-O2D
14	b	518	CLA	CAD-CBD-CGD-O2D
14	c	517	CLA	CAD-CBD-CGD-O2D
14	d	506	CLA	CAD-CBD-CGD-O2D
14	d	517	CLA	CAD-CBD-CGD-O2D
14	e	1103	CLA	CAD-CBD-CGD-O2D
14	e	1105	CLA	CAD-CBD-CGD-O2D
14	e	1107	CLA	CAD-CBD-CGD-O2D
14	e	1118	CLA	CAD-CBD-CGD-O2D
14	e	1124	CLA	CAD-CBD-CGD-O2D
14	f	1202	CLA	CAD-CBD-CGD-O2D
14	f	1208	CLA	CAD-CBD-CGD-O2D
14	f	1216	CLA	CAD-CBD-CGD-O2D
14	f	1218	CLA	CAD-CBD-CGD-O2D
14	f	1238	CLA	CAD-CBD-CGD-O2D
14	l	1303	CLA	CAD-CBD-CGD-O2D
14	q	502	CLA	CAD-CBD-CGD-O2D
14	q	512	CLA	CAD-CBD-CGD-O2D
14	q	513	CLA	CAD-CBD-CGD-O2D
14	q	516	CLA	CAD-CBD-CGD-O2D
14	r	505	CLA	CAD-CBD-CGD-O2D
14	r	511	CLA	CAD-CBD-CGD-O2D
14	s	508	CLA	CAD-CBD-CGD-O2D
14	t	518	CLA	CAD-CBD-CGD-O2D
14	u	517	CLA	CAD-CBD-CGD-O2D
14	v	506	CLA	CAD-CBD-CGD-O2D
14	v	517	CLA	CAD-CBD-CGD-O2D
18	B	1855	LHG	C6-C5-O7-C7
18	H	1855	LHG	C6-C5-O7-C7
18	f	1855	LHG	C6-C5-O7-C7
14	G	1101	CLA	C5-C6-C7-C8
14	e	1101	CLA	C5-C6-C7-C8
14	f	1227	CLA	O1D-CGD-O2D-CED
14	B	1212	CLA	CBD-CGD-O2D-CED
14	B	1220	CLA	CBA-CGA-O2A-C1
14	H	1220	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1220	CLA	CBA-CGA-O2A-C1
14	B	1227	CLA	O1D-CGD-O2D-CED
14	B	1219	CLA	C4-C3-C5-C6
14	H	1219	CLA	C4-C3-C5-C6
14	f	1219	CLA	C4-C3-C5-C6
14	A	1013	CLA	C16-C17-C18-C20
14	A	1137	CLA	C11-C12-C13-C15
14	e	1013	CLA	C16-C17-C18-C20
14	e	1137	CLA	C11-C12-C13-C15
14	B	1219	CLA	C2-C3-C5-C6
14	H	1219	CLA	C2-C3-C5-C6
14	f	1219	CLA	C2-C3-C5-C6
18	A	5009	LHG	C5-C4-O6-P
18	I	5001	LHG	C4-C5-C6-O8
18	G	5009	LHG	C5-C4-O6-P
18	S	5001	LHG	C4-C5-C6-O8
18	e	5009	LHG	C5-C4-O6-P
18	k	5001	LHG	C4-C5-C6-O8
21	B	1852	SQD	O6-C44-C45-C46
21	H	1852	SQD	O6-C44-C45-C46
21	f	1852	SQD	O6-C44-C45-C46
14	f	1212	CLA	CBD-CGD-O2D-CED
14	c	509	CLA	C5-C6-C7-C8
14	u	509	CLA	C5-C6-C7-C8
18	A	5001	LHG	C14-C15-C16-C17
18	e	5001	LHG	C14-C15-C16-C17
14	F	1302	CLA	C2A-CAA-CBA-CGA
14	R	1302	CLA	C2A-CAA-CBA-CGA
14	j	1302	CLA	C2A-CAA-CBA-CGA
14	H	1227	CLA	O1D-CGD-O2D-CED
14	5	509	CLA	C5-C6-C7-C8
14	f	1215	CLA	C5-C6-C7-C8
18	G	5001	LHG	C14-C15-C16-C17
18	e	5009	LHG	C34-C35-C36-C37
14	G	1013	CLA	C16-C17-C18-C20
14	G	1137	CLA	C11-C12-C13-C15
18	A	5009	LHG	C34-C35-C36-C37
18	A	5005	LHG	C1-C2-C3-O3
18	A	5009	LHG	C1-C2-C3-O3
18	L	5220	LHG	C1-C2-C3-O3
18	G	5005	LHG	C1-C2-C3-O3
18	G	5009	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5220	LHG	C1-C2-C3-O3
18	e	5005	LHG	C1-C2-C3-O3
18	e	5009	LHG	C1-C2-C3-O3
18	n	5220	LHG	C1-C2-C3-O3
14	A	1102	CLA	CHA-CBD-CGD-O1D
14	A	1102	CLA	CHA-CBD-CGD-O2D
14	A	1111	CLA	CHA-CBD-CGD-O1D
14	A	1120	CLA	CHA-CBD-CGD-O1D
14	A	1122	CLA	CHA-CBD-CGD-O1D
14	A	1122	CLA	CHA-CBD-CGD-O2D
14	A	1134	CLA	CHA-CBD-CGD-O1D
14	A	1137	CLA	CHA-CBD-CGD-O1D
14	A	1137	CLA	CHA-CBD-CGD-O2D
14	A	1139	CLA	CHA-CBD-CGD-O2D
14	B	1209	CLA	CHA-CBD-CGD-O1D
14	B	1213	CLA	CHA-CBD-CGD-O1D
14	B	1213	CLA	CHA-CBD-CGD-O2D
14	B	1221	CLA	CHA-CBD-CGD-O1D
14	B	1221	CLA	CHA-CBD-CGD-O2D
14	B	1226	CLA	CHA-CBD-CGD-O1D
14	B	1226	CLA	CHA-CBD-CGD-O2D
14	B	1232	CLA	CHA-CBD-CGD-O1D
14	B	1232	CLA	CHA-CBD-CGD-O2D
14	B	1234	CLA	CHA-CBD-CGD-O2D
14	B	1207	CLA	CHA-CBD-CGD-O1D
14	B	1207	CLA	CHA-CBD-CGD-O2D
14	K	1103	CLA	CHA-CBD-CGD-O1D
14	1	501	CLA	CHA-CBD-CGD-O2D
14	1	503	CLA	CHA-CBD-CGD-O1D
14	1	503	CLA	CHA-CBD-CGD-O2D
14	2	503	CLA	CHA-CBD-CGD-O1D
14	2	503	CLA	CHA-CBD-CGD-O2D
14	2	504	CLA	CHA-CBD-CGD-O1D
14	2	506	CLA	CHA-CBD-CGD-O1D
14	2	506	CLA	CHA-CBD-CGD-O2D
14	2	507	CLA	CHA-CBD-CGD-O1D
14	3	503	CLA	CHA-CBD-CGD-O1D
14	3	503	CLA	CHA-CBD-CGD-O2D
14	3	506	CLA	CHA-CBD-CGD-O1D
14	3	510	CLA	CHA-CBD-CGD-O1D
14	3	510	CLA	CHA-CBD-CGD-O2D
14	4	502	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	4	502	CLA	CHA-CBD-CGD-O2D
14	4	505	CLA	CHA-CBD-CGD-O1D
14	4	507	CLA	CHA-CBD-CGD-O1D
14	4	507	CLA	CHA-CBD-CGD-O2D
14	4	509	CLA	CHA-CBD-CGD-O1D
14	4	509	CLA	CHA-CBD-CGD-O2D
14	5	503	CLA	CHA-CBD-CGD-O1D
14	5	503	CLA	CHA-CBD-CGD-O2D
14	5	516	CLA	CHA-CBD-CGD-O1D
14	5	516	CLA	CHA-CBD-CGD-O2D
14	5	519	CLA	CHA-CBD-CGD-O1D
14	5	519	CLA	CHA-CBD-CGD-O2D
14	6	503	CLA	CHA-CBD-CGD-O1D
14	6	503	CLA	CHA-CBD-CGD-O2D
14	G	1102	CLA	CHA-CBD-CGD-O1D
14	G	1102	CLA	CHA-CBD-CGD-O2D
14	G	1111	CLA	CHA-CBD-CGD-O1D
14	G	1120	CLA	CHA-CBD-CGD-O1D
14	G	1122	CLA	CHA-CBD-CGD-O1D
14	G	1122	CLA	CHA-CBD-CGD-O2D
14	G	1134	CLA	CHA-CBD-CGD-O1D
14	G	1137	CLA	CHA-CBD-CGD-O1D
14	G	1137	CLA	CHA-CBD-CGD-O2D
14	G	1139	CLA	CHA-CBD-CGD-O2D
14	H	1209	CLA	CHA-CBD-CGD-O1D
14	H	1213	CLA	CHA-CBD-CGD-O1D
14	H	1213	CLA	CHA-CBD-CGD-O2D
14	H	1221	CLA	CHA-CBD-CGD-O1D
14	H	1221	CLA	CHA-CBD-CGD-O2D
14	H	1226	CLA	CHA-CBD-CGD-O1D
14	H	1226	CLA	CHA-CBD-CGD-O2D
14	H	1232	CLA	CHA-CBD-CGD-O1D
14	H	1232	CLA	CHA-CBD-CGD-O2D
14	H	1234	CLA	CHA-CBD-CGD-O2D
14	H	1207	CLA	CHA-CBD-CGD-O1D
14	H	1207	CLA	CHA-CBD-CGD-O2D
14	U	1103	CLA	CHA-CBD-CGD-O1D
14	Y	501	CLA	CHA-CBD-CGD-O2D
14	Y	503	CLA	CHA-CBD-CGD-O1D
14	Y	503	CLA	CHA-CBD-CGD-O2D
14	Z	503	CLA	CHA-CBD-CGD-O1D
14	Z	503	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Z	504	CLA	CHA-CBD-CGD-O1D
14	Z	506	CLA	CHA-CBD-CGD-O1D
14	Z	506	CLA	CHA-CBD-CGD-O2D
14	Z	507	CLA	CHA-CBD-CGD-O1D
14	a	503	CLA	CHA-CBD-CGD-O1D
14	a	503	CLA	CHA-CBD-CGD-O2D
14	a	506	CLA	CHA-CBD-CGD-O1D
14	a	510	CLA	CHA-CBD-CGD-O1D
14	a	510	CLA	CHA-CBD-CGD-O2D
14	b	502	CLA	CHA-CBD-CGD-O1D
14	b	502	CLA	CHA-CBD-CGD-O2D
14	b	505	CLA	CHA-CBD-CGD-O1D
14	b	507	CLA	CHA-CBD-CGD-O1D
14	b	507	CLA	CHA-CBD-CGD-O2D
14	b	509	CLA	CHA-CBD-CGD-O1D
14	b	509	CLA	CHA-CBD-CGD-O2D
14	c	503	CLA	CHA-CBD-CGD-O1D
14	c	503	CLA	CHA-CBD-CGD-O2D
14	c	516	CLA	CHA-CBD-CGD-O1D
14	c	516	CLA	CHA-CBD-CGD-O2D
14	c	519	CLA	CHA-CBD-CGD-O1D
14	c	519	CLA	CHA-CBD-CGD-O2D
14	d	503	CLA	CHA-CBD-CGD-O1D
14	d	503	CLA	CHA-CBD-CGD-O2D
14	e	1102	CLA	CHA-CBD-CGD-O1D
14	e	1102	CLA	CHA-CBD-CGD-O2D
14	e	1111	CLA	CHA-CBD-CGD-O1D
14	e	1120	CLA	CHA-CBD-CGD-O1D
14	e	1122	CLA	CHA-CBD-CGD-O1D
14	e	1122	CLA	CHA-CBD-CGD-O2D
14	e	1134	CLA	CHA-CBD-CGD-O1D
14	e	1137	CLA	CHA-CBD-CGD-O1D
14	e	1137	CLA	CHA-CBD-CGD-O2D
14	e	1139	CLA	CHA-CBD-CGD-O2D
14	f	1209	CLA	CHA-CBD-CGD-O1D
14	f	1213	CLA	CHA-CBD-CGD-O1D
14	f	1213	CLA	CHA-CBD-CGD-O2D
14	f	1221	CLA	CHA-CBD-CGD-O1D
14	f	1221	CLA	CHA-CBD-CGD-O2D
14	f	1226	CLA	CHA-CBD-CGD-O1D
14	f	1226	CLA	CHA-CBD-CGD-O2D
14	f	1232	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1232	CLA	CHA-CBD-CGD-O2D
14	f	1234	CLA	CHA-CBD-CGD-O2D
14	f	1207	CLA	CHA-CBD-CGD-O1D
14	f	1207	CLA	CHA-CBD-CGD-O2D
14	m	1103	CLA	CHA-CBD-CGD-O1D
14	q	501	CLA	CHA-CBD-CGD-O2D
14	q	503	CLA	CHA-CBD-CGD-O1D
14	q	503	CLA	CHA-CBD-CGD-O2D
14	r	503	CLA	CHA-CBD-CGD-O1D
14	r	503	CLA	CHA-CBD-CGD-O2D
14	r	504	CLA	CHA-CBD-CGD-O1D
14	r	506	CLA	CHA-CBD-CGD-O1D
14	r	506	CLA	CHA-CBD-CGD-O2D
14	r	507	CLA	CHA-CBD-CGD-O1D
14	s	503	CLA	CHA-CBD-CGD-O1D
14	s	503	CLA	CHA-CBD-CGD-O2D
14	s	506	CLA	CHA-CBD-CGD-O1D
14	s	510	CLA	CHA-CBD-CGD-O1D
14	s	510	CLA	CHA-CBD-CGD-O2D
14	t	502	CLA	CHA-CBD-CGD-O1D
14	t	502	CLA	CHA-CBD-CGD-O2D
14	t	505	CLA	CHA-CBD-CGD-O1D
14	t	507	CLA	CHA-CBD-CGD-O1D
14	t	507	CLA	CHA-CBD-CGD-O2D
14	t	509	CLA	CHA-CBD-CGD-O1D
14	t	509	CLA	CHA-CBD-CGD-O2D
14	u	503	CLA	CHA-CBD-CGD-O1D
14	u	503	CLA	CHA-CBD-CGD-O2D
14	u	516	CLA	CHA-CBD-CGD-O1D
14	u	516	CLA	CHA-CBD-CGD-O2D
14	u	519	CLA	CHA-CBD-CGD-O1D
14	u	519	CLA	CHA-CBD-CGD-O2D
14	v	503	CLA	CHA-CBD-CGD-O1D
14	v	503	CLA	CHA-CBD-CGD-O2D
18	G	5009	LHG	C34-C35-C36-C37
14	B	1215	CLA	C5-C6-C7-C8
14	H	1215	CLA	C5-C6-C7-C8
21	L	5216	SQD	C19-C20-C21-C22
21	V	5216	SQD	C19-C20-C21-C22
21	n	5216	SQD	C19-C20-C21-C22
18	L	5220	LHG	O7-C5-C6-O8
18	L	5221	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5220	LHG	O7-C5-C6-O8
18	V	5221	LHG	O7-C5-C6-O8
18	n	5220	LHG	O7-C5-C6-O8
18	n	5221	LHG	O7-C5-C6-O8
21	B	1852	SQD	O6-C44-C45-O47
21	3	822	SQD	O6-C44-C45-O47
21	4	822	SQD	O47-C45-C46-O48
21	H	1852	SQD	O6-C44-C45-O47
21	a	822	SQD	O6-C44-C45-O47
21	b	822	SQD	O47-C45-C46-O48
21	s	822	SQD	O6-C44-C45-O47
21	t	822	SQD	O47-C45-C46-O48
14	B	1223	CLA	C5-C6-C7-C8
14	H	1223	CLA	C5-C6-C7-C8
14	f	1223	CLA	C5-C6-C7-C8
14	A	1103	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	O1A-CGA-O2A-C1
14	e	1103	CLA	O1A-CGA-O2A-C1
18	A	5007	LHG	C33-C34-C35-C36
14	A	1137	CLA	C11-C12-C13-C14
14	G	1137	CLA	C11-C12-C13-C14
14	e	1137	CLA	C11-C12-C13-C14
18	A	5004	LHG	O1-C1-C2-O2
18	A	5006	LHG	O1-C1-C2-O2
18	G	5004	LHG	O1-C1-C2-O2
18	G	5006	LHG	O1-C1-C2-O2
18	e	5004	LHG	O1-C1-C2-O2
18	e	5006	LHG	O1-C1-C2-O2
18	B	1842	LHG	C27-C28-C29-C30
18	G	5007	LHG	C33-C34-C35-C36
18	f	1842	LHG	C27-C28-C29-C30
14	B	1204	CLA	C4-C3-C5-C6
14	H	1204	CLA	C4-C3-C5-C6
14	f	1204	CLA	C4-C3-C5-C6
18	L	5218	LHG	C29-C30-C31-C32
18	H	1842	LHG	C27-C28-C29-C30
18	e	5007	LHG	C33-C34-C35-C36
18	V	5218	LHG	C29-C30-C31-C32
18	n	5218	LHG	C29-C30-C31-C32
14	H	1202	CLA	C15-C16-C17-C18
14	f	1202	CLA	C15-C16-C17-C18
14	f	1234	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1203	CLA	C6-C7-C8-C9
14	B	1206	CLA	C11-C10-C8-C9
14	5	509	CLA	C11-C12-C13-C14
14	H	1203	CLA	C6-C7-C8-C9
14	H	1206	CLA	C11-C10-C8-C9
14	c	509	CLA	C11-C12-C13-C14
14	f	1203	CLA	C6-C7-C8-C9
14	f	1206	CLA	C11-C10-C8-C9
14	f	1219	CLA	C14-C13-C15-C16
14	u	509	CLA	C11-C12-C13-C14
18	A	5005	LHG	C25-C26-C27-C28
18	G	5005	LHG	C25-C26-C27-C28
14	B	1202	CLA	C15-C16-C17-C18
21	4	822	SQD	C5-C6-S-O8
21	b	822	SQD	C5-C6-S-O8
21	t	822	SQD	C5-C6-S-O8
18	e	5005	LHG	C25-C26-C27-C28
14	2	518	CLA	C2A-CAA-CBA-CGA
14	Z	518	CLA	C2A-CAA-CBA-CGA
14	r	518	CLA	C2A-CAA-CBA-CGA
14	B	1224	CLA	CAA-CBA-CGA-O2A
14	H	1224	CLA	CAA-CBA-CGA-O2A
14	f	1224	CLA	CAA-CBA-CGA-O2A
14	B	1234	CLA	C15-C16-C17-C18
14	G	1140	CLA	O1D-CGD-O2D-CED
14	c	508	CLA	O1D-CGD-O2D-CED
17	H	4010	BCR	C37-C22-C23-C24
17	v	521	BCR	C7-C8-C9-C34
18	A	5006	LHG	O1-C1-C2-C3
18	G	5006	LHG	O1-C1-C2-C3
18	e	5006	LHG	O1-C1-C2-C3
14	H	1234	CLA	C15-C16-C17-C18
17	B	4010	BCR	C21-C22-C23-C24
17	B	4014	BCR	C7-C8-C9-C10
17	3	524	BCR	C21-C22-C23-C24
17	4	521	BCR	C17-C18-C19-C20
17	H	4010	BCR	C21-C22-C23-C24
17	H	4014	BCR	C7-C8-C9-C10
17	b	521	BCR	C17-C18-C19-C20
17	f	4010	BCR	C21-C22-C23-C24
17	f	4014	BCR	C7-C8-C9-C10
17	t	521	BCR	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1240	CLA	O1D-CGD-O2D-CED
14	5	508	CLA	O1D-CGD-O2D-CED
14	A	1113	CLA	C1A-C2A-CAA-CBA
14	B	1208	CLA	C1A-C2A-CAA-CBA
14	B	1212	CLA	C1A-C2A-CAA-CBA
14	B	1229	CLA	C1A-C2A-CAA-CBA
14	B	1236	CLA	C1A-C2A-CAA-CBA
14	1	501	CLA	C1A-C2A-CAA-CBA
14	2	508	CLA	C1A-C2A-CAA-CBA
14	3	516	CLA	C1A-C2A-CAA-CBA
14	4	517	CLA	C1A-C2A-CAA-CBA
14	5	503	CLA	C1A-C2A-CAA-CBA
14	G	1113	CLA	C1A-C2A-CAA-CBA
14	H	1208	CLA	C1A-C2A-CAA-CBA
14	H	1212	CLA	C1A-C2A-CAA-CBA
14	H	1229	CLA	C1A-C2A-CAA-CBA
14	H	1236	CLA	C1A-C2A-CAA-CBA
14	Y	501	CLA	C1A-C2A-CAA-CBA
14	Z	508	CLA	C1A-C2A-CAA-CBA
14	a	516	CLA	C1A-C2A-CAA-CBA
14	b	517	CLA	C1A-C2A-CAA-CBA
14	c	503	CLA	C1A-C2A-CAA-CBA
14	e	1113	CLA	C1A-C2A-CAA-CBA
14	f	1208	CLA	C1A-C2A-CAA-CBA
14	f	1212	CLA	C1A-C2A-CAA-CBA
14	f	1229	CLA	C1A-C2A-CAA-CBA
14	f	1236	CLA	C1A-C2A-CAA-CBA
14	q	501	CLA	C1A-C2A-CAA-CBA
14	r	508	CLA	C1A-C2A-CAA-CBA
14	s	516	CLA	C1A-C2A-CAA-CBA
14	t	517	CLA	C1A-C2A-CAA-CBA
14	u	503	CLA	C1A-C2A-CAA-CBA
21	L	5216	SQD	C23-C24-C25-C26
21	V	5216	SQD	C23-C24-C25-C26
14	A	1115	CLA	C11-C12-C13-C14
14	G	1115	CLA	C11-C12-C13-C14
14	e	1115	CLA	C11-C12-C13-C14
14	G	1123	CLA	C15-C16-C17-C18
14	e	1123	CLA	C15-C16-C17-C18
14	A	1140	CLA	O1D-CGD-O2D-CED
14	e	1124	CLA	CBD-CGD-O2D-CED
18	L	5221	LHG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	V	5221	LHG	C24-C25-C26-C27
18	n	5221	LHG	C24-C25-C26-C27
17	J	4015	BCR	C15-C16-C17-C18
17	3	522	BCR	C9-C10-C11-C12
17	T	4015	BCR	C15-C16-C17-C18
17	a	522	BCR	C9-C10-C11-C12
17	s	522	BCR	C9-C10-C11-C12
14	H	1240	CLA	O1D-CGD-O2D-CED
14	e	1140	CLA	O1D-CGD-O2D-CED
14	f	1240	CLA	O1D-CGD-O2D-CED
14	A	1123	CLA	C15-C16-C17-C18
18	B	1855	LHG	O2-C2-C3-O3
18	H	1855	LHG	O2-C2-C3-O3
18	f	1855	LHG	O2-C2-C3-O3
14	u	508	CLA	O1D-CGD-O2D-CED
14	A	1124	CLA	CBD-CGD-O2D-CED
14	a	510	CLA	CBD-CGD-O2D-CED
14	s	510	CLA	CBD-CGD-O2D-CED
14	A	1108	CLA	C2-C3-C5-C6
14	A	1101	CLA	C2-C3-C5-C6
14	G	1108	CLA	C2-C3-C5-C6
14	G	1101	CLA	C2-C3-C5-C6
14	e	1108	CLA	C2-C3-C5-C6
14	e	1101	CLA	C2-C3-C5-C6
14	A	1115	CLA	C4B-C3B-CAB-CBB
14	A	1137	CLA	C4B-C3B-CAB-CBB
14	A	1140	CLA	C4B-C3B-CAB-CBB
14	B	1205	CLA	C4B-C3B-CAB-CBB
14	B	1209	CLA	C4B-C3B-CAB-CBB
14	B	1236	CLA	C4B-C3B-CAB-CBB
14	3	512	CLA	C4B-C3B-CAB-CBB
14	6	513	CLA	C4B-C3B-CAB-CBB
14	G	1115	CLA	C4B-C3B-CAB-CBB
14	G	1137	CLA	C4B-C3B-CAB-CBB
14	G	1140	CLA	C4B-C3B-CAB-CBB
14	H	1205	CLA	C4B-C3B-CAB-CBB
14	H	1209	CLA	C4B-C3B-CAB-CBB
14	H	1236	CLA	C4B-C3B-CAB-CBB
14	a	512	CLA	C4B-C3B-CAB-CBB
14	d	513	CLA	C4B-C3B-CAB-CBB
14	e	1137	CLA	C4B-C3B-CAB-CBB
14	e	1140	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1205	CLA	C4B-C3B-CAB-CBB
14	f	1209	CLA	C4B-C3B-CAB-CBB
14	f	1236	CLA	C4B-C3B-CAB-CBB
14	s	512	CLA	C4B-C3B-CAB-CBB
14	v	513	CLA	C4B-C3B-CAB-CBB
18	A	5002	LHG	C4-O6-P-O5
18	A	5005	LHG	C3-O3-P-O5
18	A	5008	LHG	C4-O6-P-O4
18	A	5003	LHG	C4-O6-P-O5
18	B	1842	LHG	C3-O3-P-O4
18	B	1855	LHG	C3-O3-P-O5
18	B	1855	LHG	C4-O6-P-O4
18	I	5001	LHG	C3-O3-P-O5
18	L	5220	LHG	C4-O6-P-O4
18	L	5221	LHG	C3-O3-P-O4
18	L	5221	LHG	C4-O6-P-O4
18	G	5002	LHG	C4-O6-P-O5
18	G	5005	LHG	C3-O3-P-O5
18	G	5008	LHG	C4-O6-P-O4
18	G	5003	LHG	C4-O6-P-O5
18	H	1842	LHG	C3-O3-P-O4
18	H	1855	LHG	C3-O3-P-O5
18	H	1855	LHG	C4-O6-P-O4
18	S	5001	LHG	C3-O3-P-O5
18	V	5220	LHG	C4-O6-P-O4
18	V	5221	LHG	C3-O3-P-O4
18	V	5221	LHG	C4-O6-P-O4
18	e	5002	LHG	C4-O6-P-O5
18	e	5005	LHG	C3-O3-P-O5
18	e	5008	LHG	C4-O6-P-O4
18	e	5003	LHG	C4-O6-P-O5
18	f	1842	LHG	C3-O3-P-O4
18	f	1855	LHG	C3-O3-P-O5
18	f	1855	LHG	C4-O6-P-O4
18	k	5001	LHG	C3-O3-P-O5
18	n	5220	LHG	C4-O6-P-O4
18	n	5221	LHG	C3-O3-P-O4
18	n	5221	LHG	C4-O6-P-O4
14	A	1117	CLA	C16-C17-C18-C20
14	G	1117	CLA	C16-C17-C18-C20
14	e	1117	CLA	C16-C17-C18-C20
21	n	5216	SQD	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1205	CLA	CBA-CGA-O2A-C1
14	H	1205	CLA	CBA-CGA-O2A-C1
14	f	1205	CLA	CBA-CGA-O2A-C1
14	3	510	CLA	CBD-CGD-O2D-CED
14	G	1124	CLA	CBD-CGD-O2D-CED
18	B	1855	LHG	O6-C4-C5-C6
18	H	1855	LHG	O6-C4-C5-C6
18	f	1855	LHG	O6-C4-C5-C6
14	B	1228	CLA	CAA-CBA-CGA-O2A
14	H	1228	CLA	CAA-CBA-CGA-O2A
14	f	1228	CLA	CAA-CBA-CGA-O2A
14	B	1213	CLA	C2A-CAA-CBA-CGA
14	2	517	CLA	C2A-CAA-CBA-CGA
14	H	1213	CLA	C2A-CAA-CBA-CGA
14	Z	517	CLA	C2A-CAA-CBA-CGA
14	f	1213	CLA	C2A-CAA-CBA-CGA
14	r	517	CLA	C2A-CAA-CBA-CGA
14	L	1502	CLA	C3-C5-C6-C7
14	V	1502	CLA	C3-C5-C6-C7
14	n	1502	CLA	C3-C5-C6-C7
18	A	5007	LHG	C28-C29-C30-C31
18	G	5007	LHG	C28-C29-C30-C31
18	e	5007	LHG	C28-C29-C30-C31
14	A	1111	CLA	CAD-CBD-CGD-O1D
14	A	1113	CLA	CAD-CBD-CGD-O1D
14	A	1801	CLA	CAD-CBD-CGD-O1D
14	B	1012	CLA	CAD-CBD-CGD-O1D
14	B	1234	CLA	CAD-CBD-CGD-O1D
14	B	1207	CLA	CAD-CBD-CGD-O1D
14	K	1103	CLA	CAD-CBD-CGD-O1D
14	K	1105	CLA	CAD-CBD-CGD-O1D
14	1	501	CLA	CAD-CBD-CGD-O1D
14	1	503	CLA	CAD-CBD-CGD-O1D
14	1	506	CLA	CAD-CBD-CGD-O1D
14	2	503	CLA	CAD-CBD-CGD-O1D
14	2	504	CLA	CAD-CBD-CGD-O1D
14	2	506	CLA	CAD-CBD-CGD-O1D
14	2	510	CLA	CAD-CBD-CGD-O1D
14	2	518	CLA	CAD-CBD-CGD-O1D
14	3	503	CLA	CAD-CBD-CGD-O1D
14	3	504	CLA	CAD-CBD-CGD-O1D
14	3	506	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	3	510	CLA	CAD-CBD-CGD-O1D
14	3	516	CLA	CAD-CBD-CGD-O1D
14	4	516	CLA	CAD-CBD-CGD-O1D
14	5	503	CLA	CAD-CBD-CGD-O1D
14	5	506	CLA	CAD-CBD-CGD-O1D
14	5	510	CLA	CAD-CBD-CGD-O1D
14	5	516	CLA	CAD-CBD-CGD-O1D
14	6	503	CLA	CAD-CBD-CGD-O1D
14	G	1111	CLA	CAD-CBD-CGD-O1D
14	G	1113	CLA	CAD-CBD-CGD-O1D
14	G	1801	CLA	CAD-CBD-CGD-O1D
14	H	1012	CLA	CAD-CBD-CGD-O1D
14	H	1234	CLA	CAD-CBD-CGD-O1D
14	H	1207	CLA	CAD-CBD-CGD-O1D
14	U	1103	CLA	CAD-CBD-CGD-O1D
14	U	1105	CLA	CAD-CBD-CGD-O1D
14	Y	501	CLA	CAD-CBD-CGD-O1D
14	Y	503	CLA	CAD-CBD-CGD-O1D
14	Y	506	CLA	CAD-CBD-CGD-O1D
14	Z	503	CLA	CAD-CBD-CGD-O1D
14	Z	504	CLA	CAD-CBD-CGD-O1D
14	Z	506	CLA	CAD-CBD-CGD-O1D
14	Z	510	CLA	CAD-CBD-CGD-O1D
14	Z	518	CLA	CAD-CBD-CGD-O1D
14	a	503	CLA	CAD-CBD-CGD-O1D
14	a	504	CLA	CAD-CBD-CGD-O1D
14	a	506	CLA	CAD-CBD-CGD-O1D
14	a	510	CLA	CAD-CBD-CGD-O1D
14	a	516	CLA	CAD-CBD-CGD-O1D
14	b	516	CLA	CAD-CBD-CGD-O1D
14	c	503	CLA	CAD-CBD-CGD-O1D
14	c	506	CLA	CAD-CBD-CGD-O1D
14	c	510	CLA	CAD-CBD-CGD-O1D
14	c	516	CLA	CAD-CBD-CGD-O1D
14	d	503	CLA	CAD-CBD-CGD-O1D
14	e	1111	CLA	CAD-CBD-CGD-O1D
14	e	1113	CLA	CAD-CBD-CGD-O1D
14	e	1801	CLA	CAD-CBD-CGD-O1D
14	f	1012	CLA	CAD-CBD-CGD-O1D
14	f	1234	CLA	CAD-CBD-CGD-O1D
14	f	1207	CLA	CAD-CBD-CGD-O1D
14	m	1103	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	m	1105	CLA	CAD-CBD-CGD-O1D
14	q	501	CLA	CAD-CBD-CGD-O1D
14	q	503	CLA	CAD-CBD-CGD-O1D
14	q	506	CLA	CAD-CBD-CGD-O1D
14	r	503	CLA	CAD-CBD-CGD-O1D
14	r	504	CLA	CAD-CBD-CGD-O1D
14	r	506	CLA	CAD-CBD-CGD-O1D
14	r	510	CLA	CAD-CBD-CGD-O1D
14	r	518	CLA	CAD-CBD-CGD-O1D
14	s	503	CLA	CAD-CBD-CGD-O1D
14	s	504	CLA	CAD-CBD-CGD-O1D
14	s	506	CLA	CAD-CBD-CGD-O1D
14	s	510	CLA	CAD-CBD-CGD-O1D
14	s	516	CLA	CAD-CBD-CGD-O1D
14	t	516	CLA	CAD-CBD-CGD-O1D
14	u	503	CLA	CAD-CBD-CGD-O1D
14	u	506	CLA	CAD-CBD-CGD-O1D
14	u	510	CLA	CAD-CBD-CGD-O1D
14	u	516	CLA	CAD-CBD-CGD-O1D
14	v	503	CLA	CAD-CBD-CGD-O1D
18	B	1842	LHG	O10-C23-O8-C6
18	f	1842	LHG	O10-C23-O8-C6
18	A	5002	LHG	C26-C27-C28-C29
18	G	5002	LHG	C26-C27-C28-C29
18	e	5002	LHG	C26-C27-C28-C29
18	n	5218	LHG	C23-C24-C25-C26
20	f	5002	LMG	C39-C40-C41-C42
18	A	5005	LHG	C24-C23-O8-C6
18	G	5005	LHG	C24-C23-O8-C6
18	e	5005	LHG	C24-C23-O8-C6
18	H	1842	LHG	O10-C23-O8-C6
20	B	5002	LMG	C39-C40-C41-C42
20	H	5002	LMG	C39-C40-C41-C42
14	A	1104	CLA	C3A-C2A-CAA-CBA
14	A	1111	CLA	C12-C13-C15-C16
14	A	1117	CLA	C11-C12-C13-C15
14	B	1203	CLA	C11-C12-C13-C15
14	B	1206	CLA	C11-C10-C8-C7
14	B	1208	CLA	C6-C7-C8-C10
14	B	1210	CLA	C2-C3-C5-C6
14	B	1210	CLA	C6-C7-C8-C10
14	B	1213	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1214	CLA	C11-C12-C13-C15
14	B	1217	CLA	C6-C7-C8-C10
14	B	1219	CLA	C6-C7-C8-C10
14	B	1227	CLA	C6-C7-C8-C10
14	G	1104	CLA	C3A-C2A-CAA-CBA
14	G	1111	CLA	C12-C13-C15-C16
14	G	1117	CLA	C11-C12-C13-C15
14	H	1203	CLA	C11-C12-C13-C15
14	H	1206	CLA	C11-C10-C8-C7
14	H	1208	CLA	C6-C7-C8-C10
14	H	1210	CLA	C2-C3-C5-C6
14	H	1210	CLA	C6-C7-C8-C10
14	H	1213	CLA	C11-C12-C13-C15
14	H	1214	CLA	C11-C12-C13-C15
14	H	1217	CLA	C6-C7-C8-C10
14	H	1219	CLA	C6-C7-C8-C10
14	H	1227	CLA	C6-C7-C8-C10
14	e	1104	CLA	C3A-C2A-CAA-CBA
14	e	1111	CLA	C12-C13-C15-C16
14	e	1117	CLA	C11-C12-C13-C15
14	f	1203	CLA	C11-C12-C13-C15
14	f	1206	CLA	C11-C10-C8-C7
14	f	1208	CLA	C6-C7-C8-C10
14	f	1210	CLA	C2-C3-C5-C6
14	f	1210	CLA	C6-C7-C8-C10
14	f	1213	CLA	C11-C12-C13-C15
14	f	1214	CLA	C11-C12-C13-C15
14	f	1217	CLA	C6-C7-C8-C10
14	f	1219	CLA	C6-C7-C8-C10
14	f	1227	CLA	C6-C7-C8-C10
18	A	5005	LHG	O6-C4-C5-O7
18	L	5218	LHG	C23-C24-C25-C26
18	G	5005	LHG	O6-C4-C5-O7
18	V	5218	LHG	C23-C24-C25-C26
18	e	5005	LHG	O6-C4-C5-O7
17	l	4015	BCR	C15-C16-C17-C18
14	3	518	CLA	CAA-CBA-CGA-O2A
14	a	518	CLA	CAA-CBA-CGA-O2A
14	s	518	CLA	CAA-CBA-CGA-O2A
14	A	1237	CLA	C5-C6-C7-C8
14	B	1234	CLA	C5-C6-C7-C8
14	G	1237	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1234	CLA	C5-C6-C7-C8
14	e	1237	CLA	C5-C6-C7-C8
14	f	1234	CLA	C5-C6-C7-C8
14	f	1234	CLA	C2C-C3C-CAC-CBC
14	B	1208	CLA	O1A-CGA-O2A-C1
14	B	1234	CLA	C2C-C3C-CAC-CBC
14	H	1234	CLA	C2C-C3C-CAC-CBC
18	B	1842	LHG	C4-C5-C6-O8
18	H	1842	LHG	C4-C5-C6-O8
18	f	1842	LHG	C4-C5-C6-O8
21	1	822	SQD	O6-C44-C45-C46
21	4	822	SQD	C44-C45-C46-O48
21	Y	822	SQD	O6-C44-C45-C46
21	b	822	SQD	C44-C45-C46-O48
21	q	822	SQD	O6-C44-C45-C46
21	t	822	SQD	C44-C45-C46-O48
14	H	1208	CLA	O1A-CGA-O2A-C1
14	f	1208	CLA	O1A-CGA-O2A-C1
18	A	5004	LHG	O7-C5-C6-O8
18	A	5005	LHG	O7-C5-C6-O8
18	A	5007	LHG	O7-C5-C6-O8
18	G	5004	LHG	O7-C5-C6-O8
18	G	5005	LHG	O7-C5-C6-O8
18	G	5007	LHG	O7-C5-C6-O8
18	e	5004	LHG	O7-C5-C6-O8
18	e	5005	LHG	O7-C5-C6-O8
18	e	5007	LHG	O7-C5-C6-O8
21	6	822	SQD	O47-C45-C46-O48
21	d	822	SQD	O47-C45-C46-O48
21	v	822	SQD	O47-C45-C46-O48
14	2	505	CLA	C5-C6-C7-C8
14	Z	505	CLA	C5-C6-C7-C8
14	r	505	CLA	C5-C6-C7-C8
14	1	516	CLA	C2C-C3C-CAC-CBC
14	Y	516	CLA	C2C-C3C-CAC-CBC
14	q	516	CLA	C2C-C3C-CAC-CBC
14	B	1021	CLA	O1A-CGA-O2A-C1
14	H	1021	CLA	O1A-CGA-O2A-C1
14	f	1021	CLA	O1A-CGA-O2A-C1
14	B	1202	CLA	C4-C3-C5-C6
14	H	1202	CLA	C4-C3-C5-C6
14	A	1128	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1128	CLA	C10-C11-C12-C13
14	e	1128	CLA	C10-C11-C12-C13
14	A	1013	CLA	C14-C13-C15-C16
14	A	1104	CLA	C14-C13-C15-C16
14	A	1106	CLA	C14-C13-C15-C16
14	A	1131	CLA	C14-C13-C15-C16
14	B	1012	CLA	C11-C10-C8-C9
14	B	1208	CLA	C14-C13-C15-C16
14	B	1214	CLA	C11-C12-C13-C14
14	B	1225	CLA	C14-C13-C15-C16
14	B	1239	CLA	C14-C13-C15-C16
14	B	1240	CLA	C11-C12-C13-C14
14	B	1230	CLA	C6-C7-C8-C9
14	5	509	CLA	C6-C7-C8-C9
14	G	1013	CLA	C14-C13-C15-C16
14	G	1104	CLA	C14-C13-C15-C16
14	G	1106	CLA	C14-C13-C15-C16
14	G	1131	CLA	C14-C13-C15-C16
14	H	1012	CLA	C11-C10-C8-C9
14	H	1208	CLA	C14-C13-C15-C16
14	H	1214	CLA	C11-C12-C13-C14
14	H	1225	CLA	C14-C13-C15-C16
14	H	1239	CLA	C14-C13-C15-C16
14	H	1240	CLA	C11-C12-C13-C14
14	H	1230	CLA	C6-C7-C8-C9
14	c	509	CLA	C6-C7-C8-C9
14	e	1013	CLA	C14-C13-C15-C16
14	e	1104	CLA	C14-C13-C15-C16
14	e	1106	CLA	C14-C13-C15-C16
14	e	1131	CLA	C14-C13-C15-C16
14	f	1012	CLA	C11-C10-C8-C9
14	f	1208	CLA	C6-C7-C8-C9
14	f	1208	CLA	C14-C13-C15-C16
14	f	1214	CLA	C11-C12-C13-C14
14	f	1225	CLA	C14-C13-C15-C16
14	f	1239	CLA	C14-C13-C15-C16
14	f	1240	CLA	C11-C12-C13-C14
14	f	1230	CLA	C6-C7-C8-C9
14	u	509	CLA	C6-C7-C8-C9
21	1	822	SQD	O48-C23-C24-C25
21	Y	822	SQD	O48-C23-C24-C25
21	q	822	SQD	O48-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	4010	BCR	C11-C12-C13-C35
17	6	521	BCR	C7-C8-C9-C34
17	H	4010	BCR	C11-C12-C13-C35
17	d	521	BCR	C7-C8-C9-C34
17	f	4010	BCR	C11-C12-C13-C35
18	n	5221	LHG	C29-C30-C31-C32
18	L	5221	LHG	C29-C30-C31-C32
18	V	5221	LHG	C29-C30-C31-C32
14	B	1229	CLA	CAA-CBA-CGA-O2A
14	H	1229	CLA	CAA-CBA-CGA-O2A
14	A	1106	CLA	C2B-C3B-CAB-CBB
14	A	1109	CLA	C2B-C3B-CAB-CBB
14	A	1110	CLA	C2B-C3B-CAB-CBB
14	A	1111	CLA	C2B-C3B-CAB-CBB
14	A	1115	CLA	C2B-C3B-CAB-CBB
14	A	1140	CLA	C2B-C3B-CAB-CBB
14	B	1203	CLA	C2B-C3B-CAB-CBB
14	B	1205	CLA	C2B-C3B-CAB-CBB
14	B	1208	CLA	C2B-C3B-CAB-CBB
14	B	1210	CLA	C2B-C3B-CAB-CBB
14	B	1240	CLA	C2B-C3B-CAB-CBB
14	K	1401	CLA	C2B-C3B-CAB-CBB
14	L	1502	CLA	C2B-C3B-CAB-CBB
14	1	507	CLA	C2B-C3B-CAB-CBB
14	1	511	CLA	C2B-C3B-CAB-CBB
14	1	513	CLA	C2B-C3B-CAB-CBB
14	2	508	CLA	C2B-C3B-CAB-CBB
14	2	518	CLA	C2B-C3B-CAB-CBB
14	3	507	CLA	C2B-C3B-CAB-CBB
14	3	508	CLA	C2B-C3B-CAB-CBB
14	3	516	CLA	C2B-C3B-CAB-CBB
14	4	504	CLA	C2B-C3B-CAB-CBB
14	4	506	CLA	C2B-C3B-CAB-CBB
14	4	510	CLA	C2B-C3B-CAB-CBB
14	4	511	CLA	C2B-C3B-CAB-CBB
14	4	512	CLA	C2B-C3B-CAB-CBB
14	4	513	CLA	C2B-C3B-CAB-CBB
14	5	505	CLA	C2B-C3B-CAB-CBB
14	5	508	CLA	C2B-C3B-CAB-CBB
14	6	508	CLA	C2B-C3B-CAB-CBB
14	6	511	CLA	C2B-C3B-CAB-CBB
14	6	513	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1106	CLA	C2B-C3B-CAB-CBB
14	G	1109	CLA	C2B-C3B-CAB-CBB
14	G	1110	CLA	C2B-C3B-CAB-CBB
14	G	1111	CLA	C2B-C3B-CAB-CBB
14	G	1115	CLA	C2B-C3B-CAB-CBB
14	G	1140	CLA	C2B-C3B-CAB-CBB
14	H	1203	CLA	C2B-C3B-CAB-CBB
14	H	1205	CLA	C2B-C3B-CAB-CBB
14	H	1208	CLA	C2B-C3B-CAB-CBB
14	H	1210	CLA	C2B-C3B-CAB-CBB
14	H	1240	CLA	C2B-C3B-CAB-CBB
14	U	1401	CLA	C2B-C3B-CAB-CBB
14	V	1502	CLA	C2B-C3B-CAB-CBB
14	Y	507	CLA	C2B-C3B-CAB-CBB
14	Y	511	CLA	C2B-C3B-CAB-CBB
14	Y	513	CLA	C2B-C3B-CAB-CBB
14	Z	508	CLA	C2B-C3B-CAB-CBB
14	Z	518	CLA	C2B-C3B-CAB-CBB
14	a	507	CLA	C2B-C3B-CAB-CBB
14	a	508	CLA	C2B-C3B-CAB-CBB
14	a	516	CLA	C2B-C3B-CAB-CBB
14	b	504	CLA	C2B-C3B-CAB-CBB
14	b	506	CLA	C2B-C3B-CAB-CBB
14	b	510	CLA	C2B-C3B-CAB-CBB
14	b	511	CLA	C2B-C3B-CAB-CBB
14	b	512	CLA	C2B-C3B-CAB-CBB
14	b	513	CLA	C2B-C3B-CAB-CBB
14	c	505	CLA	C2B-C3B-CAB-CBB
14	c	508	CLA	C2B-C3B-CAB-CBB
14	d	508	CLA	C2B-C3B-CAB-CBB
14	d	511	CLA	C2B-C3B-CAB-CBB
14	d	513	CLA	C2B-C3B-CAB-CBB
14	e	1106	CLA	C2B-C3B-CAB-CBB
14	e	1109	CLA	C2B-C3B-CAB-CBB
14	e	1110	CLA	C2B-C3B-CAB-CBB
14	e	1111	CLA	C2B-C3B-CAB-CBB
14	e	1115	CLA	C2B-C3B-CAB-CBB
14	e	1140	CLA	C2B-C3B-CAB-CBB
14	f	1203	CLA	C2B-C3B-CAB-CBB
14	f	1205	CLA	C2B-C3B-CAB-CBB
14	f	1208	CLA	C2B-C3B-CAB-CBB
14	f	1210	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1240	CLA	C2B-C3B-CAB-CBB
14	m	1401	CLA	C2B-C3B-CAB-CBB
14	n	1502	CLA	C2B-C3B-CAB-CBB
14	q	507	CLA	C2B-C3B-CAB-CBB
14	q	511	CLA	C2B-C3B-CAB-CBB
14	q	513	CLA	C2B-C3B-CAB-CBB
14	r	508	CLA	C2B-C3B-CAB-CBB
14	r	518	CLA	C2B-C3B-CAB-CBB
14	s	507	CLA	C2B-C3B-CAB-CBB
14	s	508	CLA	C2B-C3B-CAB-CBB
14	s	516	CLA	C2B-C3B-CAB-CBB
14	t	504	CLA	C2B-C3B-CAB-CBB
14	t	506	CLA	C2B-C3B-CAB-CBB
14	t	510	CLA	C2B-C3B-CAB-CBB
14	t	511	CLA	C2B-C3B-CAB-CBB
14	t	512	CLA	C2B-C3B-CAB-CBB
14	t	513	CLA	C2B-C3B-CAB-CBB
14	u	505	CLA	C2B-C3B-CAB-CBB
14	u	508	CLA	C2B-C3B-CAB-CBB
14	v	504	CLA	C2B-C3B-CAB-CBB
14	v	508	CLA	C2B-C3B-CAB-CBB
14	v	511	CLA	C2B-C3B-CAB-CBB
14	v	513	CLA	C2B-C3B-CAB-CBB
18	e	5006	LHG	C29-C30-C31-C32
14	A	1132	CLA	C8-C10-C11-C12
14	e	1132	CLA	C8-C10-C11-C12
18	A	5006	LHG	C29-C30-C31-C32
14	A	1107	CLA	C4-C3-C5-C6
14	3	505	CLA	C4-C3-C5-C6
14	G	1107	CLA	C4-C3-C5-C6
14	e	1107	CLA	C4-C3-C5-C6
14	f	1202	CLA	C4-C3-C5-C6
14	f	1229	CLA	CAA-CBA-CGA-O2A
14	B	1204	CLA	C2-C3-C5-C6
14	H	1204	CLA	C2-C3-C5-C6
14	f	1204	CLA	C2-C3-C5-C6
18	G	5006	LHG	C29-C30-C31-C32
14	G	1132	CLA	C8-C10-C11-C12
14	2	501	CLA	C2A-CAA-CBA-CGA
14	3	518	CLA	C2A-CAA-CBA-CGA
14	5	501	CLA	C2A-CAA-CBA-CGA
14	Z	501	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	518	CLA	C2A-CAA-CBA-CGA
14	c	501	CLA	C2A-CAA-CBA-CGA
14	r	501	CLA	C2A-CAA-CBA-CGA
14	s	518	CLA	C2A-CAA-CBA-CGA
14	u	501	CLA	C2A-CAA-CBA-CGA
18	L	5221	LHG	O9-C7-O7-C5
18	V	5221	LHG	O9-C7-O7-C5
18	n	5221	LHG	O9-C7-O7-C5
20	J	5104	LMG	O9-C10-O7-C8
20	T	5104	LMG	O9-C10-O7-C8
20	l	5104	LMG	O9-C10-O7-C8
14	A	1106	CLA	C2-C1-O2A-CGA
14	A	1107	CLA	C2-C1-O2A-CGA
14	A	1138	CLA	C2-C1-O2A-CGA
14	A	1237	CLA	C2-C1-O2A-CGA
14	B	1212	CLA	C2-C1-O2A-CGA
14	3	505	CLA	C2-C1-O2A-CGA
14	6	505	CLA	C2-C1-O2A-CGA
14	G	1106	CLA	C2-C1-O2A-CGA
14	G	1107	CLA	C2-C1-O2A-CGA
14	G	1138	CLA	C2-C1-O2A-CGA
14	G	1237	CLA	C2-C1-O2A-CGA
14	H	1212	CLA	C2-C1-O2A-CGA
14	a	505	CLA	C2-C1-O2A-CGA
14	d	505	CLA	C2-C1-O2A-CGA
14	e	1106	CLA	C2-C1-O2A-CGA
14	e	1107	CLA	C2-C1-O2A-CGA
14	e	1138	CLA	C2-C1-O2A-CGA
14	e	1237	CLA	C2-C1-O2A-CGA
14	f	1212	CLA	C2-C1-O2A-CGA
14	s	505	CLA	C2-C1-O2A-CGA
14	v	505	CLA	C2-C1-O2A-CGA
21	B	1852	SQD	O10-C23-O48-C46
21	H	1852	SQD	O10-C23-O48-C46
21	n	5216	SQD	C16-C17-C18-C19
21	L	5216	SQD	C16-C17-C18-C19
14	H	1212	CLA	O1D-CGD-O2D-CED
14	f	1220	CLA	O1A-CGA-O2A-C1
21	f	1852	SQD	O10-C23-O48-C46
18	A	5007	LHG	O6-C4-C5-O7
18	G	5007	LHG	O6-C4-C5-O7
18	e	5007	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	V	5216	SQD	C16-C17-C18-C19
14	a	505	CLA	C4-C3-C5-C6
14	s	505	CLA	C4-C3-C5-C6
14	f	1212	CLA	O1D-CGD-O2D-CED
17	3	522	BCR	C1-C6-C7-C8
17	a	522	BCR	C1-C6-C7-C8
17	s	522	BCR	C1-C6-C7-C8
14	B	1220	CLA	O1A-CGA-O2A-C1
14	B	1212	CLA	O1D-CGD-O2D-CED
14	A	1124	CLA	CBA-CGA-O2A-C1
14	G	1124	CLA	CBA-CGA-O2A-C1
14	e	1124	CLA	CBA-CGA-O2A-C1
14	5	503	CLA	C2A-CAA-CBA-CGA
14	c	503	CLA	C2A-CAA-CBA-CGA
14	u	503	CLA	C2A-CAA-CBA-CGA
17	L	4020	BCR	C20-C21-C22-C23
17	V	4020	BCR	C20-C21-C22-C23
17	n	4020	BCR	C20-C21-C22-C23
14	H	1220	CLA	O1A-CGA-O2A-C1
18	A	5002	LHG	O7-C5-C6-O8
18	G	5002	LHG	O7-C5-C6-O8
18	e	5002	LHG	O7-C5-C6-O8
14	B	1207	CLA	C15-C16-C17-C18
14	H	1207	CLA	C15-C16-C17-C18
14	f	1207	CLA	C15-C16-C17-C18
18	A	5002	LHG	C3-O3-P-O6
18	A	5007	LHG	C3-O3-P-O6
18	A	5001	LHG	C3-O3-P-O6
18	A	5003	LHG	C3-O3-P-O6
18	A	5003	LHG	C4-O6-P-O3
18	I	5001	LHG	C4-O6-P-O3
18	G	5002	LHG	C3-O3-P-O6
18	G	5007	LHG	C3-O3-P-O6
18	G	5001	LHG	C3-O3-P-O6
18	G	5003	LHG	C3-O3-P-O6
18	G	5003	LHG	C4-O6-P-O3
18	S	5001	LHG	C4-O6-P-O3
18	e	5002	LHG	C3-O3-P-O6
18	e	5007	LHG	C3-O3-P-O6
18	e	5001	LHG	C3-O3-P-O6
18	e	5003	LHG	C3-O3-P-O6
18	e	5003	LHG	C4-O6-P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	k	5001	LHG	C4-O6-P-O3
20	B	5002	LMG	C7-C8-C9-O8
20	H	5002	LMG	C7-C8-C9-O8
20	f	5002	LMG	C7-C8-C9-O8
14	A	1022	CLA	C4-C3-C5-C6
14	G	1022	CLA	C4-C3-C5-C6
14	e	1022	CLA	C4-C3-C5-C6
14	A	1103	CLA	C12-C13-C15-C16
14	A	1101	CLA	C6-C7-C8-C10
14	B	1023	CLA	C11-C10-C8-C7
14	B	1208	CLA	C12-C13-C15-C16
14	2	505	CLA	C12-C13-C15-C16
14	G	1103	CLA	C12-C13-C15-C16
14	G	1101	CLA	C6-C7-C8-C10
14	H	1023	CLA	C11-C10-C8-C7
14	H	1208	CLA	C12-C13-C15-C16
14	Z	505	CLA	C12-C13-C15-C16
14	e	1103	CLA	C12-C13-C15-C16
14	e	1101	CLA	C6-C7-C8-C10
14	f	1023	CLA	C11-C10-C8-C7
14	f	1208	CLA	C12-C13-C15-C16
14	r	505	CLA	C12-C13-C15-C16
14	A	1107	CLA	C11-C10-C8-C9
14	A	1139	CLA	C14-C13-C15-C16
14	A	1101	CLA	C11-C10-C8-C9
14	B	1208	CLA	C6-C7-C8-C9
14	B	1210	CLA	C11-C12-C13-C14
14	B	1217	CLA	C6-C7-C8-C9
14	B	1219	CLA	C11-C10-C8-C9
14	B	1229	CLA	C6-C7-C8-C9
14	G	1107	CLA	C11-C10-C8-C9
14	G	1139	CLA	C14-C13-C15-C16
14	G	1101	CLA	C11-C10-C8-C9
14	H	1208	CLA	C6-C7-C8-C9
14	H	1210	CLA	C11-C12-C13-C14
14	H	1217	CLA	C6-C7-C8-C9
14	H	1219	CLA	C11-C10-C8-C9
14	H	1229	CLA	C6-C7-C8-C9
14	e	1107	CLA	C11-C10-C8-C9
14	e	1139	CLA	C14-C13-C15-C16
14	e	1101	CLA	C11-C10-C8-C9
14	f	1210	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1217	CLA	C6-C7-C8-C9
14	f	1219	CLA	C11-C10-C8-C9
14	f	1229	CLA	C6-C7-C8-C9
17	J	4012	BCR	C9-C10-C11-C12
17	T	4012	BCR	C9-C10-C11-C12
17	l	4012	BCR	C9-C10-C11-C12
14	B	1021	CLA	C16-C17-C18-C20
14	H	1021	CLA	C16-C17-C18-C20
14	f	1021	CLA	C16-C17-C18-C20
14	A	1128	CLA	CBA-CGA-O2A-C1
14	G	1128	CLA	CBA-CGA-O2A-C1
14	2	503	CLA	C13-C15-C16-C17
14	Z	503	CLA	C13-C15-C16-C17
14	r	503	CLA	C13-C15-C16-C17
14	A	1128	CLA	O1A-CGA-O2A-C1
14	G	1128	CLA	O1A-CGA-O2A-C1
14	e	1128	CLA	O1A-CGA-O2A-C1
17	1	524	BCR	C11-C12-C13-C35
17	Y	524	BCR	C11-C12-C13-C35
17	q	524	BCR	C11-C12-C13-C35
14	B	1210	CLA	CBA-CGA-O2A-C1
14	H	1210	CLA	CBA-CGA-O2A-C1
14	e	1128	CLA	CBA-CGA-O2A-C1
14	f	1210	CLA	CBA-CGA-O2A-C1
18	L	5220	LHG	C2-C3-O3-P
18	V	5220	LHG	C2-C3-O3-P
18	n	5220	LHG	C2-C3-O3-P
18	V	5220	LHG	C25-C26-C27-C28
18	L	5220	LHG	C25-C26-C27-C28
14	B	1213	CLA	C12-C13-C15-C16
14	H	1213	CLA	C12-C13-C15-C16
14	f	1213	CLA	C12-C13-C15-C16
18	n	5220	LHG	C25-C26-C27-C28
14	B	1021	CLA	C16-C17-C18-C19
14	H	1021	CLA	C16-C17-C18-C19
14	f	1021	CLA	C16-C17-C18-C19
14	A	1011	CLA	CBA-CGA-O2A-C1
14	G	1011	CLA	CBA-CGA-O2A-C1
14	e	1011	CLA	CBA-CGA-O2A-C1
14	e	1130	CLA	C3-C5-C6-C7
14	A	1126	CLA	CAA-CBA-CGA-O2A
14	G	1126	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1126	CLA	CAA-CBA-CGA-O2A
18	G	5003	LHG	C11-C12-C13-C14
18	e	5003	LHG	C11-C12-C13-C14
14	A	1109	CLA	C15-C16-C17-C18
14	G	1109	CLA	C15-C16-C17-C18
14	G	1135	CLA	C5-C6-C7-C8
18	A	5003	LHG	C11-C12-C13-C14
19	A	1848	LMU	O1'-C1-C2-C3
19	G	1848	LMU	O1'-C1-C2-C3
19	e	1848	LMU	O1'-C1-C2-C3
14	A	1106	CLA	C4B-C3B-CAB-CBB
14	A	1108	CLA	C4B-C3B-CAB-CBB
14	A	1109	CLA	C4B-C3B-CAB-CBB
14	A	1133	CLA	C4B-C3B-CAB-CBB
14	B	1203	CLA	C4B-C3B-CAB-CBB
14	F	1301	CLA	C4B-C3B-CAB-CBB
14	1	511	CLA	C4B-C3B-CAB-CBB
14	2	508	CLA	C4B-C3B-CAB-CBB
14	2	518	CLA	C4B-C3B-CAB-CBB
14	3	501	CLA	C4B-C3B-CAB-CBB
14	3	504	CLA	C4B-C3B-CAB-CBB
14	4	504	CLA	C4B-C3B-CAB-CBB
14	4	510	CLA	C4B-C3B-CAB-CBB
14	5	505	CLA	C4B-C3B-CAB-CBB
14	5	506	CLA	C4B-C3B-CAB-CBB
14	5	508	CLA	C4B-C3B-CAB-CBB
14	6	504	CLA	C4B-C3B-CAB-CBB
14	6	506	CLA	C4B-C3B-CAB-CBB
14	G	1106	CLA	C4B-C3B-CAB-CBB
14	G	1108	CLA	C4B-C3B-CAB-CBB
14	G	1109	CLA	C4B-C3B-CAB-CBB
14	G	1133	CLA	C4B-C3B-CAB-CBB
14	H	1203	CLA	C4B-C3B-CAB-CBB
14	R	1301	CLA	C4B-C3B-CAB-CBB
14	Y	511	CLA	C4B-C3B-CAB-CBB
14	Z	508	CLA	C4B-C3B-CAB-CBB
14	Z	518	CLA	C4B-C3B-CAB-CBB
14	a	501	CLA	C4B-C3B-CAB-CBB
14	a	504	CLA	C4B-C3B-CAB-CBB
14	b	504	CLA	C4B-C3B-CAB-CBB
14	b	510	CLA	C4B-C3B-CAB-CBB
14	c	505	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	c	506	CLA	C4B-C3B-CAB-CBB
14	c	508	CLA	C4B-C3B-CAB-CBB
14	d	504	CLA	C4B-C3B-CAB-CBB
14	d	506	CLA	C4B-C3B-CAB-CBB
14	e	1106	CLA	C4B-C3B-CAB-CBB
14	e	1108	CLA	C4B-C3B-CAB-CBB
14	e	1109	CLA	C4B-C3B-CAB-CBB
14	e	1133	CLA	C4B-C3B-CAB-CBB
14	f	1203	CLA	C4B-C3B-CAB-CBB
14	j	1301	CLA	C4B-C3B-CAB-CBB
14	q	511	CLA	C4B-C3B-CAB-CBB
14	r	508	CLA	C4B-C3B-CAB-CBB
14	r	518	CLA	C4B-C3B-CAB-CBB
14	s	501	CLA	C4B-C3B-CAB-CBB
14	s	504	CLA	C4B-C3B-CAB-CBB
14	t	504	CLA	C4B-C3B-CAB-CBB
14	t	510	CLA	C4B-C3B-CAB-CBB
14	u	505	CLA	C4B-C3B-CAB-CBB
14	u	506	CLA	C4B-C3B-CAB-CBB
14	u	508	CLA	C4B-C3B-CAB-CBB
14	v	504	CLA	C4B-C3B-CAB-CBB
14	v	506	CLA	C4B-C3B-CAB-CBB
14	4	513	CLA	C2A-CAA-CBA-CGA
14	b	513	CLA	C2A-CAA-CBA-CGA
14	t	513	CLA	C2A-CAA-CBA-CGA
17	A	4001	BCR	C13-C14-C15-C16
17	3	524	BCR	C9-C10-C11-C12
17	G	4001	BCR	C13-C14-C15-C16
17	a	524	BCR	C9-C10-C11-C12
17	e	4001	BCR	C13-C14-C15-C16
17	s	524	BCR	C9-C10-C11-C12
18	A	5009	LHG	O6-C4-C5-C6
18	G	5009	LHG	O6-C4-C5-C6
18	e	5009	LHG	O6-C4-C5-C6
14	A	1130	CLA	C3-C5-C6-C7
14	G	1130	CLA	C3-C5-C6-C7
14	A	1135	CLA	C5-C6-C7-C8
14	e	1109	CLA	C15-C16-C17-C18
14	e	1135	CLA	C5-C6-C7-C8
18	A	5009	LHG	O6-C4-C5-O7
18	G	5009	LHG	O6-C4-C5-O7
18	e	5009	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1205	CLA	O1A-CGA-O2A-C1
14	H	1205	CLA	O1A-CGA-O2A-C1
14	f	1205	CLA	O1A-CGA-O2A-C1
14	f	1210	CLA	O1A-CGA-O2A-C1
14	B	1210	CLA	O1A-CGA-O2A-C1
14	H	1210	CLA	O1A-CGA-O2A-C1
14	a	510	CLA	O1D-CGD-O2D-CED
18	L	5220	LHG	C26-C27-C28-C29
18	n	5220	LHG	C26-C27-C28-C29
14	A	1801	CLA	CAA-CBA-CGA-O1A
14	1	508	CLA	CAA-CBA-CGA-O2A
14	G	1801	CLA	CAA-CBA-CGA-O1A
14	e	1801	CLA	CAA-CBA-CGA-O1A
14	A	1132	CLA	C2C-C3C-CAC-CBC
14	G	1132	CLA	C2C-C3C-CAC-CBC
14	e	1132	CLA	C2C-C3C-CAC-CBC
18	V	5220	LHG	C26-C27-C28-C29
19	l	5105	LMU	C5-C6-C7-C8
14	Y	508	CLA	CAA-CBA-CGA-O2A
14	q	508	CLA	CAA-CBA-CGA-O2A
14	A	1137	CLA	C2A-CAA-CBA-CGA
14	A	1237	CLA	C2A-CAA-CBA-CGA
14	B	1204	CLA	C2A-CAA-CBA-CGA
14	B	1210	CLA	C2A-CAA-CBA-CGA
14	6	501	CLA	C2A-CAA-CBA-CGA
14	G	1137	CLA	C2A-CAA-CBA-CGA
14	G	1237	CLA	C2A-CAA-CBA-CGA
14	H	1204	CLA	C2A-CAA-CBA-CGA
14	H	1210	CLA	C2A-CAA-CBA-CGA
14	d	501	CLA	C2A-CAA-CBA-CGA
14	e	1137	CLA	C2A-CAA-CBA-CGA
14	e	1237	CLA	C2A-CAA-CBA-CGA
14	f	1204	CLA	C2A-CAA-CBA-CGA
14	f	1210	CLA	C2A-CAA-CBA-CGA
14	v	501	CLA	C2A-CAA-CBA-CGA
19	J	5105	LMU	C5-C6-C7-C8
19	T	5105	LMU	C5-C6-C7-C8
14	G	1011	CLA	CAA-CBA-CGA-O2A
14	3	510	CLA	O1D-CGD-O2D-CED
14	B	1206	CLA	C3A-C2A-CAA-CBA
14	B	1228	CLA	C3A-C2A-CAA-CBA
14	2	512	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	4	517	CLA	C3A-C2A-CAA-CBA
14	H	1206	CLA	C3A-C2A-CAA-CBA
14	H	1228	CLA	C3A-C2A-CAA-CBA
14	Z	512	CLA	C3A-C2A-CAA-CBA
14	b	517	CLA	C3A-C2A-CAA-CBA
14	f	1206	CLA	C3A-C2A-CAA-CBA
14	f	1228	CLA	C3A-C2A-CAA-CBA
14	r	512	CLA	C3A-C2A-CAA-CBA
14	t	517	CLA	C3A-C2A-CAA-CBA
14	e	1124	CLA	O1D-CGD-O2D-CED
14	Y	504	CLA	CBD-CGD-O2D-CED
17	4	521	BCR	C13-C14-C15-C16
17	a	521	BCR	C9-C10-C11-C12
17	b	521	BCR	C13-C14-C15-C16
17	s	521	BCR	C9-C10-C11-C12
17	t	521	BCR	C13-C14-C15-C16
14	u	501	CLA	CAA-CBA-CGA-O2A
14	B	1224	CLA	C4-C3-C5-C6
14	J	1302	CLA	C4-C3-C5-C6
14	H	1224	CLA	C4-C3-C5-C6
14	T	1302	CLA	C4-C3-C5-C6
14	f	1224	CLA	C4-C3-C5-C6
14	l	1302	CLA	C4-C3-C5-C6
14	s	510	CLA	O1D-CGD-O2D-CED
14	1	504	CLA	CBD-CGD-O2D-CED
14	J	1302	CLA	C2-C3-C5-C6
14	T	1302	CLA	C2-C3-C5-C6
14	l	1302	CLA	C2-C3-C5-C6
14	A	1011	CLA	CAA-CBA-CGA-O2A
14	e	1011	CLA	CAA-CBA-CGA-O2A
14	A	1106	CLA	C11-C10-C8-C9
14	A	1126	CLA	C14-C13-C15-C16
14	A	1139	CLA	C11-C12-C13-C14
14	A	1237	CLA	C14-C13-C15-C16
14	G	1106	CLA	C11-C10-C8-C9
14	G	1126	CLA	C14-C13-C15-C16
14	G	1139	CLA	C11-C12-C13-C14
14	G	1237	CLA	C14-C13-C15-C16
14	e	1106	CLA	C11-C10-C8-C9
14	e	1126	CLA	C14-C13-C15-C16
14	e	1139	CLA	C11-C12-C13-C14
14	e	1237	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	k	5001	LHG	C24-C25-C26-C27
14	A	1801	CLA	CAA-CBA-CGA-O2A
14	2	519	CLA	CAA-CBA-CGA-O2A
14	G	1801	CLA	CAA-CBA-CGA-O2A
14	Z	519	CLA	CAA-CBA-CGA-O2A
14	e	1801	CLA	CAA-CBA-CGA-O2A
14	r	519	CLA	CAA-CBA-CGA-O2A
14	G	1129	CLA	CBD-CGD-O2D-CED
18	I	5001	LHG	C24-C25-C26-C27
18	L	5220	LHG	C31-C32-C33-C34
18	S	5001	LHG	C24-C25-C26-C27
18	V	5220	LHG	C31-C32-C33-C34
18	n	5220	LHG	C31-C32-C33-C34
17	A	4011	BCR	C11-C10-C9-C34
17	A	4011	BCR	C16-C17-C18-C36
17	B	4006	BCR	C11-C10-C9-C34
17	B	4006	BCR	C20-C21-C22-C37
17	F	4016	BCR	C35-C13-C14-C15
17	L	4020	BCR	C20-C21-C22-C37
17	G	4011	BCR	C11-C10-C9-C34
17	G	4011	BCR	C16-C17-C18-C36
17	H	4006	BCR	C11-C10-C9-C34
17	H	4006	BCR	C20-C21-C22-C37
17	R	4016	BCR	C35-C13-C14-C15
17	V	4020	BCR	C20-C21-C22-C37
17	e	4011	BCR	C11-C10-C9-C34
17	e	4011	BCR	C16-C17-C18-C36
17	f	4006	BCR	C11-C10-C9-C34
17	f	4006	BCR	C20-C21-C22-C37
17	j	4016	BCR	C35-C13-C14-C15
17	n	4020	BCR	C20-C21-C22-C37
21	B	1852	SQD	C44-C45-C46-O48
21	L	5216	SQD	O6-C44-C45-C46
21	2	822	SQD	C44-C45-C46-O48
21	4	822	SQD	O6-C44-C45-C46
21	H	1852	SQD	C44-C45-C46-O48
21	V	5216	SQD	O6-C44-C45-C46
21	Z	822	SQD	C44-C45-C46-O48
21	b	822	SQD	O6-C44-C45-C46
21	f	1852	SQD	C44-C45-C46-O48
21	n	5216	SQD	O6-C44-C45-C46
21	r	822	SQD	C44-C45-C46-O48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	t	822	SQD	O6-C44-C45-C46
14	3	518	CLA	C3-C5-C6-C7
14	a	518	CLA	C3-C5-C6-C7
14	s	518	CLA	C3-C5-C6-C7
14	1	508	CLA	CAA-CBA-CGA-O1A
14	4	508	CLA	CAA-CBA-CGA-O1A
14	b	508	CLA	CAA-CBA-CGA-O1A
14	c	501	CLA	CAA-CBA-CGA-O2A
14	q	508	CLA	CAA-CBA-CGA-O1A
14	t	508	CLA	CAA-CBA-CGA-O1A
14	B	1216	CLA	C2A-CAA-CBA-CGA
14	3	503	CLA	C2A-CAA-CBA-CGA
14	4	502	CLA	C2A-CAA-CBA-CGA
14	H	1216	CLA	C2A-CAA-CBA-CGA
14	a	503	CLA	C2A-CAA-CBA-CGA
14	b	502	CLA	C2A-CAA-CBA-CGA
14	f	1216	CLA	C2A-CAA-CBA-CGA
14	t	502	CLA	C2A-CAA-CBA-CGA
14	A	1124	CLA	O1D-CGD-O2D-CED
20	B	5002	LMG	C40-C41-C42-C43
20	H	5002	LMG	C40-C41-C42-C43
14	A	1117	CLA	C16-C17-C18-C19
14	B	1229	CLA	C16-C17-C18-C19
14	G	1117	CLA	C16-C17-C18-C19
14	H	1229	CLA	C16-C17-C18-C19
14	e	1117	CLA	C16-C17-C18-C19
14	f	1229	CLA	C16-C17-C18-C19
14	A	1126	CLA	O2A-C1-C2-C3
14	B	1216	CLA	O2A-C1-C2-C3
14	G	1126	CLA	O2A-C1-C2-C3
14	H	1216	CLA	O2A-C1-C2-C3
14	e	1126	CLA	O2A-C1-C2-C3
14	f	1216	CLA	O2A-C1-C2-C3
18	A	5004	LHG	O2-C2-C3-O3
18	G	5004	LHG	O2-C2-C3-O3
18	e	5004	LHG	O2-C2-C3-O3
14	B	1236	CLA	CBA-CGA-O2A-C1
14	H	1236	CLA	CBA-CGA-O2A-C1
14	f	1236	CLA	CBA-CGA-O2A-C1
14	G	1124	CLA	O1D-CGD-O2D-CED
20	f	5002	LMG	C40-C41-C42-C43
14	5	501	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Y	508	CLA	CAA-CBA-CGA-O1A
17	A	4011	BCR	C7-C8-C9-C34
17	G	4011	BCR	C7-C8-C9-C34
17	e	4011	BCR	C7-C8-C9-C34
14	A	1123	CLA	C13-C15-C16-C17
14	G	1123	CLA	C13-C15-C16-C17
14	q	504	CLA	CBD-CGD-O2D-CED
18	e	5004	LHG	C28-C29-C30-C31
18	A	5004	LHG	C28-C29-C30-C31
18	G	5004	LHG	C28-C29-C30-C31
14	4	508	CLA	CAA-CBA-CGA-O2A
14	5	501	CLA	CAA-CBA-CGA-O1A
14	6	510	CLA	CAA-CBA-CGA-O2A
14	6	517	CLA	CAA-CBA-CGA-O1A
14	b	508	CLA	CAA-CBA-CGA-O2A
14	d	510	CLA	CAA-CBA-CGA-O2A
14	d	517	CLA	CAA-CBA-CGA-O1A
14	t	508	CLA	CAA-CBA-CGA-O2A
14	v	510	CLA	CAA-CBA-CGA-O2A
14	v	517	CLA	CAA-CBA-CGA-O1A
21	5	822	SQD	C46-C45-O47-C7
21	c	822	SQD	C46-C45-O47-C7
21	u	822	SQD	C46-C45-O47-C7
14	A	1022	CLA	C15-C16-C17-C18
14	G	1022	CLA	C15-C16-C17-C18
14	e	1123	CLA	C13-C15-C16-C17
14	A	1111	CLA	C1A-C2A-CAA-CBA
14	A	1128	CLA	C1A-C2A-CAA-CBA
14	B	1206	CLA	C1A-C2A-CAA-CBA
14	B	1228	CLA	C1A-C2A-CAA-CBA
14	L	1502	CLA	C1A-C2A-CAA-CBA
14	2	504	CLA	C1A-C2A-CAA-CBA
14	2	512	CLA	C1A-C2A-CAA-CBA
14	3	508	CLA	C1A-C2A-CAA-CBA
14	4	516	CLA	C1A-C2A-CAA-CBA
14	5	506	CLA	C1A-C2A-CAA-CBA
14	6	517	CLA	C1A-C2A-CAA-CBA
14	G	1111	CLA	C1A-C2A-CAA-CBA
14	G	1128	CLA	C1A-C2A-CAA-CBA
14	H	1206	CLA	C1A-C2A-CAA-CBA
14	H	1228	CLA	C1A-C2A-CAA-CBA
14	V	1502	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Z	504	CLA	C1A-C2A-CAA-CBA
14	Z	512	CLA	C1A-C2A-CAA-CBA
14	a	508	CLA	C1A-C2A-CAA-CBA
14	b	516	CLA	C1A-C2A-CAA-CBA
14	c	506	CLA	C1A-C2A-CAA-CBA
14	d	517	CLA	C1A-C2A-CAA-CBA
14	e	1111	CLA	C1A-C2A-CAA-CBA
14	e	1128	CLA	C1A-C2A-CAA-CBA
14	f	1206	CLA	C1A-C2A-CAA-CBA
14	f	1228	CLA	C1A-C2A-CAA-CBA
14	n	1502	CLA	C1A-C2A-CAA-CBA
14	r	504	CLA	C1A-C2A-CAA-CBA
14	r	512	CLA	C1A-C2A-CAA-CBA
14	s	508	CLA	C1A-C2A-CAA-CBA
14	t	516	CLA	C1A-C2A-CAA-CBA
14	u	506	CLA	C1A-C2A-CAA-CBA
14	v	517	CLA	C1A-C2A-CAA-CBA
14	A	1137	CLA	C11-C10-C8-C7
14	A	1101	CLA	C12-C13-C15-C16
14	B	1215	CLA	C6-C7-C8-C10
14	B	1235	CLA	C6-C7-C8-C10
14	G	1137	CLA	C11-C10-C8-C7
14	G	1101	CLA	C12-C13-C15-C16
14	H	1215	CLA	C6-C7-C8-C10
14	H	1235	CLA	C6-C7-C8-C10
14	e	1137	CLA	C11-C10-C8-C7
14	e	1101	CLA	C12-C13-C15-C16
14	f	1215	CLA	C6-C7-C8-C10
14	f	1235	CLA	C6-C7-C8-C10
14	A	1237	CLA	C8-C10-C11-C12
14	G	1237	CLA	C8-C10-C11-C12
14	e	1237	CLA	C8-C10-C11-C12
14	1	501	CLA	CAA-CBA-CGA-O2A
14	2	519	CLA	CAA-CBA-CGA-O1A
14	Y	501	CLA	CAA-CBA-CGA-O2A
14	q	501	CLA	CAA-CBA-CGA-O2A
14	r	519	CLA	CAA-CBA-CGA-O1A
17	3	521	BCR	C9-C10-C11-C12
14	A	1129	CLA	CBD-CGD-O2D-CED
14	A	1011	CLA	O1A-CGA-O2A-C1
14	Z	519	CLA	CAA-CBA-CGA-O1A
14	c	501	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	501	CLA	CAA-CBA-CGA-O1A
14	e	1022	CLA	C15-C16-C17-C18
14	A	1109	CLA	C3-C5-C6-C7
14	A	1110	CLA	C3-C5-C6-C7
14	G	1109	CLA	C3-C5-C6-C7
14	G	1110	CLA	C3-C5-C6-C7
14	e	1110	CLA	C3-C5-C6-C7
14	2	503	CLA	C2A-CAA-CBA-CGA
14	Z	503	CLA	C2A-CAA-CBA-CGA
14	r	503	CLA	C2A-CAA-CBA-CGA
14	s	503	CLA	C2A-CAA-CBA-CGA
14	A	1116	CLA	C8-C10-C11-C12
14	G	1116	CLA	C8-C10-C11-C12
19	J	5105	LMU	C2-C3-C4-C5
19	T	5105	LMU	C2-C3-C4-C5
19	l	5105	LMU	C2-C3-C4-C5
14	G	1011	CLA	O1A-CGA-O2A-C1
14	5	519	CLA	CAA-CBA-CGA-O2A
14	c	519	CLA	CAA-CBA-CGA-O1A
14	c	519	CLA	CAA-CBA-CGA-O2A
14	q	501	CLA	CAA-CBA-CGA-O1A
14	u	519	CLA	CAA-CBA-CGA-O2A
14	e	1116	CLA	C8-C10-C11-C12
18	L	5221	LHG	C12-C13-C14-C15
18	V	5221	LHG	C12-C13-C14-C15
18	n	5221	LHG	C12-C13-C14-C15
15	G	2001	PQN	C23-C25-C26-C27
15	e	2001	PQN	C23-C25-C26-C27
14	1	501	CLA	CAA-CBA-CGA-O1A
14	5	510	CLA	CAA-CBA-CGA-O2A
14	5	519	CLA	CAA-CBA-CGA-O1A
14	c	510	CLA	CAA-CBA-CGA-O2A
14	u	510	CLA	CAA-CBA-CGA-O2A
14	u	519	CLA	CAA-CBA-CGA-O1A
15	A	2001	PQN	C23-C25-C26-C27
14	e	1129	CLA	CBD-CGD-O2D-CED
14	G	1022	CLA	C2-C3-C5-C6
14	A	1108	CLA	C2B-C3B-CAB-CBB
14	A	1124	CLA	C2B-C3B-CAB-CBB
14	A	1133	CLA	C2B-C3B-CAB-CBB
14	A	1137	CLA	C2B-C3B-CAB-CBB
14	B	1209	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1236	CLA	C2B-C3B-CAB-CBB
14	2	507	CLA	C2B-C3B-CAB-CBB
14	3	501	CLA	C2B-C3B-CAB-CBB
14	3	504	CLA	C2B-C3B-CAB-CBB
14	5	506	CLA	C2B-C3B-CAB-CBB
14	6	504	CLA	C2B-C3B-CAB-CBB
14	G	1108	CLA	C2B-C3B-CAB-CBB
14	G	1124	CLA	C2B-C3B-CAB-CBB
14	G	1133	CLA	C2B-C3B-CAB-CBB
14	G	1137	CLA	C2B-C3B-CAB-CBB
14	H	1209	CLA	C2B-C3B-CAB-CBB
14	H	1236	CLA	C2B-C3B-CAB-CBB
14	Z	507	CLA	C2B-C3B-CAB-CBB
14	a	501	CLA	C2B-C3B-CAB-CBB
14	a	504	CLA	C2B-C3B-CAB-CBB
14	c	506	CLA	C2B-C3B-CAB-CBB
14	d	504	CLA	C2B-C3B-CAB-CBB
14	e	1108	CLA	C2B-C3B-CAB-CBB
14	e	1124	CLA	C2B-C3B-CAB-CBB
14	e	1133	CLA	C2B-C3B-CAB-CBB
14	e	1137	CLA	C2B-C3B-CAB-CBB
14	f	1209	CLA	C2B-C3B-CAB-CBB
14	f	1236	CLA	C2B-C3B-CAB-CBB
14	r	507	CLA	C2B-C3B-CAB-CBB
14	s	501	CLA	C2B-C3B-CAB-CBB
14	s	504	CLA	C2B-C3B-CAB-CBB
14	u	506	CLA	C2B-C3B-CAB-CBB
14	4	510	CLA	CAA-CBA-CGA-O1A
14	6	510	CLA	CAA-CBA-CGA-O1A
14	Y	501	CLA	CAA-CBA-CGA-O1A
14	b	510	CLA	CAA-CBA-CGA-O1A
14	d	510	CLA	CAA-CBA-CGA-O1A
14	t	510	CLA	CAA-CBA-CGA-O1A
14	u	510	CLA	CAA-CBA-CGA-O1A
14	v	510	CLA	CAA-CBA-CGA-O1A
14	G	1124	CLA	O1A-CGA-O2A-C1
14	e	1011	CLA	O1A-CGA-O2A-C1
14	e	1124	CLA	O1A-CGA-O2A-C1
14	e	1109	CLA	C3-C5-C6-C7
17	A	4011	BCR	C11-C10-C9-C8
17	A	4011	BCR	C16-C17-C18-C19
17	B	4006	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	4006	BCR	C20-C21-C22-C23
17	F	4016	BCR	C12-C13-C14-C15
17	G	4011	BCR	C11-C10-C9-C8
17	G	4011	BCR	C16-C17-C18-C19
17	H	4006	BCR	C11-C10-C9-C8
17	H	4006	BCR	C20-C21-C22-C23
17	R	4016	BCR	C12-C13-C14-C15
17	e	4011	BCR	C11-C10-C9-C8
17	e	4011	BCR	C16-C17-C18-C19
17	f	4006	BCR	C11-C10-C9-C8
17	f	4006	BCR	C20-C21-C22-C23
17	j	4016	BCR	C12-C13-C14-C15
14	4	510	CLA	CAA-CBA-CGA-O2A
14	5	510	CLA	CAA-CBA-CGA-O1A
14	b	501	CLA	CAA-CBA-CGA-O1A
14	b	510	CLA	CAA-CBA-CGA-O2A
14	c	510	CLA	CAA-CBA-CGA-O1A
14	t	510	CLA	CAA-CBA-CGA-O2A
21	L	5216	SQD	O6-C44-C45-O47
21	V	5216	SQD	O6-C44-C45-O47
21	n	5216	SQD	O6-C44-C45-O47
18	A	5001	LHG	C24-C25-C26-C27
17	A	4008	BCR	C19-C20-C21-C22
17	G	4008	BCR	C19-C20-C21-C22
17	e	4008	BCR	C19-C20-C21-C22
14	4	501	CLA	CAA-CBA-CGA-O1A
14	d	519	CLA	CAA-CBA-CGA-O1A
14	t	501	CLA	CAA-CBA-CGA-O1A
14	A	1101	CLA	C15-C16-C17-C18
14	G	1101	CLA	C15-C16-C17-C18
14	e	1101	CLA	C15-C16-C17-C18
14	A	1124	CLA	O1A-CGA-O2A-C1
18	e	5001	LHG	C24-C25-C26-C27
14	B	1220	CLA	C6-C7-C8-C10
14	H	1220	CLA	C6-C7-C8-C10
18	I	5001	LHG	C30-C31-C32-C33
18	G	5001	LHG	C24-C25-C26-C27
18	k	5001	LHG	C30-C31-C32-C33
18	S	5001	LHG	C30-C31-C32-C33
14	1	510	CLA	CAA-CBA-CGA-O2A
14	3	519	CLA	CAA-CBA-CGA-O2A
14	4	512	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	6	519	CLA	CAA-CBA-CGA-O1A
14	Y	510	CLA	CAA-CBA-CGA-O2A
14	a	519	CLA	CAA-CBA-CGA-O2A
14	b	512	CLA	CAA-CBA-CGA-O2A
14	d	517	CLA	CAA-CBA-CGA-O2A
14	q	510	CLA	CAA-CBA-CGA-O2A
14	s	519	CLA	CAA-CBA-CGA-O2A
14	t	512	CLA	CAA-CBA-CGA-O1A
14	t	512	CLA	CAA-CBA-CGA-O2A
14	v	519	CLA	CAA-CBA-CGA-O1A
18	B	1842	LHG	C24-C25-C26-C27
18	H	1842	LHG	C24-C25-C26-C27
18	f	1842	LHG	C24-C25-C26-C27
14	B	1207	CLA	C2-C1-O2A-CGA
14	H	1207	CLA	C2-C1-O2A-CGA
14	f	1207	CLA	C2-C1-O2A-CGA
14	q	504	CLA	O1D-CGD-O2D-CED
14	A	1022	CLA	C2-C3-C5-C6
14	B	1224	CLA	C2-C3-C5-C6
14	H	1224	CLA	C2-C3-C5-C6
14	e	1022	CLA	C2-C3-C5-C6
14	f	1224	CLA	C2-C3-C5-C6
19	B	1843	LMU	C6-C7-C8-C9
19	H	1843	LMU	C6-C7-C8-C9
19	f	1843	LMU	C6-C7-C8-C9
14	4	512	CLA	CAA-CBA-CGA-O1A
14	6	517	CLA	CAA-CBA-CGA-O2A
14	Y	510	CLA	CAA-CBA-CGA-O1A
14	b	512	CLA	CAA-CBA-CGA-O1A
14	q	510	CLA	CAA-CBA-CGA-O1A
14	v	517	CLA	CAA-CBA-CGA-O2A
14	B	1202	CLA	CAA-CBA-CGA-O2A
14	e	1116	CLA	CAA-CBA-CGA-O2A
14	f	1202	CLA	CAA-CBA-CGA-O2A
14	f	1220	CLA	C6-C7-C8-C10
14	A	1103	CLA	C14-C13-C15-C16
14	B	1023	CLA	C11-C10-C8-C9
14	B	1204	CLA	C11-C10-C8-C9
14	B	1215	CLA	C14-C13-C15-C16
14	G	1103	CLA	C14-C13-C15-C16
14	H	1023	CLA	C11-C10-C8-C9
14	H	1204	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1215	CLA	C14-C13-C15-C16
14	e	1103	CLA	C14-C13-C15-C16
14	f	1023	CLA	C11-C10-C8-C9
14	f	1204	CLA	C11-C10-C8-C9
14	f	1215	CLA	C14-C13-C15-C16
14	2	509	CLA	O1A-CGA-O2A-C1
14	Z	509	CLA	O1A-CGA-O2A-C1
14	r	509	CLA	O1A-CGA-O2A-C1
14	1	510	CLA	CAA-CBA-CGA-O1A
14	A	1116	CLA	CAA-CBA-CGA-O2A
14	2	518	CLA	CAA-CBA-CGA-O2A
14	H	1202	CLA	CAA-CBA-CGA-O2A
14	Z	518	CLA	CAA-CBA-CGA-O2A
14	r	518	CLA	CAA-CBA-CGA-O2A
18	A	5008	LHG	C9-C10-C11-C12
18	G	5008	LHG	C9-C10-C11-C12
18	e	5005	LHG	C30-C31-C32-C33
14	1	504	CLA	O1D-CGD-O2D-CED
18	A	5005	LHG	C30-C31-C32-C33
18	G	5005	LHG	C30-C31-C32-C33
18	e	5008	LHG	C9-C10-C11-C12
14	A	1013	CLA	C2A-CAA-CBA-CGA
14	G	1013	CLA	C2A-CAA-CBA-CGA
14	e	1013	CLA	C2A-CAA-CBA-CGA
14	H	1202	CLA	C16-C17-C18-C20
14	6	519	CLA	CAA-CBA-CGA-O2A
14	d	519	CLA	CAA-CBA-CGA-O2A
14	v	519	CLA	CAA-CBA-CGA-O2A
14	B	1236	CLA	O1A-CGA-O2A-C1
14	H	1236	CLA	O1A-CGA-O2A-C1
14	f	1236	CLA	O1A-CGA-O2A-C1
17	A	4001	BCR	C1-C6-C7-C8
17	A	4008	BCR	C1-C6-C7-C8
17	B	4014	BCR	C1-C6-C7-C8
17	B	4014	BCR	C5-C6-C7-C8
17	L	4022	BCR	C23-C24-C25-C30
17	L	4020	BCR	C23-C24-C25-C30
17	4	523	BCR	C1-C6-C7-C8
17	5	521	BCR	C1-C6-C7-C8
17	6	524	BCR	C1-C6-C7-C8
17	G	4001	BCR	C1-C6-C7-C8
17	G	4008	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	4014	BCR	C1-C6-C7-C8
17	V	4022	BCR	C23-C24-C25-C30
17	V	4020	BCR	C23-C24-C25-C30
17	b	523	BCR	C1-C6-C7-C8
17	c	521	BCR	C1-C6-C7-C8
17	d	524	BCR	C1-C6-C7-C8
17	d	524	BCR	C23-C24-C25-C30
17	e	4001	BCR	C1-C6-C7-C8
17	e	4008	BCR	C1-C6-C7-C8
17	f	4014	BCR	C1-C6-C7-C8
17	f	4014	BCR	C5-C6-C7-C8
17	n	4022	BCR	C23-C24-C25-C30
17	n	4020	BCR	C23-C24-C25-C30
17	t	523	BCR	C1-C6-C7-C8
17	u	521	BCR	C1-C6-C7-C8
17	v	524	BCR	C1-C6-C7-C8
14	Y	504	CLA	O1D-CGD-O2D-CED
14	G	1116	CLA	CAA-CBA-CGA-O2A
21	3	822	SQD	O6-C44-C45-C46
21	a	822	SQD	O6-C44-C45-C46
21	s	822	SQD	O6-C44-C45-C46
18	A	5007	LHG	O1-C1-C2-C3
18	G	5007	LHG	O1-C1-C2-C3
18	e	5007	LHG	O1-C1-C2-C3
14	B	1228	CLA	O1A-CGA-O2A-C1
17	A	4011	BCR	C19-C20-C21-C22
17	1	522	BCR	C15-C16-C17-C18
17	4	521	BCR	C15-C16-C17-C18
17	G	4011	BCR	C19-C20-C21-C22
17	Y	522	BCR	C15-C16-C17-C18
17	b	521	BCR	C15-C16-C17-C18
17	e	4011	BCR	C19-C20-C21-C22
17	q	522	BCR	C15-C16-C17-C18
17	t	521	BCR	C15-C16-C17-C18
14	A	1106	CLA	C4-C3-C5-C6
14	G	1106	CLA	C4-C3-C5-C6
14	e	1106	CLA	C4-C3-C5-C6
17	B	4010	BCR	C11-C12-C13-C14
17	J	4015	BCR	C7-C8-C9-C10
17	2	523	BCR	C7-C8-C9-C10
17	H	4010	BCR	C11-C12-C13-C14
17	T	4015	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	Z	523	BCR	C7-C8-C9-C10
17	f	4010	BCR	C11-C12-C13-C14
17	l	4015	BCR	C7-C8-C9-C10
17	r	523	BCR	C7-C8-C9-C10
14	A	1107	CLA	C2-C3-C5-C6
14	B	1202	CLA	C2-C3-C5-C6
14	G	1107	CLA	C2-C3-C5-C6
14	H	1202	CLA	C2-C3-C5-C6
14	e	1107	CLA	C2-C3-C5-C6
14	f	1202	CLA	C2-C3-C5-C6
14	1	505	CLA	CAA-CBA-CGA-O2A
14	4	501	CLA	CAA-CBA-CGA-O2A
14	5	507	CLA	CAA-CBA-CGA-O2A
14	6	501	CLA	CAA-CBA-CGA-O2A
14	b	501	CLA	CAA-CBA-CGA-O2A
14	c	507	CLA	CAA-CBA-CGA-O2A
14	d	501	CLA	CAA-CBA-CGA-O2A
14	q	505	CLA	CAA-CBA-CGA-O2A
14	t	501	CLA	CAA-CBA-CGA-O2A
14	u	507	CLA	CAA-CBA-CGA-O2A
14	H	1201	CLA	C8-C10-C11-C12
18	A	5001	LHG	C19-C20-C21-C22
18	e	5001	LHG	C19-C20-C21-C22
14	B	1201	CLA	C8-C10-C11-C12
14	1	507	CLA	CAA-CBA-CGA-O2A
14	6	509	CLA	CAA-CBA-CGA-O2A
14	Y	505	CLA	CAA-CBA-CGA-O2A
14	Y	507	CLA	CAA-CBA-CGA-O2A
14	d	509	CLA	CAA-CBA-CGA-O2A
14	q	507	CLA	CAA-CBA-CGA-O2A
14	v	501	CLA	CAA-CBA-CGA-O2A
14	v	509	CLA	CAA-CBA-CGA-O2A
14	H	1228	CLA	O1A-CGA-O2A-C1
14	f	1228	CLA	O1A-CGA-O2A-C1
18	G	5001	LHG	C19-C20-C21-C22
14	B	1202	CLA	C16-C17-C18-C20
14	f	1202	CLA	C16-C17-C18-C20
18	A	5005	LHG	C26-C27-C28-C29
18	G	5005	LHG	C26-C27-C28-C29
18	e	5005	LHG	C26-C27-C28-C29
14	e	1129	CLA	O1D-CGD-O2D-CED
14	f	1201	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	L	5221	LHG	C23-C24-C25-C26
18	V	5221	LHG	C23-C24-C25-C26
18	n	5221	LHG	C23-C24-C25-C26
14	5	512	CLA	CAA-CBA-CGA-O2A
14	u	512	CLA	CAA-CBA-CGA-O2A
20	B	5002	LMG	C38-C39-C40-C41
14	G	1126	CLA	O1A-CGA-O2A-C1
20	H	5002	LMG	C38-C39-C40-C41
20	f	5002	LMG	C38-C39-C40-C41
14	2	507	CLA	CAA-CBA-CGA-O2A
14	2	510	CLA	CAA-CBA-CGA-O1A
14	4	513	CLA	CAA-CBA-CGA-O2A
14	Z	507	CLA	CAA-CBA-CGA-O2A
14	Z	510	CLA	CAA-CBA-CGA-O1A
14	b	513	CLA	CAA-CBA-CGA-O2A
14	c	512	CLA	CAA-CBA-CGA-O2A
14	r	507	CLA	CAA-CBA-CGA-O2A
14	t	513	CLA	CAA-CBA-CGA-O2A
14	G	1129	CLA	O1D-CGD-O2D-CED
14	A	1117	CLA	C4B-C3B-CAB-CBB
14	A	1119	CLA	C4B-C3B-CAB-CBB
14	A	1124	CLA	C4B-C3B-CAB-CBB
14	B	1204	CLA	C4B-C3B-CAB-CBB
14	B	1210	CLA	C4B-C3B-CAB-CBB
14	2	503	CLA	C4B-C3B-CAB-CBB
14	2	507	CLA	C4B-C3B-CAB-CBB
14	2	512	CLA	C4B-C3B-CAB-CBB
14	4	511	CLA	C4B-C3B-CAB-CBB
14	6	508	CLA	C4B-C3B-CAB-CBB
14	G	1117	CLA	C4B-C3B-CAB-CBB
14	G	1119	CLA	C4B-C3B-CAB-CBB
14	G	1124	CLA	C4B-C3B-CAB-CBB
14	H	1204	CLA	C4B-C3B-CAB-CBB
14	H	1210	CLA	C4B-C3B-CAB-CBB
14	Z	503	CLA	C4B-C3B-CAB-CBB
14	Z	507	CLA	C4B-C3B-CAB-CBB
14	Z	512	CLA	C4B-C3B-CAB-CBB
14	b	511	CLA	C4B-C3B-CAB-CBB
14	d	508	CLA	C4B-C3B-CAB-CBB
14	e	1117	CLA	C4B-C3B-CAB-CBB
14	e	1119	CLA	C4B-C3B-CAB-CBB
14	e	1124	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	f	1204	CLA	C4B-C3B-CAB-CBB
14	f	1210	CLA	C4B-C3B-CAB-CBB
14	r	503	CLA	C4B-C3B-CAB-CBB
14	r	507	CLA	C4B-C3B-CAB-CBB
14	r	512	CLA	C4B-C3B-CAB-CBB
14	t	511	CLA	C4B-C3B-CAB-CBB
14	v	508	CLA	C4B-C3B-CAB-CBB
14	A	1126	CLA	O1A-CGA-O2A-C1
14	e	1126	CLA	O1A-CGA-O2A-C1
14	B	1240	CLA	C4-C3-C5-C6
14	H	1240	CLA	C4-C3-C5-C6
14	f	1240	CLA	C4-C3-C5-C6
14	A	1129	CLA	O1D-CGD-O2D-CED
14	A	1101	CLA	C11-C10-C8-C7
14	B	1203	CLA	C11-C10-C8-C7
14	B	1205	CLA	C12-C13-C15-C16
14	B	1213	CLA	C6-C7-C8-C10
14	B	1229	CLA	C6-C7-C8-C10
14	L	1501	CLA	C11-C10-C8-C7
14	G	1101	CLA	C11-C10-C8-C7
14	H	1203	CLA	C11-C10-C8-C7
14	H	1205	CLA	C12-C13-C15-C16
14	H	1213	CLA	C6-C7-C8-C10
14	H	1229	CLA	C6-C7-C8-C10
14	V	1501	CLA	C11-C10-C8-C7
14	e	1101	CLA	C11-C10-C8-C7
14	f	1203	CLA	C11-C10-C8-C7
14	f	1205	CLA	C12-C13-C15-C16
14	f	1213	CLA	C6-C7-C8-C10
14	f	1229	CLA	C6-C7-C8-C10
14	n	1501	CLA	C11-C10-C8-C7
14	2	510	CLA	CAA-CBA-CGA-O2A
14	6	511	CLA	CAA-CBA-CGA-O2A
14	Z	510	CLA	CAA-CBA-CGA-O2A
14	d	511	CLA	CAA-CBA-CGA-O2A
14	r	510	CLA	CAA-CBA-CGA-O1A
14	r	510	CLA	CAA-CBA-CGA-O2A
14	s	519	CLA	CAA-CBA-CGA-O1A
14	v	511	CLA	CAA-CBA-CGA-O2A
21	H	1852	SQD	C26-C27-C28-C29
21	B	1852	SQD	C26-C27-C28-C29
17	6	521	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	d	521	BCR	C9-C10-C11-C12
17	v	521	BCR	C9-C10-C11-C12
14	3	519	CLA	CAA-CBA-CGA-O1A
21	f	1852	SQD	C26-C27-C28-C29
14	6	509	CLA	CAA-CBA-CGA-O1A
14	6	512	CLA	CAA-CBA-CGA-O2A
14	a	519	CLA	CAA-CBA-CGA-O1A
14	B	1203	CLA	CAA-CBA-CGA-O2A
14	H	1203	CLA	CAA-CBA-CGA-O2A
14	f	1203	CLA	CAA-CBA-CGA-O2A
14	1	508	CLA	C2A-CAA-CBA-CGA
14	Y	508	CLA	C2A-CAA-CBA-CGA
14	q	508	CLA	C2A-CAA-CBA-CGA
14	4	507	CLA	CAA-CBA-CGA-O2A
14	b	507	CLA	CAA-CBA-CGA-O2A
14	d	509	CLA	CAA-CBA-CGA-O1A
14	d	512	CLA	CAA-CBA-CGA-O2A
14	v	507	CLA	CAA-CBA-CGA-O2A
14	v	509	CLA	CAA-CBA-CGA-O1A
14	v	512	CLA	CAA-CBA-CGA-O2A
14	s	509	CLA	O1D-CGD-O2D-CED
14	A	1013	CLA	C4-C3-C5-C6
14	A	1126	CLA	C4-C3-C5-C6
14	A	1127	CLA	C4-C3-C5-C6
14	G	1013	CLA	C4-C3-C5-C6
14	G	1126	CLA	C4-C3-C5-C6
14	G	1127	CLA	C4-C3-C5-C6
14	e	1013	CLA	C4-C3-C5-C6
14	e	1126	CLA	C4-C3-C5-C6
14	e	1127	CLA	C4-C3-C5-C6
14	6	507	CLA	CAA-CBA-CGA-O2A
14	Y	516	CLA	CAA-CBA-CGA-O2A
14	d	507	CLA	CAA-CBA-CGA-O2A
14	t	507	CLA	CAA-CBA-CGA-O2A
14	3	505	CLA	C2-C3-C5-C6
14	a	505	CLA	C2-C3-C5-C6
14	s	505	CLA	C2-C3-C5-C6
14	H	1228	CLA	CBA-CGA-O2A-C1
14	A	1123	CLA	CAA-CBA-CGA-O2A
14	A	1138	CLA	C11-C12-C13-C14
14	B	1227	CLA	C6-C7-C8-C9
14	B	1235	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	2	505	CLA	C6-C7-C8-C9
14	2	505	CLA	C14-C13-C15-C16
14	G	1138	CLA	C11-C12-C13-C14
14	H	1227	CLA	C6-C7-C8-C9
14	H	1235	CLA	C6-C7-C8-C9
14	Z	505	CLA	C6-C7-C8-C9
14	Z	505	CLA	C14-C13-C15-C16
14	e	1138	CLA	C11-C12-C13-C14
14	f	1227	CLA	C6-C7-C8-C9
14	f	1235	CLA	C6-C7-C8-C9
14	r	505	CLA	C6-C7-C8-C9
14	r	505	CLA	C14-C13-C15-C16
18	L	5218	LHG	C9-C10-C11-C12
18	V	5218	LHG	C9-C10-C11-C12
14	1	512	CLA	CAA-CBA-CGA-O2A
14	4	519	CLA	CAA-CBA-CGA-O2A
14	Y	512	CLA	CAA-CBA-CGA-O2A
14	Y	513	CLA	CAA-CBA-CGA-O2A
14	b	519	CLA	CAA-CBA-CGA-O2A
14	q	512	CLA	CAA-CBA-CGA-O2A
14	t	519	CLA	CAA-CBA-CGA-O2A
18	n	5218	LHG	C9-C10-C11-C12
14	A	1111	CLA	C3A-C2A-CAA-CBA
14	4	516	CLA	C3A-C2A-CAA-CBA
14	G	1111	CLA	C3A-C2A-CAA-CBA
14	b	516	CLA	C3A-C2A-CAA-CBA
14	e	1111	CLA	C3A-C2A-CAA-CBA
14	t	516	CLA	C3A-C2A-CAA-CBA
14	3	509	CLA	O1D-CGD-O2D-CED
20	J	5104	LMG	O10-C28-O8-C9
20	T	5104	LMG	O10-C28-O8-C9
20	l	5104	LMG	O10-C28-O8-C9
14	G	1123	CLA	CAA-CBA-CGA-O2A
14	e	1123	CLA	CAA-CBA-CGA-O2A
14	1	509	CLA	CAA-CBA-CGA-O2A
14	1	513	CLA	CAA-CBA-CGA-O2A
14	1	516	CLA	CAA-CBA-CGA-O2A
14	1	517	CLA	CAA-CBA-CGA-O2A
14	2	512	CLA	CAA-CBA-CGA-O2A
14	3	507	CLA	CAA-CBA-CGA-O2A
14	6	504	CLA	CAA-CBA-CGA-O2A
14	Y	509	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Z	512	CLA	CAA-CBA-CGA-O2A
14	a	507	CLA	CAA-CBA-CGA-O2A
14	d	516	CLA	CAA-CBA-CGA-O2A
14	q	509	CLA	CAA-CBA-CGA-O2A
14	q	513	CLA	CAA-CBA-CGA-O2A
14	q	516	CLA	CAA-CBA-CGA-O2A
14	q	517	CLA	CAA-CBA-CGA-O2A
14	r	512	CLA	CAA-CBA-CGA-O2A
14	s	507	CLA	CAA-CBA-CGA-O2A
14	v	504	CLA	CAA-CBA-CGA-O2A
14	A	1109	CLA	CAD-CBD-CGD-O2D
14	A	1114	CLA	CAD-CBD-CGD-O2D
14	A	1129	CLA	CAD-CBD-CGD-O2D
14	A	1138	CLA	CAD-CBD-CGD-O2D
14	B	1210	CLA	CAD-CBD-CGD-O2D
14	B	1229	CLA	CAD-CBD-CGD-O2D
14	1	507	CLA	CAD-CBD-CGD-O2D
14	1	509	CLA	CAD-CBD-CGD-O2D
14	1	519	CLA	CAD-CBD-CGD-O2D
14	2	501	CLA	CAD-CBD-CGD-O2D
14	2	502	CLA	CAD-CBD-CGD-O2D
14	2	508	CLA	CAD-CBD-CGD-O2D
14	3	502	CLA	CAD-CBD-CGD-O2D
14	4	505	CLA	CAD-CBD-CGD-O2D
14	4	510	CLA	CAD-CBD-CGD-O2D
14	5	502	CLA	CAD-CBD-CGD-O2D
14	5	505	CLA	CAD-CBD-CGD-O2D
14	5	509	CLA	CAD-CBD-CGD-O2D
14	6	501	CLA	CAD-CBD-CGD-O2D
14	6	504	CLA	CAD-CBD-CGD-O2D
14	6	507	CLA	CAD-CBD-CGD-O2D
14	G	1109	CLA	CAD-CBD-CGD-O2D
14	G	1114	CLA	CAD-CBD-CGD-O2D
14	G	1129	CLA	CAD-CBD-CGD-O2D
14	G	1138	CLA	CAD-CBD-CGD-O2D
14	H	1210	CLA	CAD-CBD-CGD-O2D
14	H	1229	CLA	CAD-CBD-CGD-O2D
14	Y	507	CLA	CAD-CBD-CGD-O2D
14	Y	509	CLA	CAD-CBD-CGD-O2D
14	Y	519	CLA	CAD-CBD-CGD-O2D
14	Z	501	CLA	CAD-CBD-CGD-O2D
14	Z	502	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	Z	508	CLA	CAD-CBD-CGD-O2D
14	a	502	CLA	CAD-CBD-CGD-O2D
14	b	505	CLA	CAD-CBD-CGD-O2D
14	b	510	CLA	CAD-CBD-CGD-O2D
14	c	502	CLA	CAD-CBD-CGD-O2D
14	c	505	CLA	CAD-CBD-CGD-O2D
14	c	509	CLA	CAD-CBD-CGD-O2D
14	d	501	CLA	CAD-CBD-CGD-O2D
14	d	504	CLA	CAD-CBD-CGD-O2D
14	d	507	CLA	CAD-CBD-CGD-O2D
14	e	1109	CLA	CAD-CBD-CGD-O2D
14	e	1114	CLA	CAD-CBD-CGD-O2D
14	e	1129	CLA	CAD-CBD-CGD-O2D
14	e	1138	CLA	CAD-CBD-CGD-O2D
14	f	1210	CLA	CAD-CBD-CGD-O2D
14	f	1229	CLA	CAD-CBD-CGD-O2D
14	q	507	CLA	CAD-CBD-CGD-O2D
14	q	509	CLA	CAD-CBD-CGD-O2D
14	q	519	CLA	CAD-CBD-CGD-O2D
14	r	501	CLA	CAD-CBD-CGD-O2D
14	r	502	CLA	CAD-CBD-CGD-O2D
14	r	508	CLA	CAD-CBD-CGD-O2D
14	r	509	CLA	CAD-CBD-CGD-O2D
14	s	502	CLA	CAD-CBD-CGD-O2D
14	t	505	CLA	CAD-CBD-CGD-O2D
14	t	510	CLA	CAD-CBD-CGD-O2D
14	u	502	CLA	CAD-CBD-CGD-O2D
14	u	505	CLA	CAD-CBD-CGD-O2D
14	u	509	CLA	CAD-CBD-CGD-O2D
14	v	501	CLA	CAD-CBD-CGD-O2D
14	v	504	CLA	CAD-CBD-CGD-O2D
14	v	507	CLA	CAD-CBD-CGD-O2D
14	A	1022	CLA	C16-C17-C18-C19
14	G	1022	CLA	C16-C17-C18-C19
14	e	1022	CLA	C16-C17-C18-C19
14	f	1215	CLA	C15-C16-C17-C18
14	A	1114	CLA	CAA-CBA-CGA-O2A
14	5	513	CLA	CAA-CBA-CGA-O2A
14	6	516	CLA	CAA-CBA-CGA-O2A
14	Y	517	CLA	CAA-CBA-CGA-O2A
14	c	513	CLA	CAA-CBA-CGA-O2A
14	d	504	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1114	CLA	CAA-CBA-CGA-O2A
14	u	513	CLA	CAA-CBA-CGA-O2A
14	v	516	CLA	CAA-CBA-CGA-O2A
14	B	1206	CLA	CAA-CBA-CGA-O2A
14	H	1206	CLA	CAA-CBA-CGA-O2A
14	f	1206	CLA	CAA-CBA-CGA-O2A
14	B	1228	CLA	CBA-CGA-O2A-C1
14	f	1228	CLA	CBA-CGA-O2A-C1
14	a	509	CLA	O1D-CGD-O2D-CED
14	1	505	CLA	CAA-CBA-CGA-O1A
14	1	507	CLA	CAA-CBA-CGA-O1A
14	5	512	CLA	CAA-CBA-CGA-O1A
14	G	1114	CLA	CAA-CBA-CGA-O2A
14	Y	505	CLA	CAA-CBA-CGA-O1A
14	c	512	CLA	CAA-CBA-CGA-O1A
14	q	505	CLA	CAA-CBA-CGA-O1A
14	q	507	CLA	CAA-CBA-CGA-O1A
14	t	513	CLA	CAA-CBA-CGA-O1A
14	u	512	CLA	CAA-CBA-CGA-O1A
14	B	1215	CLA	C15-C16-C17-C18
14	A	1126	CLA	C2-C3-C5-C6
14	G	1126	CLA	C2-C3-C5-C6
14	e	1126	CLA	C2-C3-C5-C6
18	A	5002	LHG	O7-C7-C8-C9
18	L	5220	LHG	O8-C23-C24-C25
18	G	5002	LHG	O7-C7-C8-C9
18	V	5220	LHG	O8-C23-C24-C25
18	e	5002	LHG	O7-C7-C8-C9
17	1	524	BCR	C11-C12-C13-C14
17	6	521	BCR	C7-C8-C9-C10
17	Y	524	BCR	C11-C12-C13-C14
17	d	521	BCR	C7-C8-C9-C10
17	v	521	BCR	C7-C8-C9-C10
18	A	5009	LHG	C4-C5-C6-O8
18	G	5009	LHG	C4-C5-C6-O8
18	e	5009	LHG	C4-C5-C6-O8
14	F	1302	CLA	CAA-CBA-CGA-O2A
14	2	507	CLA	CAA-CBA-CGA-O1A
14	4	513	CLA	CAA-CBA-CGA-O1A
14	R	1302	CLA	CAA-CBA-CGA-O2A
14	Y	507	CLA	CAA-CBA-CGA-O1A
14	Z	507	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	513	CLA	CAA-CBA-CGA-O1A
14	c	517	CLA	CAA-CBA-CGA-O2A
14	d	511	CLA	CAA-CBA-CGA-O1A
14	j	1302	CLA	CAA-CBA-CGA-O2A
14	q	513	CLA	CAA-CBA-CGA-O1A
14	r	507	CLA	CAA-CBA-CGA-O1A
14	r	516	CLA	CAA-CBA-CGA-O2A
14	u	517	CLA	CAA-CBA-CGA-O2A
14	v	511	CLA	CAA-CBA-CGA-O1A
18	A	5001	LHG	O6-C4-C5-O7
18	G	5001	LHG	O6-C4-C5-O7
18	e	5001	LHG	O6-C4-C5-O7
14	A	1123	CLA	C8-C10-C11-C12
14	G	1123	CLA	C8-C10-C11-C12
14	H	1215	CLA	C15-C16-C17-C18
18	n	5220	LHG	O8-C23-C24-C25
20	B	5002	LMG	O7-C10-C11-C12
20	H	5002	LMG	O7-C10-C11-C12
20	f	5002	LMG	O7-C10-C11-C12
21	B	1852	SQD	O47-C7-C8-C9
21	H	1852	SQD	O47-C7-C8-C9
21	f	1852	SQD	O47-C7-C8-C9
14	1	513	CLA	CAA-CBA-CGA-O1A
14	2	516	CLA	CAA-CBA-CGA-O2A
14	3	501	CLA	CAA-CBA-CGA-O1A
14	5	507	CLA	CAA-CBA-CGA-O1A
14	5	517	CLA	CAA-CBA-CGA-O2A
14	6	511	CLA	CAA-CBA-CGA-O1A
14	Y	513	CLA	CAA-CBA-CGA-O1A
14	Z	516	CLA	CAA-CBA-CGA-O2A
14	c	507	CLA	CAA-CBA-CGA-O1A
14	s	501	CLA	CAA-CBA-CGA-O2A
14	v	501	CLA	CAA-CBA-CGA-O1A
14	H	1216	CLA	C8-C10-C11-C12
14	e	1123	CLA	C8-C10-C11-C12
14	f	1216	CLA	C8-C10-C11-C12
14	A	1125	CLA	O2A-C1-C2-C3
14	G	1125	CLA	O2A-C1-C2-C3
14	e	1125	CLA	O2A-C1-C2-C3
14	J	1302	CLA	C2A-CAA-CBA-CGA
14	T	1302	CLA	C2A-CAA-CBA-CGA
14	l	1302	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	1216	CLA	C8-C10-C11-C12
14	K	1401	CLA	CAA-CBA-CGA-O2A
14	U	1401	CLA	CAA-CBA-CGA-O2A
14	m	1401	CLA	CAA-CBA-CGA-O2A
18	A	5001	LHG	O8-C23-C24-C25
18	G	5001	LHG	O8-C23-C24-C25
18	e	5001	LHG	O8-C23-C24-C25
14	1	509	CLA	CAA-CBA-CGA-O1A
14	1	512	CLA	CAA-CBA-CGA-O1A
14	2	512	CLA	CAA-CBA-CGA-O1A
14	3	501	CLA	CAA-CBA-CGA-O2A
14	3	506	CLA	CAA-CBA-CGA-O2A
14	3	507	CLA	CAA-CBA-CGA-O1A
14	4	519	CLA	CAA-CBA-CGA-O1A
14	6	501	CLA	CAA-CBA-CGA-O1A
14	6	507	CLA	CAA-CBA-CGA-O1A
14	Y	509	CLA	CAA-CBA-CGA-O1A
14	Y	512	CLA	CAA-CBA-CGA-O1A
14	Z	512	CLA	CAA-CBA-CGA-O1A
14	a	501	CLA	CAA-CBA-CGA-O1A
14	a	501	CLA	CAA-CBA-CGA-O2A
14	a	506	CLA	CAA-CBA-CGA-O2A
14	a	507	CLA	CAA-CBA-CGA-O1A
14	b	519	CLA	CAA-CBA-CGA-O1A
14	d	501	CLA	CAA-CBA-CGA-O1A
14	d	507	CLA	CAA-CBA-CGA-O1A
14	q	509	CLA	CAA-CBA-CGA-O1A
14	q	512	CLA	CAA-CBA-CGA-O1A
14	r	512	CLA	CAA-CBA-CGA-O1A
14	s	501	CLA	CAA-CBA-CGA-O1A
14	s	506	CLA	CAA-CBA-CGA-O2A
14	t	519	CLA	CAA-CBA-CGA-O1A
14	u	507	CLA	CAA-CBA-CGA-O1A
14	v	507	CLA	CAA-CBA-CGA-O1A
18	A	5006	LHG	C10-C11-C12-C13
18	e	5006	LHG	C10-C11-C12-C13
14	A	1011	CLA	CHA-CBD-CGD-O2D
14	A	1106	CLA	CHA-CBD-CGD-O1D
14	A	1106	CLA	CHA-CBD-CGD-O2D
14	A	1111	CLA	CHA-CBD-CGD-O2D
14	A	1112	CLA	CHA-CBD-CGD-O1D
14	A	1112	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1123	CLA	CHA-CBD-CGD-O2D
14	A	1127	CLA	CHA-CBD-CGD-O1D
14	A	1127	CLA	CHA-CBD-CGD-O2D
14	A	1128	CLA	CHA-CBD-CGD-O1D
14	A	1128	CLA	CHA-CBD-CGD-O2D
14	A	1134	CLA	CHA-CBD-CGD-O2D
14	B	1201	CLA	CHA-CBD-CGD-O2D
14	B	1212	CLA	CHA-CBD-CGD-O1D
14	B	1222	CLA	CHA-CBD-CGD-O1D
14	B	1222	CLA	CHA-CBD-CGD-O2D
14	B	1235	CLA	CHA-CBD-CGD-O2D
14	K	1103	CLA	CHA-CBD-CGD-O2D
14	L	1501	CLA	CHA-CBD-CGD-O1D
14	L	1501	CLA	CHA-CBD-CGD-O2D
14	1	517	CLA	CHA-CBD-CGD-O1D
14	1	518	CLA	CHA-CBD-CGD-O1D
14	1	518	CLA	CHA-CBD-CGD-O2D
14	2	504	CLA	CHA-CBD-CGD-O2D
14	2	507	CLA	CHA-CBD-CGD-O2D
14	2	517	CLA	CHA-CBD-CGD-O1D
14	2	517	CLA	CHA-CBD-CGD-O2D
14	2	519	CLA	CHA-CBD-CGD-O1D
14	3	506	CLA	CHA-CBD-CGD-O2D
14	3	517	CLA	CHA-CBD-CGD-O1D
14	3	517	CLA	CHA-CBD-CGD-O2D
14	3	518	CLA	CHA-CBD-CGD-O2D
14	3	519	CLA	CHA-CBD-CGD-O1D
14	4	503	CLA	CHA-CBD-CGD-O1D
14	4	503	CLA	CHA-CBD-CGD-O2D
14	4	506	CLA	CHA-CBD-CGD-O1D
14	4	512	CLA	CHA-CBD-CGD-O1D
14	4	517	CLA	CHA-CBD-CGD-O2D
14	5	507	CLA	CHA-CBD-CGD-O1D
14	5	507	CLA	CHA-CBD-CGD-O2D
14	5	512	CLA	CHA-CBD-CGD-O2D
14	6	502	CLA	CHA-CBD-CGD-O2D
14	6	511	CLA	CHA-CBD-CGD-O2D
14	6	512	CLA	CHA-CBD-CGD-O1D
14	6	516	CLA	CHA-CBD-CGD-O1D
14	6	519	CLA	CHA-CBD-CGD-O1D
14	G	1011	CLA	CHA-CBD-CGD-O2D
14	G	1106	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	1106	CLA	CHA-CBD-CGD-O2D
14	G	1111	CLA	CHA-CBD-CGD-O2D
14	G	1112	CLA	CHA-CBD-CGD-O1D
14	G	1112	CLA	CHA-CBD-CGD-O2D
14	G	1123	CLA	CHA-CBD-CGD-O2D
14	G	1127	CLA	CHA-CBD-CGD-O1D
14	G	1127	CLA	CHA-CBD-CGD-O2D
14	G	1128	CLA	CHA-CBD-CGD-O1D
14	G	1128	CLA	CHA-CBD-CGD-O2D
14	G	1134	CLA	CHA-CBD-CGD-O2D
14	H	1201	CLA	CHA-CBD-CGD-O2D
14	H	1212	CLA	CHA-CBD-CGD-O1D
14	H	1222	CLA	CHA-CBD-CGD-O1D
14	H	1222	CLA	CHA-CBD-CGD-O2D
14	H	1235	CLA	CHA-CBD-CGD-O2D
14	U	1103	CLA	CHA-CBD-CGD-O2D
14	V	1501	CLA	CHA-CBD-CGD-O1D
14	V	1501	CLA	CHA-CBD-CGD-O2D
14	Y	517	CLA	CHA-CBD-CGD-O1D
14	Y	518	CLA	CHA-CBD-CGD-O1D
14	Y	518	CLA	CHA-CBD-CGD-O2D
14	Z	504	CLA	CHA-CBD-CGD-O2D
14	Z	507	CLA	CHA-CBD-CGD-O2D
14	Z	517	CLA	CHA-CBD-CGD-O1D
14	Z	517	CLA	CHA-CBD-CGD-O2D
14	Z	519	CLA	CHA-CBD-CGD-O1D
14	a	506	CLA	CHA-CBD-CGD-O2D
14	a	517	CLA	CHA-CBD-CGD-O1D
14	a	517	CLA	CHA-CBD-CGD-O2D
14	a	518	CLA	CHA-CBD-CGD-O2D
14	a	519	CLA	CHA-CBD-CGD-O1D
14	b	503	CLA	CHA-CBD-CGD-O1D
14	b	503	CLA	CHA-CBD-CGD-O2D
14	b	506	CLA	CHA-CBD-CGD-O1D
14	b	512	CLA	CHA-CBD-CGD-O1D
14	b	517	CLA	CHA-CBD-CGD-O2D
14	c	507	CLA	CHA-CBD-CGD-O1D
14	c	507	CLA	CHA-CBD-CGD-O2D
14	c	512	CLA	CHA-CBD-CGD-O2D
14	d	502	CLA	CHA-CBD-CGD-O2D
14	d	511	CLA	CHA-CBD-CGD-O2D
14	d	512	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	d	516	CLA	CHA-CBD-CGD-O1D
14	d	519	CLA	CHA-CBD-CGD-O1D
14	e	1011	CLA	CHA-CBD-CGD-O2D
14	e	1106	CLA	CHA-CBD-CGD-O1D
14	e	1106	CLA	CHA-CBD-CGD-O2D
14	e	1111	CLA	CHA-CBD-CGD-O2D
14	e	1112	CLA	CHA-CBD-CGD-O1D
14	e	1112	CLA	CHA-CBD-CGD-O2D
14	e	1123	CLA	CHA-CBD-CGD-O2D
14	e	1127	CLA	CHA-CBD-CGD-O1D
14	e	1127	CLA	CHA-CBD-CGD-O2D
14	e	1128	CLA	CHA-CBD-CGD-O1D
14	e	1128	CLA	CHA-CBD-CGD-O2D
14	e	1134	CLA	CHA-CBD-CGD-O2D
14	f	1201	CLA	CHA-CBD-CGD-O2D
14	f	1212	CLA	CHA-CBD-CGD-O1D
14	f	1222	CLA	CHA-CBD-CGD-O1D
14	f	1222	CLA	CHA-CBD-CGD-O2D
14	f	1223	CLA	CHA-CBD-CGD-O2D
14	f	1235	CLA	CHA-CBD-CGD-O2D
14	m	1103	CLA	CHA-CBD-CGD-O2D
14	n	1501	CLA	CHA-CBD-CGD-O1D
14	n	1501	CLA	CHA-CBD-CGD-O2D
14	q	517	CLA	CHA-CBD-CGD-O1D
14	q	518	CLA	CHA-CBD-CGD-O1D
14	q	518	CLA	CHA-CBD-CGD-O2D
14	r	504	CLA	CHA-CBD-CGD-O2D
14	r	507	CLA	CHA-CBD-CGD-O2D
14	r	517	CLA	CHA-CBD-CGD-O1D
14	r	517	CLA	CHA-CBD-CGD-O2D
14	r	519	CLA	CHA-CBD-CGD-O1D
14	s	506	CLA	CHA-CBD-CGD-O2D
14	s	517	CLA	CHA-CBD-CGD-O1D
14	s	517	CLA	CHA-CBD-CGD-O2D
14	s	518	CLA	CHA-CBD-CGD-O2D
14	s	519	CLA	CHA-CBD-CGD-O1D
14	t	503	CLA	CHA-CBD-CGD-O1D
14	t	503	CLA	CHA-CBD-CGD-O2D
14	t	506	CLA	CHA-CBD-CGD-O1D
14	t	512	CLA	CHA-CBD-CGD-O1D
14	t	517	CLA	CHA-CBD-CGD-O2D
14	u	507	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	507	CLA	CHA-CBD-CGD-O2D
14	u	512	CLA	CHA-CBD-CGD-O2D
14	v	502	CLA	CHA-CBD-CGD-O2D
14	v	511	CLA	CHA-CBD-CGD-O2D
14	v	512	CLA	CHA-CBD-CGD-O1D
14	v	516	CLA	CHA-CBD-CGD-O1D
14	v	519	CLA	CHA-CBD-CGD-O1D
14	F	1302	CLA	CAA-CBA-CGA-O1A
14	4	507	CLA	CAA-CBA-CGA-O1A
14	5	517	CLA	CAA-CBA-CGA-O1A
14	R	1302	CLA	CAA-CBA-CGA-O1A
14	Z	516	CLA	CAA-CBA-CGA-O1A
14	b	507	CLA	CAA-CBA-CGA-O1A
14	c	513	CLA	CAA-CBA-CGA-O1A
14	c	517	CLA	CAA-CBA-CGA-O1A
14	d	504	CLA	CAA-CBA-CGA-O1A
14	j	1302	CLA	CAA-CBA-CGA-O1A
14	r	516	CLA	CAA-CBA-CGA-O1A
14	s	507	CLA	CAA-CBA-CGA-O1A
14	t	507	CLA	CAA-CBA-CGA-O1A
14	u	508	CLA	CAA-CBA-CGA-O2A
14	u	517	CLA	CAA-CBA-CGA-O1A
14	v	504	CLA	CAA-CBA-CGA-O1A
14	A	1106	CLA	CAA-CBA-CGA-O2A
14	A	1108	CLA	CAA-CBA-CGA-O2A
14	A	1120	CLA	CAA-CBA-CGA-O2A
14	A	1137	CLA	CAA-CBA-CGA-O2A
14	G	1106	CLA	CAA-CBA-CGA-O2A
14	G	1120	CLA	CAA-CBA-CGA-O2A
14	e	1106	CLA	CAA-CBA-CGA-O2A
14	e	1108	CLA	CAA-CBA-CGA-O2A
14	e	1120	CLA	CAA-CBA-CGA-O2A
18	G	5006	LHG	C10-C11-C12-C13
18	A	5003	LHG	O6-C4-C5-C6
18	G	5003	LHG	O6-C4-C5-C6
18	e	5003	LHG	O6-C4-C5-C6
14	2	516	CLA	CAA-CBA-CGA-O1A
14	4	509	CLA	CAA-CBA-CGA-O2A
14	5	513	CLA	CAA-CBA-CGA-O1A
14	6	504	CLA	CAA-CBA-CGA-O1A
14	b	509	CLA	CAA-CBA-CGA-O2A
14	t	509	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	513	CLA	CAA-CBA-CGA-O1A
19	G	1848	LMU	C7-C8-C9-C10
14	G	1108	CLA	CAA-CBA-CGA-O2A
14	G	1137	CLA	CAA-CBA-CGA-O2A
14	H	1221	CLA	CAA-CBA-CGA-O2A
14	e	1137	CLA	CAA-CBA-CGA-O2A
18	A	5006	LHG	O8-C23-C24-C25
18	G	5006	LHG	O8-C23-C24-C25
18	e	5006	LHG	O8-C23-C24-C25
19	e	1848	LMU	C7-C8-C9-C10
20	J	5104	LMG	O1-C7-C8-O7
20	T	5104	LMG	O1-C7-C8-O7
20	l	5104	LMG	O1-C7-C8-O7
21	4	822	SQD	O6-C44-C45-O47
21	b	822	SQD	O6-C44-C45-O47
21	t	822	SQD	O6-C44-C45-O47
19	A	1848	LMU	C7-C8-C9-C10
14	5	508	CLA	CAA-CBA-CGA-O2A
14	6	512	CLA	CAA-CBA-CGA-O1A
14	6	516	CLA	CAA-CBA-CGA-O1A
14	Y	516	CLA	CAA-CBA-CGA-O1A
14	c	508	CLA	CAA-CBA-CGA-O2A
14	v	512	CLA	CAA-CBA-CGA-O1A
14	A	1107	CLA	CAA-CBA-CGA-O2A
14	A	1135	CLA	CAA-CBA-CGA-O2A
14	A	1237	CLA	CAA-CBA-CGA-O2A
14	B	1221	CLA	CAA-CBA-CGA-O2A
14	G	1107	CLA	CAA-CBA-CGA-O2A
14	G	1135	CLA	CAA-CBA-CGA-O2A
14	G	1237	CLA	CAA-CBA-CGA-O2A
14	e	1107	CLA	CAA-CBA-CGA-O2A
14	e	1135	CLA	CAA-CBA-CGA-O2A
14	e	1237	CLA	CAA-CBA-CGA-O2A
14	f	1221	CLA	CAA-CBA-CGA-O2A
14	1	516	CLA	CAA-CBA-CGA-O1A
14	1	519	CLA	CAA-CBA-CGA-O2A
14	Y	519	CLA	CAA-CBA-CGA-O2A
14	d	512	CLA	CAA-CBA-CGA-O1A
14	q	516	CLA	CAA-CBA-CGA-O1A
14	q	519	CLA	CAA-CBA-CGA-O2A
14	v	516	CLA	CAA-CBA-CGA-O1A
14	4	516	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	t	516	CLA	CAA-CBA-CGA-O1A
18	B	1855	LHG	C16-C17-C18-C19
18	f	1855	LHG	C16-C17-C18-C19
14	A	1013	CLA	C12-C13-C15-C16
14	A	1126	CLA	C12-C13-C15-C16
14	A	1136	CLA	C12-C13-C15-C16
14	A	1137	CLA	C6-C7-C8-C10
14	A	1237	CLA	C6-C7-C8-C10
14	B	1204	CLA	C11-C10-C8-C7
14	6	505	CLA	C11-C12-C13-C15
14	G	1013	CLA	C12-C13-C15-C16
14	G	1126	CLA	C12-C13-C15-C16
14	G	1136	CLA	C12-C13-C15-C16
14	G	1137	CLA	C6-C7-C8-C10
14	G	1237	CLA	C6-C7-C8-C10
14	H	1204	CLA	C11-C10-C8-C7
14	d	505	CLA	C11-C12-C13-C15
14	e	1013	CLA	C12-C13-C15-C16
14	e	1126	CLA	C12-C13-C15-C16
14	e	1136	CLA	C12-C13-C15-C16
14	e	1137	CLA	C6-C7-C8-C10
14	e	1237	CLA	C6-C7-C8-C10
14	f	1204	CLA	C11-C10-C8-C7
14	v	505	CLA	C11-C12-C13-C15
18	H	1855	LHG	C16-C17-C18-C19
14	r	505	CLA	C13-C15-C16-C17
18	B	1842	LHG	O8-C23-C24-C25
18	H	1842	LHG	O8-C23-C24-C25
18	f	1842	LHG	O8-C23-C24-C25
14	b	516	CLA	CAA-CBA-CGA-O1A
14	d	516	CLA	CAA-CBA-CGA-O1A
14	A	1109	CLA	C6-C7-C8-C9
14	B	1207	CLA	C11-C12-C13-C14
14	6	505	CLA	C11-C12-C13-C14
14	H	1207	CLA	C11-C12-C13-C14
14	d	505	CLA	C11-C12-C13-C14
14	e	1109	CLA	C6-C7-C8-C9
14	f	1207	CLA	C11-C12-C13-C14
14	v	505	CLA	C11-C12-C13-C14
21	3	822	SQD	O48-C23-C24-C25
21	a	822	SQD	O48-C23-C24-C25
21	s	822	SQD	O48-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	2	505	CLA	C13-C15-C16-C17
14	Z	505	CLA	C13-C15-C16-C17
14	A	1011	CLA	C2B-C3B-CAB-CBB
14	6	506	CLA	C2B-C3B-CAB-CBB
14	G	1011	CLA	C2B-C3B-CAB-CBB
14	d	506	CLA	C2B-C3B-CAB-CBB
14	e	1011	CLA	C2B-C3B-CAB-CBB
14	v	506	CLA	C2B-C3B-CAB-CBB
18	G	5007	LHG	O9-C7-C8-C9
18	A	5006	LHG	C31-C32-C33-C34
18	L	5218	LHG	C33-C34-C35-C36
18	V	5218	LHG	C33-C34-C35-C36
18	e	5006	LHG	C31-C32-C33-C34
18	n	5218	LHG	C33-C34-C35-C36
14	1	517	CLA	CAA-CBA-CGA-O1A
14	q	517	CLA	CAA-CBA-CGA-O1A
14	A	1117	CLA	C2A-CAA-CBA-CGA
14	1	502	CLA	C2A-CAA-CBA-CGA
14	G	1117	CLA	C2A-CAA-CBA-CGA
14	Y	502	CLA	C2A-CAA-CBA-CGA
14	e	1117	CLA	C2A-CAA-CBA-CGA
14	q	502	CLA	C2A-CAA-CBA-CGA
18	A	5007	LHG	O9-C7-C8-C9
18	e	5007	LHG	O9-C7-C8-C9
18	G	5006	LHG	C31-C32-C33-C34
14	Y	517	CLA	CAA-CBA-CGA-O1A
14	B	1206	CLA	CAA-CBA-CGA-O1A
14	H	1206	CLA	CAA-CBA-CGA-O1A
14	f	1206	CLA	CAA-CBA-CGA-O1A
14	B	1220	CLA	C6-C7-C8-C9
14	H	1220	CLA	C6-C7-C8-C9
14	f	1220	CLA	C6-C7-C8-C9
21	B	1852	SQD	O48-C23-C24-C25
21	H	1852	SQD	O48-C23-C24-C25
21	f	1852	SQD	O48-C23-C24-C25
14	3	506	CLA	CAA-CBA-CGA-O1A
14	a	506	CLA	CAA-CBA-CGA-O1A
14	s	506	CLA	CAA-CBA-CGA-O1A
17	q	524	BCR	C11-C12-C13-C14
18	A	5001	LHG	C28-C29-C30-C31
18	G	5001	LHG	C28-C29-C30-C31
14	B	1204	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1204	CLA	CBA-CGA-O2A-C1
14	f	1204	CLA	CBA-CGA-O2A-C1
14	A	1107	CLA	C8-C10-C11-C12
14	G	1107	CLA	C8-C10-C11-C12
14	e	1107	CLA	C8-C10-C11-C12
14	A	1105	CLA	C1A-C2A-CAA-CBA
14	B	1012	CLA	C1A-C2A-CAA-CBA
14	B	1223	CLA	C1A-C2A-CAA-CBA
14	2	507	CLA	C1A-C2A-CAA-CBA
14	2	511	CLA	C1A-C2A-CAA-CBA
14	3	504	CLA	C1A-C2A-CAA-CBA
14	3	506	CLA	C1A-C2A-CAA-CBA
14	3	512	CLA	C1A-C2A-CAA-CBA
14	3	517	CLA	C1A-C2A-CAA-CBA
14	4	506	CLA	C1A-C2A-CAA-CBA
14	5	511	CLA	C1A-C2A-CAA-CBA
14	5	517	CLA	C1A-C2A-CAA-CBA
14	6	519	CLA	C1A-C2A-CAA-CBA
14	G	1105	CLA	C1A-C2A-CAA-CBA
14	H	1012	CLA	C1A-C2A-CAA-CBA
14	H	1223	CLA	C1A-C2A-CAA-CBA
14	Z	507	CLA	C1A-C2A-CAA-CBA
14	Z	511	CLA	C1A-C2A-CAA-CBA
14	a	504	CLA	C1A-C2A-CAA-CBA
14	a	506	CLA	C1A-C2A-CAA-CBA
14	a	512	CLA	C1A-C2A-CAA-CBA
14	a	517	CLA	C1A-C2A-CAA-CBA
14	b	506	CLA	C1A-C2A-CAA-CBA
14	c	511	CLA	C1A-C2A-CAA-CBA
14	c	517	CLA	C1A-C2A-CAA-CBA
14	d	519	CLA	C1A-C2A-CAA-CBA
14	e	1105	CLA	C1A-C2A-CAA-CBA
14	f	1012	CLA	C1A-C2A-CAA-CBA
14	f	1223	CLA	C1A-C2A-CAA-CBA
14	r	507	CLA	C1A-C2A-CAA-CBA
14	r	511	CLA	C1A-C2A-CAA-CBA
14	s	504	CLA	C1A-C2A-CAA-CBA
14	s	506	CLA	C1A-C2A-CAA-CBA
14	s	512	CLA	C1A-C2A-CAA-CBA
14	s	517	CLA	C1A-C2A-CAA-CBA
14	t	506	CLA	C1A-C2A-CAA-CBA
14	u	511	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	u	517	CLA	C1A-C2A-CAA-CBA
14	v	519	CLA	C1A-C2A-CAA-CBA
18	e	5001	LHG	C28-C29-C30-C31
14	G	1123	CLA	CAA-CBA-CGA-O1A
14	e	1123	CLA	CAA-CBA-CGA-O1A
14	f	1023	CLA	C8-C10-C11-C12
14	n	1502	CLA	C8-C10-C11-C12
14	2	518	CLA	C2-C1-O2A-CGA
14	Z	518	CLA	C2-C1-O2A-CGA
14	r	518	CLA	C2-C1-O2A-CGA
14	B	1023	CLA	C8-C10-C11-C12
14	L	1502	CLA	C8-C10-C11-C12
14	A	1123	CLA	CAA-CBA-CGA-O1A
18	A	5007	LHG	C17-C18-C19-C20
17	B	4009	BCR	C19-C20-C21-C22
21	6	822	SQD	O6-C44-C45-C46
21	d	822	SQD	O6-C44-C45-C46
21	v	822	SQD	O6-C44-C45-C46
18	G	5007	LHG	C17-C18-C19-C20
14	H	1023	CLA	C8-C10-C11-C12
14	V	1502	CLA	C8-C10-C11-C12
14	f	1023	CLA	C13-C15-C16-C17
18	e	5007	LHG	C17-C18-C19-C20
14	H	1203	CLA	CAA-CBA-CGA-O1A
18	A	5003	LHG	O9-C7-C8-C9
18	G	5003	LHG	O9-C7-C8-C9
18	e	5006	LHG	O10-C23-C24-C25
18	e	5003	LHG	O9-C7-C8-C9
14	H	1023	CLA	C13-C15-C16-C17
14	1	519	CLA	CAA-CBA-CGA-O1A
18	A	5008	LHG	O7-C7-C8-C9
18	G	5008	LHG	O7-C7-C8-C9
18	e	5008	LHG	O7-C7-C8-C9
14	A	1011	CLA	C8-C10-C11-C12
14	B	1023	CLA	C13-C15-C16-C17
14	e	1138	CLA	C15-C16-C17-C18
14	B	1203	CLA	CAA-CBA-CGA-O1A
14	B	1221	CLA	CAA-CBA-CGA-O1A
14	H	1221	CLA	CAA-CBA-CGA-O1A
14	f	1203	CLA	CAA-CBA-CGA-O1A
18	A	5006	LHG	O10-C23-C24-C25
18	G	5006	LHG	O10-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1204	CLA	O1A-CGA-O2A-C1
14	5	508	CLA	CAA-CBA-CGA-O1A
14	Y	519	CLA	CAA-CBA-CGA-O1A
14	b	509	CLA	CAA-CBA-CGA-O1A
14	c	508	CLA	CAA-CBA-CGA-O1A
14	t	509	CLA	CAA-CBA-CGA-O1A
14	u	508	CLA	CAA-CBA-CGA-O1A
14	G	1011	CLA	C8-C10-C11-C12
14	e	1011	CLA	C8-C10-C11-C12
14	A	1111	CLA	C4B-C3B-CAB-CBB
14	G	1111	CLA	C4B-C3B-CAB-CBB
14	Z	511	CLA	C4B-C3B-CAB-CBB
14	e	1111	CLA	C4B-C3B-CAB-CBB
18	A	5002	LHG	C3-O3-P-O5
18	A	5006	LHG	C3-O3-P-O5
18	A	5007	LHG	C3-O3-P-O5
18	A	5009	LHG	C4-O6-P-O5
18	A	5001	LHG	C3-O3-P-O5
18	A	5003	LHG	C3-O3-P-O5
18	B	1842	LHG	C4-O6-P-O5
18	I	5001	LHG	C4-O6-P-O4
18	I	5001	LHG	C4-O6-P-O5
18	G	5002	LHG	C3-O3-P-O5
18	G	5006	LHG	C3-O3-P-O5
18	G	5007	LHG	C3-O3-P-O5
18	G	5009	LHG	C4-O6-P-O5
18	G	5001	LHG	C3-O3-P-O5
18	G	5003	LHG	C3-O3-P-O5
18	H	1842	LHG	C4-O6-P-O5
18	S	5001	LHG	C4-O6-P-O4
18	S	5001	LHG	C4-O6-P-O5
18	e	5002	LHG	C3-O3-P-O5
18	e	5006	LHG	C3-O3-P-O5
18	e	5007	LHG	C3-O3-P-O5
18	e	5009	LHG	C4-O6-P-O5
18	e	5001	LHG	C3-O3-P-O5
18	e	5003	LHG	C3-O3-P-O5
18	f	1842	LHG	C4-O6-P-O5
18	k	5001	LHG	C4-O6-P-O4
18	k	5001	LHG	C4-O6-P-O5
14	A	1108	CLA	CAA-CBA-CGA-O1A
14	A	1120	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	K	1401	CLA	CAA-CBA-CGA-O1A
14	G	1120	CLA	CAA-CBA-CGA-O1A
14	U	1401	CLA	CAA-CBA-CGA-O1A
14	e	1108	CLA	CAA-CBA-CGA-O1A
14	e	1120	CLA	CAA-CBA-CGA-O1A
14	f	1221	CLA	CAA-CBA-CGA-O1A
14	m	1401	CLA	CAA-CBA-CGA-O1A
18	A	5007	LHG	O7-C7-C8-C9
18	G	5007	LHG	O7-C7-C8-C9
18	e	5007	LHG	O7-C7-C8-C9
20	J	5104	LMG	O6-C1-O1-C7
20	T	5104	LMG	O6-C1-O1-C7
20	l	5104	LMG	O6-C1-O1-C7
14	A	1138	CLA	C15-C16-C17-C18
14	f	1204	CLA	O1A-CGA-O2A-C1
14	4	509	CLA	CAA-CBA-CGA-O1A
14	q	519	CLA	CAA-CBA-CGA-O1A
17	A	4008	BCR	C5-C6-C7-C8
17	6	524	BCR	C23-C24-C25-C30
17	G	4008	BCR	C5-C6-C7-C8
17	H	4014	BCR	C5-C6-C7-C8
17	e	4008	BCR	C5-C6-C7-C8
17	v	524	BCR	C23-C24-C25-C30
14	A	1123	CLA	C10-C11-C12-C13
14	B	1021	CLA	C13-C15-C16-C17
14	G	1123	CLA	C10-C11-C12-C13
14	G	1138	CLA	C15-C16-C17-C18
14	H	1021	CLA	C13-C15-C16-C17
14	e	1123	CLA	C10-C11-C12-C13
14	f	1021	CLA	C13-C15-C16-C17
14	G	1108	CLA	CAA-CBA-CGA-O1A
14	B	1204	CLA	O1A-CGA-O2A-C1
14	v	508	CLA	O1D-CGD-O2D-CED
20	B	5002	LMG	O8-C28-C29-C30
20	H	5002	LMG	O8-C28-C29-C30
21	L	5216	SQD	O47-C7-C8-C9
21	V	5216	SQD	O47-C7-C8-C9
21	n	5216	SQD	O47-C7-C8-C9
14	d	518	CLA	CAA-CBA-CGA-O1A
14	v	518	CLA	CAA-CBA-CGA-O1A
14	L	1501	CLA	C11-C12-C13-C14
14	V	1501	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	n	1501	CLA	C11-C12-C13-C14
18	I	5001	LHG	C26-C27-C28-C29
18	e	5006	LHG	C33-C34-C35-C36
14	A	1106	CLA	CAA-CBA-CGA-O1A
14	A	1237	CLA	CAA-CBA-CGA-O1A
14	G	1237	CLA	CAA-CBA-CGA-O1A
14	e	1237	CLA	CAA-CBA-CGA-O1A
20	B	5002	LMG	O10-C28-C29-C30
20	H	5002	LMG	O10-C28-C29-C30
20	f	5002	LMG	O10-C28-C29-C30
18	A	5006	LHG	C33-C34-C35-C36
18	k	5001	LHG	C26-C27-C28-C29
18	G	5006	LHG	C33-C34-C35-C36
18	S	5001	LHG	C26-C27-C28-C29
14	A	1114	CLA	CAA-CBA-CGA-O1A
14	G	1114	CLA	CAA-CBA-CGA-O1A
14	e	1114	CLA	CAA-CBA-CGA-O1A
18	A	5006	LHG	O7-C7-C8-C9
18	G	5006	LHG	O7-C7-C8-C9
20	f	5002	LMG	O8-C28-C29-C30
14	6	508	CLA	O1D-CGD-O2D-CED
14	G	1106	CLA	CAA-CBA-CGA-O1A
14	e	1106	CLA	CAA-CBA-CGA-O1A
17	H	4009	BCR	C19-C20-C21-C22
17	f	4009	BCR	C19-C20-C21-C22
14	d	508	CLA	O1D-CGD-O2D-CED
14	4	516	CLA	CAA-CBA-CGA-O2A
14	6	518	CLA	CAA-CBA-CGA-O1A
14	b	516	CLA	CAA-CBA-CGA-O2A
14	A	1011	CLA	CAD-CBD-CGD-O1D
14	A	1132	CLA	CAD-CBD-CGD-O1D
14	A	1135	CLA	CAD-CBD-CGD-O1D
14	B	1210	CLA	CAD-CBD-CGD-O1D
14	B	1212	CLA	CAD-CBD-CGD-O1D
14	L	1501	CLA	CAD-CBD-CGD-O1D
14	1	517	CLA	CAD-CBD-CGD-O1D
14	4	504	CLA	CAD-CBD-CGD-O1D
14	6	504	CLA	CAD-CBD-CGD-O1D
14	6	516	CLA	CAD-CBD-CGD-O1D
14	G	1011	CLA	CAD-CBD-CGD-O1D
14	G	1132	CLA	CAD-CBD-CGD-O1D
14	G	1135	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	1210	CLA	CAD-CBD-CGD-O1D
14	H	1212	CLA	CAD-CBD-CGD-O1D
14	V	1501	CLA	CAD-CBD-CGD-O1D
14	Y	517	CLA	CAD-CBD-CGD-O1D
14	b	504	CLA	CAD-CBD-CGD-O1D
14	d	504	CLA	CAD-CBD-CGD-O1D
14	d	511	CLA	CAD-CBD-CGD-O1D
14	d	516	CLA	CAD-CBD-CGD-O1D
14	e	1011	CLA	CAD-CBD-CGD-O1D
14	e	1132	CLA	CAD-CBD-CGD-O1D
14	e	1135	CLA	CAD-CBD-CGD-O1D
14	f	1210	CLA	CAD-CBD-CGD-O1D
14	f	1212	CLA	CAD-CBD-CGD-O1D
14	n	1501	CLA	CAD-CBD-CGD-O1D
14	q	517	CLA	CAD-CBD-CGD-O1D
14	t	504	CLA	CAD-CBD-CGD-O1D
14	v	504	CLA	CAD-CBD-CGD-O1D
14	v	516	CLA	CAD-CBD-CGD-O1D
14	A	1103	CLA	CAA-CBA-CGA-O2A
14	2	501	CLA	CAA-CBA-CGA-O2A
14	G	1103	CLA	CAA-CBA-CGA-O2A
14	Z	501	CLA	CAA-CBA-CGA-O2A
14	e	1103	CLA	CAA-CBA-CGA-O2A
14	r	501	CLA	CAA-CBA-CGA-O2A
18	e	5006	LHG	O7-C7-C8-C9
18	f	1855	LHG	O7-C7-C8-C9
14	B	1229	CLA	C10-C11-C12-C13
14	H	1229	CLA	C10-C11-C12-C13
14	f	1229	CLA	C10-C11-C12-C13
14	A	1013	CLA	C11-C12-C13-C14
14	A	1111	CLA	C14-C13-C15-C16
14	A	1119	CLA	C14-C13-C15-C16
14	A	1136	CLA	C11-C10-C8-C9
14	A	1136	CLA	C14-C13-C15-C16
14	G	1013	CLA	C11-C12-C13-C14
14	G	1109	CLA	C6-C7-C8-C9
14	G	1111	CLA	C14-C13-C15-C16
14	G	1136	CLA	C11-C10-C8-C9
14	G	1136	CLA	C14-C13-C15-C16
14	e	1013	CLA	C11-C12-C13-C14
14	e	1111	CLA	C14-C13-C15-C16
14	e	1119	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1136	CLA	C11-C10-C8-C9
14	e	1136	CLA	C14-C13-C15-C16
14	t	516	CLA	CAA-CBA-CGA-O2A
14	A	1135	CLA	CAA-CBA-CGA-O1A
14	G	1135	CLA	CAA-CBA-CGA-O1A
14	e	1135	CLA	CAA-CBA-CGA-O1A
18	B	1855	LHG	O7-C7-C8-C9
18	H	1855	LHG	O7-C7-C8-C9
14	A	1110	CLA	CAA-CBA-CGA-O2A
14	A	1111	CLA	CAA-CBA-CGA-O2A
14	A	1115	CLA	CAA-CBA-CGA-O2A
14	B	1213	CLA	CAA-CBA-CGA-O2A
14	G	1110	CLA	CAA-CBA-CGA-O2A
14	G	1111	CLA	CAA-CBA-CGA-O2A
14	G	1115	CLA	CAA-CBA-CGA-O2A
14	e	1110	CLA	CAA-CBA-CGA-O2A
14	e	1111	CLA	CAA-CBA-CGA-O2A
14	e	1115	CLA	CAA-CBA-CGA-O2A
14	f	1213	CLA	CAA-CBA-CGA-O2A
14	1	518	CLA	CAA-CBA-CGA-O2A
14	Y	518	CLA	CAA-CBA-CGA-O2A
14	q	518	CLA	CAA-CBA-CGA-O2A
14	A	1118	CLA	C3A-C2A-CAA-CBA
14	A	1119	CLA	C12-C13-C15-C16
14	A	1125	CLA	C11-C12-C13-C15
14	B	1201	CLA	C6-C7-C8-C10
14	B	1215	CLA	C11-C12-C13-C15
14	B	1215	CLA	C12-C13-C15-C16
14	B	1229	CLA	C11-C10-C8-C7
14	B	1207	CLA	C11-C12-C13-C15
14	B	1230	CLA	C11-C10-C8-C7
14	5	518	CLA	C3A-C2A-CAA-CBA
14	G	1118	CLA	C3A-C2A-CAA-CBA
14	G	1119	CLA	C12-C13-C15-C16
14	G	1125	CLA	C11-C12-C13-C15
14	H	1201	CLA	C6-C7-C8-C10
14	H	1215	CLA	C11-C12-C13-C15
14	H	1215	CLA	C12-C13-C15-C16
14	H	1207	CLA	C11-C12-C13-C15
14	H	1230	CLA	C11-C10-C8-C7
14	c	518	CLA	C3A-C2A-CAA-CBA
14	e	1118	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	e	1119	CLA	C12-C13-C15-C16
14	e	1125	CLA	C11-C12-C13-C15
14	f	1201	CLA	C6-C7-C8-C10
14	f	1215	CLA	C11-C12-C13-C15
14	f	1215	CLA	C12-C13-C15-C16
14	f	1207	CLA	C11-C12-C13-C15
14	f	1230	CLA	C11-C10-C8-C7
14	u	518	CLA	C3A-C2A-CAA-CBA
14	A	1107	CLA	CAA-CBA-CGA-O1A
14	G	1107	CLA	CAA-CBA-CGA-O1A
14	G	1137	CLA	CAA-CBA-CGA-O1A
14	e	1137	CLA	CAA-CBA-CGA-O1A
18	A	5007	LHG	O10-C23-C24-C25
18	G	5007	LHG	O10-C23-C24-C25
18	e	5007	LHG	O10-C23-C24-C25
14	A	1013	CLA	CAA-CBA-CGA-O2A
14	G	1013	CLA	CAA-CBA-CGA-O2A
14	H	1213	CLA	CAA-CBA-CGA-O2A
14	s	509	CLA	CBD-CGD-O2D-CED
18	e	5009	LHG	C12-C13-C14-C15
17	A	4011	BCR	C7-C8-C9-C10
17	1	521	BCR	C17-C18-C19-C20
17	G	4011	BCR	C7-C8-C9-C10
17	Y	521	BCR	C17-C18-C19-C20
17	e	4011	BCR	C7-C8-C9-C10
17	q	521	BCR	C17-C18-C19-C20
14	A	1137	CLA	CAA-CBA-CGA-O1A
14	e	1107	CLA	CAA-CBA-CGA-O1A
17	2	522	BCR	C15-C16-C17-C18
17	2	524	BCR	C9-C10-C11-C12
17	5	521	BCR	C9-C10-C11-C12
17	Z	522	BCR	C15-C16-C17-C18
17	Z	524	BCR	C9-C10-C11-C12
17	c	521	BCR	C9-C10-C11-C12
17	r	522	BCR	C15-C16-C17-C18
17	r	524	BCR	C9-C10-C11-C12
17	u	521	BCR	C9-C10-C11-C12
18	A	5009	LHG	C12-C13-C14-C15
18	G	5009	LHG	C12-C13-C14-C15
19	A	1849	LMU	C2-C1-O1'-C1'
19	G	1849	LMU	C2-C1-O1'-C1'
19	e	1849	LMU	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	1111	CLA	CAA-CBA-CGA-O1A
14	G	1111	CLA	CAA-CBA-CGA-O1A
14	e	1111	CLA	CAA-CBA-CGA-O1A
14	e	1125	CLA	CAA-CBA-CGA-O1A
20	J	5104	LMG	O10-C28-C29-C30
20	l	5104	LMG	O10-C28-C29-C30
14	3	509	CLA	CBD-CGD-O2D-CED
14	a	509	CLA	CBD-CGD-O2D-CED
14	A	1125	CLA	CAA-CBA-CGA-O2A
14	G	1125	CLA	CAA-CBA-CGA-O2A
14	e	1013	CLA	CAA-CBA-CGA-O2A
14	e	1125	CLA	CAA-CBA-CGA-O2A
14	A	1125	CLA	CAA-CBA-CGA-O1A
14	G	1125	CLA	CAA-CBA-CGA-O1A
14	2	504	CLA	C2A-CAA-CBA-CGA
14	3	513	CLA	C2A-CAA-CBA-CGA
14	Z	504	CLA	C2A-CAA-CBA-CGA
14	a	513	CLA	C2A-CAA-CBA-CGA
14	r	504	CLA	C2A-CAA-CBA-CGA
14	s	513	CLA	C2A-CAA-CBA-CGA
14	G	1105	CLA	C5-C6-C7-C8
14	G	1237	CLA	C13-C15-C16-C17
14	e	1237	CLA	C13-C15-C16-C17
14	A	1115	CLA	CAA-CBA-CGA-O1A
14	G	1013	CLA	CAA-CBA-CGA-O1A
14	G	1115	CLA	CAA-CBA-CGA-O1A
20	T	5104	LMG	O10-C28-C29-C30
14	A	1131	CLA	C4-C3-C5-C6
14	G	1131	CLA	C4-C3-C5-C6
14	e	1131	CLA	C4-C3-C5-C6
14	K	1105	CLA	CAA-CBA-CGA-O2A
14	3	510	CLA	CAA-CBA-CGA-O1A
14	U	1105	CLA	CAA-CBA-CGA-O2A
14	a	510	CLA	CAA-CBA-CGA-O1A
14	m	1105	CLA	CAA-CBA-CGA-O2A
14	s	510	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

661 monomers are involved in 1532 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	W	4021	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1212	CLA	1	0
14	V	1501	CLA	8	0
17	J	4012	BCR	3	0
17	r	522	BCR	1	0
14	f	1012	CLA	4	0
17	d	521	BCR	2	0
14	Z	509	CLA	2	0
18	G	5009	LHG	3	0
17	n	4022	BCR	9	0
17	V	4019	BCR	3	0
14	G	1131	CLA	2	0
18	B	1855	LHG	3	0
20	T	5104	LMG	1	0
14	e	1114	CLA	1	0
18	e	5008	LHG	7	0
14	B	1228	CLA	4	0
14	A	1127	CLA	1	0
17	H	4009	BCR	2	0
19	G	1849	LMU	1	0
14	A	1137	CLA	5	0
14	5	511	CLA	1	0
14	4	512	CLA	2	0
17	b	524	BCR	3	0
17	a	524	BCR	1	0
14	U	1105	CLA	2	0
14	5	507	CLA	1	0
14	m	1105	CLA	2	0
14	H	1226	CLA	5	0
14	A	1115	CLA	2	0
14	f	1216	CLA	4	0
14	H	1238	CLA	1	0
14	f	1236	CLA	3	0
14	f	1205	CLA	2	0
14	G	1137	CLA	5	0
17	G	4008	BCR	3	0
17	f	4017	BCR	5	0
14	A	1013	CLA	8	0
14	c	502	CLA	2	0
14	H	1206	CLA	5	0
14	B	1208	CLA	5	0
14	A	1101	CLA	5	0
14	J	1302	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1124	CLA	3	0
14	f	1207	CLA	8	0
14	d	518	CLA	1	0
14	f	1206	CLA	5	0
14	e	1125	CLA	5	0
14	b	502	CLA	3	0
14	G	1134	CLA	1	0
18	n	5220	LHG	4	0
14	A	1138	CLA	1	0
14	e	1011	CLA	2	0
17	A	4008	BCR	5	0
14	t	512	CLA	3	0
17	t	522	BCR	1	0
14	e	1237	CLA	6	0
14	H	1208	CLA	4	0
14	F	1302	CLA	3	0
14	A	1801	CLA	3	0
14	B	1235	CLA	4	0
14	H	1225	CLA	4	0
14	v	509	CLA	1	0
17	A	4003	BCR	1	0
17	n	4219	BCR	10	0
18	e	5003	LHG	2	0
14	A	1134	CLA	2	0
14	4	504	CLA	1	0
14	q	513	CLA	2	0
14	Z	513	CLA	2	0
14	u	502	CLA	2	0
14	4	507	CLA	1	0
17	H	4017	BCR	3	0
17	a	522	BCR	1	0
14	R	1302	CLA	3	0
14	B	1221	CLA	9	0
14	a	513	CLA	2	0
14	1	510	CLA	1	0
14	G	1104	CLA	6	0
14	G	1138	CLA	1	0
14	r	510	CLA	1	0
17	3	522	BCR	1	0
14	e	1121	CLA	3	0
14	F	1301	CLA	1	0
14	t	511	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1229	CLA	5	0
14	2	513	CLA	2	0
14	f	1229	CLA	6	0
20	B	5002	LMG	5	0
17	A	4011	BCR	3	0
18	A	5006	LHG	3	0
14	t	507	CLA	1	0
14	Y	516	CLA	6	0
14	B	1205	CLA	2	0
17	6	524	BCR	4	0
14	v	512	CLA	3	0
14	G	1118	CLA	2	0
15	B	2002	PQN	4	0
14	H	1215	CLA	4	0
17	J	4013	BCR	6	0
17	B	4006	BCR	4	0
14	H	1204	CLA	2	0
14	H	1228	CLA	3	0
14	f	1215	CLA	3	0
14	u	513	CLA	2	0
17	q	522	BCR	2	0
14	v	510	CLA	1	0
17	Y	521	BCR	6	0
14	e	1013	CLA	7	0
17	Z	523	BCR	2	0
14	A	1118	CLA	2	0
18	L	5218	LHG	2	0
14	A	1133	CLA	2	0
14	q	505	CLA	2	0
17	L	4019	BCR	3	0
14	5	502	CLA	2	0
14	G	1140	CLA	3	0
17	v	524	BCR	3	0
14	d	511	CLA	2	0
14	f	1231	CLA	3	0
14	a	517	CLA	1	0
18	G	5004	LHG	2	0
18	e	5009	LHG	4	0
17	B	4010	BCR	6	0
14	e	1131	CLA	2	0
14	A	1114	CLA	1	0
17	2	522	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	6	512	CLA	4	0
17	f	4014	BCR	3	0
14	B	1204	CLA	3	0
14	B	1224	CLA	3	0
14	f	1214	CLA	2	0
17	b	523	BCR	1	0
14	e	1140	CLA	3	0
17	f	4005	BCR	4	0
14	G	1106	CLA	4	0
14	B	1234	CLA	5	0
18	A	5005	LHG	7	0
17	J	4015	BCR	5	0
17	T	4012	BCR	3	0
21	1	822	SQD	1	0
18	G	5007	LHG	2	0
14	d	506	CLA	2	0
14	B	1238	CLA	1	0
18	e	5001	LHG	4	0
14	A	1106	CLA	4	0
14	e	1101	CLA	5	0
14	G	1119	CLA	7	0
14	G	1105	CLA	2	0
14	H	1219	CLA	2	0
18	A	5007	LHG	2	0
19	A	1848	LMU	2	0
14	H	1203	CLA	2	0
14	3	503	CLA	1	0
14	H	1221	CLA	9	0
17	4	522	BCR	1	0
14	r	509	CLA	2	0
18	A	5008	LHG	7	0
14	6	519	CLA	1	0
14	B	1012	CLA	5	0
14	f	1218	CLA	2	0
19	e	1848	LMU	2	0
21	Y	822	SQD	1	0
18	f	1842	LHG	2	0
17	a	521	BCR	1	0
21	L	5216	SQD	6	0
14	A	1119	CLA	5	0
14	H	1214	CLA	2	0
14	1	513	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	d	523	BCR	4	0
14	G	1116	CLA	6	0
14	f	1212	CLA	1	0
14	j	1301	CLA	1	0
14	r	501	CLA	2	0
14	t	502	CLA	3	0
14	e	1109	CLA	2	0
17	Z	524	BCR	6	0
14	e	1124	CLA	2	0
14	f	1210	CLA	7	0
14	b	503	CLA	1	0
17	Z	522	BCR	2	0
14	6	506	CLA	2	0
17	u	524	BCR	2	0
14	G	1133	CLA	2	0
14	e	1104	CLA	5	0
14	e	1120	CLA	2	0
14	a	503	CLA	1	0
17	n	4020	BCR	2	0
14	A	1116	CLA	4	0
14	e	1137	CLA	6	0
14	e	1117	CLA	4	0
17	A	4007	BCR	2	0
17	e	4008	BCR	5	0
14	G	1120	CLA	2	0
22	P	170	FMN	1	0
14	Y	512	CLA	4	0
14	2	510	CLA	1	0
21	f	1852	SQD	9	0
14	d	517	CLA	2	0
14	G	1022	CLA	2	0
14	L	1501	CLA	7	0
14	Y	502	CLA	2	0
14	H	1217	CLA	1	0
17	3	524	BCR	1	0
14	B	1209	CLA	2	0
14	e	1110	CLA	2	0
14	f	1220	CLA	2	0
14	f	1226	CLA	5	0
14	K	1105	CLA	2	0
17	b	521	BCR	1	0
14	f	1217	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	e	1849	LMU	1	0
14	H	1209	CLA	2	0
14	A	1120	CLA	2	0
17	G	4002	BCR	2	0
17	G	4011	BCR	4	0
14	e	1130	CLA	4	0
14	A	1022	CLA	2	0
14	H	1222	CLA	2	0
14	e	1129	CLA	5	0
17	B	4014	BCR	5	0
14	f	1222	CLA	1	0
14	v	519	CLA	2	0
14	q	510	CLA	1	0
17	G	4007	BCR	3	0
17	a	523	BCR	1	0
14	5	505	CLA	1	0
14	Z	501	CLA	3	0
14	a	502	CLA	3	0
17	A	4002	BCR	5	0
19	A	1849	LMU	1	0
14	q	502	CLA	2	0
14	2	517	CLA	1	0
17	n	4019	BCR	4	0
14	H	1201	CLA	2	0
17	e	4011	BCR	3	0
17	S	4018	BCR	3	0
14	u	505	CLA	1	0
14	B	1202	CLA	2	0
14	1	509	CLA	1	0
14	v	506	CLA	2	0
17	T	4015	BCR	4	0
14	4	510	CLA	2	0
14	A	1108	CLA	1	0
14	4	516	CLA	2	0
14	6	518	CLA	1	0
18	I	5001	LHG	2	0
14	q	507	CLA	1	0
14	f	1239	CLA	4	0
17	s	521	BCR	1	0
14	v	502	CLA	2	0
14	2	509	CLA	2	0
21	3	822	SQD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	f	1227	CLA	2	0
14	Z	519	CLA	1	0
17	u	522	BCR	1	0
14	Z	510	CLA	1	0
14	r	502	CLA	3	0
14	G	1128	CLA	7	0
14	Y	511	CLA	1	0
19	H	1843	LMU	1	0
14	f	1203	CLA	2	0
14	1	516	CLA	6	0
14	G	1130	CLA	4	0
14	a	512	CLA	5	0
14	b	510	CLA	2	0
14	e	1122	CLA	3	0
17	K	4104	BCR	3	0
18	L	5220	LHG	4	0
18	V	5221	LHG	8	0
17	B	4017	BCR	4	0
14	B	1201	CLA	2	0
14	f	1223	CLA	4	0
14	u	506	CLA	2	0
14	A	1128	CLA	7	0
14	G	1801	CLA	3	0
18	n	5221	LHG	6	0
17	Y	523	BCR	1	0
14	t	510	CLA	1	0
17	1	521	BCR	6	0
14	V	1502	CLA	3	0
14	B	1231	CLA	3	0
14	H	1212	CLA	1	0
14	e	1118	CLA	2	0
14	t	501	CLA	1	0
14	A	1136	CLA	1	0
14	B	1229	CLA	7	0
14	e	1103	CLA	4	0
14	t	505	CLA	1	0
18	B	1842	LHG	2	0
14	3	505	CLA	1	0
17	2	523	BCR	2	0
14	b	512	CLA	2	0
18	A	5004	LHG	3	0
22	p	170	FMN	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1205	CLA	2	0
14	r	503	CLA	3	0
14	H	1223	CLA	4	0
17	f	4006	BCR	4	0
14	V	1503	CLA	2	0
14	Z	502	CLA	3	0
14	G	1115	CLA	3	0
17	6	523	BCR	3	0
14	G	1136	CLA	2	0
14	d	513	CLA	2	0
14	A	1131	CLA	2	0
14	b	511	CLA	2	0
14	e	1105	CLA	2	0
14	e	1112	CLA	1	0
17	B	4004	BCR	3	0
14	b	517	CLA	1	0
14	f	1238	CLA	1	0
14	G	1108	CLA	1	0
14	t	516	CLA	2	0
14	f	1201	CLA	4	0
14	T	1302	CLA	1	0
14	a	511	CLA	1	0
14	b	504	CLA	1	0
14	c	509	CLA	1	0
18	L	5221	LHG	6	0
17	H	4010	BCR	7	0
17	T	4013	BCR	6	0
14	f	1202	CLA	3	0
14	B	1222	CLA	1	0
17	L	4219	BCR	7	0
17	f	4010	BCR	6	0
14	b	509	CLA	2	0
14	A	1105	CLA	2	0
14	u	512	CLA	5	0
14	H	1012	CLA	4	0
17	r	524	BCR	5	0
14	5	513	CLA	2	0
14	s	512	CLA	5	0
14	r	519	CLA	1	0
17	2	524	BCR	6	0
18	e	5002	LHG	1	0
17	q	524	BCR	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	4	513	CLA	2	0
14	2	502	CLA	3	0
14	f	1234	CLA	4	0
14	s	502	CLA	2	0
14	4	517	CLA	1	0
14	f	1209	CLA	2	0
14	f	1225	CLA	4	0
17	f	4009	BCR	3	0
14	3	510	CLA	2	0
14	6	511	CLA	2	0
14	2	501	CLA	3	0
14	B	1021	CLA	1	0
21	a	822	SQD	2	0
14	B	1207	CLA	10	0
21	V	5216	SQD	6	0
17	o	4021	BCR	1	0
21	q	822	SQD	1	0
17	v	523	BCR	3	0
14	B	1226	CLA	5	0
14	e	1119	CLA	7	0
14	q	516	CLA	6	0
14	G	1101	CLA	5	0
14	B	1223	CLA	4	0
14	B	1219	CLA	2	0
14	G	1135	CLA	3	0
14	d	505	CLA	4	0
14	e	1135	CLA	3	0
21	n	5216	SQD	6	0
14	e	1116	CLA	5	0
14	1	512	CLA	4	0
14	A	1237	CLA	6	0
17	1	522	BCR	2	0
18	e	5006	LHG	3	0
14	v	511	CLA	2	0
14	e	1107	CLA	1	0
14	5	510	CLA	1	0
14	H	1207	CLA	8	0
17	H	4014	BCR	3	0
14	B	1211	CLA	1	0
14	H	1234	CLA	6	0
17	e	4003	BCR	3	0
14	H	1230	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1135	CLA	3	0
17	L	4020	BCR	2	0
17	4	524	BCR	3	0
17	G	4003	BCR	3	0
14	s	503	CLA	1	0
17	q	521	BCR	5	0
17	v	521	BCR	2	0
19	G	1848	LMU	2	0
14	Y	505	CLA	4	0
14	f	1208	CLA	4	0
14	e	1022	CLA	2	0
14	f	1228	CLA	4	0
14	d	519	CLA	2	0
14	B	1240	CLA	1	0
17	M	4021	BCR	2	0
14	A	1110	CLA	2	0
14	A	1102	CLA	1	0
14	r	505	CLA	3	0
14	a	510	CLA	2	0
14	t	503	CLA	1	0
17	u	523	BCR	2	0
14	A	1109	CLA	1	0
15	A	2001	PQN	3	0
14	1	504	CLA	1	0
17	4	523	BCR	2	0
15	f	2002	PQN	5	0
14	b	505	CLA	1	0
14	H	1235	CLA	4	0
14	c	507	CLA	1	0
14	1	507	CLA	1	0
14	j	1302	CLA	3	0
14	q	511	CLA	1	0
14	s	511	CLA	1	0
17	t	524	BCR	3	0
14	Z	512	CLA	6	0
17	c	521	BCR	4	0
14	c	512	CLA	4	0
17	e	4007	BCR	2	0
14	H	1236	CLA	3	0
14	e	1128	CLA	5	0
14	R	1301	CLA	1	0
17	r	521	BCR	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	e	1108	CLA	1	0
14	q	504	CLA	1	0
14	u	509	CLA	3	0
17	1	523	BCR	2	0
14	6	509	CLA	1	0
14	2	503	CLA	3	0
17	s	523	BCR	2	0
14	v	505	CLA	4	0
18	G	5005	LHG	6	0
14	c	513	CLA	2	0
14	q	518	CLA	1	0
14	B	1214	CLA	2	0
14	G	1110	CLA	1	0
17	u	521	BCR	6	0
14	d	510	CLA	1	0
18	G	5006	LHG	3	0
17	H	4005	BCR	3	0
15	G	2001	PQN	2	0
14	G	1127	CLA	1	0
14	B	1210	CLA	7	0
14	r	506	CLA	2	0
14	c	511	CLA	1	0
14	1	511	CLA	1	0
21	s	822	SQD	2	0
14	B	1215	CLA	3	0
14	f	1021	CLA	2	0
17	A	4001	BCR	4	0
14	f	1204	CLA	2	0
14	s	513	CLA	2	0
17	U	4104	BCR	3	0
14	f	1224	CLA	4	0
14	6	513	CLA	2	0
14	H	1216	CLA	5	0
14	B	1236	CLA	3	0
17	5	523	BCR	2	0
15	H	2002	PQN	4	0
14	G	1123	CLA	3	0
14	4	503	CLA	1	0
17	4	521	BCR	2	0
14	G	1114	CLA	1	0
17	H	4004	BCR	5	0
14	5	509	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1125	CLA	3	0
14	Y	510	CLA	1	0
17	l	4013	BCR	5	0
18	V	5218	LHG	2	0
18	V	5220	LHG	4	0
14	H	1231	CLA	3	0
17	F	4016	BCR	6	0
17	G	4001	BCR	3	0
14	t	513	CLA	2	0
14	3	502	CLA	3	0
17	B	4005	BCR	4	0
14	3	513	CLA	2	0
14	e	1134	CLA	2	0
14	Z	518	CLA	2	0
20	f	5002	LMG	6	0
14	A	1126	CLA	9	0
17	V	4022	BCR	8	0
14	4	501	CLA	1	0
14	A	1123	CLA	1	0
18	n	5218	LHG	2	0
14	t	504	CLA	1	0
14	u	507	CLA	1	0
14	H	1227	CLA	2	0
14	f	1219	CLA	1	0
14	B	1239	CLA	4	0
17	c	523	BCR	2	0
14	e	1115	CLA	2	0
14	G	1117	CLA	4	0
14	e	1136	CLA	1	0
14	4	511	CLA	2	0
14	e	1801	CLA	3	0
17	Z	521	BCR	7	0
18	S	5001	LHG	2	0
17	B	4009	BCR	3	0
17	1	524	BCR	5	0
14	B	1227	CLA	2	0
14	B	1225	CLA	4	0
14	G	1129	CLA	5	0
14	d	502	CLA	2	0
18	e	5004	LHG	2	0
14	n	1501	CLA	7	0
14	A	1130	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	513	CLA	2	0
14	n	1502	CLA	3	0
14	Z	503	CLA	3	0
14	G	1125	CLA	3	0
14	e	1126	CLA	8	0
14	l	1302	CLA	1	0
14	A	1117	CLA	5	0
14	B	1220	CLA	3	0
14	A	1139	CLA	2	0
14	e	1123	CLA	2	0
14	B	1216	CLA	4	0
17	V	4219	BCR	8	0
17	d	524	BCR	4	0
14	v	513	CLA	2	0
14	b	501	CLA	1	0
14	Y	507	CLA	1	0
14	Z	511	CLA	1	0
18	f	1855	LHG	3	0
14	6	505	CLA	4	0
14	6	517	CLA	2	0
14	n	1503	CLA	3	0
17	5	521	BCR	3	0
14	B	1218	CLA	2	0
14	e	1139	CLA	2	0
14	A	1122	CLA	2	0
14	G	1237	CLA	6	0
18	G	5008	LHG	8	0
14	B	1206	CLA	4	0
14	Y	509	CLA	1	0
17	2	521	BCR	7	0
18	G	5003	LHG	2	0
14	2	518	CLA	2	0
14	H	1220	CLA	3	0
18	H	1842	LHG	2	0
17	R	4016	BCR	6	0
14	A	1011	CLA	2	0
14	t	508	CLA	1	0
17	c	522	BCR	1	0
14	5	506	CLA	3	0
14	G	1103	CLA	4	0
14	v	518	CLA	1	0
17	t	523	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	5003	LHG	2	0
14	L	1502	CLA	3	0
17	V	4020	BCR	2	0
14	G	1121	CLA	3	0
14	2	505	CLA	4	0
18	H	1855	LHG	3	0
14	G	1011	CLA	3	0
17	s	522	BCR	2	0
14	c	505	CLA	1	0
17	v	522	BCR	2	0
17	H	4006	BCR	4	0
14	A	1103	CLA	3	0
17	6	522	BCR	4	0
14	4	509	CLA	3	0
14	1	502	CLA	2	0
14	H	1021	CLA	2	0
14	f	1235	CLA	4	0
14	A	1121	CLA	3	0
21	B	1852	SQD	8	0
14	L	1503	CLA	1	0
14	t	517	CLA	2	0
14	b	508	CLA	1	0
21	H	1852	SQD	9	0
14	B	1217	CLA	2	0
14	r	512	CLA	5	0
20	H	5002	LMG	6	0
15	e	2001	PQN	2	0
14	4	502	CLA	3	0
14	H	1239	CLA	4	0
18	k	5001	LHG	2	0
14	G	1124	CLA	3	0
14	6	510	CLA	1	0
14	A	1104	CLA	6	0
17	l	4012	BCR	3	0
14	e	1106	CLA	5	0
14	t	509	CLA	1	0
14	v	517	CLA	2	0
14	b	507	CLA	1	0
19	f	1843	LMU	1	0
14	2	506	CLA	2	0
17	r	523	BCR	1	0
17	t	521	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	c	506	CLA	3	0
14	A	1129	CLA	5	0
14	3	512	CLA	5	0
17	q	523	BCR	1	0
14	H	1224	CLA	3	0
14	f	1023	CLA	2	0
18	A	5001	LHG	5	0
14	d	512	CLA	3	0
17	d	522	BCR	2	0
17	k	4018	BCR	5	0
14	b	516	CLA	2	0
14	u	510	CLA	1	0
17	I	4018	BCR	4	0
14	Y	518	CLA	1	0
14	e	1138	CLA	3	0
14	G	1112	CLA	1	0
14	Z	505	CLA	4	0
14	G	1013	CLA	7	0
14	f	1221	CLA	7	0
14	r	517	CLA	1	0
14	c	510	CLA	1	0
14	u	511	CLA	1	0
14	5	512	CLA	4	0
17	5	522	BCR	2	0
17	j	4016	BCR	6	0
17	Y	524	BCR	5	0
14	H	1218	CLA	2	0
14	A	1140	CLA	3	0
14	B	1023	CLA	2	0
22	X	170	FMN	2	0
14	2	519	CLA	1	0
14	H	1210	CLA	7	0
14	q	512	CLA	4	0
14	Y	513	CLA	2	0
14	A	1112	CLA	1	0
18	G	5001	LHG	5	0
14	r	513	CLA	2	0
14	s	510	CLA	2	0
17	L	4022	BCR	8	0
14	Y	504	CLA	1	0
14	A	1107	CLA	1	0
17	l	4015	BCR	6	0

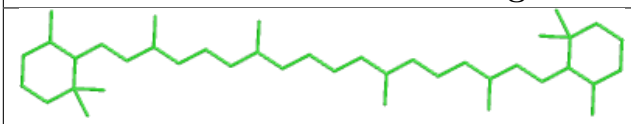
Continued on next page...

Continued from previous page...

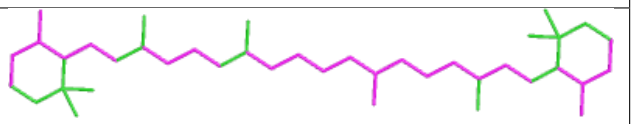
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	3	517	CLA	1	0
14	q	509	CLA	1	0
18	e	5007	LHG	2	0
14	H	1023	CLA	5	0
14	r	511	CLA	1	0
17	3	521	BCR	1	0
14	4	508	CLA	1	0
18	A	5009	LHG	3	0
14	6	502	CLA	2	0
14	1	505	CLA	2	0
17	m	4104	BCR	3	0
14	1	518	CLA	1	0
17	3	523	BCR	2	0
19	B	1843	LMU	1	0
14	Z	506	CLA	2	0
17	e	4001	BCR	3	0
14	G	1122	CLA	3	0
18	e	5005	LHG	6	0
14	G	1126	CLA	10	0
14	G	1107	CLA	1	0
14	G	1109	CLA	1	0
14	B	1203	CLA	2	0
14	Z	517	CLA	1	0
14	r	518	CLA	2	0
14	2	512	CLA	5	0
14	3	511	CLA	1	0
17	e	4002	BCR	1	0
14	d	509	CLA	1	0
14	H	1202	CLA	3	0
17	f	4004	BCR	2	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.

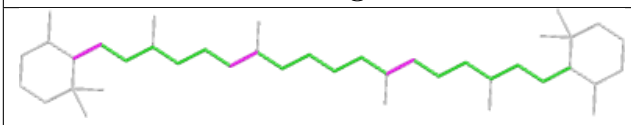
Ligand BCR W 4021



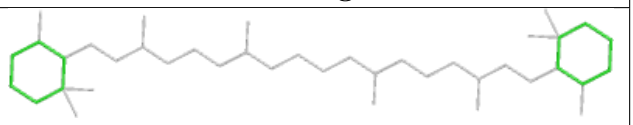
Bond lengths



Bond angles

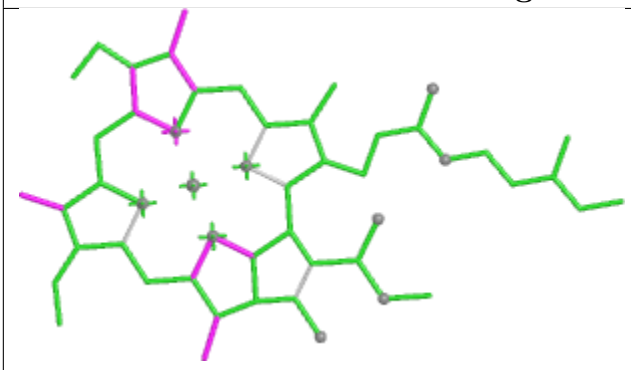


Torsions

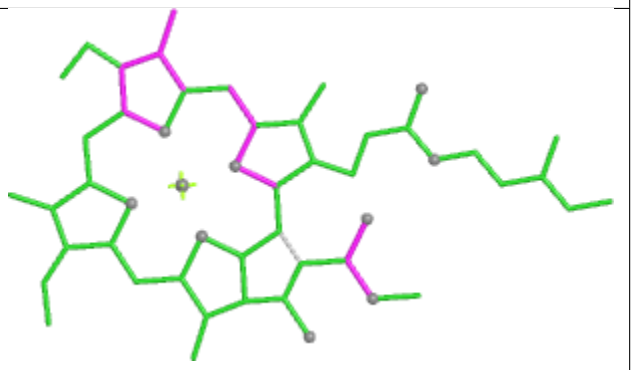


Rings

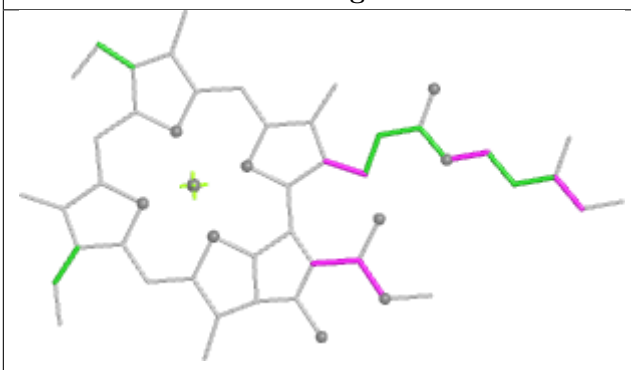
Ligand CLA B 1212



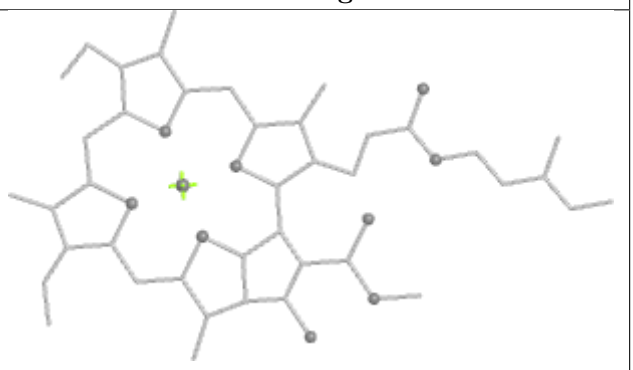
Bond lengths



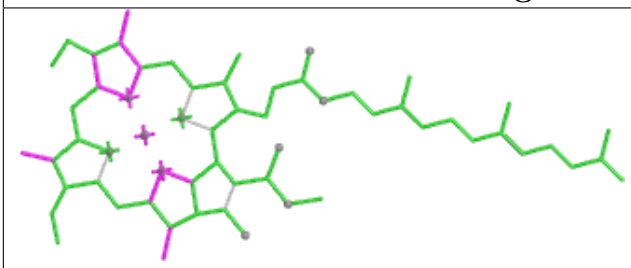
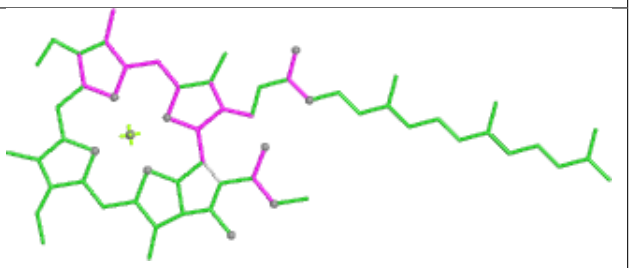
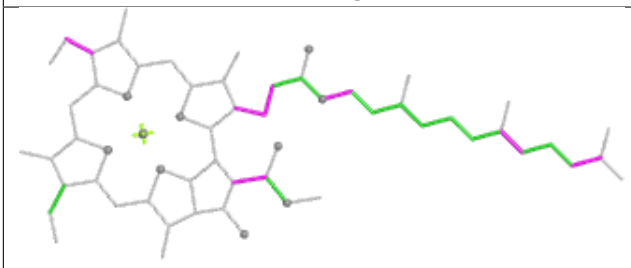
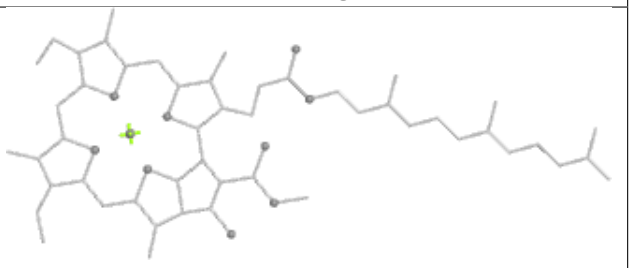
Bond angles

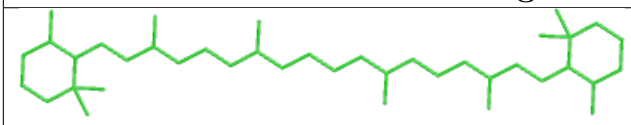
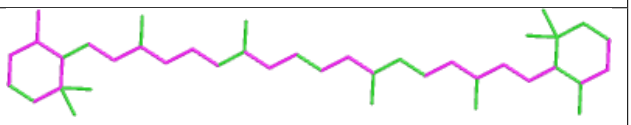
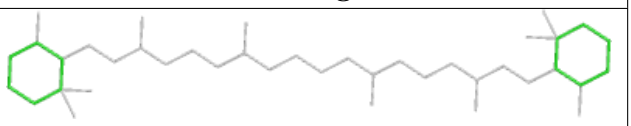


Torsions

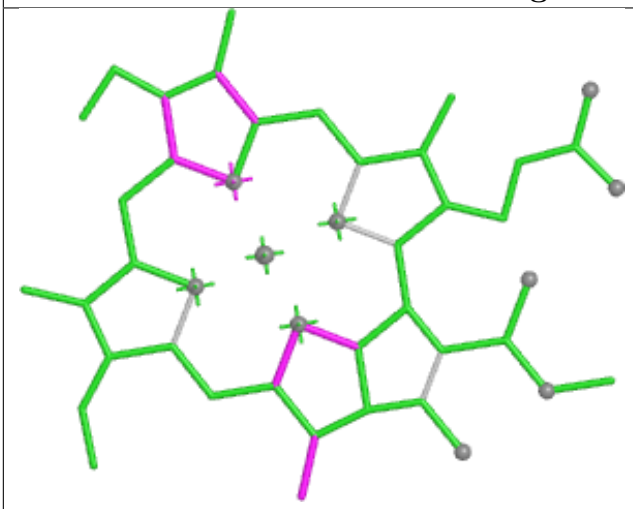


Rings

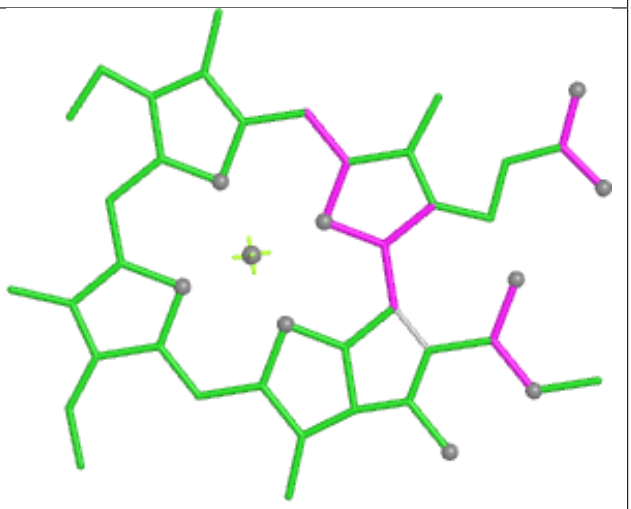
Ligand CLA V 1501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 4012	
	
Bond lengths	Bond angles
	
Torsions	Rings

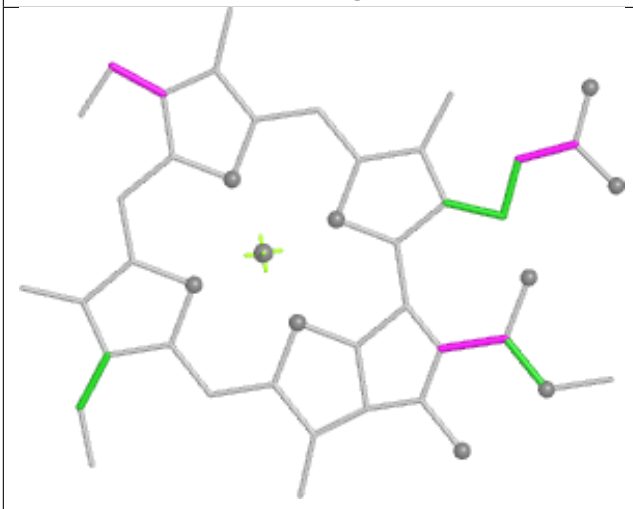
Ligand CLA s 507



Bond lengths



Bond angles

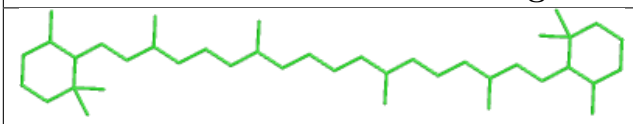


Torsions

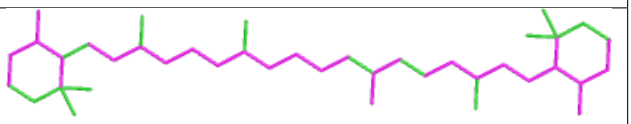


Rings

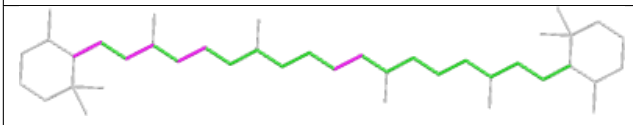
Ligand BCR r 522



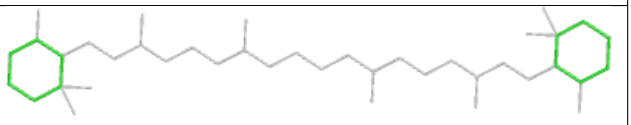
Bond lengths



Bond angles

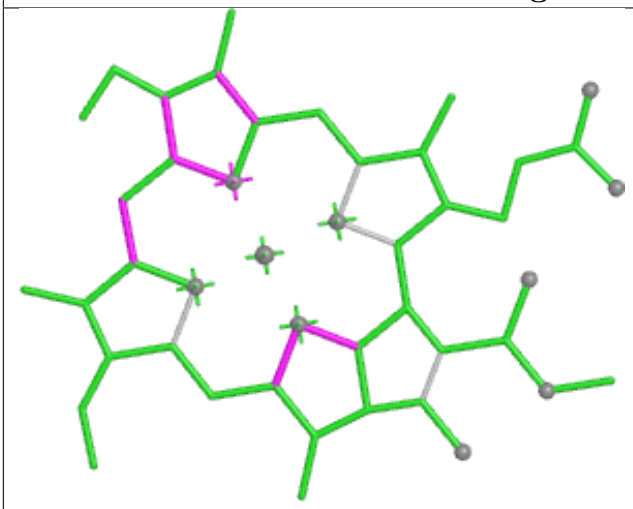


Torsions

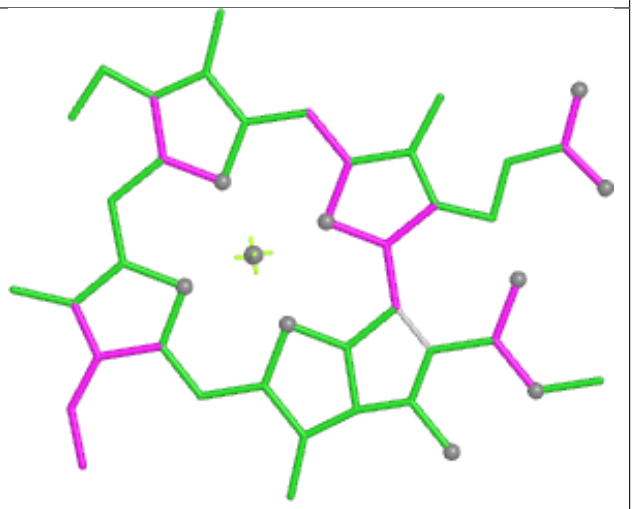


Rings

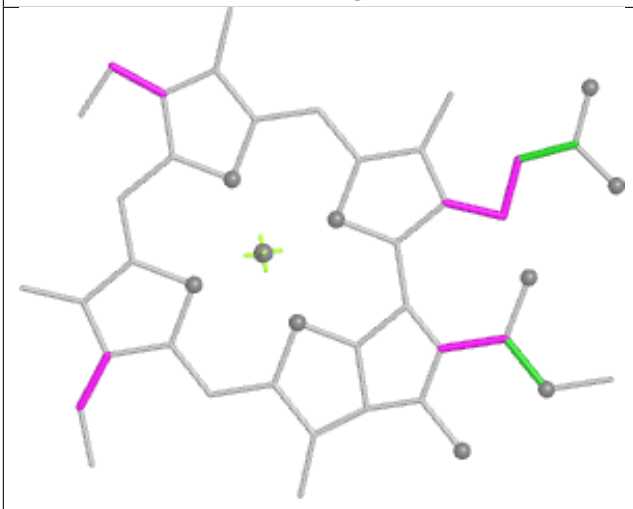
Ligand CLA s 516



Bond lengths



Bond angles

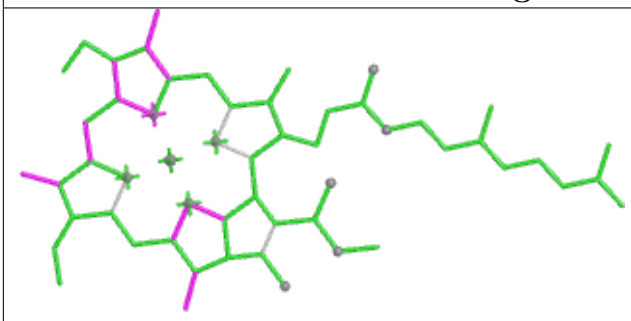


Torsions

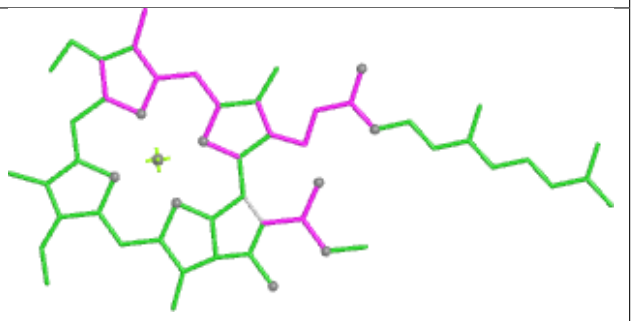


Rings

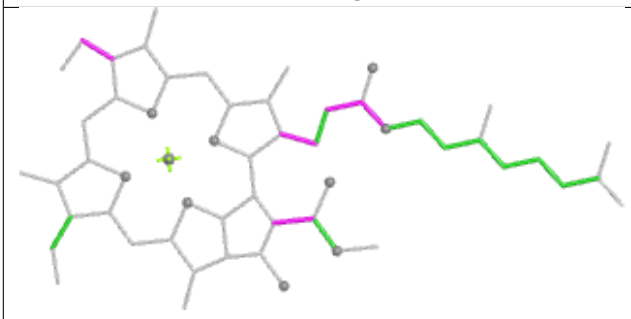
Ligand CLA m 1401



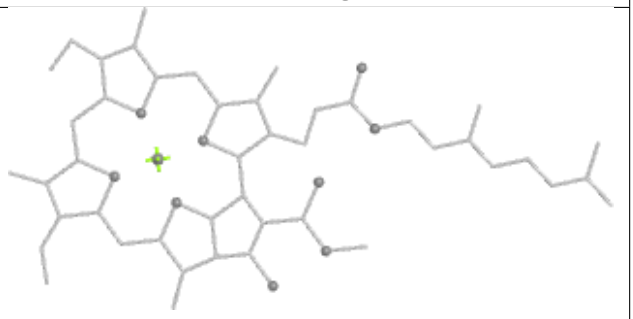
Bond lengths



Bond angles

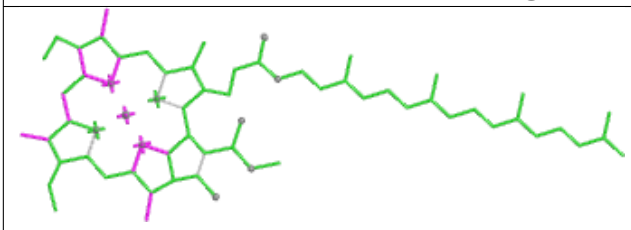


Torsions

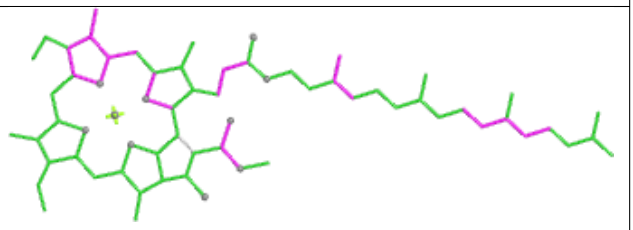


Rings

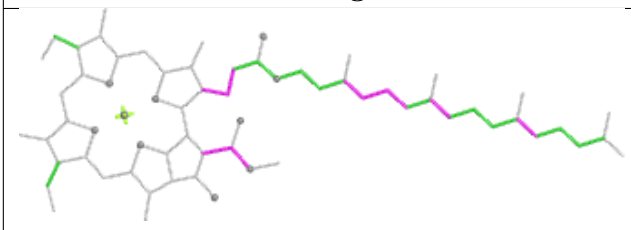
Ligand CLA f 1012



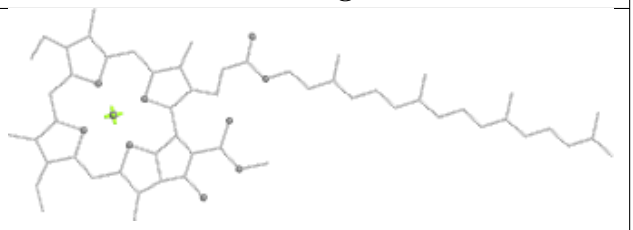
Bond lengths



Bond angles

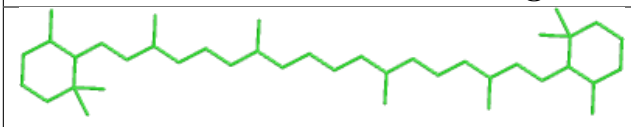


Torsions

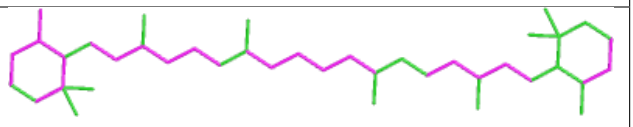


Rings

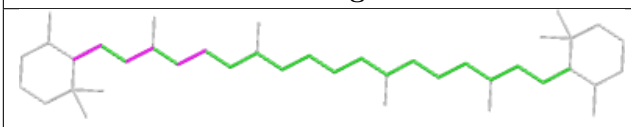
Ligand BCR d 521



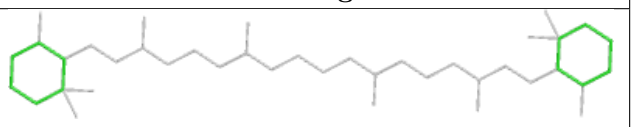
Bond lengths



Bond angles

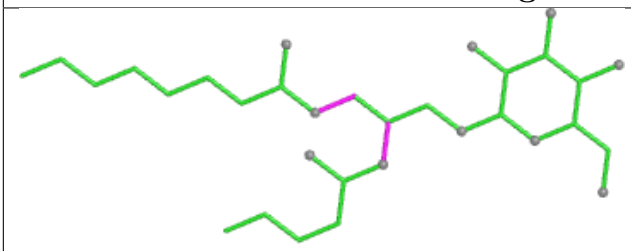


Torsions

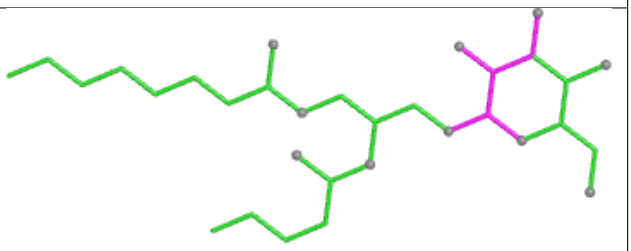


Rings

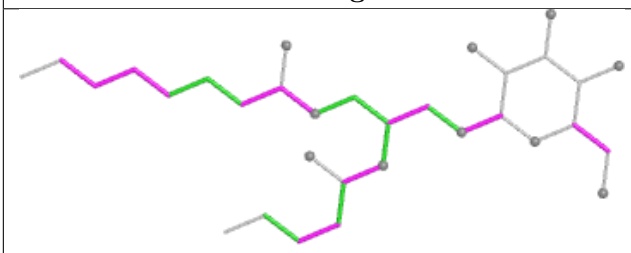
Ligand LMG l 5104



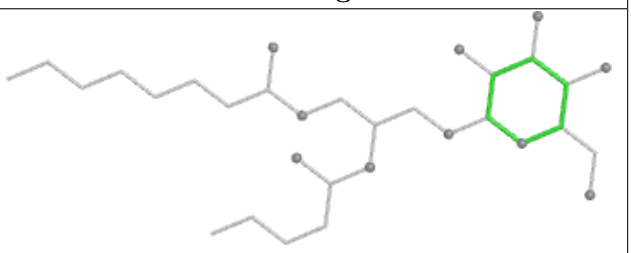
Bond lengths



Bond angles

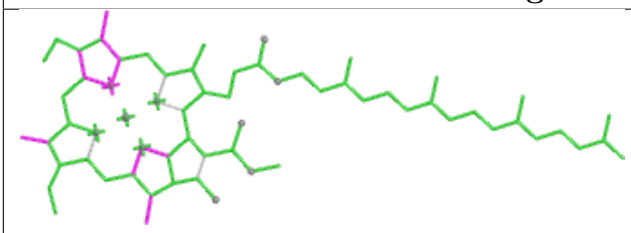


Torsions

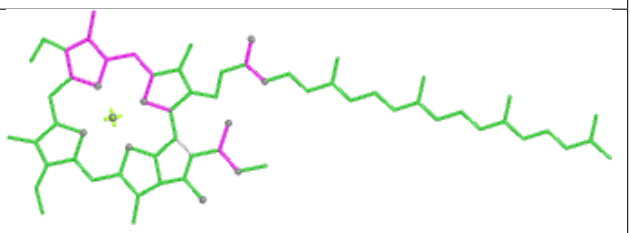


Rings

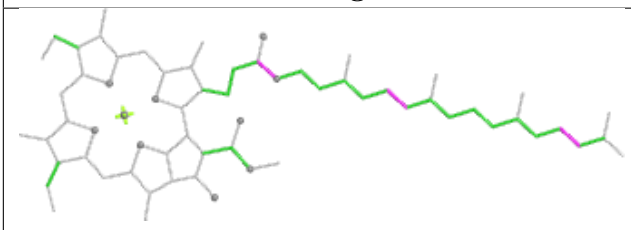
Ligand CLA Z 509



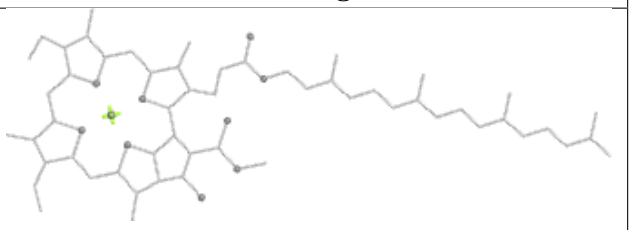
Bond lengths



Bond angles

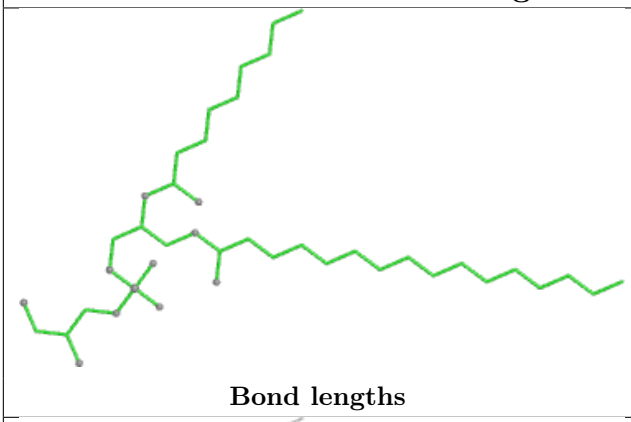


Torsions

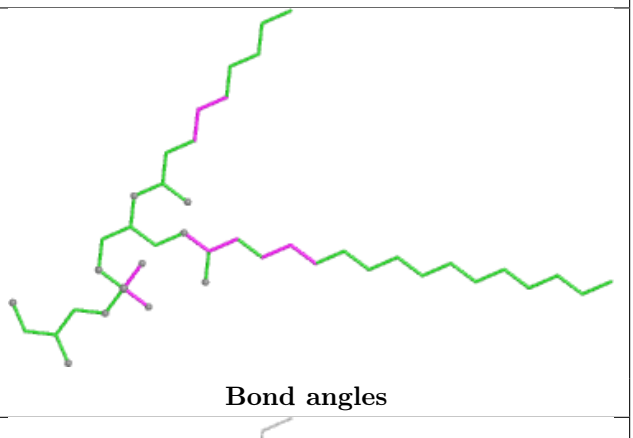


Rings

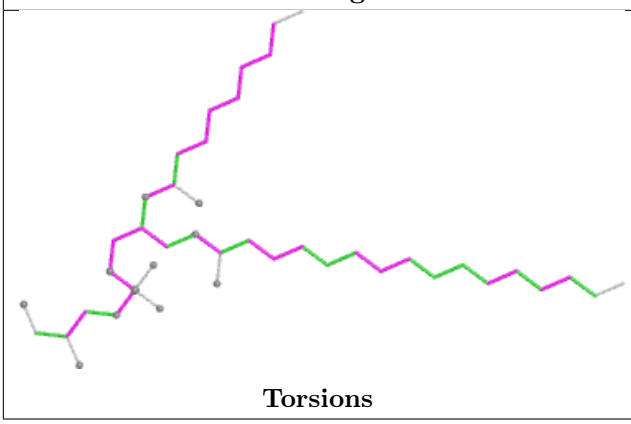
Ligand LHG G 5009



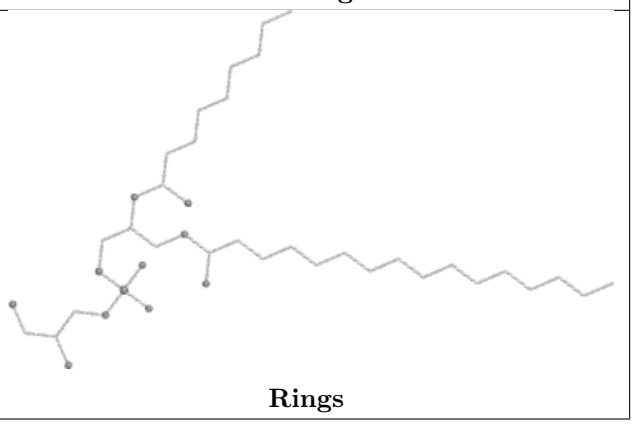
Bond lengths



Bond angles

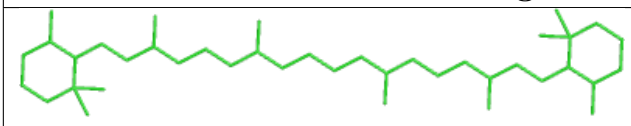


Torsions

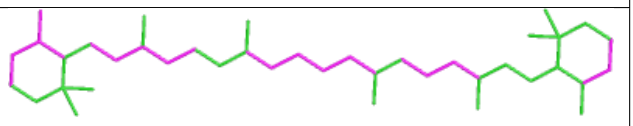


Rings

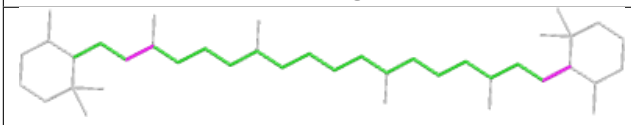
Ligand BCR n 4022



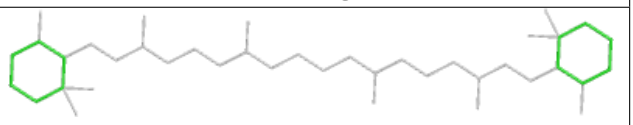
Bond lengths



Bond angles

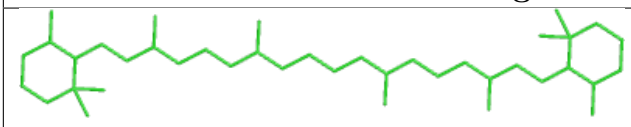


Torsions

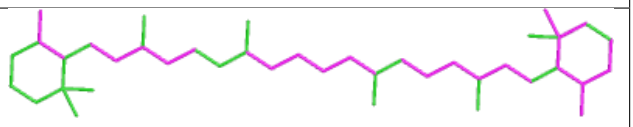


Rings

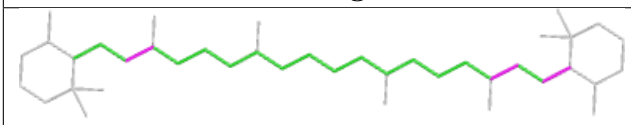
Ligand BCR V 4019



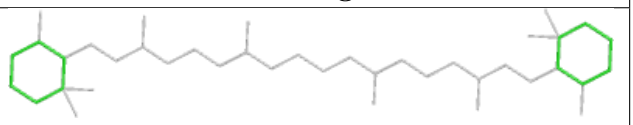
Bond lengths



Bond angles

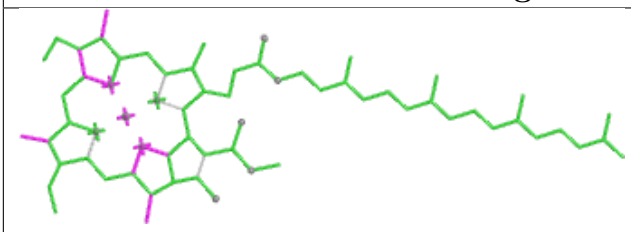


Torsions

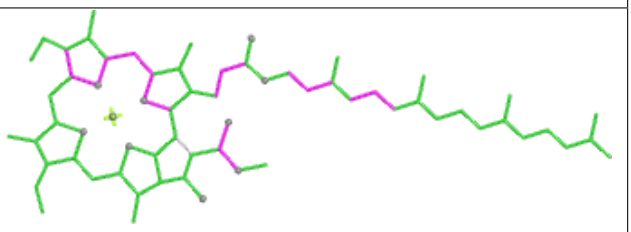


Rings

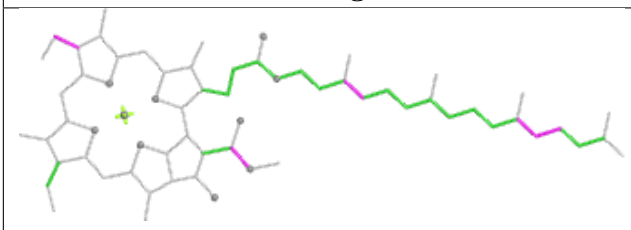
Ligand CLA G 1131



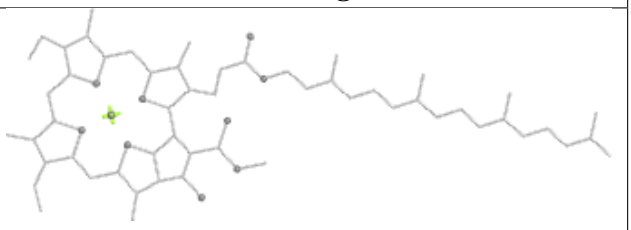
Bond lengths



Bond angles

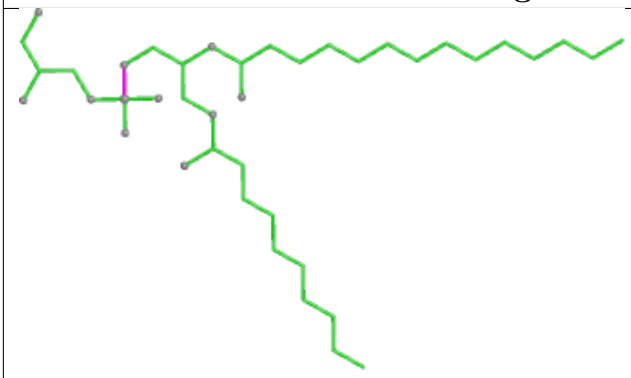


Torsions

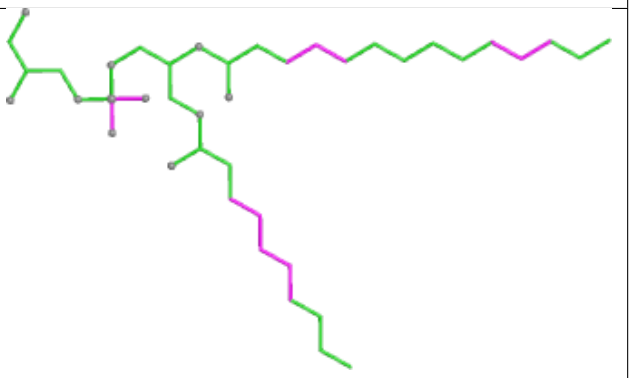


Rings

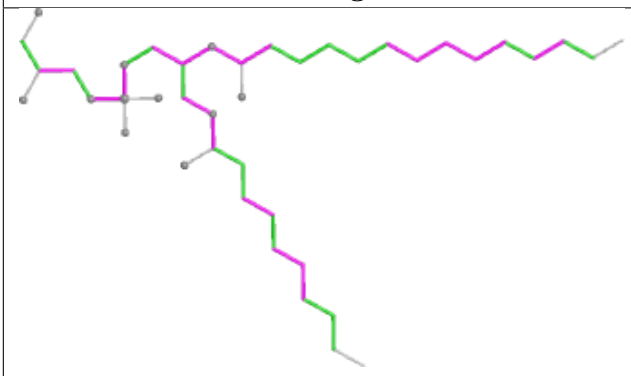
Ligand LHG B 1855



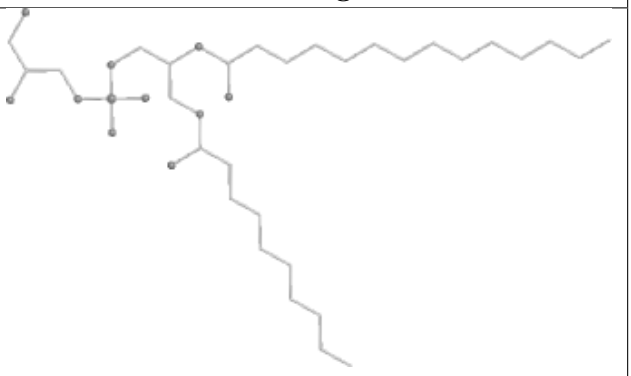
Bond lengths



Bond angles

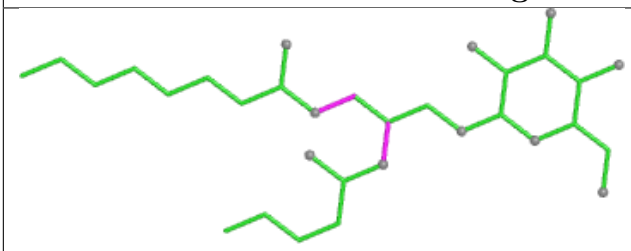


Torsions

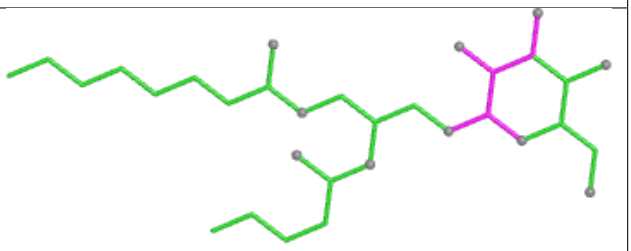


Rings

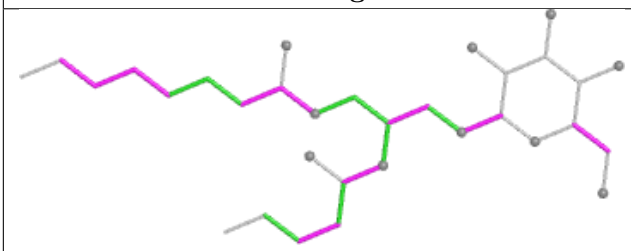
Ligand LMG T 5104



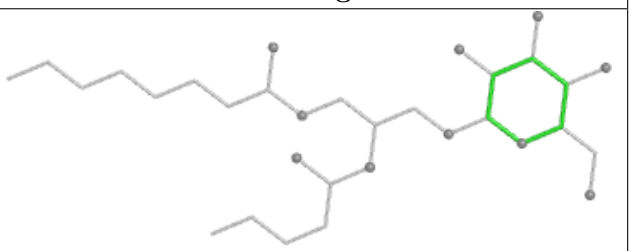
Bond lengths



Bond angles

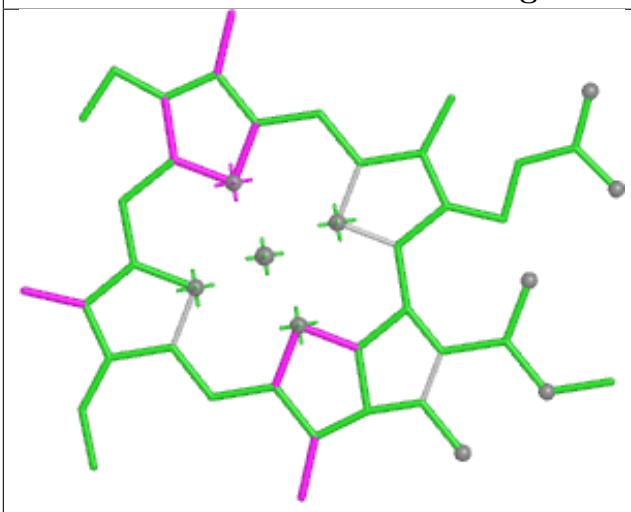


Torsions

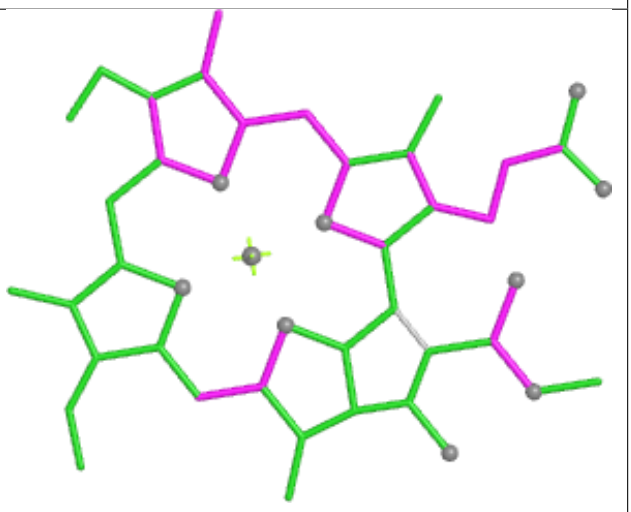


Rings

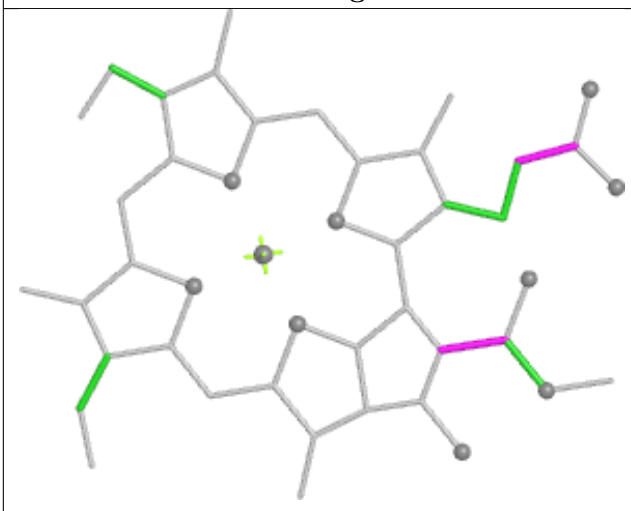
Ligand CLA e 1114



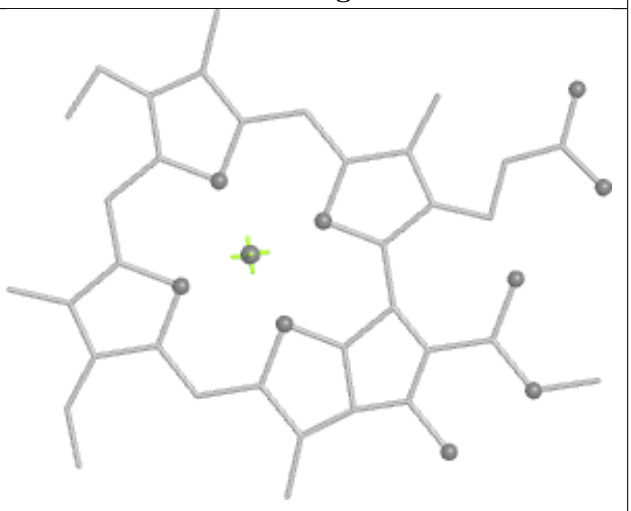
Bond lengths



Bond angles

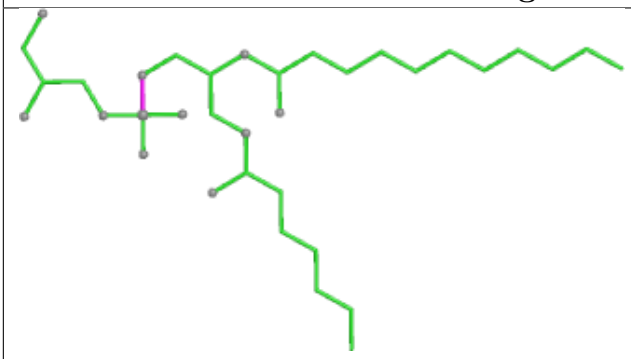


Torsions

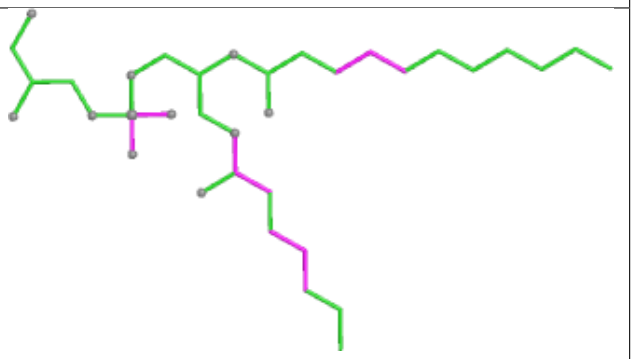


Rings

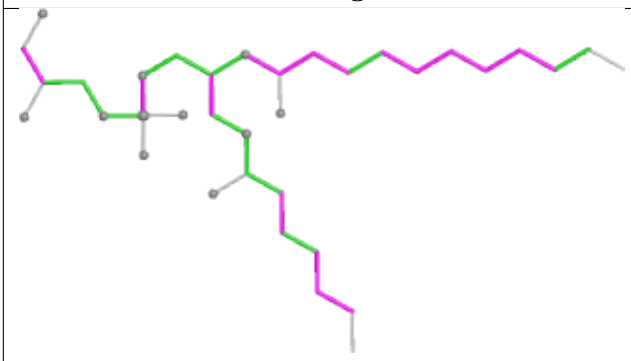
Ligand LHG e 5008



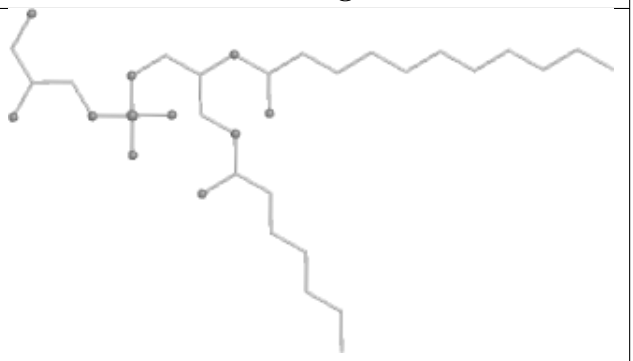
Bond lengths



Bond angles

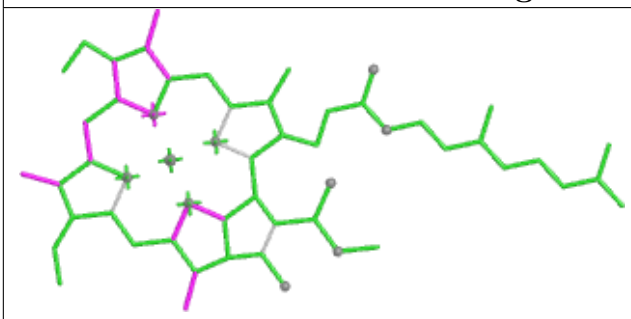


Torsions

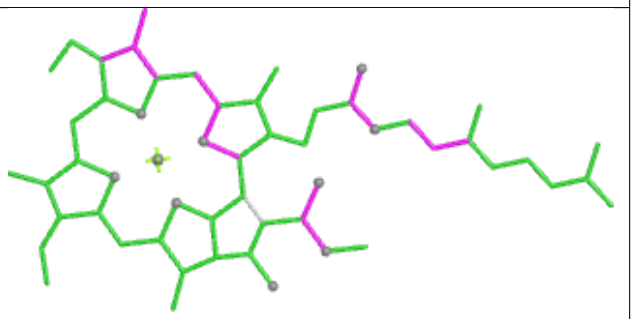


Rings

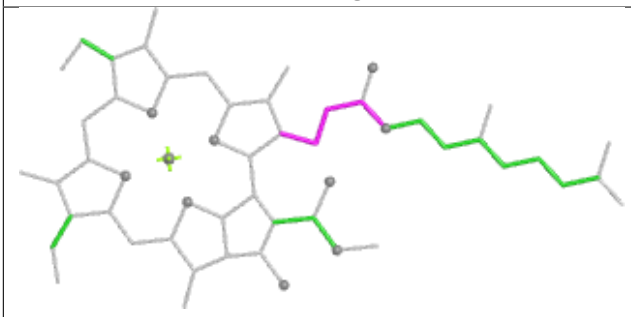
Ligand CLA B 1228



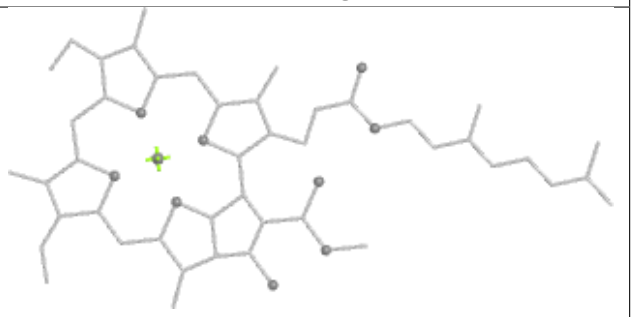
Bond lengths



Bond angles

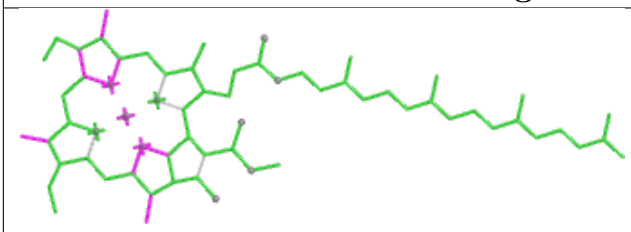


Torsions

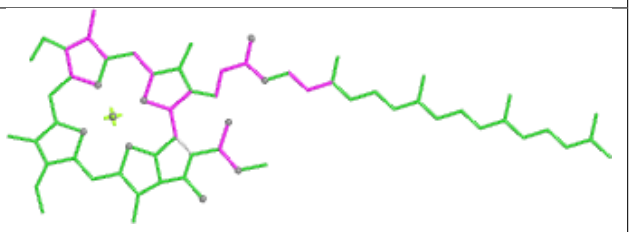


Rings

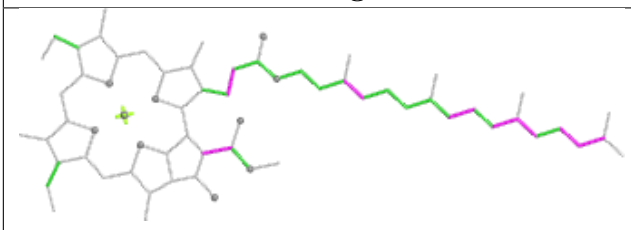
Ligand CLA A 1127



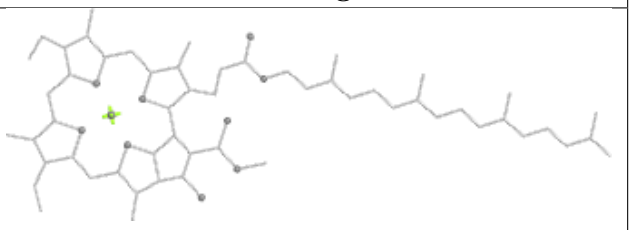
Bond lengths



Bond angles



Torsions



Rings

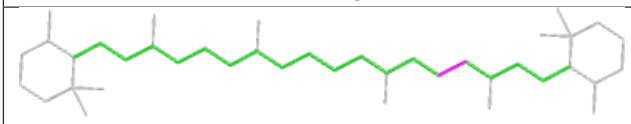
Ligand BCR H 4009



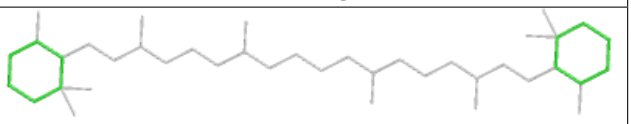
Bond lengths



Bond angles

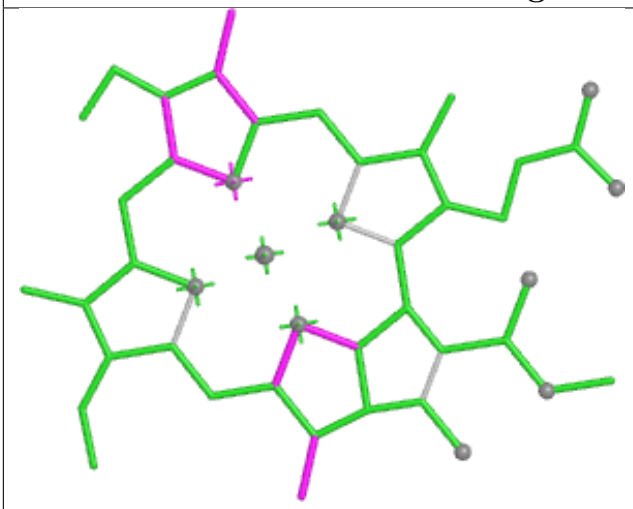


Torsions

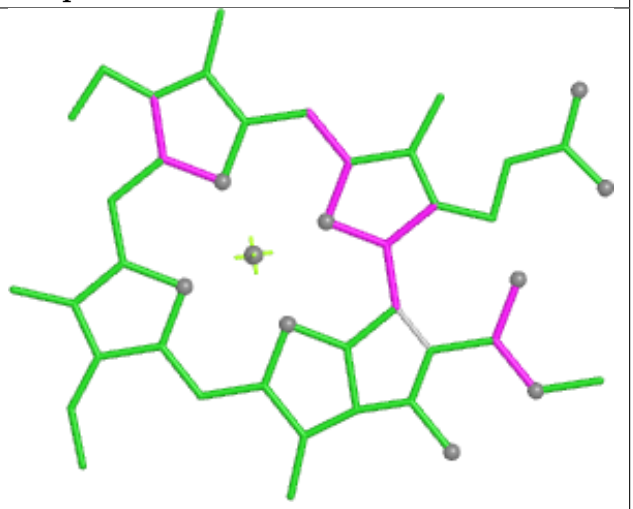


Rings

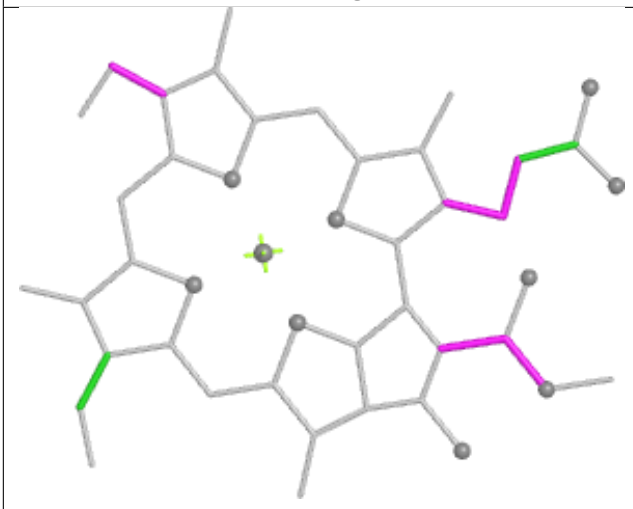
Ligand CLA q 503



Bond lengths



Bond angles

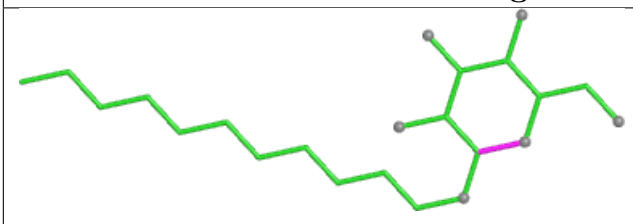


Torsions

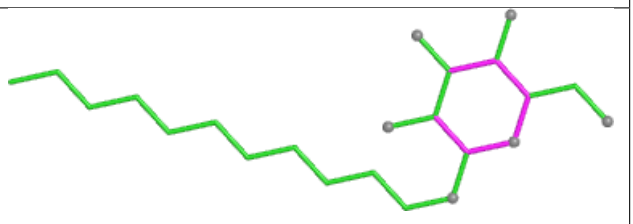


Rings

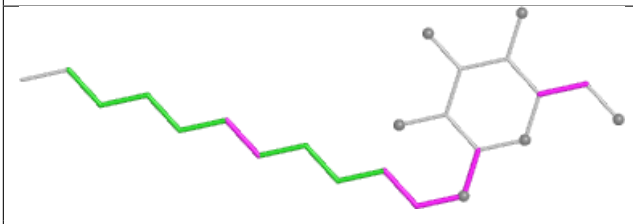
Ligand LMU G 1849



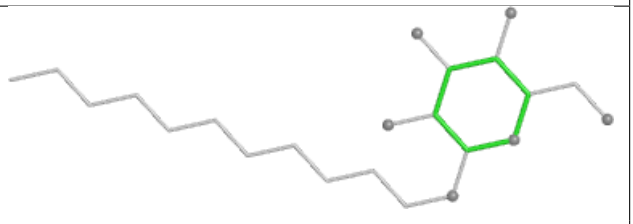
Bond lengths



Bond angles

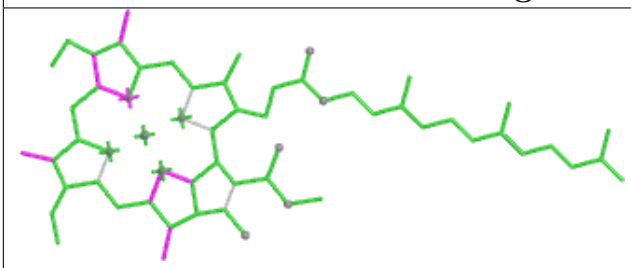


Torsions

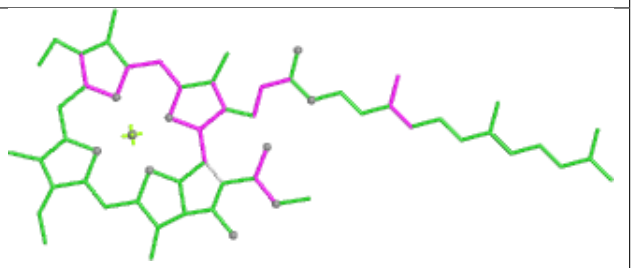


Rings

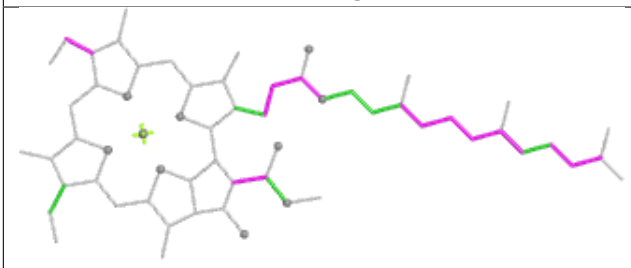
Ligand CLA A 1137



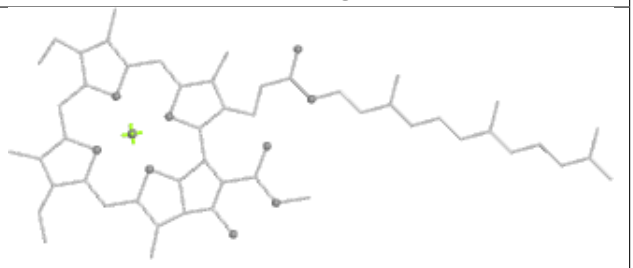
Bond lengths



Bond angles

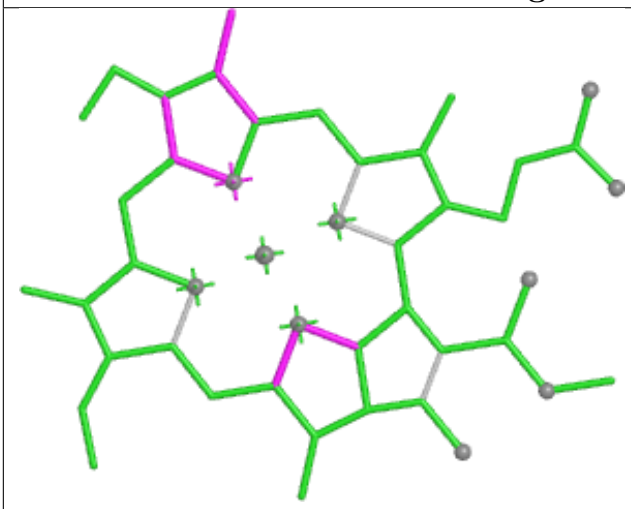


Torsions

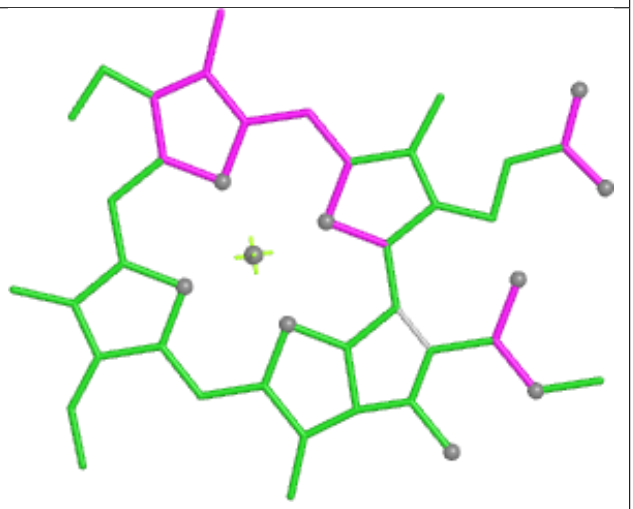


Rings

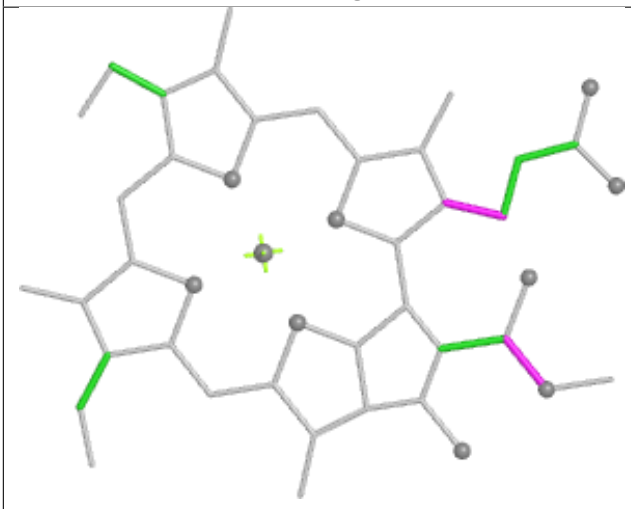
Ligand CLA 5 511



Bond lengths



Bond angles

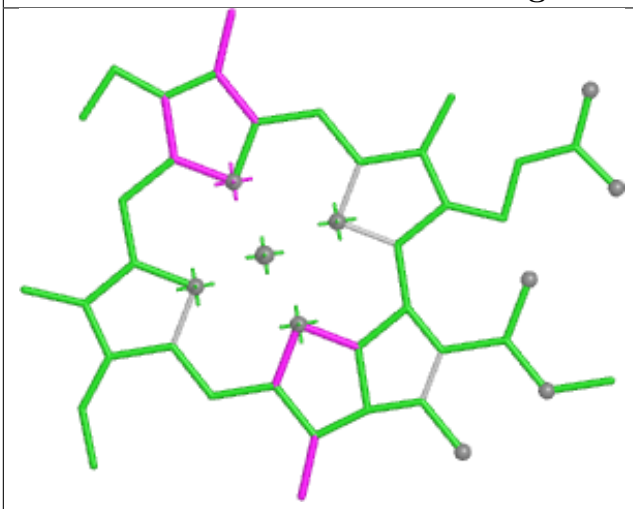


Torsions

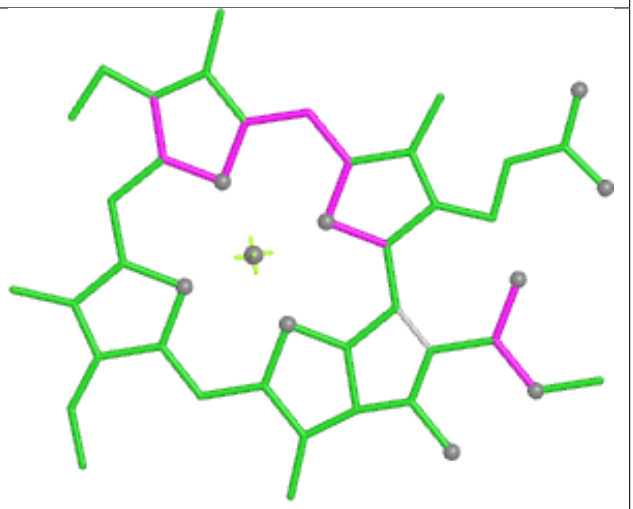


Rings

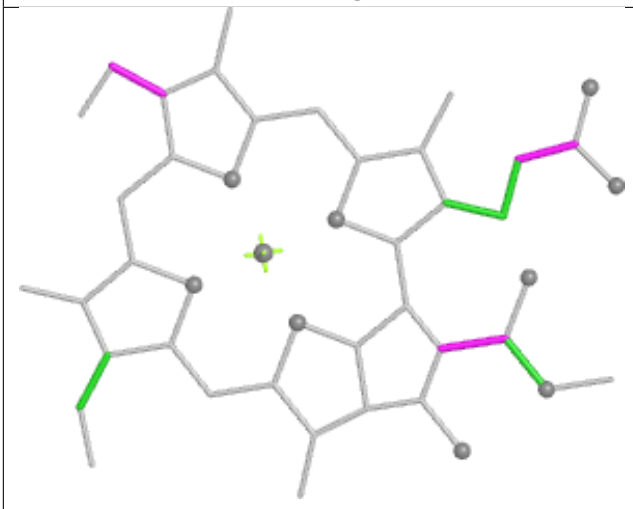
Ligand CLA 4 512



Bond lengths



Bond angles

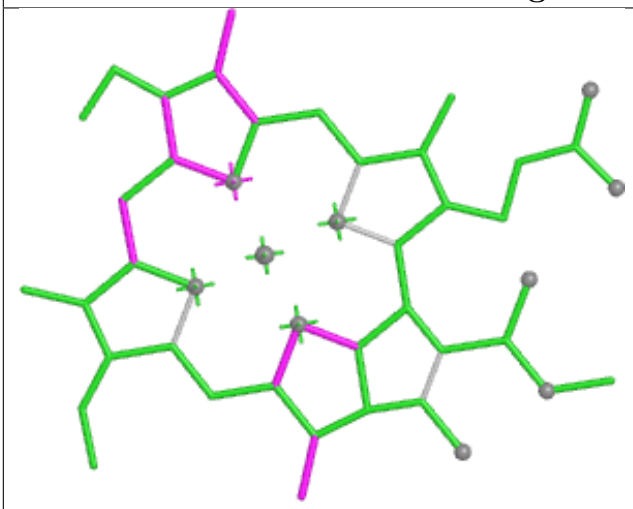


Torsions

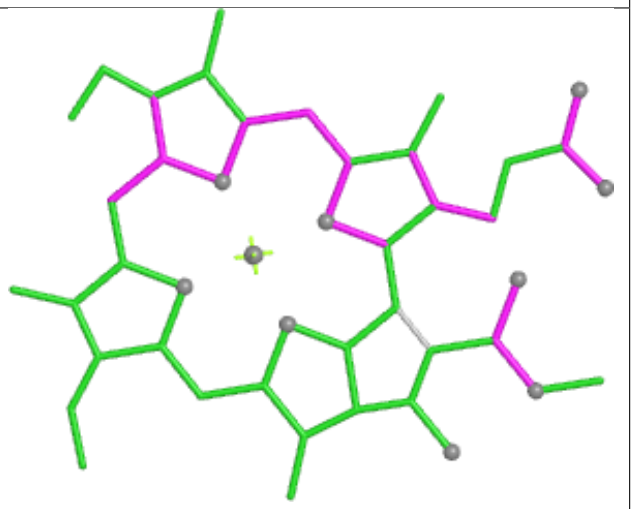


Rings

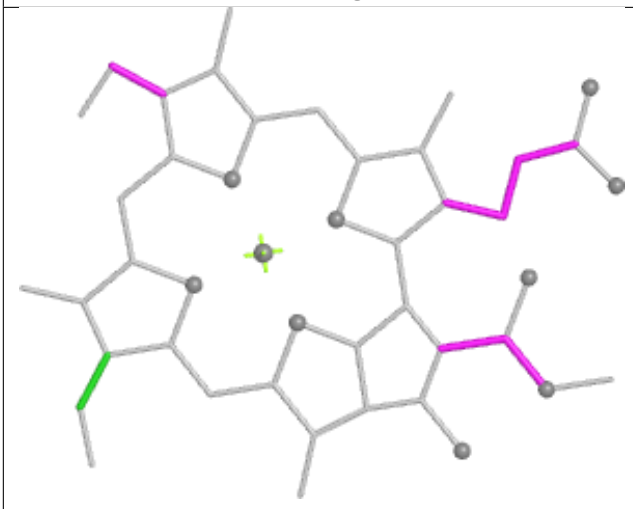
Ligand CLA 6 516



Bond lengths



Bond angles

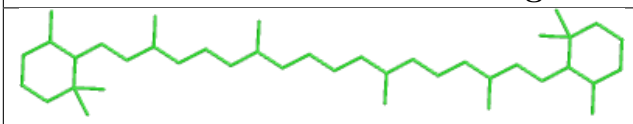


Torsions

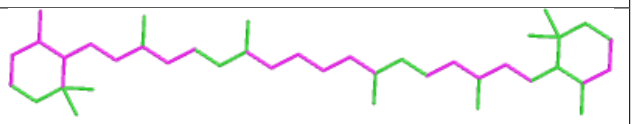


Rings

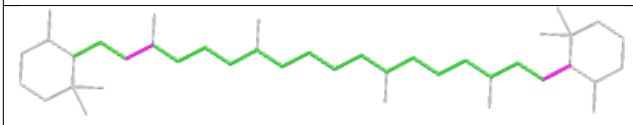
Ligand BCR b 524



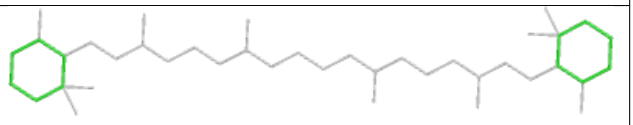
Bond lengths



Bond angles

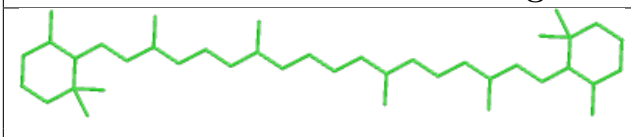


Torsions

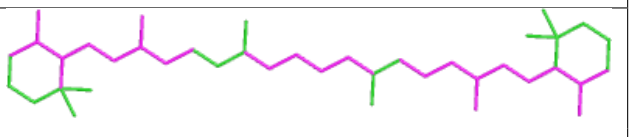


Rings

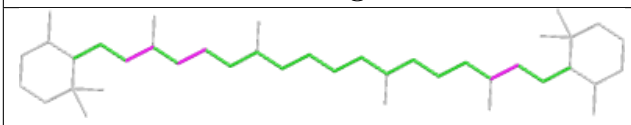
Ligand BCR a 524



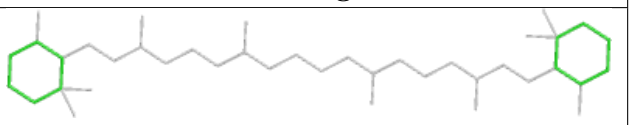
Bond lengths



Bond angles

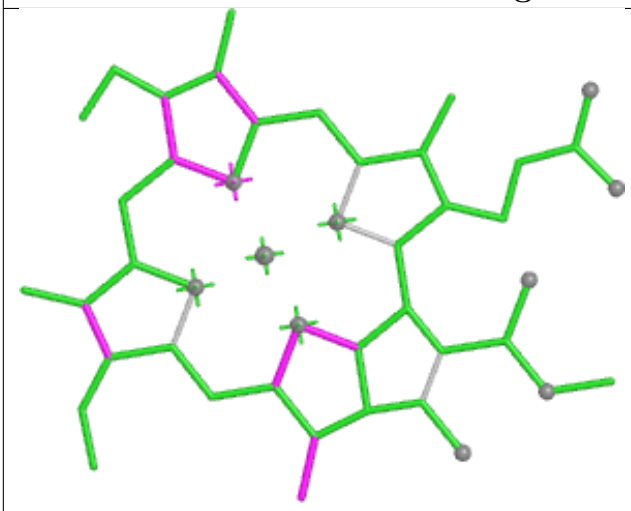


Torsions

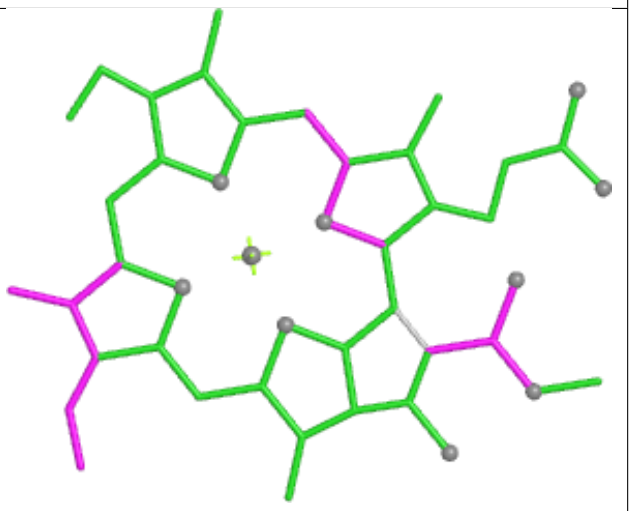


Rings

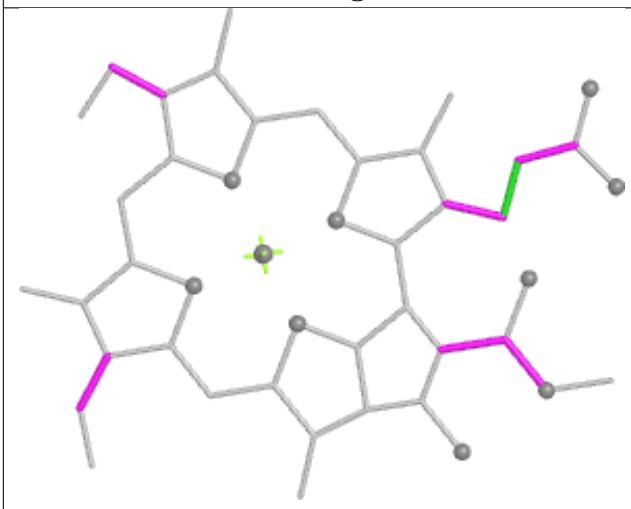
Ligand CLA U 1105



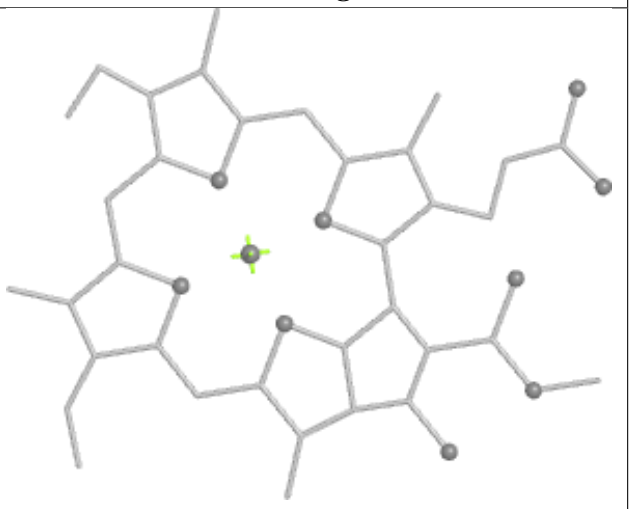
Bond lengths



Bond angles

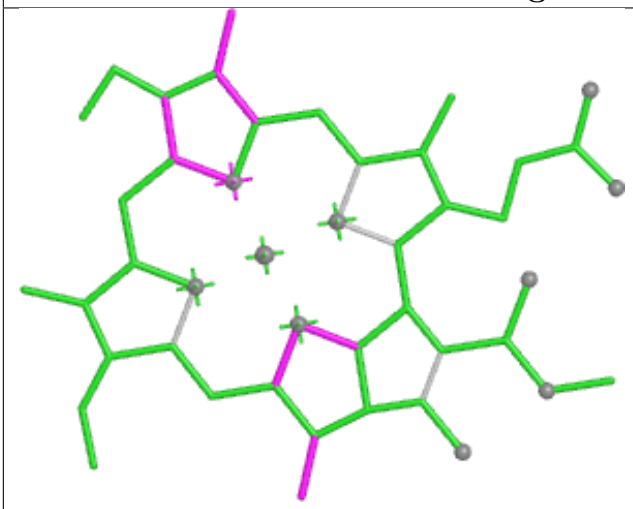


Torsions

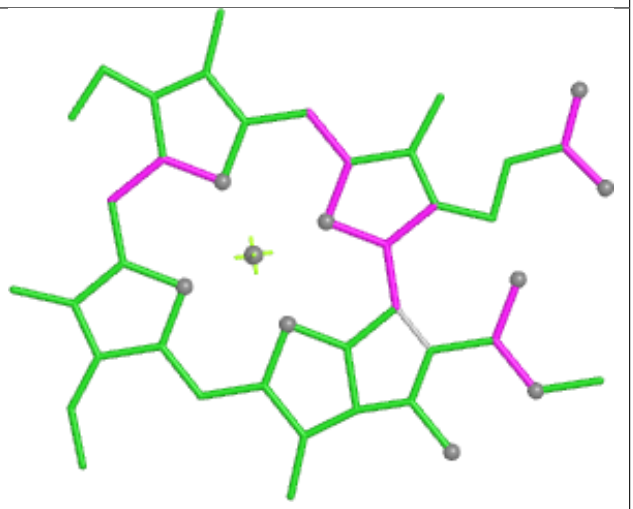


Rings

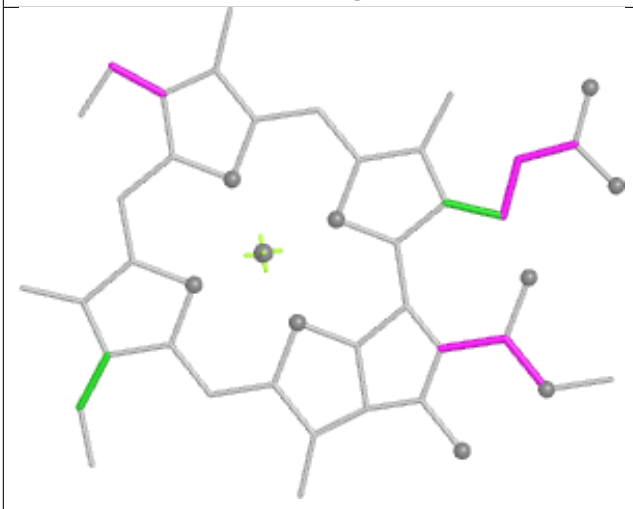
Ligand CLA 5 507



Bond lengths



Bond angles

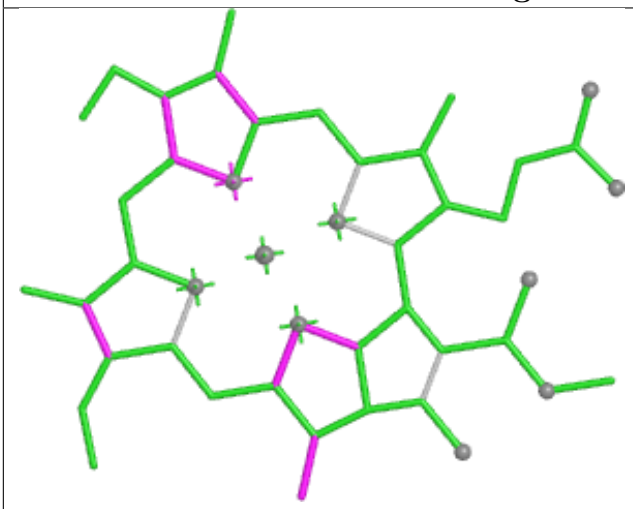


Torsions

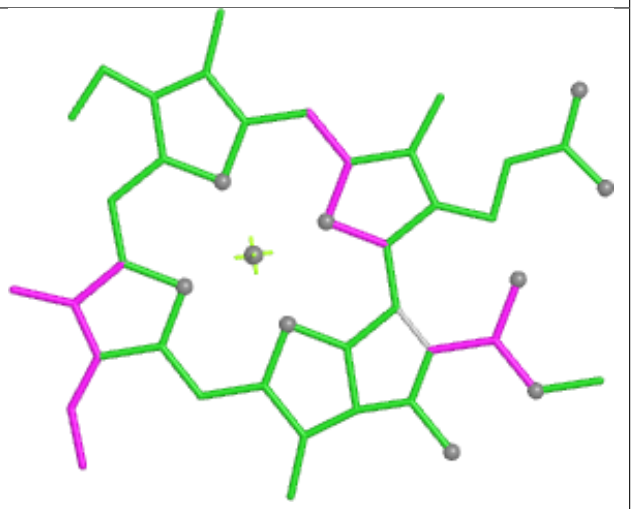


Rings

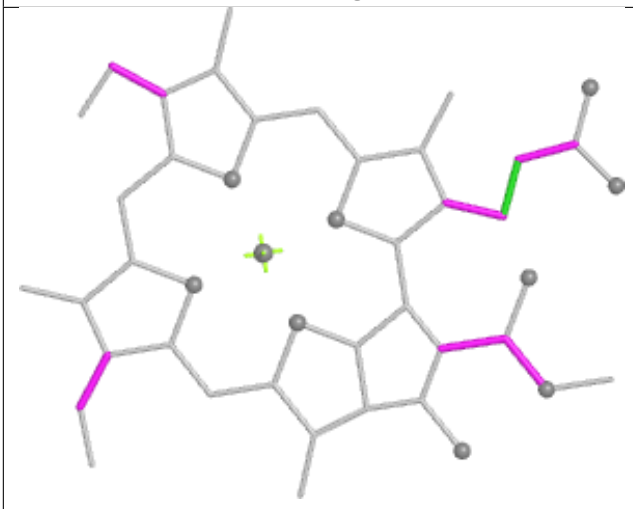
Ligand CLA m 1105



Bond lengths



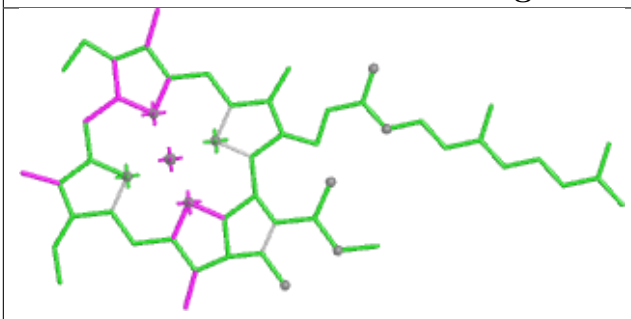
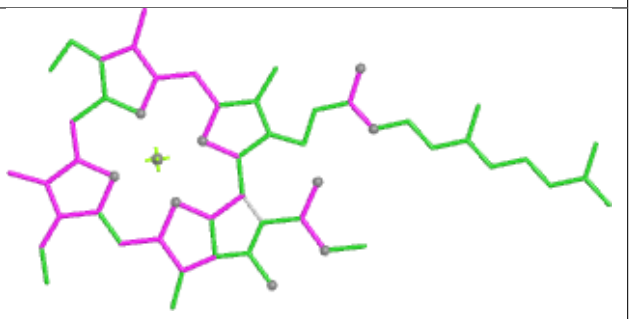
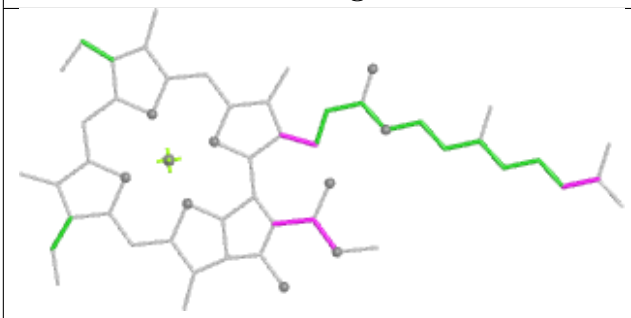
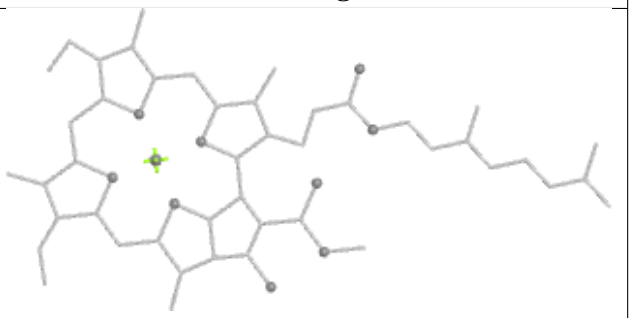
Bond angles

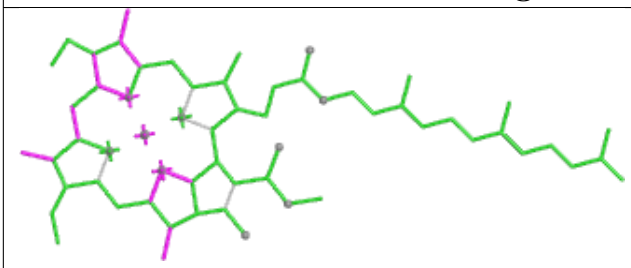
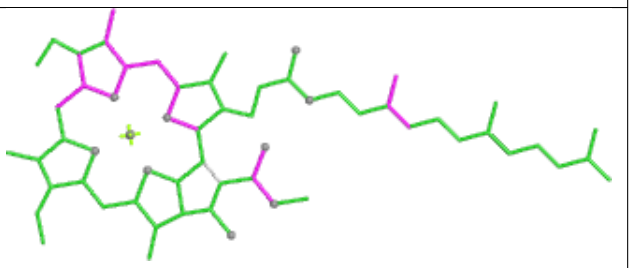
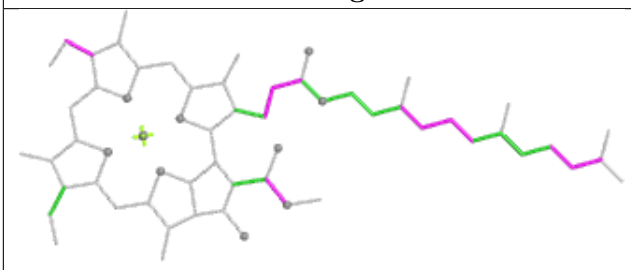
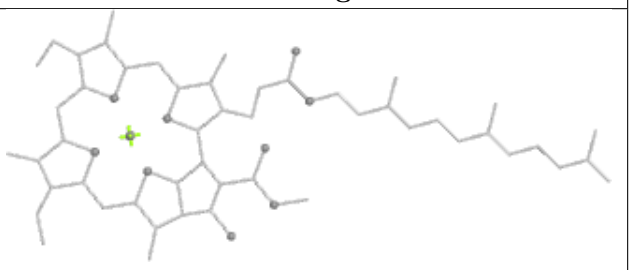


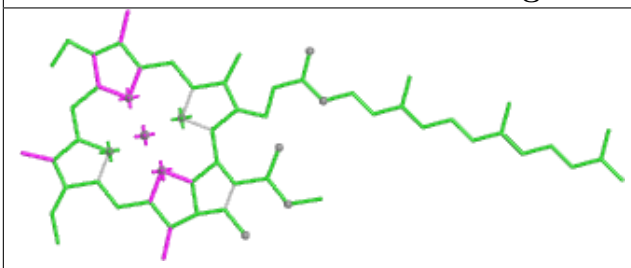
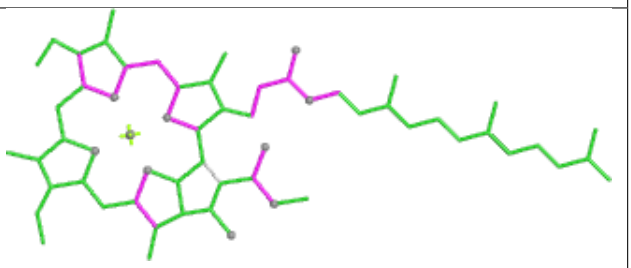
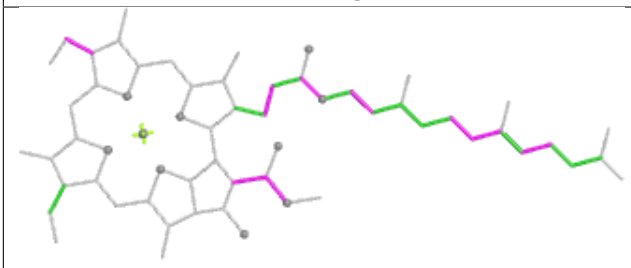
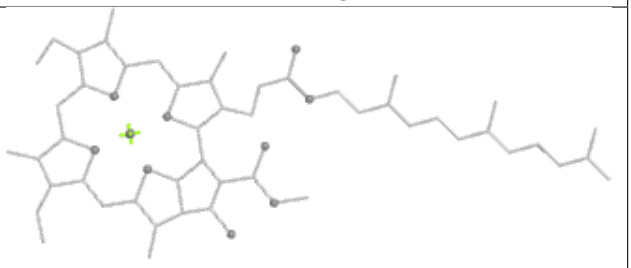
Torsions

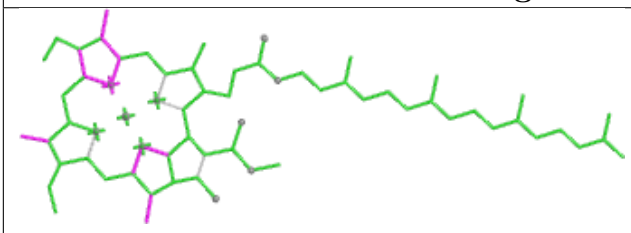
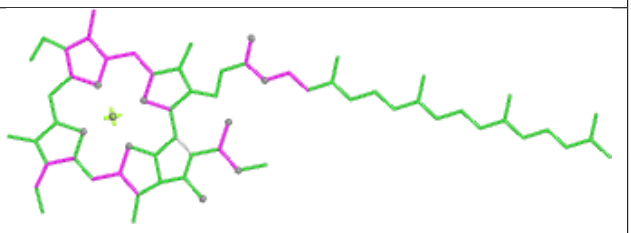
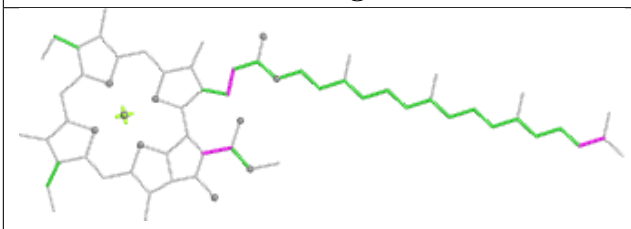
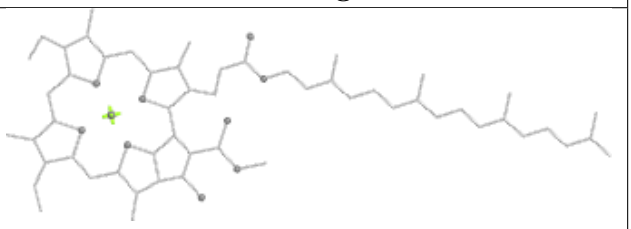


Rings

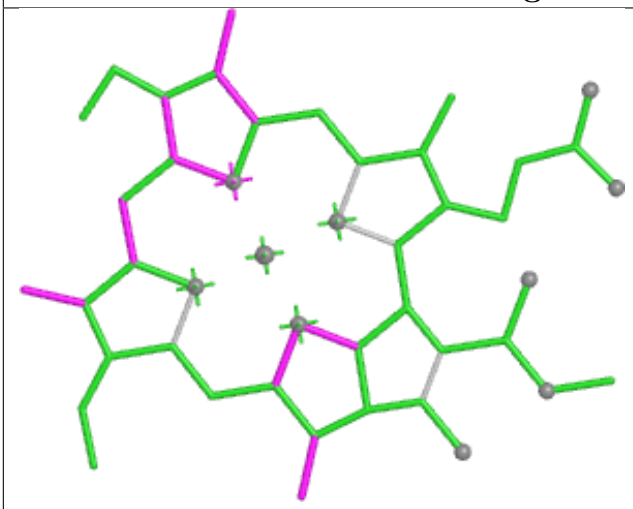
Ligand CLA H 1226	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1115	
	
Bond lengths	Bond angles
	
Torsions	Rings

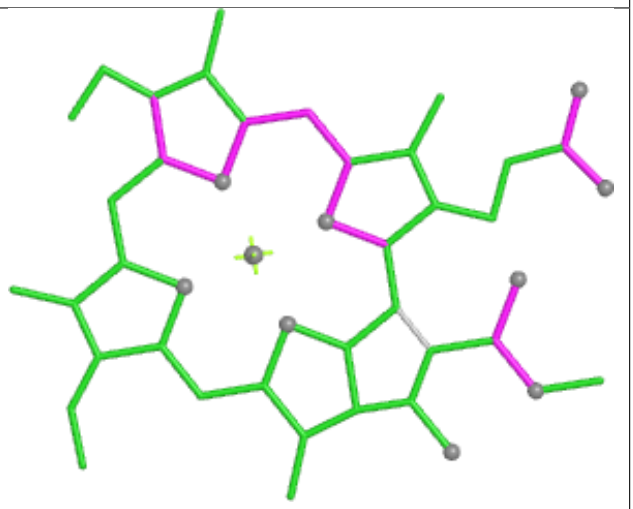
Ligand CLA f 1216	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1238	
	
Bond lengths	Bond angles
	
Torsions	Rings

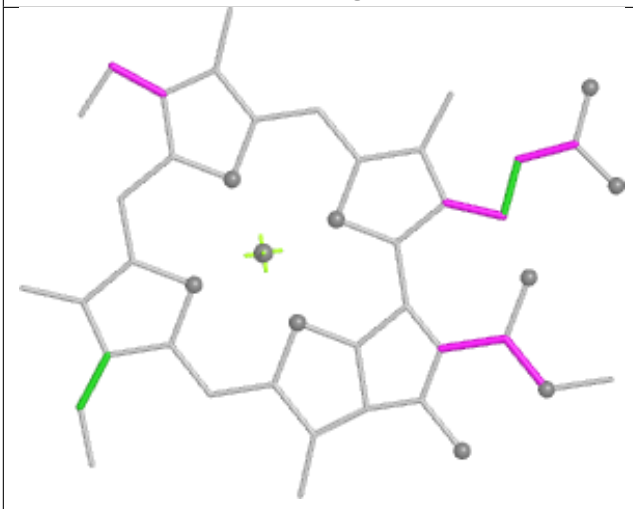
Ligand CLA Y 519



Bond lengths



Bond angles

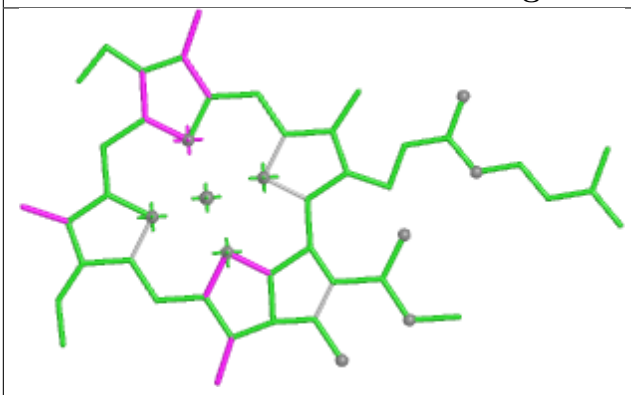


Torsions

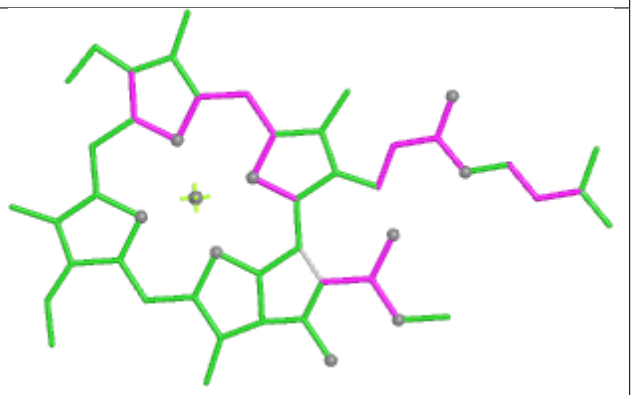


Rings

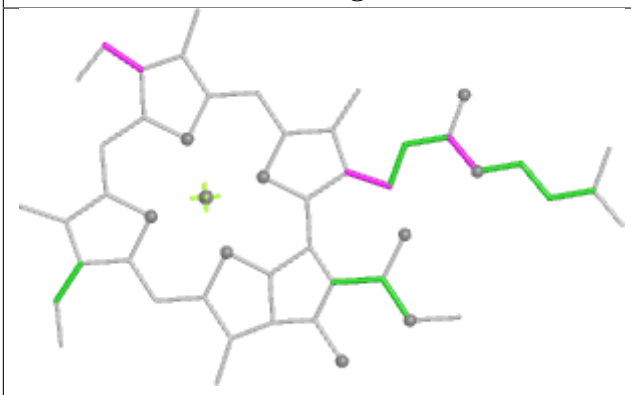
Ligand CLA f 1236



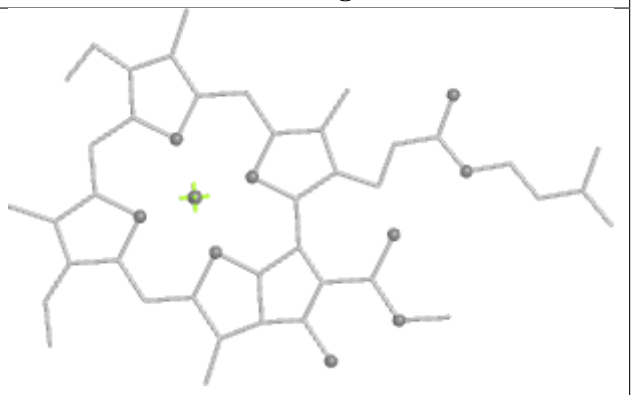
Bond lengths



Bond angles

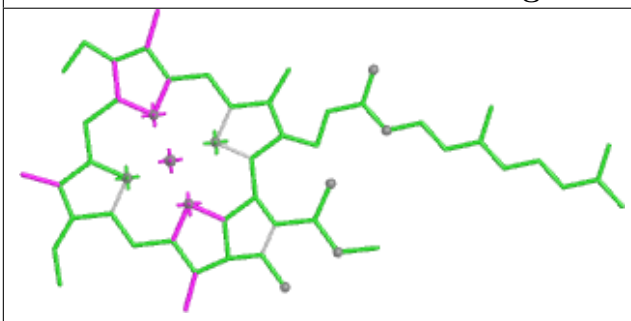


Torsions

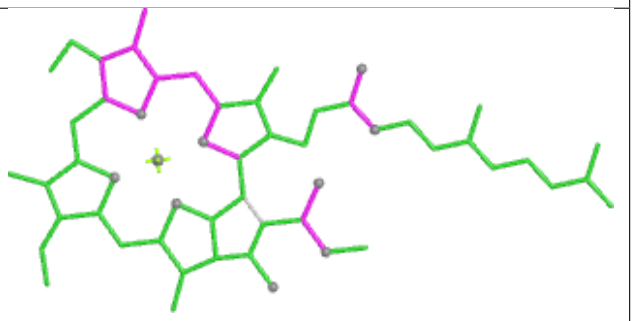


Rings

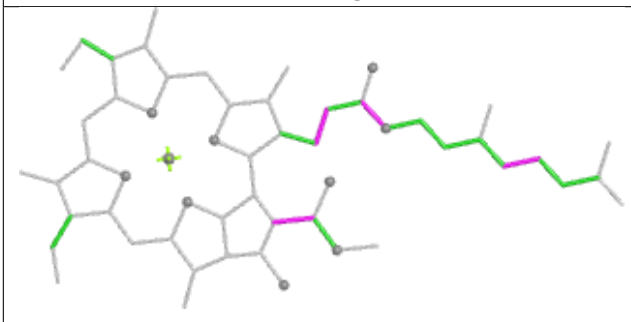
Ligand CLA f 1232



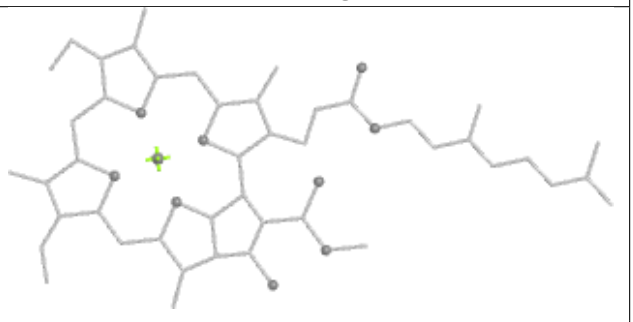
Bond lengths



Bond angles

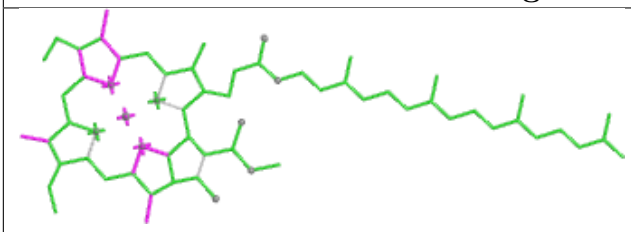


Torsions

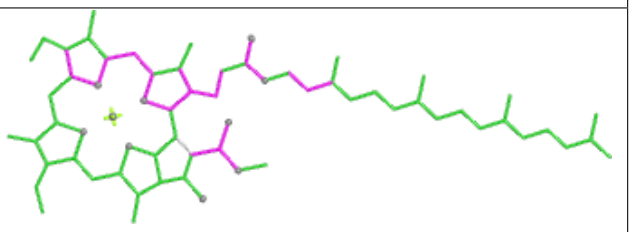


Rings

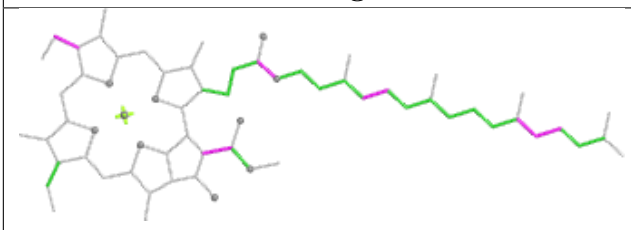
Ligand CLA f 1205



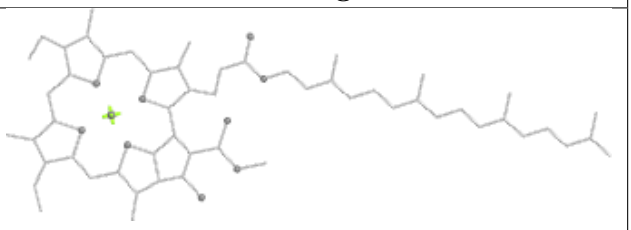
Bond lengths



Bond angles

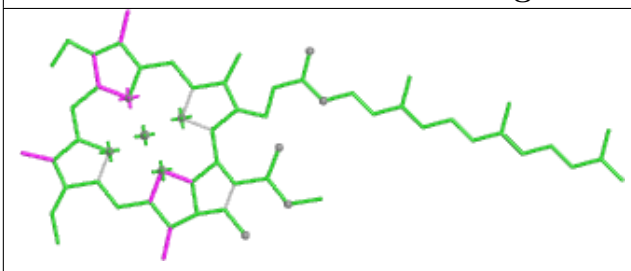


Torsions

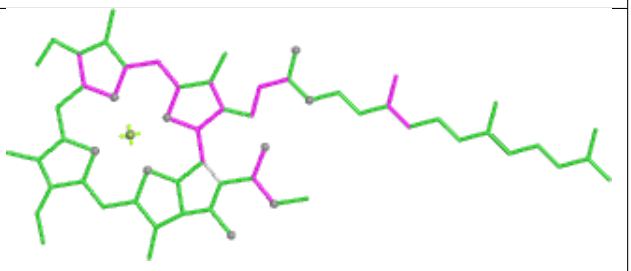


Rings

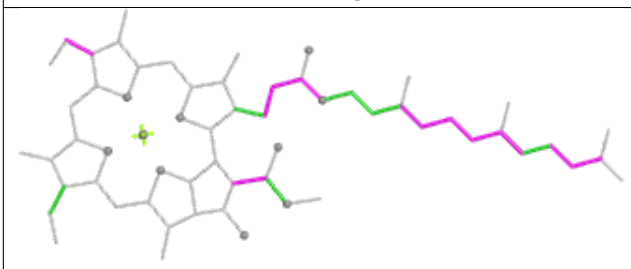
Ligand CLA G 1137



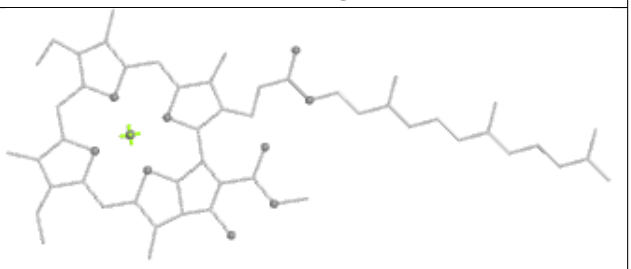
Bond lengths



Bond angles



Torsions

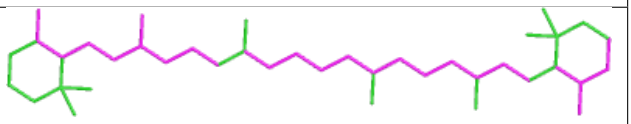


Rings

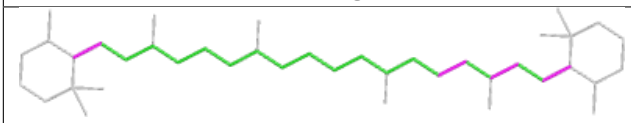
Ligand BCR G 4008



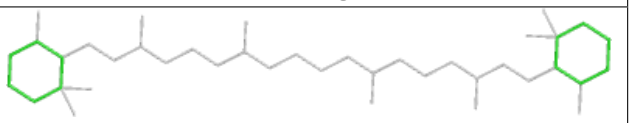
Bond lengths



Bond angles

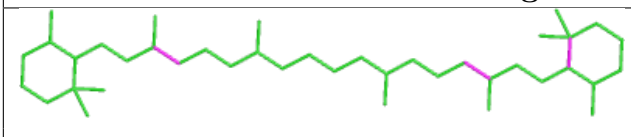


Torsions

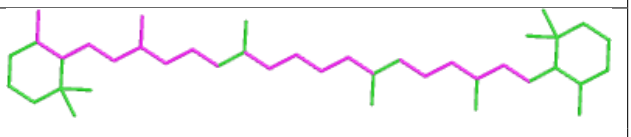


Rings

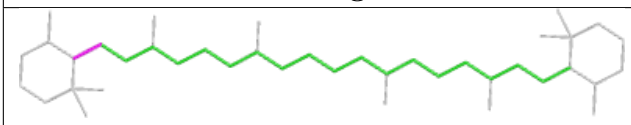
Ligand BCR f 4017



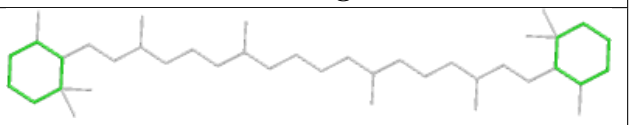
Bond lengths



Bond angles

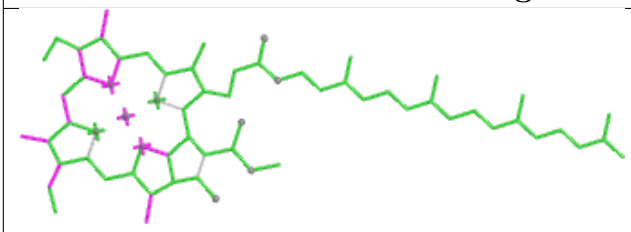


Torsions

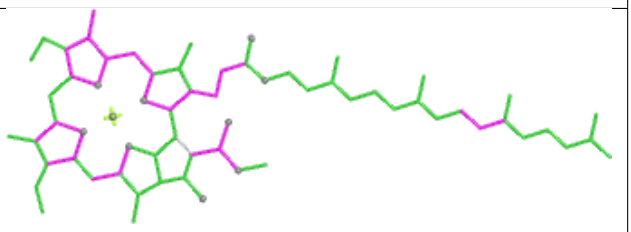


Rings

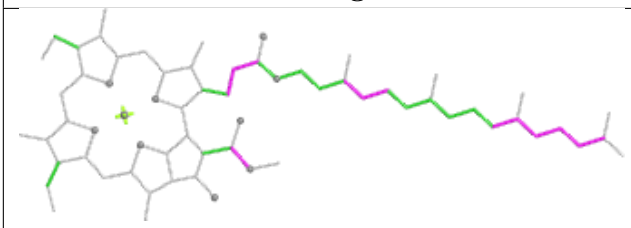
Ligand CLA A 1013



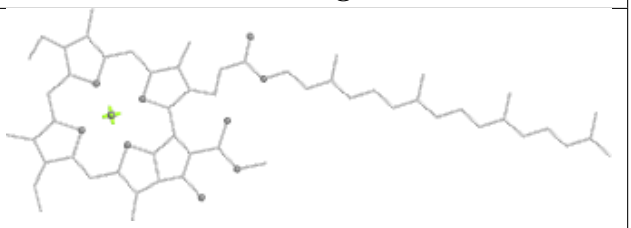
Bond lengths



Bond angles

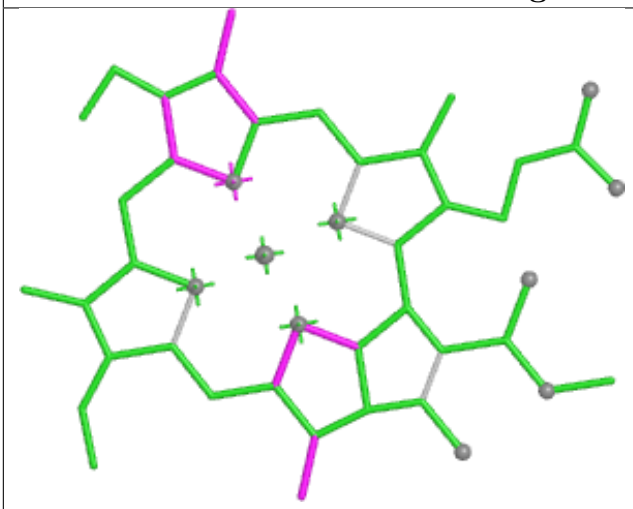


Torsions

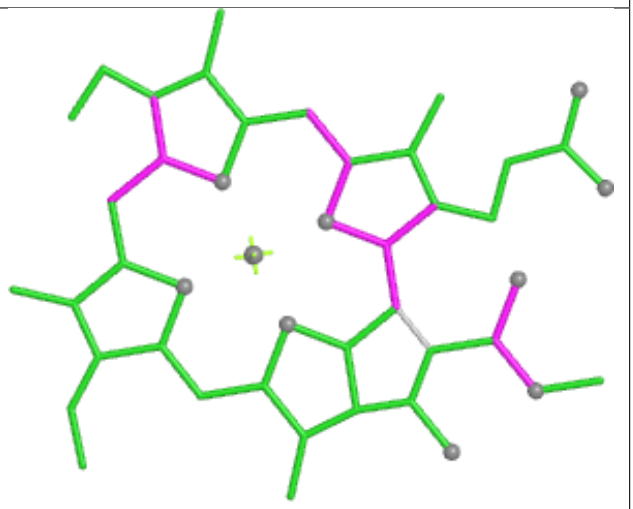


Rings

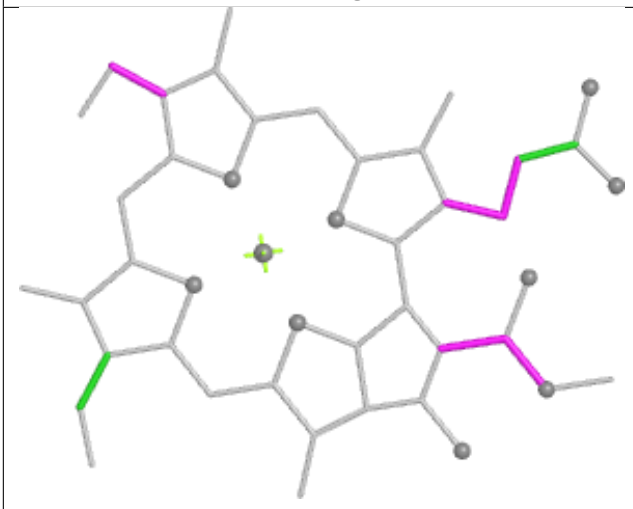
Ligand CLA c 502



Bond lengths



Bond angles

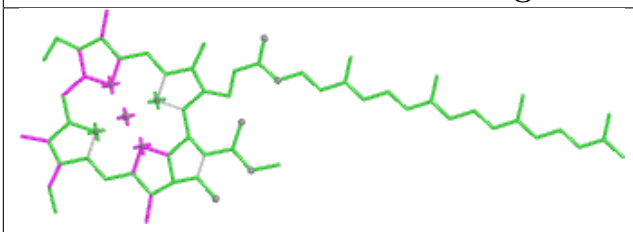


Torsions

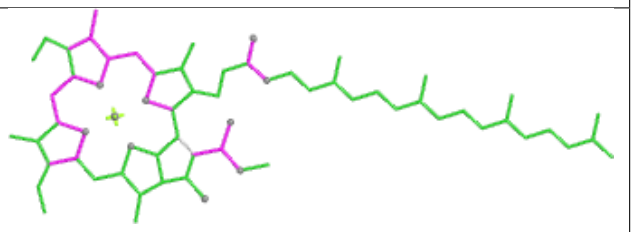


Rings

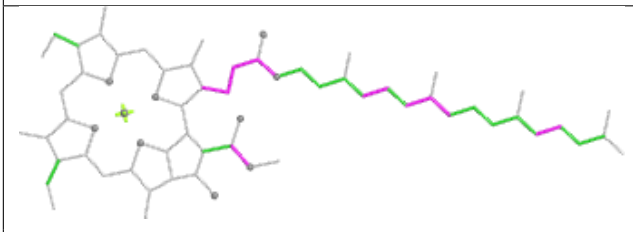
Ligand CLA H 1206



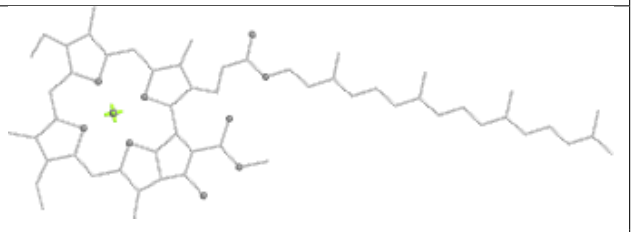
Bond lengths



Bond angles

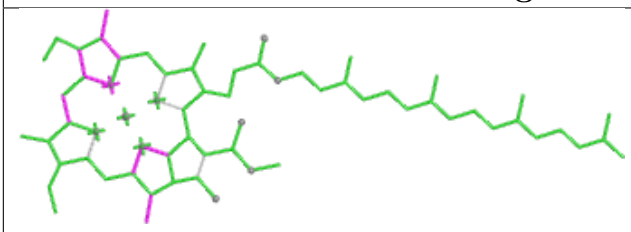


Torsions

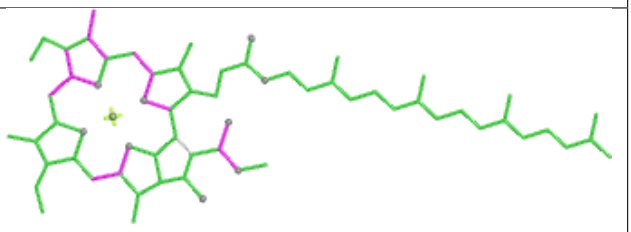


Rings

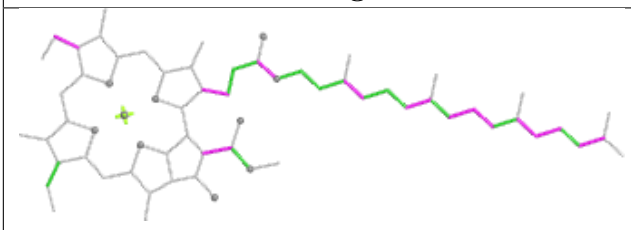
Ligand CLA B 1208



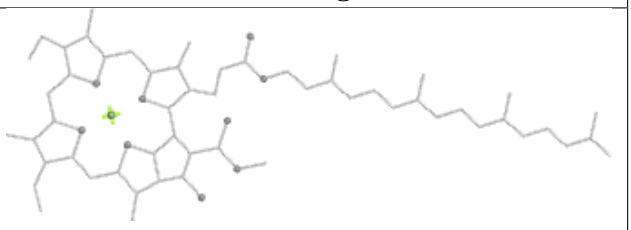
Bond lengths



Bond angles

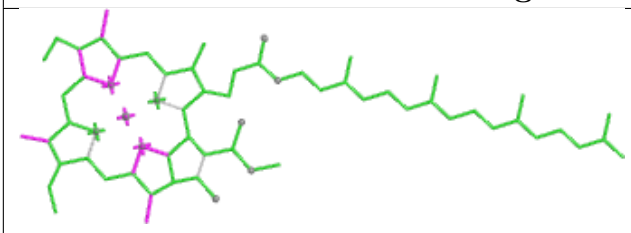


Torsions

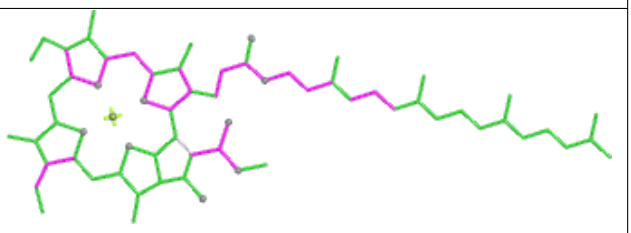


Rings

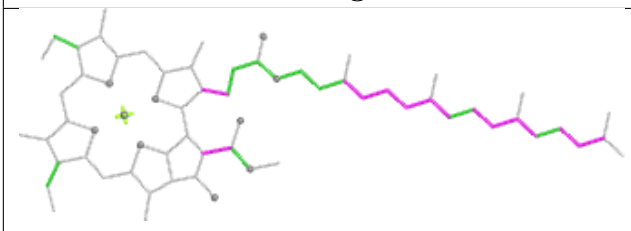
Ligand CLA A 1101



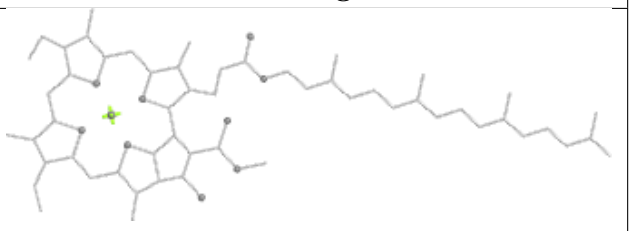
Bond lengths



Bond angles

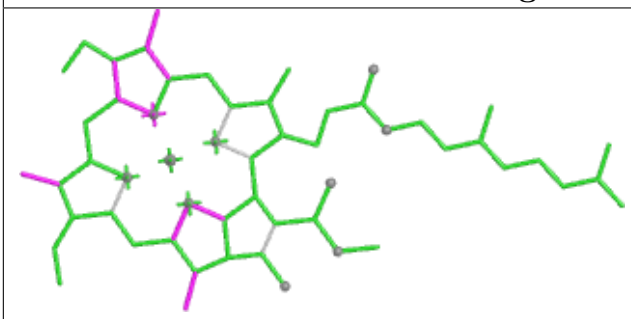


Torsions

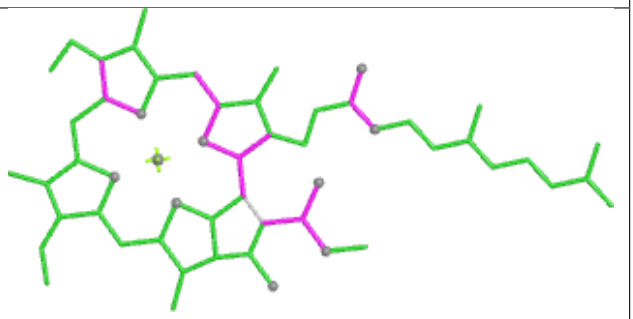


Rings

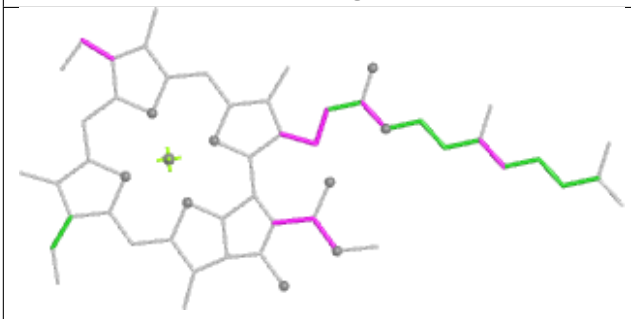
Ligand CLA J 1302



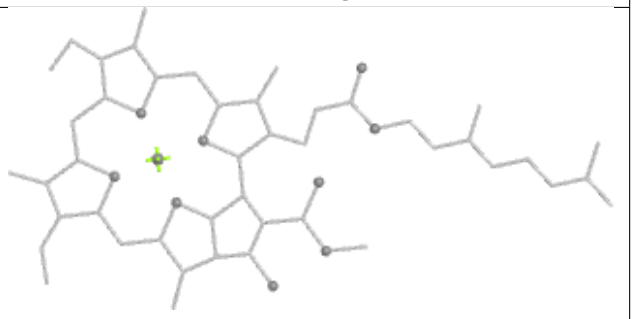
Bond lengths



Bond angles

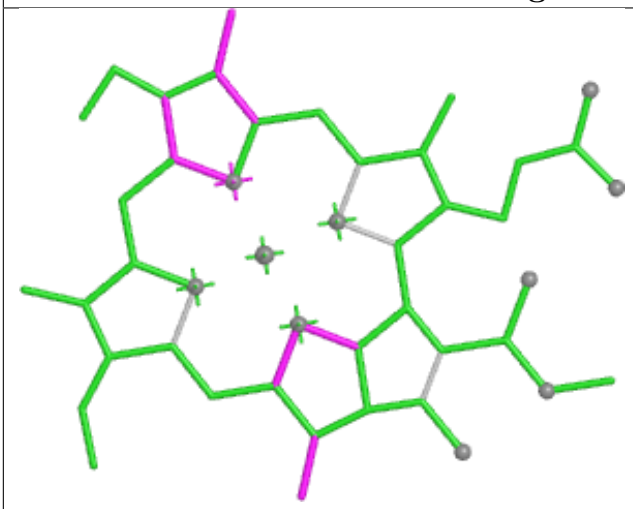


Torsions

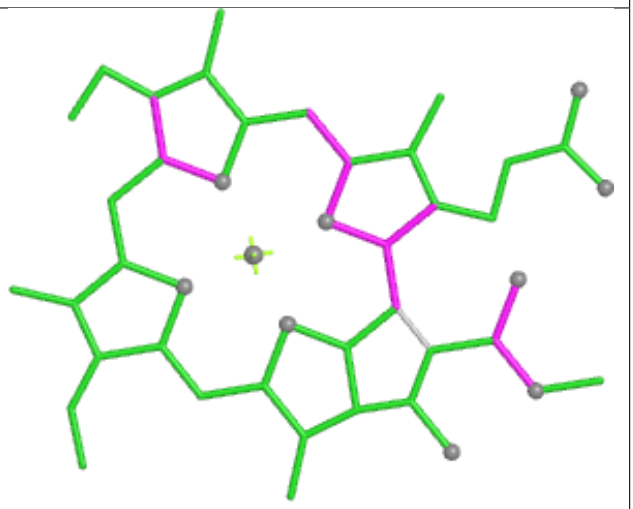


Rings

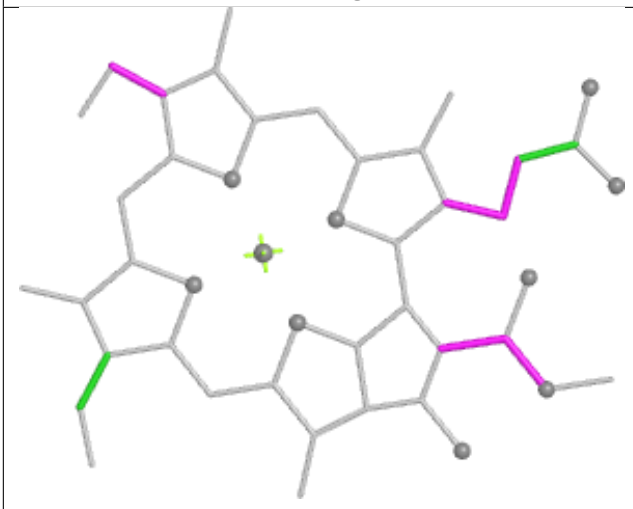
Ligand CLA 1 503



Bond lengths



Bond angles

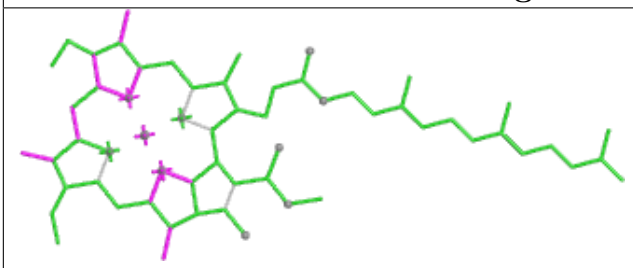


Torsions

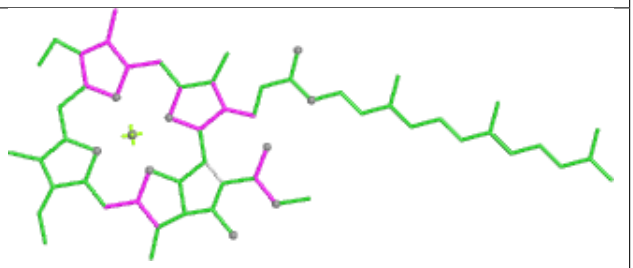


Rings

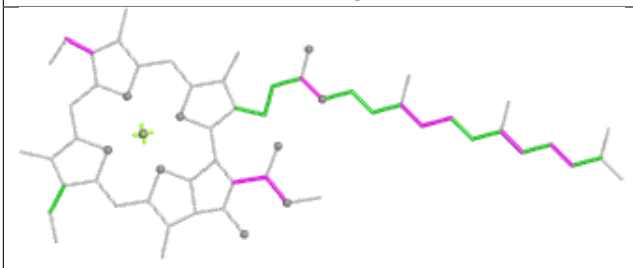
Ligand CLA A 1124



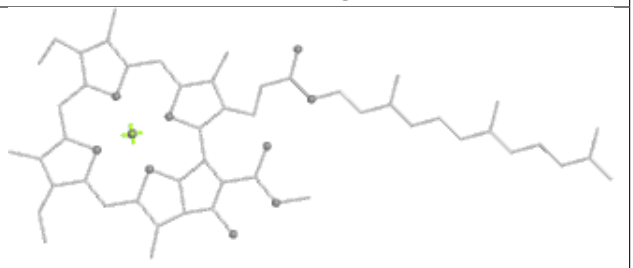
Bond lengths



Bond angles

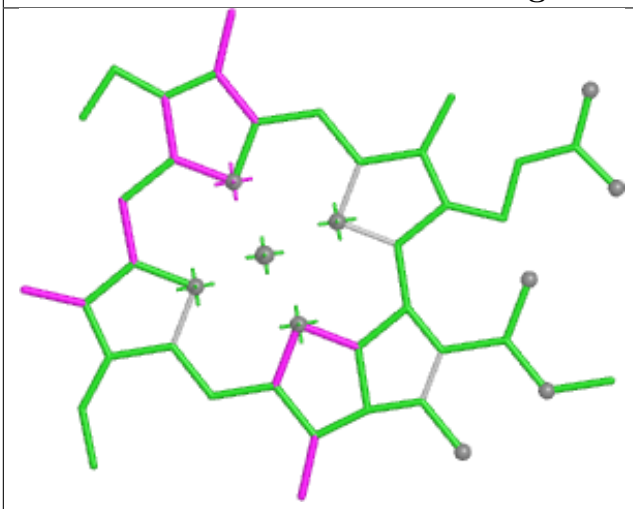


Torsions

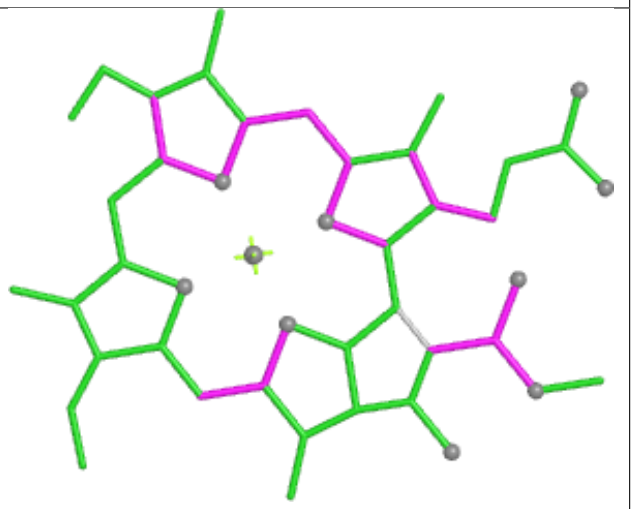


Rings

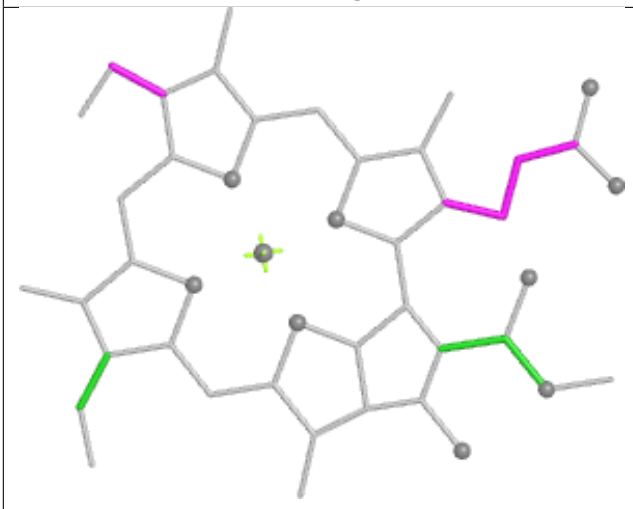
Ligand CLA 3 501



Bond lengths



Bond angles

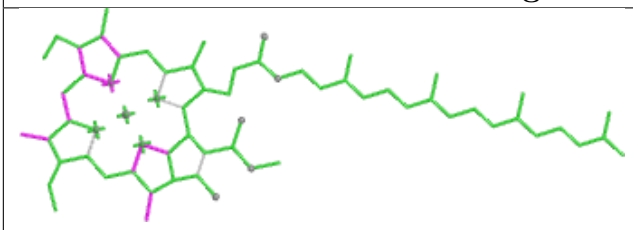


Torsions

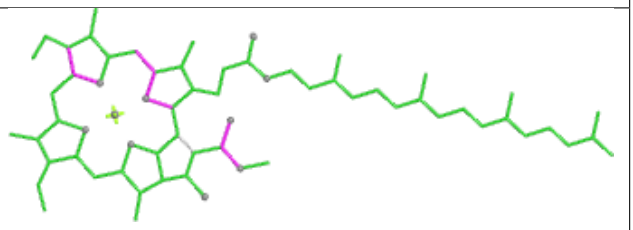


Rings

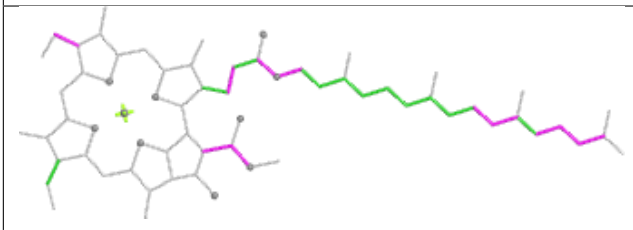
Ligand CLA f 1207



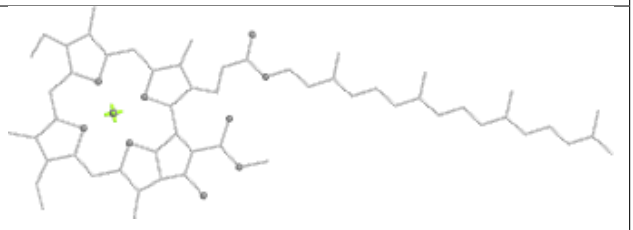
Bond lengths



Bond angles

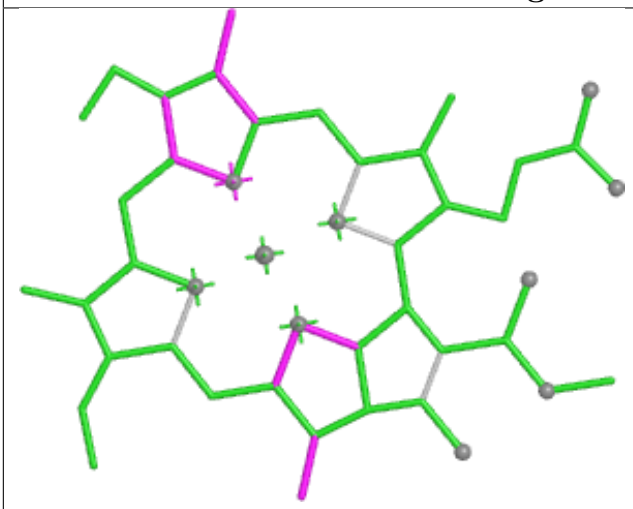


Torsions

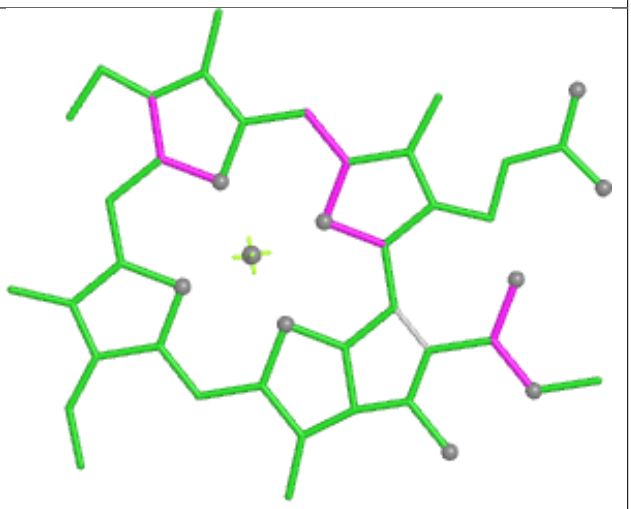


Rings

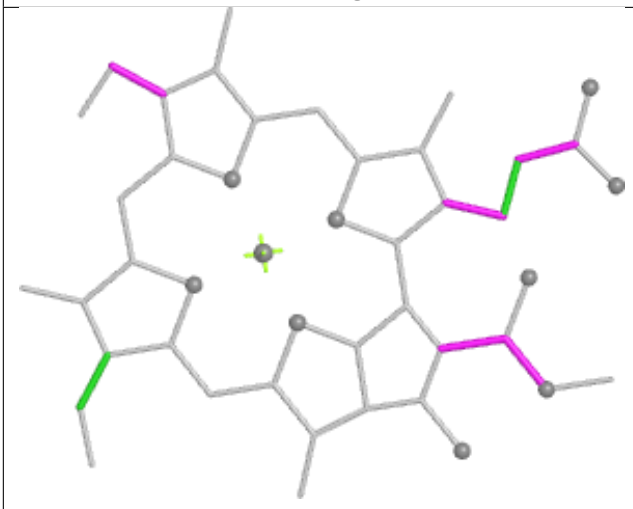
Ligand CLA d 518



Bond lengths



Bond angles

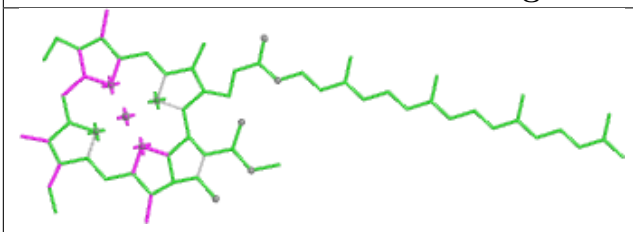


Torsions

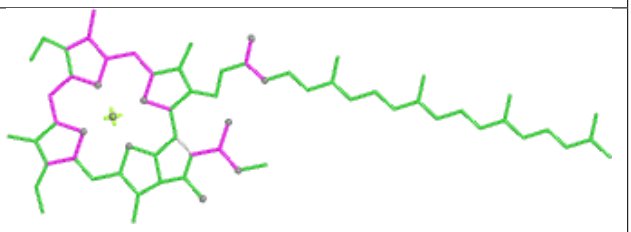


Rings

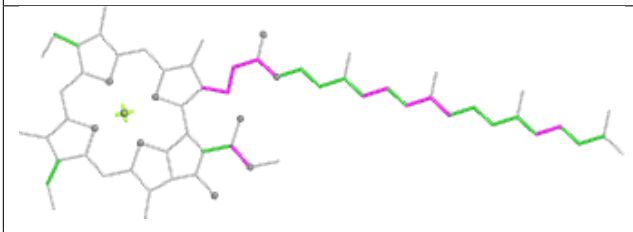
Ligand CLA f 1206



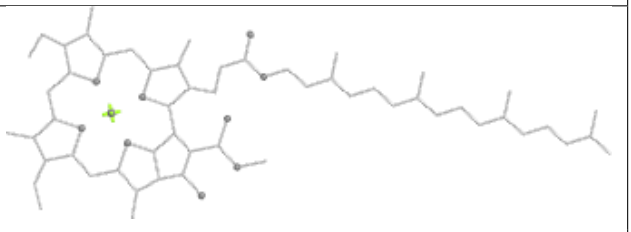
Bond lengths



Bond angles

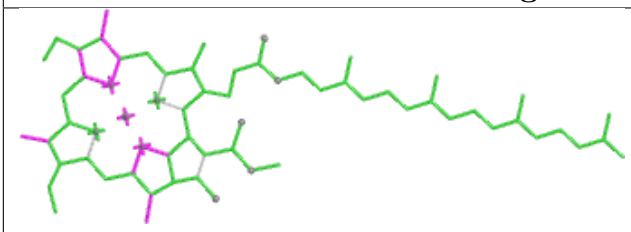


Torsions

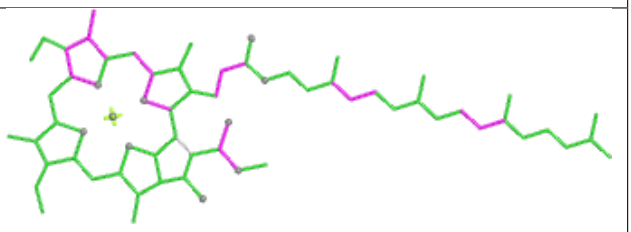


Rings

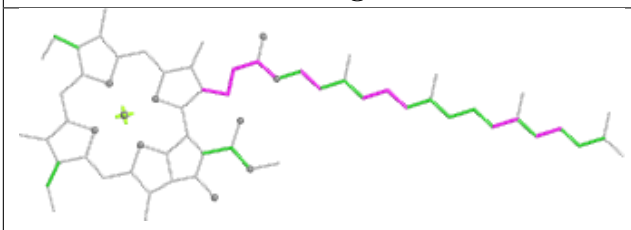
Ligand CLA e 1125



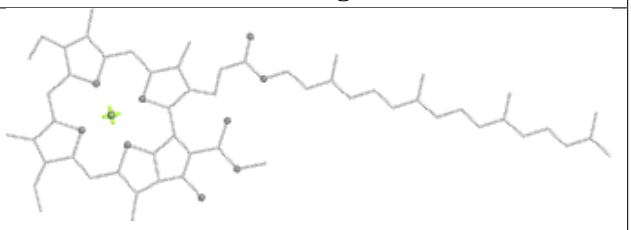
Bond lengths



Bond angles

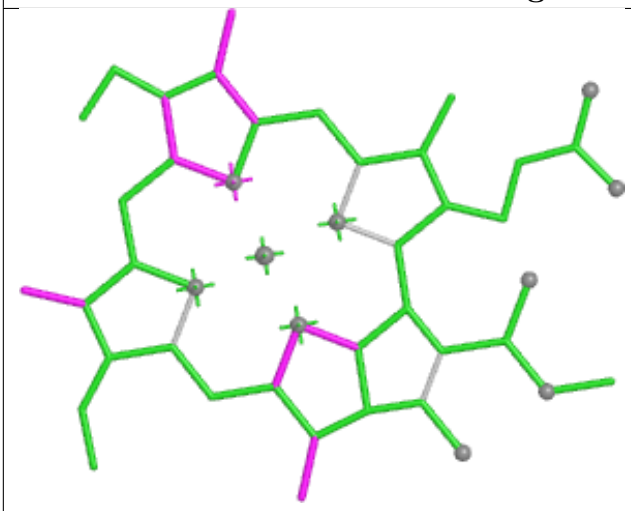


Torsions

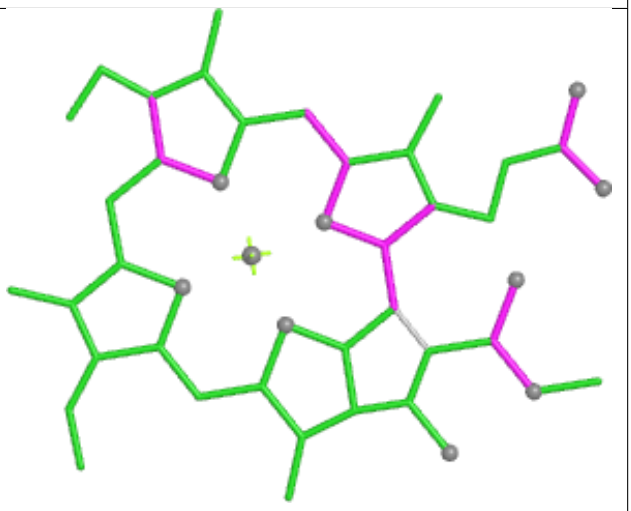


Rings

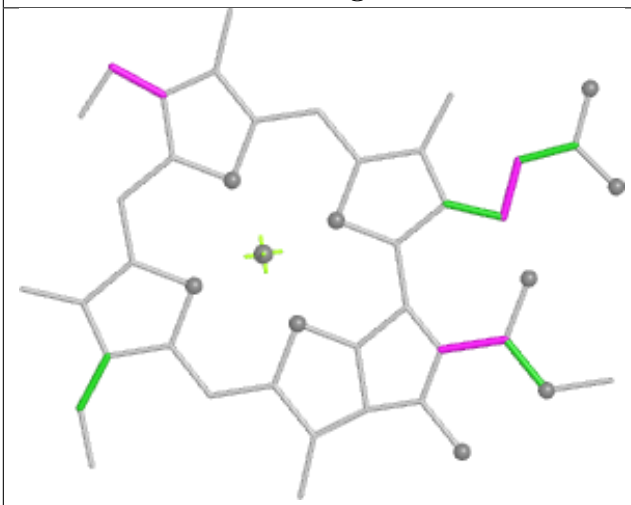
Ligand CLA b 502



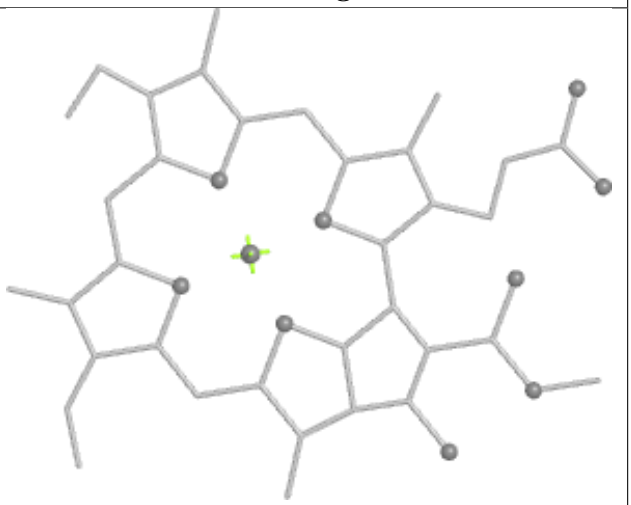
Bond lengths



Bond angles

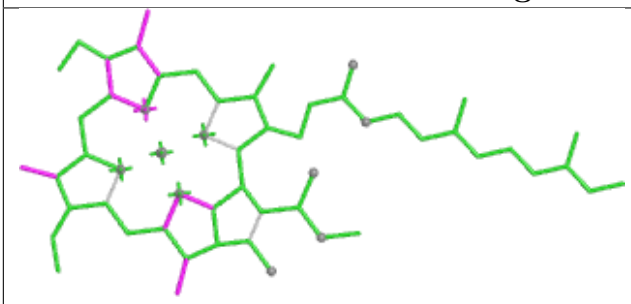


Torsions

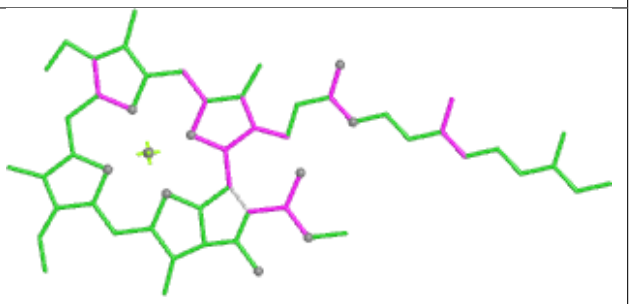


Rings

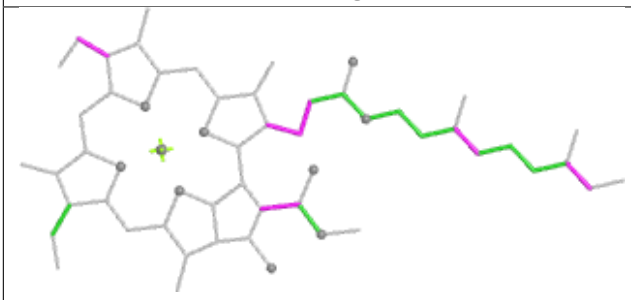
Ligand CLA G 1134



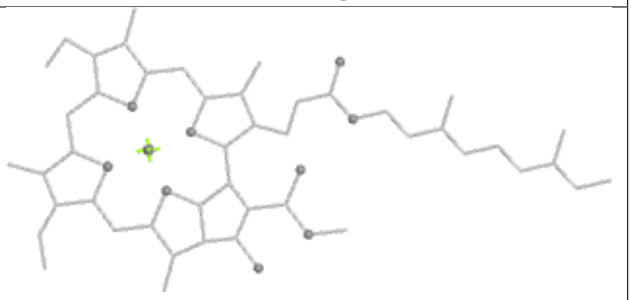
Bond lengths



Bond angles

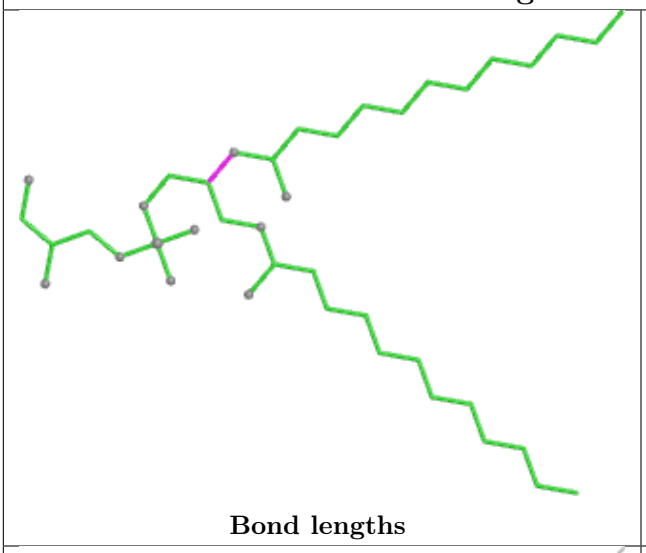


Torsions

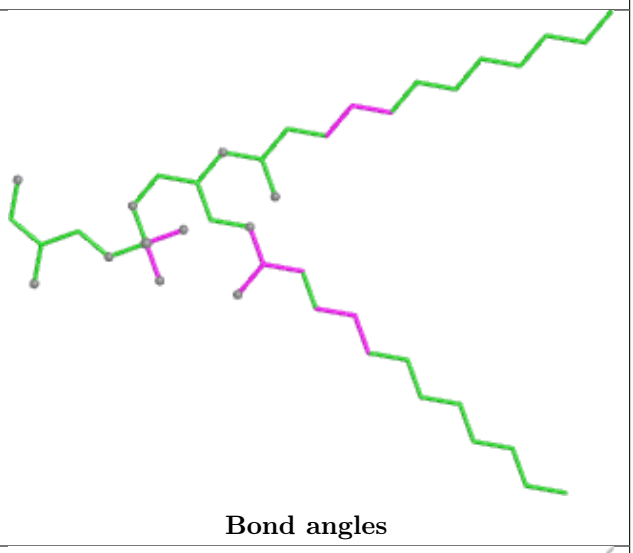


Rings

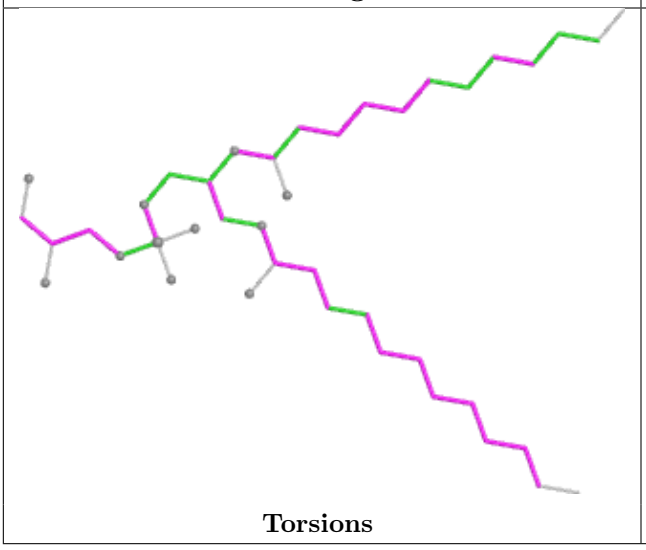
Ligand LHG n 5220



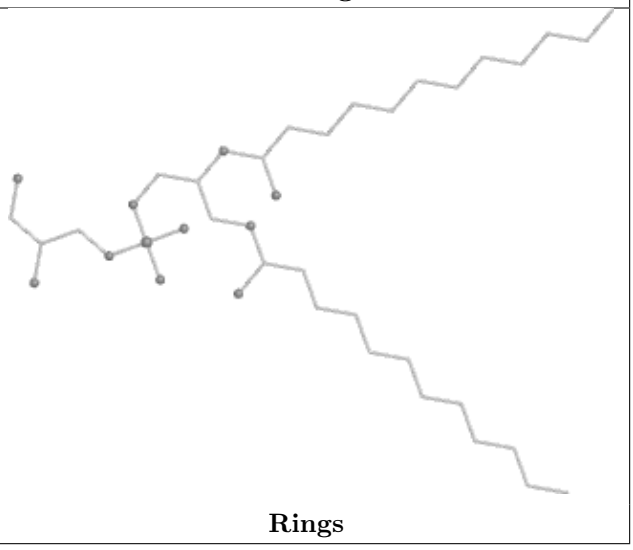
Bond lengths



Bond angles

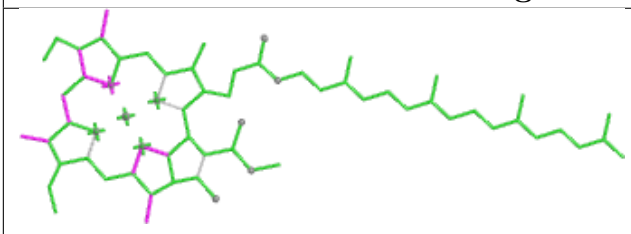


Torsions

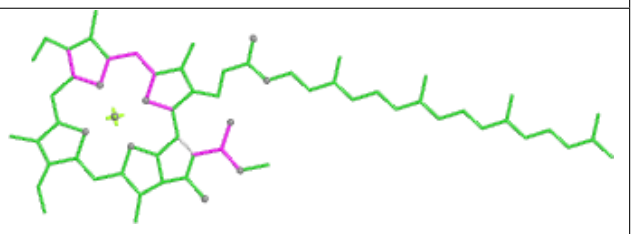


Rings

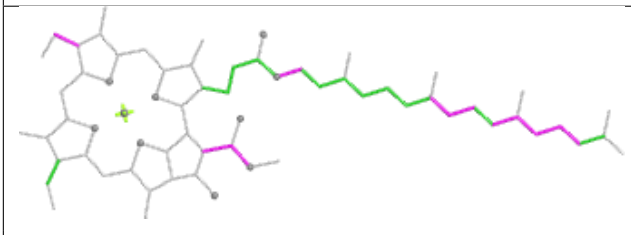
Ligand CLA A 1138



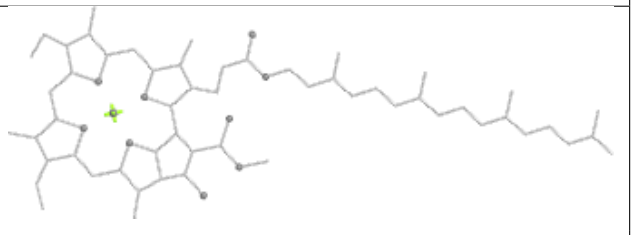
Bond lengths



Bond angles

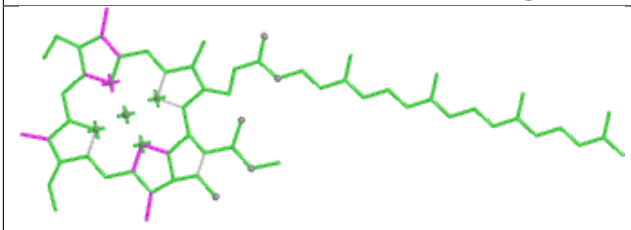


Torsions

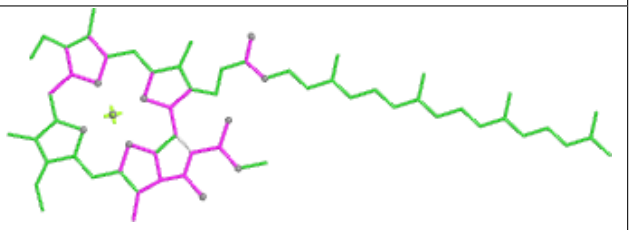


Rings

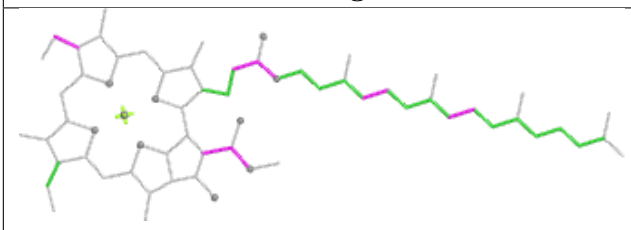
Ligand CLA e 1011



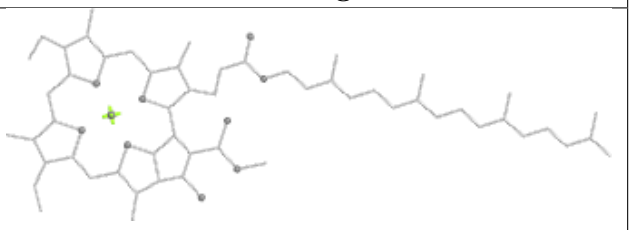
Bond lengths



Bond angles

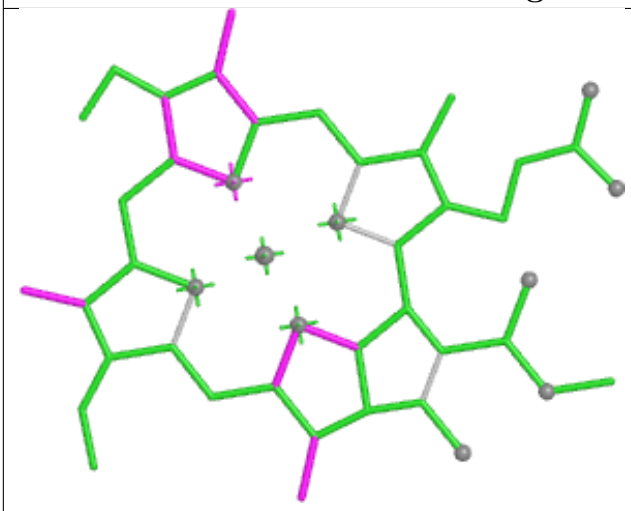


Torsions

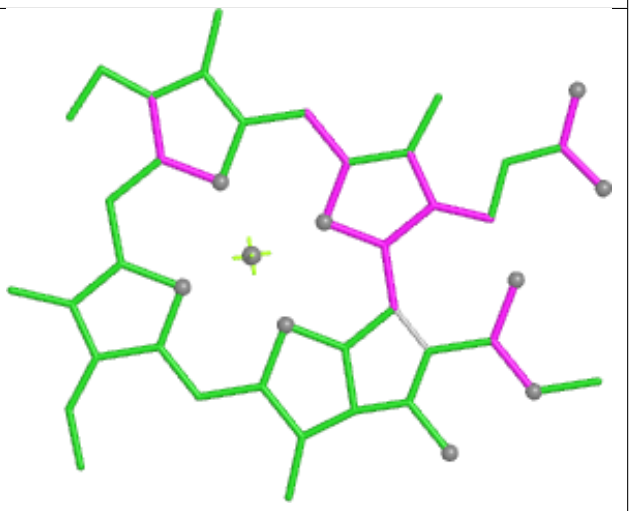


Rings

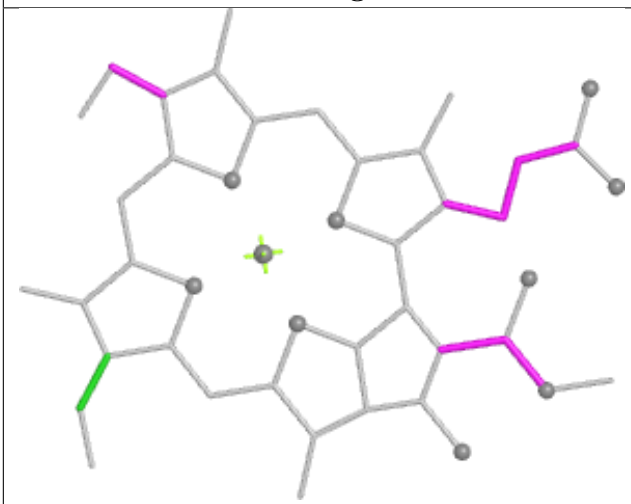
Ligand CLA Z 507



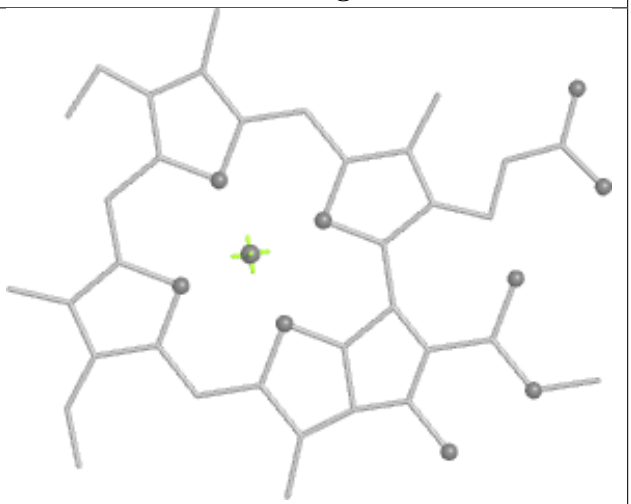
Bond lengths



Bond angles

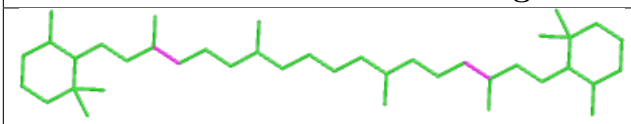


Torsions

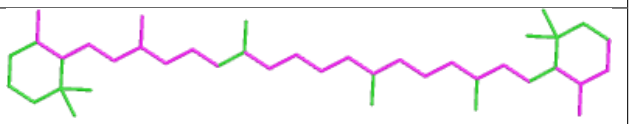


Rings

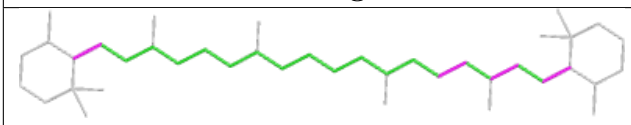
Ligand BCR A 4008



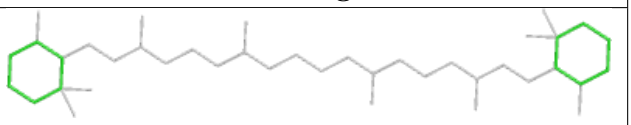
Bond lengths



Bond angles

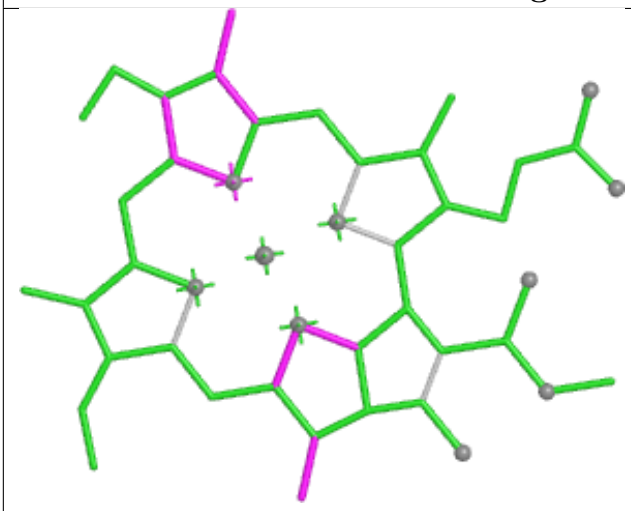


Torsions

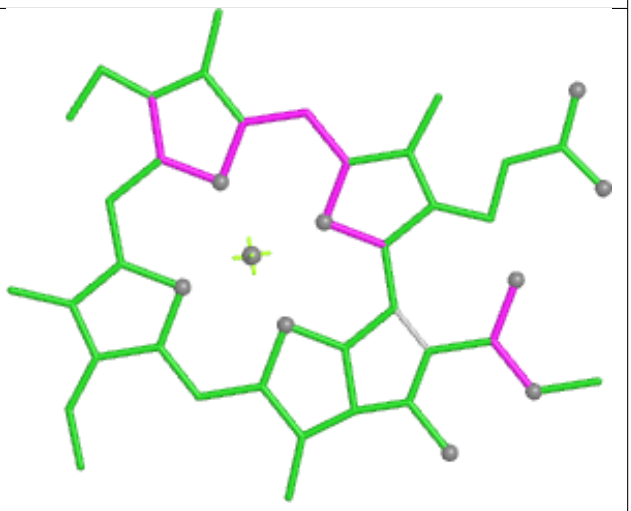


Rings

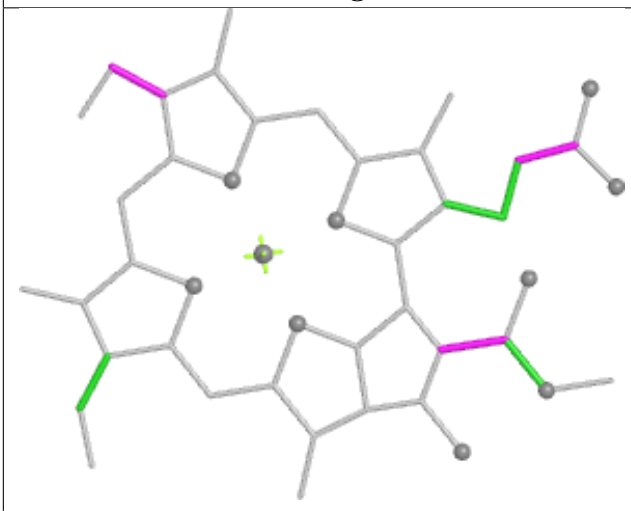
Ligand CLA t 512



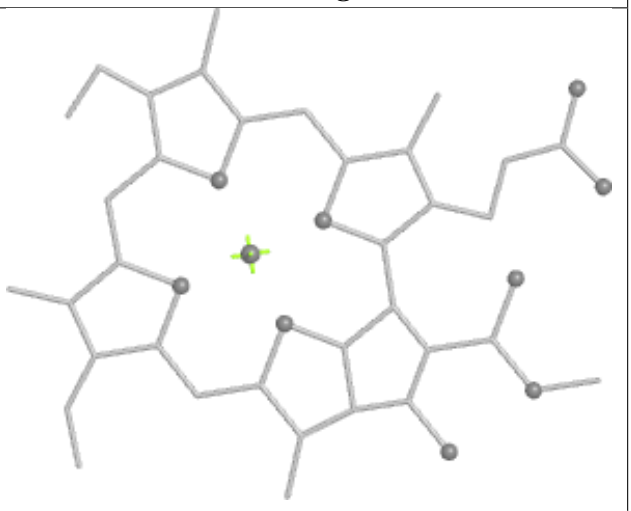
Bond lengths



Bond angles

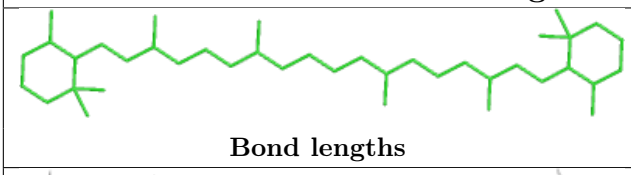


Torsions

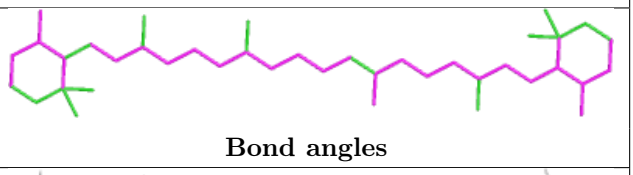


Rings

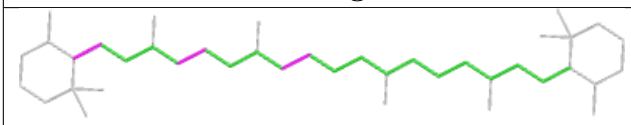
Ligand BCR t 522



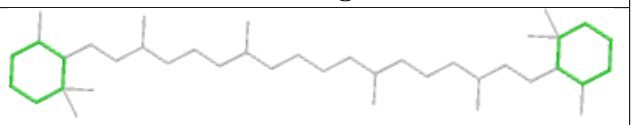
Bond lengths



Bond angles

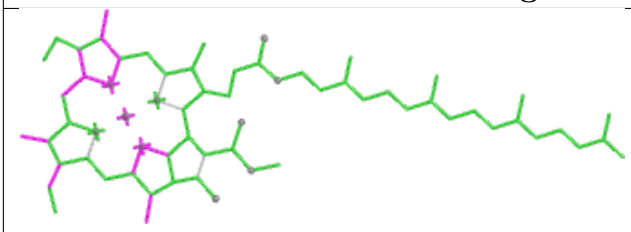


Torsions

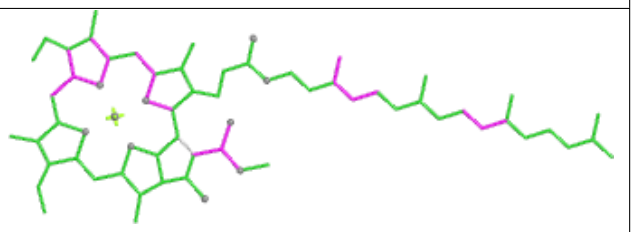


Rings

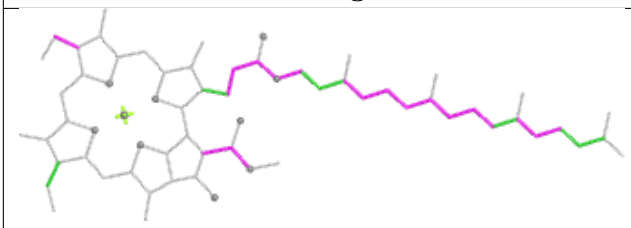
Ligand CLA e 1237



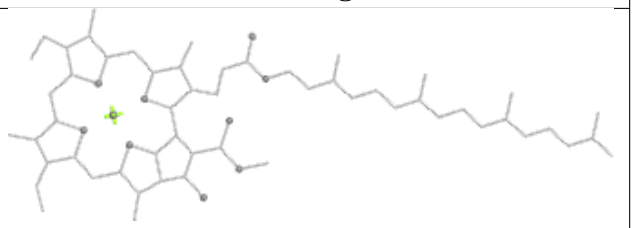
Bond lengths



Bond angles

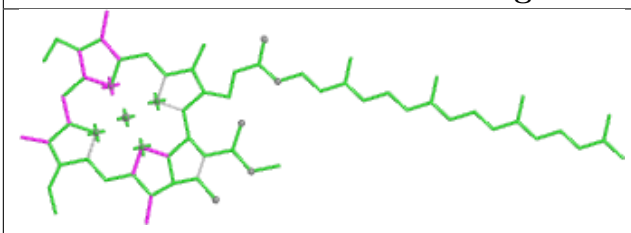


Torsions

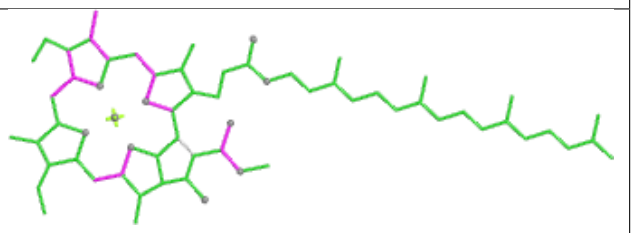


Rings

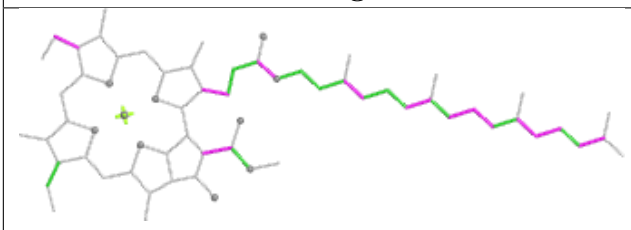
Ligand CLA H 1208



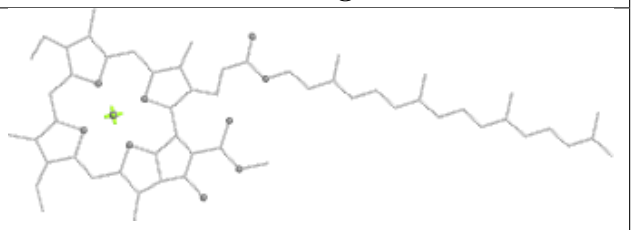
Bond lengths



Bond angles

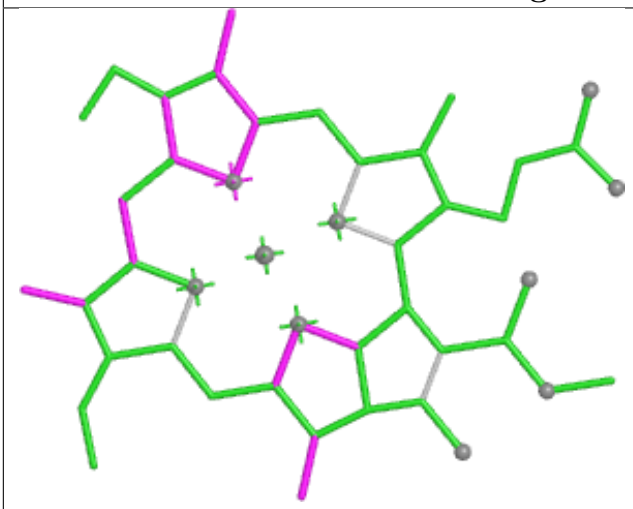


Torsions

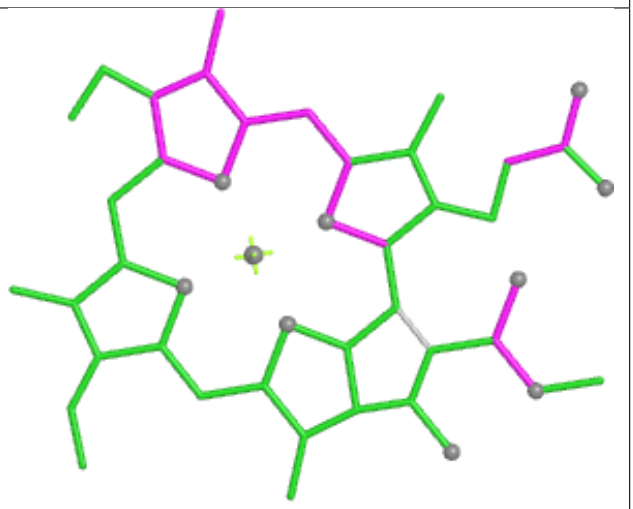


Rings

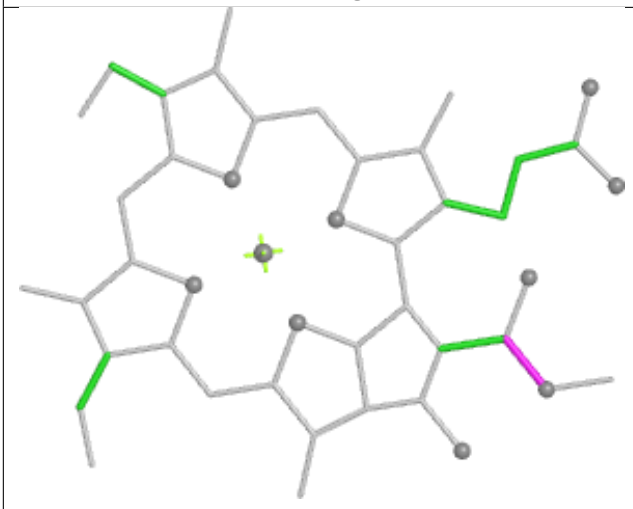
Ligand CLA s 509



Bond lengths



Bond angles

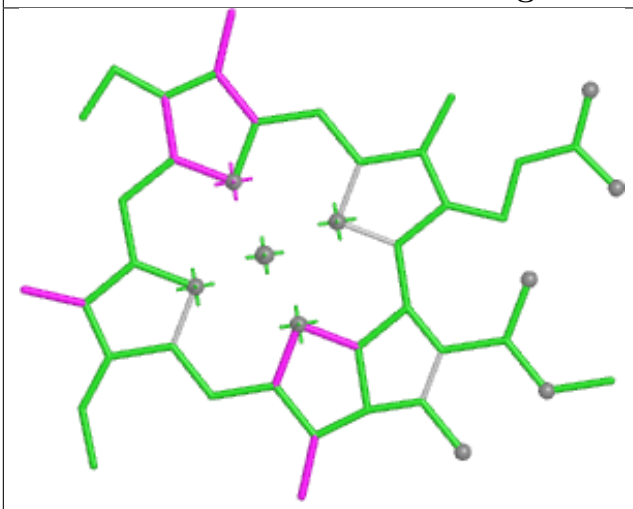


Torsions

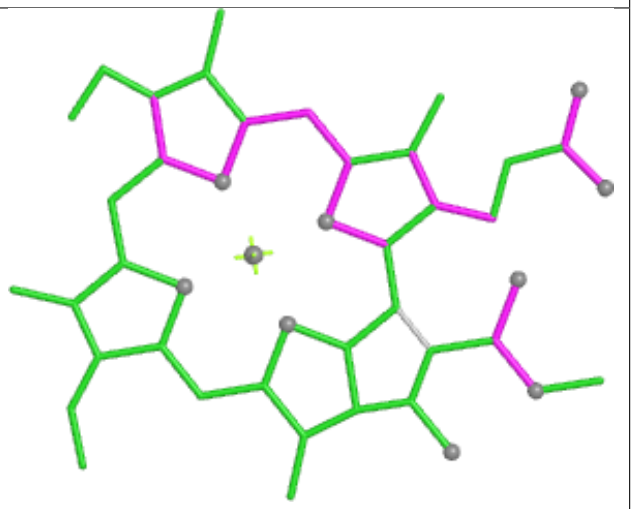


Rings

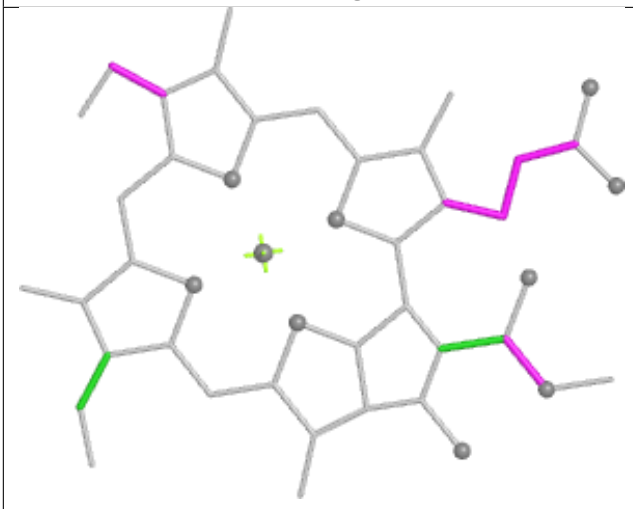
Ligand CLA F 1302



Bond lengths



Bond angles

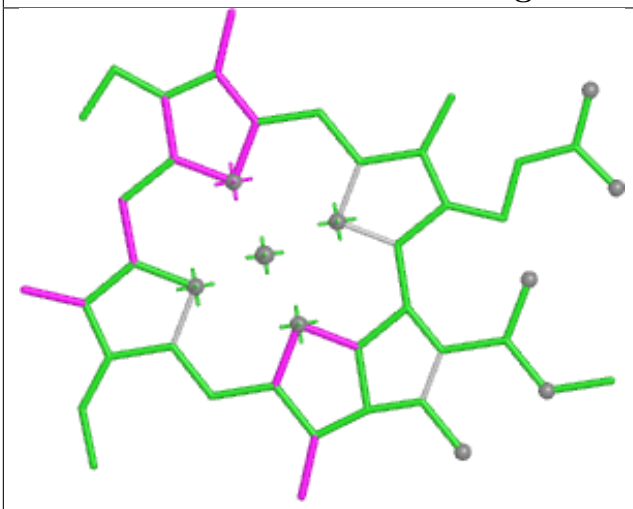


Torsions

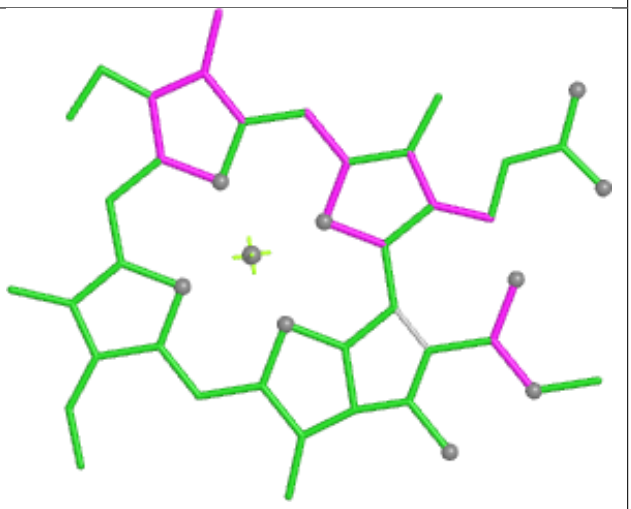


Rings

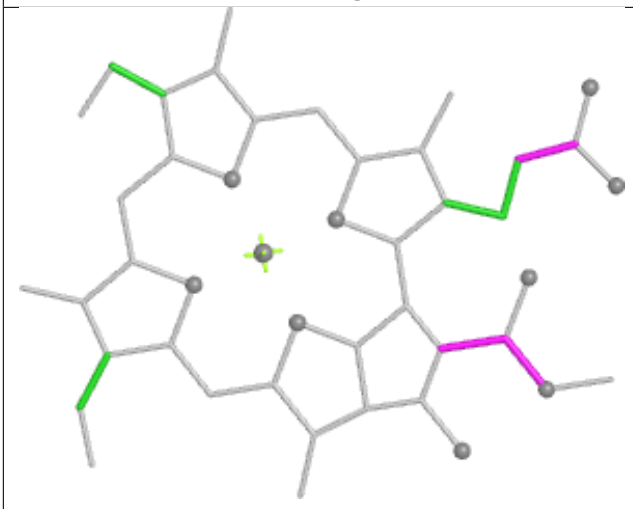
Ligand CLA A 1801



Bond lengths



Bond angles

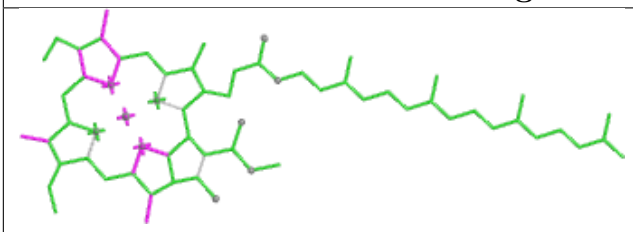


Torsions

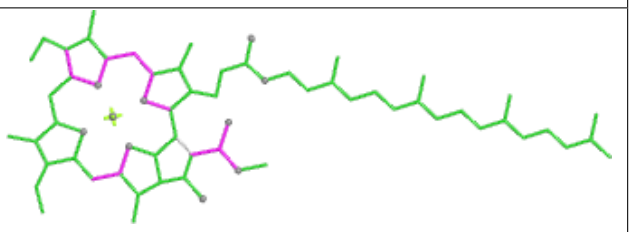


Rings

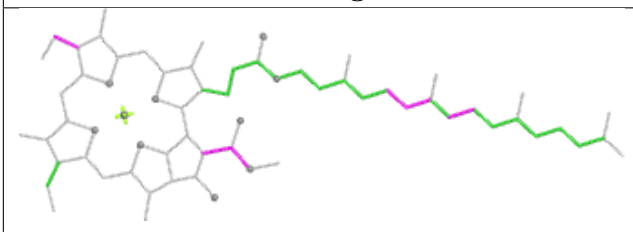
Ligand CLA B 1235



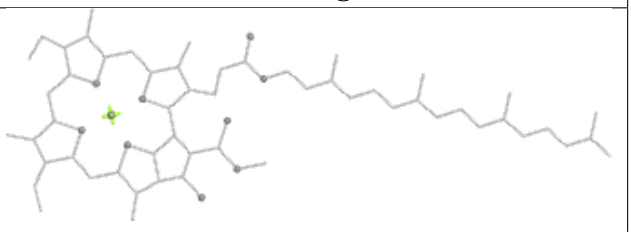
Bond lengths



Bond angles

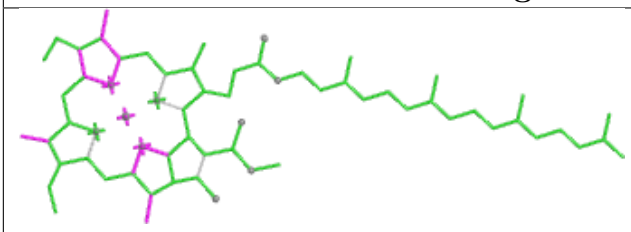


Torsions

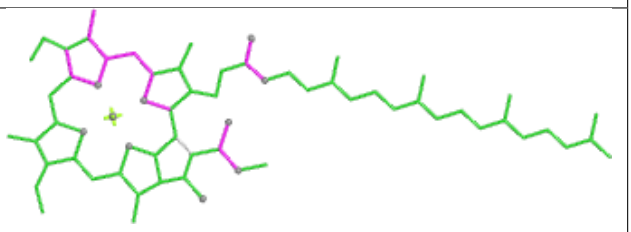


Rings

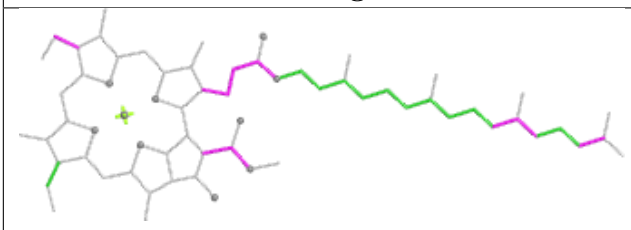
Ligand CLA G 1111



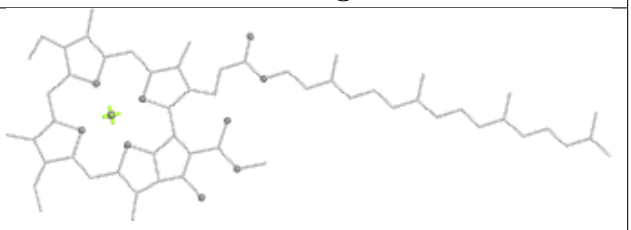
Bond lengths



Bond angles

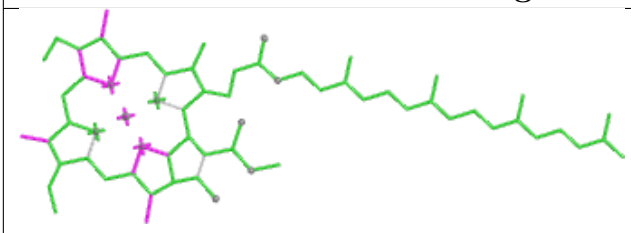


Torsions

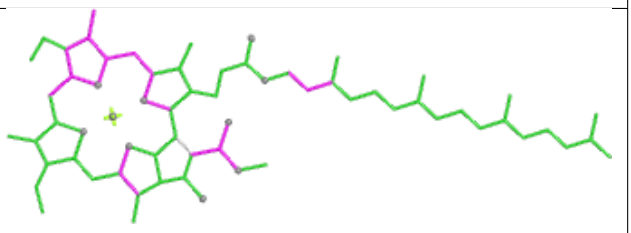


Rings

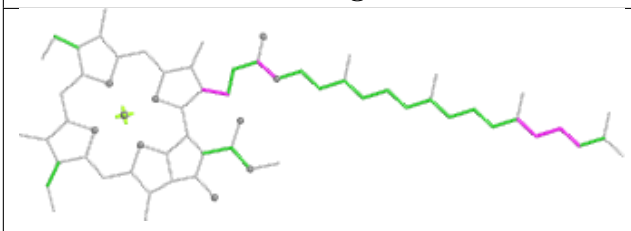
Ligand CLA H 1225



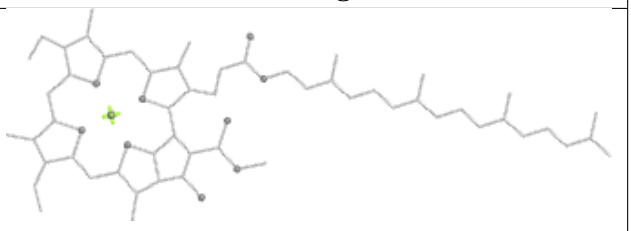
Bond lengths



Bond angles

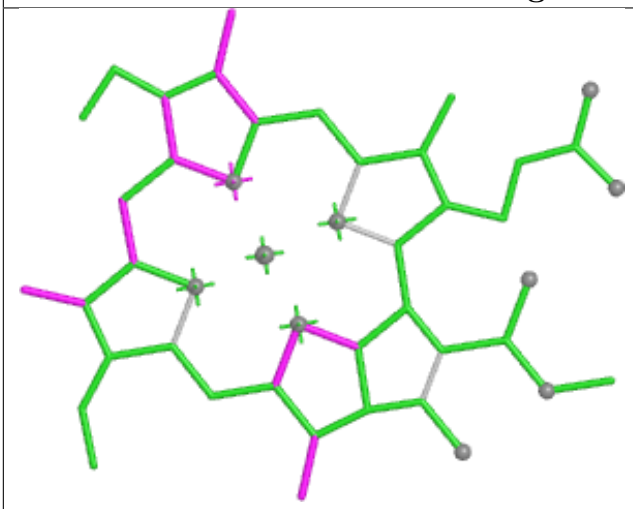


Torsions

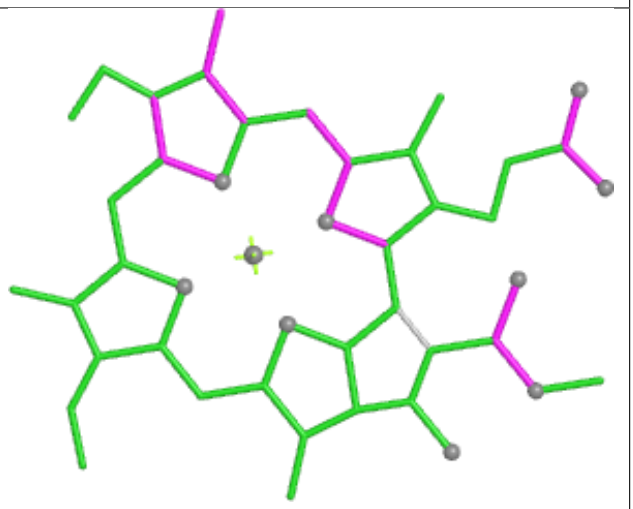


Rings

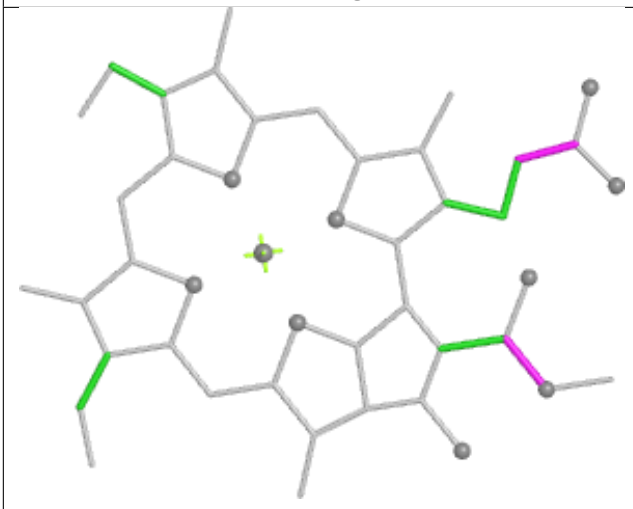
Ligand CLA v 509



Bond lengths



Bond angles

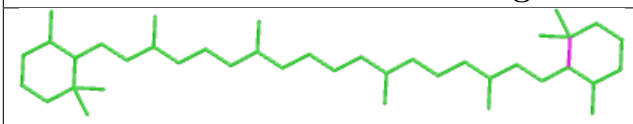


Torsions

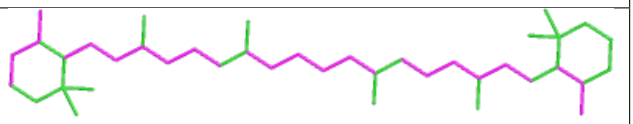


Rings

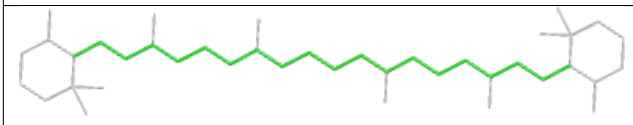
Ligand BCR A 4003



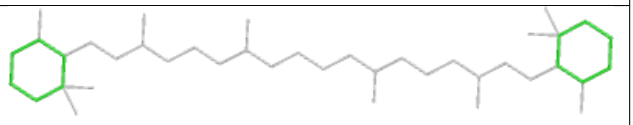
Bond lengths



Bond angles

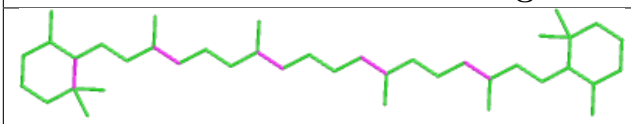


Torsions

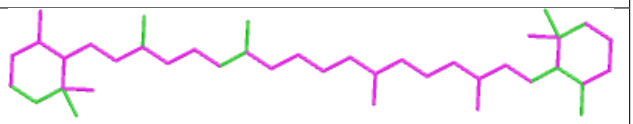


Rings

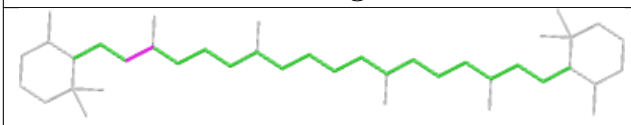
Ligand BCR n 4219



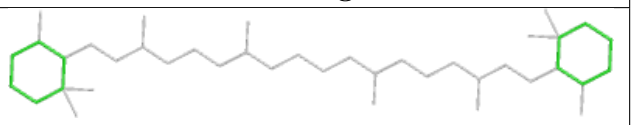
Bond lengths



Bond angles

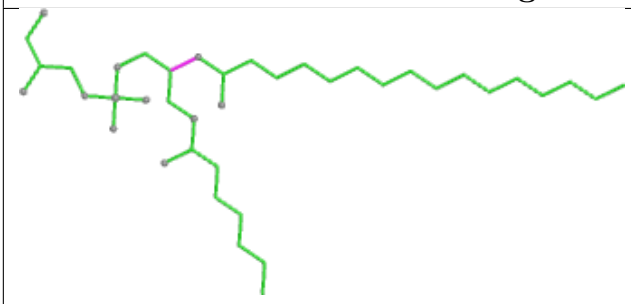


Torsions

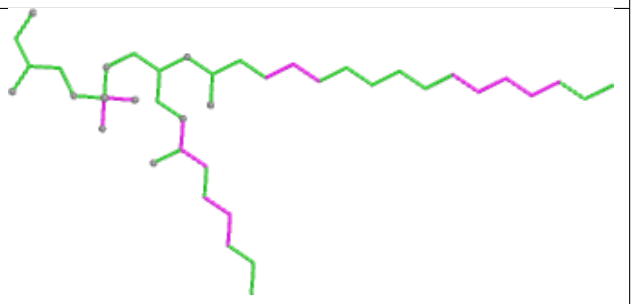


Rings

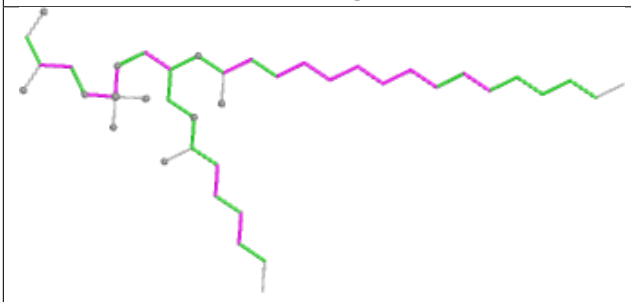
Ligand LHG e 5003



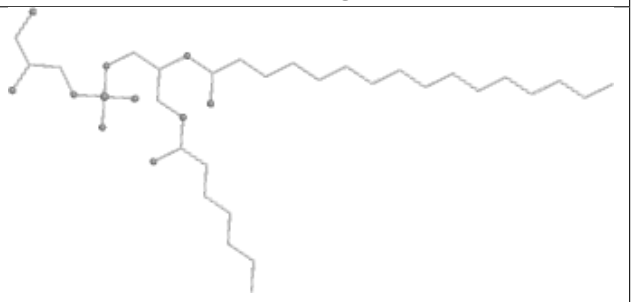
Bond lengths



Bond angles

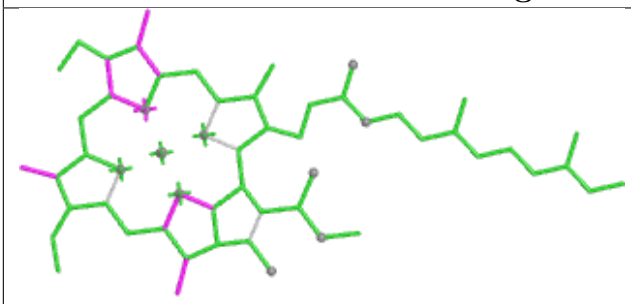


Torsions

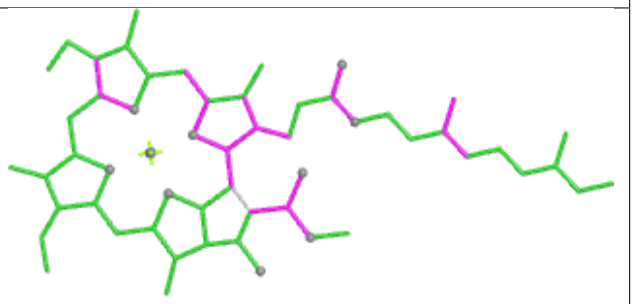


Rings

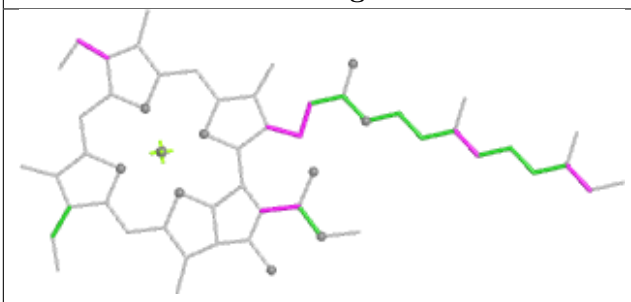
Ligand CLA A 1134



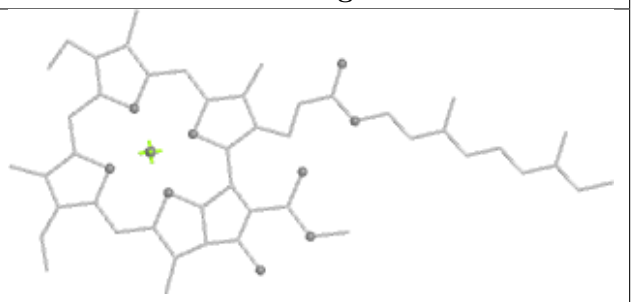
Bond lengths



Bond angles

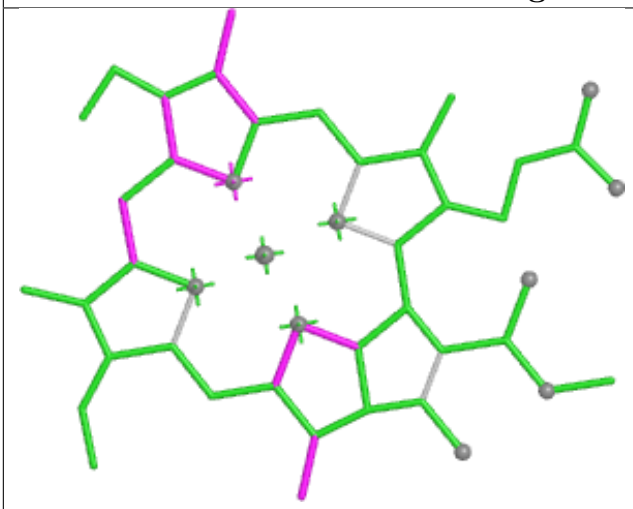


Torsions

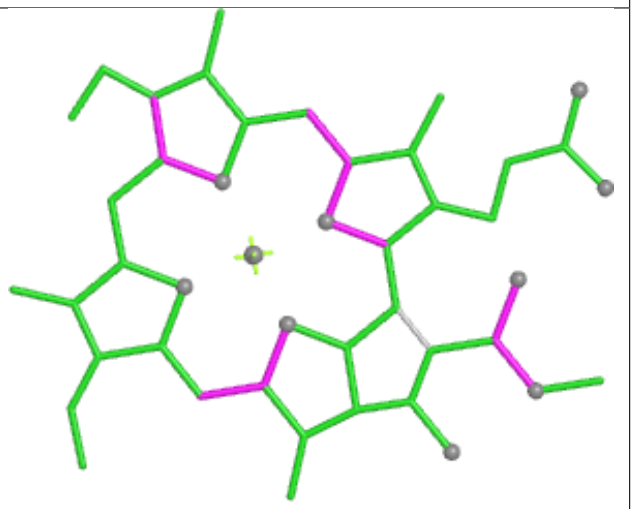


Rings

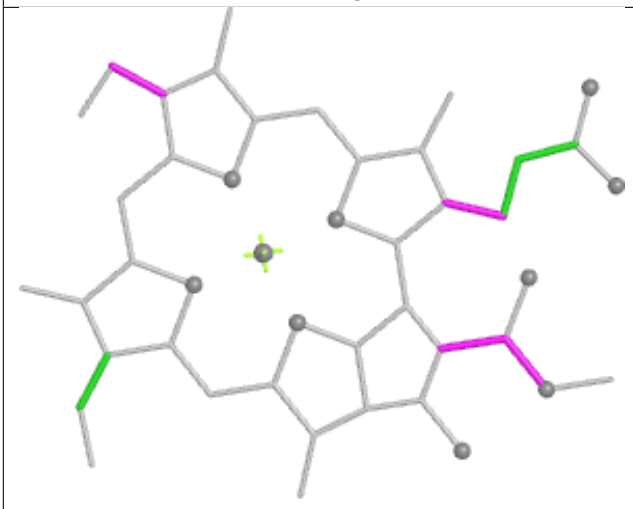
Ligand CLA 4 504



Bond lengths



Bond angles

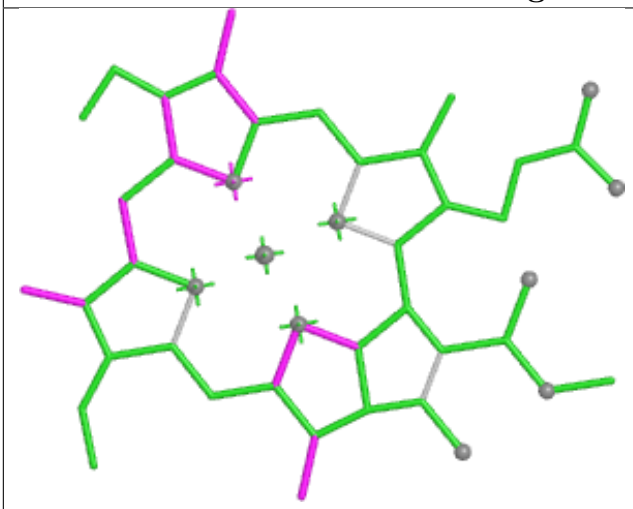


Torsions

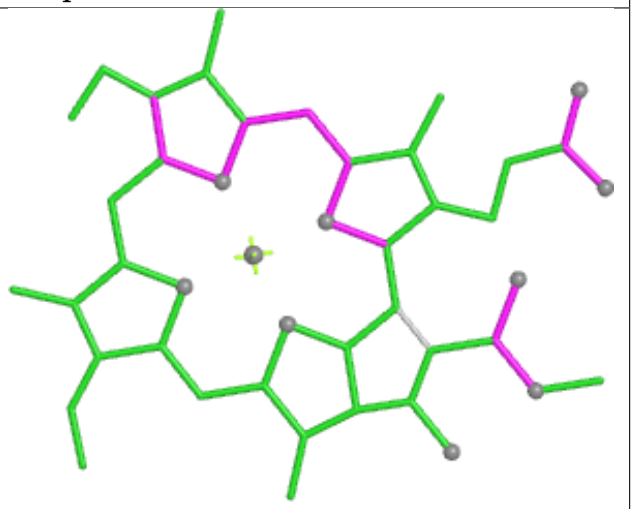


Rings

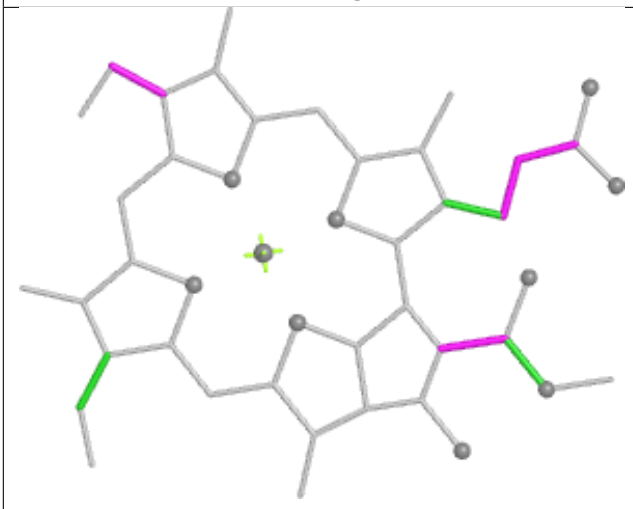
Ligand CLA q 513



Bond lengths



Bond angles

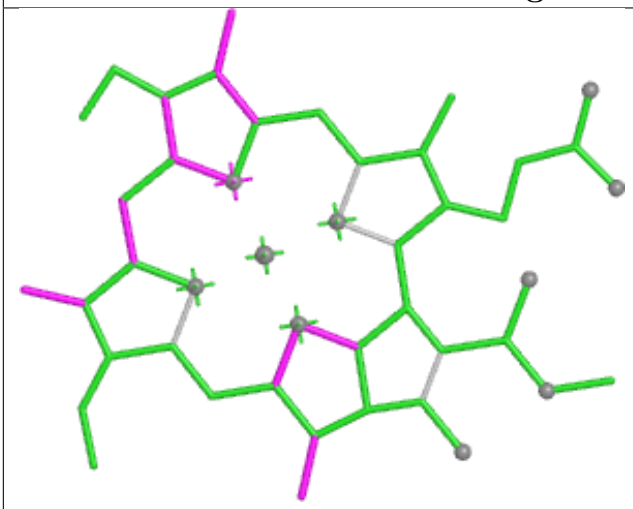


Torsions

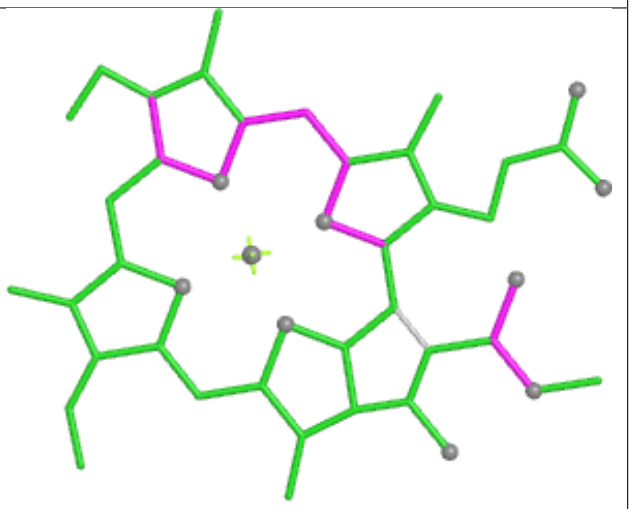


Rings

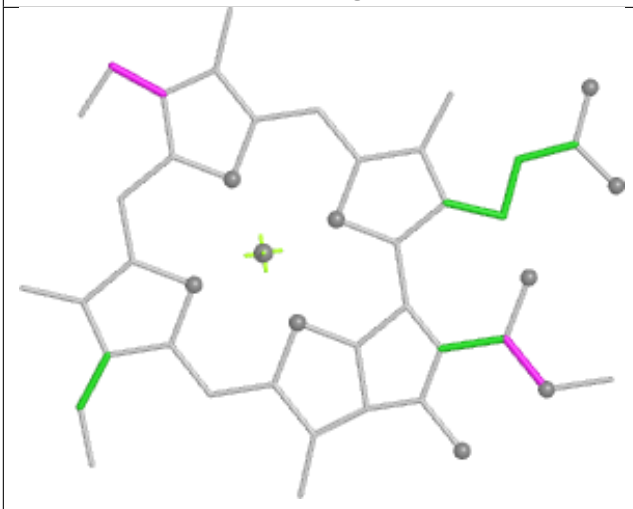
Ligand CLA Z 513



Bond lengths



Bond angles

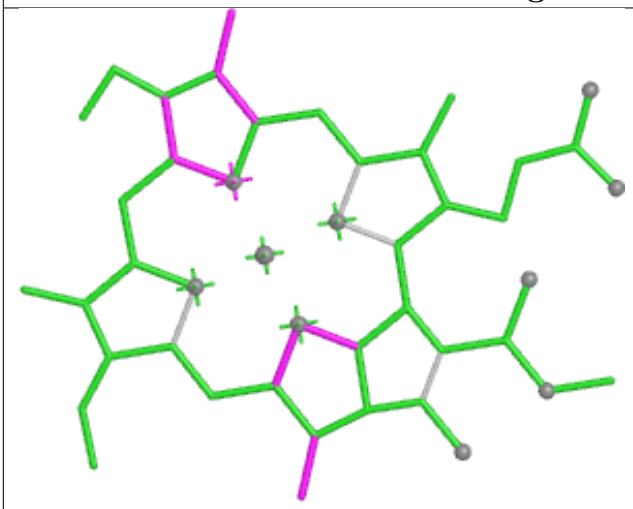


Torsions

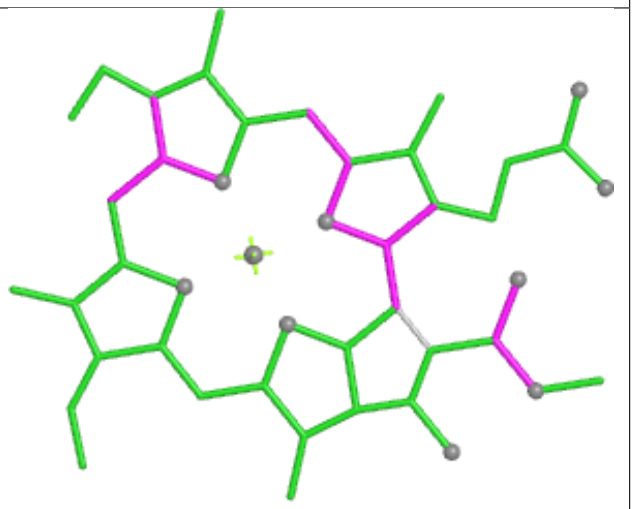


Rings

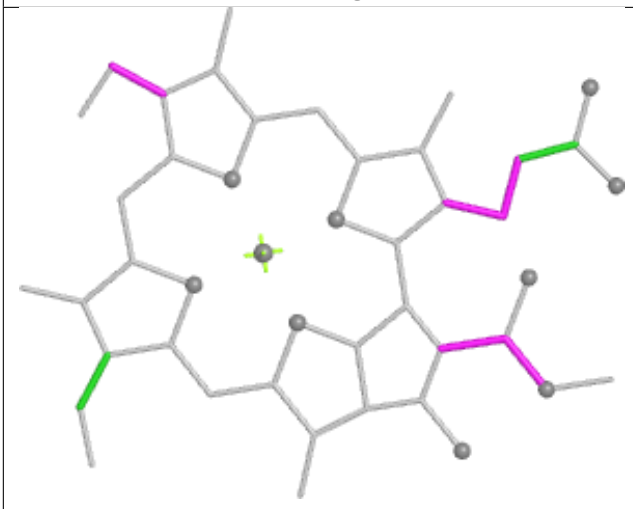
Ligand CLA u 502



Bond lengths



Bond angles

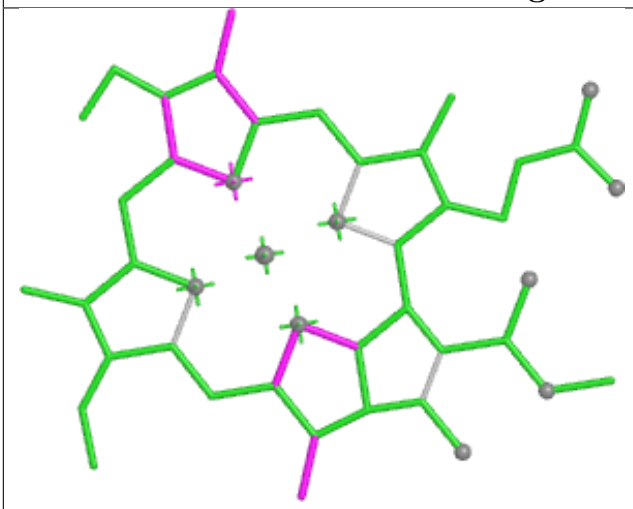


Torsions

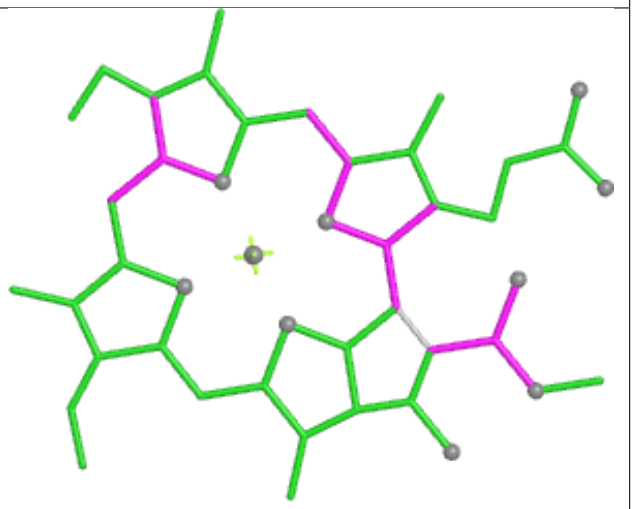


Rings

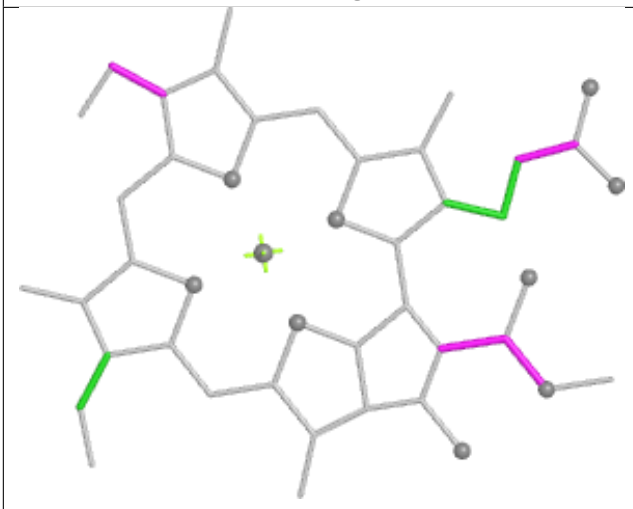
Ligand CLA 4 507



Bond lengths



Bond angles

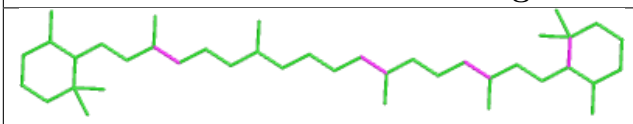


Torsions

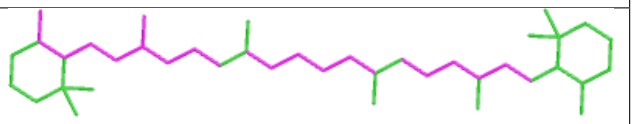


Rings

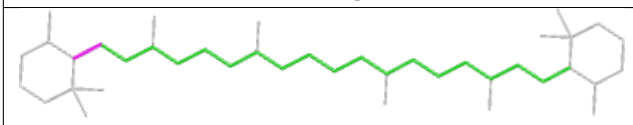
Ligand BCR H 4017



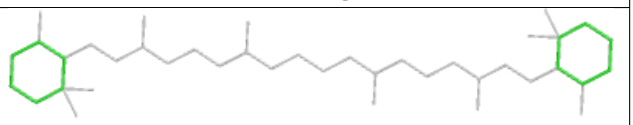
Bond lengths



Bond angles

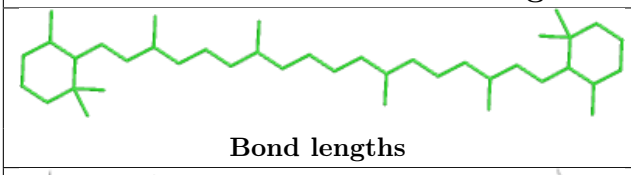


Torsions

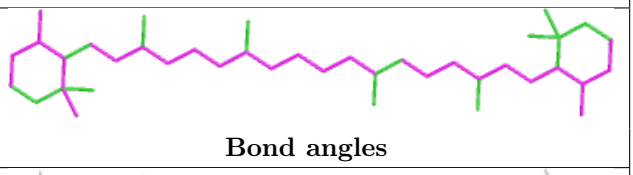


Rings

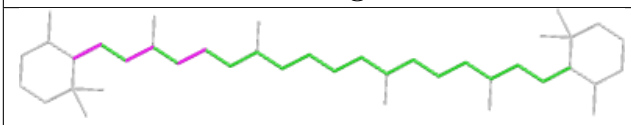
Ligand BCR a 522



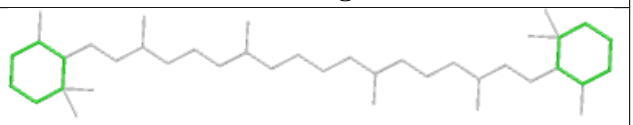
Bond lengths



Bond angles

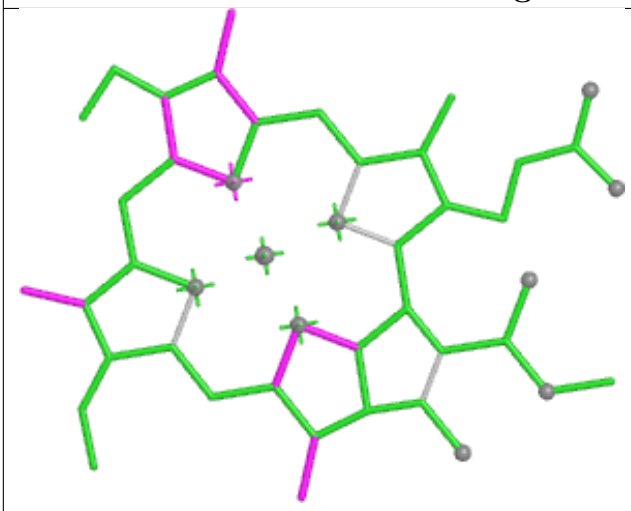


Torsions

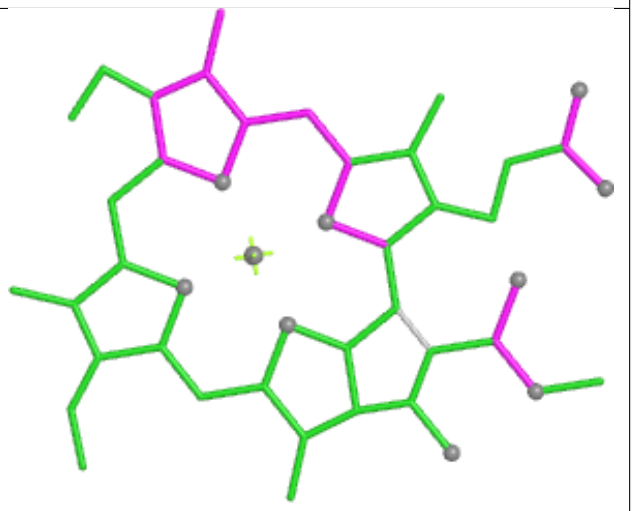


Rings

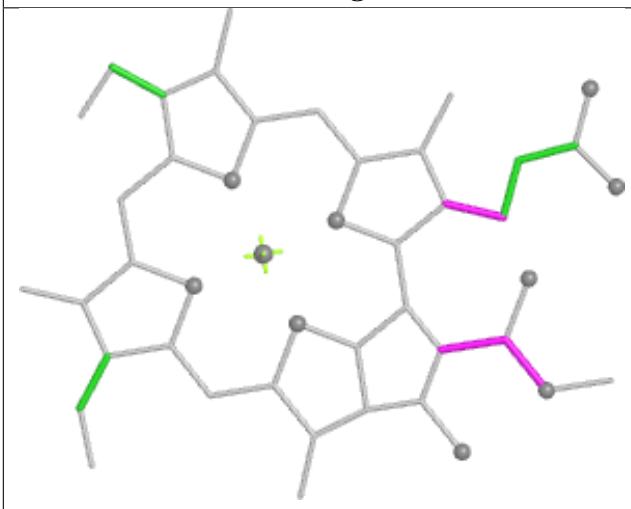
Ligand CLA G 1113



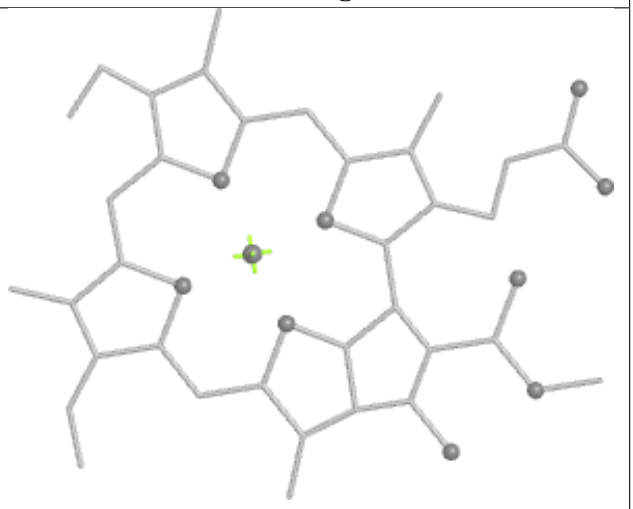
Bond lengths



Bond angles

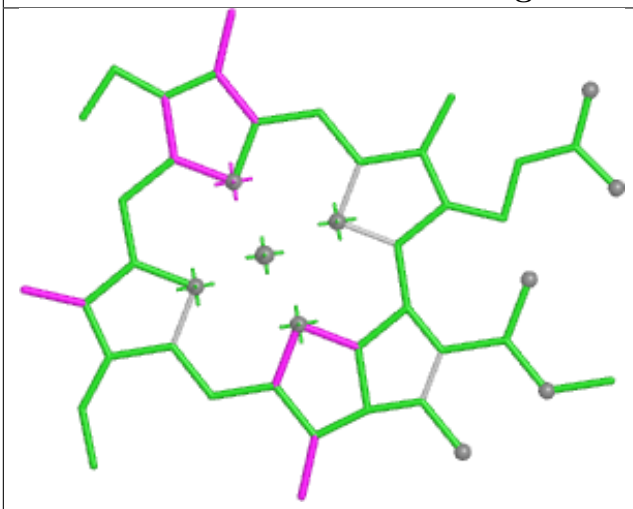


Torsions

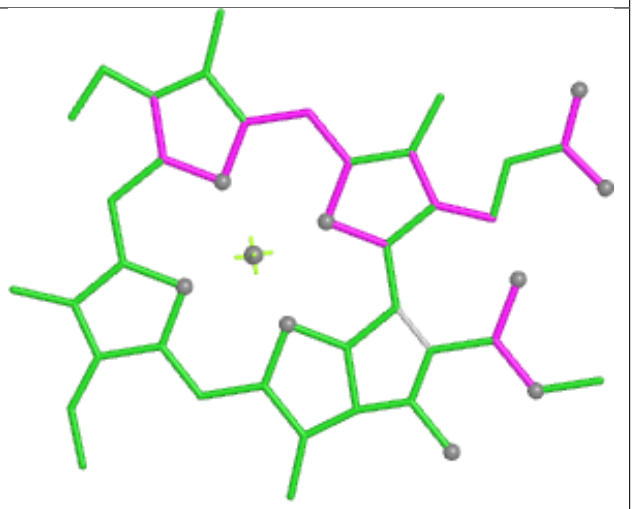


Rings

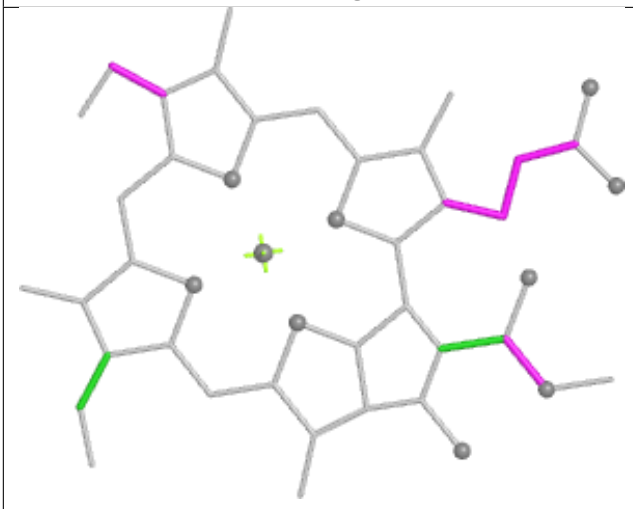
Ligand CLA R 1302



Bond lengths



Bond angles

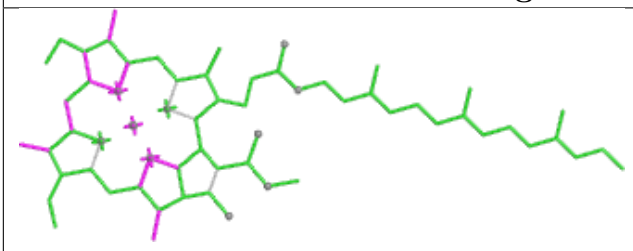


Torsions

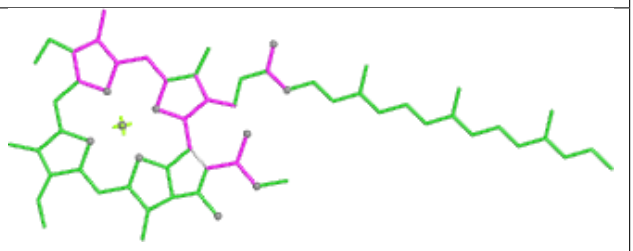


Rings

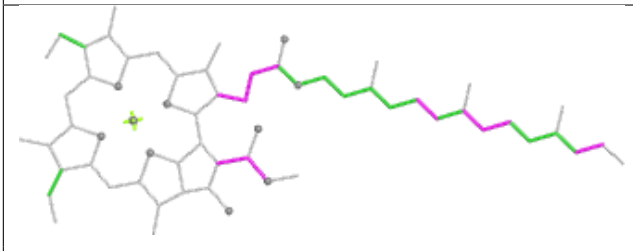
Ligand CLA B 1221



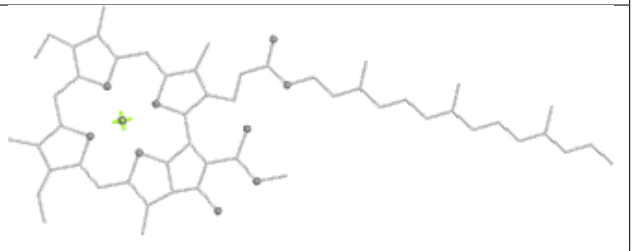
Bond lengths



Bond angles

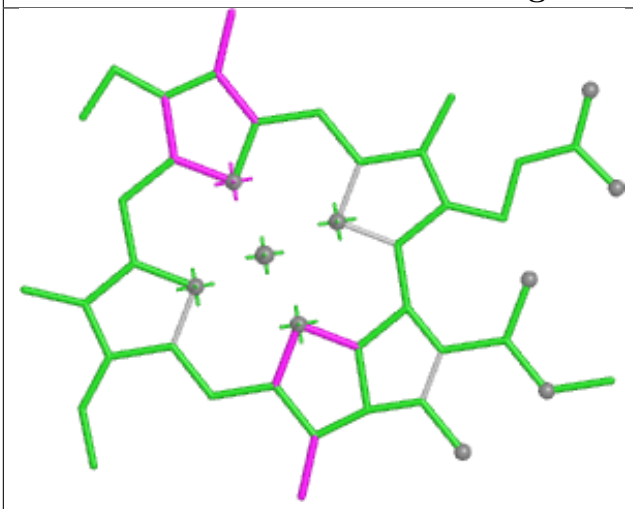


Torsions

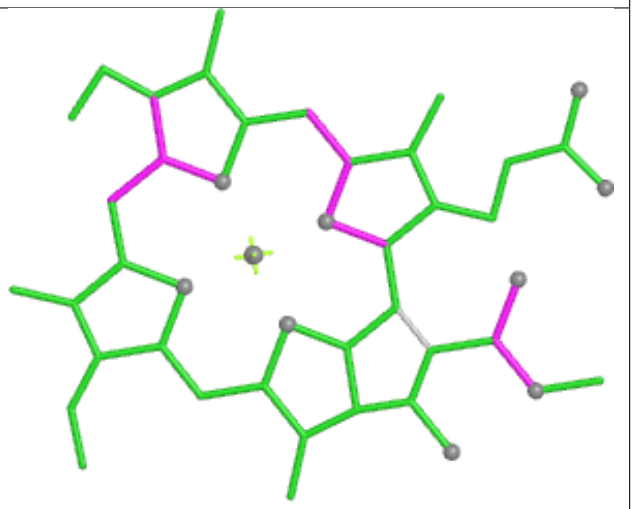


Rings

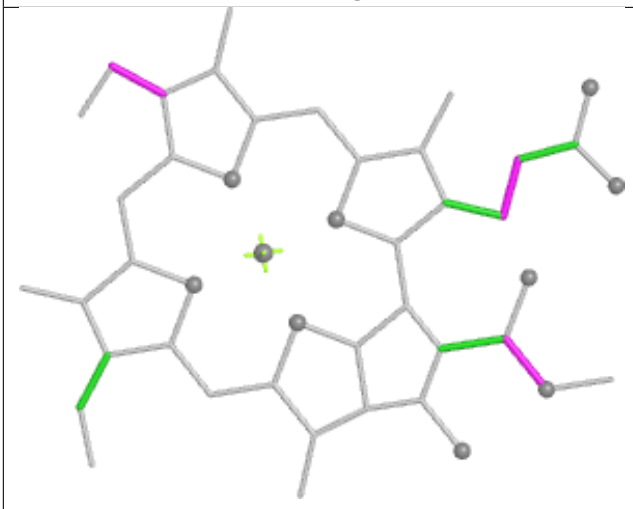
Ligand CLA a 513



Bond lengths



Bond angles

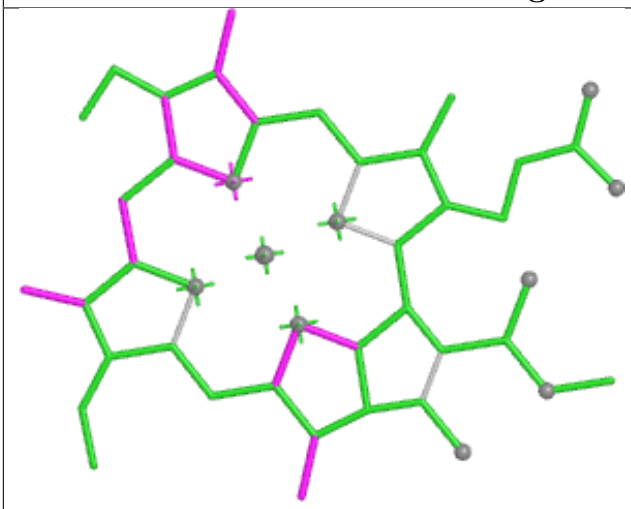


Torsions

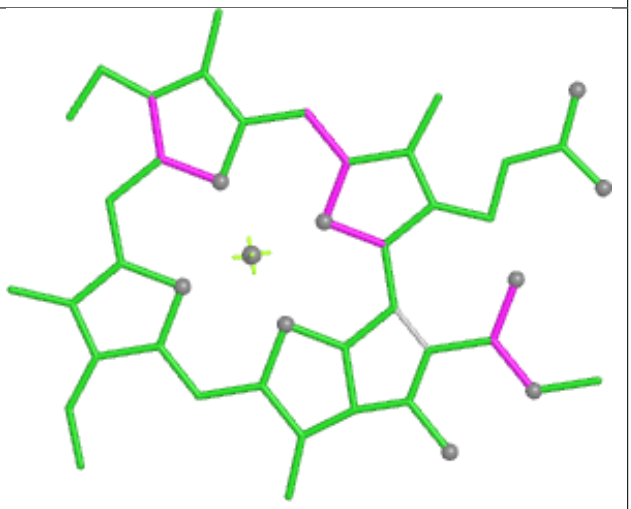


Rings

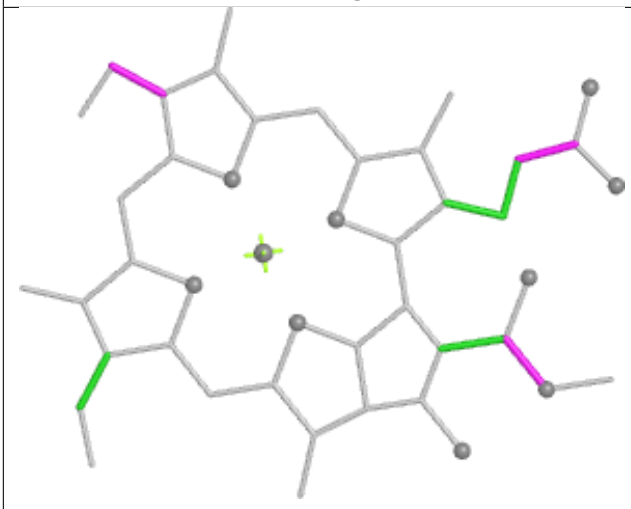
Ligand CLA 1 510



Bond lengths



Bond angles

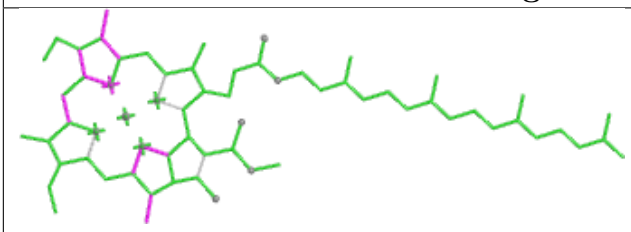


Torsions

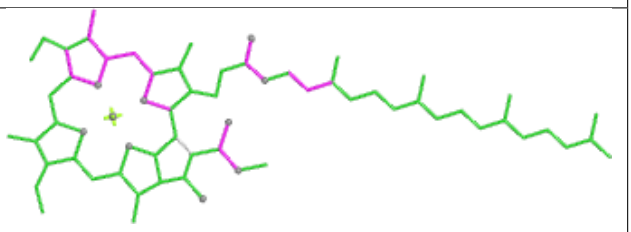


Rings

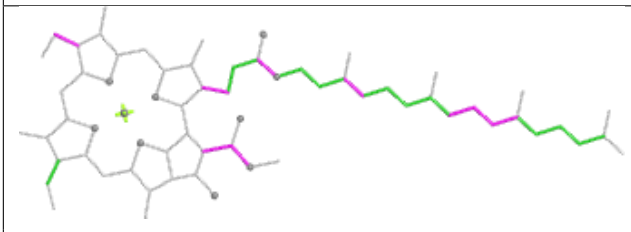
Ligand CLA f 1240



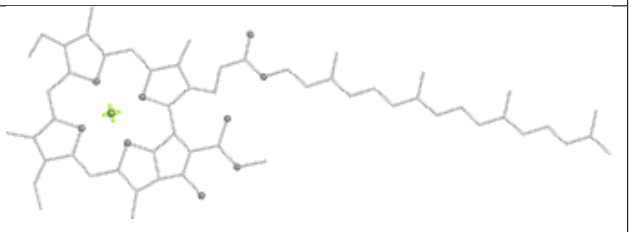
Bond lengths



Bond angles

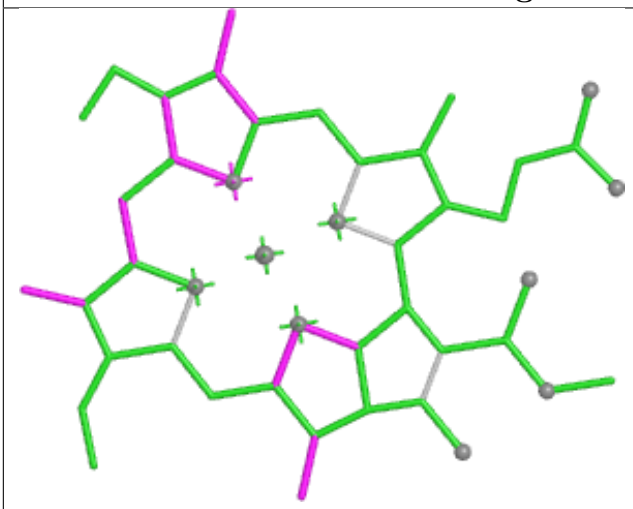


Torsions

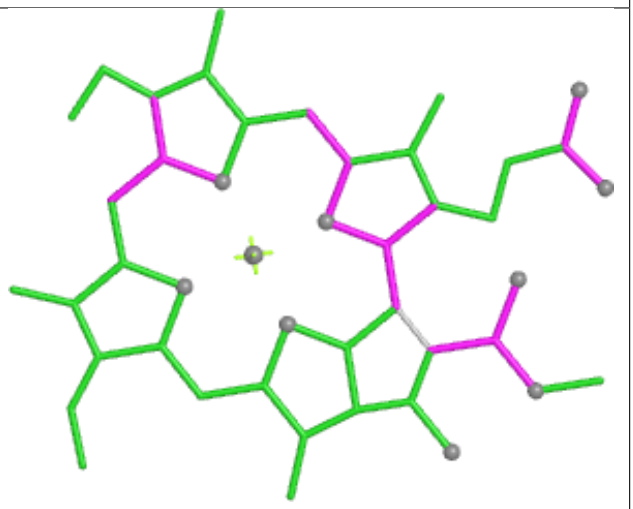


Rings

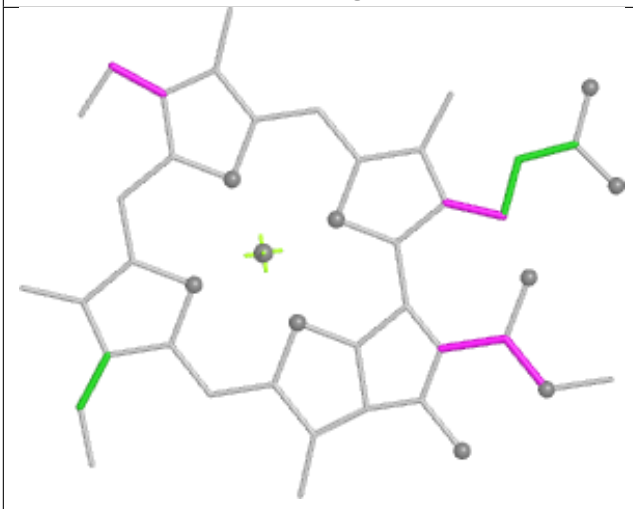
Ligand CLA T 1303



Bond lengths



Bond angles

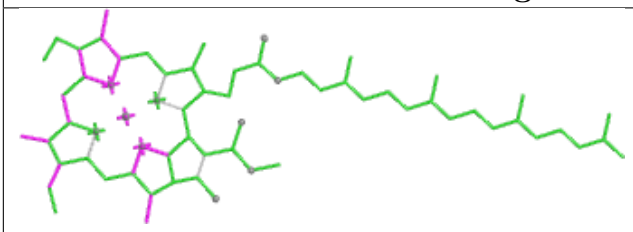


Torsions

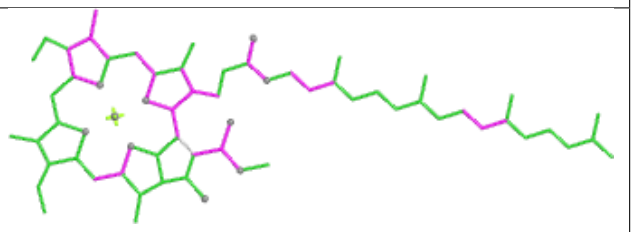


Rings

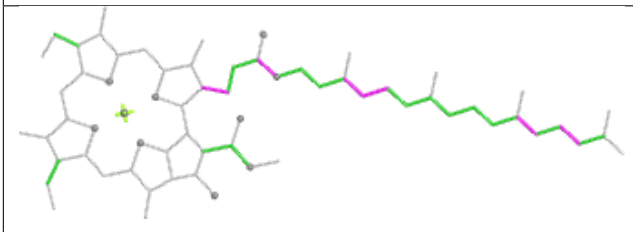
Ligand CLA G 1104



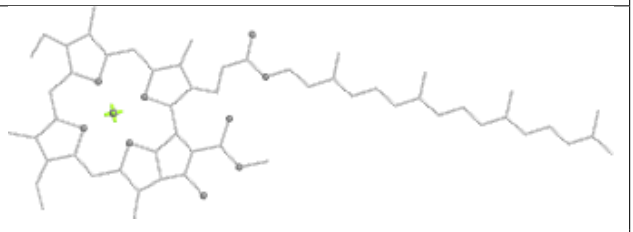
Bond lengths



Bond angles

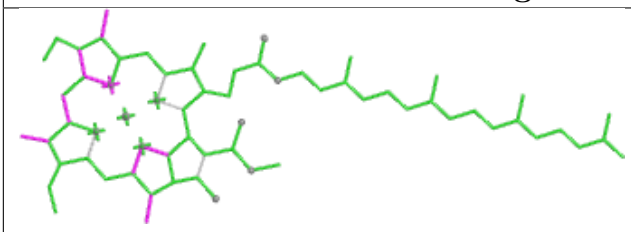


Torsions

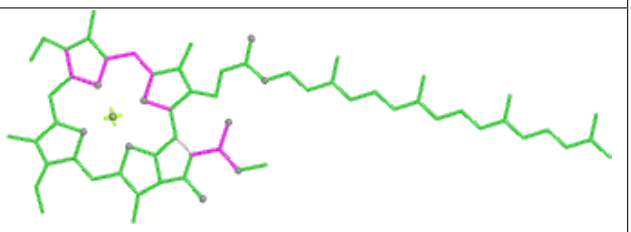


Rings

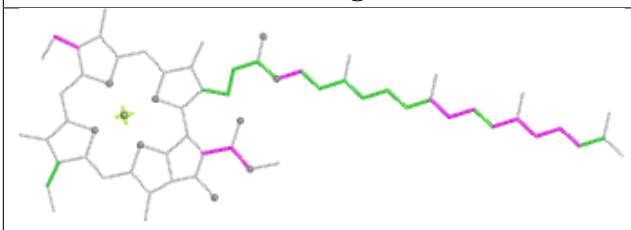
Ligand CLA G 1138



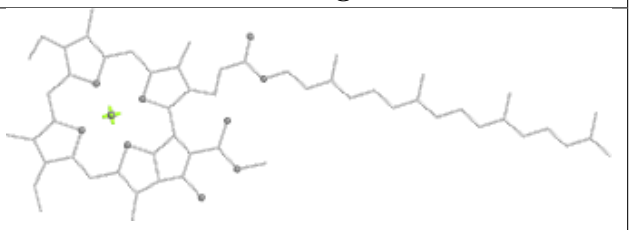
Bond lengths



Bond angles

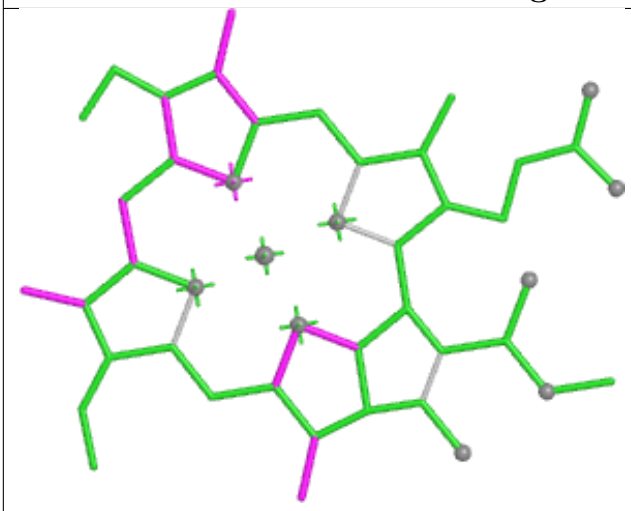


Torsions

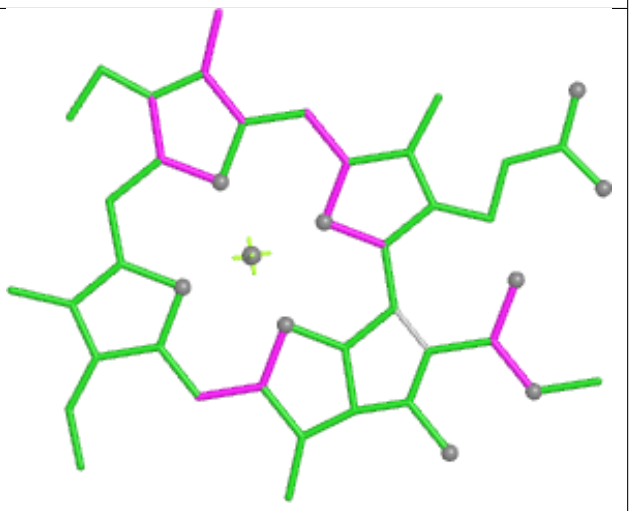


Rings

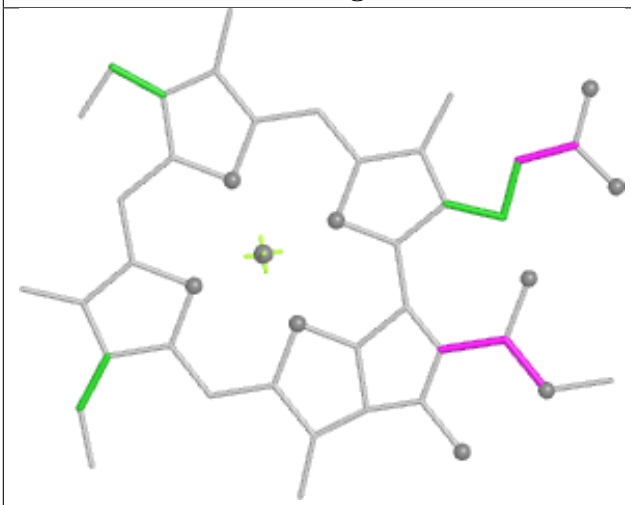
Ligand CLA r 510



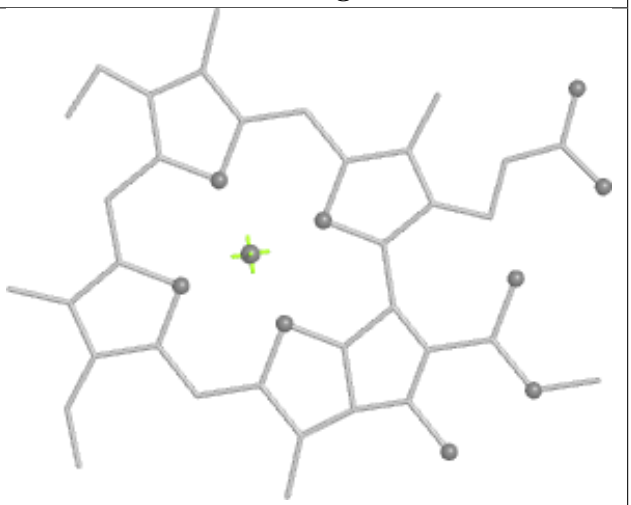
Bond lengths



Bond angles

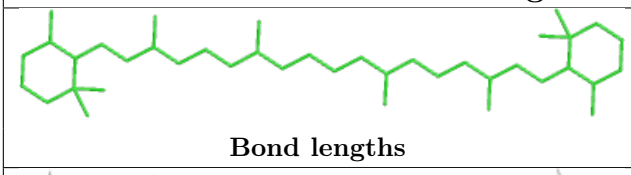


Torsions

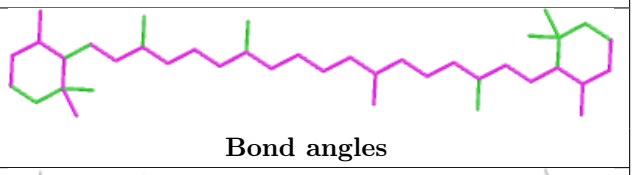


Rings

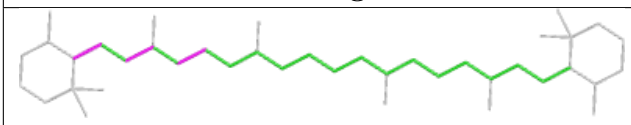
Ligand BCR 3 522



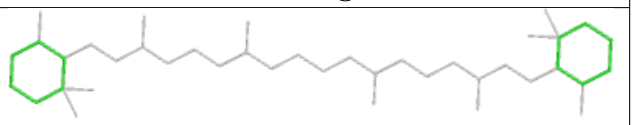
Bond lengths



Bond angles

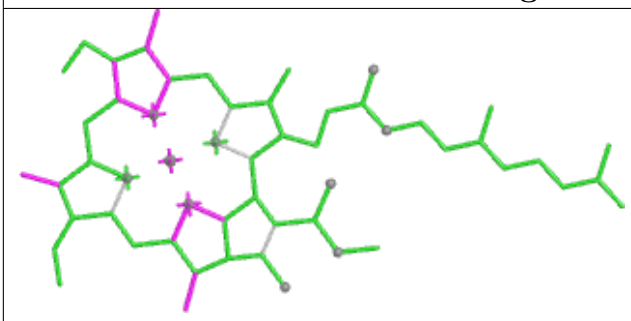


Torsions

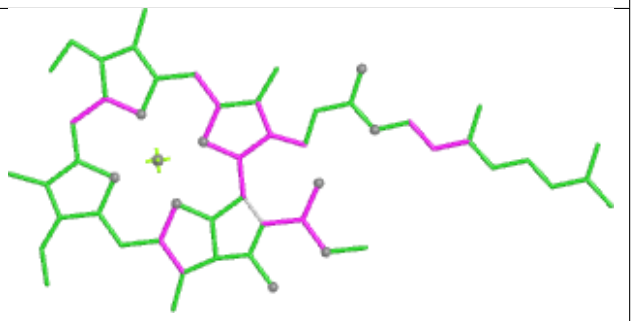


Rings

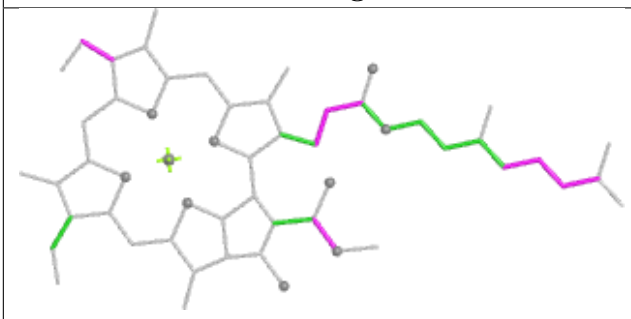
Ligand CLA e 1121



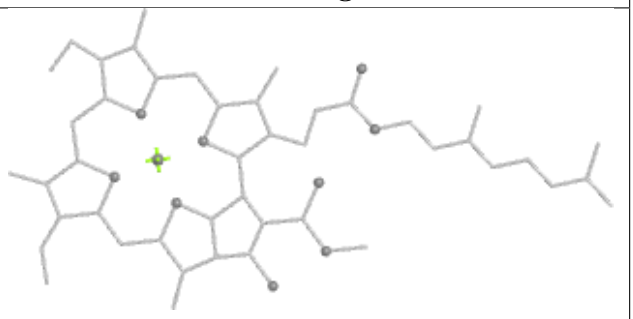
Bond lengths



Bond angles

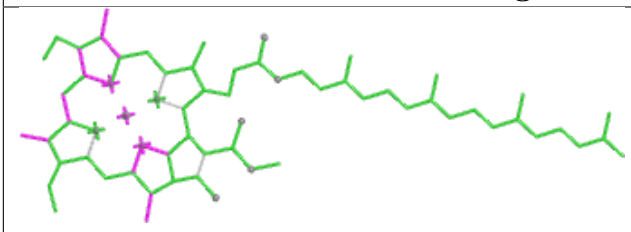


Torsions

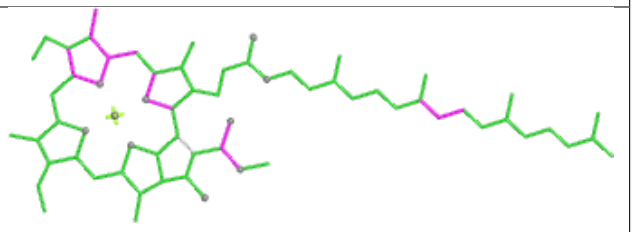


Rings

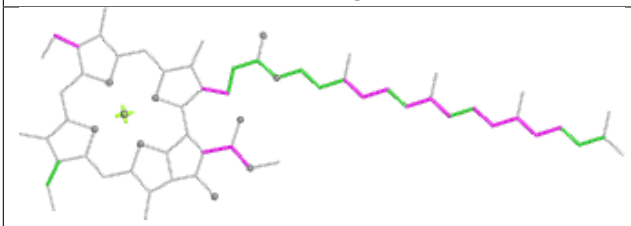
Ligand CLA G 1139



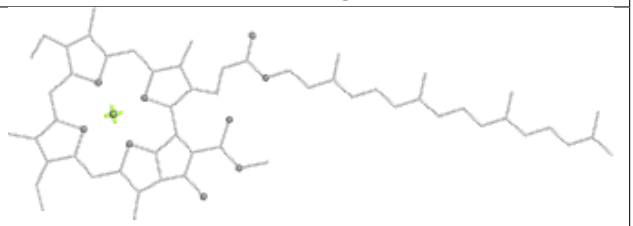
Bond lengths



Bond angles

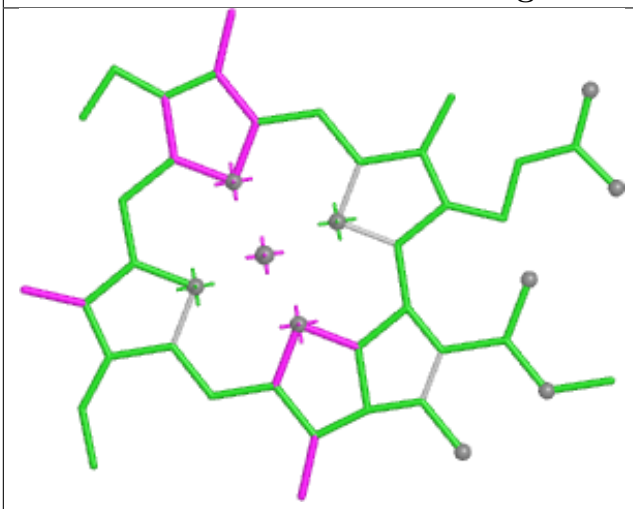


Torsions

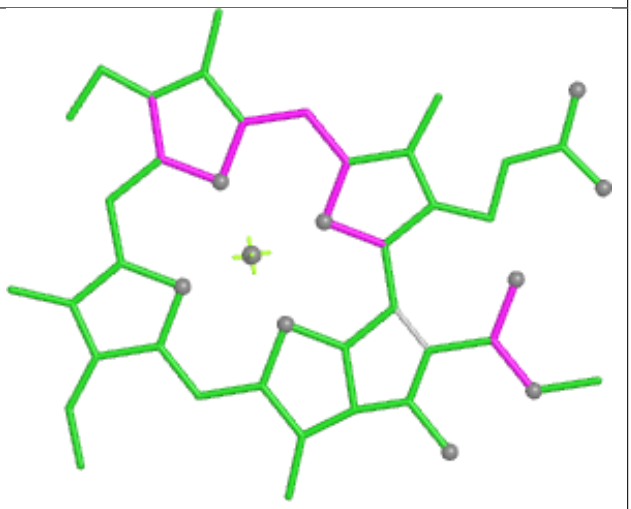


Rings

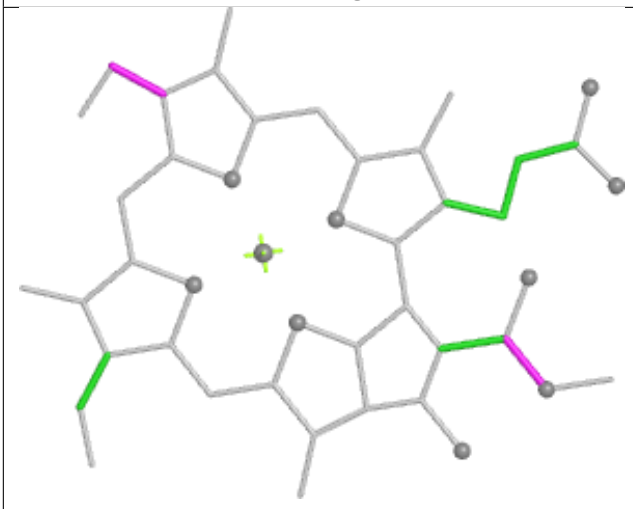
Ligand CLA F 1301



Bond lengths



Bond angles

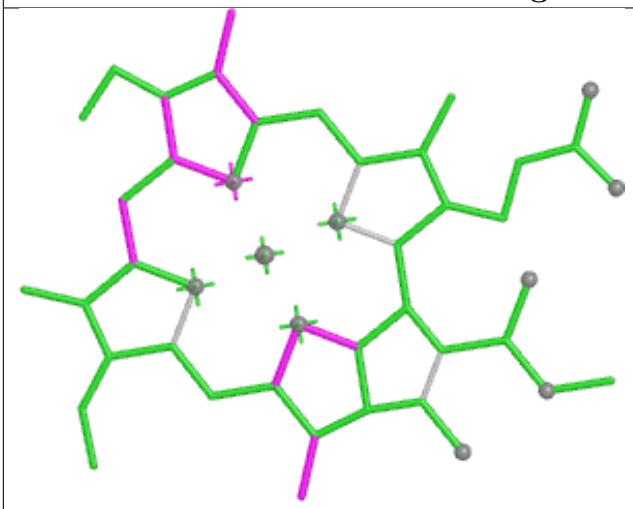


Torsions

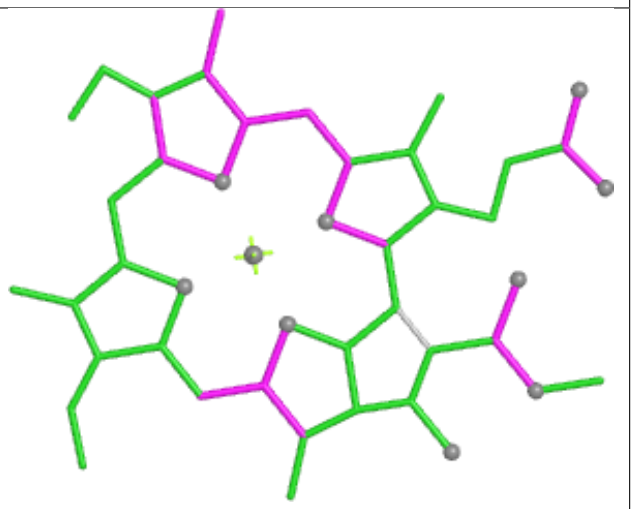


Rings

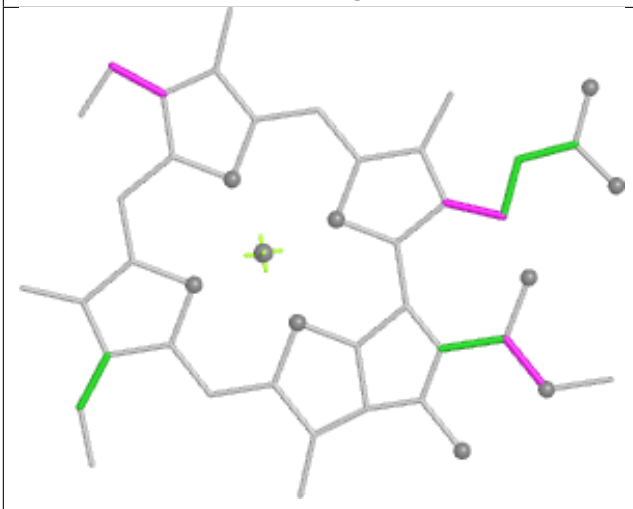
Ligand CLA t 511



Bond lengths



Bond angles

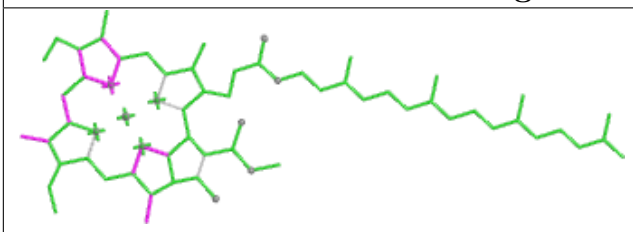


Torsions

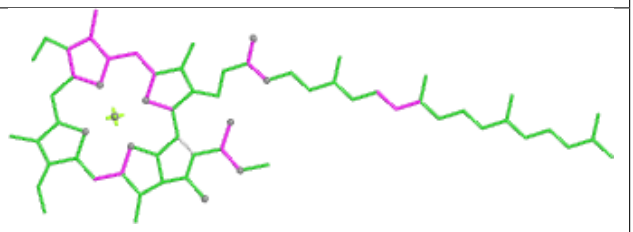


Rings

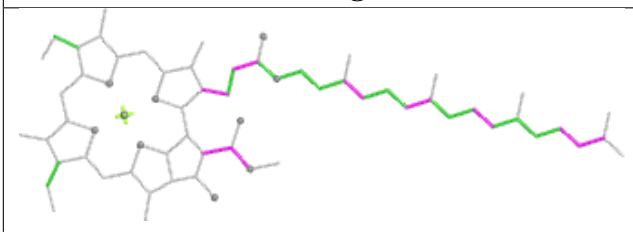
Ligand CLA H 1229



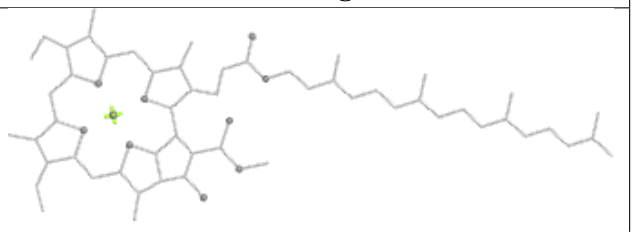
Bond lengths



Bond angles

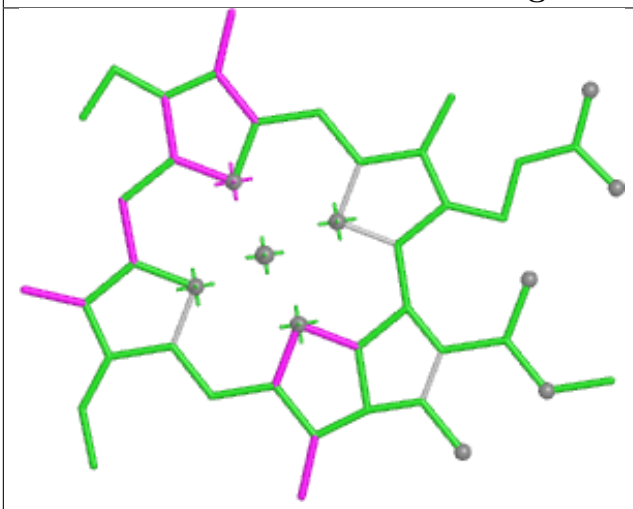


Torsions

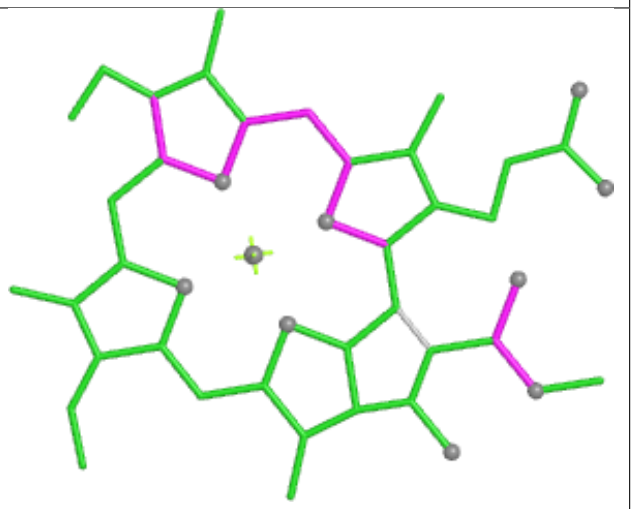


Rings

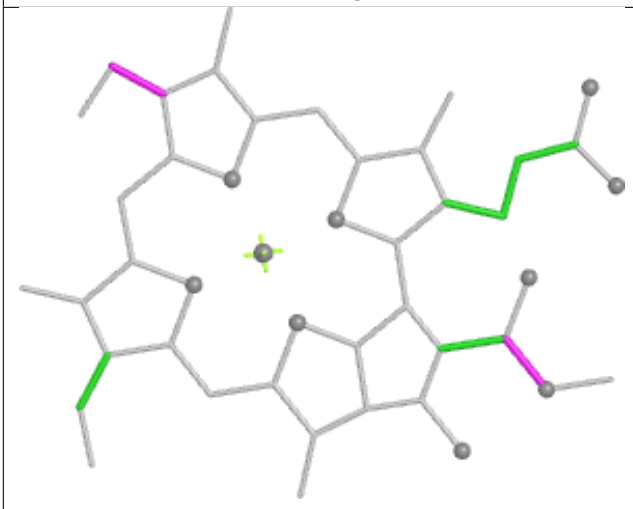
Ligand CLA 2 513



Bond lengths



Bond angles

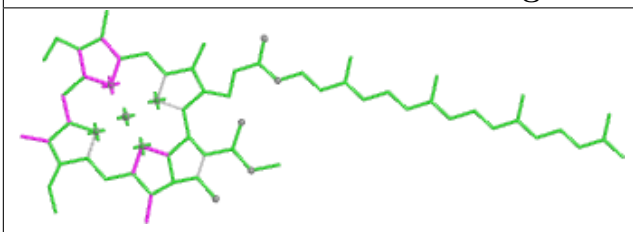


Torsions

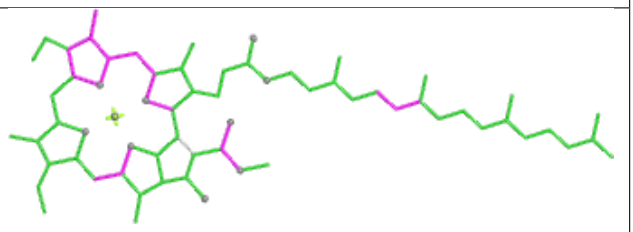


Rings

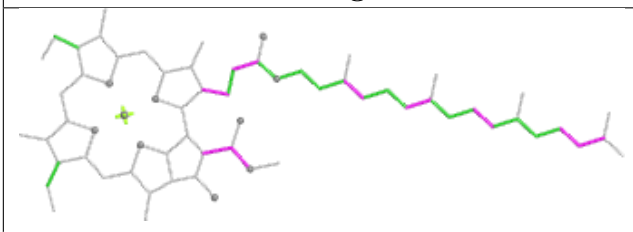
Ligand CLA f 1229



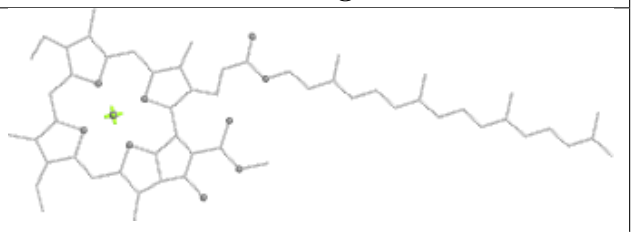
Bond lengths



Bond angles

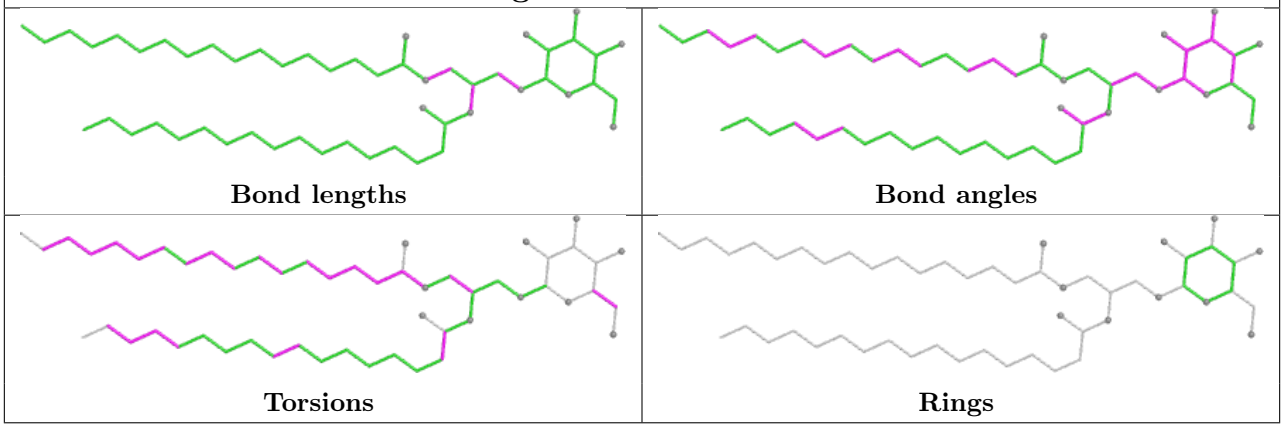


Torsions

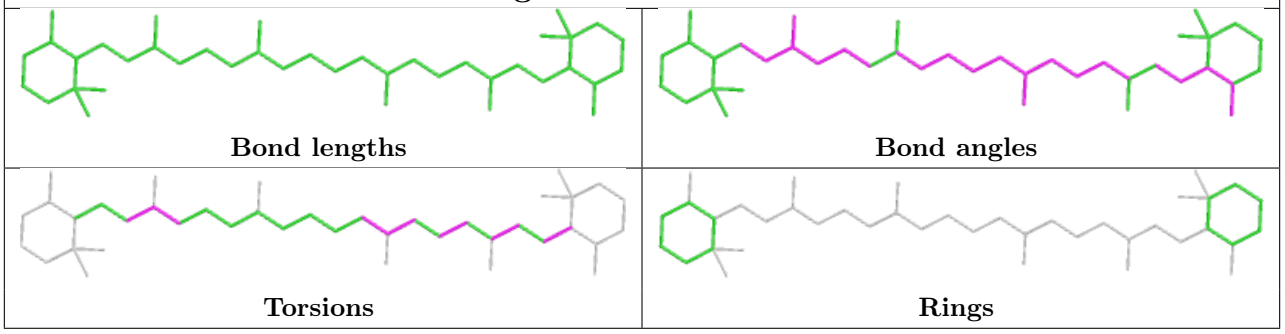


Rings

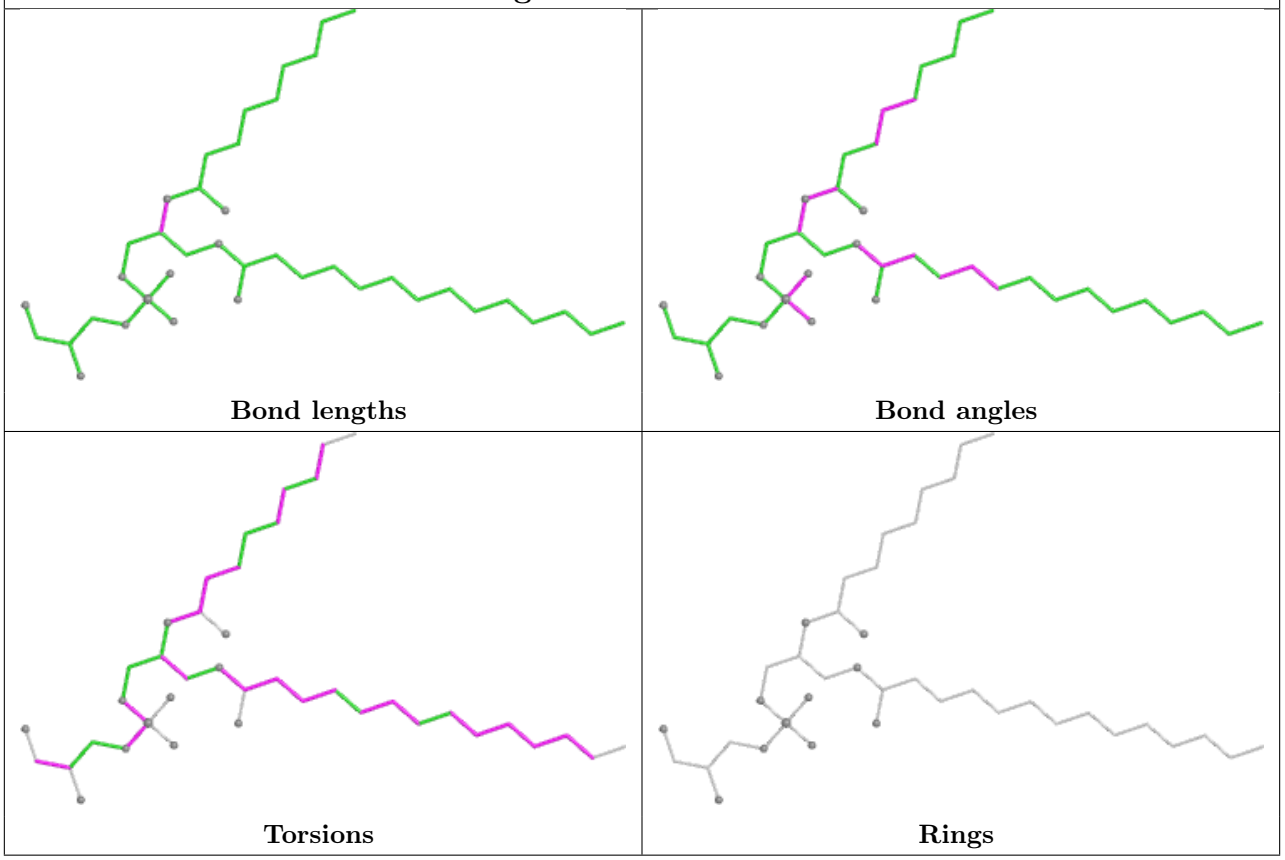
Ligand LMG B 5002



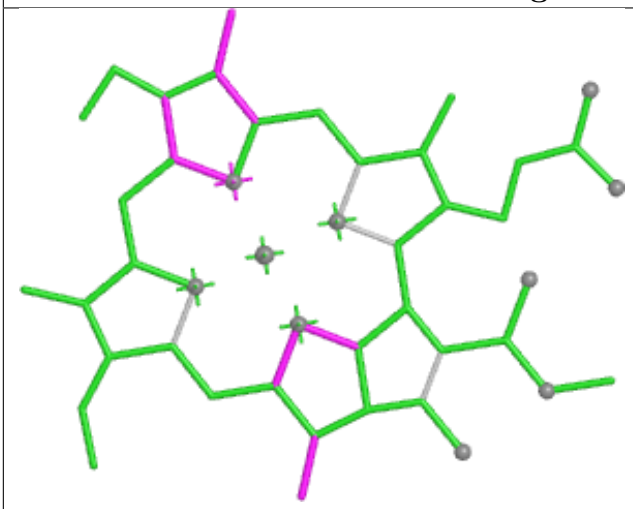
Ligand BCR A 4011



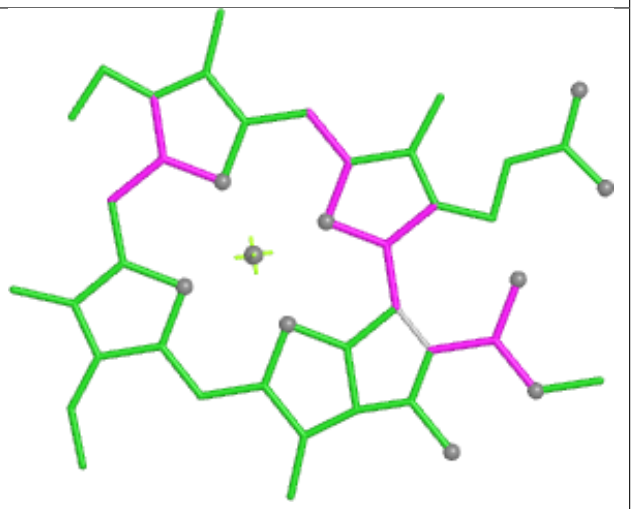
Ligand LHG A 5006



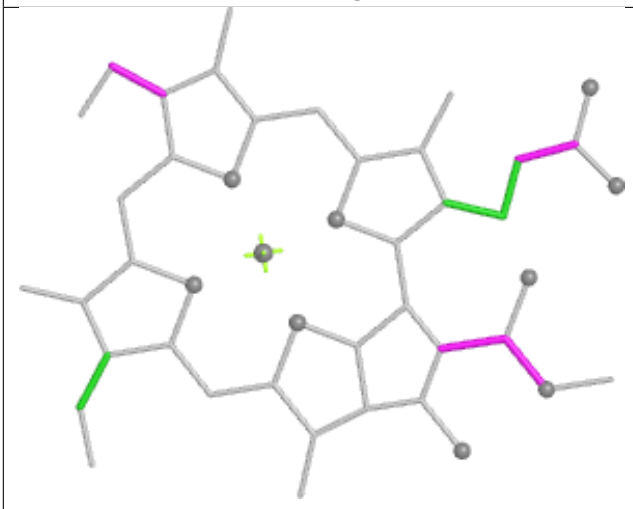
Ligand CLA t 507



Bond lengths



Bond angles

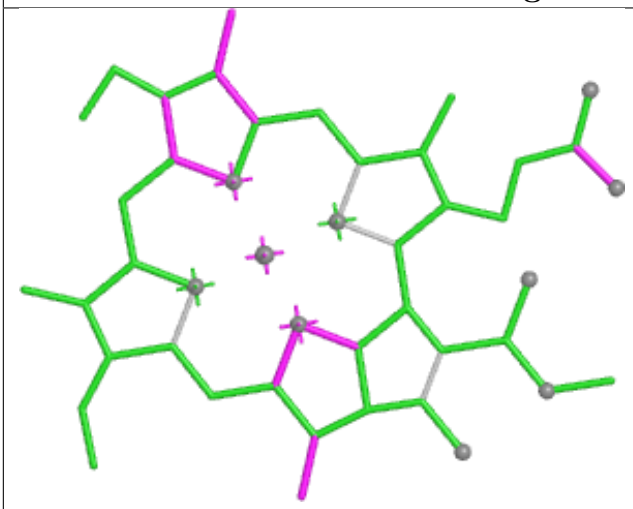


Torsions

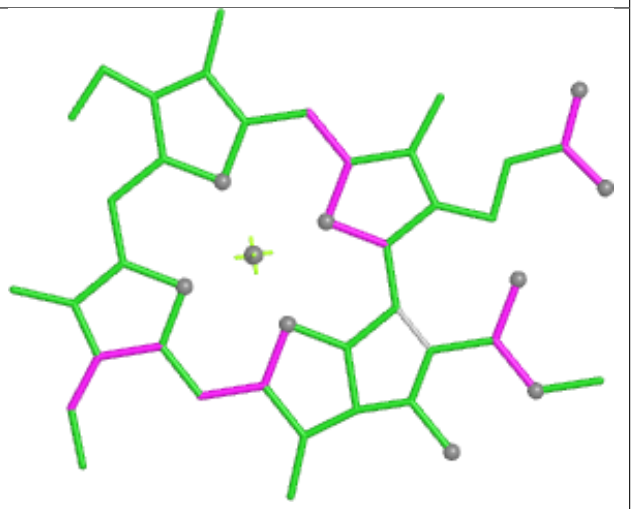


Rings

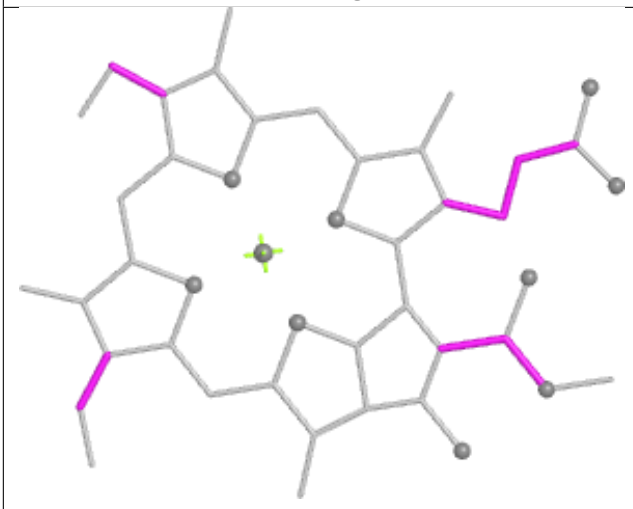
Ligand CLA Y 516



Bond lengths



Bond angles

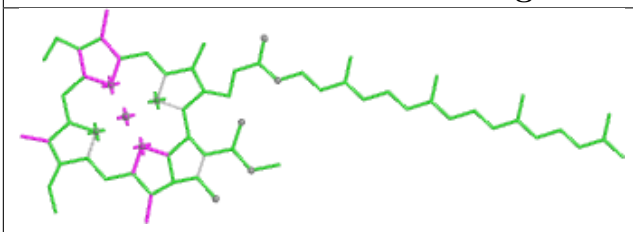


Torsions

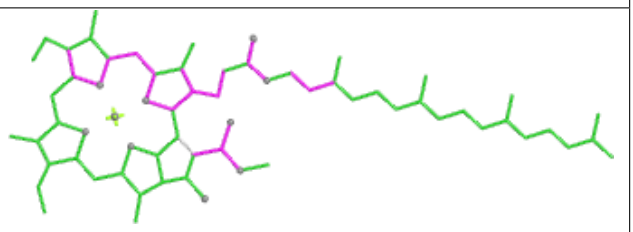


Rings

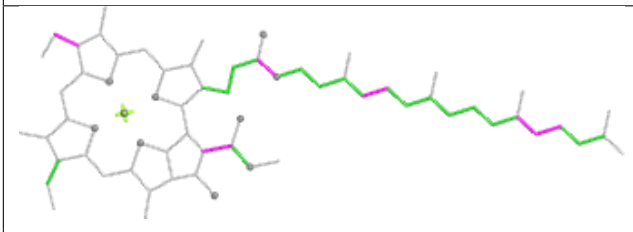
Ligand CLA B 1205



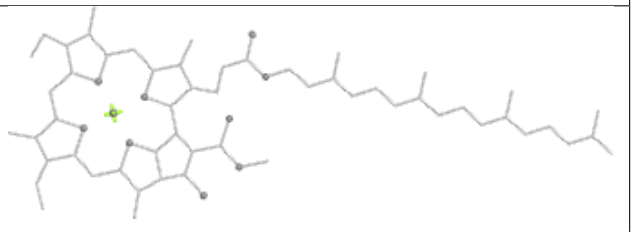
Bond lengths



Bond angles

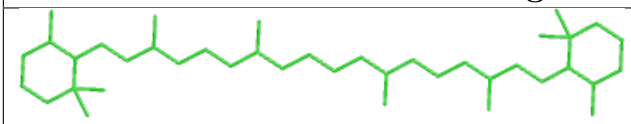


Torsions

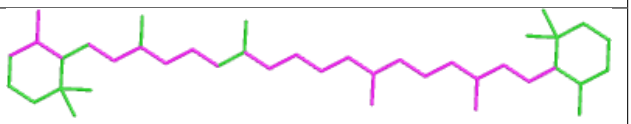


Rings

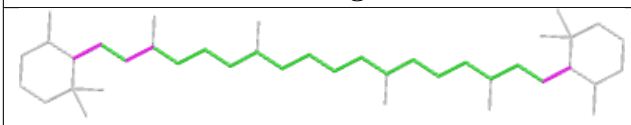
Ligand BCR 6 524



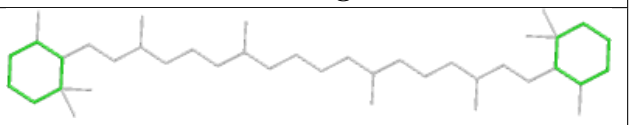
Bond lengths



Bond angles

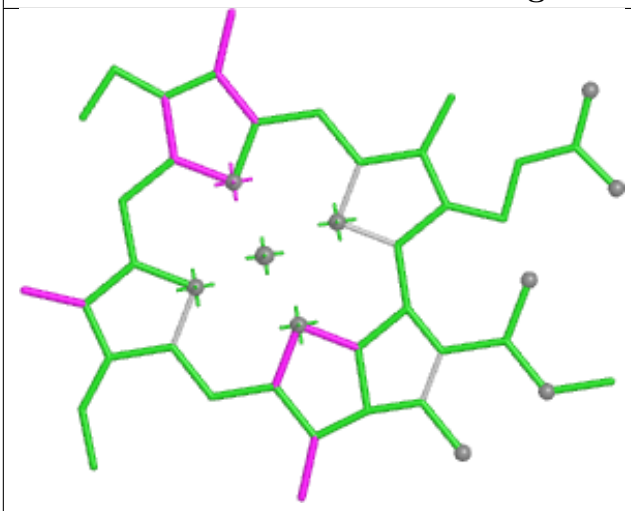


Torsions

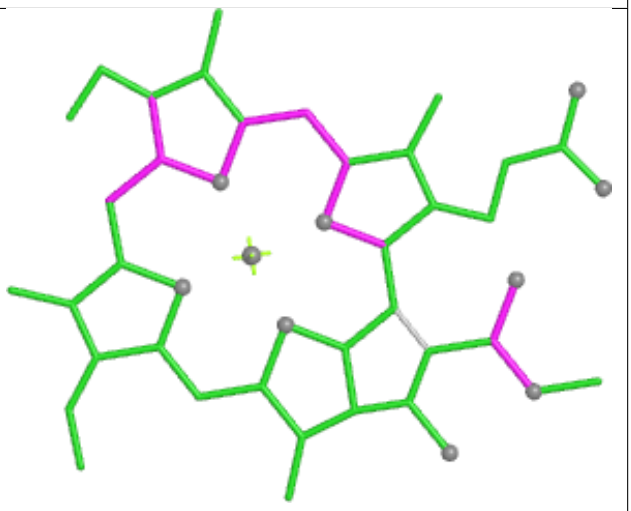


Rings

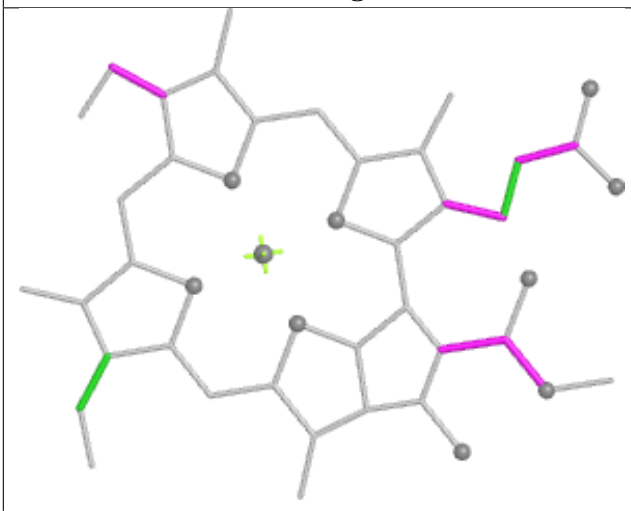
Ligand CLA v 512



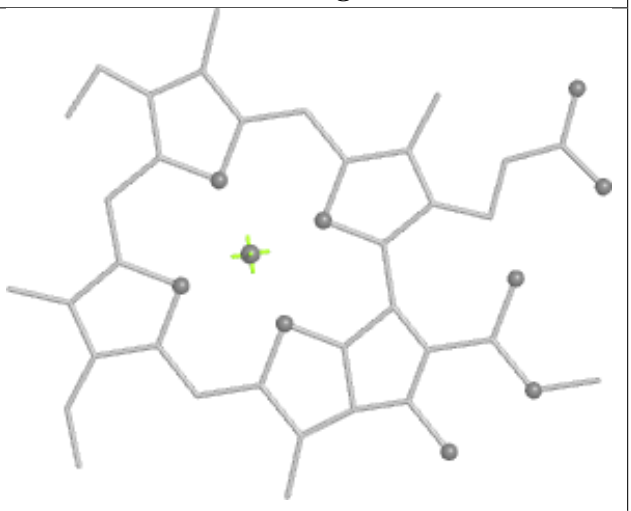
Bond lengths



Bond angles

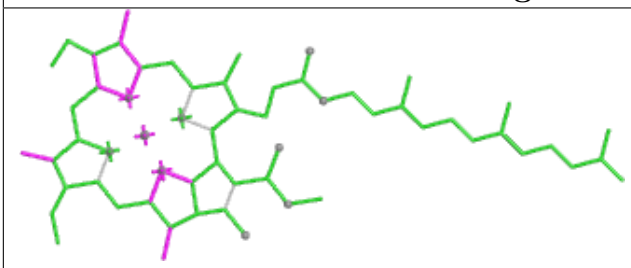


Torsions

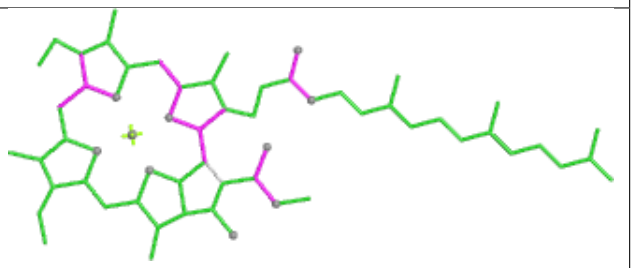


Rings

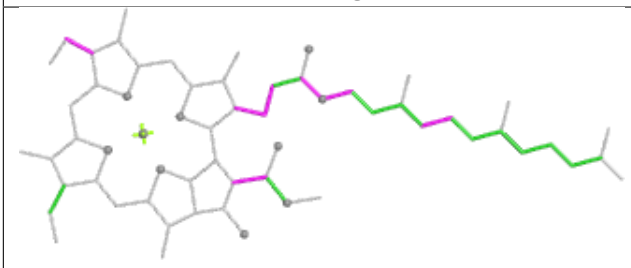
Ligand CLA G 1118



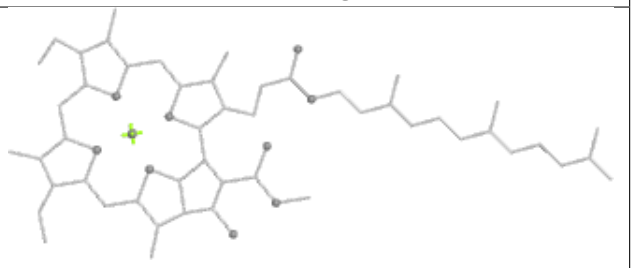
Bond lengths



Bond angles

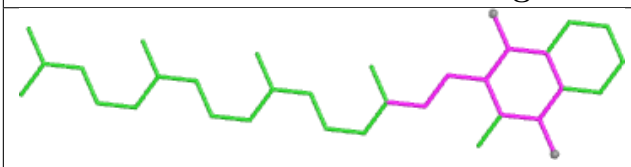


Torsions

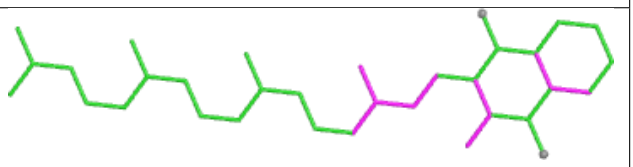


Rings

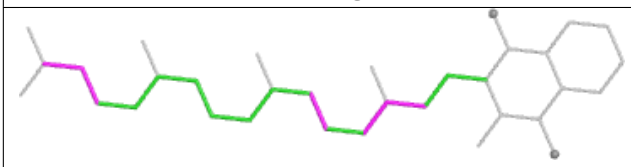
Ligand PQN B 2002



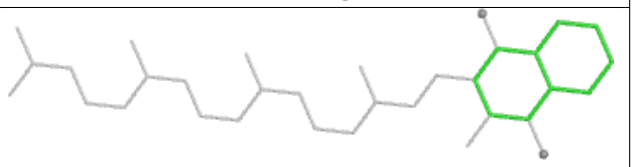
Bond lengths



Bond angles

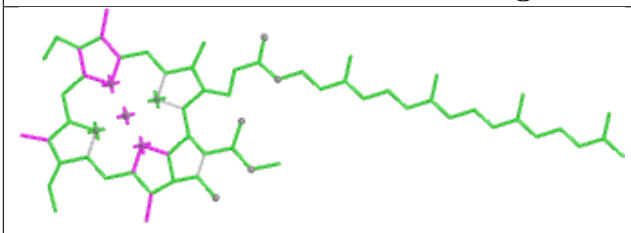


Torsions

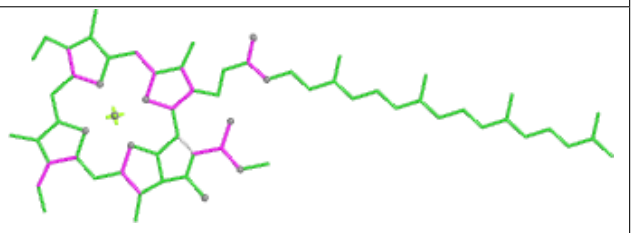


Rings

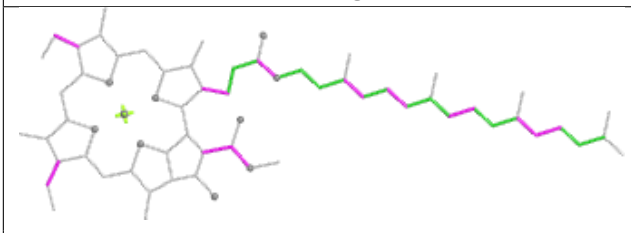
Ligand CLA A 1132



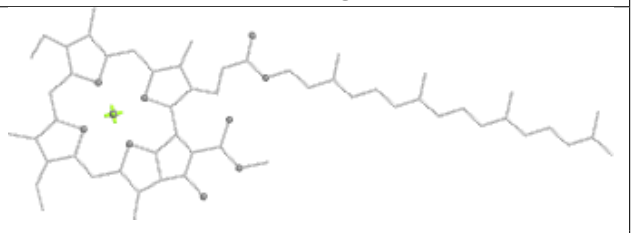
Bond lengths



Bond angles

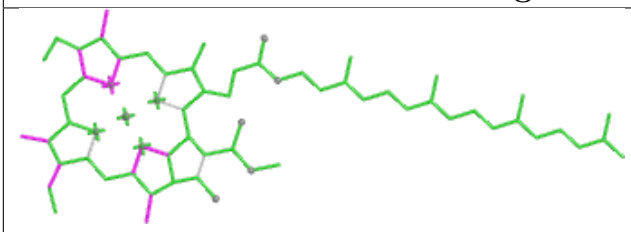


Torsions

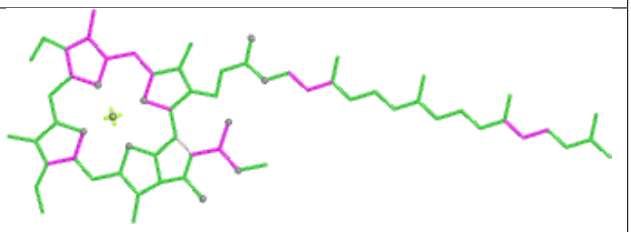


Rings

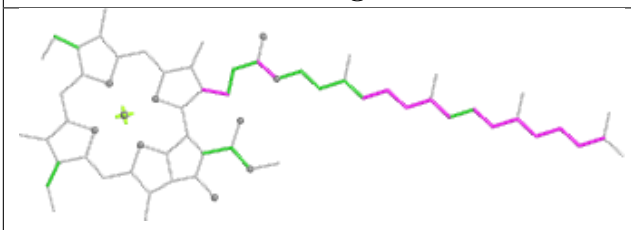
Ligand CLA H 1215



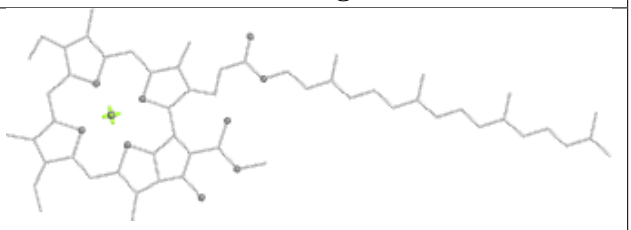
Bond lengths



Bond angles



Torsions

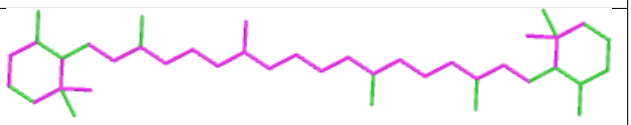


Rings

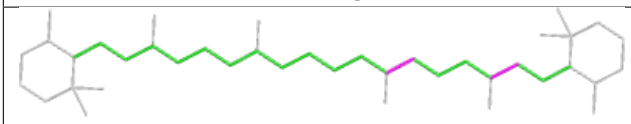
Ligand BCR J 4013



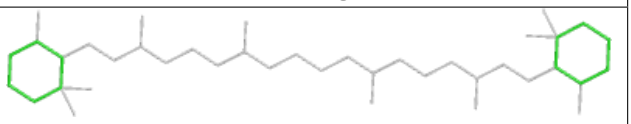
Bond lengths



Bond angles

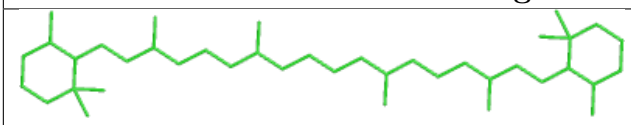


Torsions

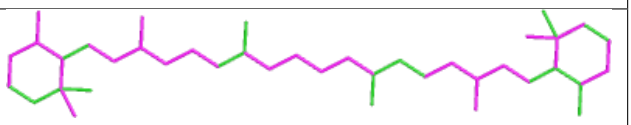


Rings

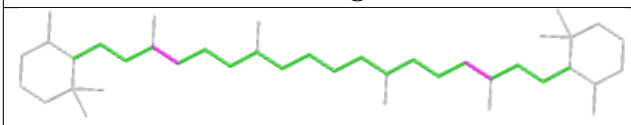
Ligand BCR B 4006



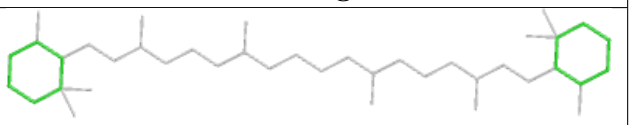
Bond lengths



Bond angles

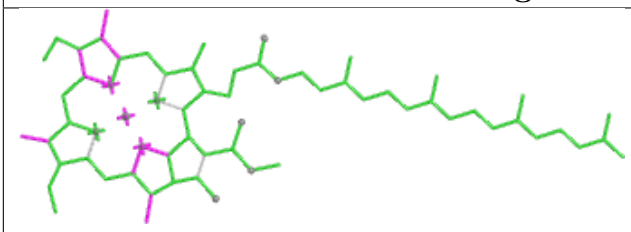


Torsions

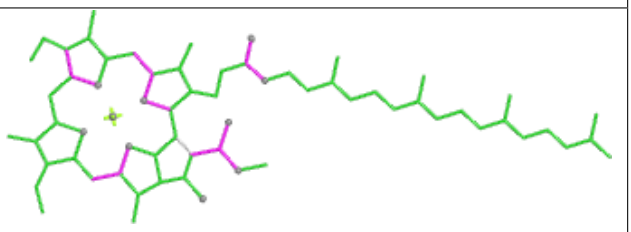


Rings

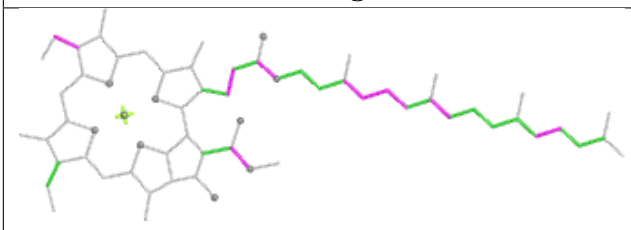
Ligand CLA H 1204



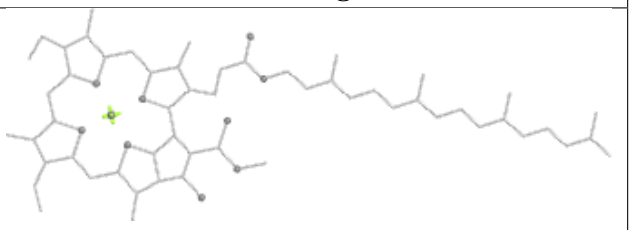
Bond lengths



Bond angles



Torsions

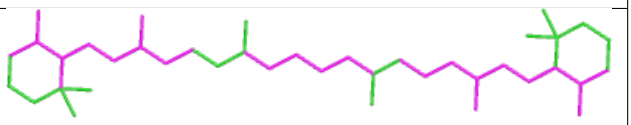


Rings

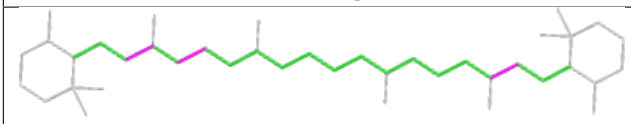
Ligand BCR s 524



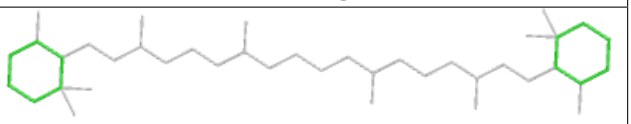
Bond lengths



Bond angles

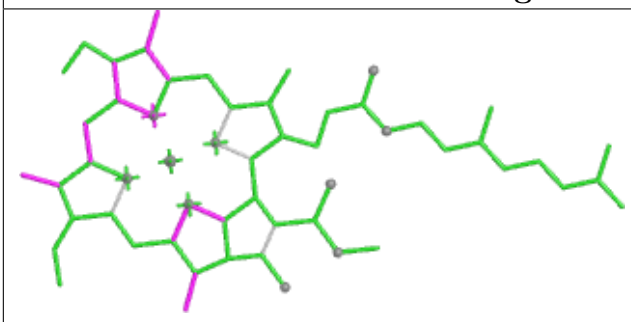


Torsions

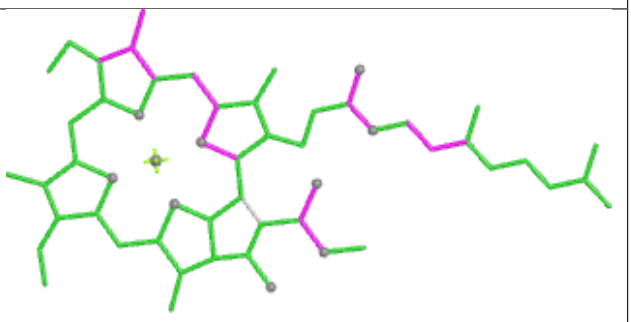


Rings

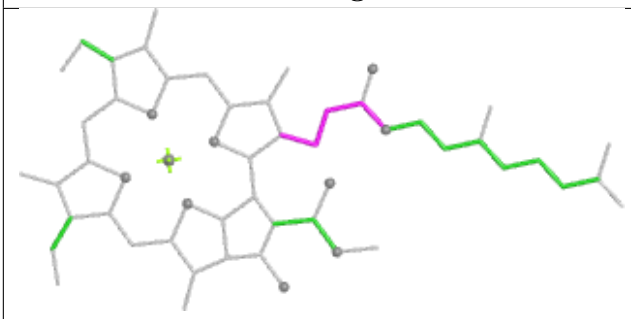
Ligand CLA H 1228



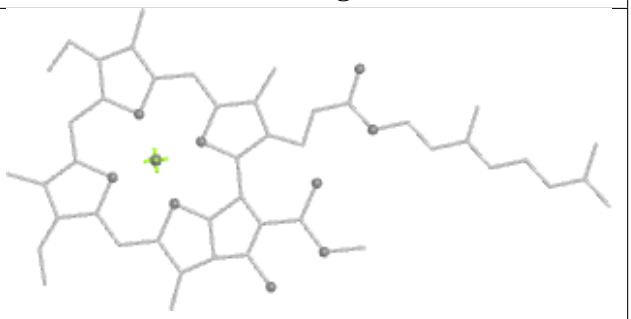
Bond lengths



Bond angles

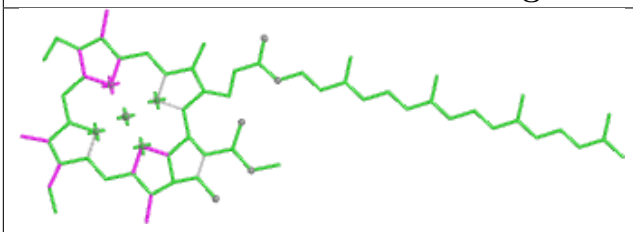


Torsions

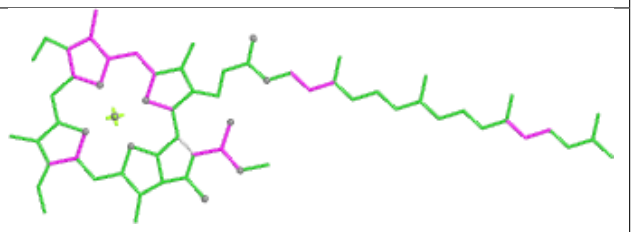


Rings

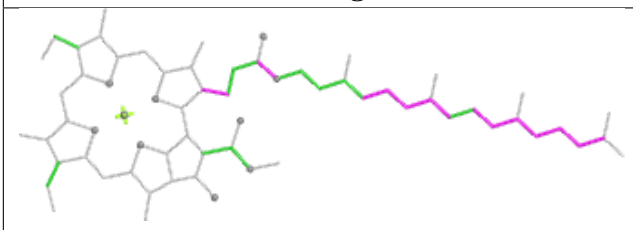
Ligand CLA f 1215



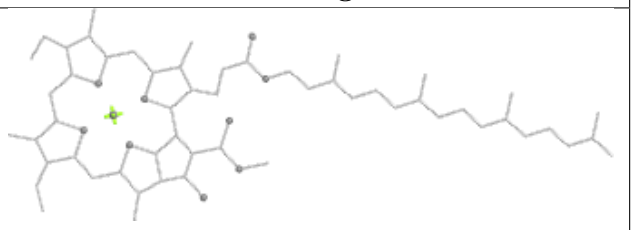
Bond lengths



Bond angles

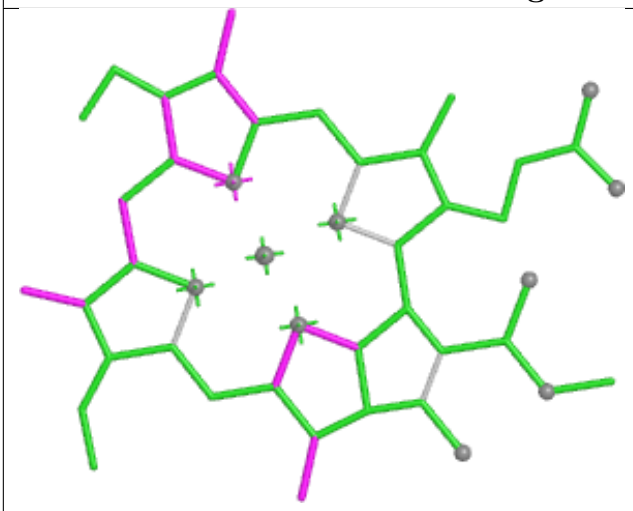


Torsions

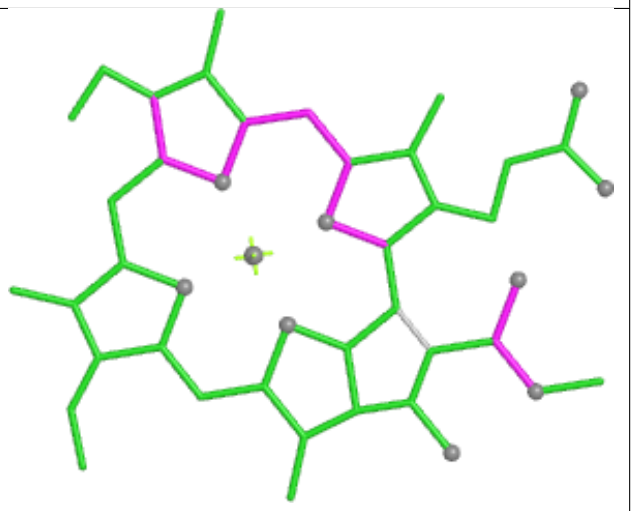


Rings

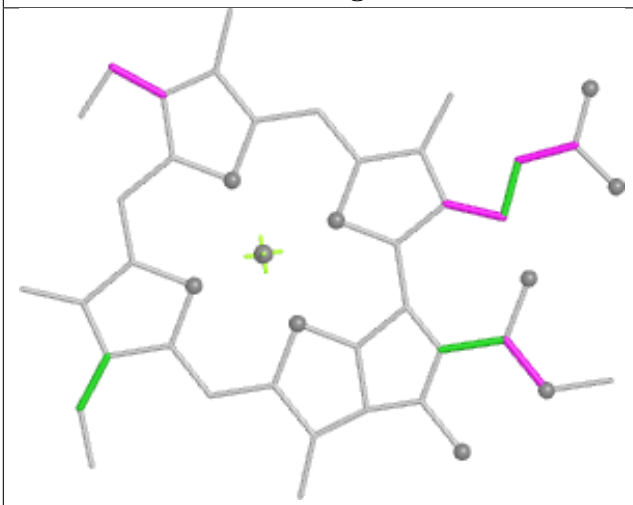
Ligand CLA u 513



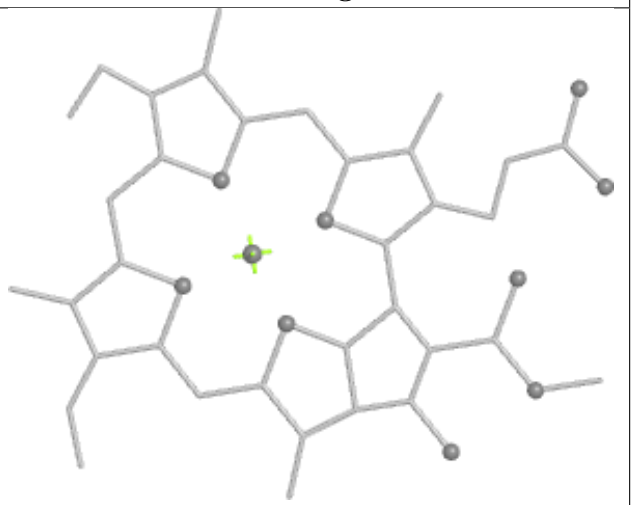
Bond lengths



Bond angles

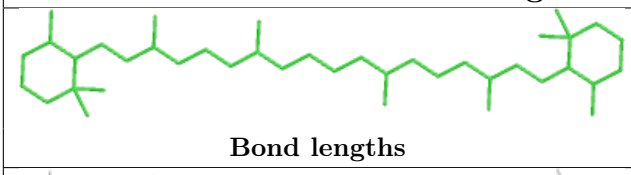


Torsions

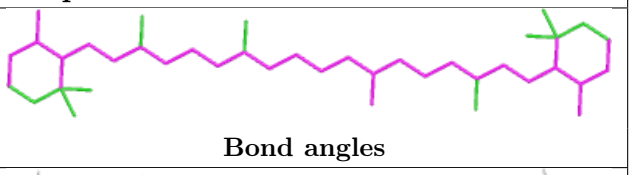


Rings

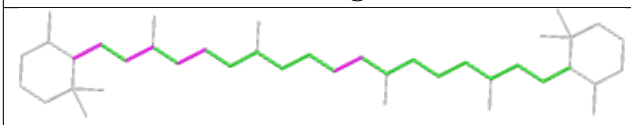
Ligand BCR q 522



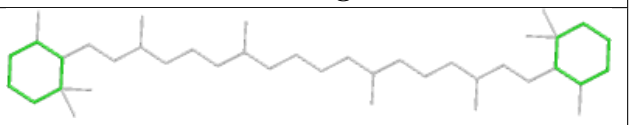
Bond lengths



Bond angles

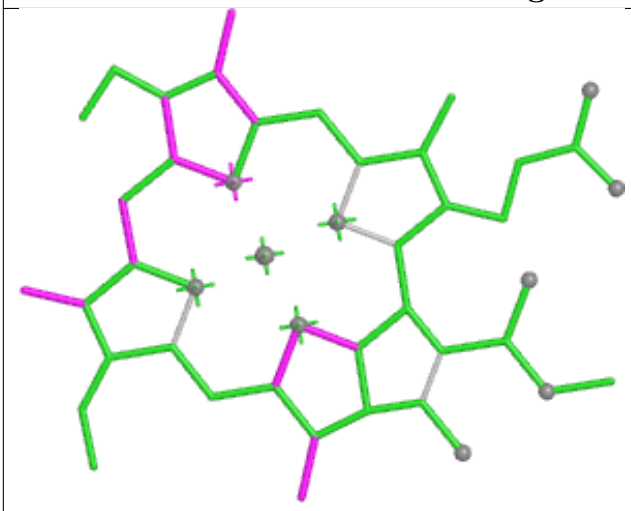


Torsions

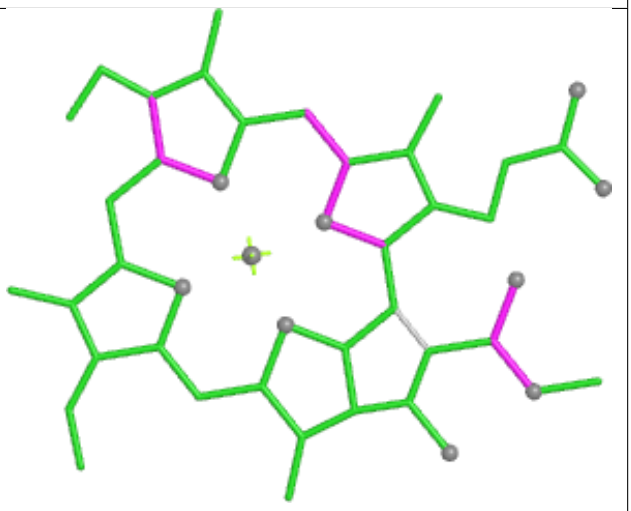


Rings

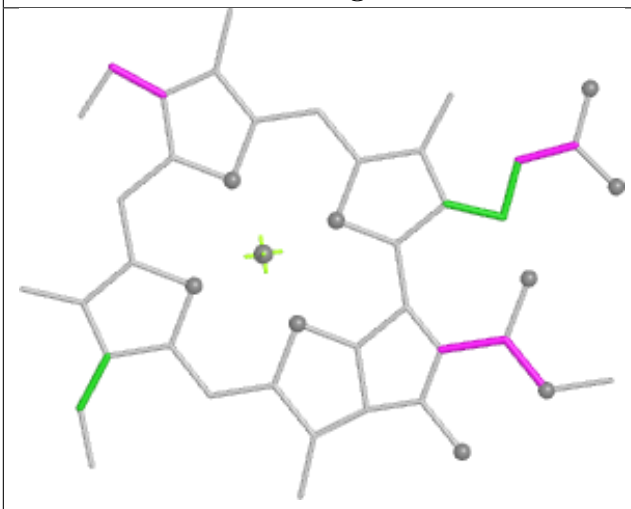
Ligand CLA v 510



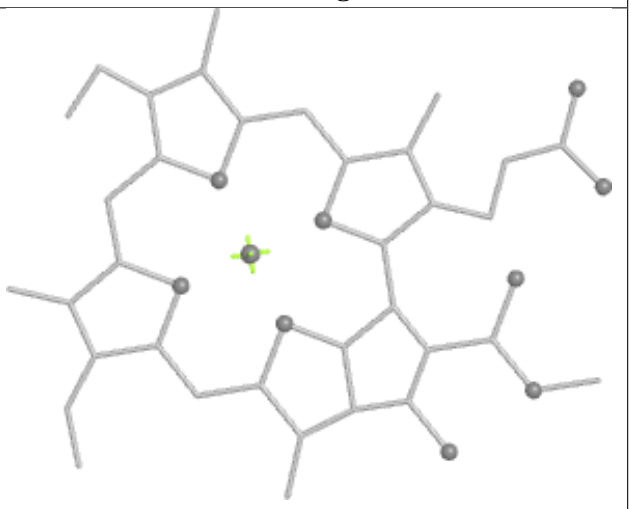
Bond lengths



Bond angles

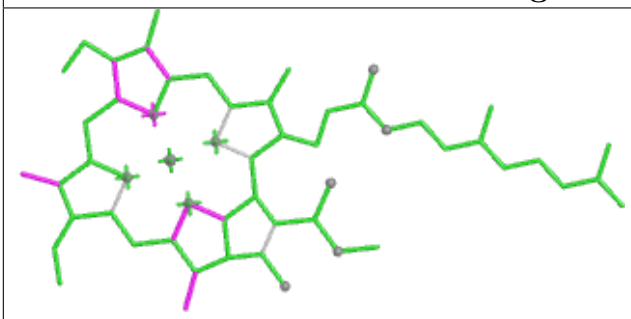


Torsions

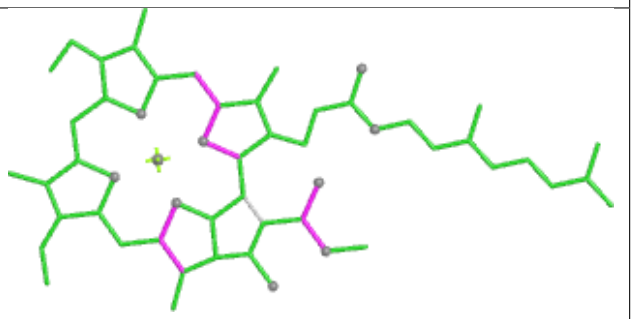


Rings

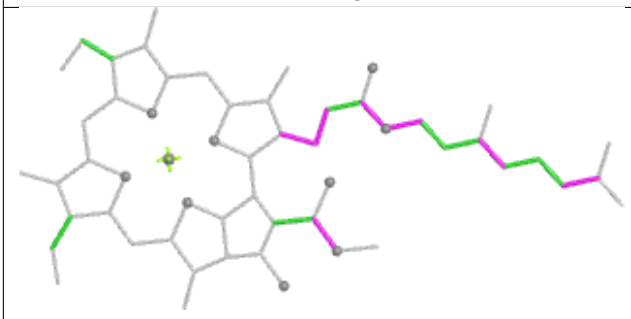
Ligand CLA s 505



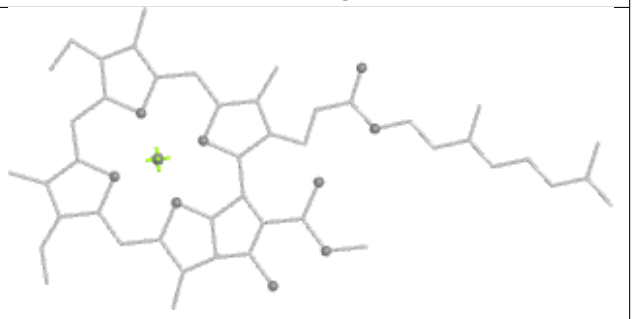
Bond lengths



Bond angles

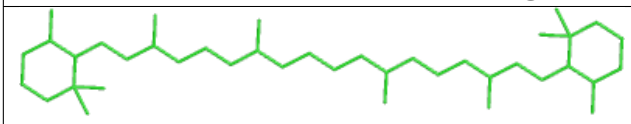


Torsions

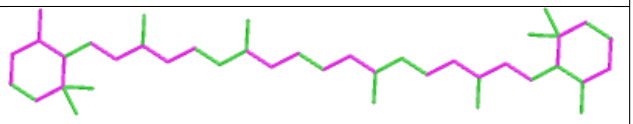


Rings

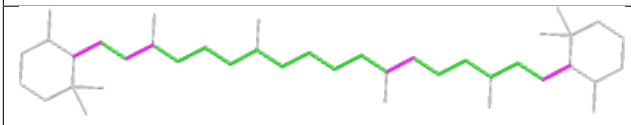
Ligand BCR Y 521



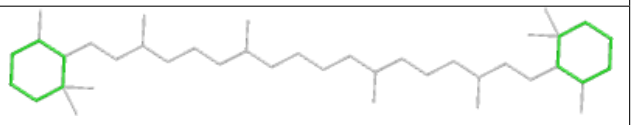
Bond lengths



Bond angles

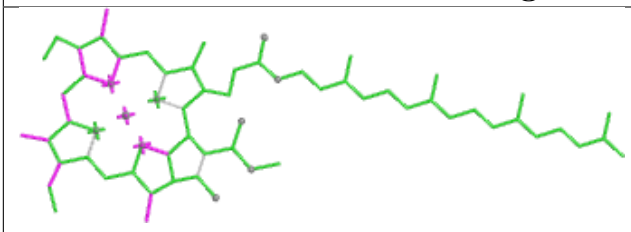


Torsions

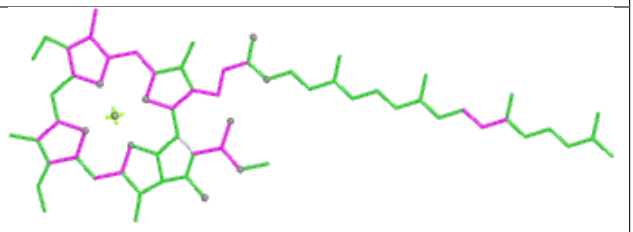


Rings

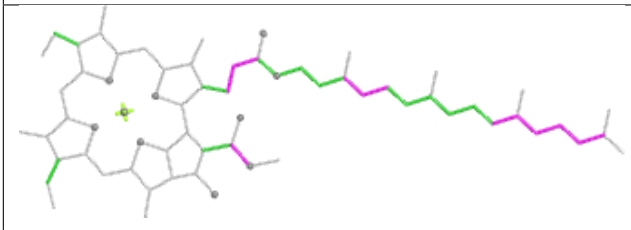
Ligand CLA e 1013



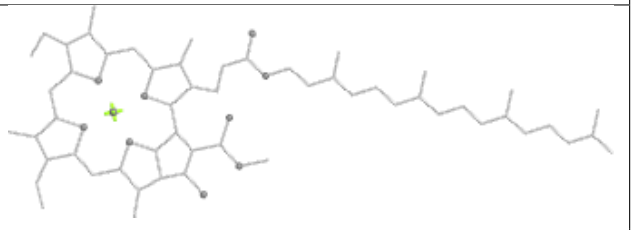
Bond lengths



Bond angles

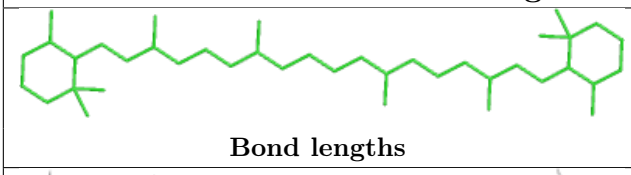


Torsions

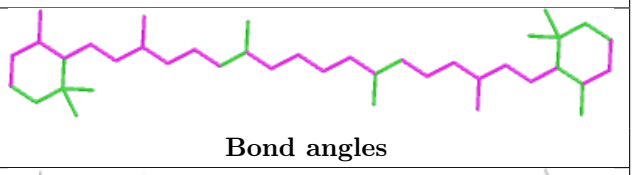


Rings

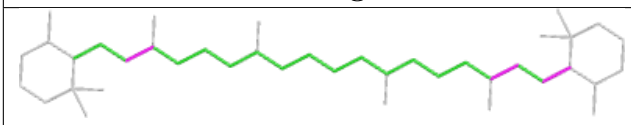
Ligand BCR Z 523



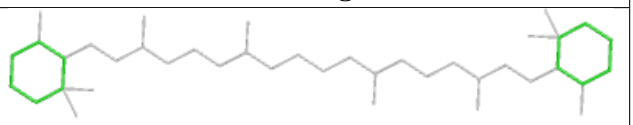
Bond lengths



Bond angles

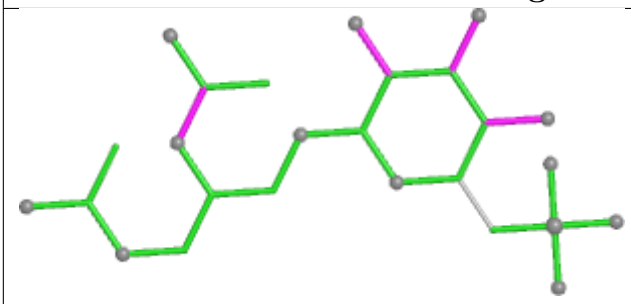


Torsions

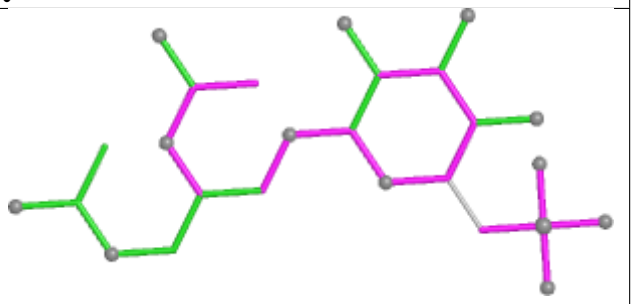


Rings

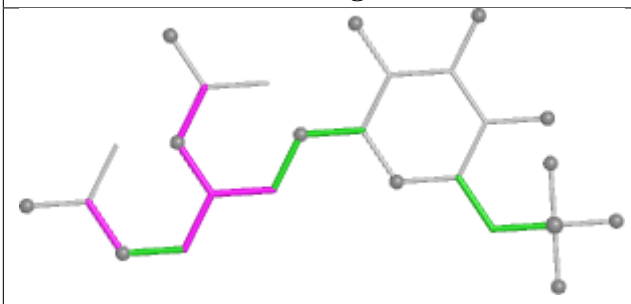
Ligand SQD 6 822



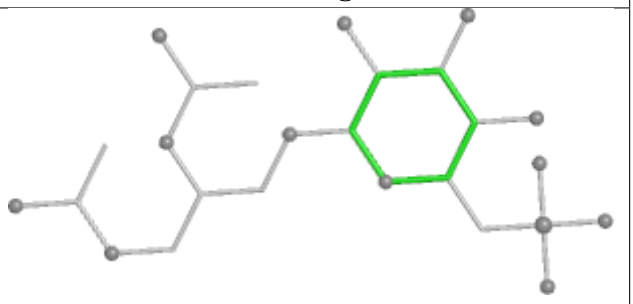
Bond lengths



Bond angles

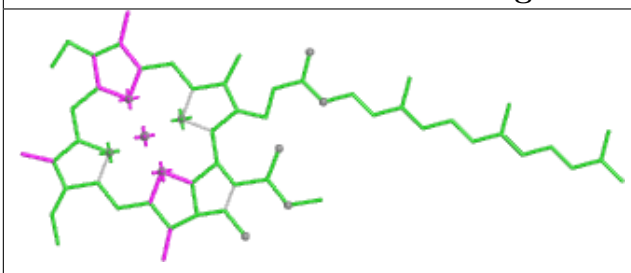


Torsions

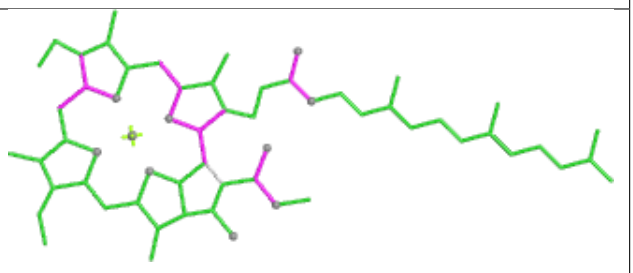


Rings

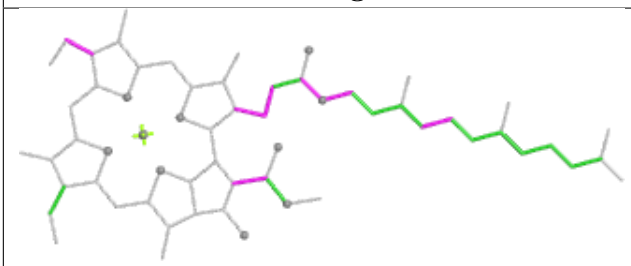
Ligand CLA A 1118



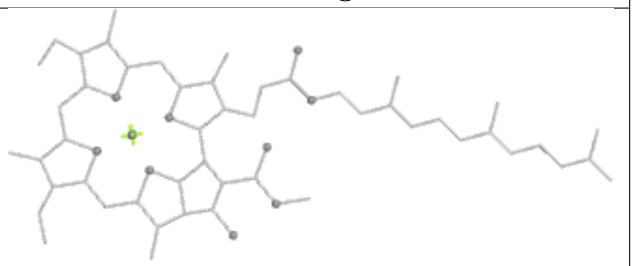
Bond lengths



Bond angles

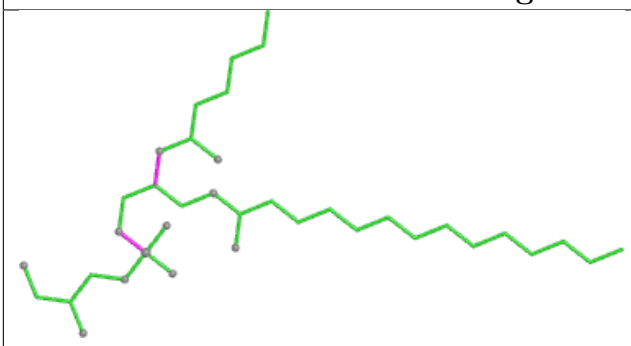


Torsions

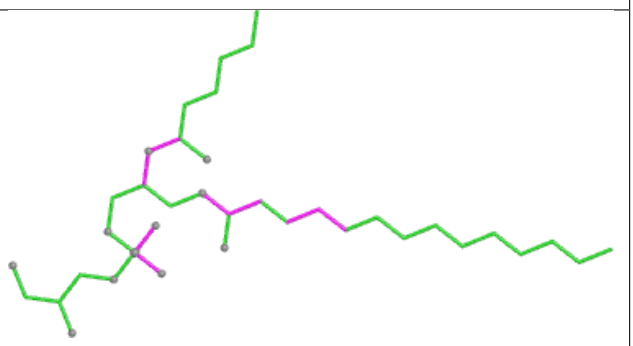


Rings

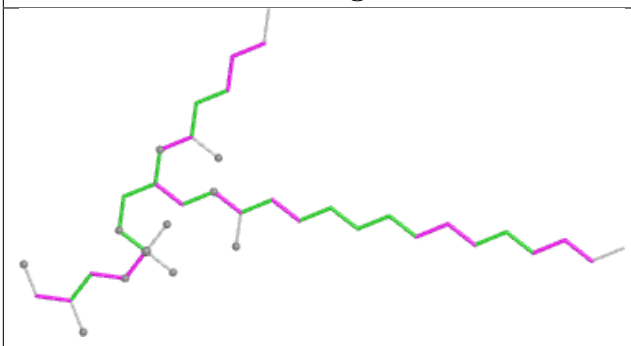
Ligand LHG L 5218



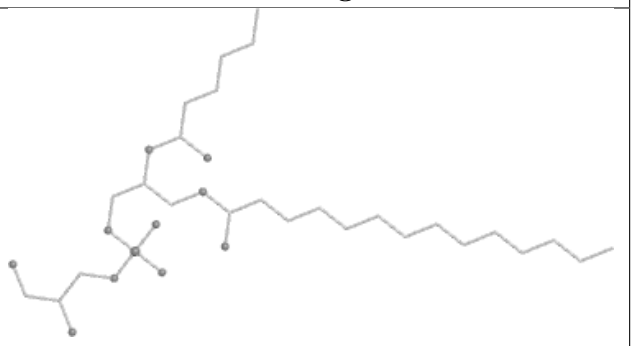
Bond lengths



Bond angles

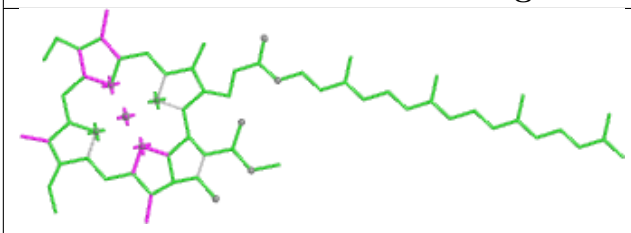


Torsions

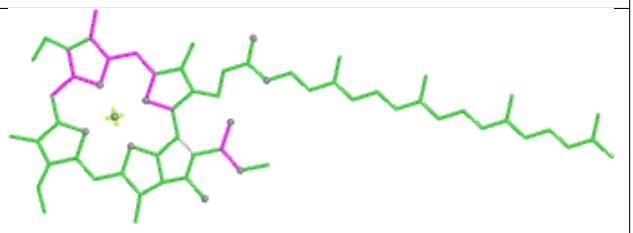


Rings

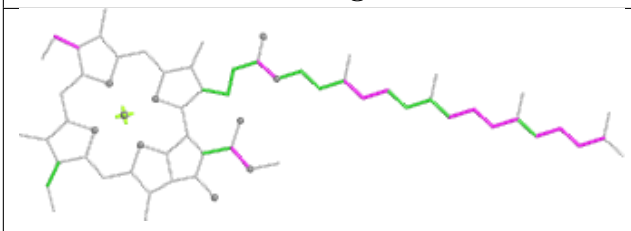
Ligand CLA A 1133



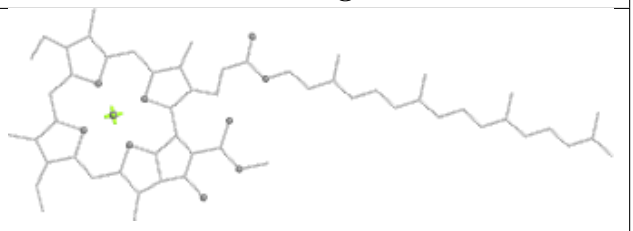
Bond lengths



Bond angles

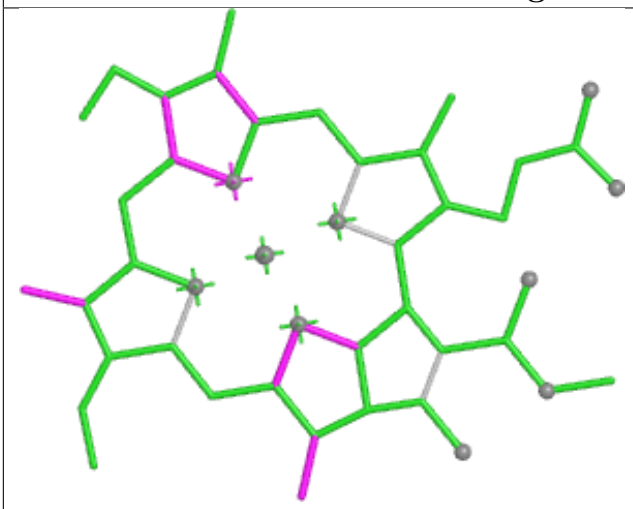


Torsions

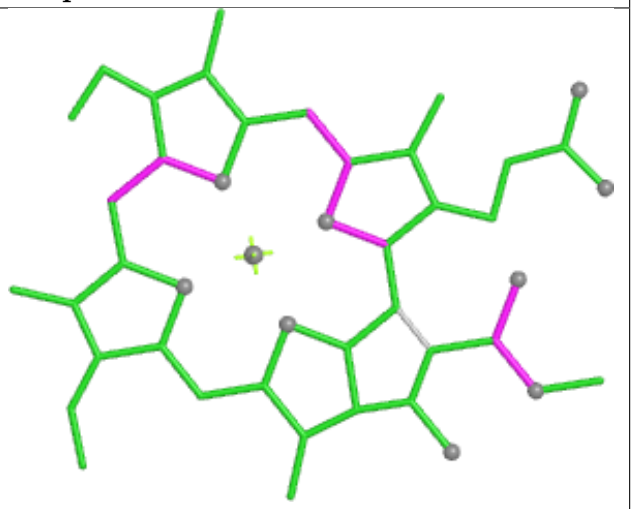


Rings

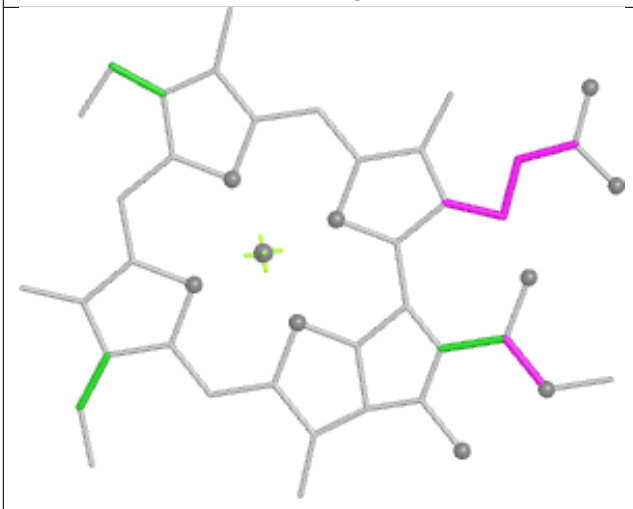
Ligand CLA q 505



Bond lengths



Bond angles

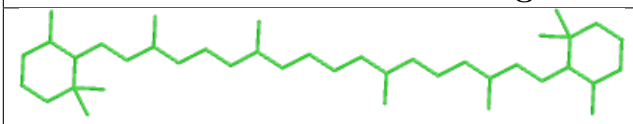


Torsions

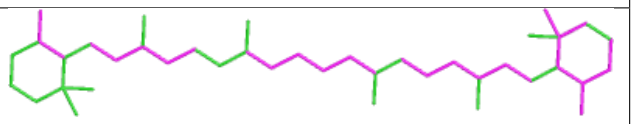


Rings

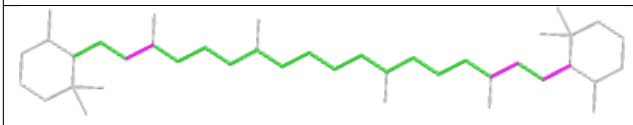
Ligand BCR L 4019



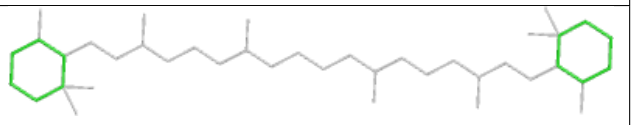
Bond lengths



Bond angles

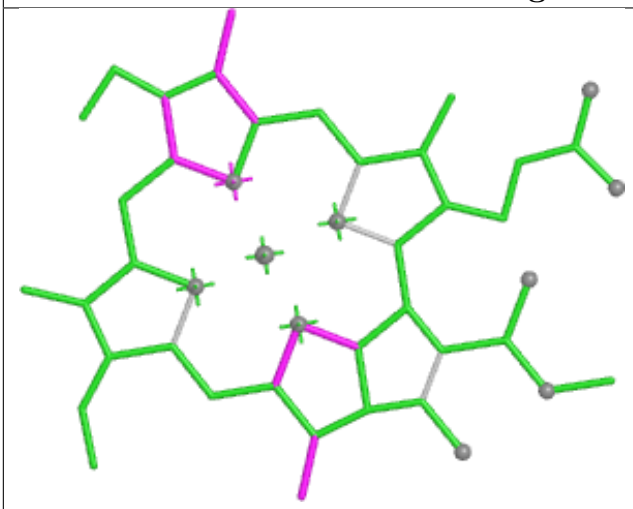


Torsions

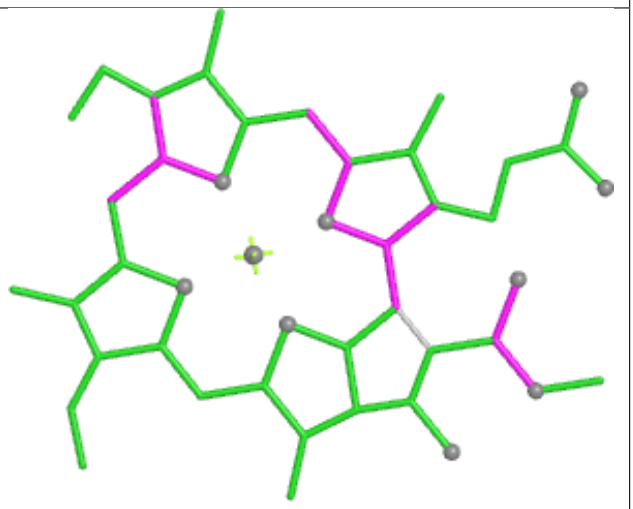


Rings

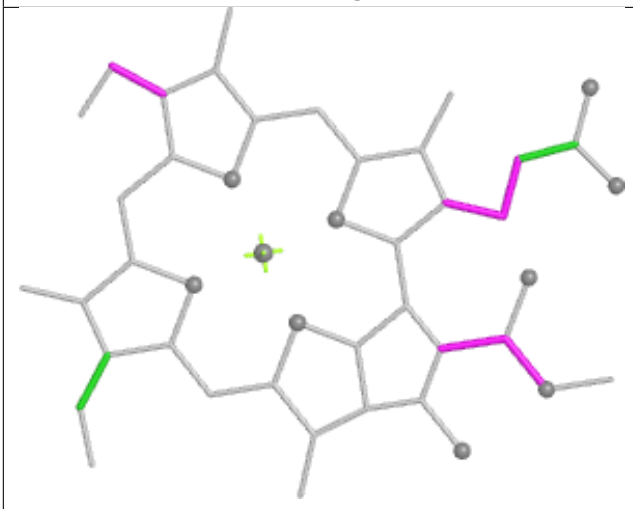
Ligand CLA 5 502



Bond lengths



Bond angles

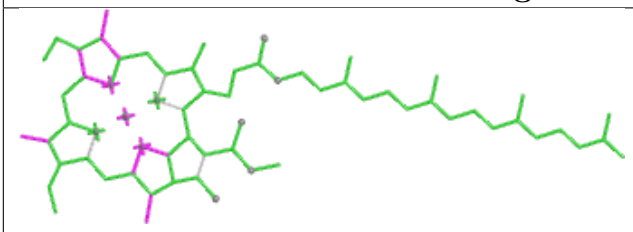


Torsions

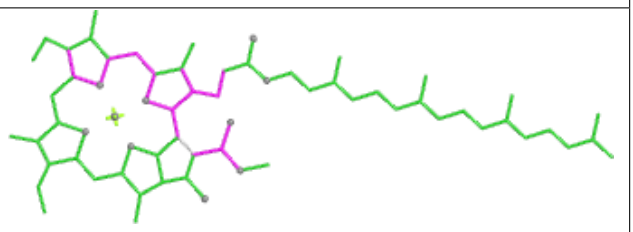


Rings

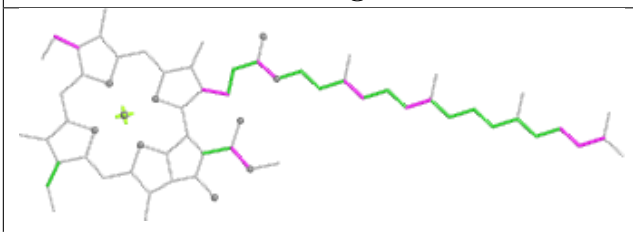
Ligand CLA G 1140



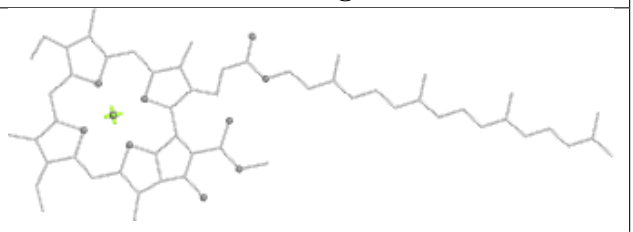
Bond lengths



Bond angles

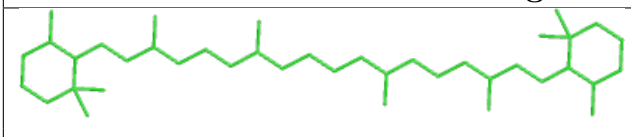


Torsions

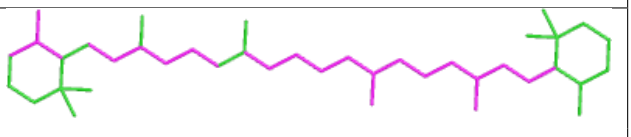


Rings

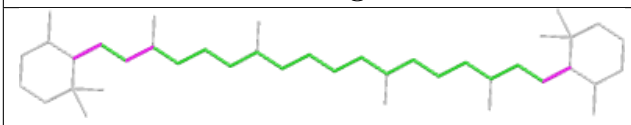
Ligand BCR v 524



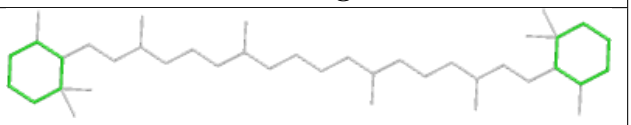
Bond lengths



Bond angles

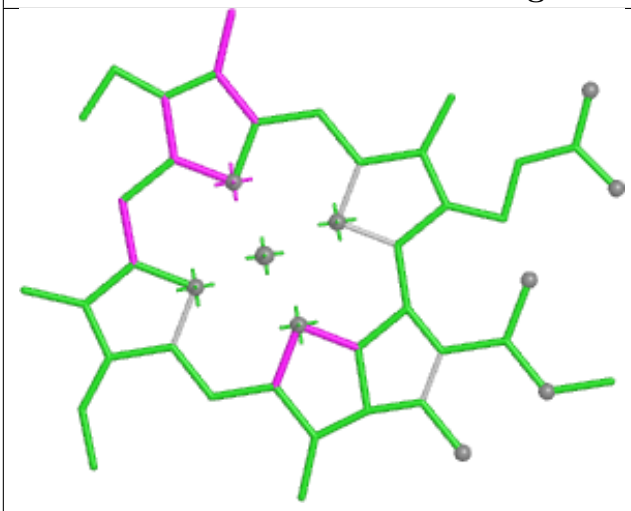


Torsions

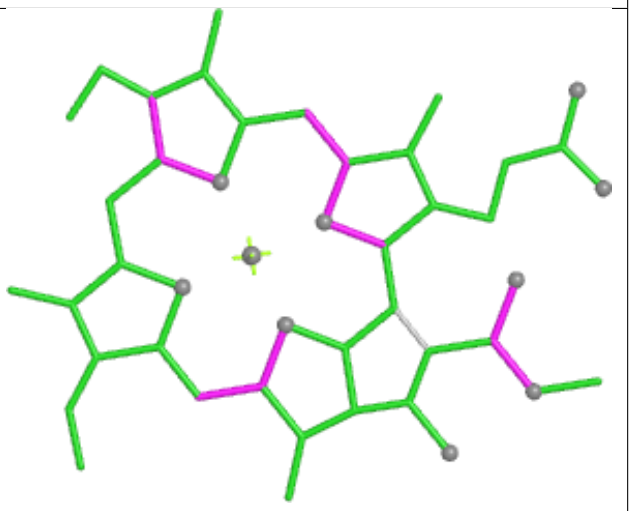


Rings

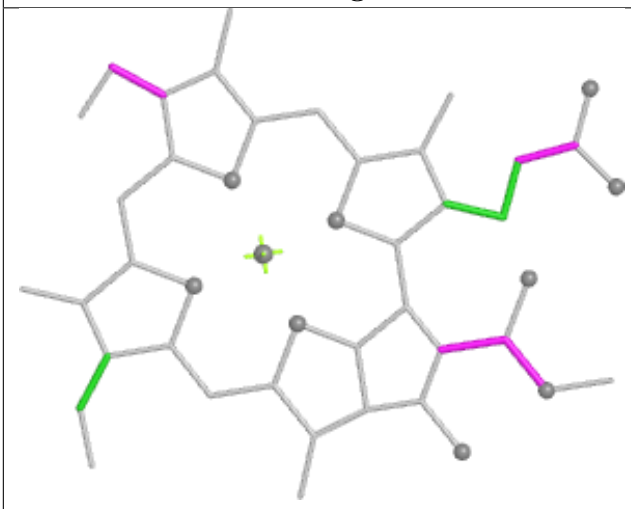
Ligand CLA d 511



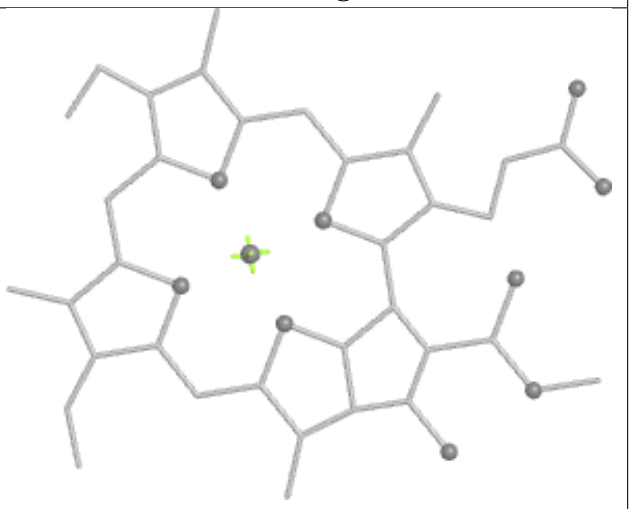
Bond lengths



Bond angles

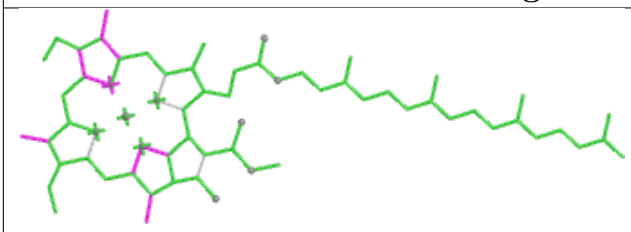


Torsions

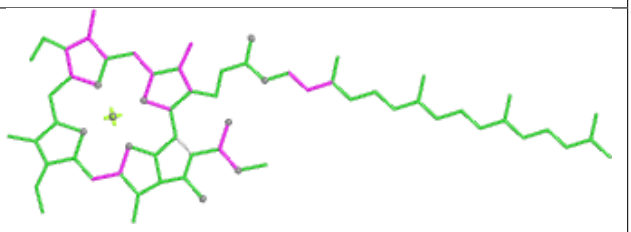


Rings

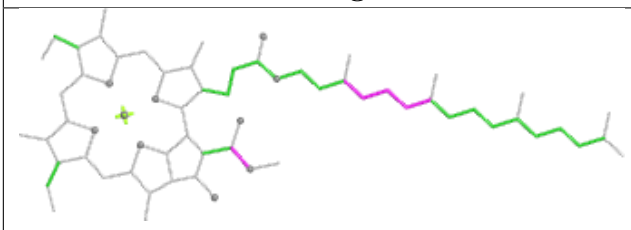
Ligand CLA f 1231



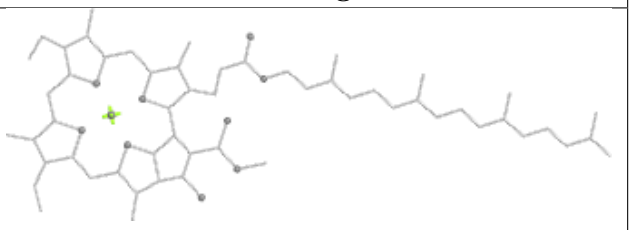
Bond lengths



Bond angles

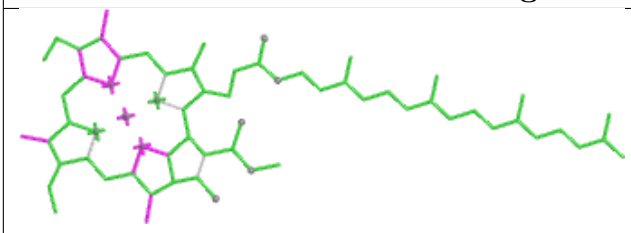


Torsions

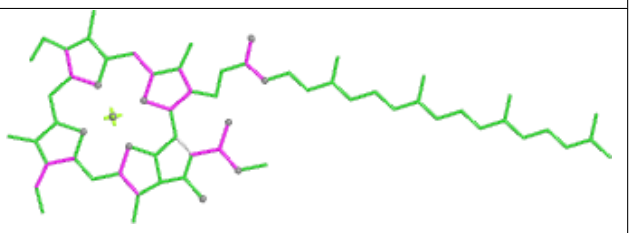


Rings

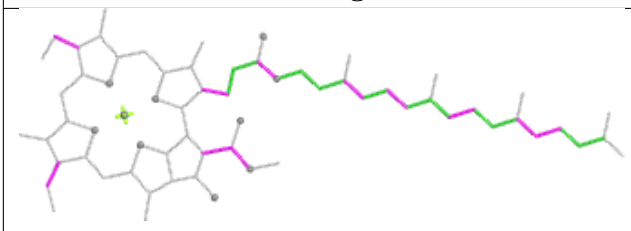
Ligand CLA e 1132



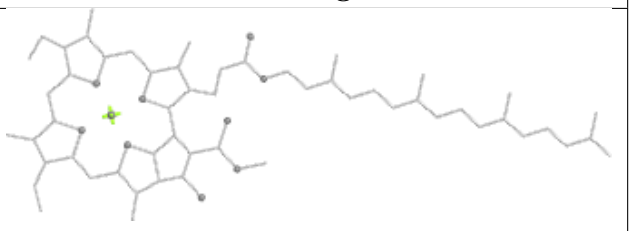
Bond lengths



Bond angles

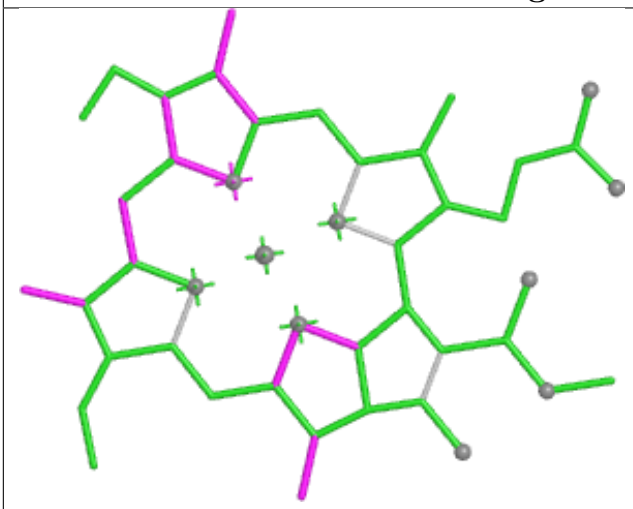


Torsions

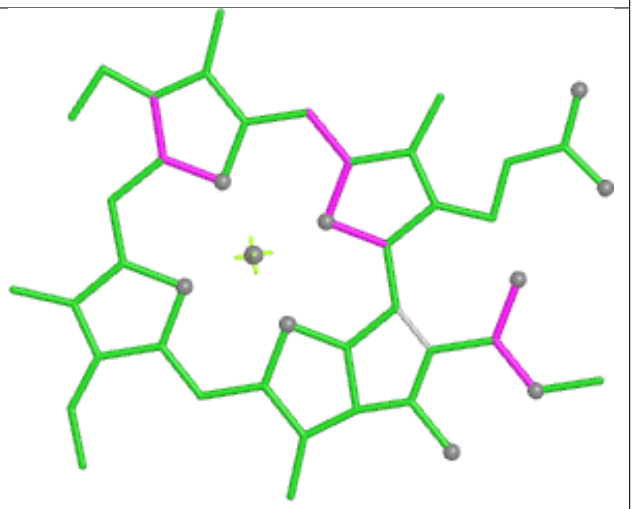


Rings

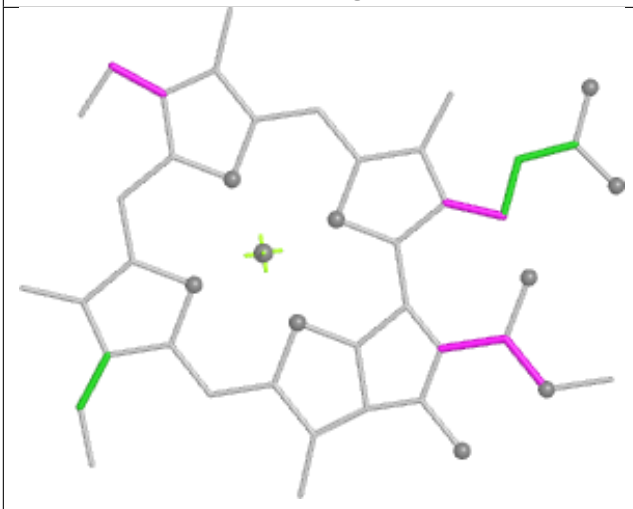
Ligand CLA a 517



Bond lengths



Bond angles

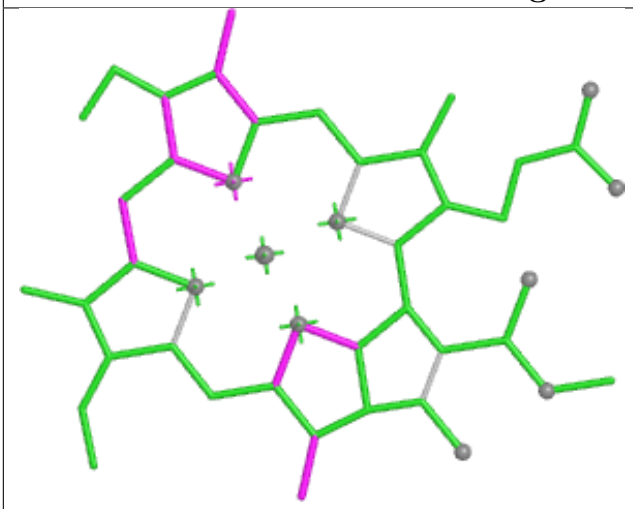


Torsions

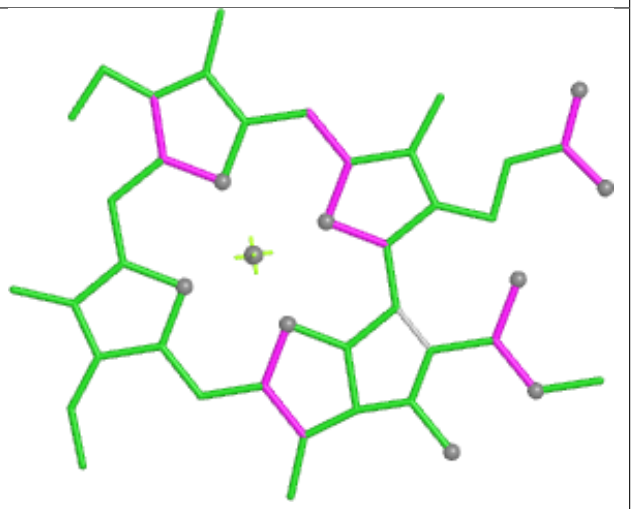


Rings

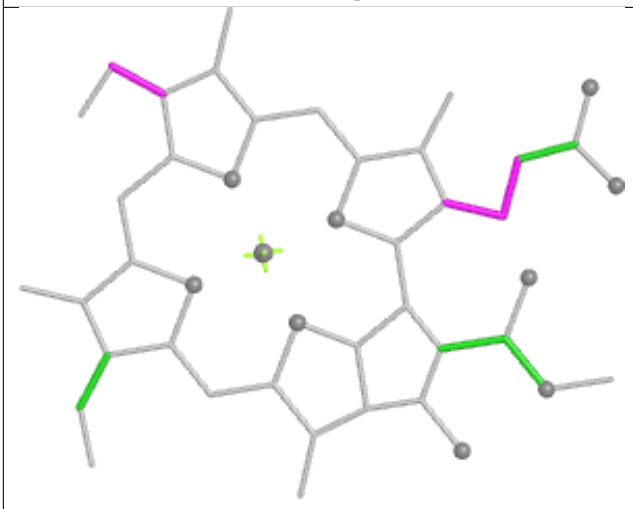
Ligand CLA c 518



Bond lengths



Bond angles

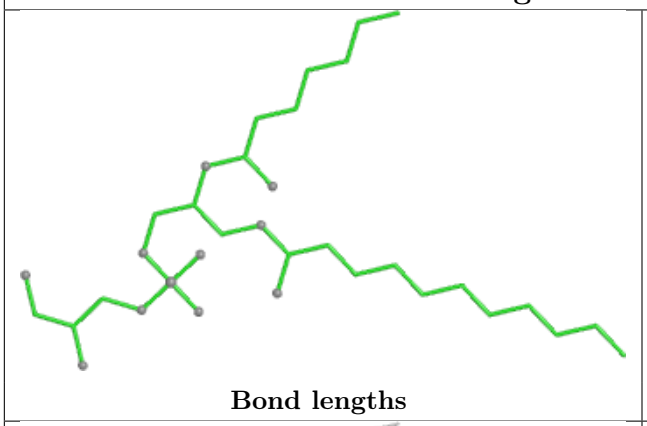


Torsions

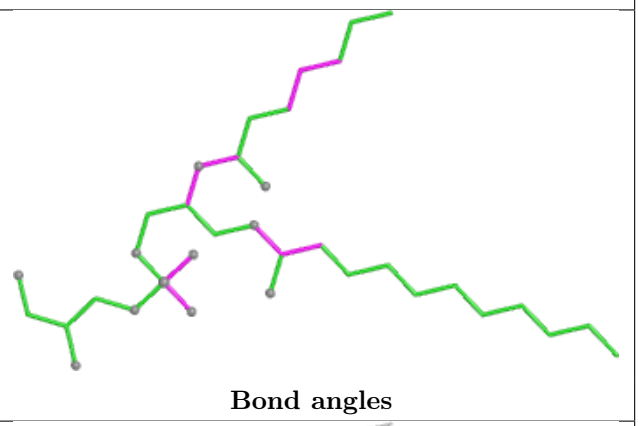


Rings

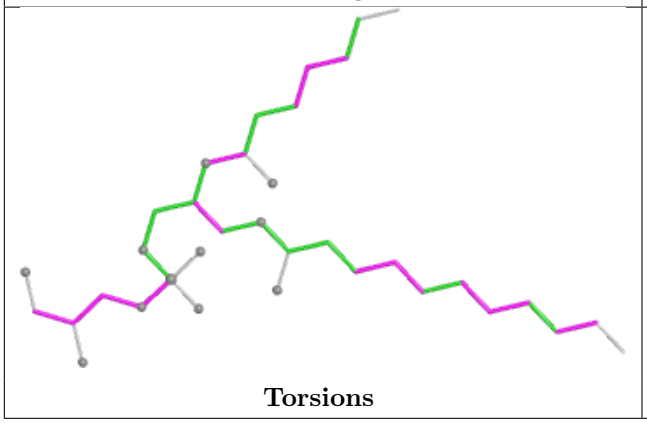
Ligand LHG G 5004



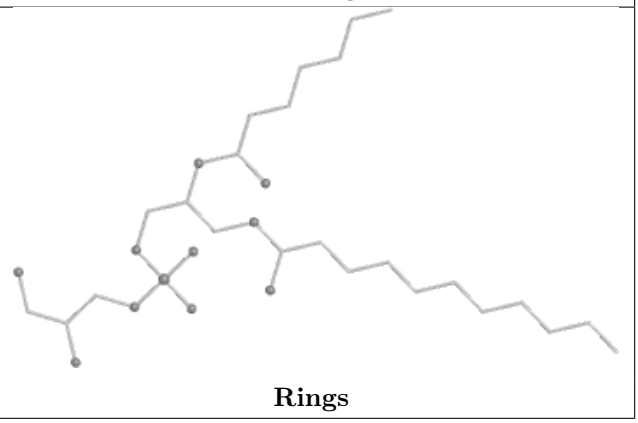
Bond lengths



Bond angles

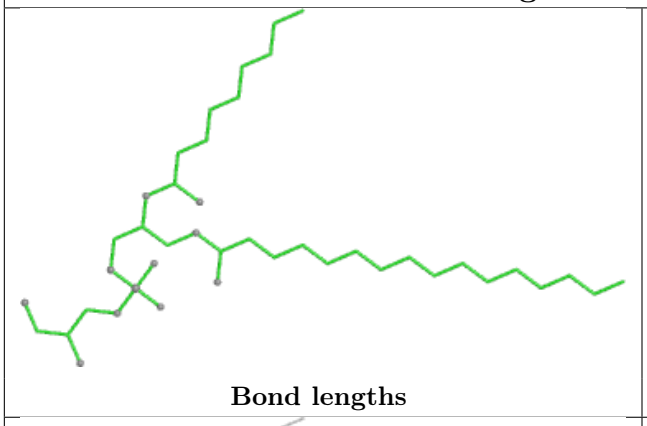


Torsions

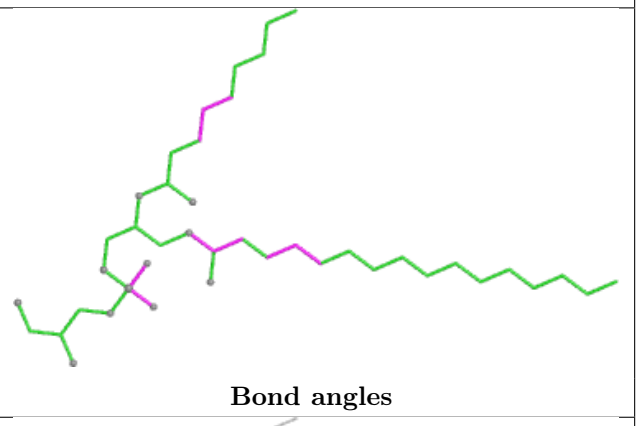


Rings

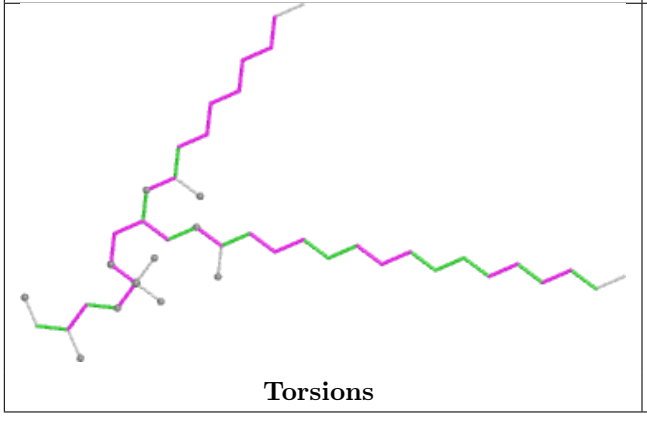
Ligand LHG e 5009



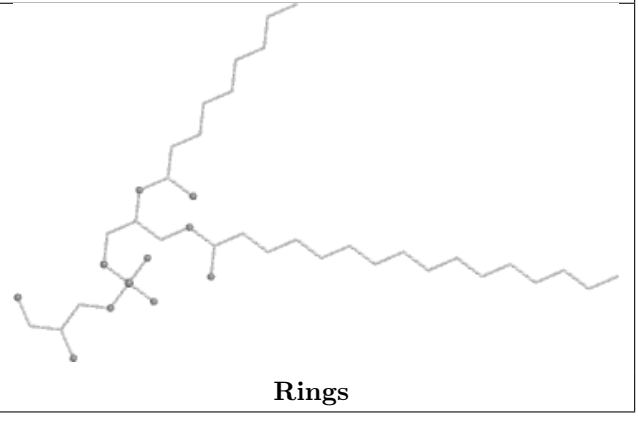
Bond lengths



Bond angles

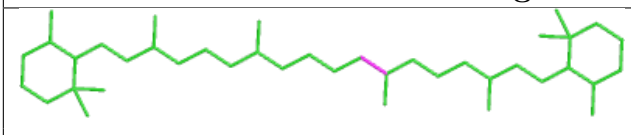


Torsions

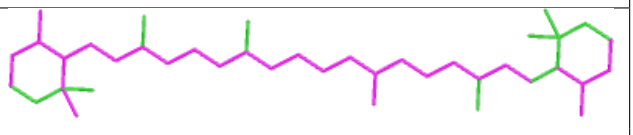


Rings

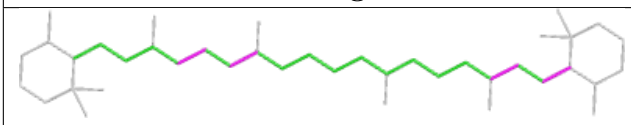
Ligand BCR B 4010



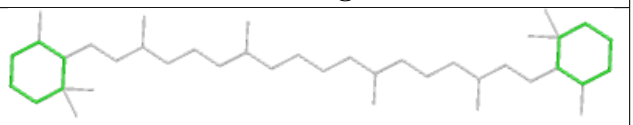
Bond lengths



Bond angles

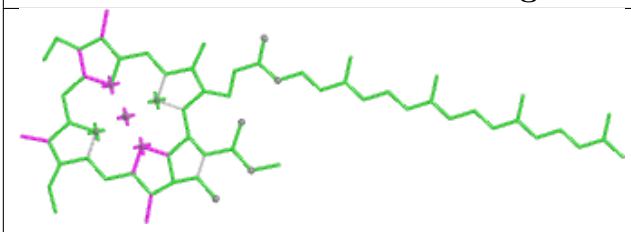


Torsions

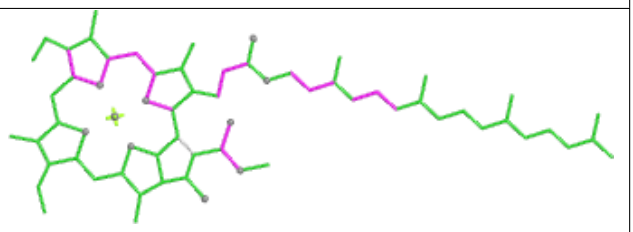


Rings

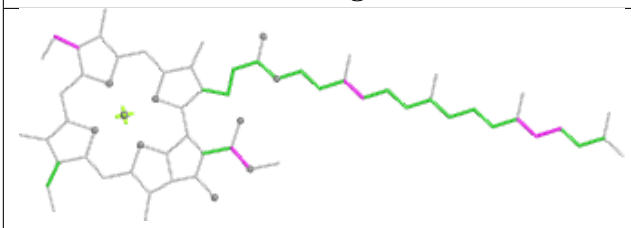
Ligand CLA e 1131



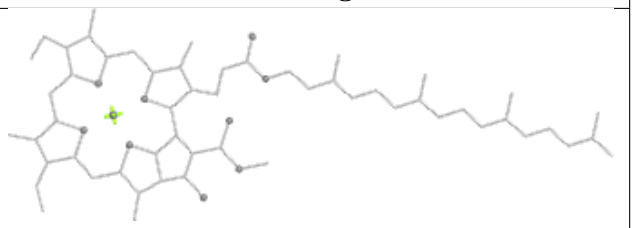
Bond lengths



Bond angles

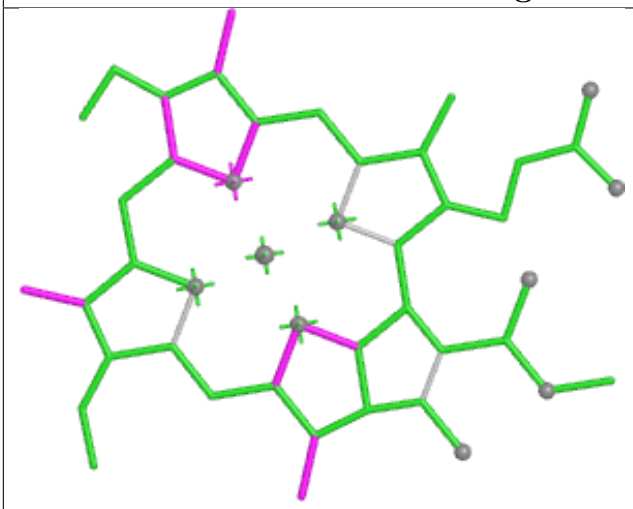


Torsions

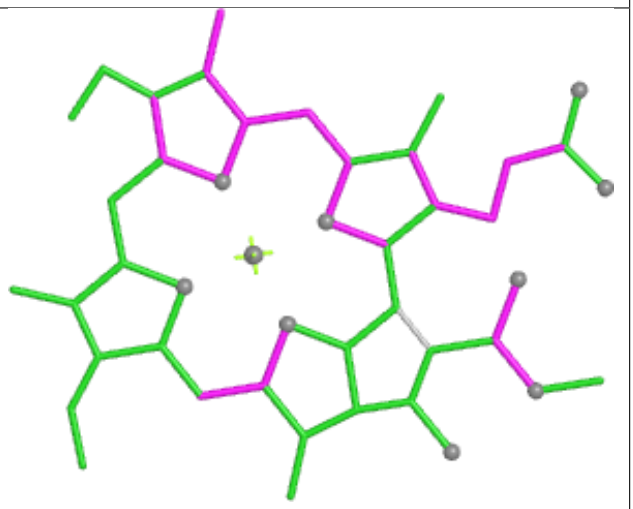


Rings

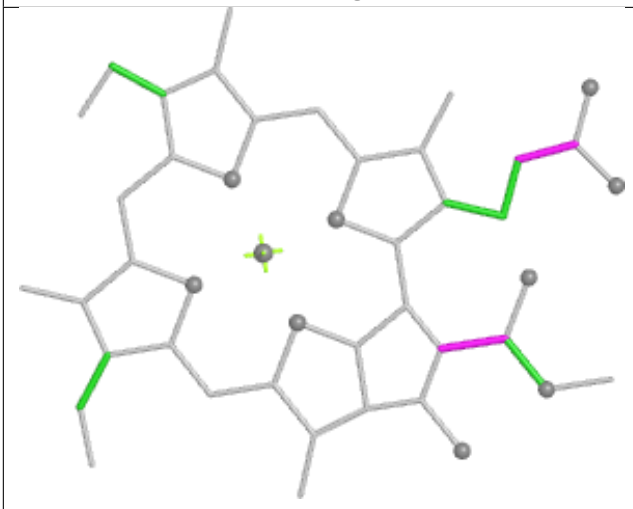
Ligand CLA A 1114



Bond lengths



Bond angles

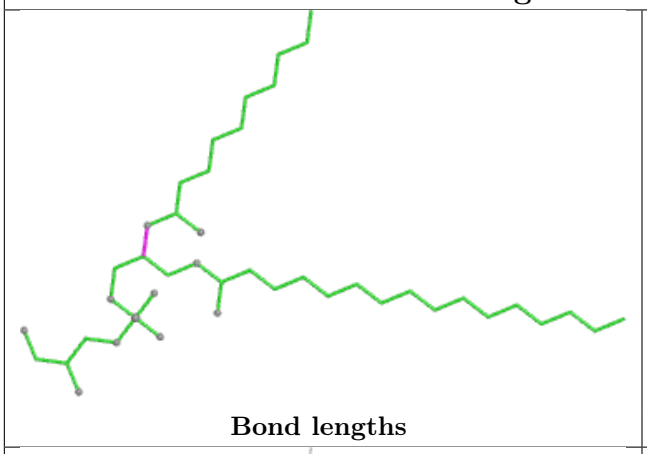


Torsions

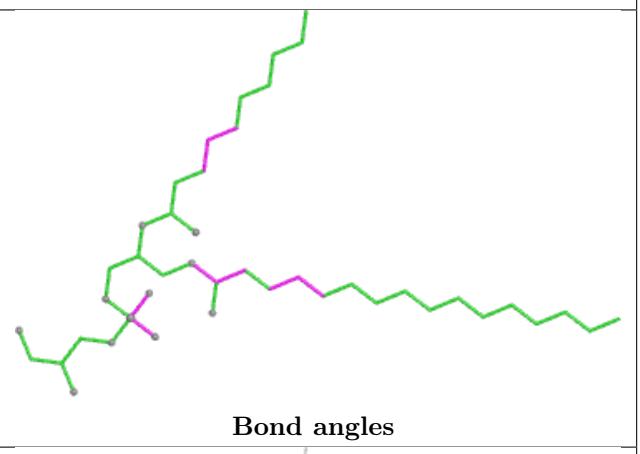


Rings

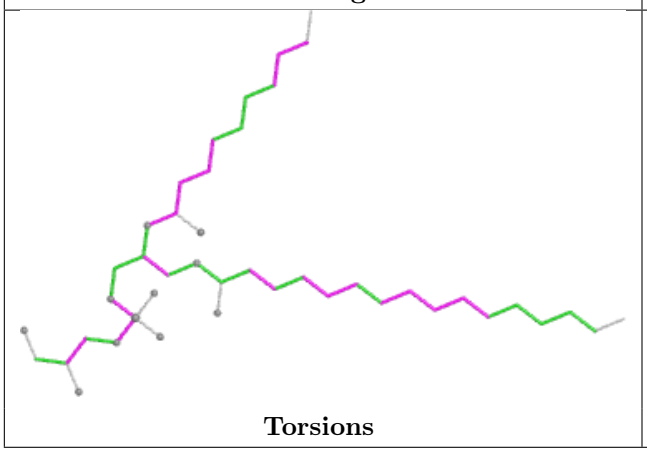
Ligand LHG A 5002



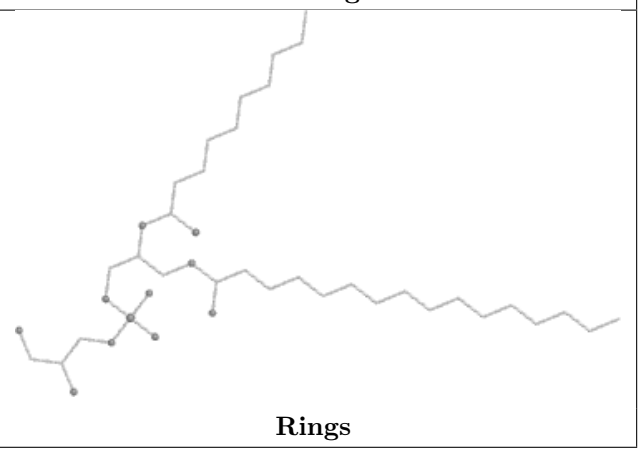
Bond lengths



Bond angles

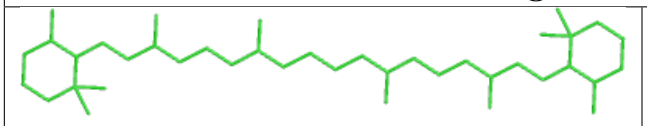


Torsions

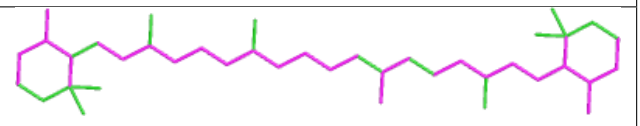


Rings

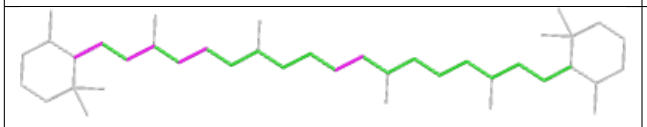
Ligand BCR 2 522



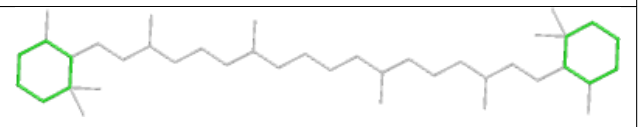
Bond lengths



Bond angles

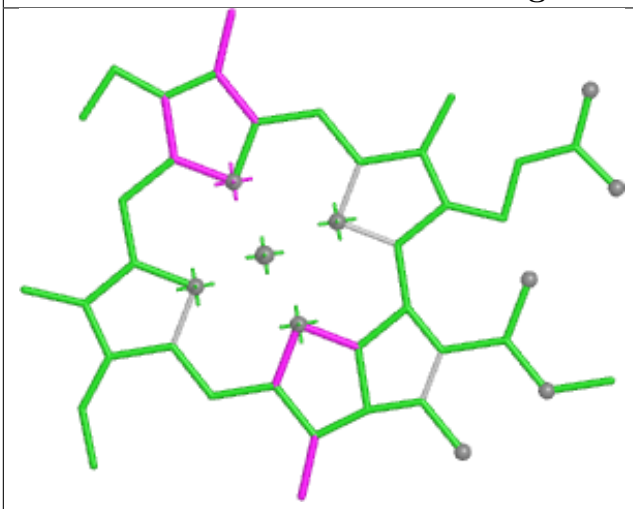


Torsions

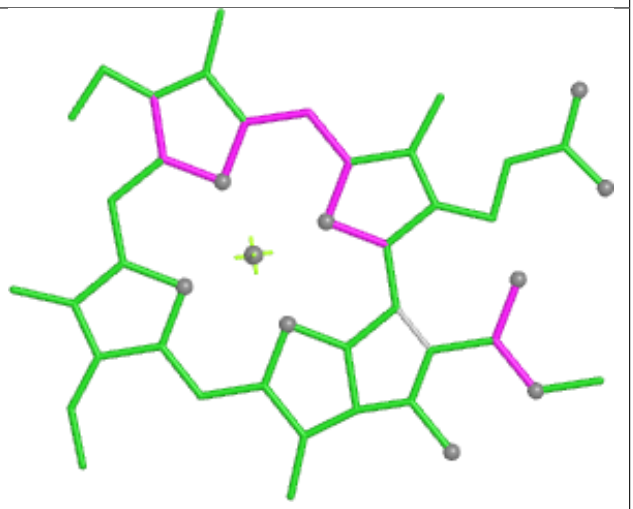


Rings

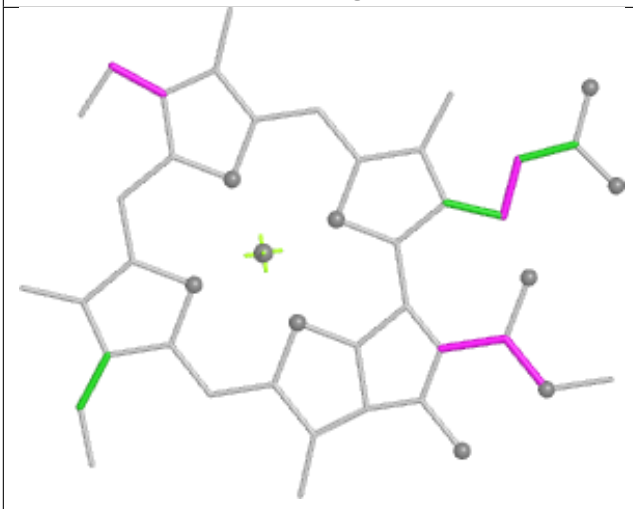
Ligand CLA 6 503



Bond lengths



Bond angles

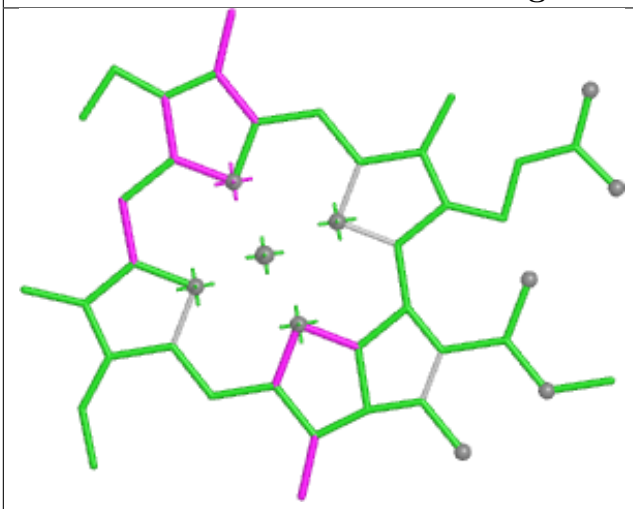


Torsions

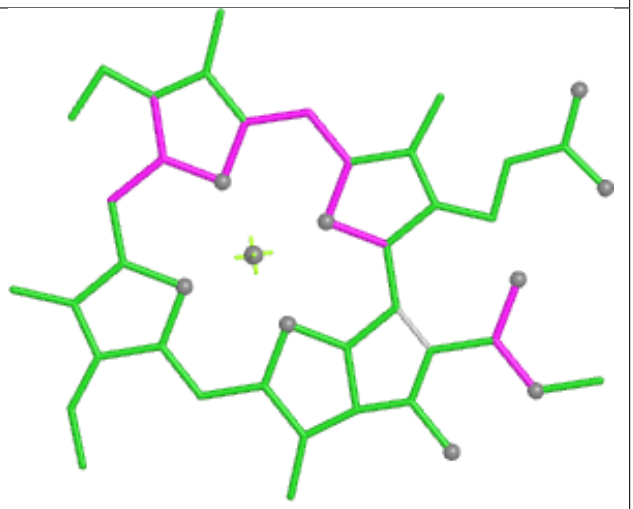


Rings

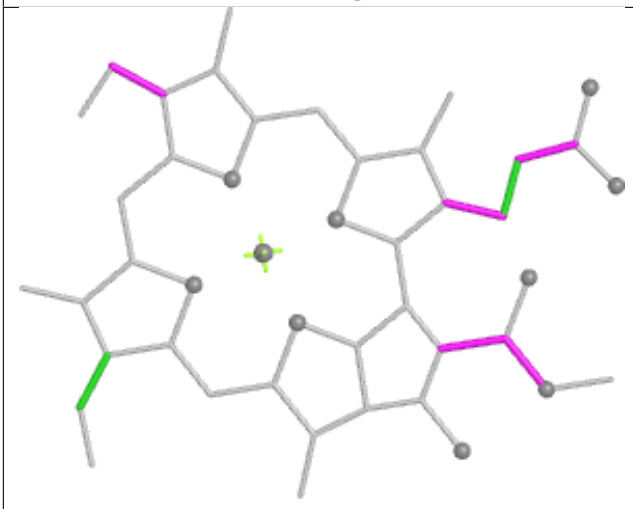
Ligand CLA 6 512



Bond lengths



Bond angles

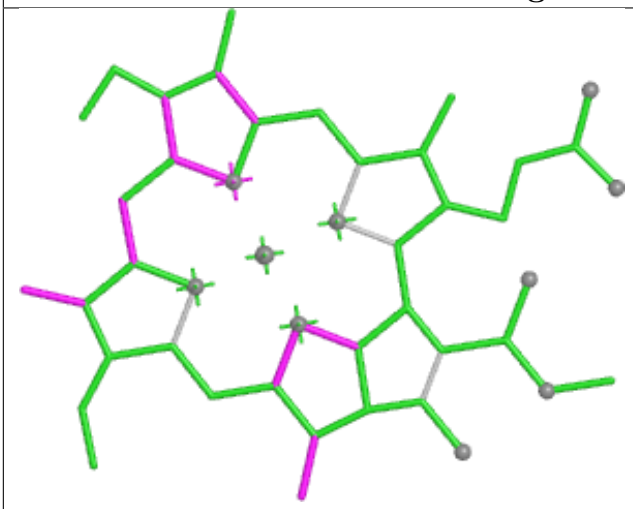


Torsions

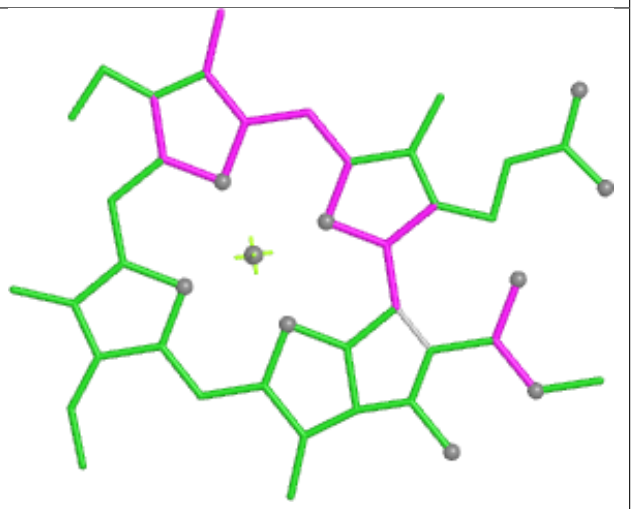


Rings

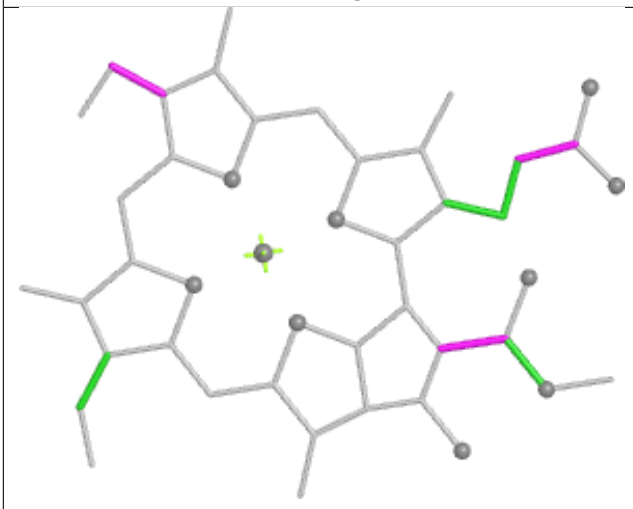
Ligand CLA v 504



Bond lengths



Bond angles

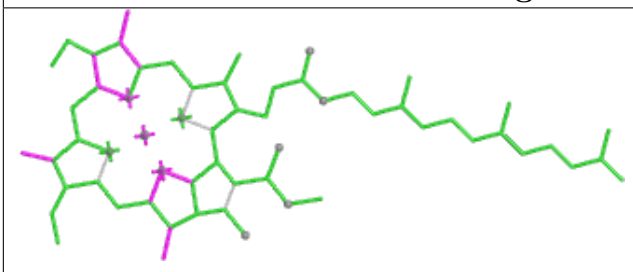


Torsions

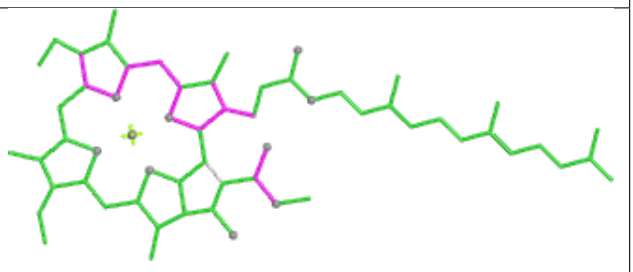


Rings

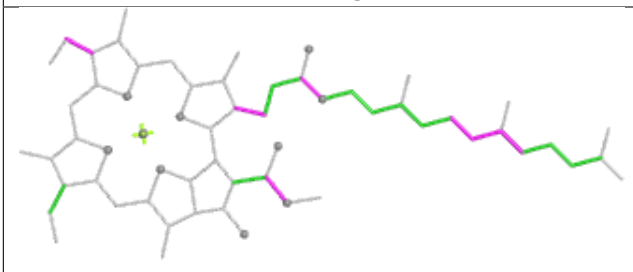
Ligand CLA B 1230



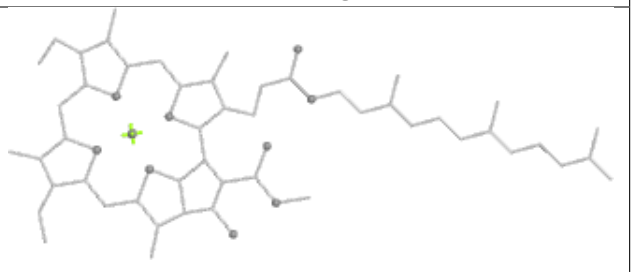
Bond lengths



Bond angles

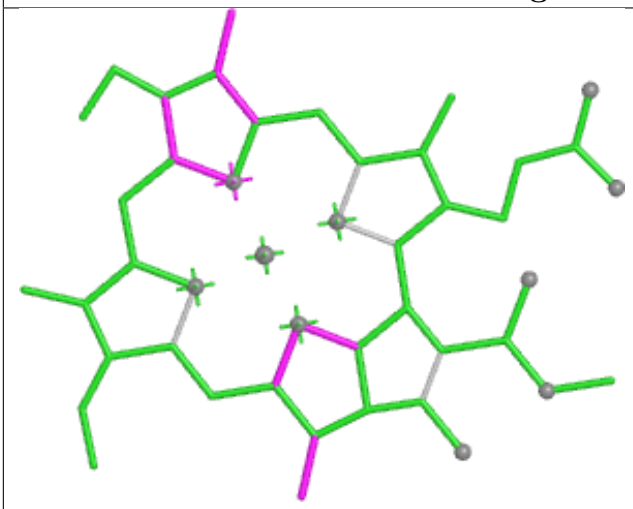


Torsions

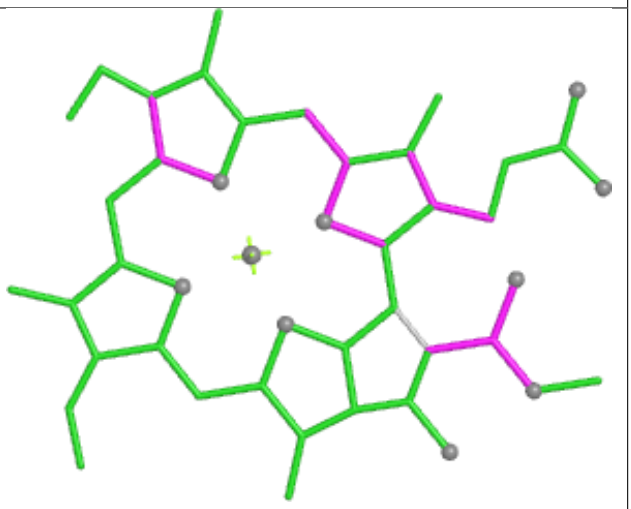


Rings

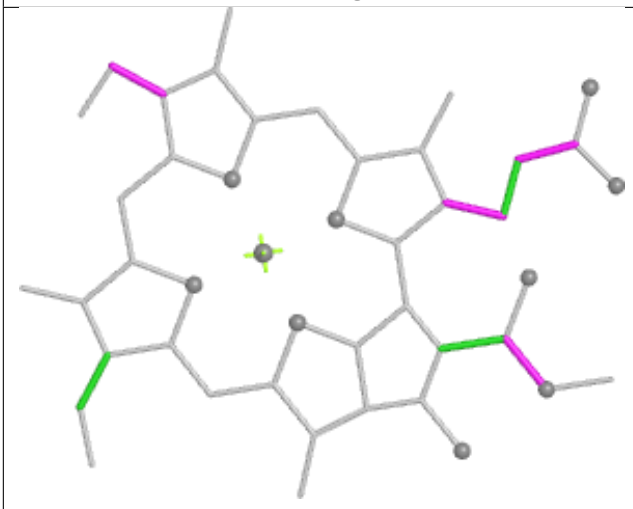
Ligand CLA r 516



Bond lengths



Bond angles

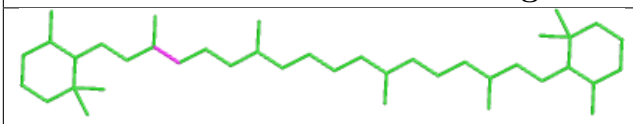


Torsions

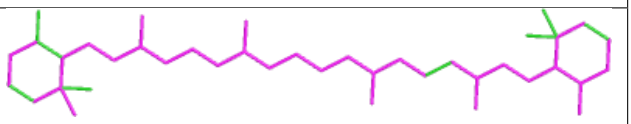


Rings

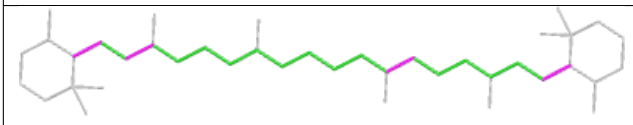
Ligand BCR f 4014



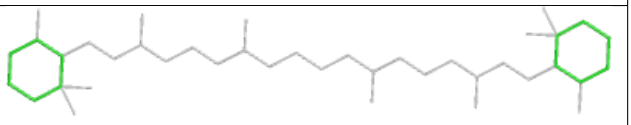
Bond lengths



Bond angles

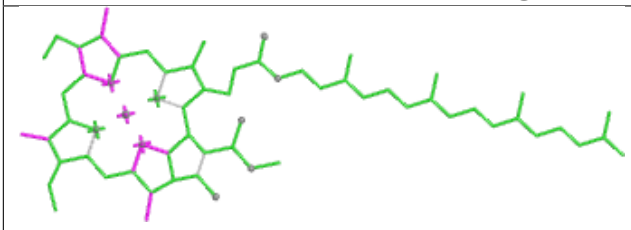


Torsions

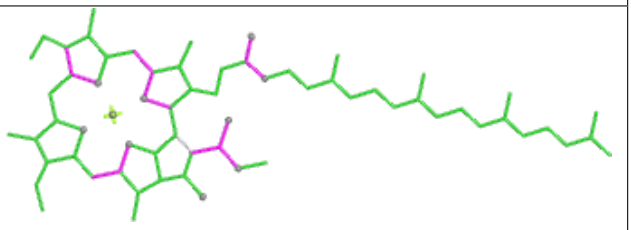


Rings

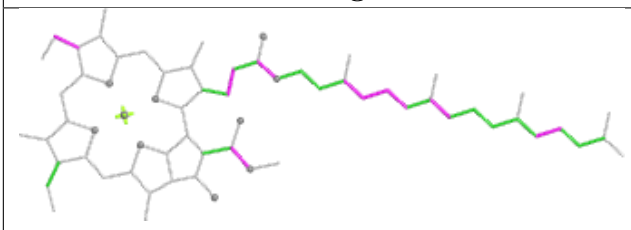
Ligand CLA B 1204



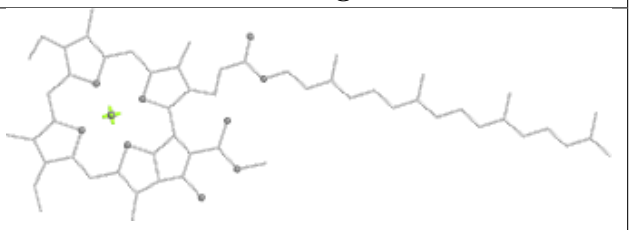
Bond lengths



Bond angles

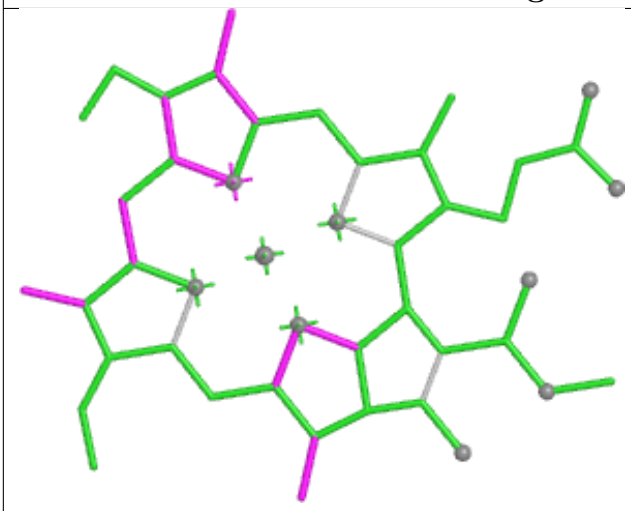


Torsions

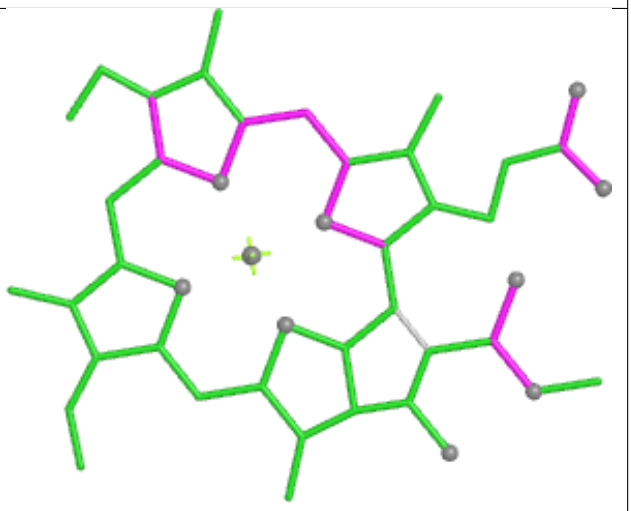


Rings

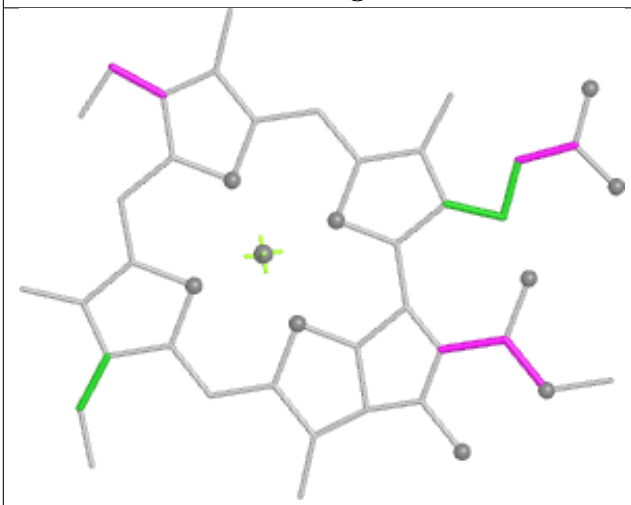
Ligand CLA b 519



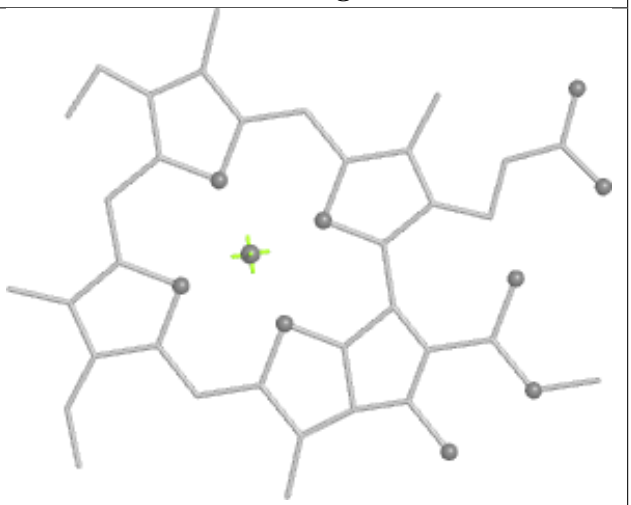
Bond lengths



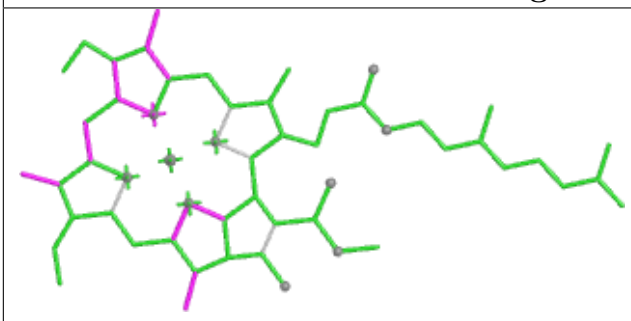
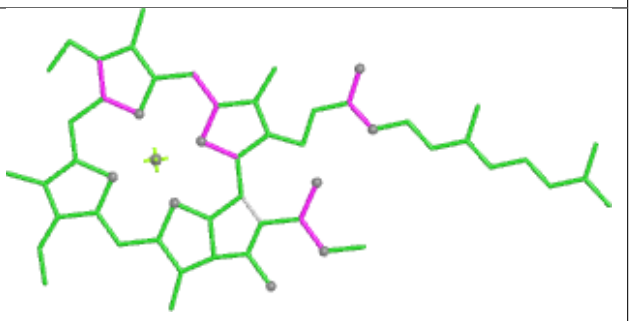
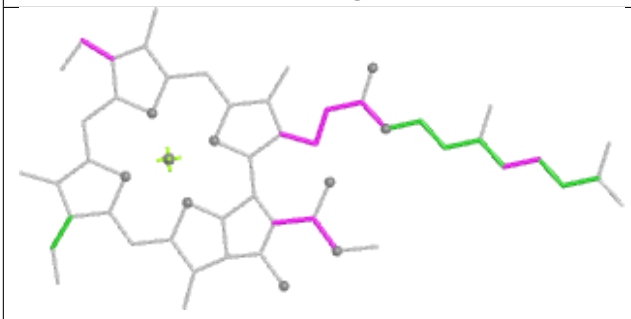
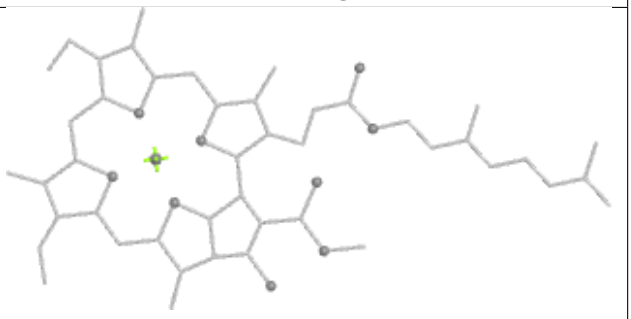
Bond angles

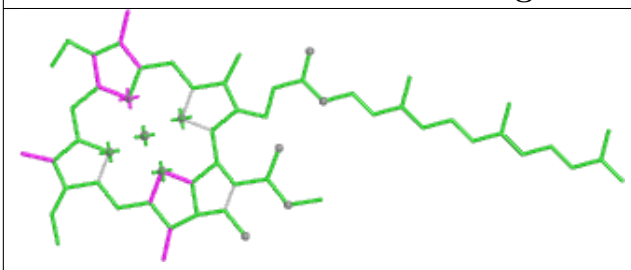
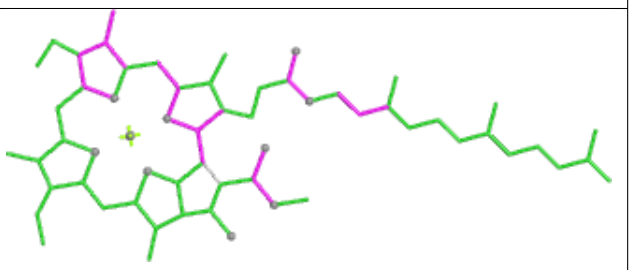
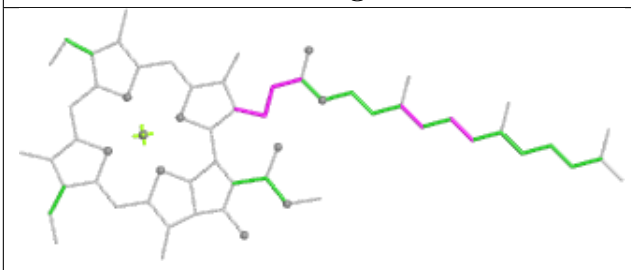
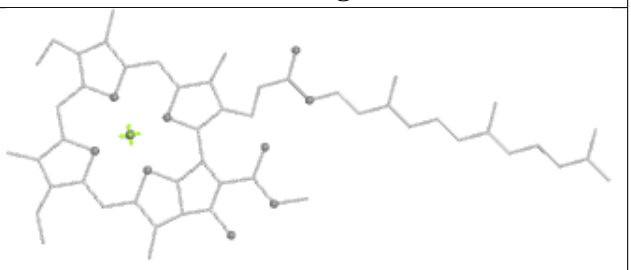


Torsions

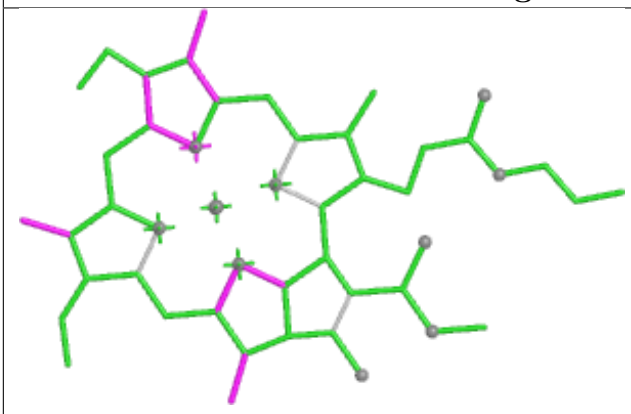


Rings

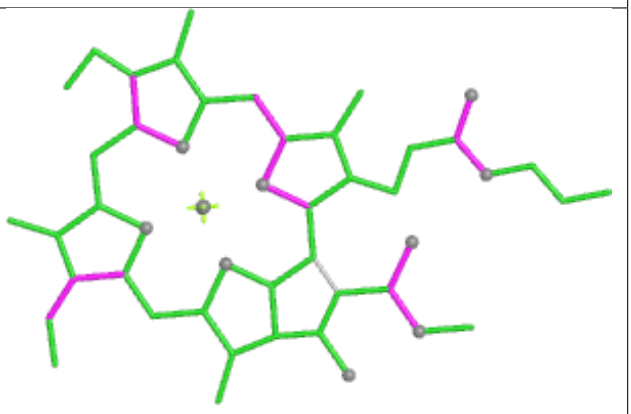
Ligand CLA s 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1224	
	
Bond lengths	Bond angles
	
Torsions	Rings

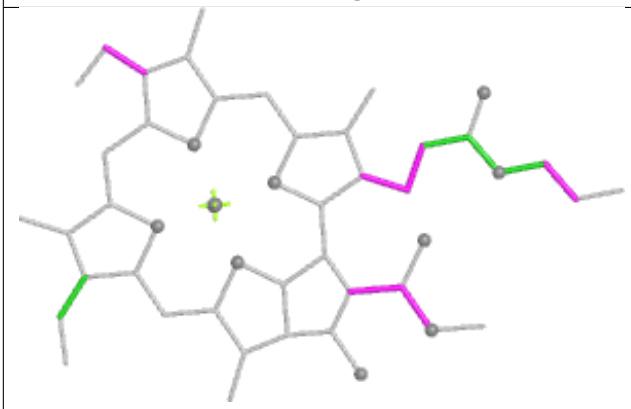
Ligand CLA K 1103



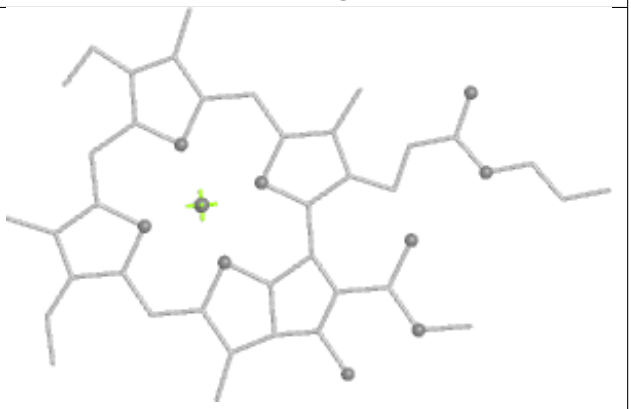
Bond lengths



Bond angles

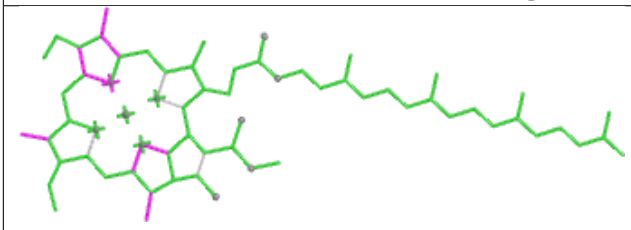


Torsions

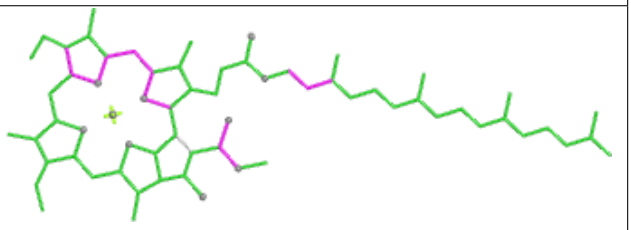


Rings

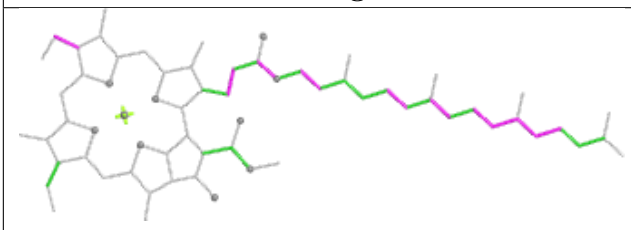
Ligand CLA f 1214



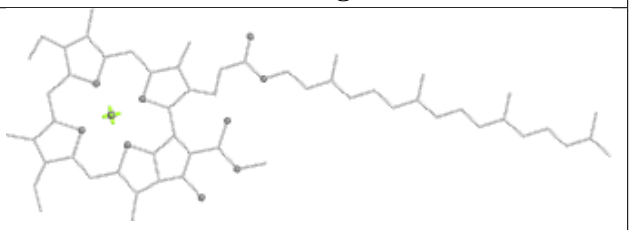
Bond lengths



Bond angles

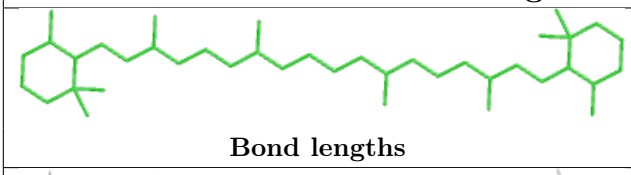


Torsions

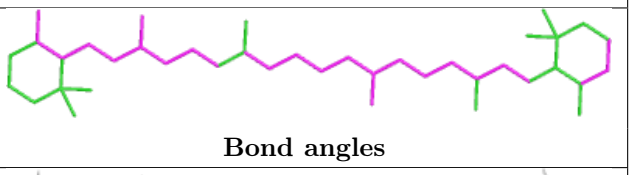


Rings

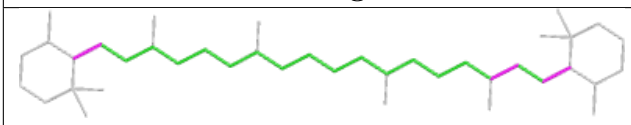
Ligand BCR b 523



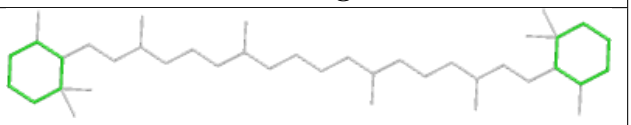
Bond lengths



Bond angles

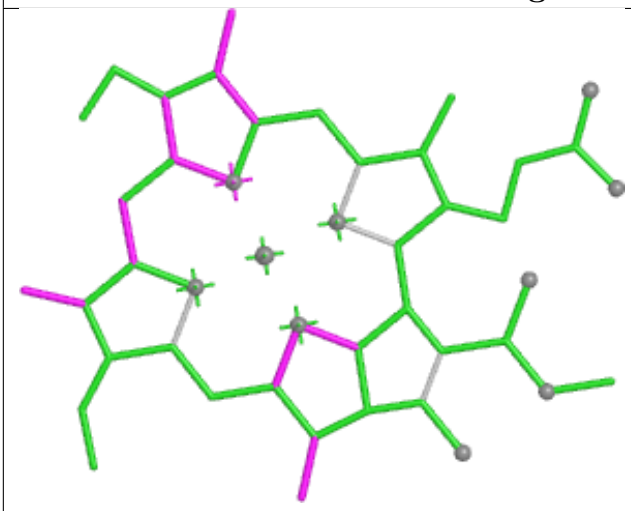


Torsions

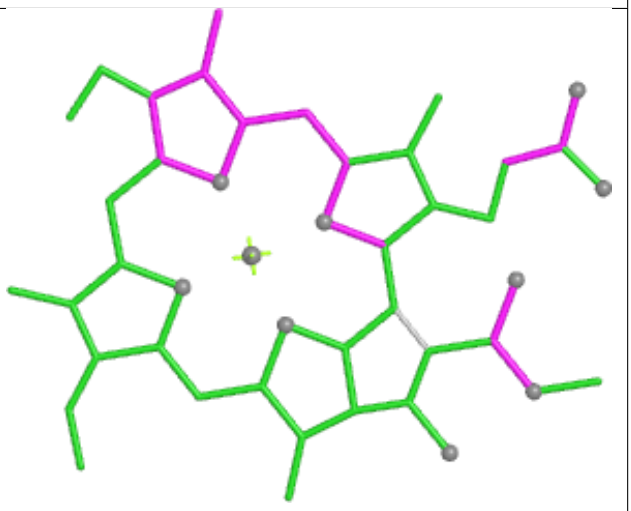


Rings

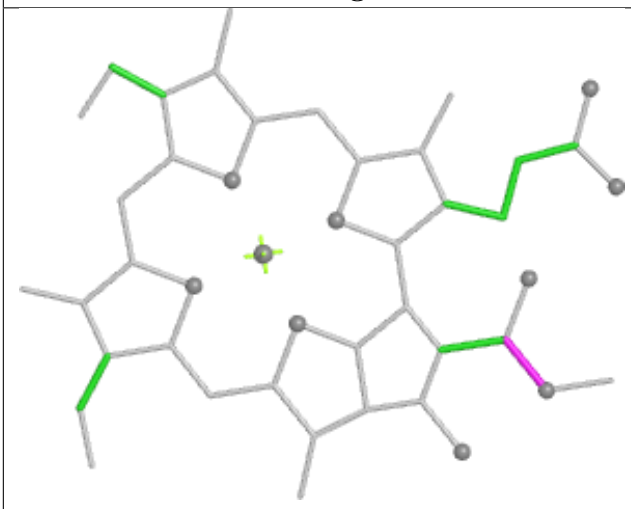
Ligand CLA a 509



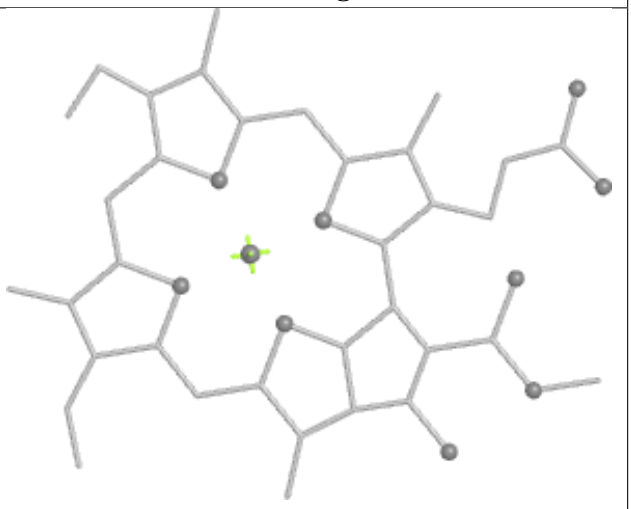
Bond lengths



Bond angles

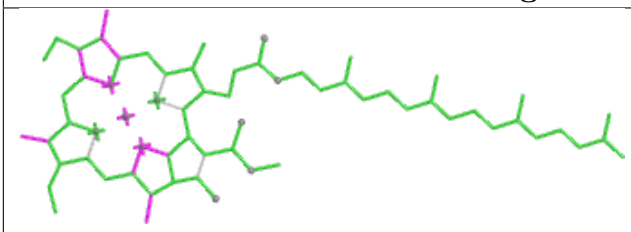


Torsions

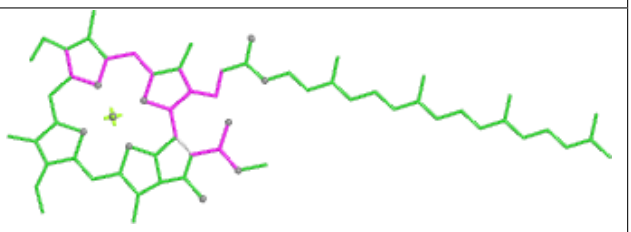


Rings

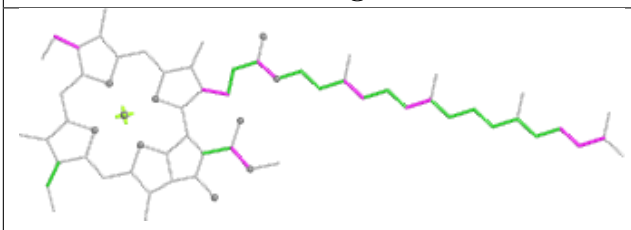
Ligand CLA e 1140



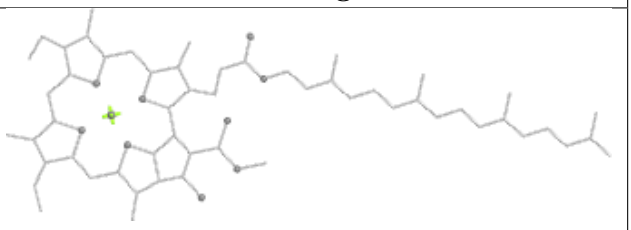
Bond lengths



Bond angles

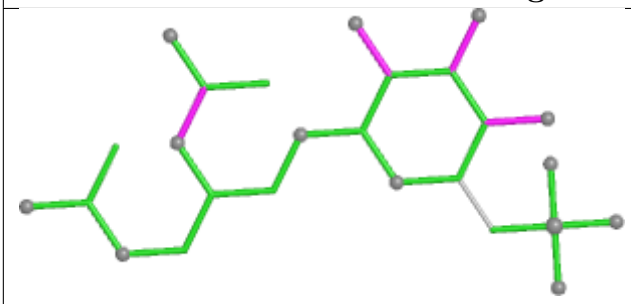


Torsions

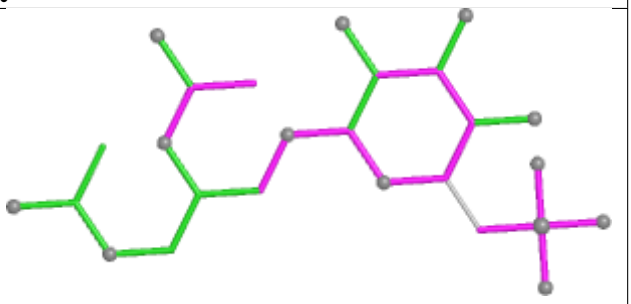


Rings

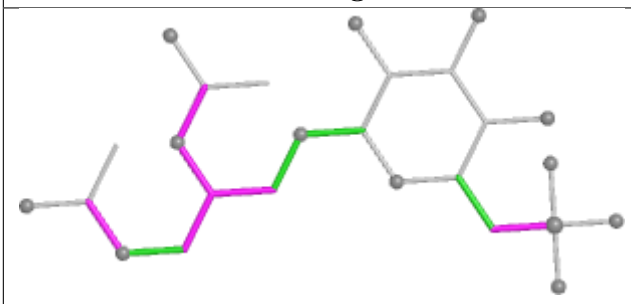
Ligand SQD b 822



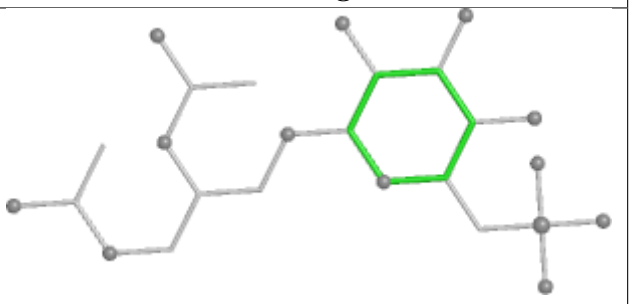
Bond lengths



Bond angles

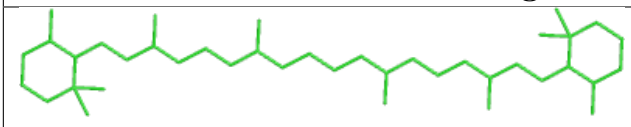


Torsions

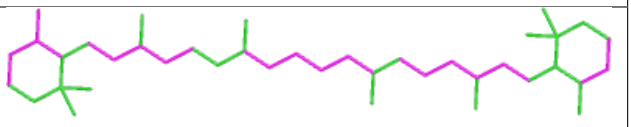


Rings

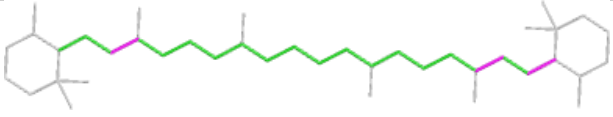
Ligand BCR f 4005



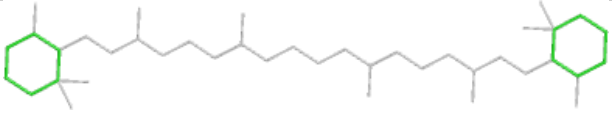
Bond lengths



Bond angles

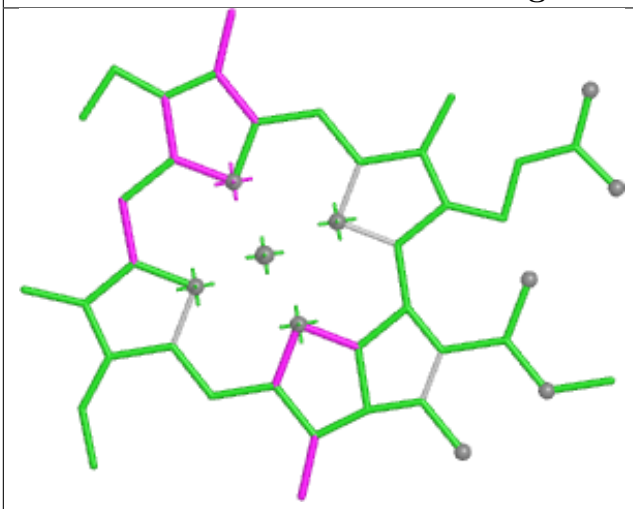


Torsions

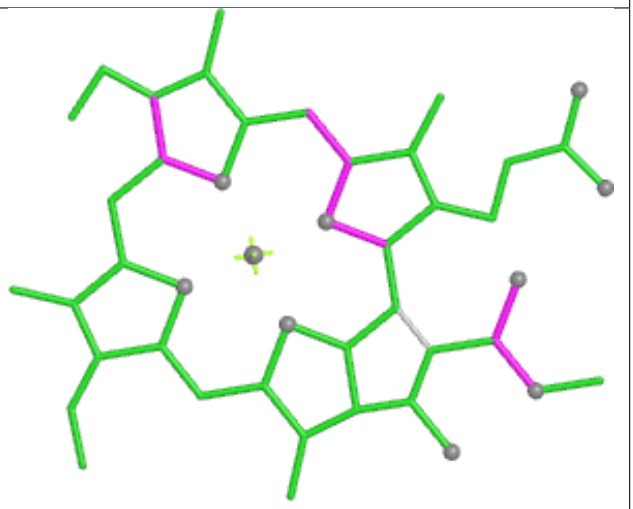


Rings

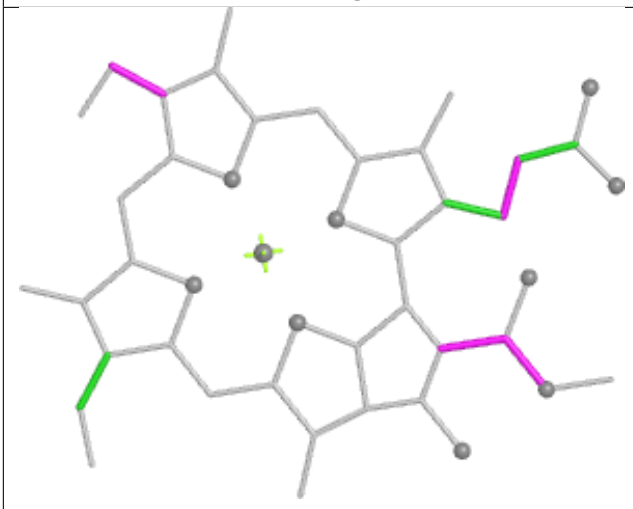
Ligand CLA 4 518



Bond lengths



Bond angles

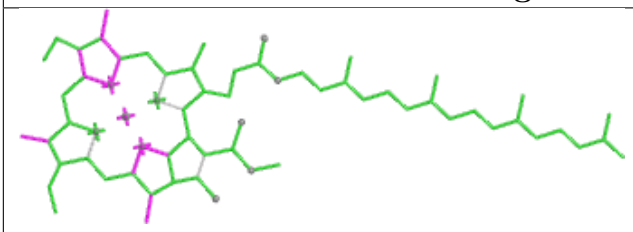


Torsions

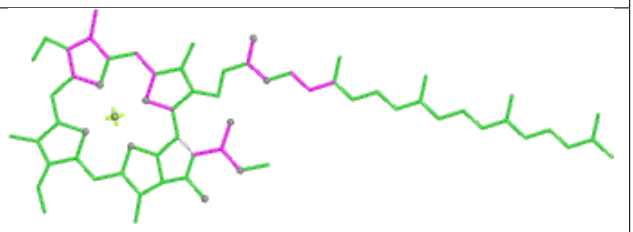


Rings

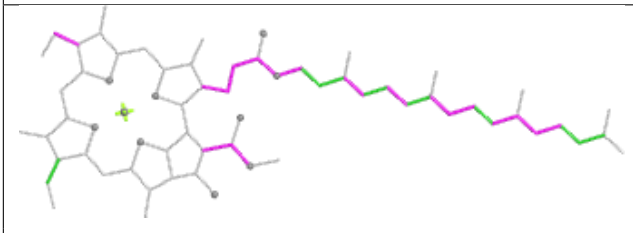
Ligand CLA G 1106



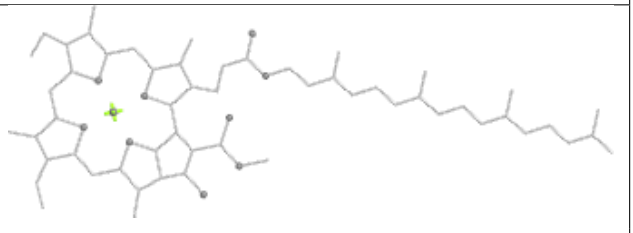
Bond lengths



Bond angles

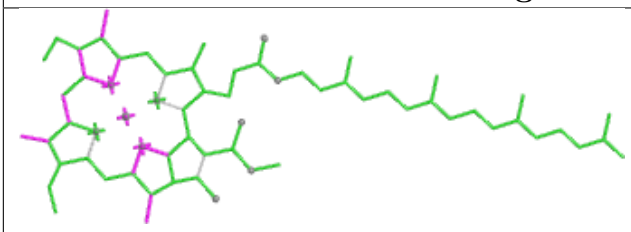


Torsions

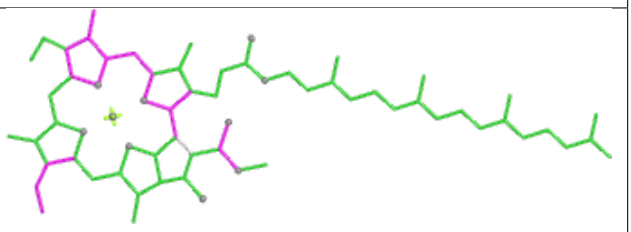


Rings

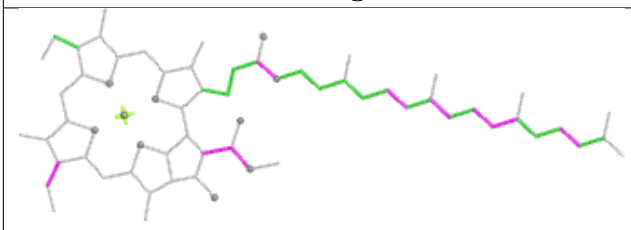
Ligand CLA B 1234



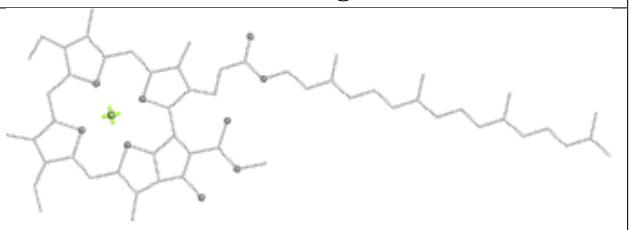
Bond lengths



Bond angles

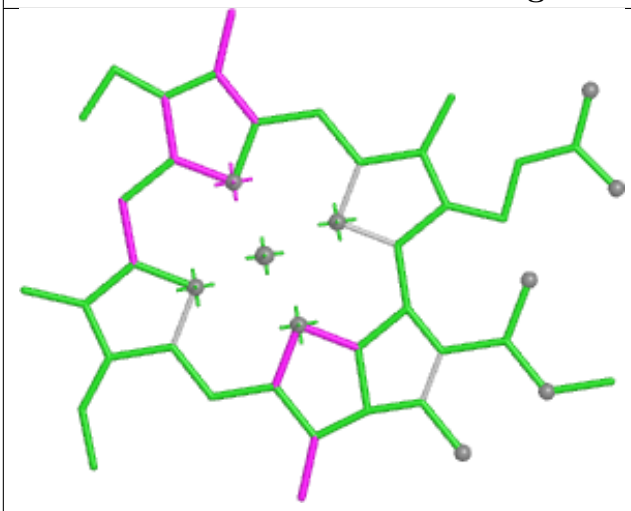


Torsions

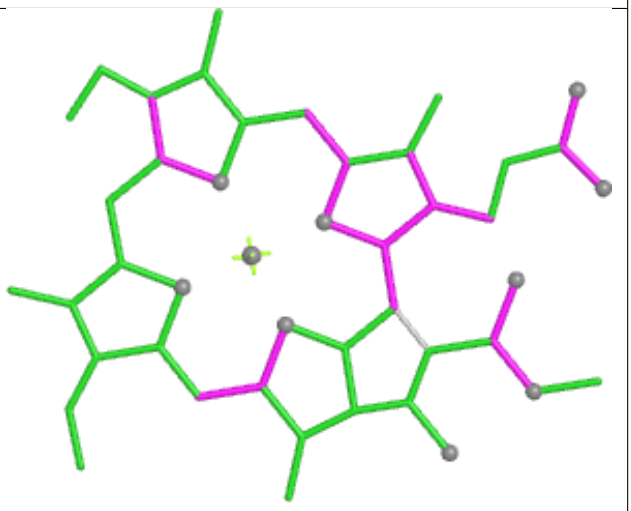


Rings

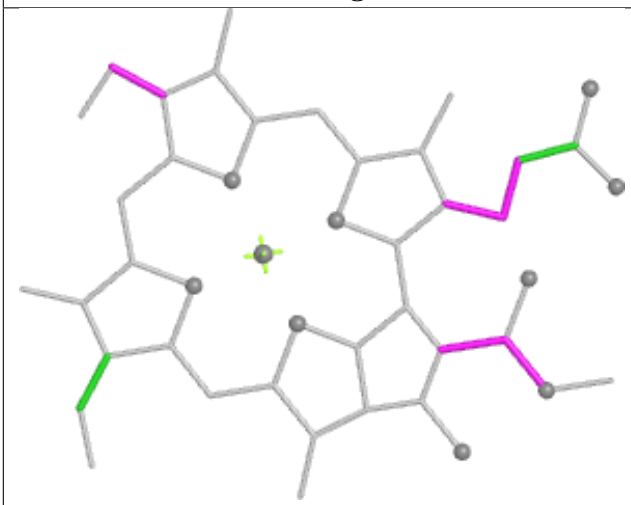
Ligand CLA u 503



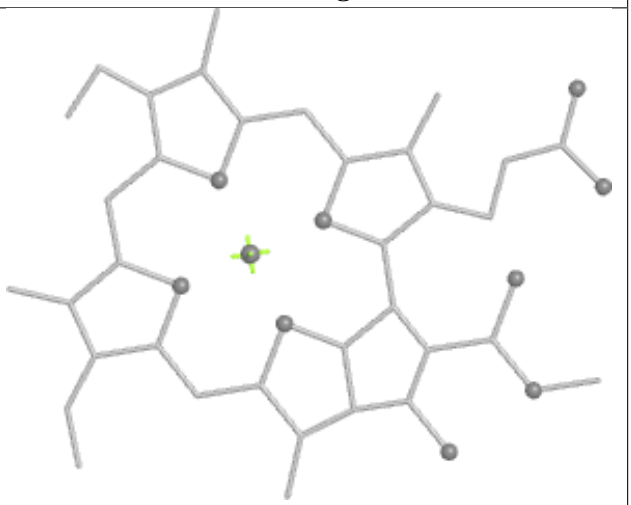
Bond lengths



Bond angles

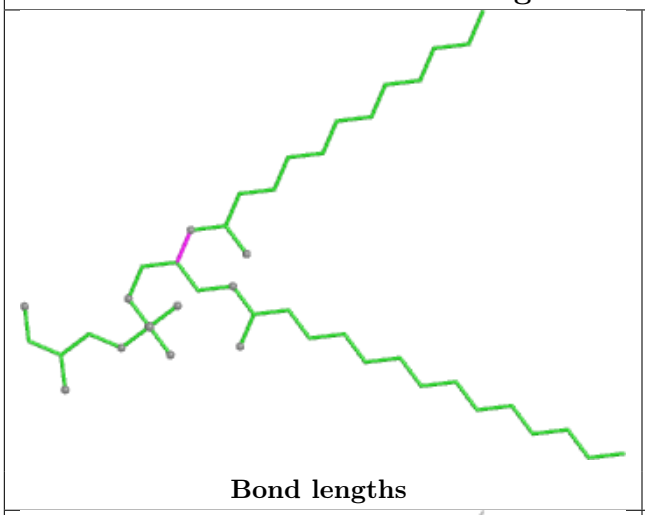


Torsions

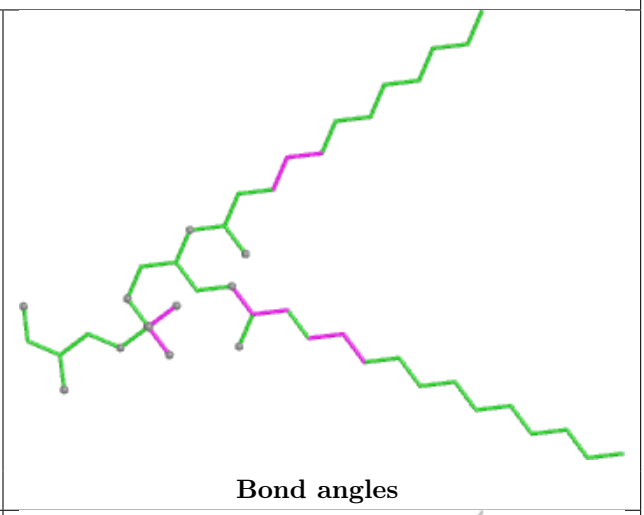


Rings

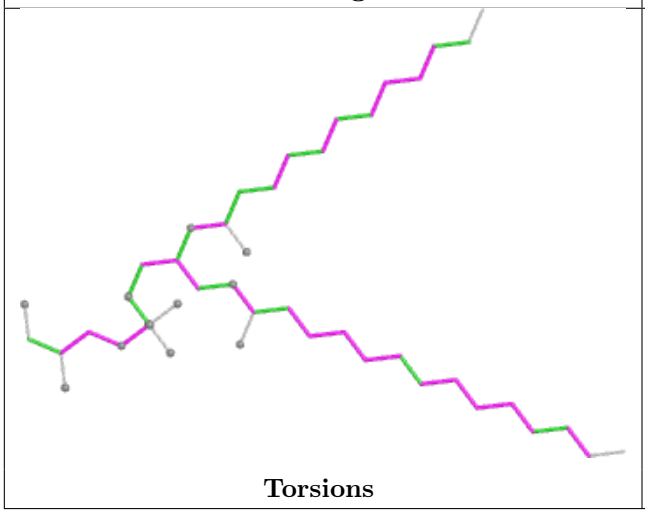
Ligand LHG A 5005



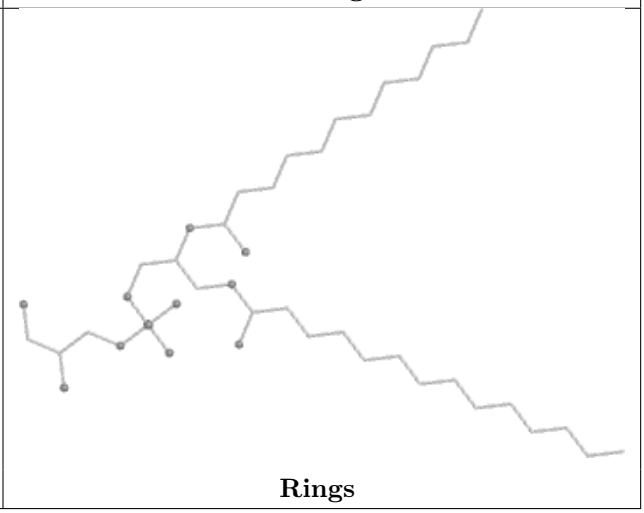
Bond lengths



Bond angles

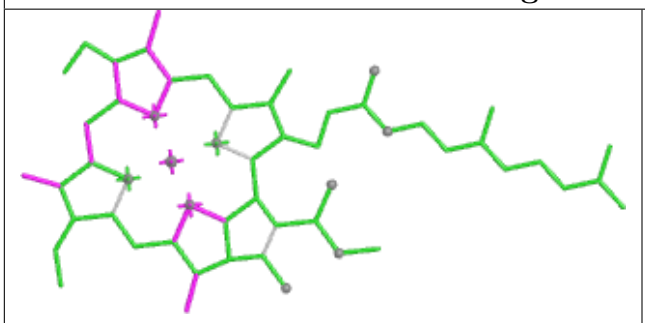


Torsions

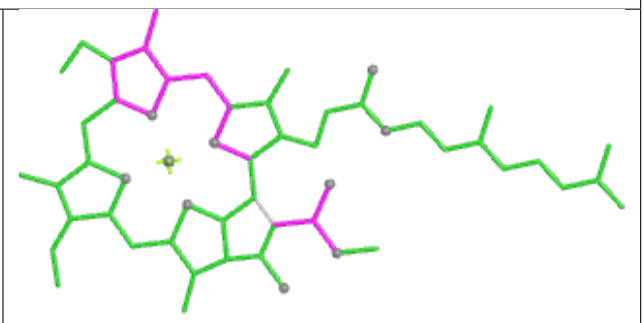


Rings

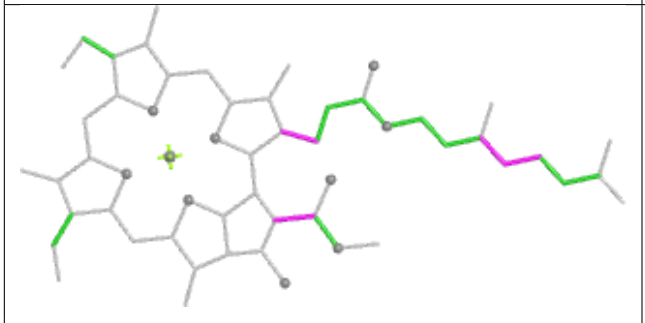
Ligand CLA e 1102



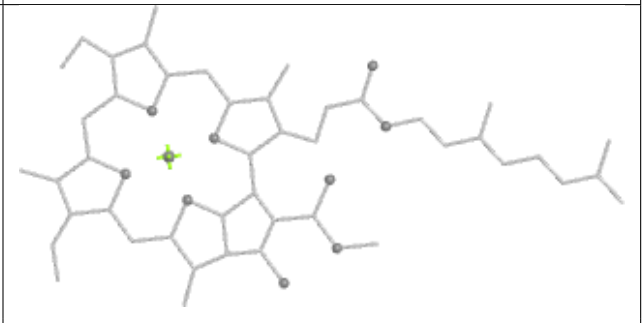
Bond lengths



Bond angles

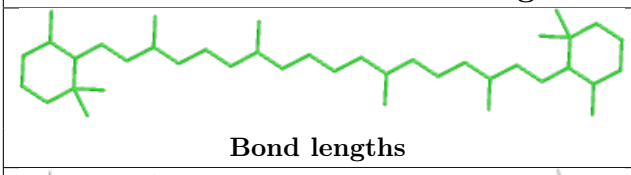


Torsions

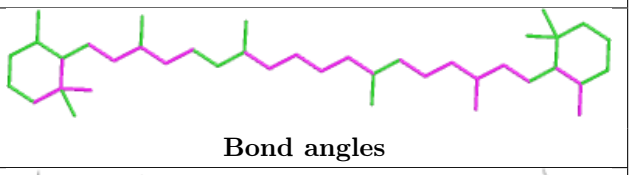


Rings

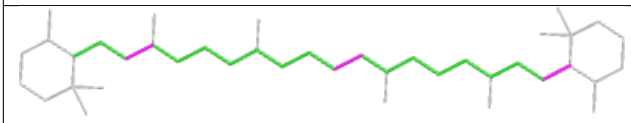
Ligand BCR J 4015



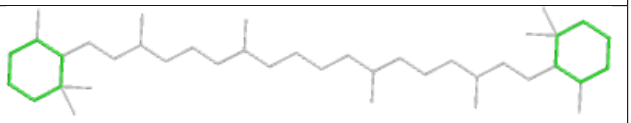
Bond lengths



Bond angles



Torsions

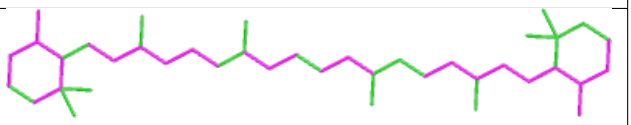


Rings

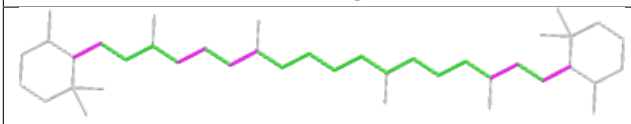
Ligand BCR T 4012



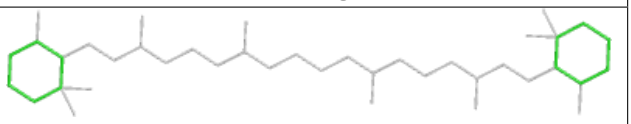
Bond lengths



Bond angles

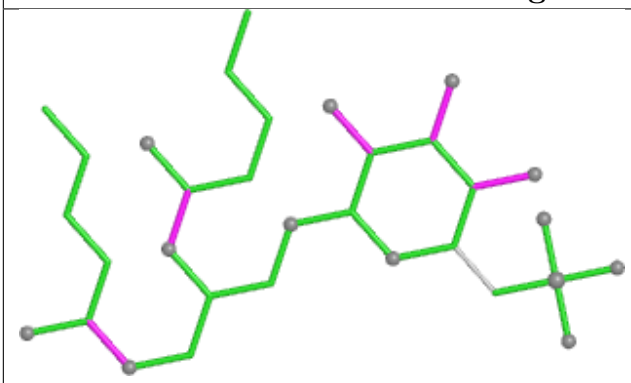


Torsions

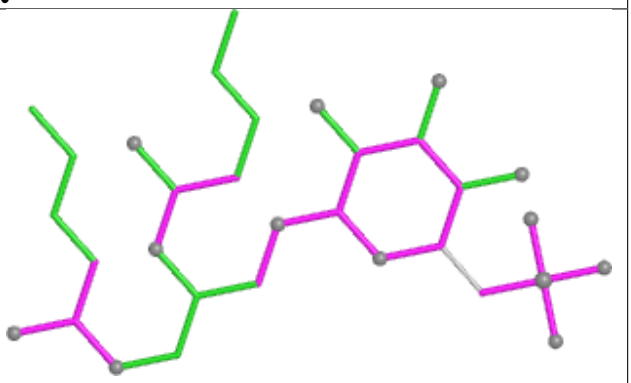


Rings

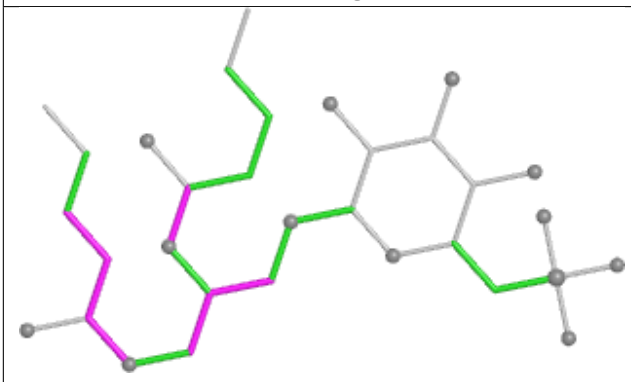
Ligand SQD 1 822



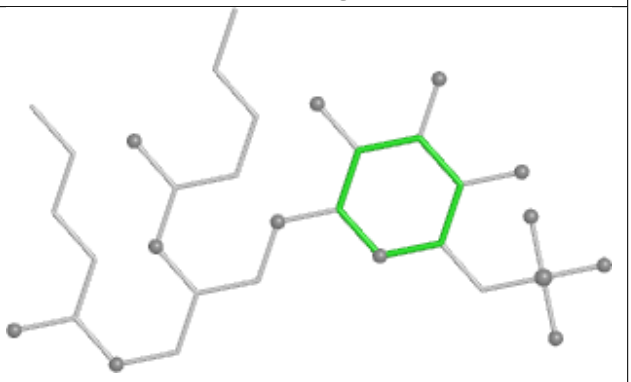
Bond lengths



Bond angles

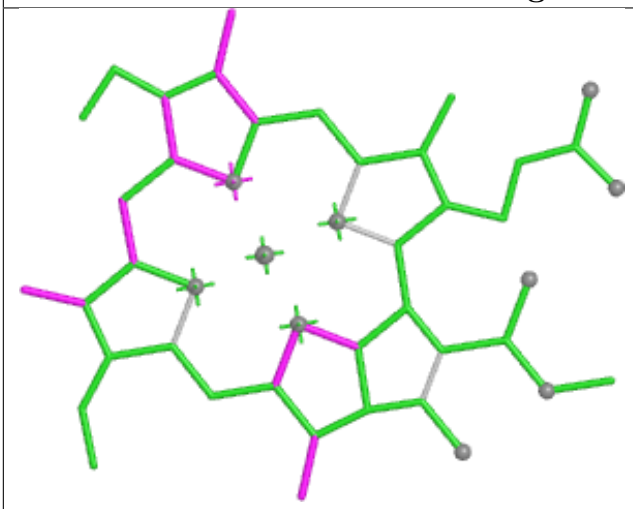


Torsions

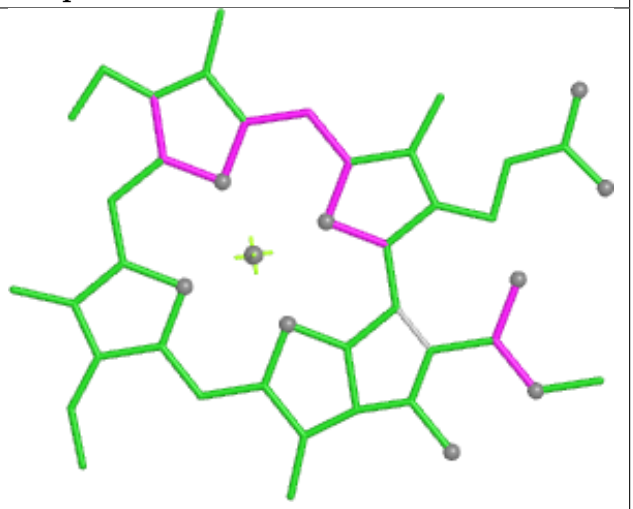


Rings

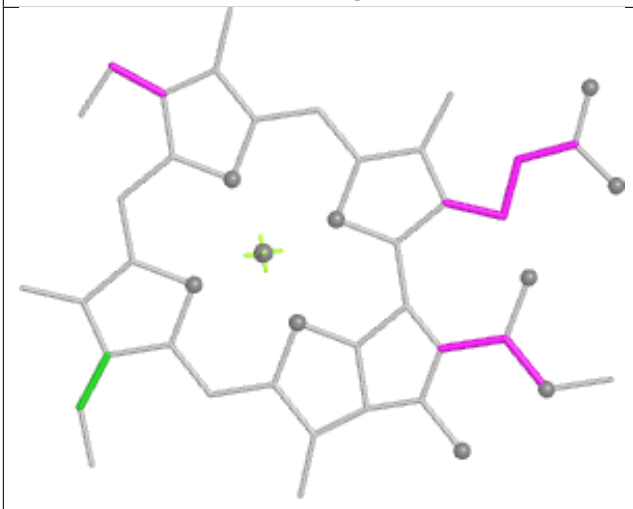
Ligand CLA q 501



Bond lengths



Bond angles

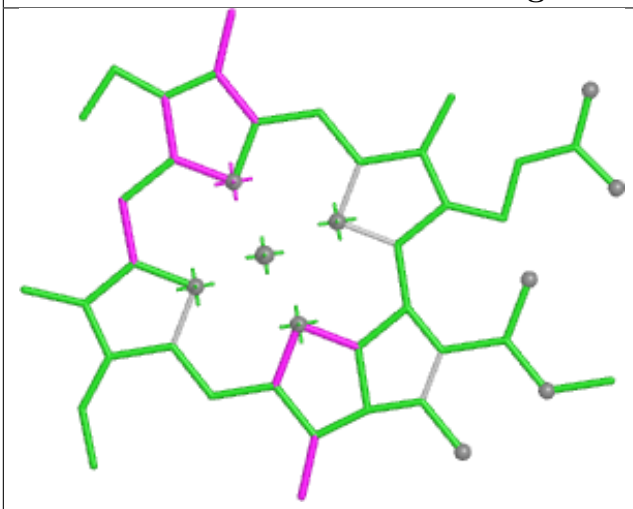


Torsions

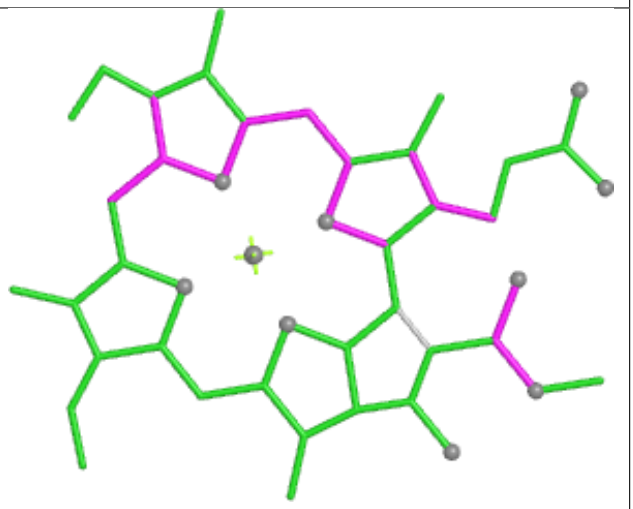


Rings

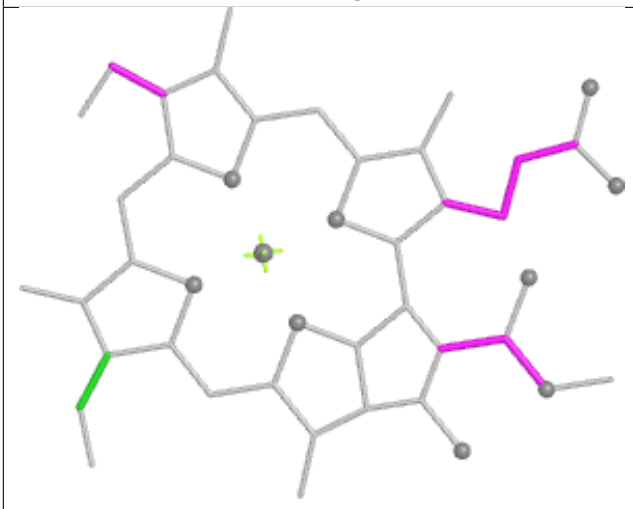
Ligand CLA d 516



Bond lengths



Bond angles

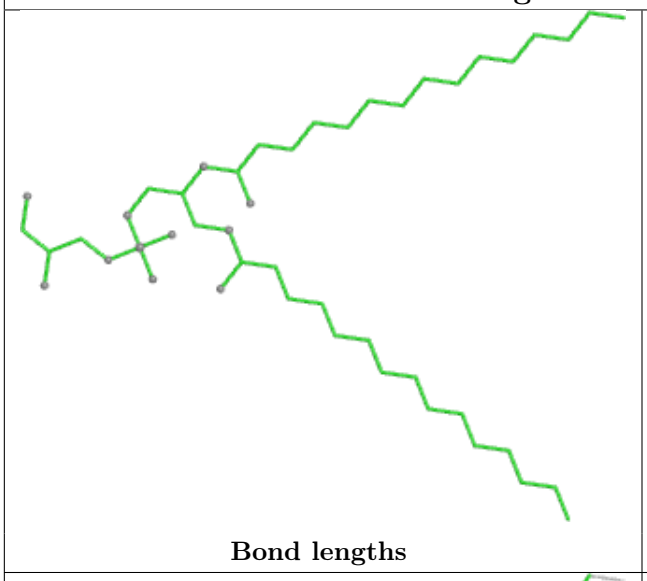


Torsions

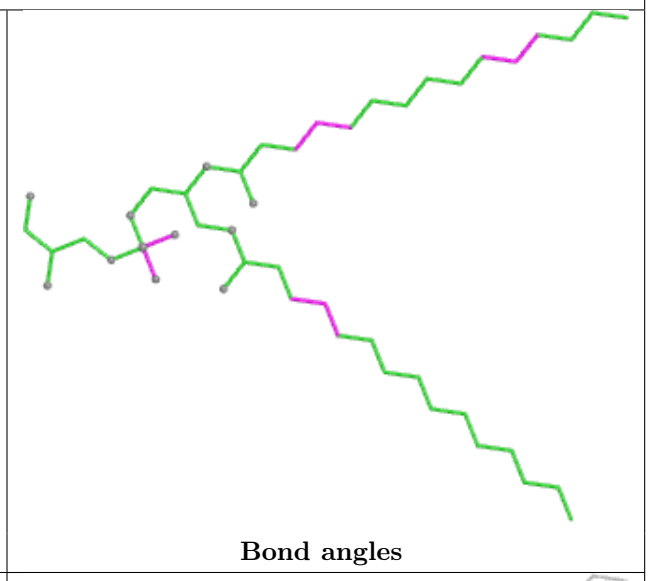


Rings

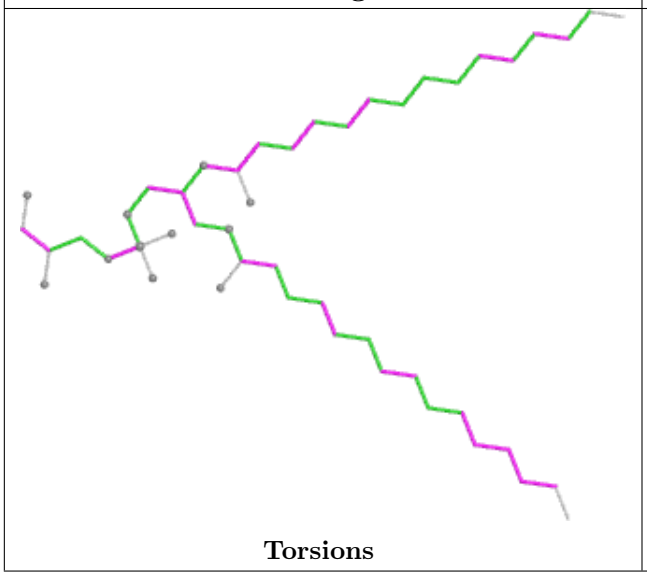
Ligand LHG G 5007



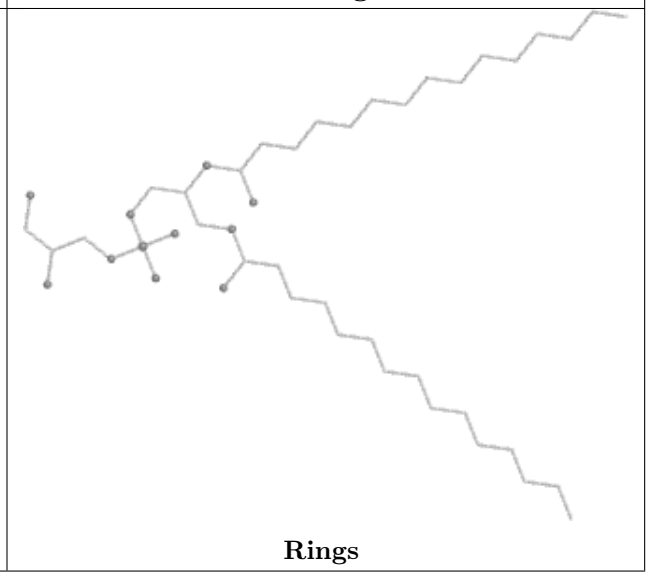
Bond lengths



Bond angles

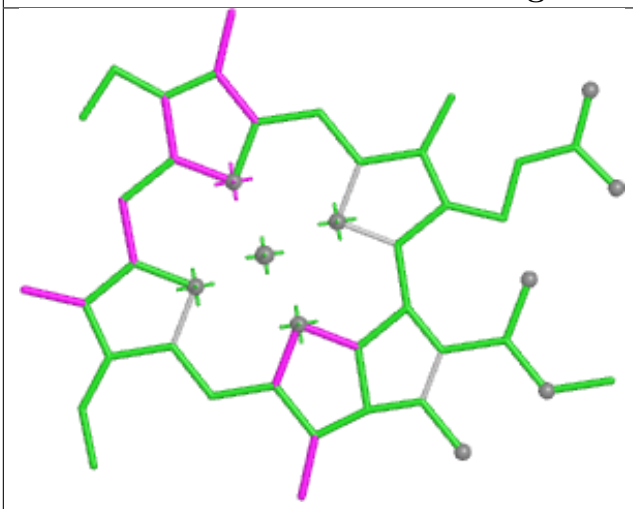


Torsions

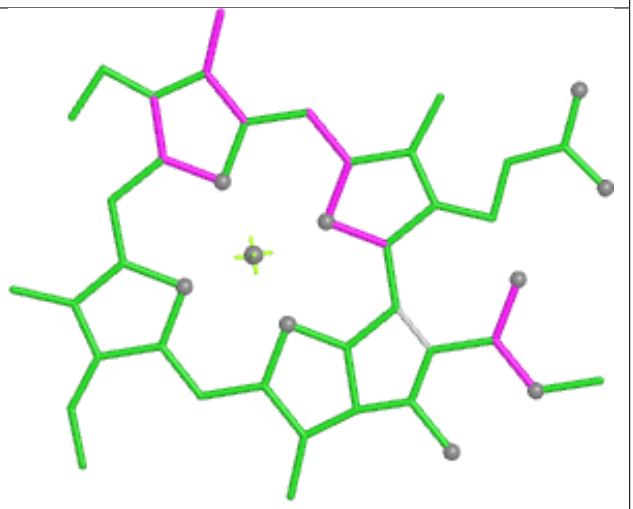


Rings

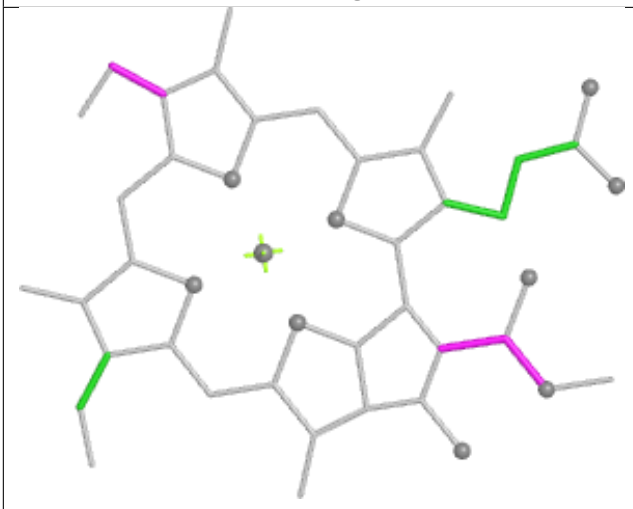
Ligand CLA d 506



Bond lengths



Bond angles

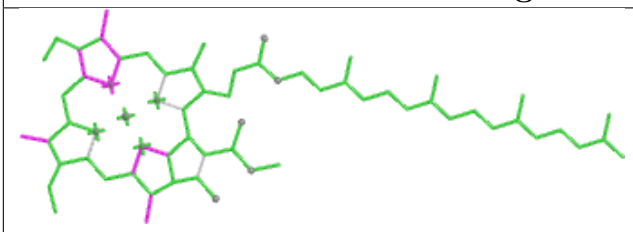


Torsions

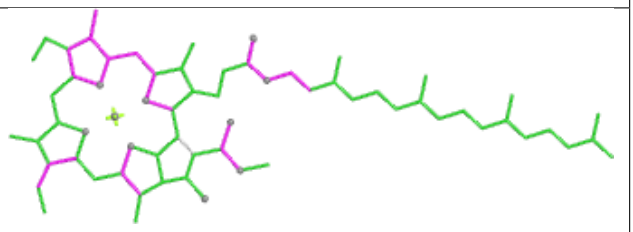


Rings

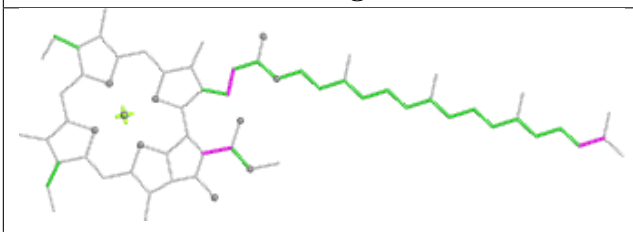
Ligand CLA B 1238



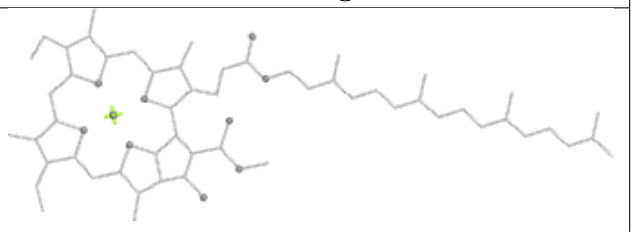
Bond lengths



Bond angles

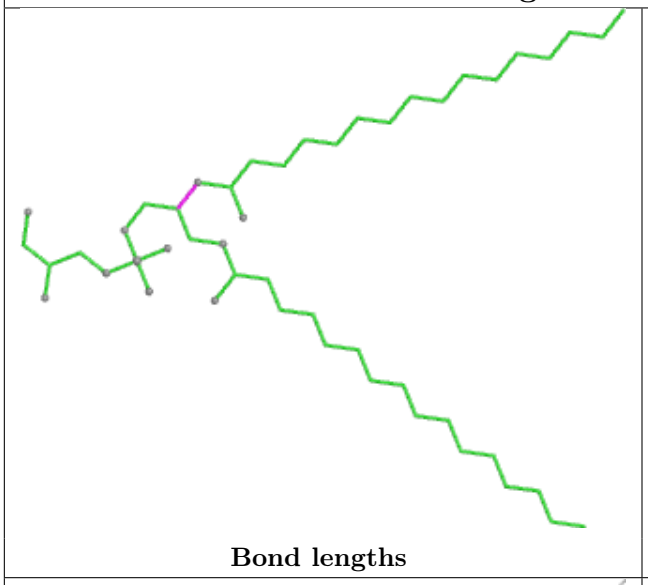


Torsions

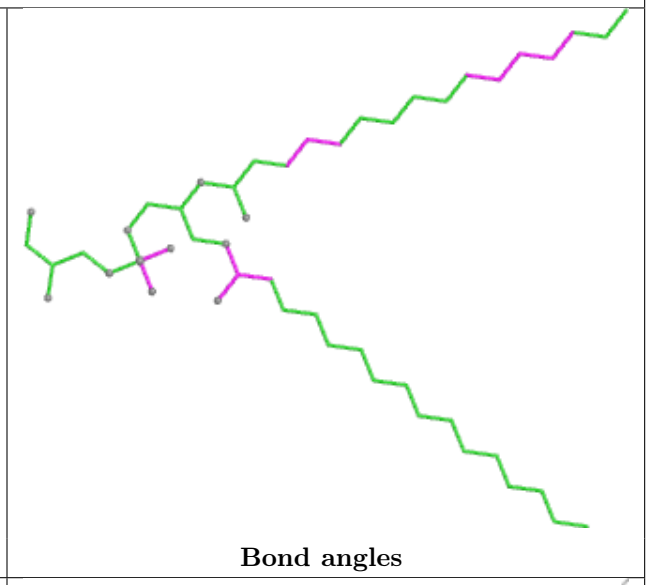


Rings

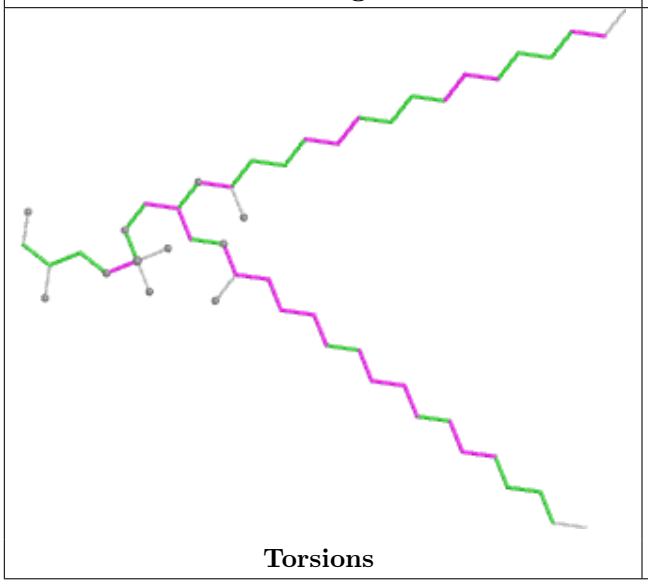
Ligand LHG e 5001



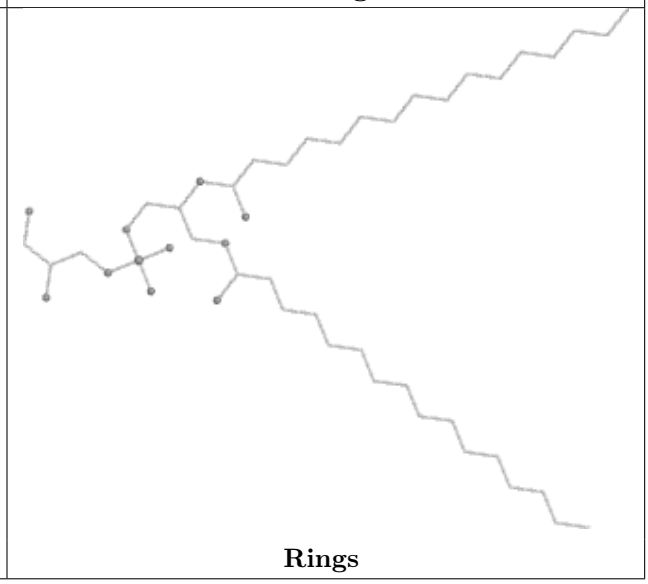
Bond lengths



Bond angles

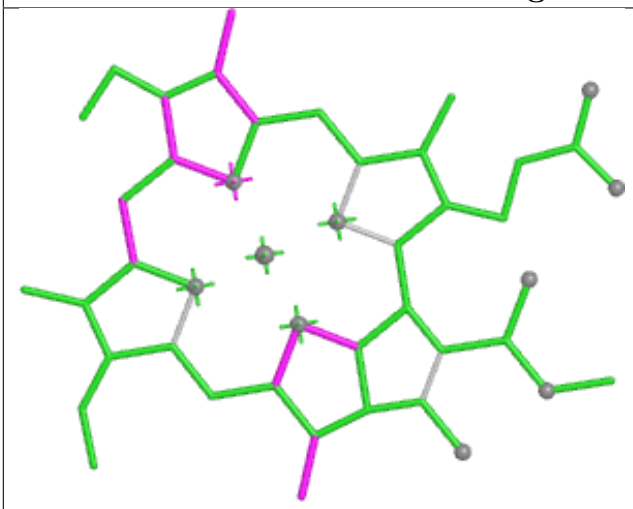


Torsions

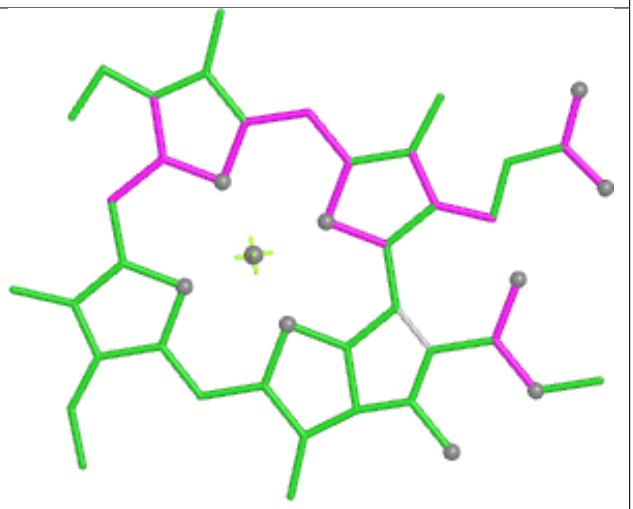


Rings

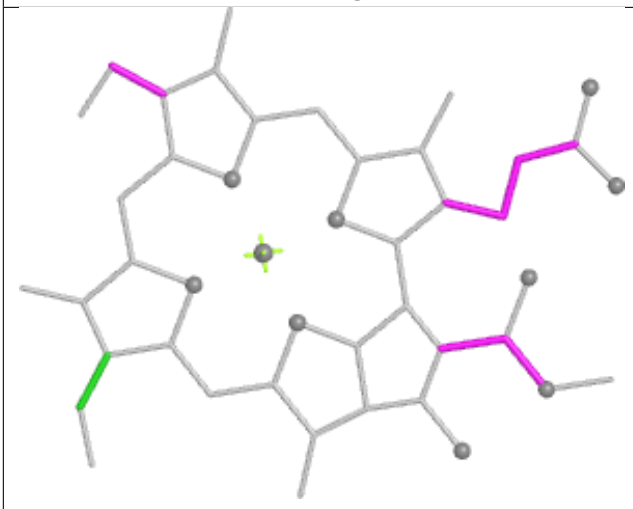
Ligand CLA v 516



Bond lengths



Bond angles

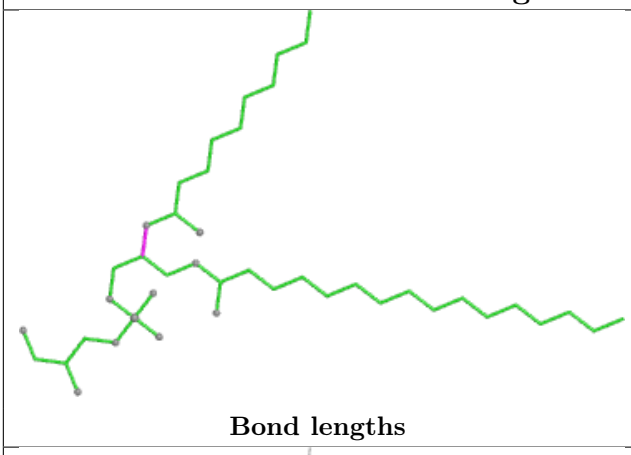


Torsions

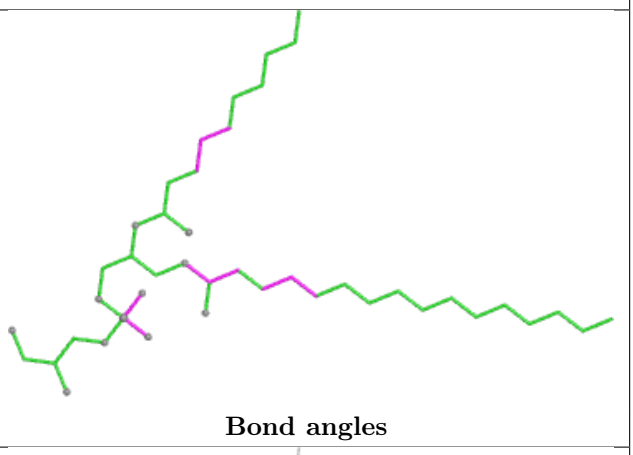


Rings

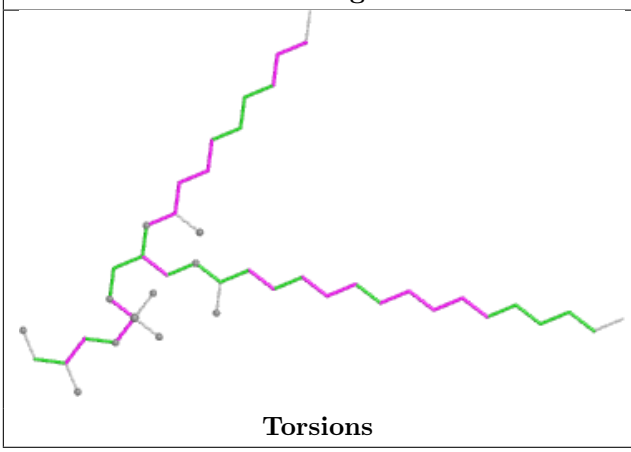
Ligand LHG G 5002



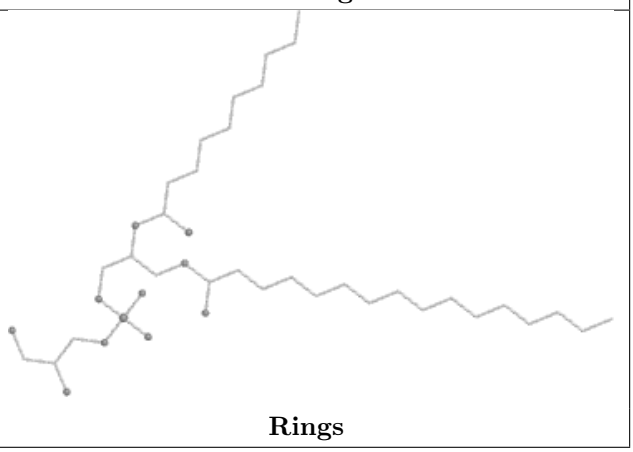
Bond lengths



Bond angles

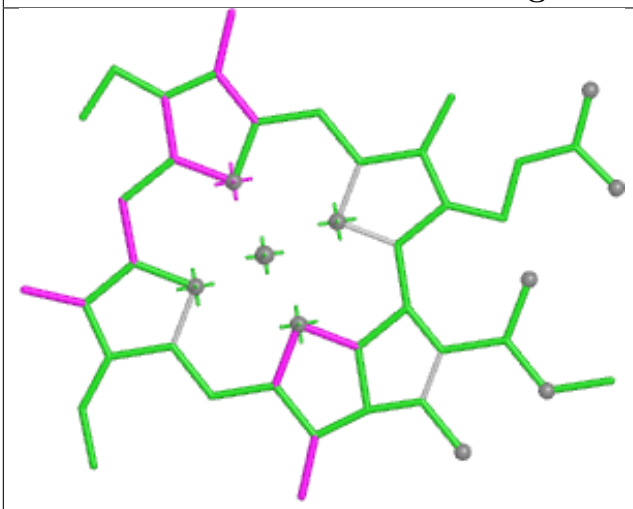


Torsions

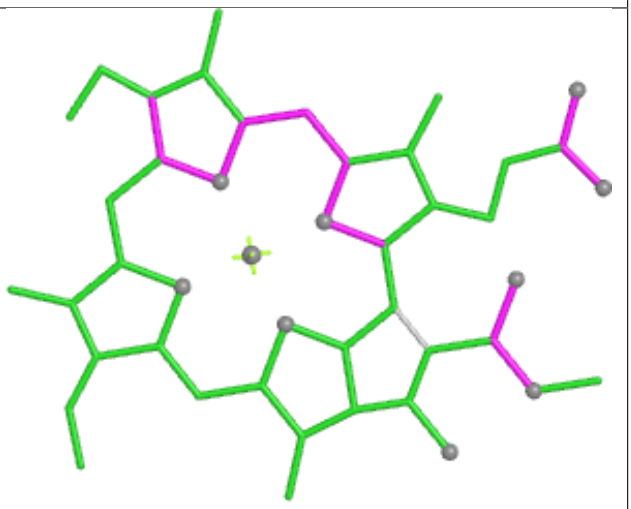


Rings

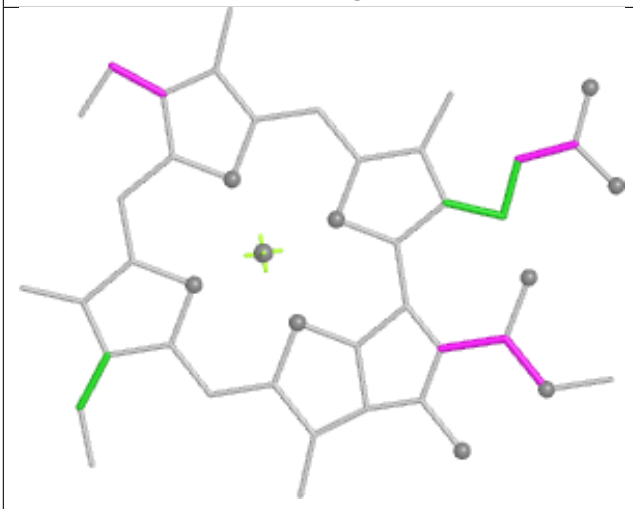
Ligand CLA 4 519



Bond lengths



Bond angles

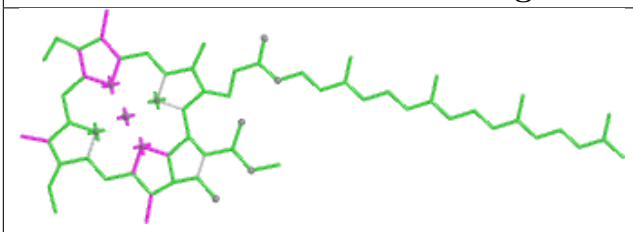


Torsions

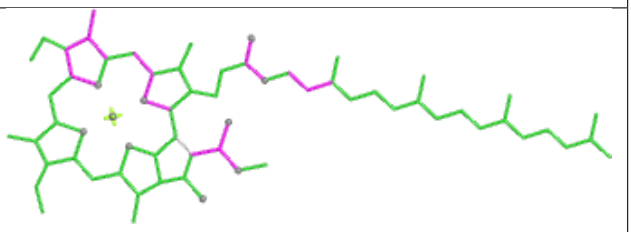


Rings

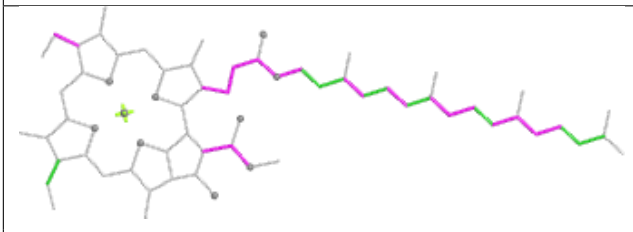
Ligand CLA A 1106



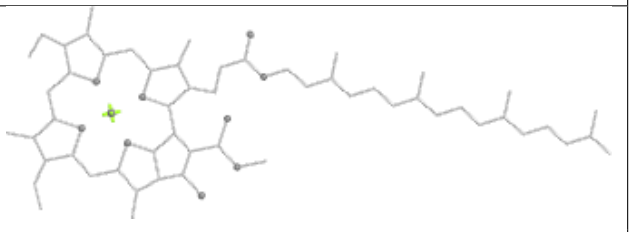
Bond lengths



Bond angles

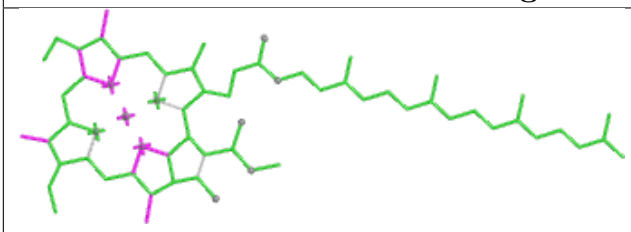


Torsions

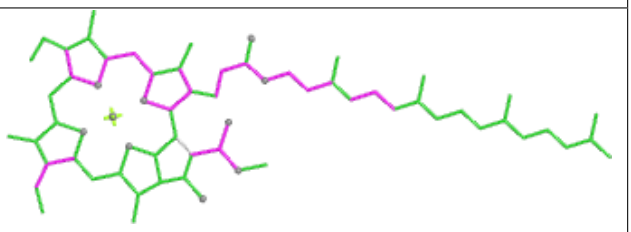


Rings

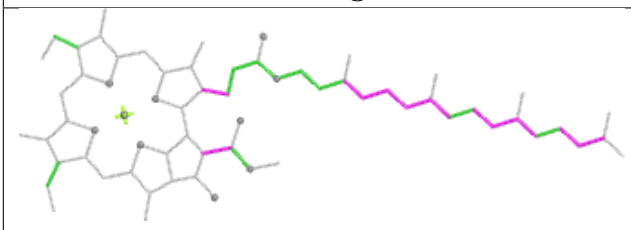
Ligand CLA e 1101



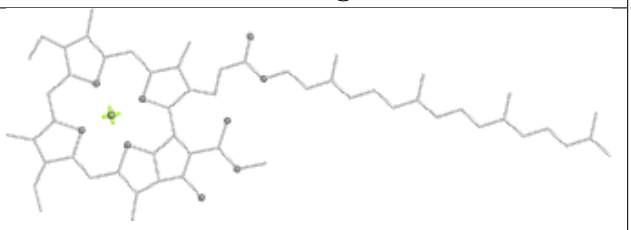
Bond lengths



Bond angles

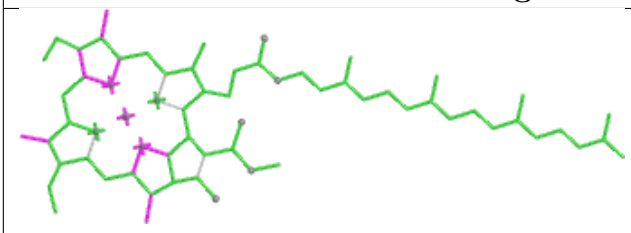


Torsions

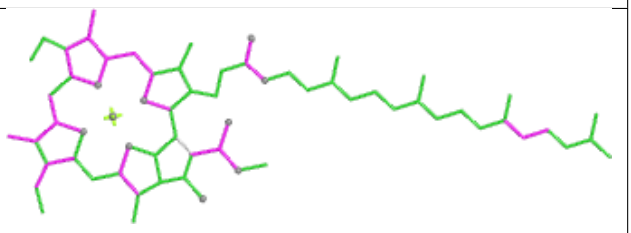


Rings

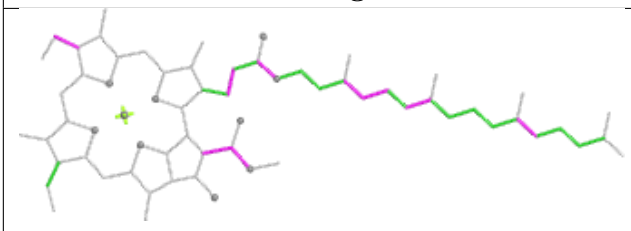
Ligand CLA G 1119



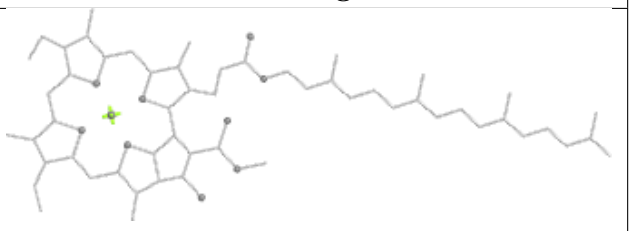
Bond lengths



Bond angles

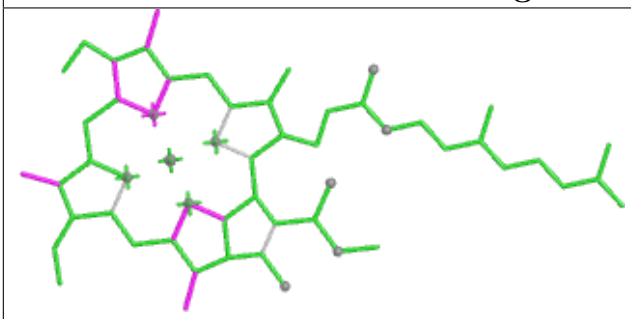


Torsions

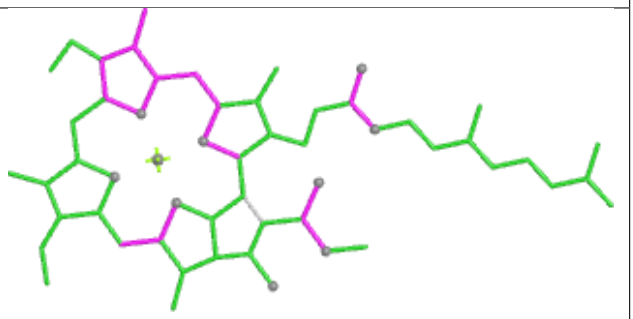


Rings

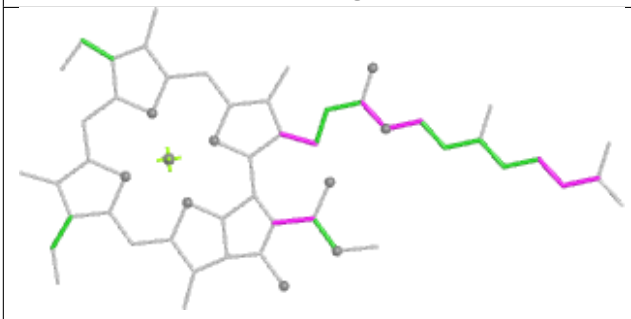
Ligand CLA G 1105



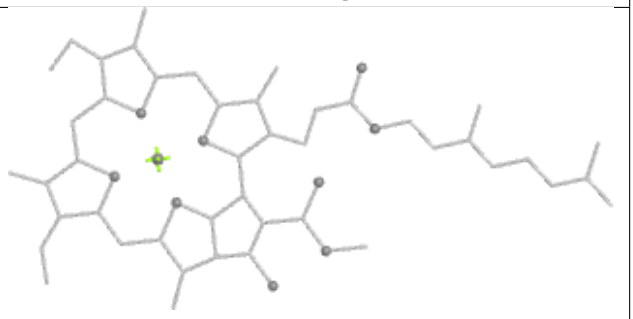
Bond lengths



Bond angles

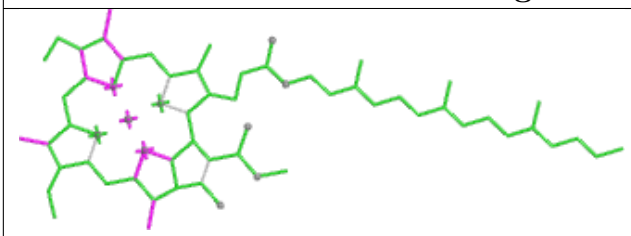


Torsions

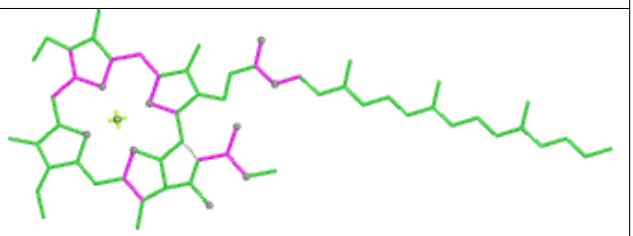


Rings

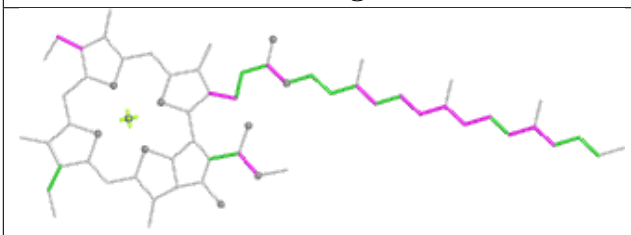
Ligand CLA H 1219



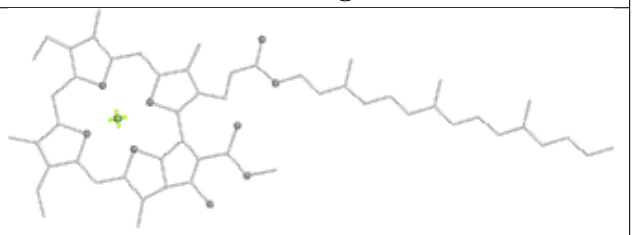
Bond lengths



Bond angles

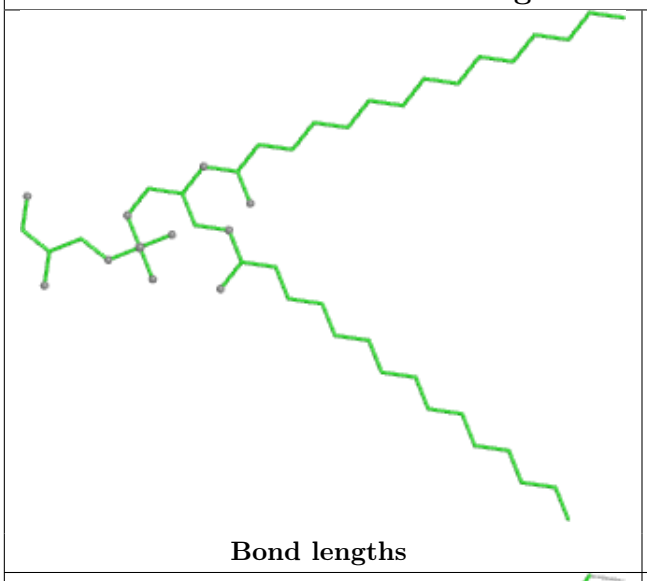


Torsions

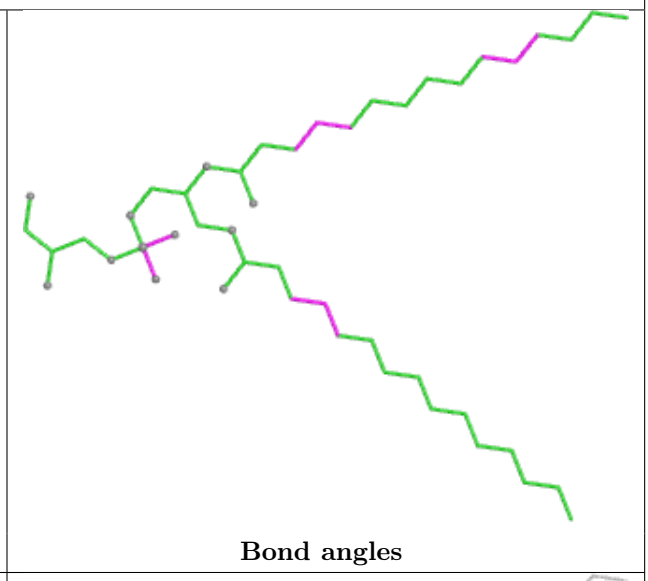


Rings

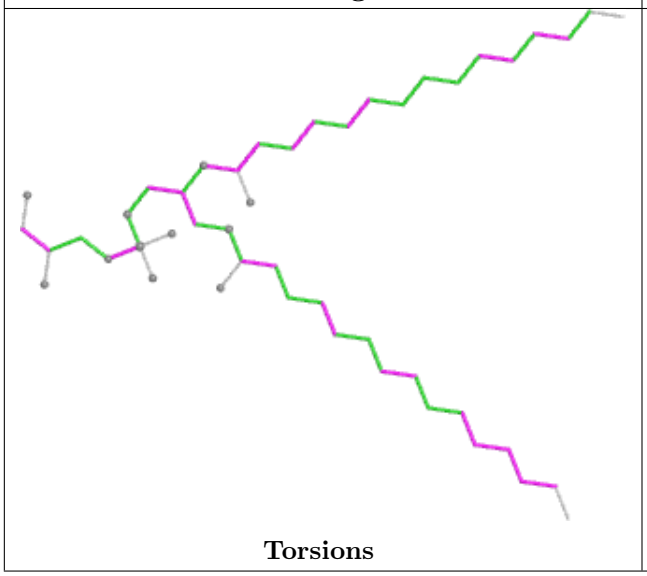
Ligand LHG A 5007



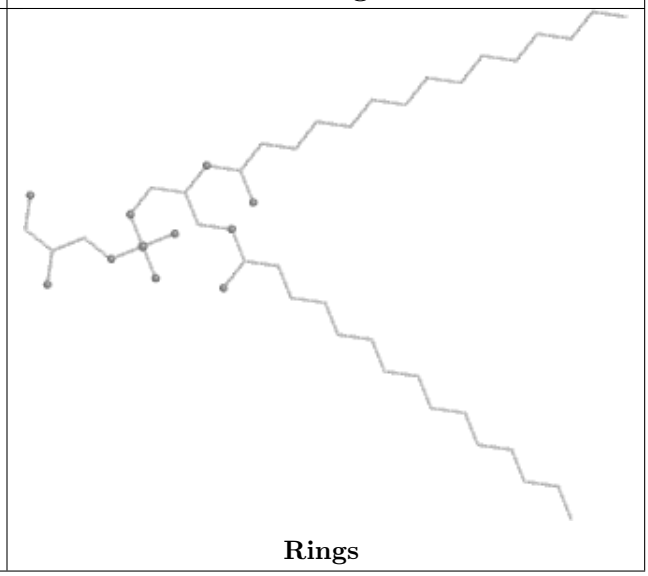
Bond lengths



Bond angles

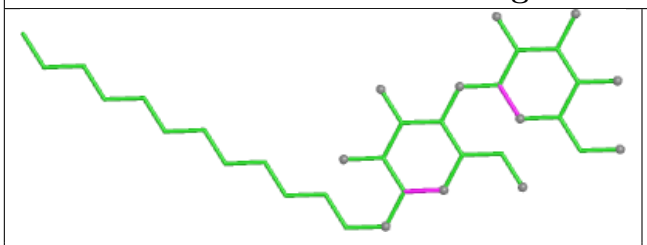


Torsions

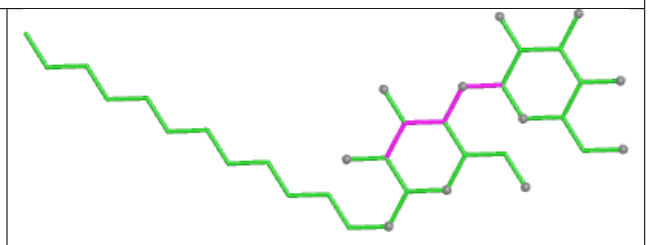


Rings

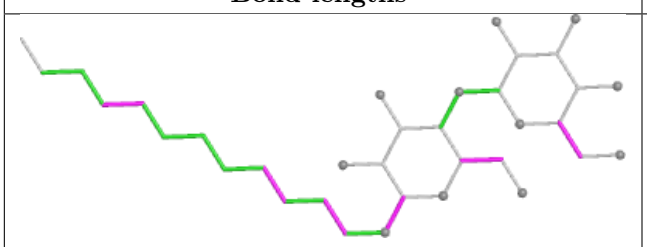
Ligand LMU A 1848



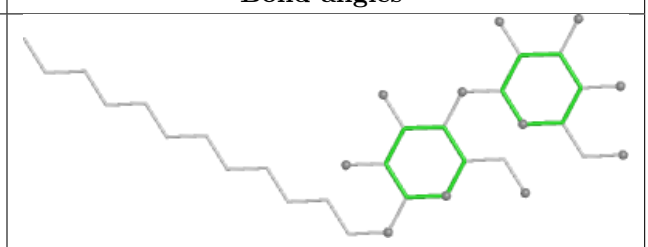
Bond lengths



Bond angles

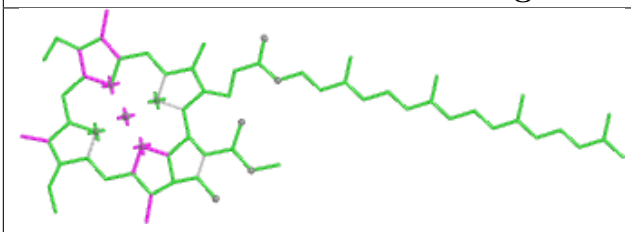


Torsions

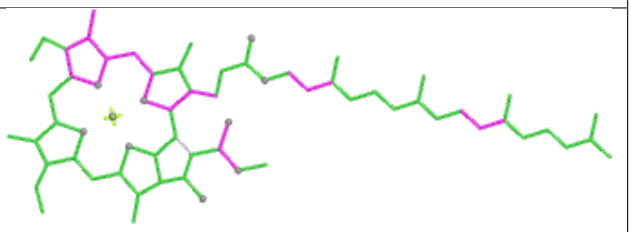


Rings

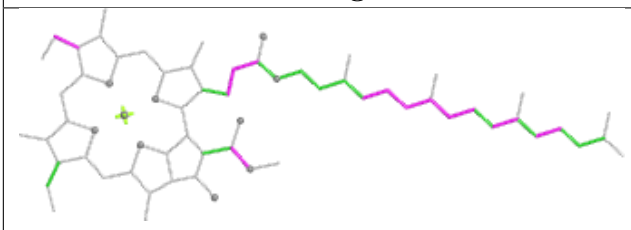
Ligand CLA H 1203



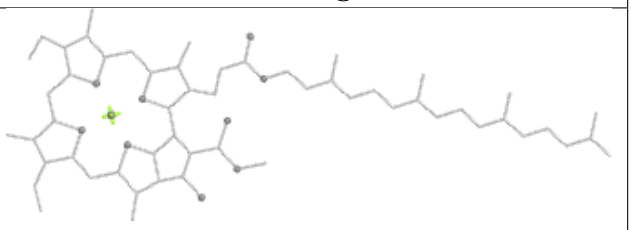
Bond lengths



Bond angles

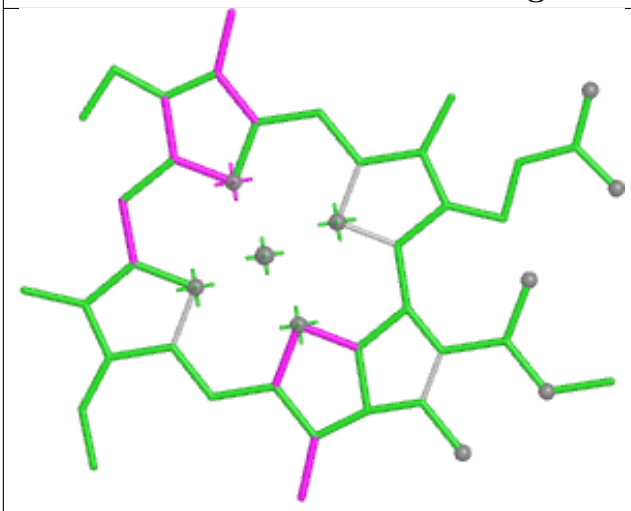


Torsions

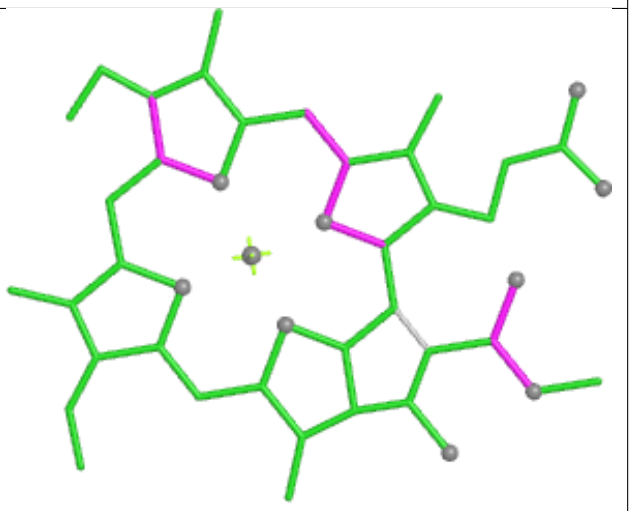


Rings

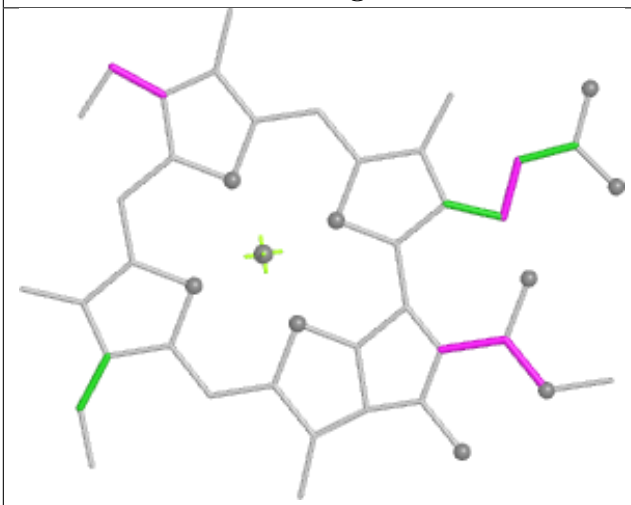
Ligand CLA b 518



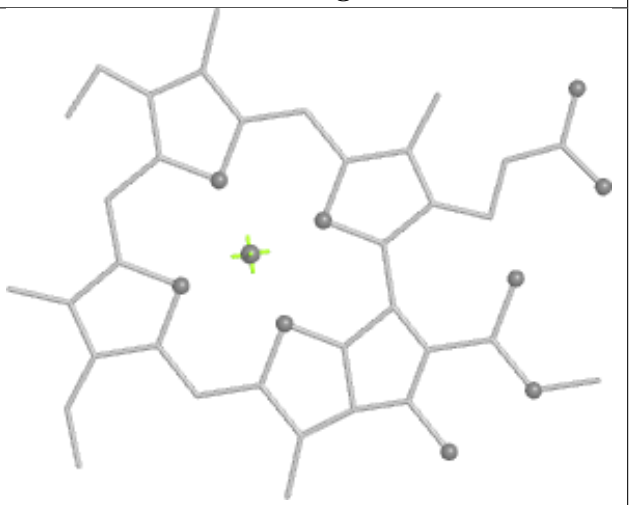
Bond lengths



Bond angles

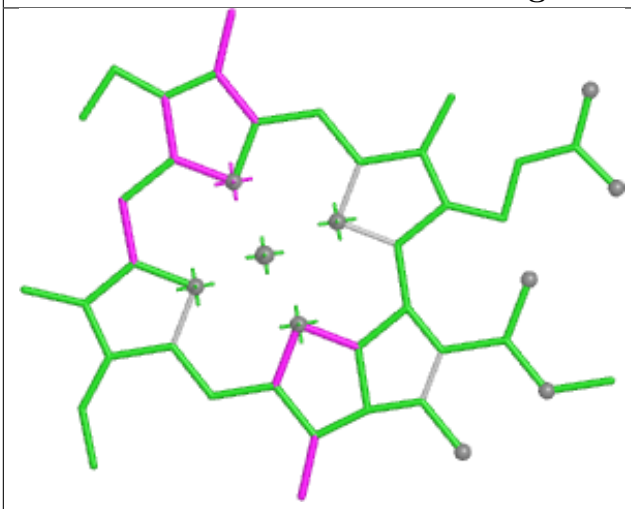


Torsions

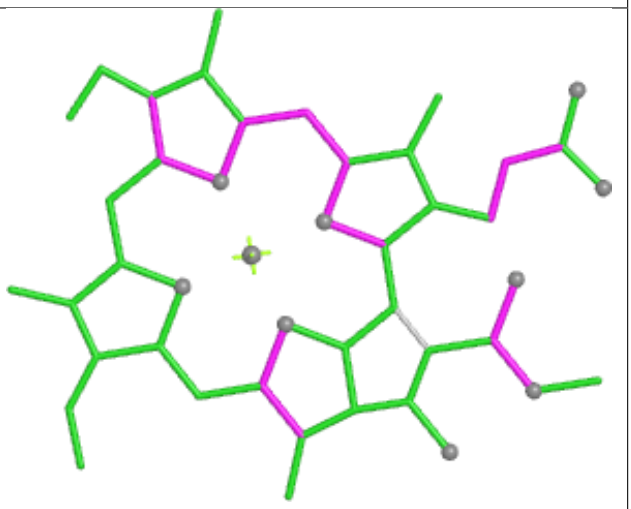


Rings

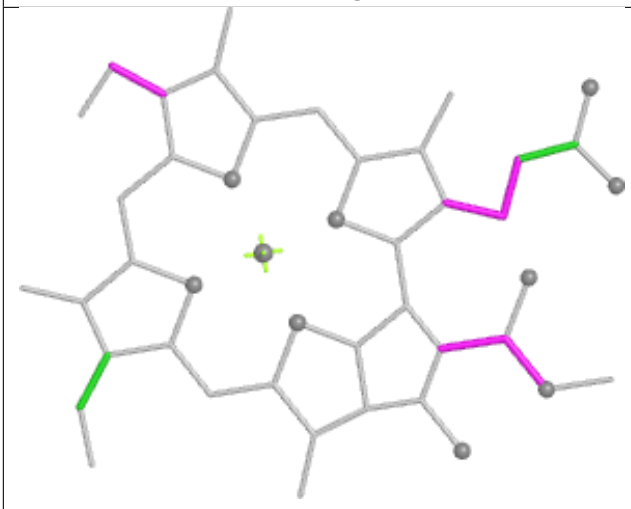
Ligand CLA 3 503



Bond lengths



Bond angles

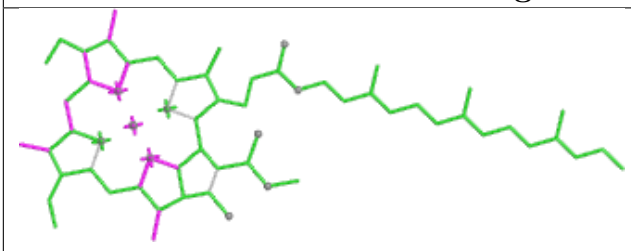


Torsions

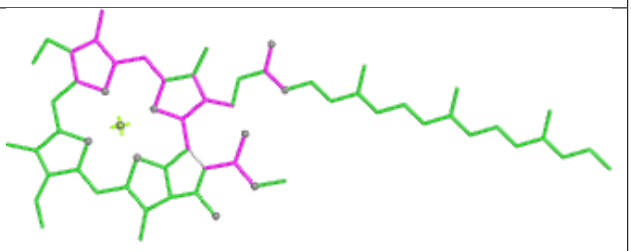


Rings

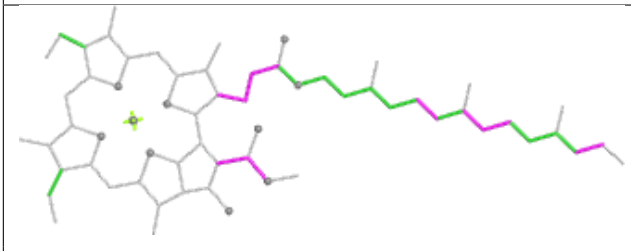
Ligand CLA H 1221



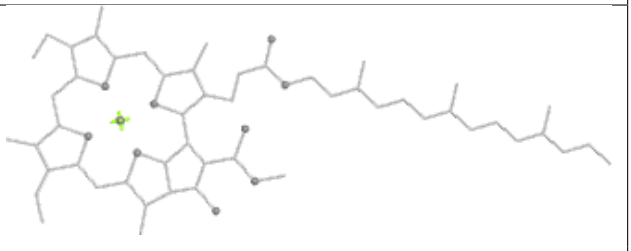
Bond lengths



Bond angles

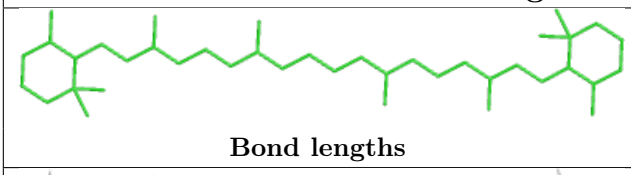


Torsions

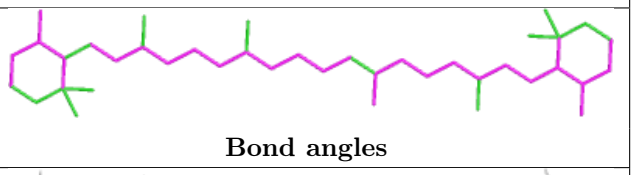


Rings

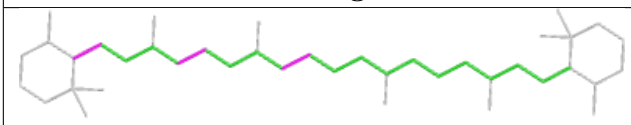
Ligand BCR 4 522



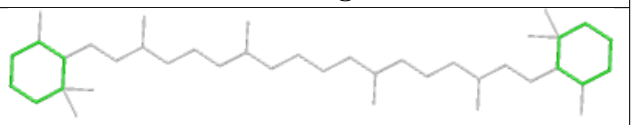
Bond lengths



Bond angles

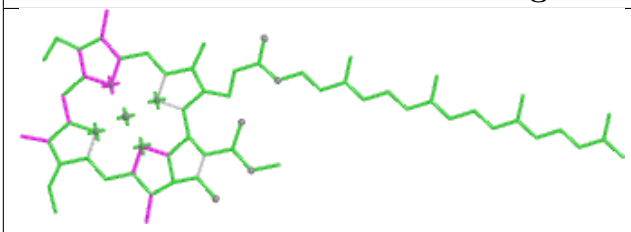


Torsions

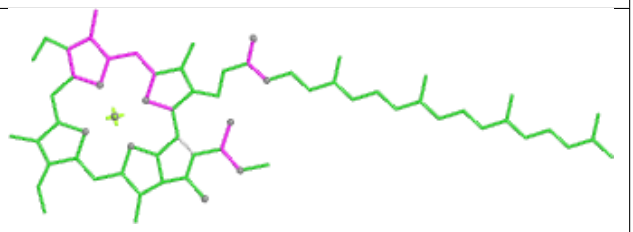


Rings

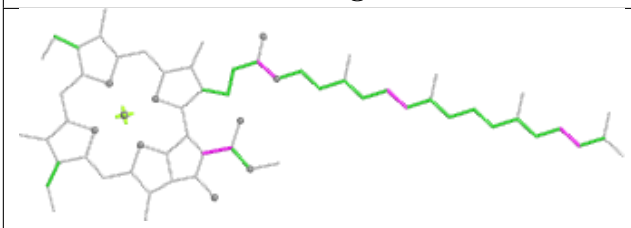
Ligand CLA r 509



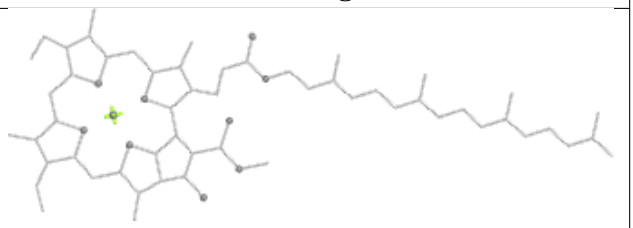
Bond lengths



Bond angles

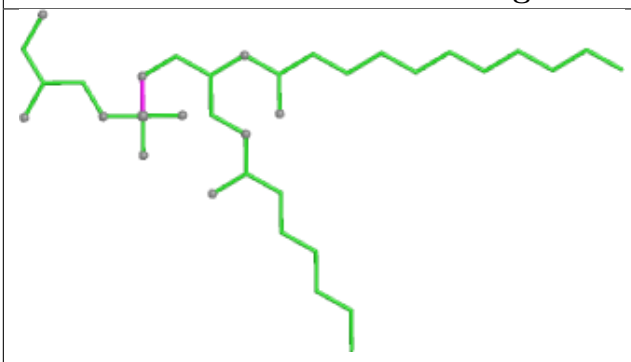


Torsions

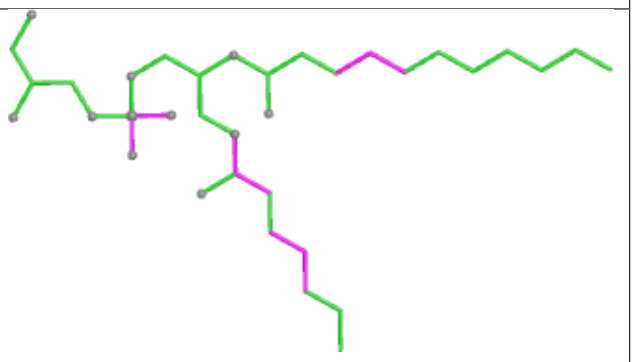


Rings

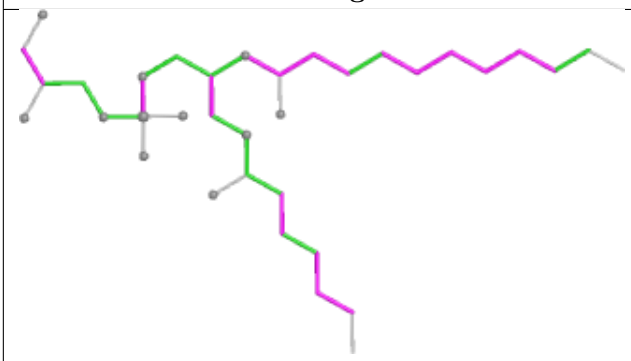
Ligand LHG A 5008



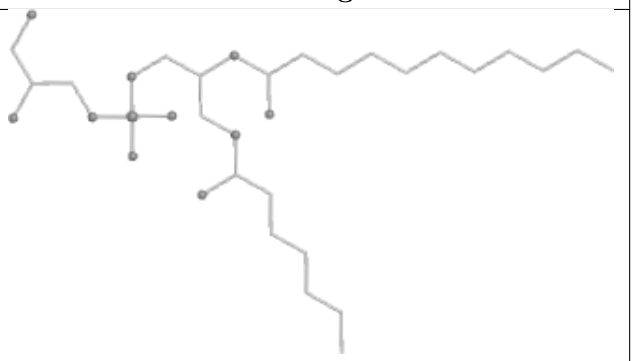
Bond lengths



Bond angles

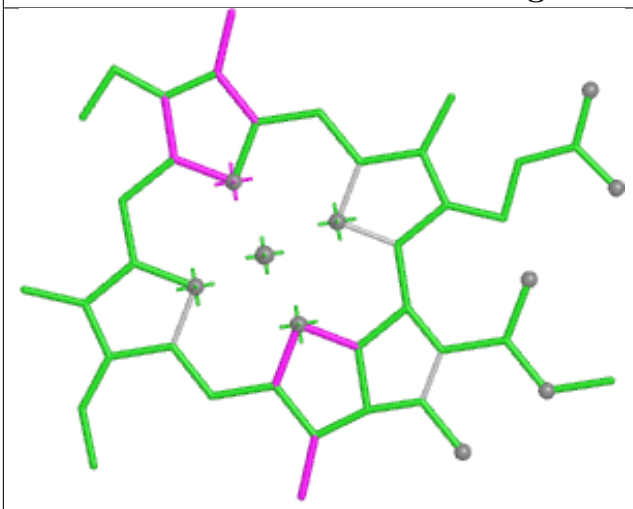


Torsions

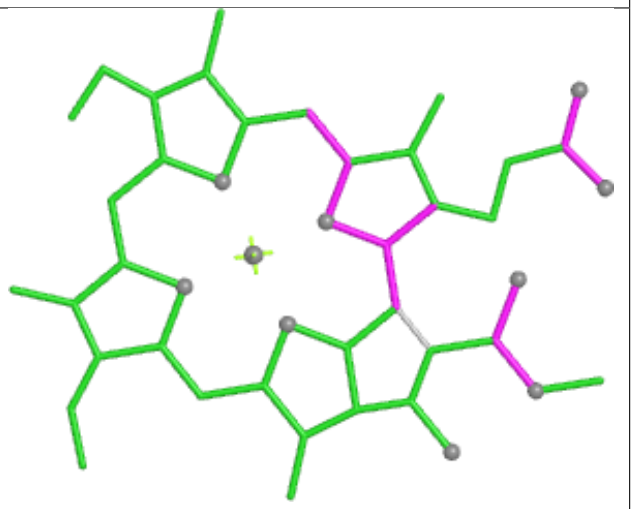


Rings

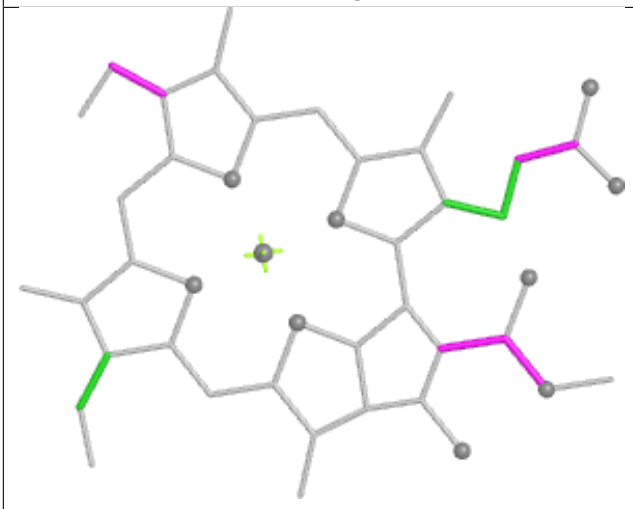
Ligand CLA d 507



Bond lengths



Bond angles

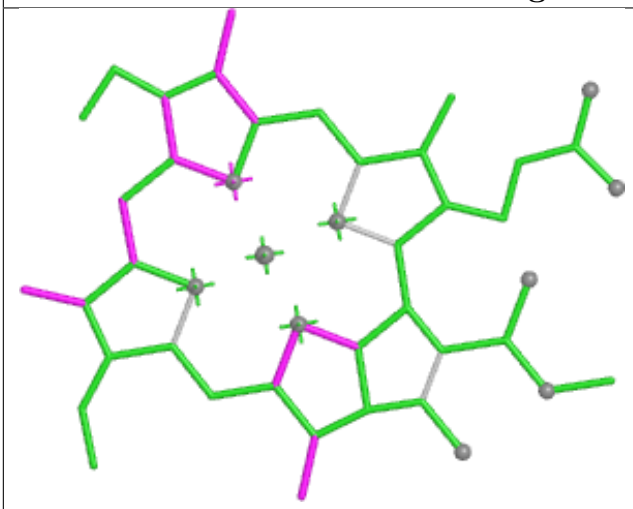


Torsions

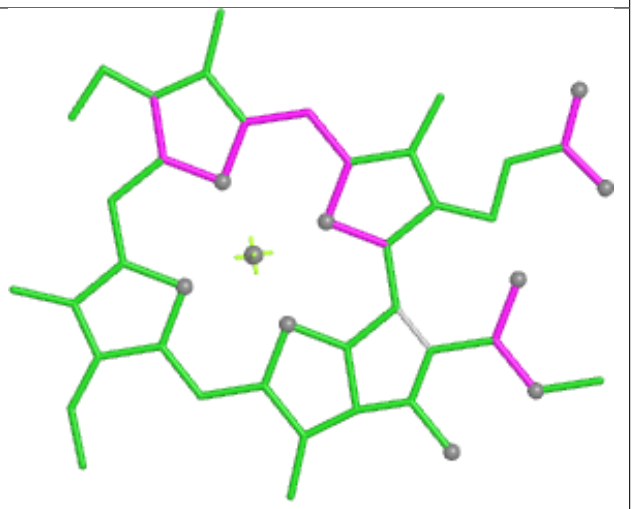


Rings

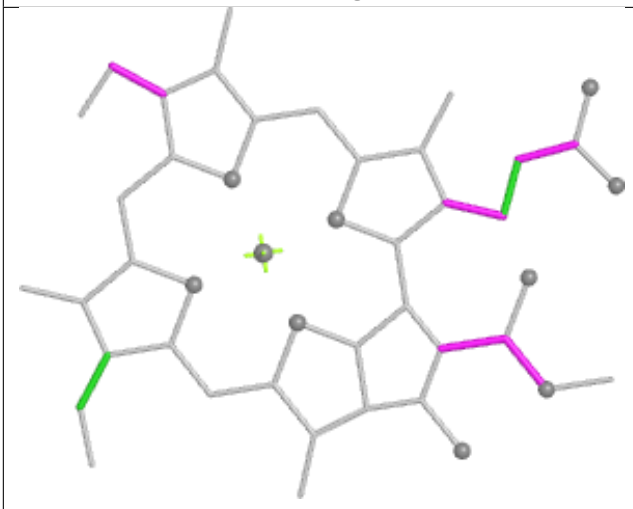
Ligand CLA 6 519



Bond lengths



Bond angles

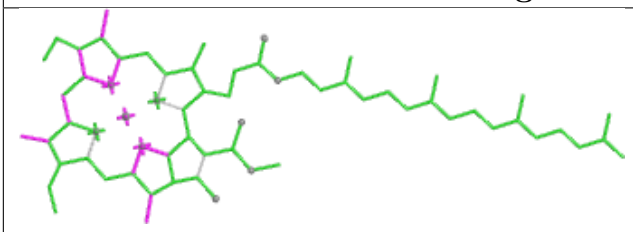


Torsions

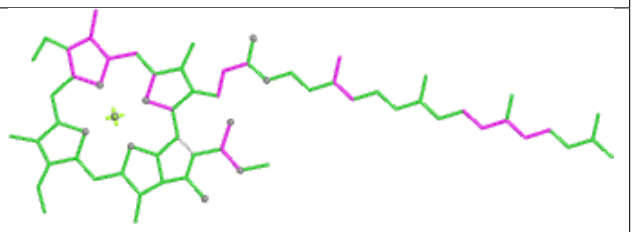


Rings

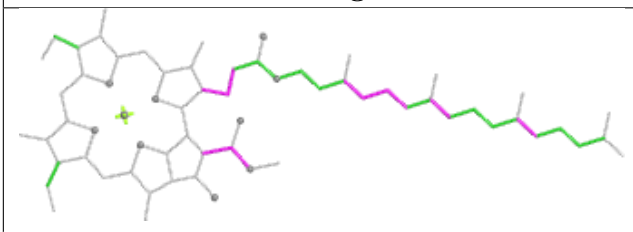
Ligand CLA B 1012



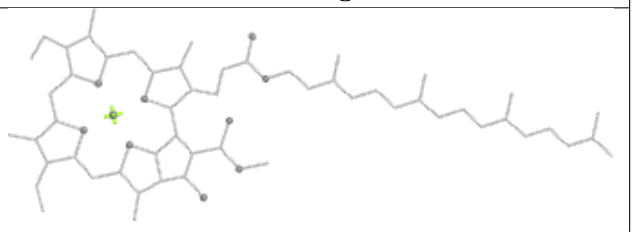
Bond lengths



Bond angles

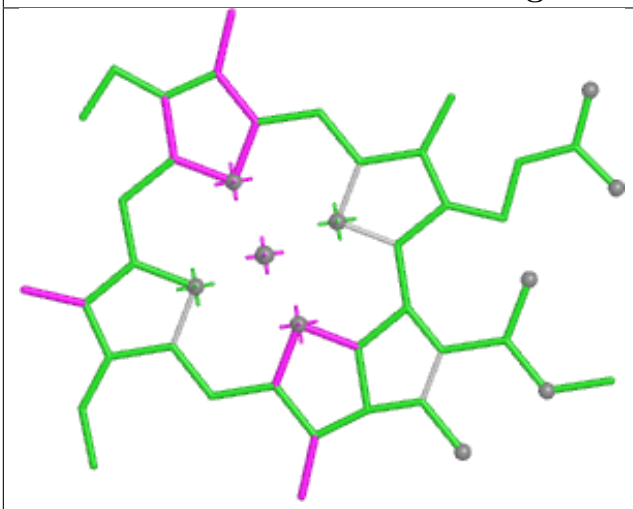


Torsions

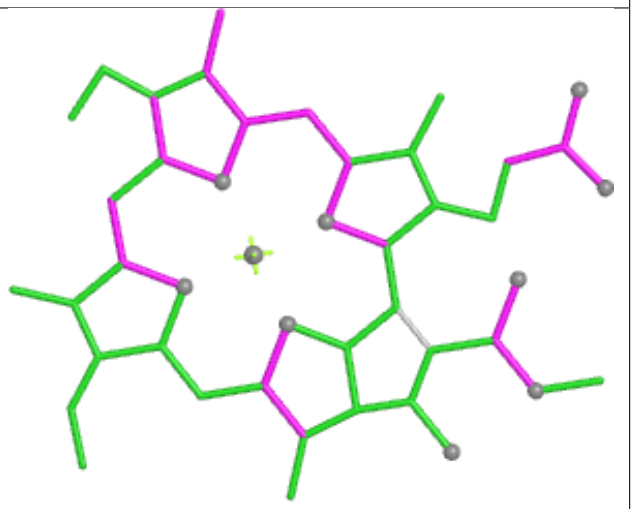


Rings

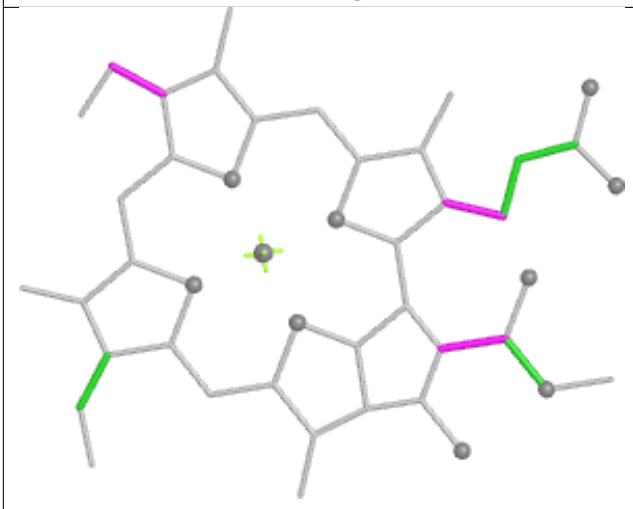
Ligand CLA Z 508



Bond lengths



Bond angles

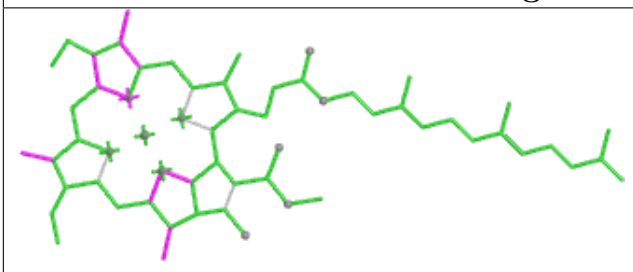


Torsions

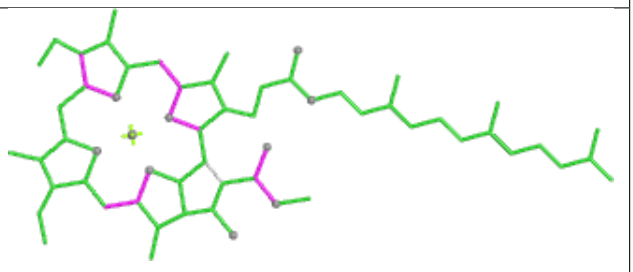


Rings

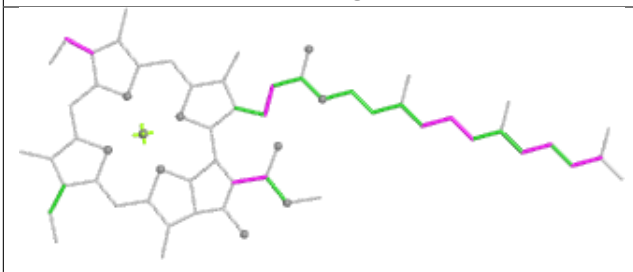
Ligand CLA f 1218



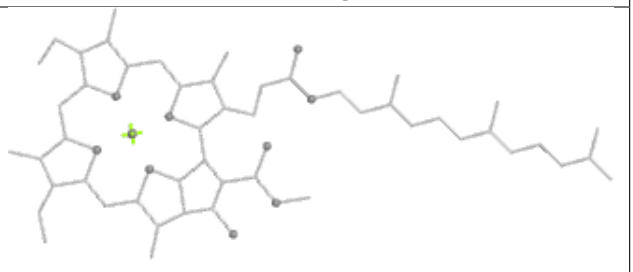
Bond lengths



Bond angles

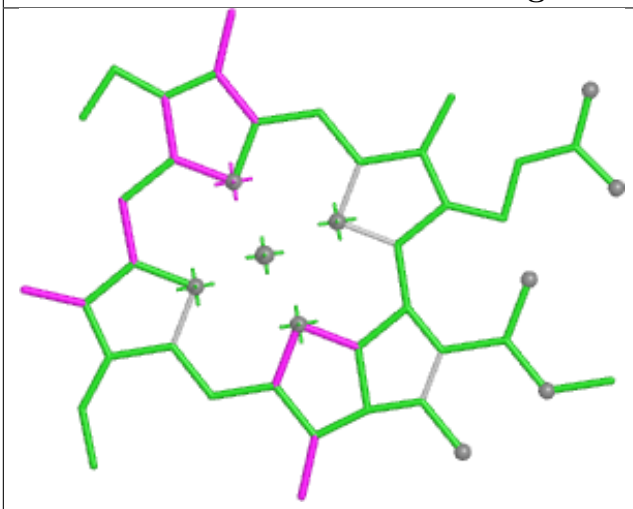


Torsions

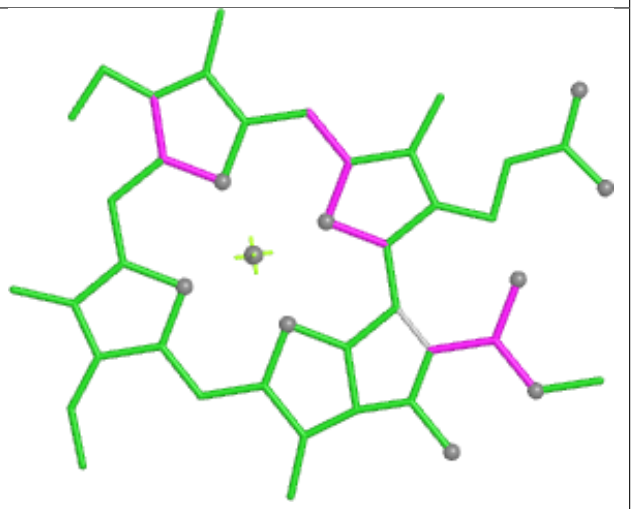


Rings

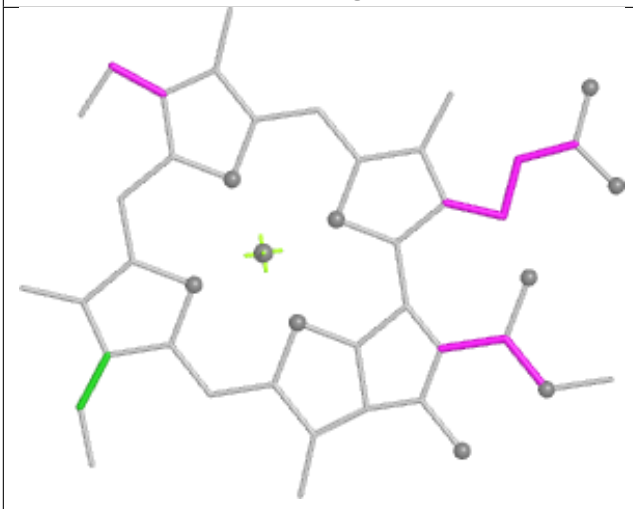
Ligand CLA v 501



Bond lengths



Bond angles

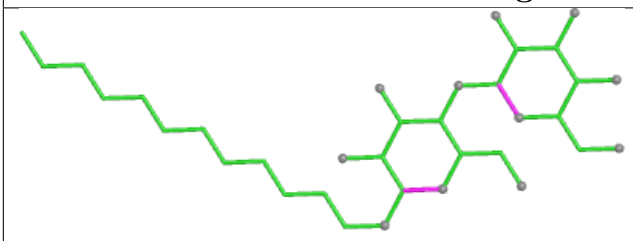


Torsions

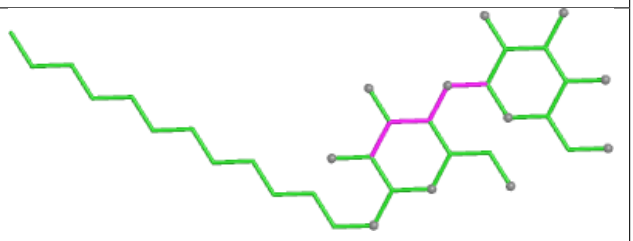


Rings

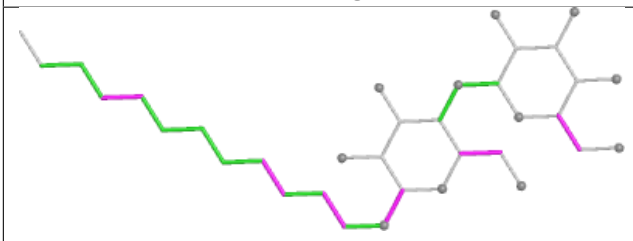
Ligand LMU e 1848



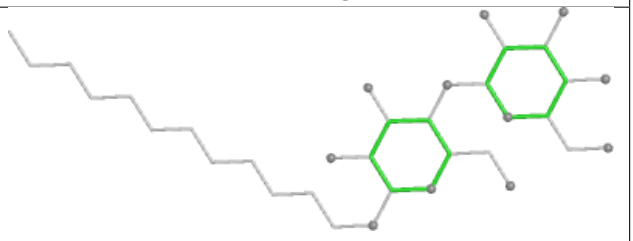
Bond lengths



Bond angles

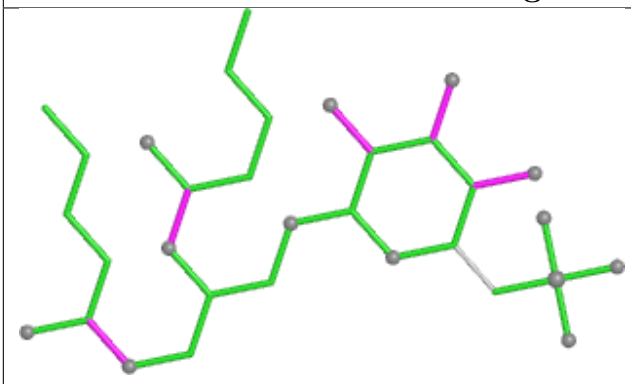


Torsions

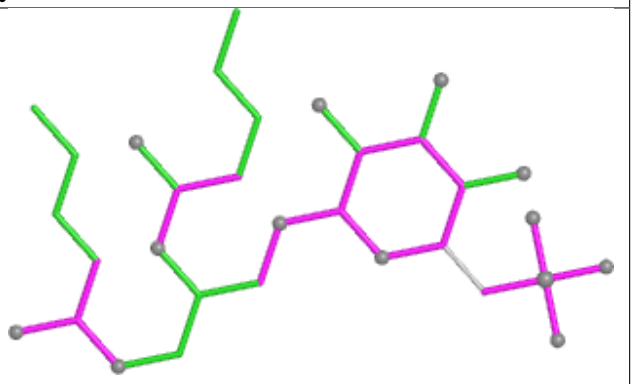


Rings

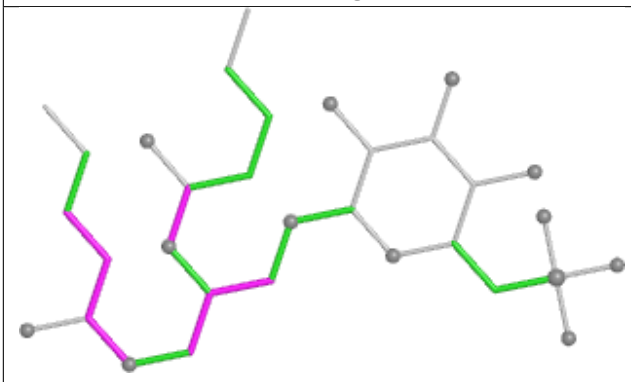
Ligand SQD Y 822



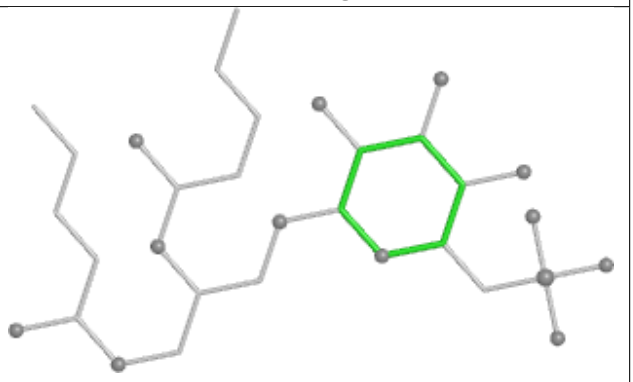
Bond lengths



Bond angles

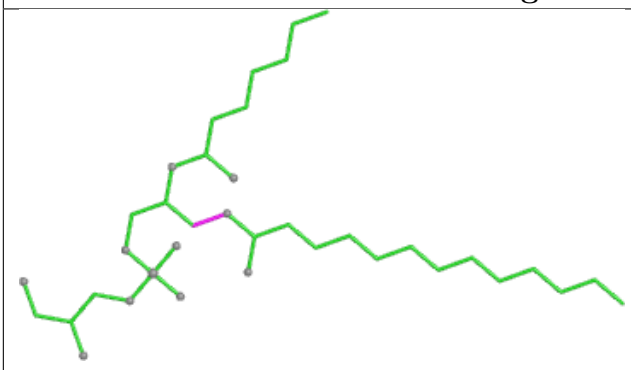


Torsions

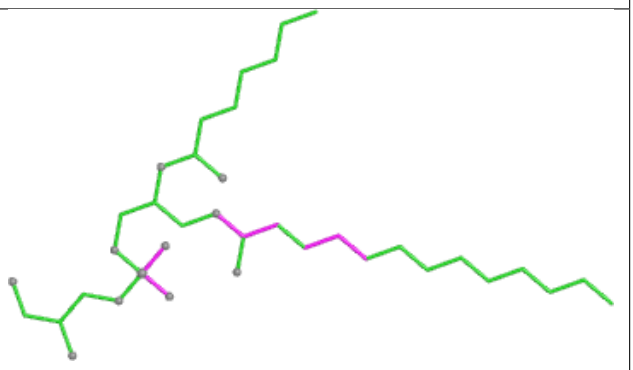


Rings

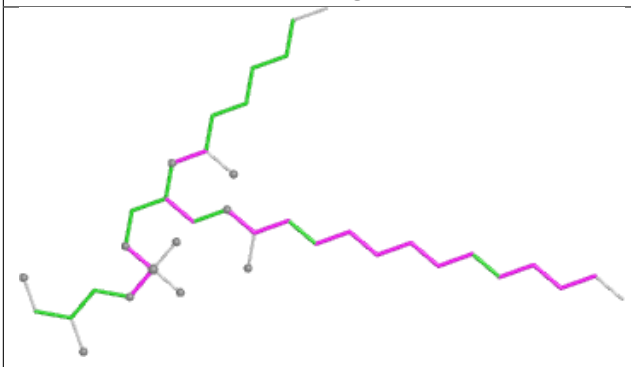
Ligand LHG f 1842



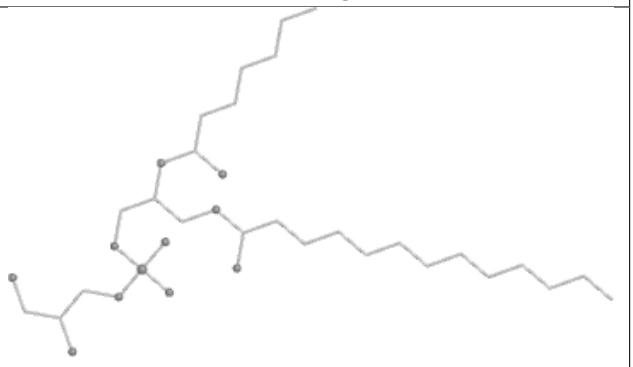
Bond lengths



Bond angles

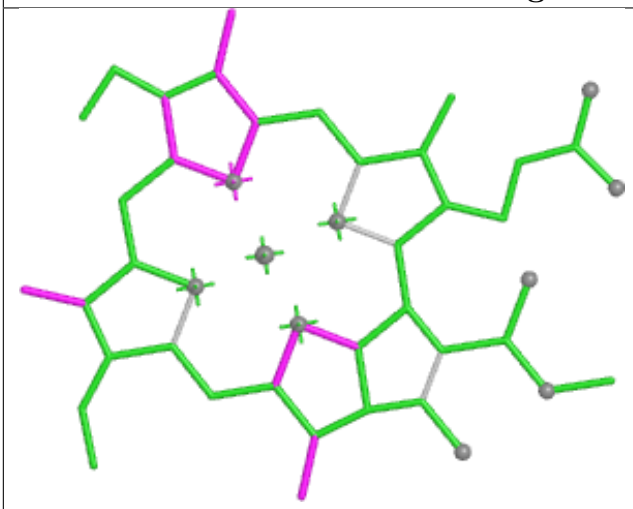


Torsions

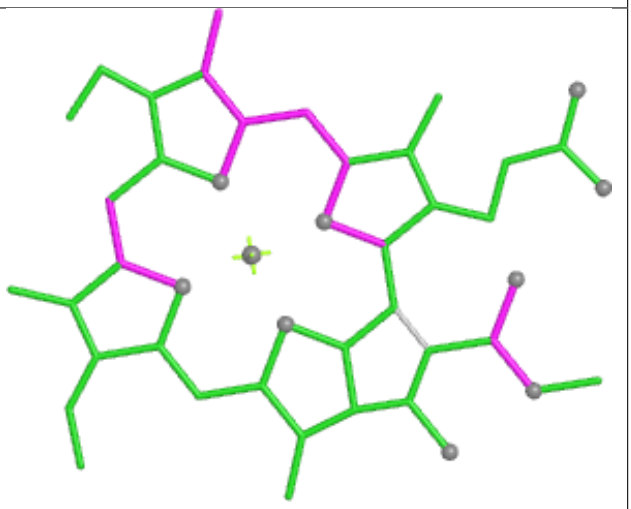


Rings

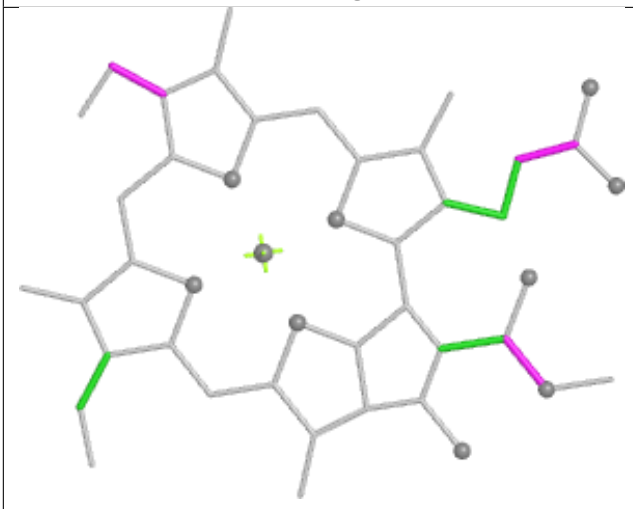
Ligand CLA u 508



Bond lengths



Bond angles

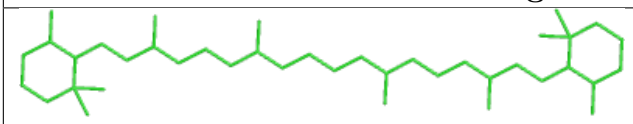


Torsions

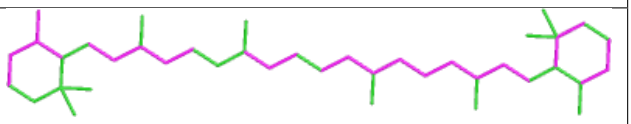


Rings

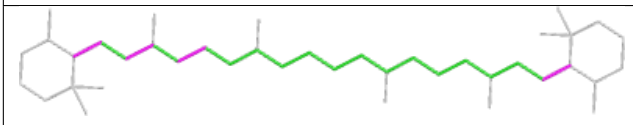
Ligand BCR a 521



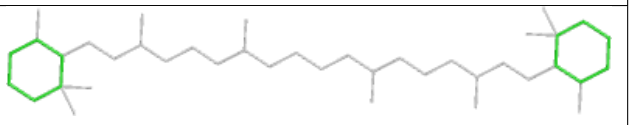
Bond lengths



Bond angles

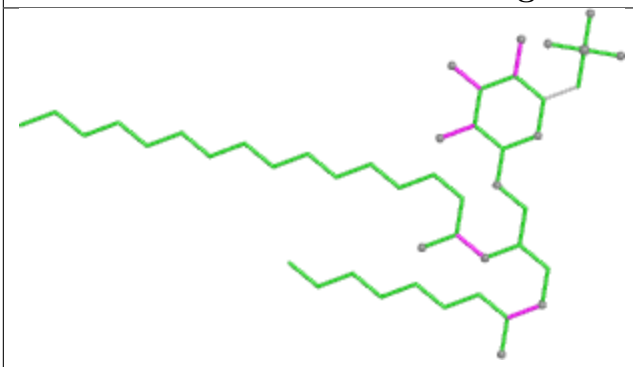


Torsions

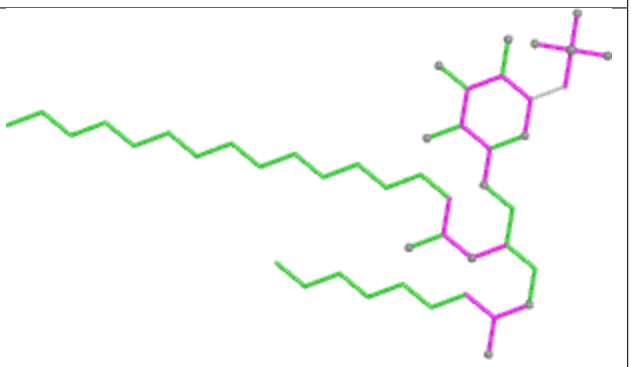


Rings

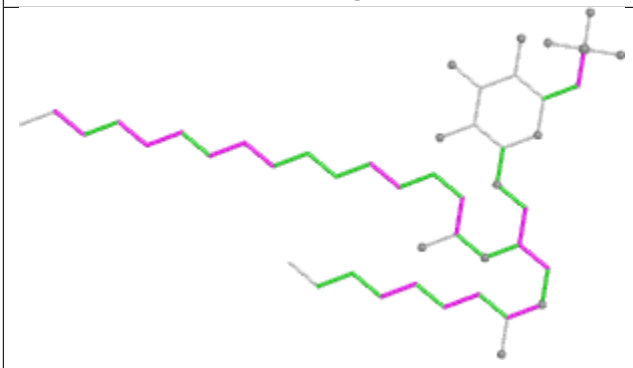
Ligand SQD L 5216



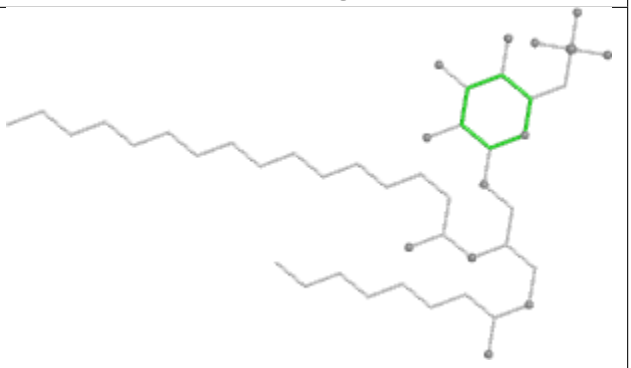
Bond lengths



Bond angles

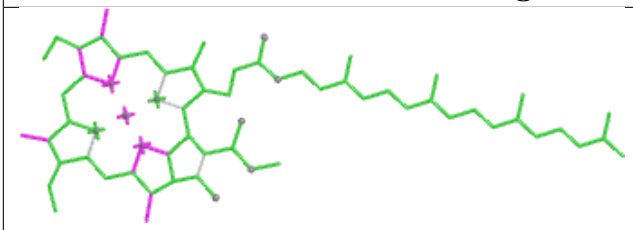


Torsions

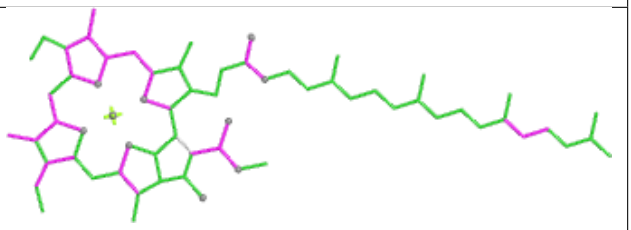


Rings

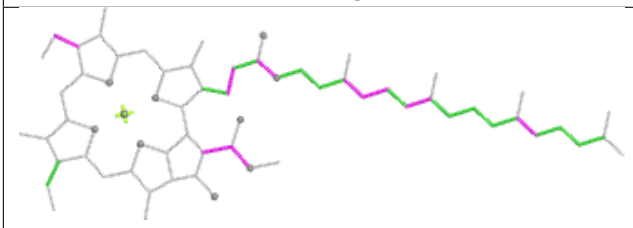
Ligand CLA A 1119



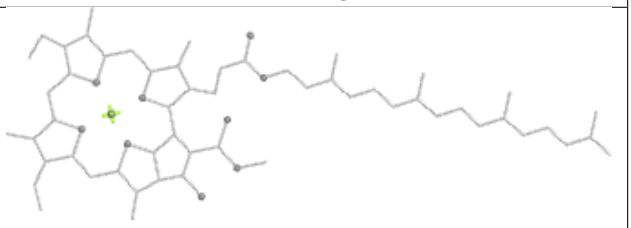
Bond lengths



Bond angles

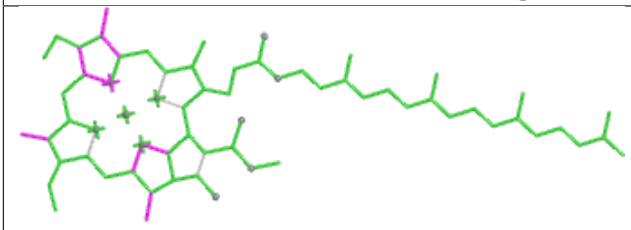


Torsions

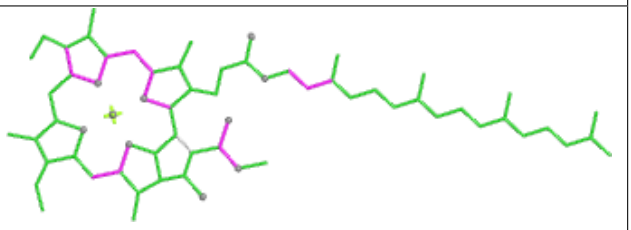


Rings

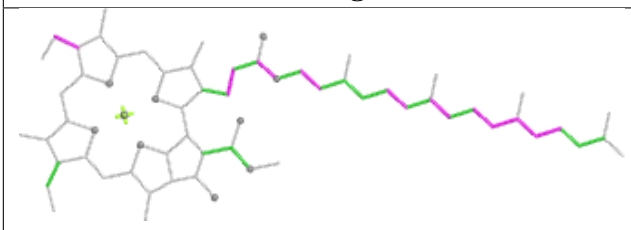
Ligand CLA H 1214



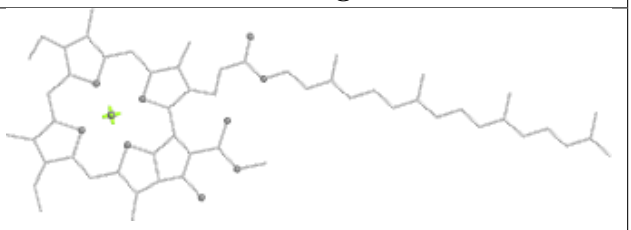
Bond lengths



Bond angles

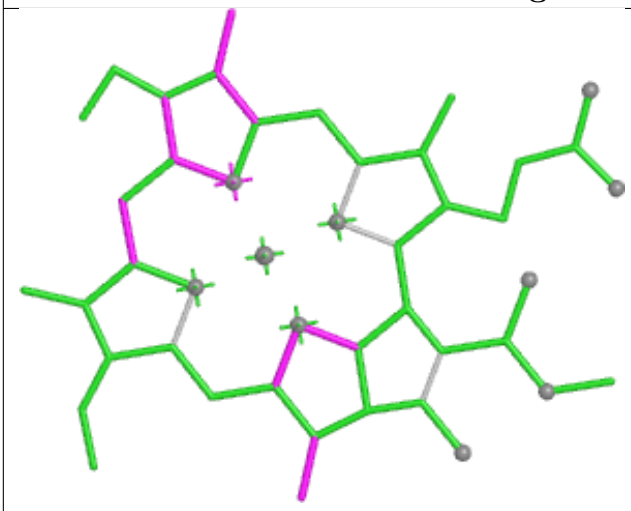


Torsions

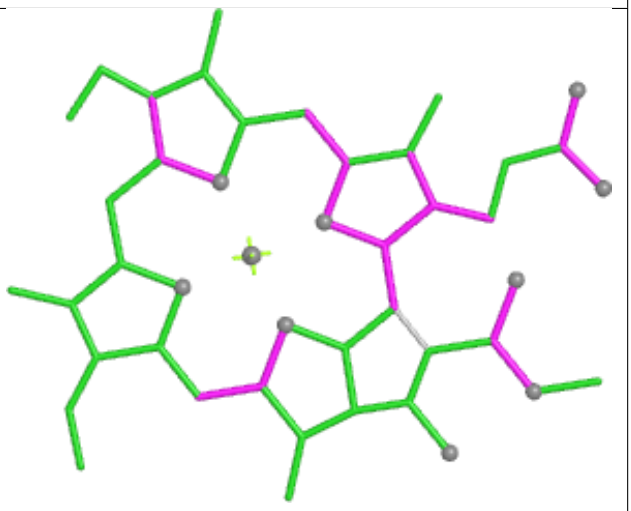


Rings

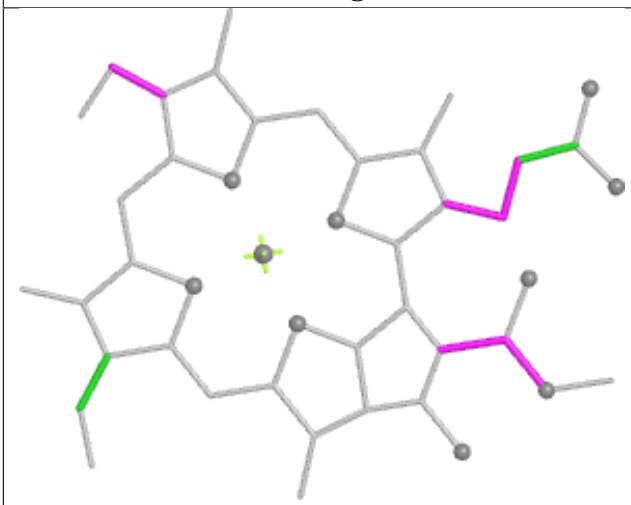
Ligand CLA c 503



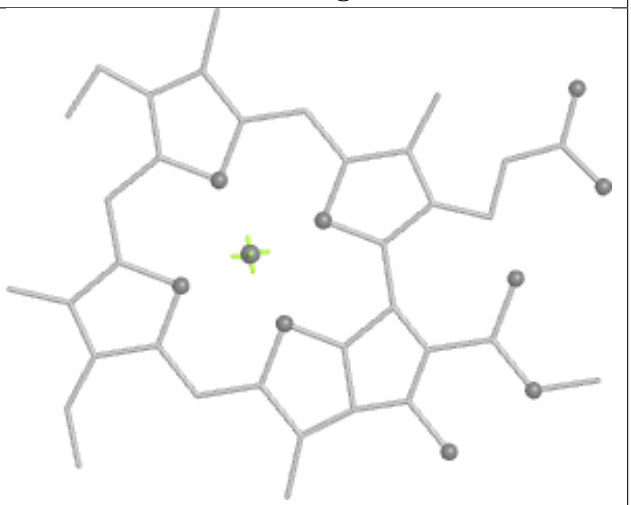
Bond lengths



Bond angles

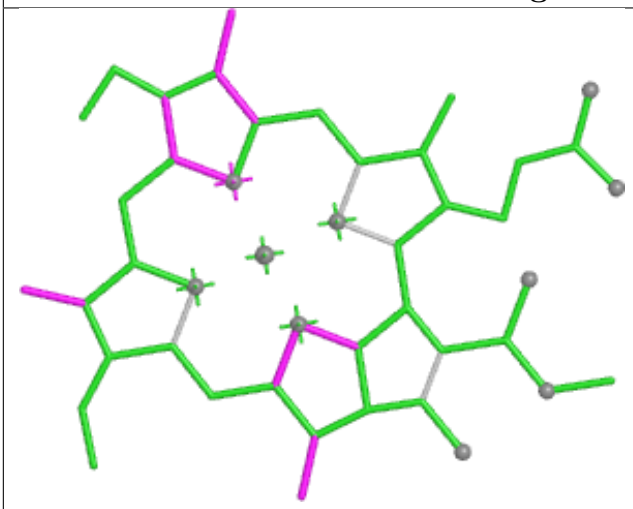


Torsions

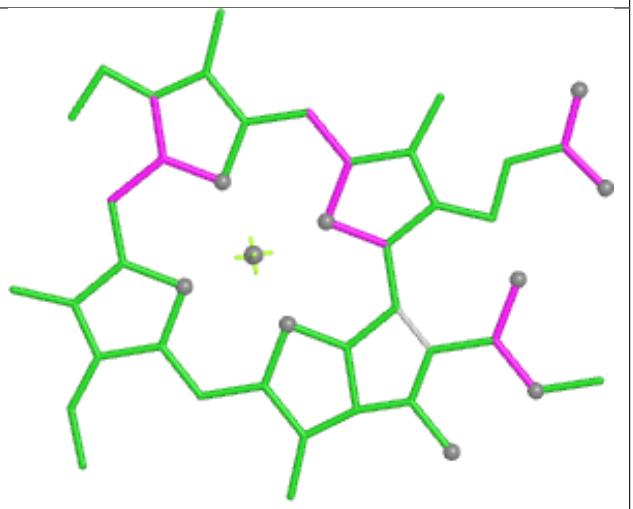


Rings

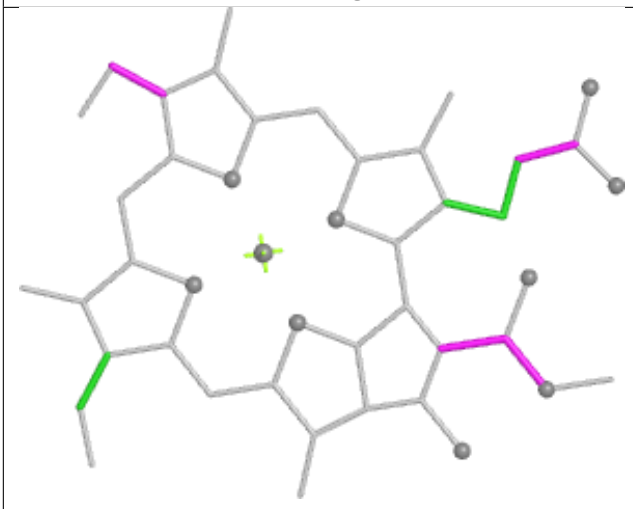
Ligand CLA s 519



Bond lengths



Bond angles

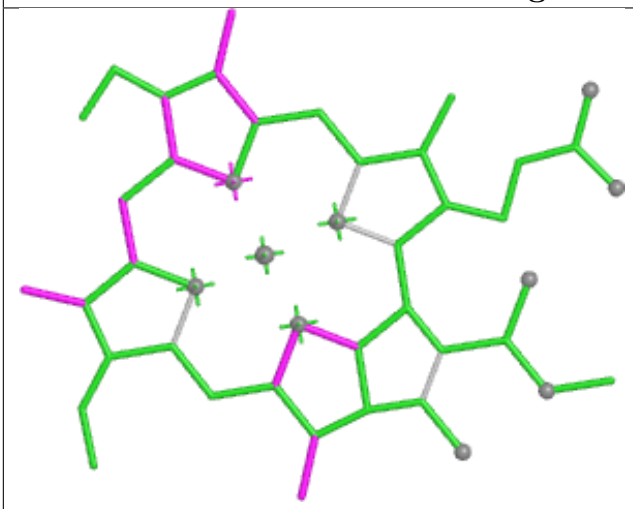


Torsions

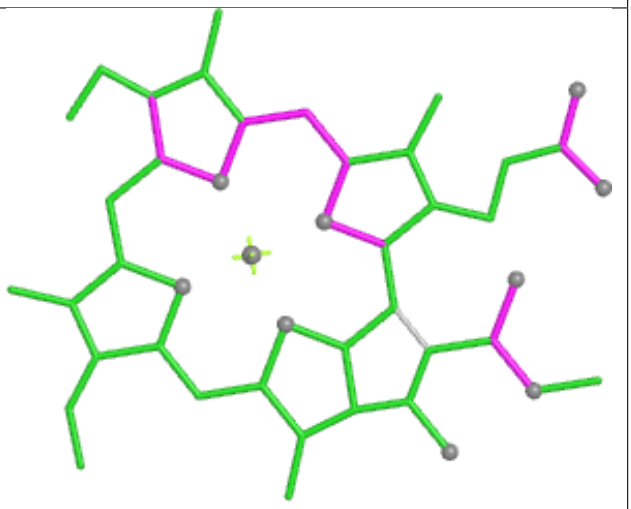


Rings

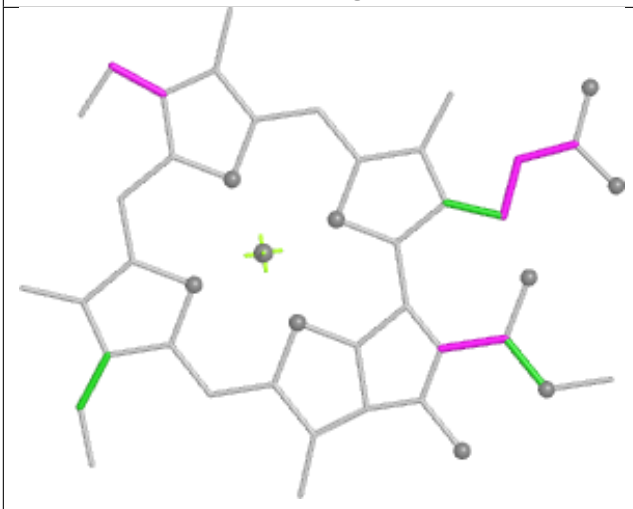
Ligand CLA 1 513



Bond lengths



Bond angles

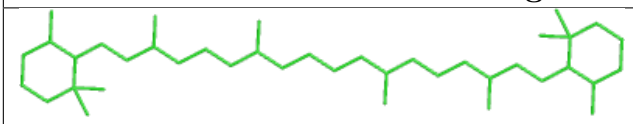


Torsions

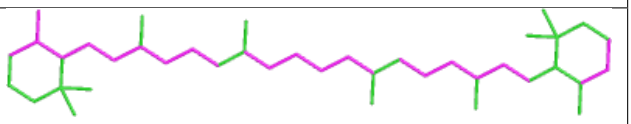


Rings

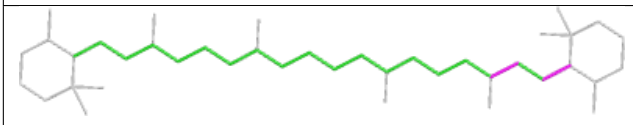
Ligand BCR d 523



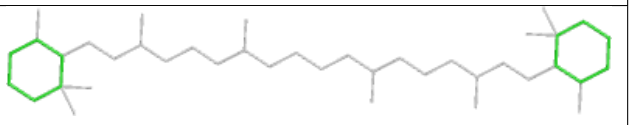
Bond lengths



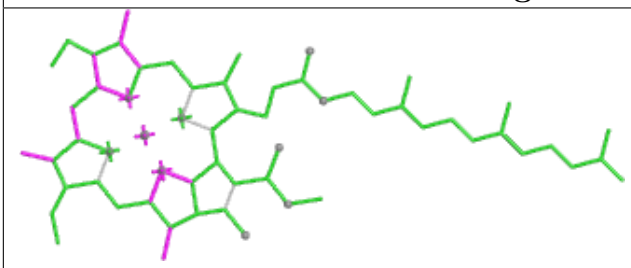
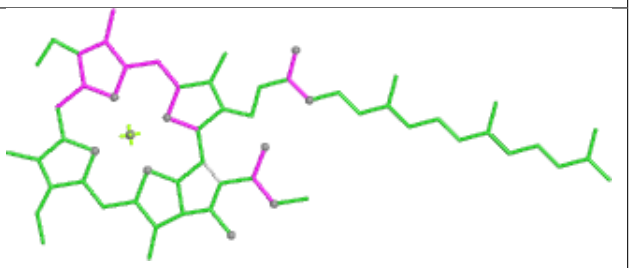
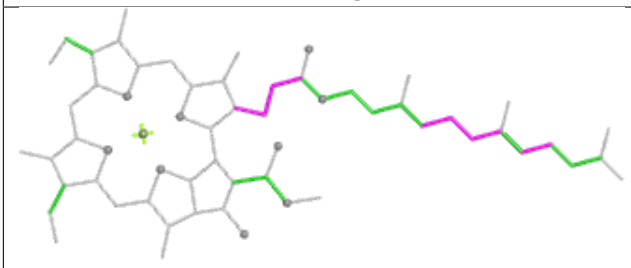
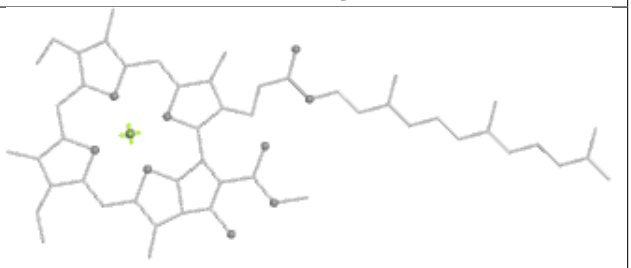
Bond angles

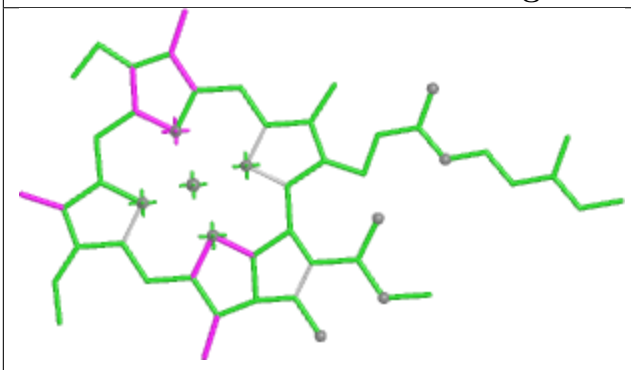
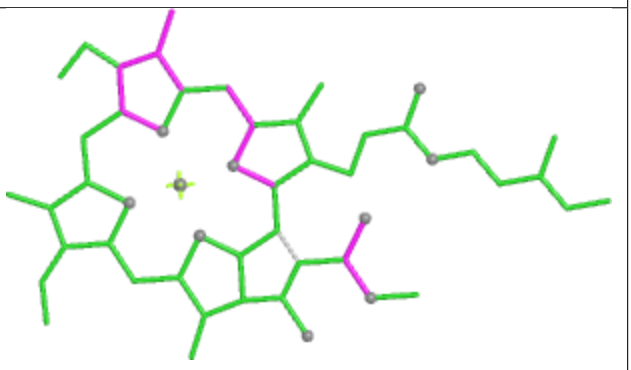
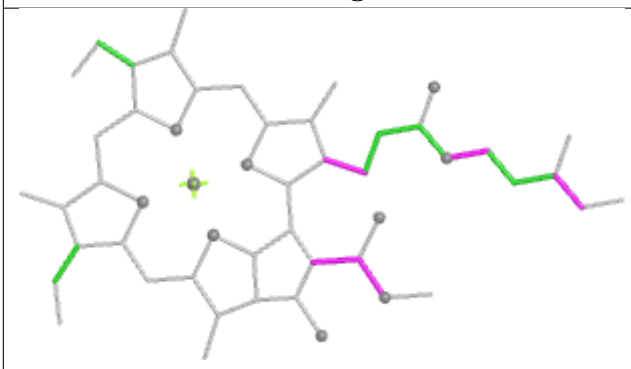
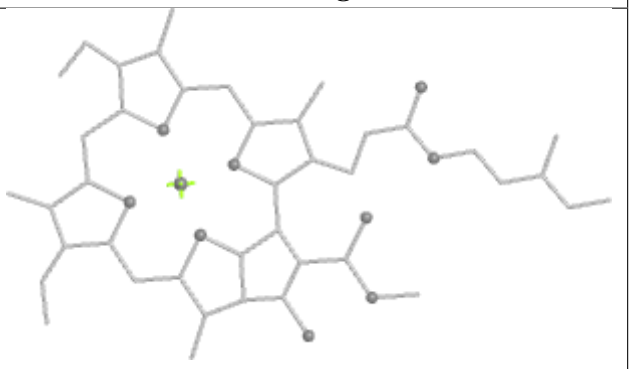


Torsions

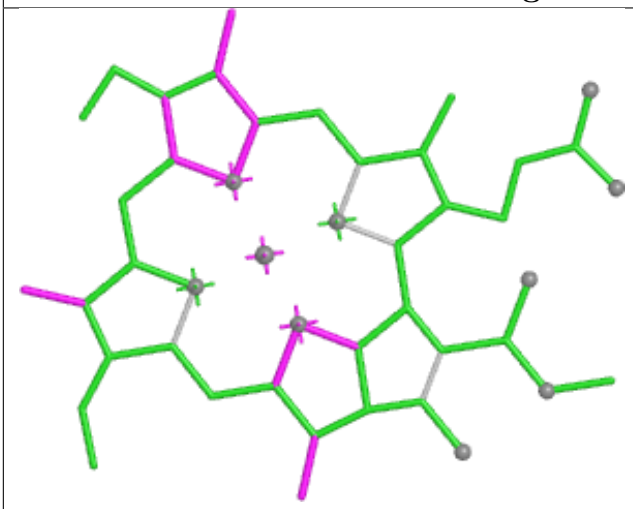


Rings

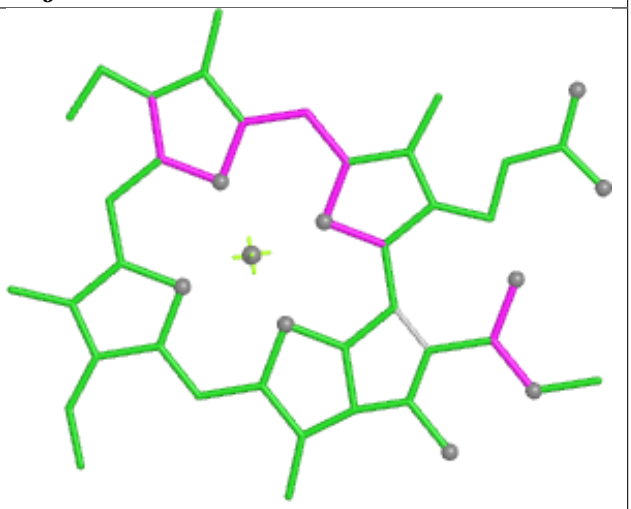
Ligand CLA G 1116	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 1212	
	
Bond lengths	Bond angles
	
Torsions	Rings

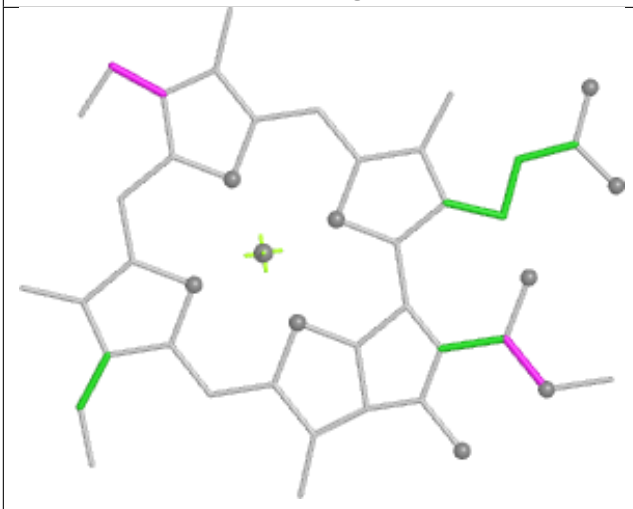
Ligand CLA j 1301



Bond lengths



Bond angles

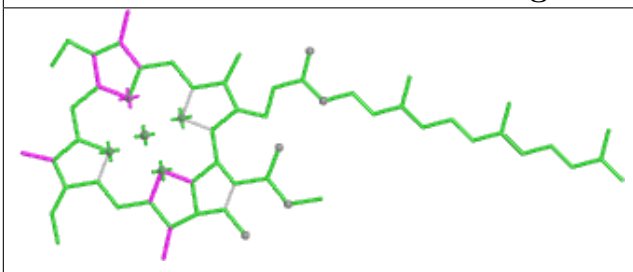


Torsions

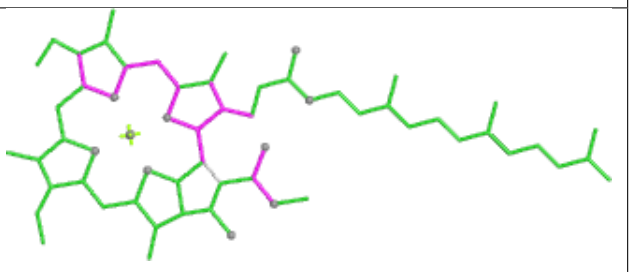


Rings

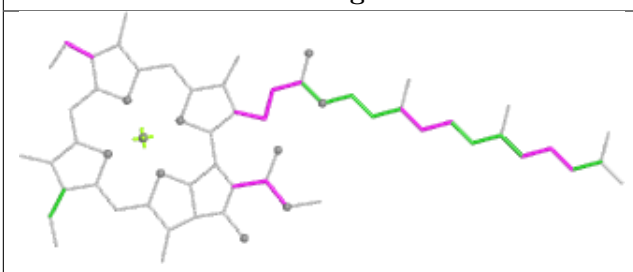
Ligand CLA r 501



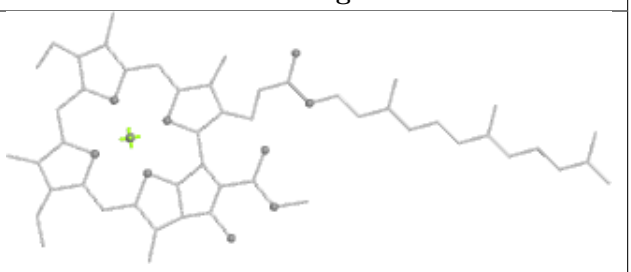
Bond lengths



Bond angles

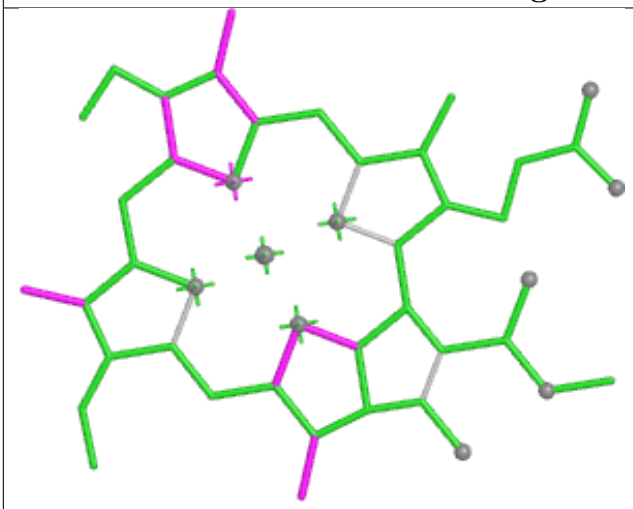


Torsions

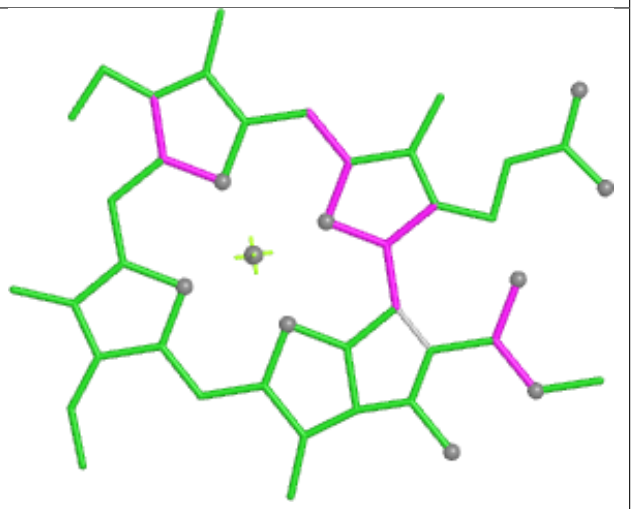


Rings

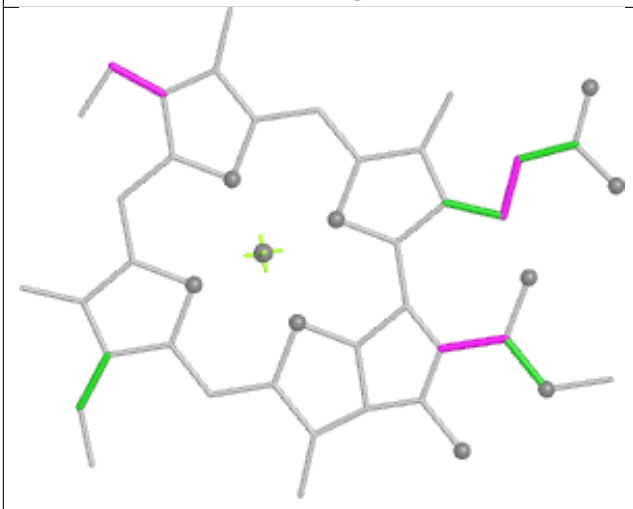
Ligand CLA t 502



Bond lengths



Bond angles

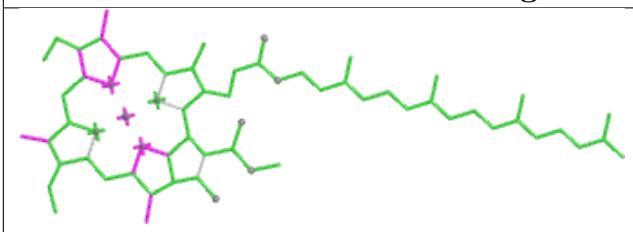


Torsions

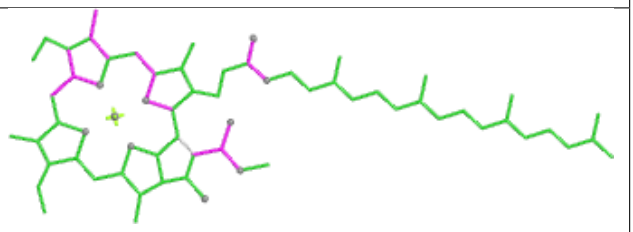


Rings

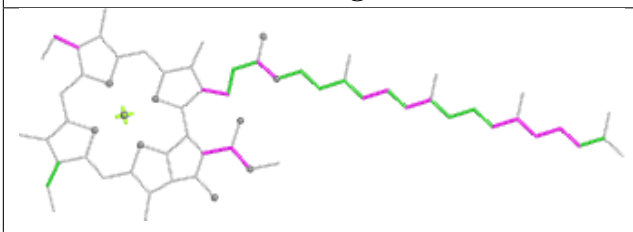
Ligand CLA e 1109



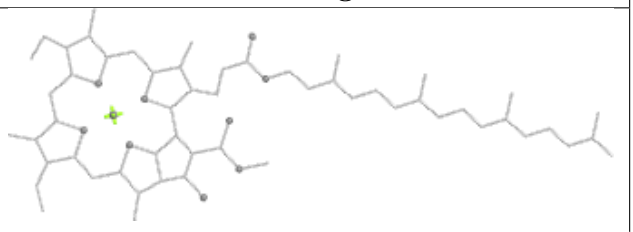
Bond lengths



Bond angles

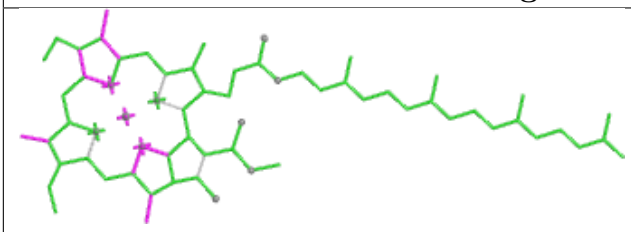


Torsions

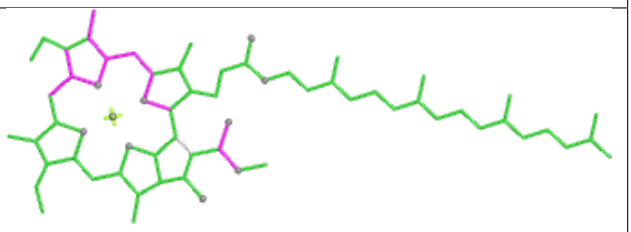


Rings

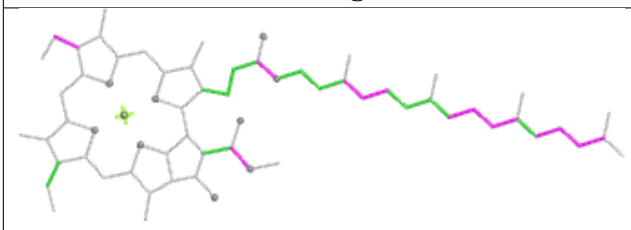
Ligand CLA e 1133



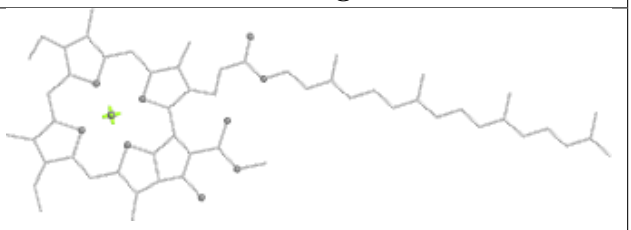
Bond lengths



Bond angles



Torsions

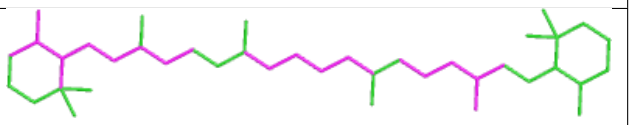


Rings

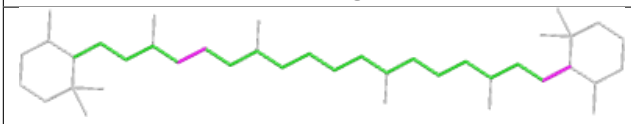
Ligand BCR Z 524



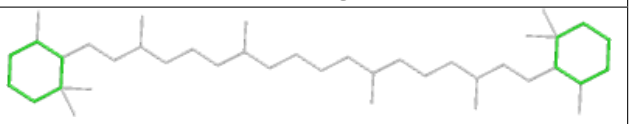
Bond lengths



Bond angles

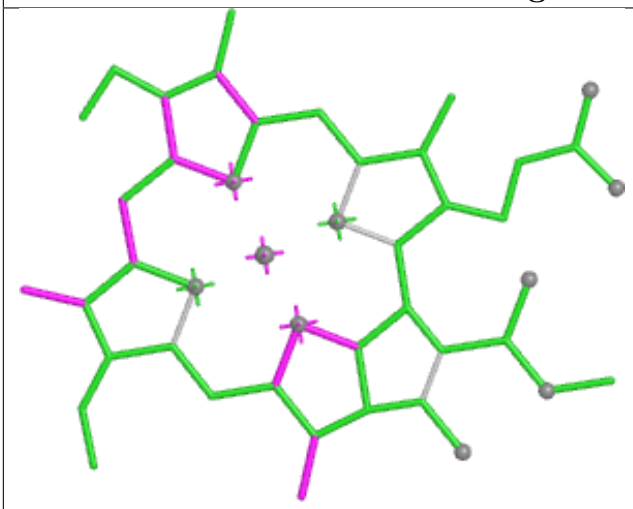


Torsions

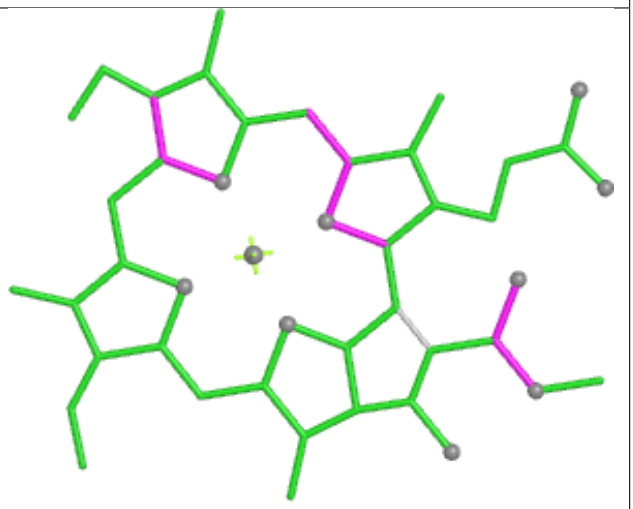


Rings

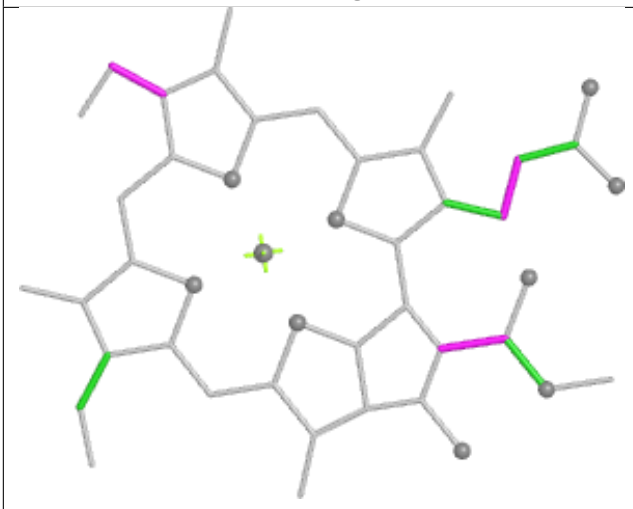
Ligand CLA 4 505



Bond lengths



Bond angles

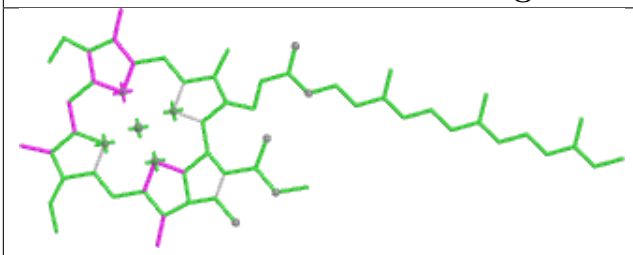


Torsions

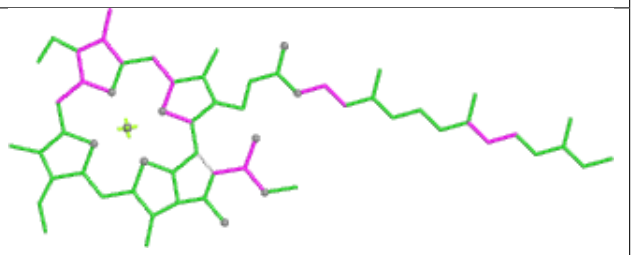


Rings

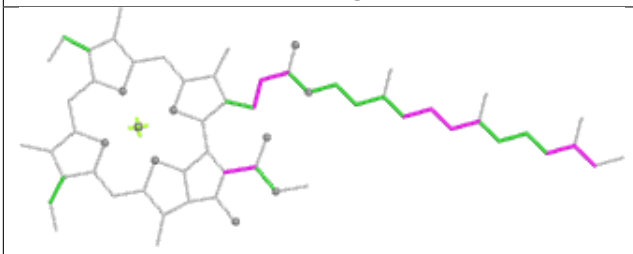
Ligand CLA H 1213



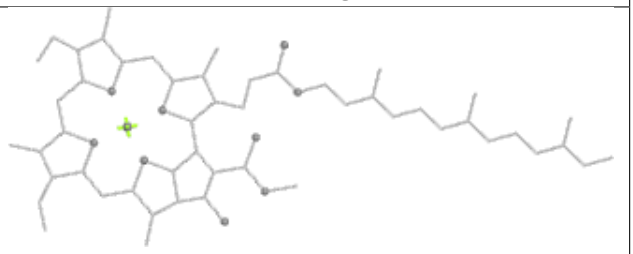
Bond lengths



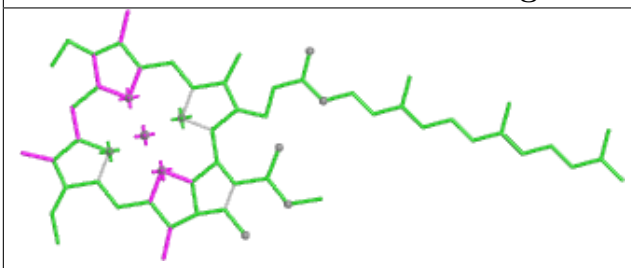
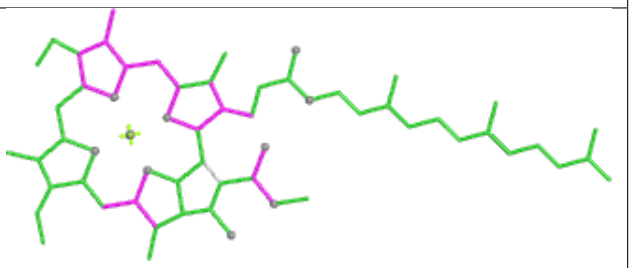
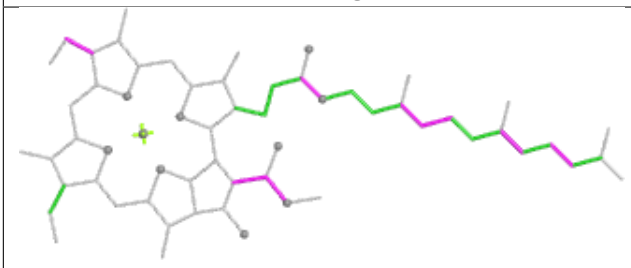
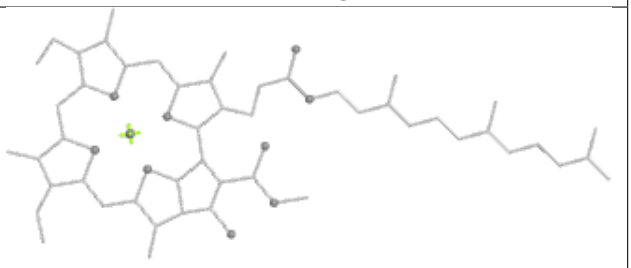
Bond angles

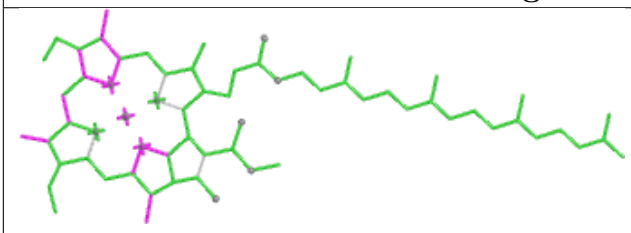
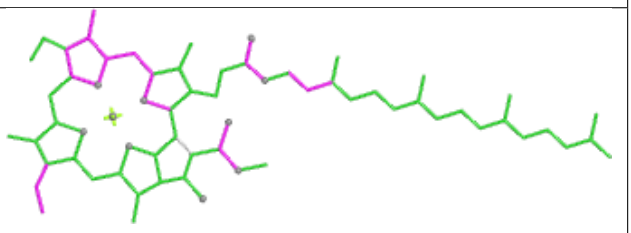
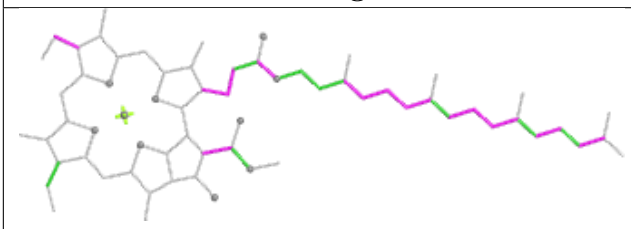
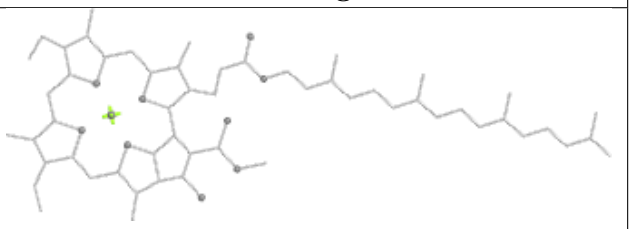


Torsions

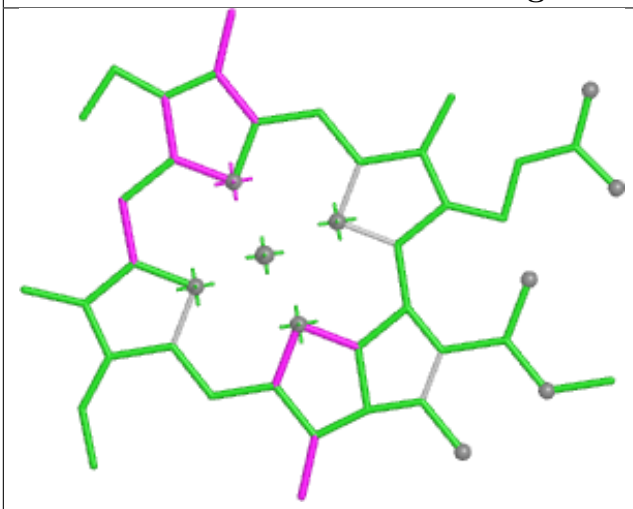


Rings

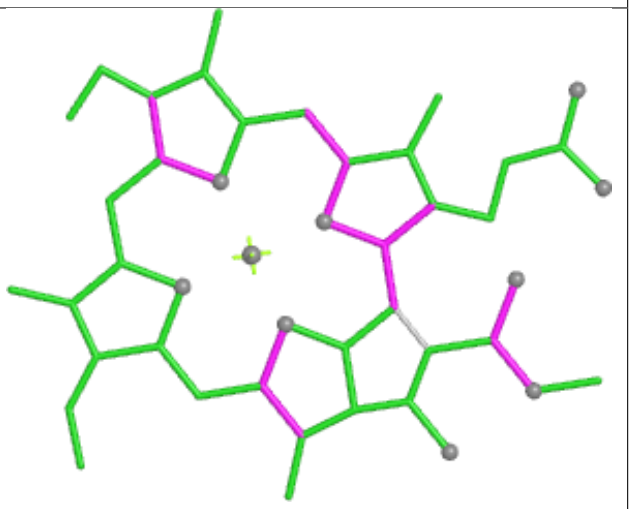
Ligand CLA e 1124	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings

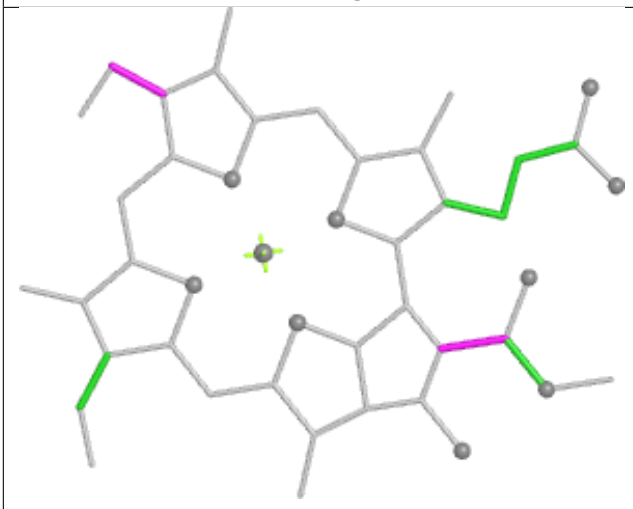
Ligand CLA b 503



Bond lengths



Bond angles

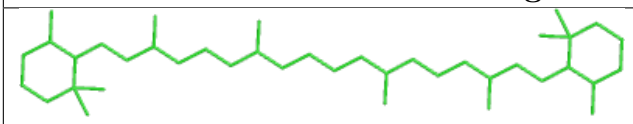


Torsions

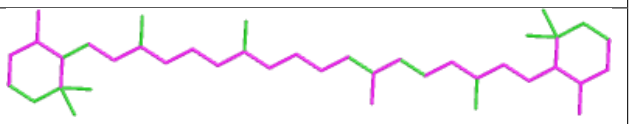


Rings

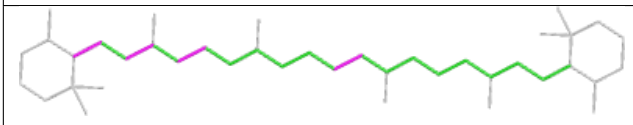
Ligand BCR Z 522



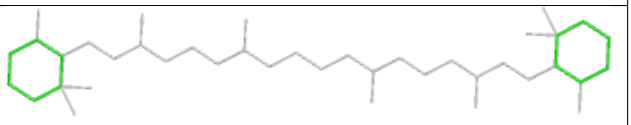
Bond lengths



Bond angles

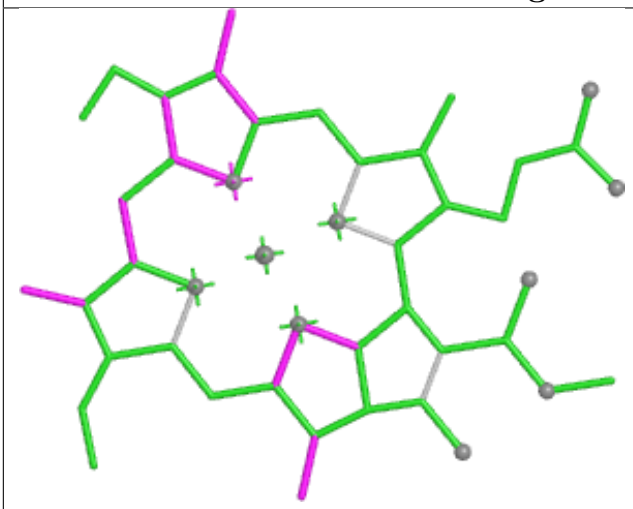


Torsions

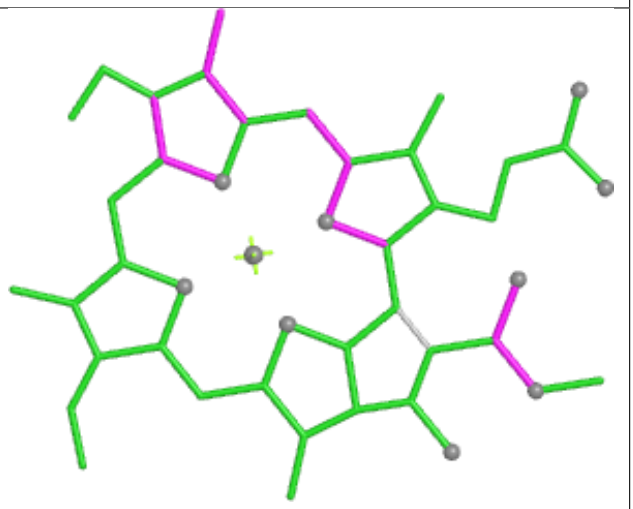


Rings

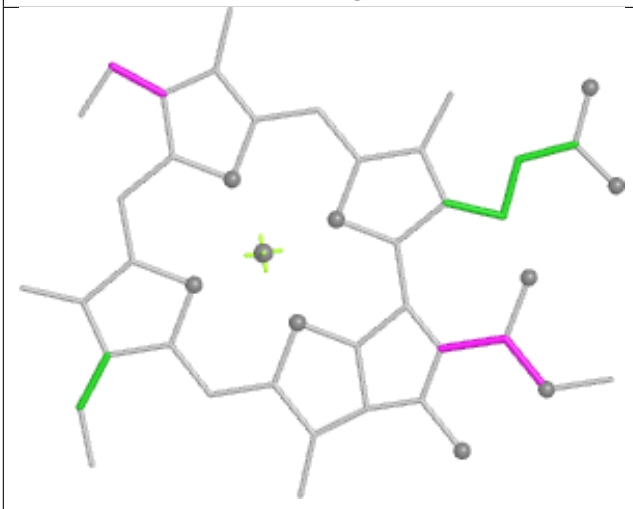
Ligand CLA 6 506



Bond lengths



Bond angles

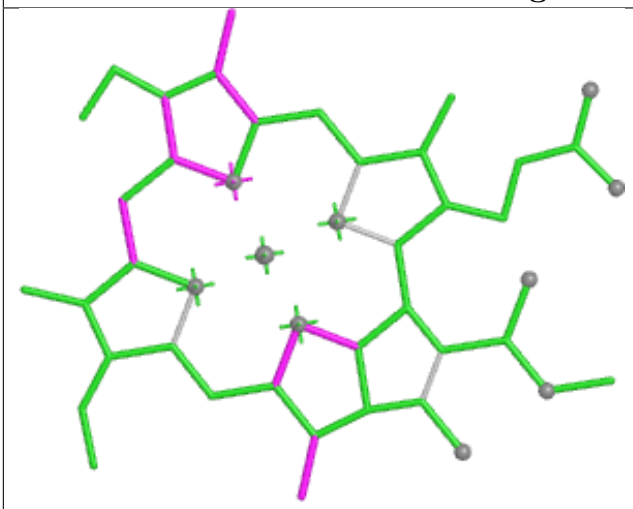


Torsions

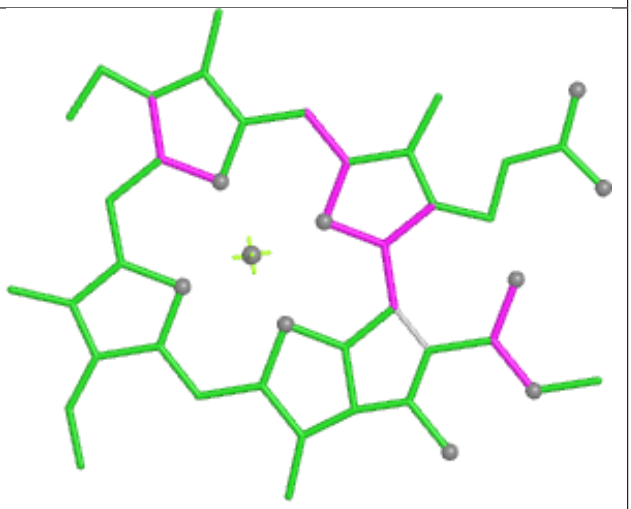


Rings

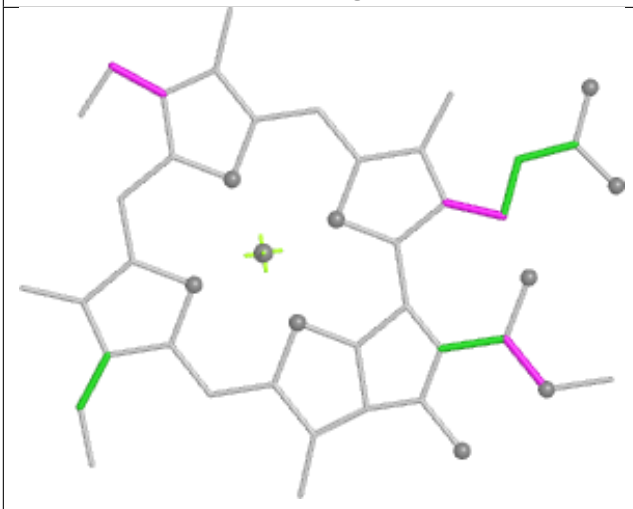
Ligand CLA c 504



Bond lengths



Bond angles

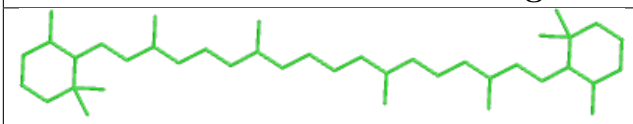


Torsions

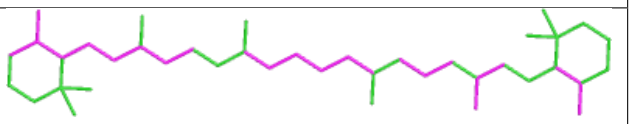


Rings

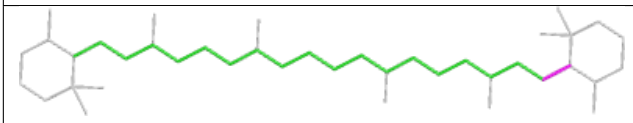
Ligand BCR u 524



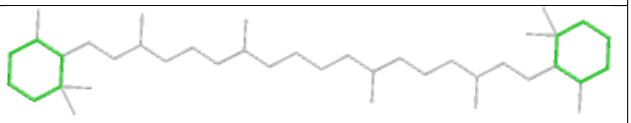
Bond lengths



Bond angles

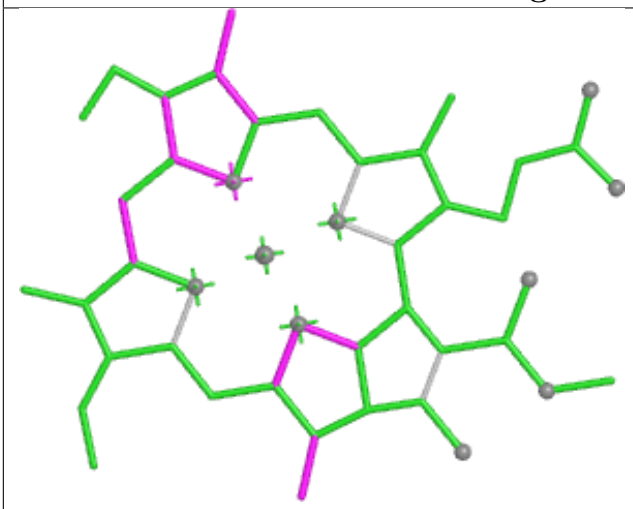


Torsions

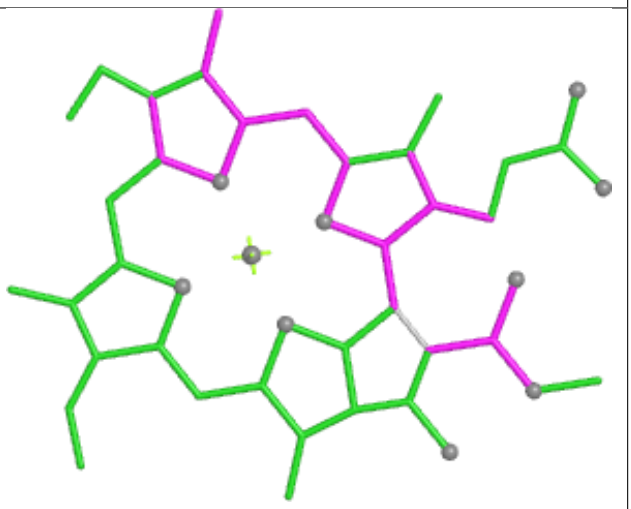


Rings

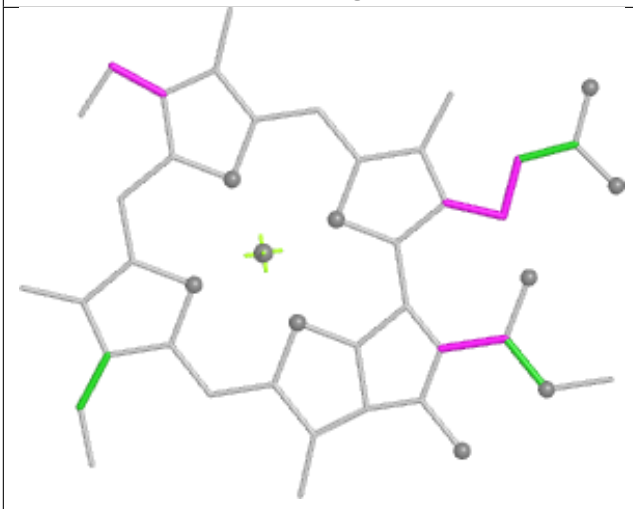
Ligand CLA s 504



Bond lengths



Bond angles

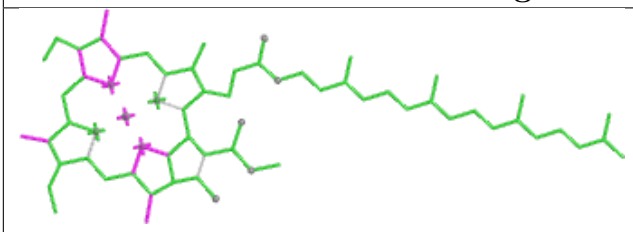


Torsions

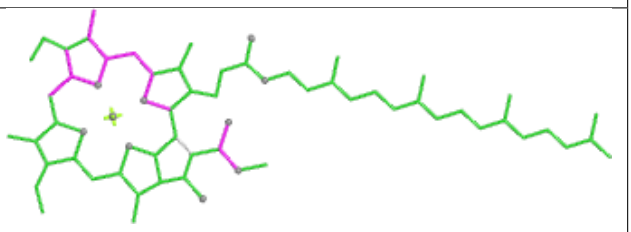


Rings

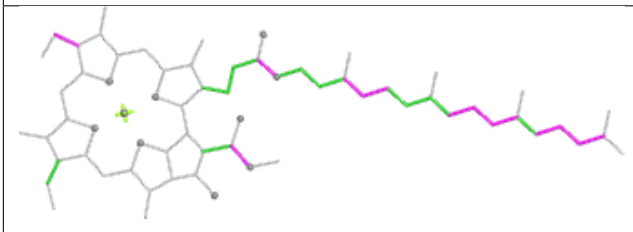
Ligand CLA G 1133



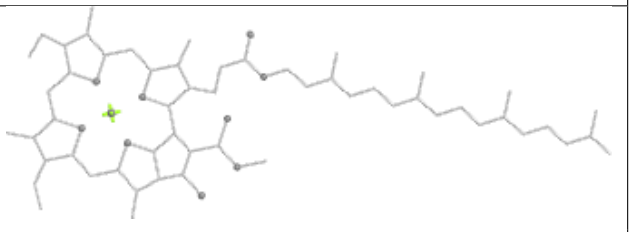
Bond lengths



Bond angles

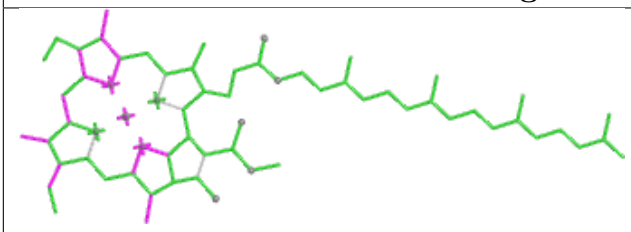


Torsions

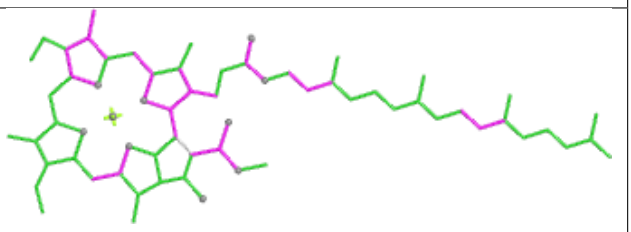


Rings

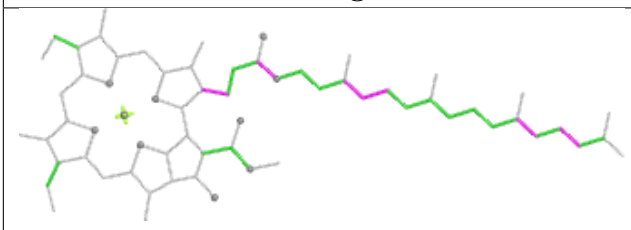
Ligand CLA e 1104



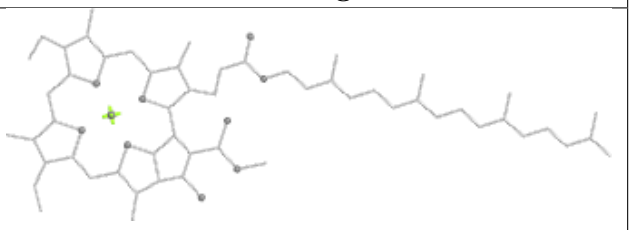
Bond lengths



Bond angles

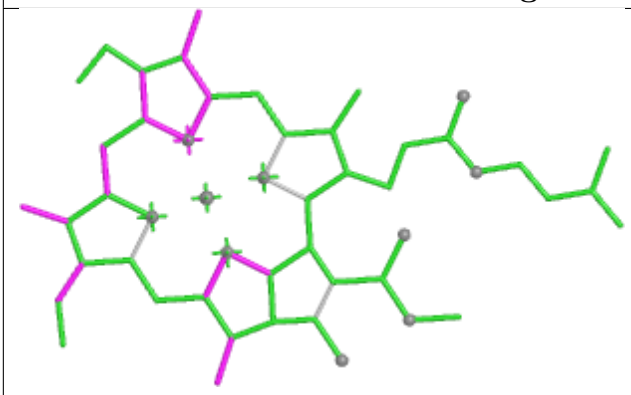


Torsions

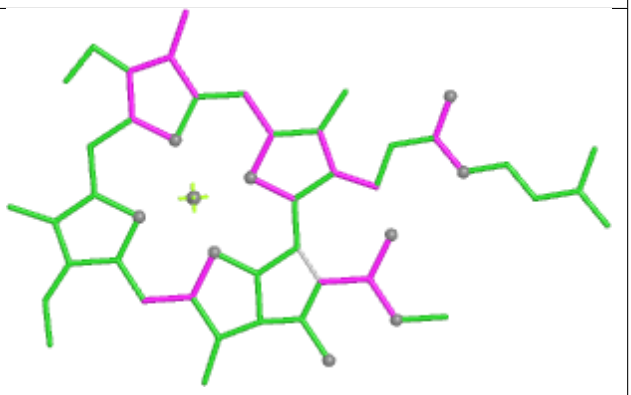


Rings

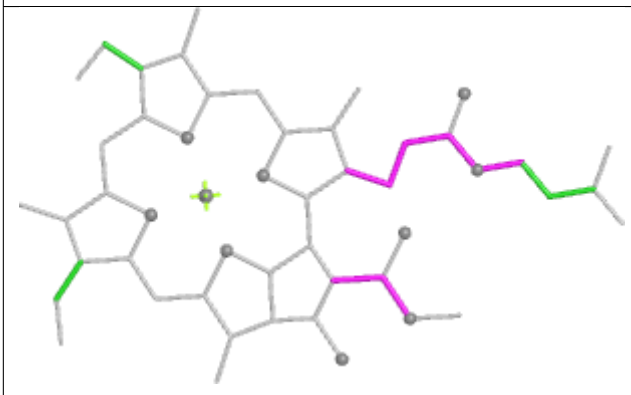
Ligand CLA e 1120



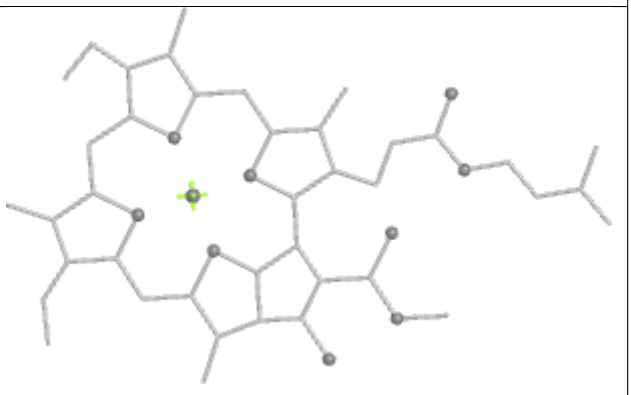
Bond lengths



Bond angles

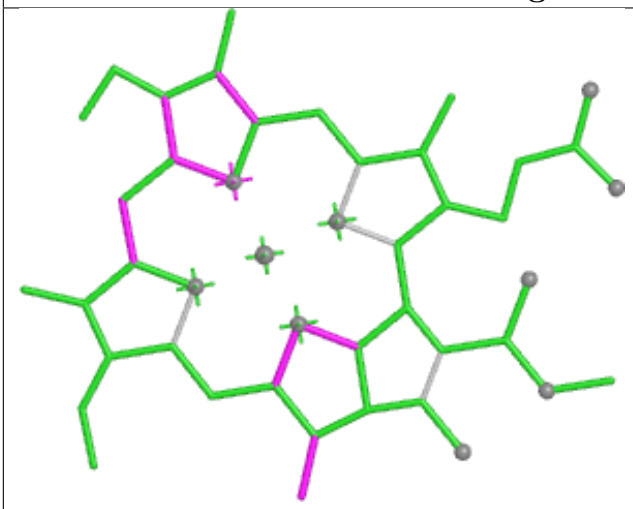


Torsions

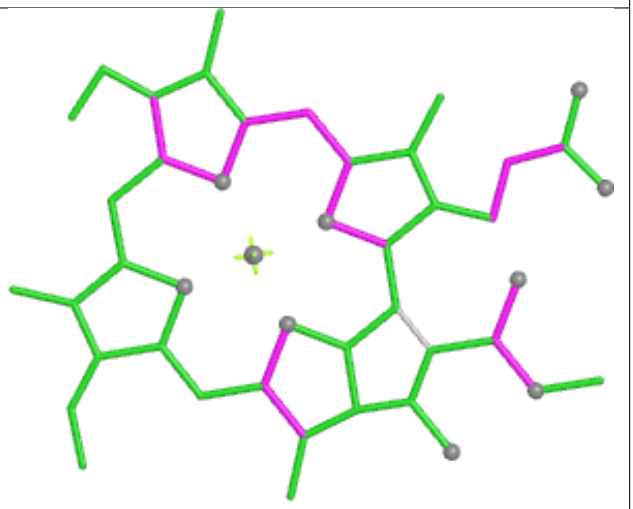


Rings

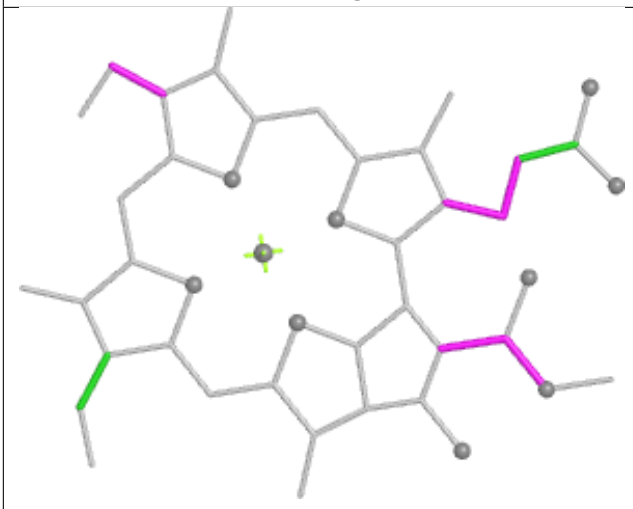
Ligand CLA a 503



Bond lengths



Bond angles

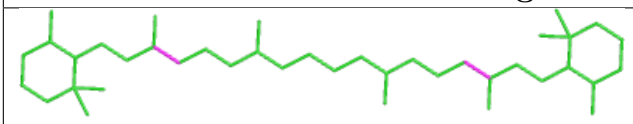


Torsions

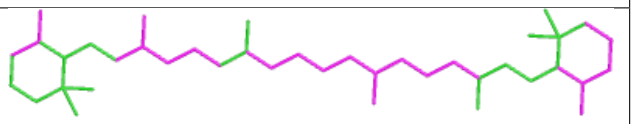


Rings

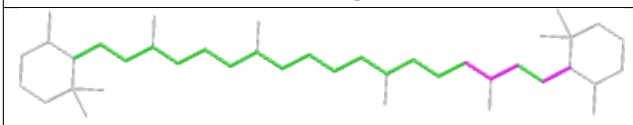
Ligand BCR n 4020



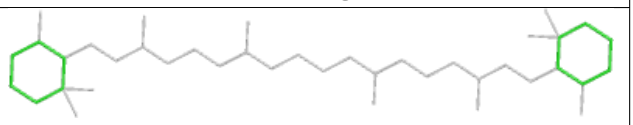
Bond lengths



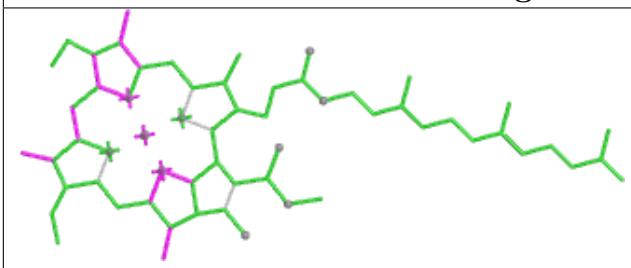
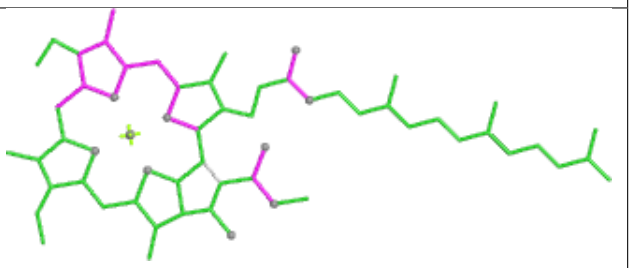
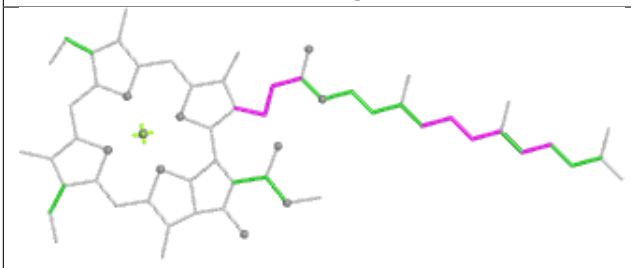
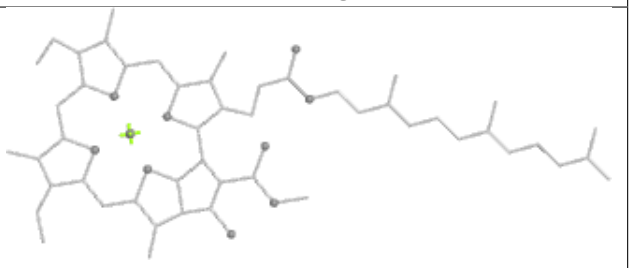
Bond angles

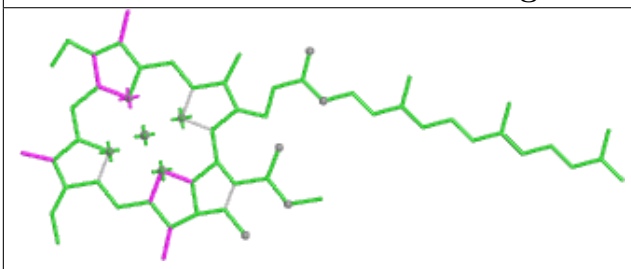
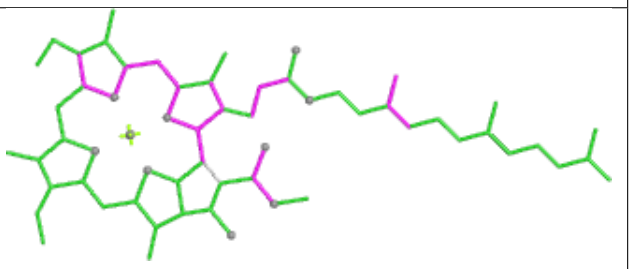
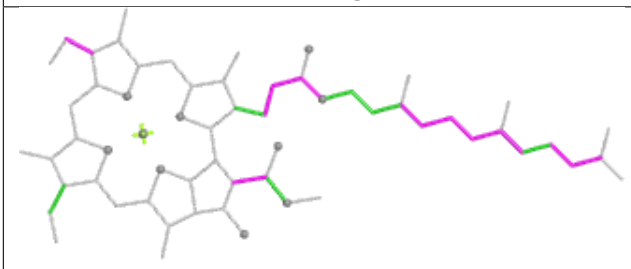
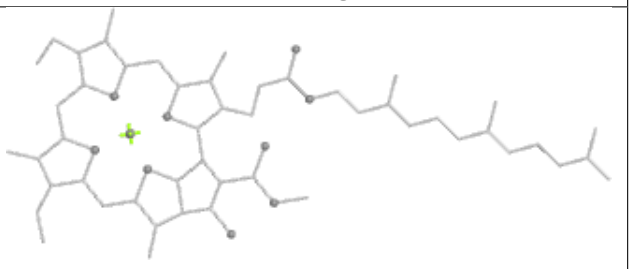


Torsions

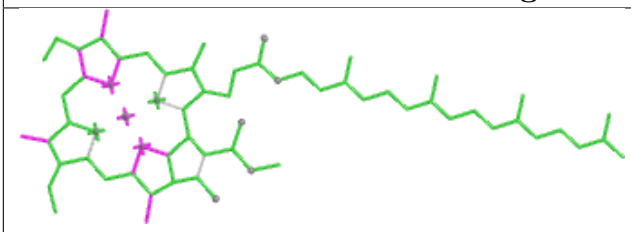


Rings

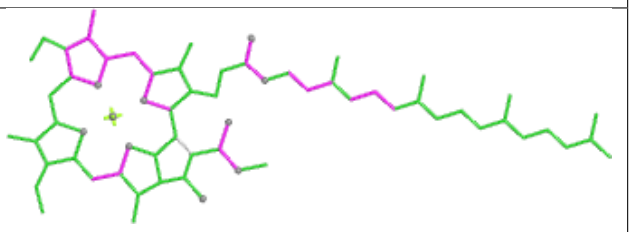
Ligand CLA A 1116	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 1137	
	
Bond lengths	Bond angles
	
Torsions	Rings

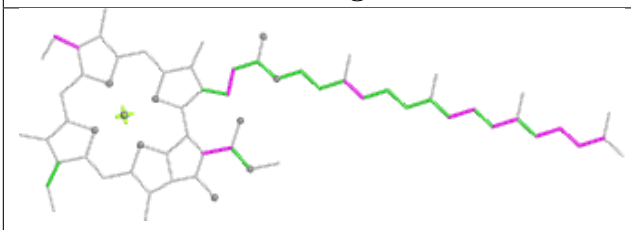
Ligand CLA e 1117



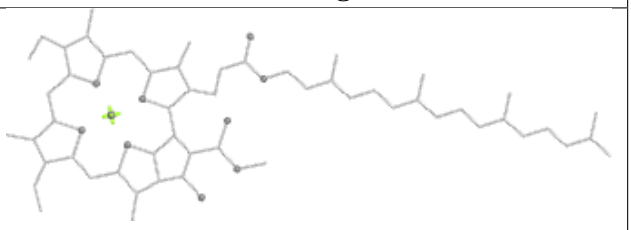
Bond lengths



Bond angles



Torsions



Rings

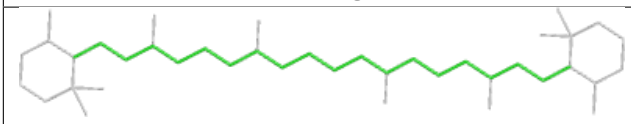
Ligand BCR A 4007



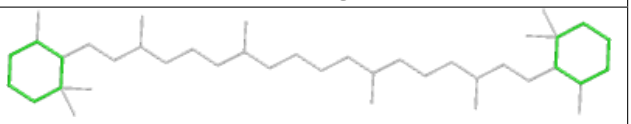
Bond lengths



Bond angles

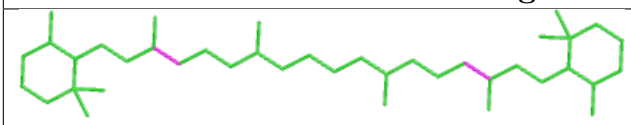


Torsions

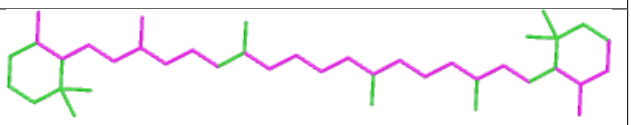


Rings

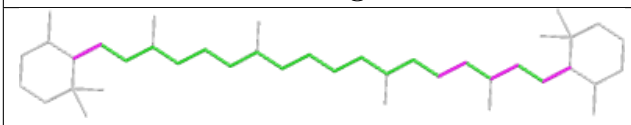
Ligand BCR e 4008



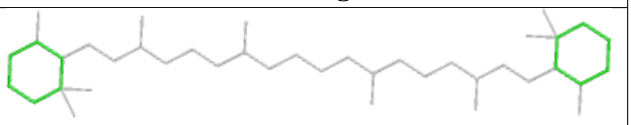
Bond lengths



Bond angles

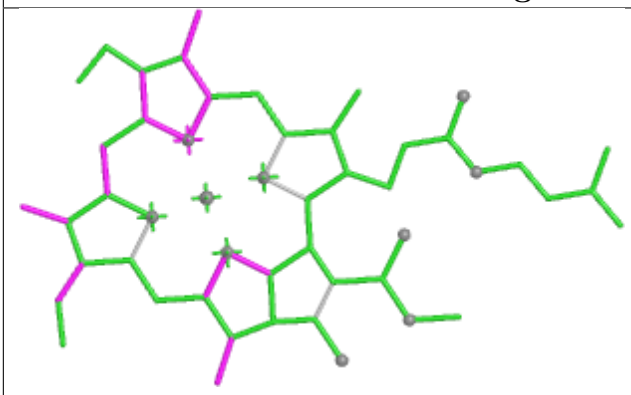


Torsions

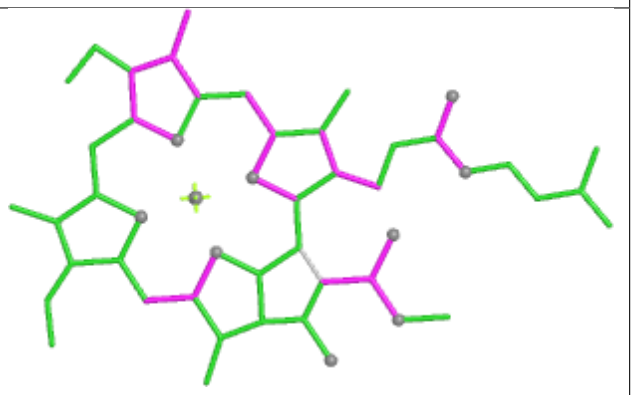


Rings

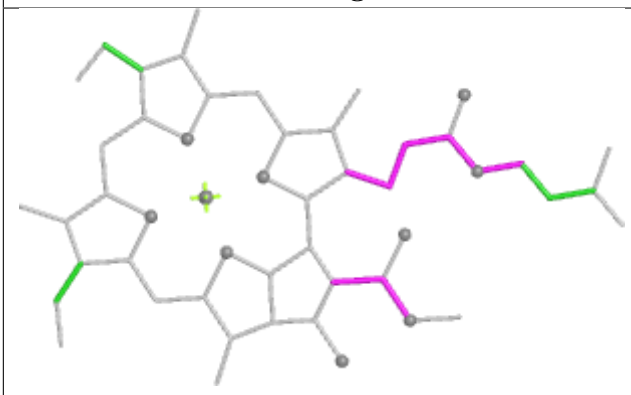
Ligand CLA G 1120



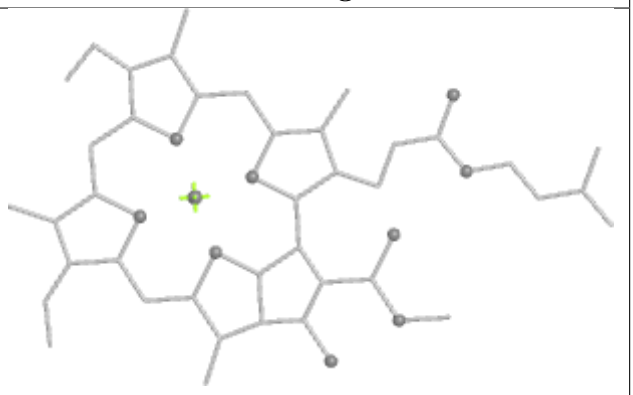
Bond lengths



Bond angles

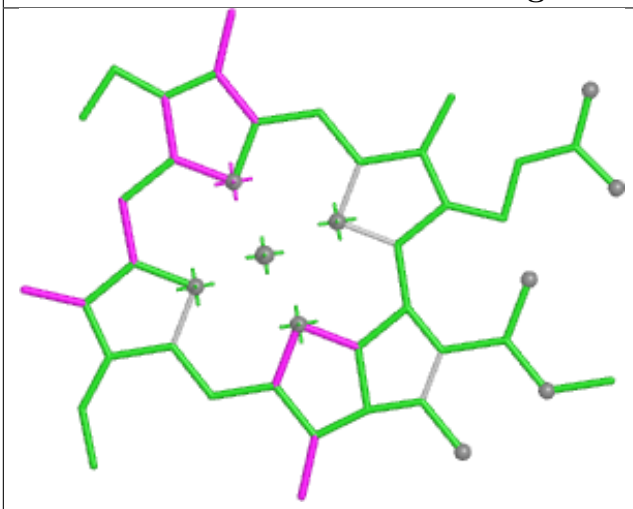


Torsions

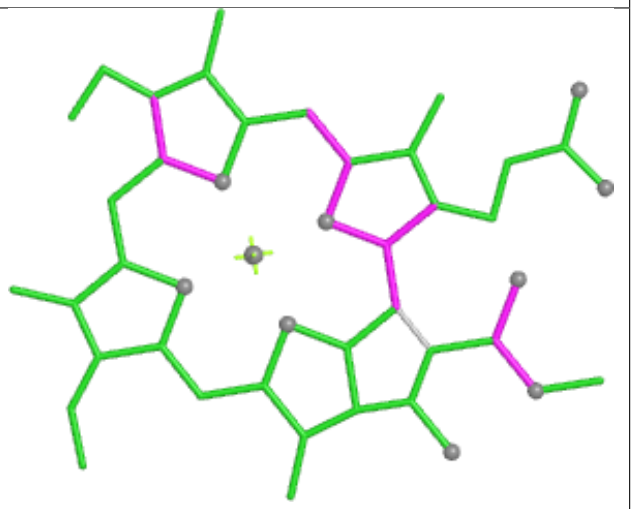


Rings

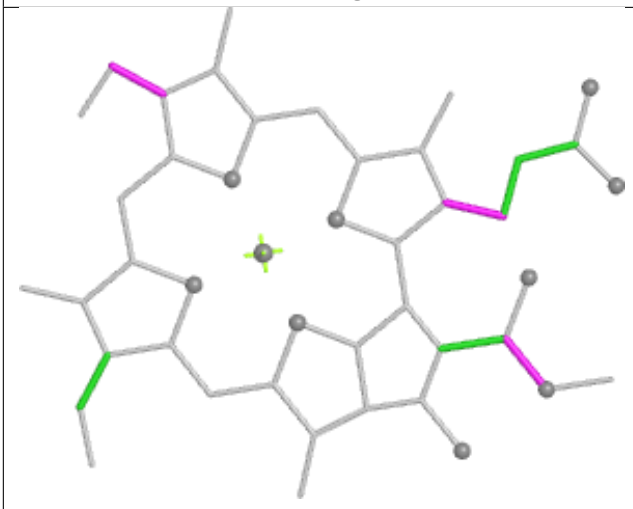
Ligand CLA u 504



Bond lengths



Bond angles

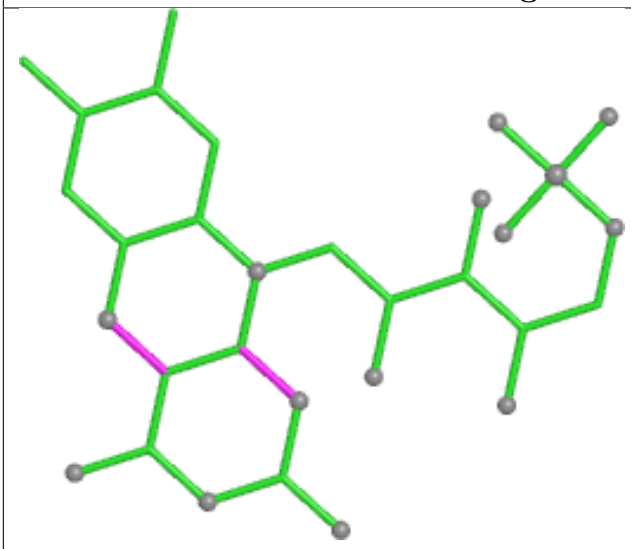


Torsions

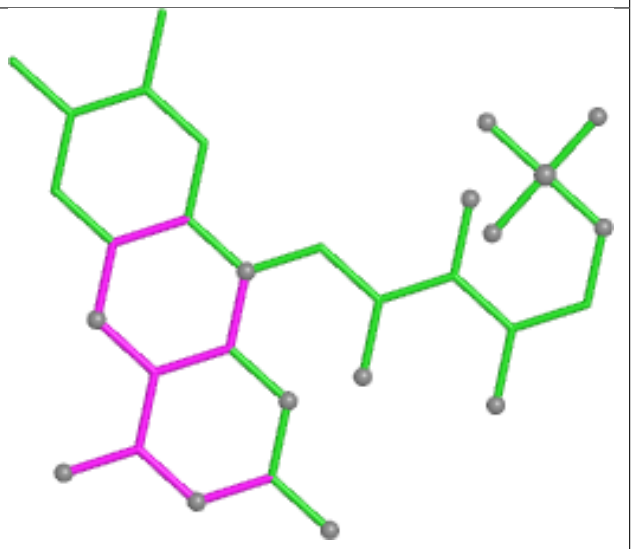


Rings

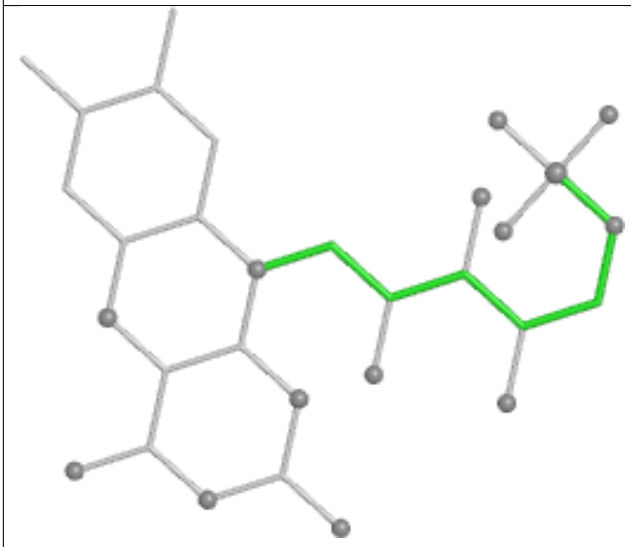
Ligand FMN P 170



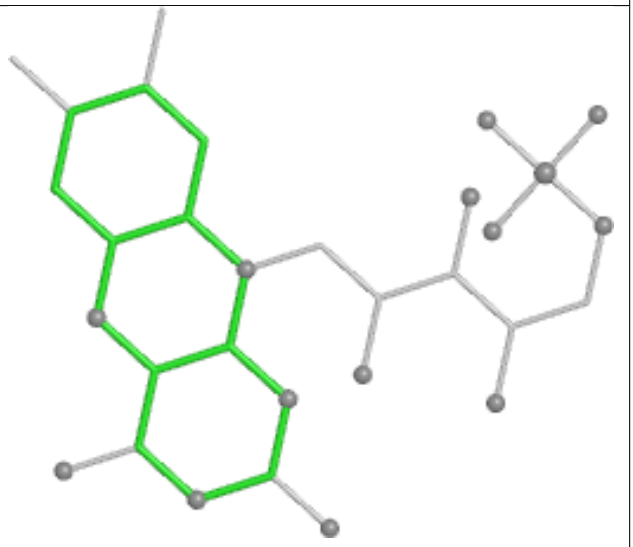
Bond lengths



Bond angles

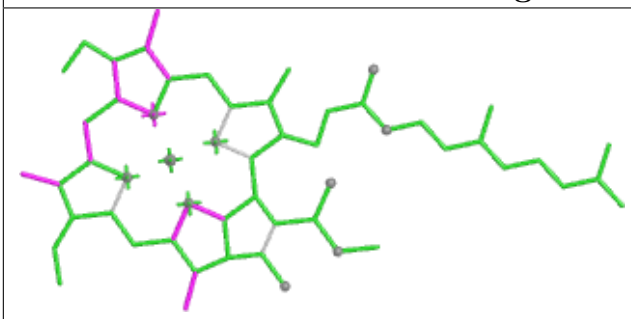


Torsions

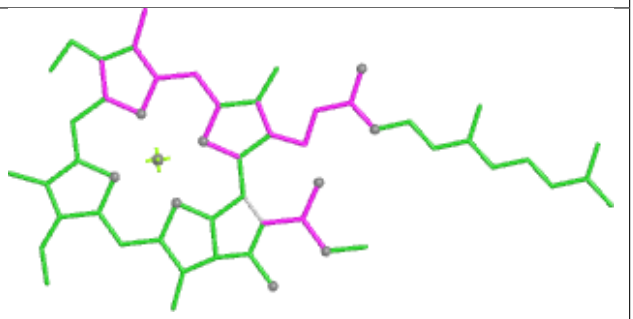


Rings

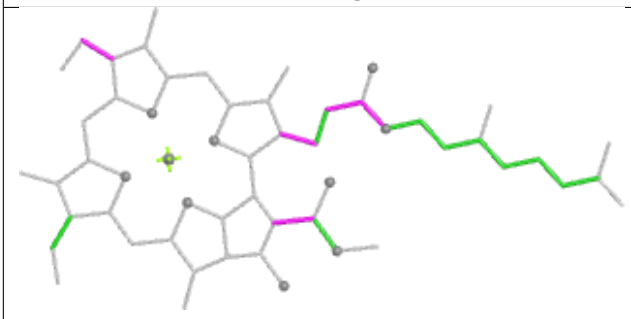
Ligand CLA K 1401



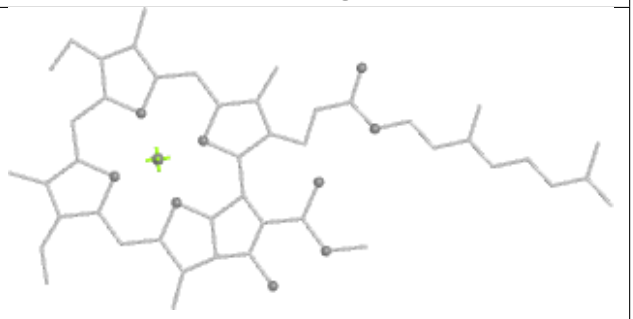
Bond lengths



Bond angles

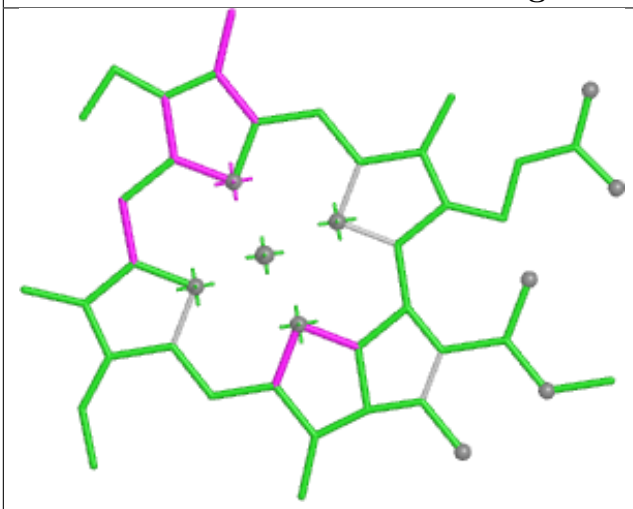


Torsions

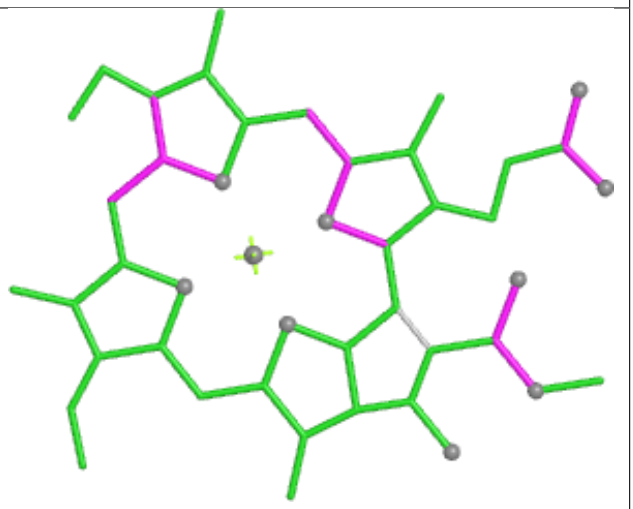


Rings

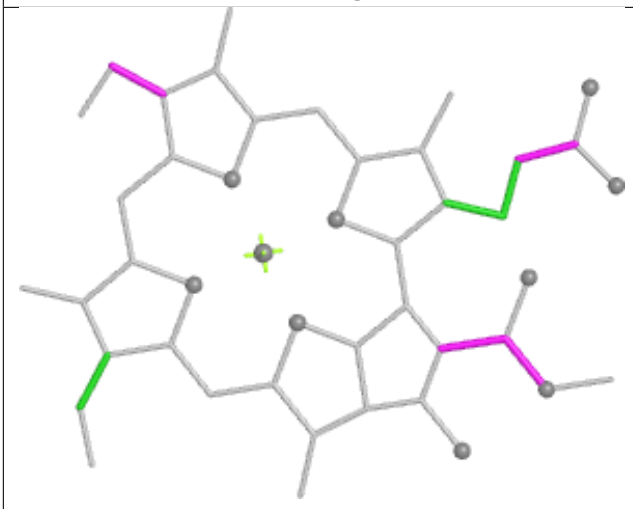
Ligand CLA 5 519



Bond lengths



Bond angles

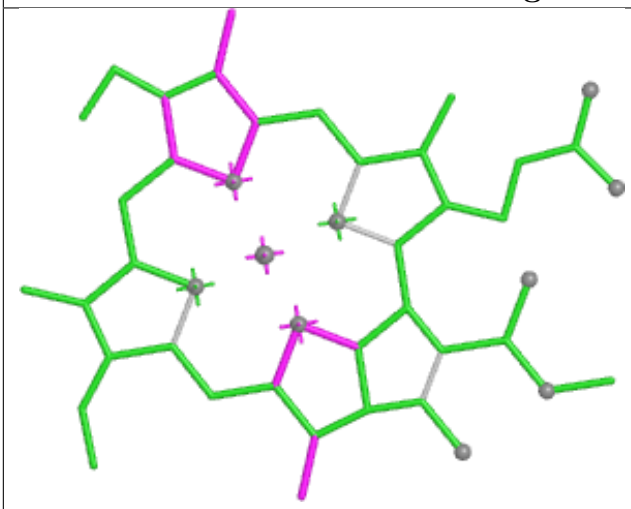


Torsions

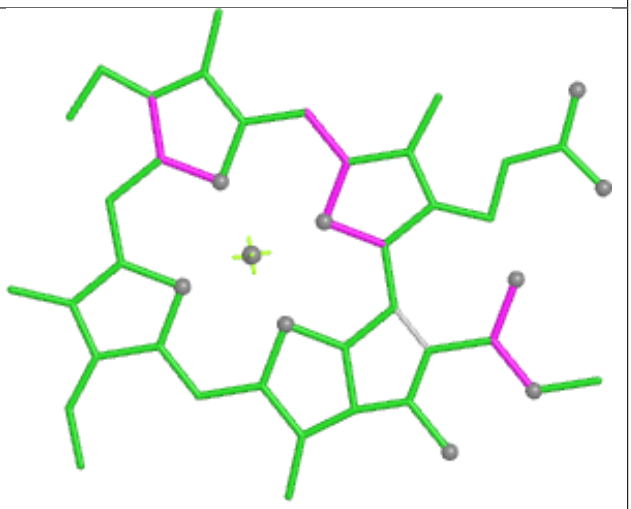


Rings

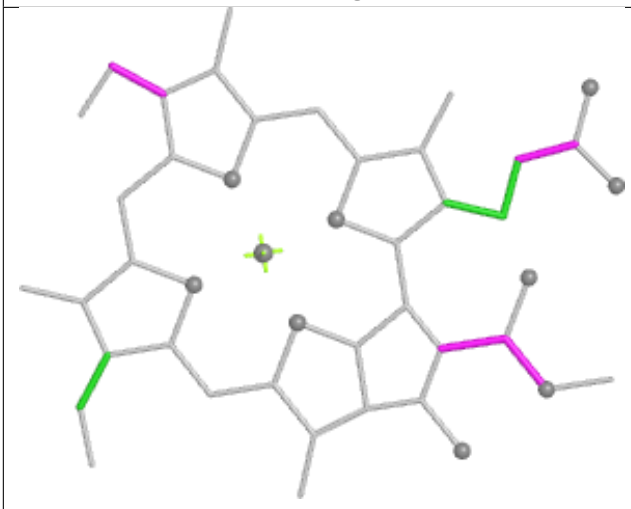
Ligand CLA Y 512



Bond lengths



Bond angles

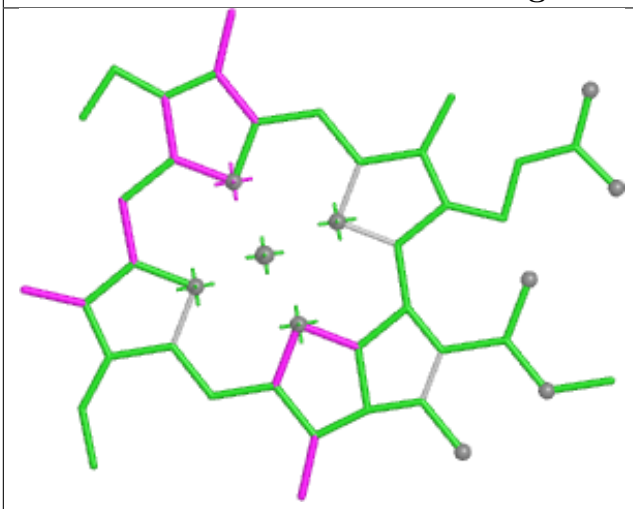


Torsions

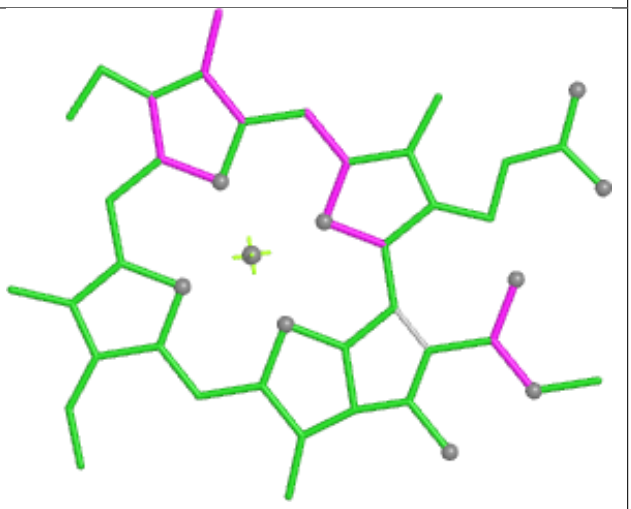


Rings

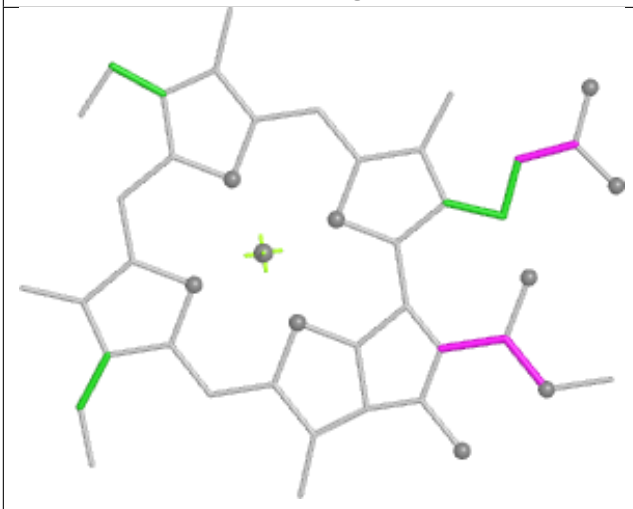
Ligand CLA 2 510



Bond lengths



Bond angles

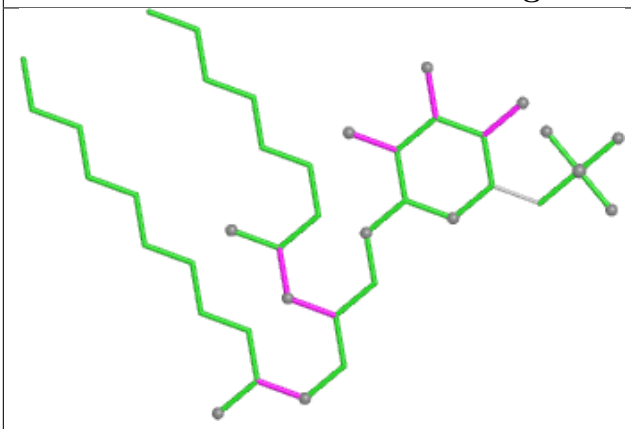


Torsions

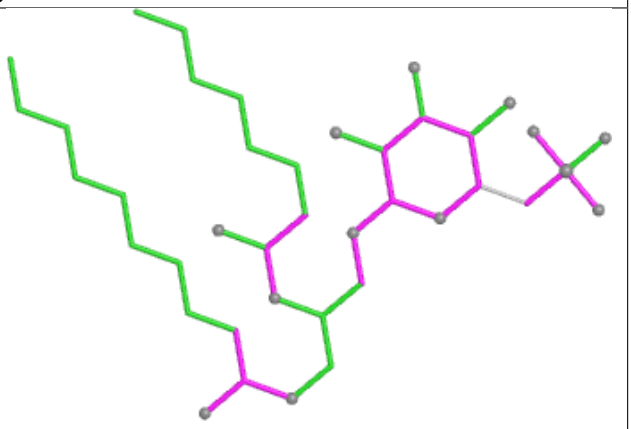


Rings

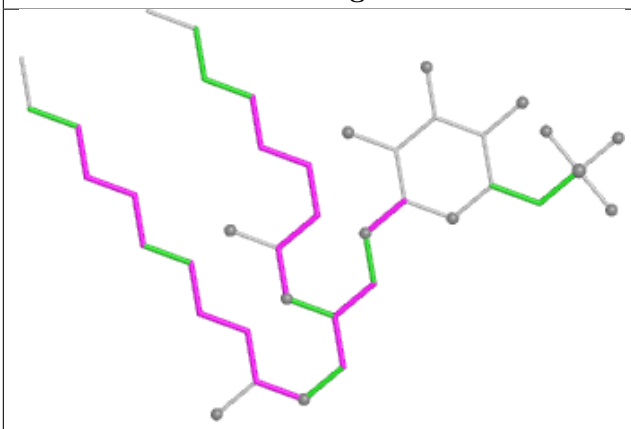
Ligand SQD f 1852



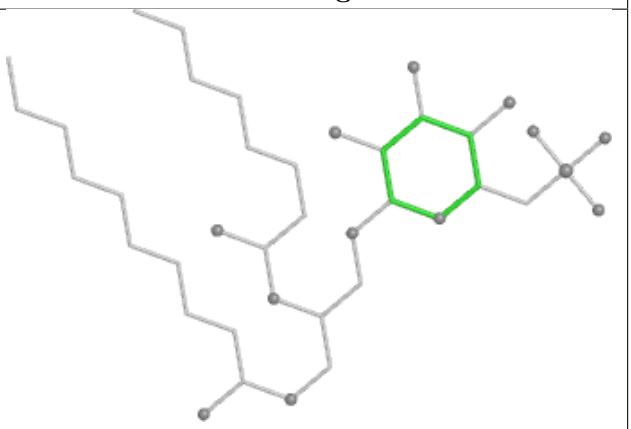
Bond lengths



Bond angles

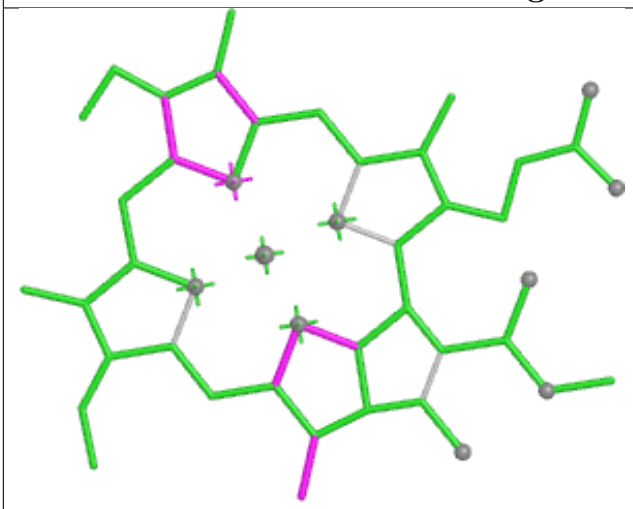


Torsions

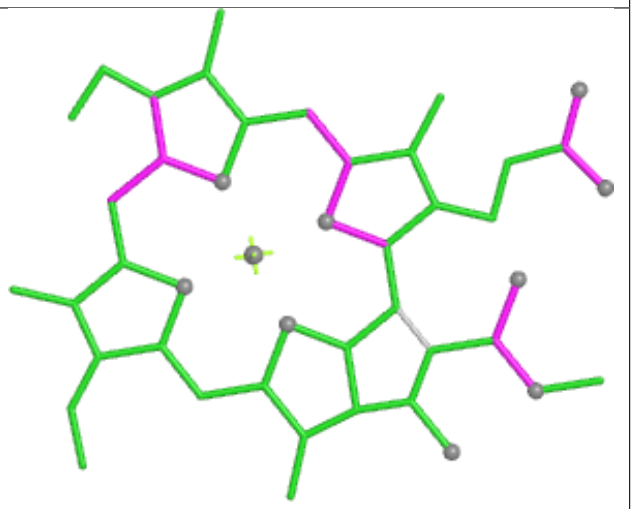


Rings

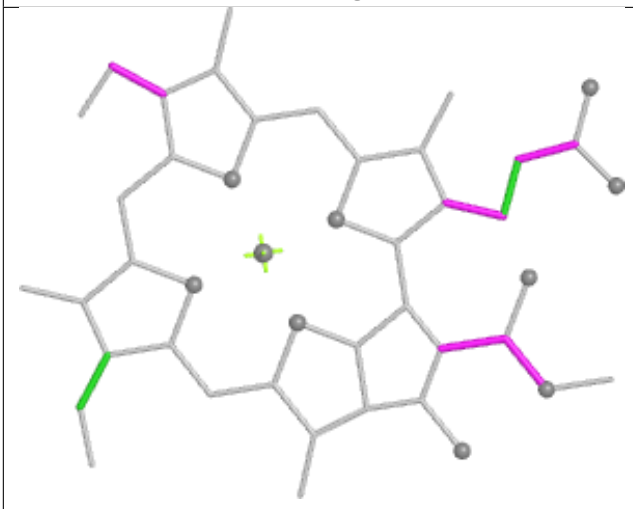
Ligand CLA d 517



Bond lengths



Bond angles

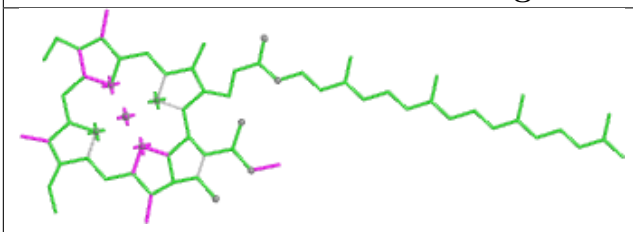


Torsions

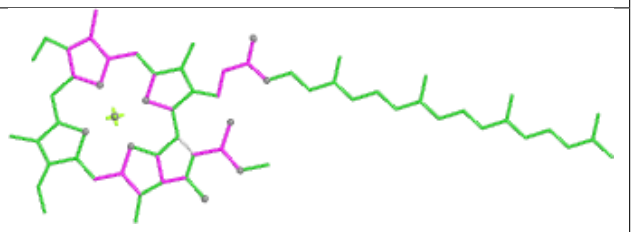


Rings

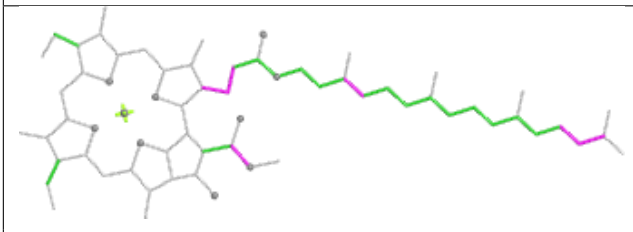
Ligand CLA G 1022



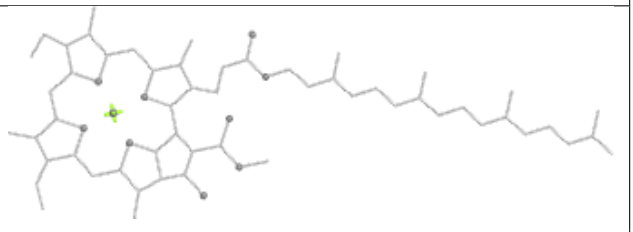
Bond lengths



Bond angles

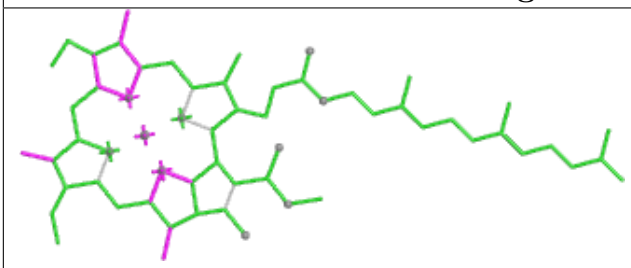


Torsions

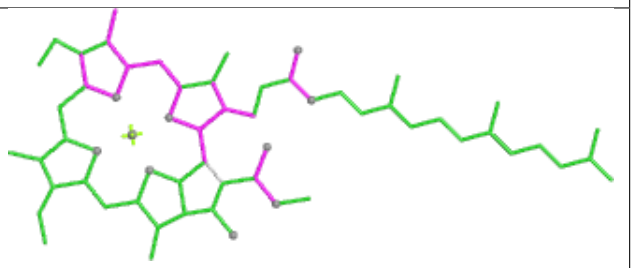


Rings

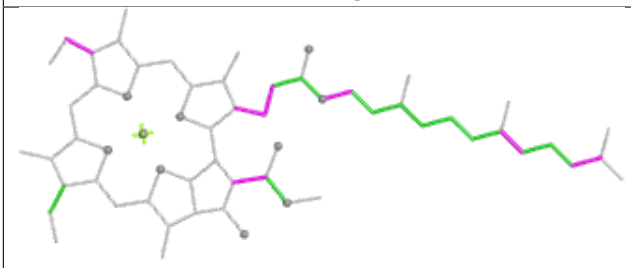
Ligand CLA L 1501



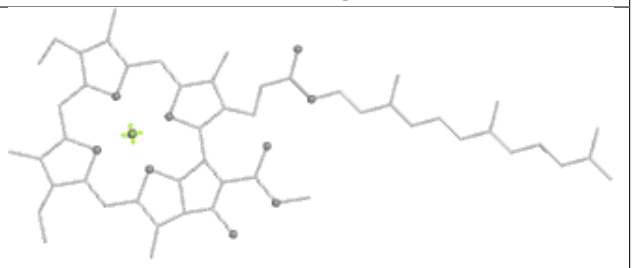
Bond lengths



Bond angles

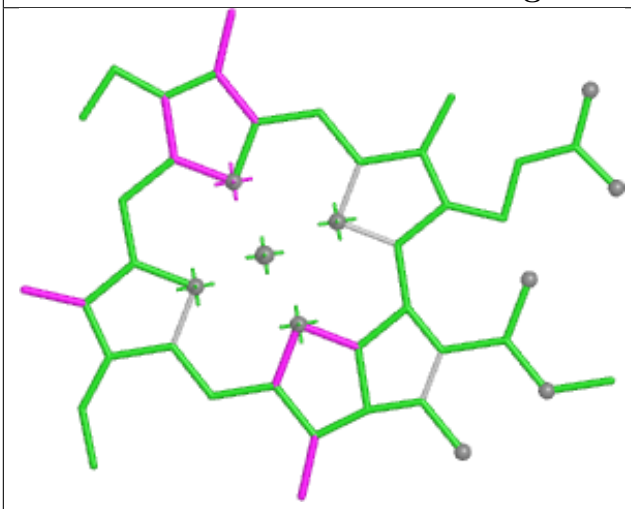


Torsions

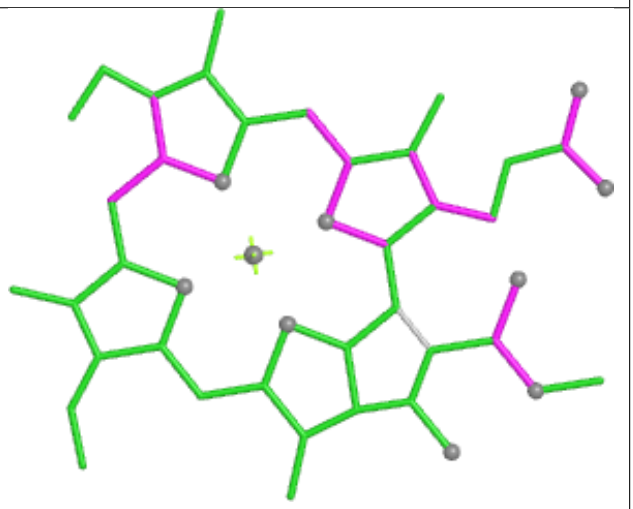


Rings

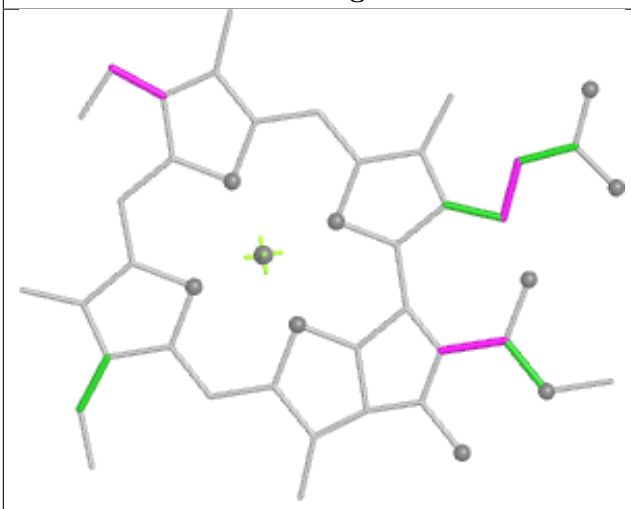
Ligand CLA Y 502



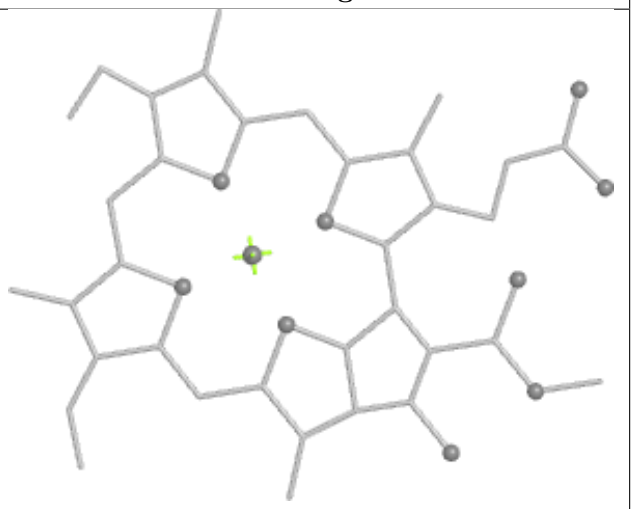
Bond lengths



Bond angles

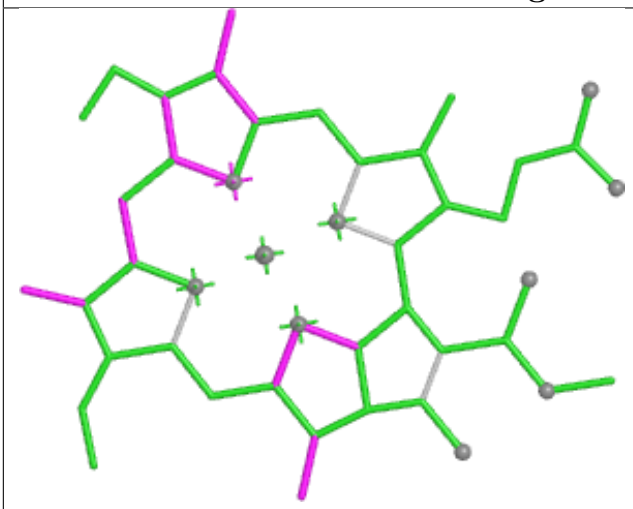


Torsions

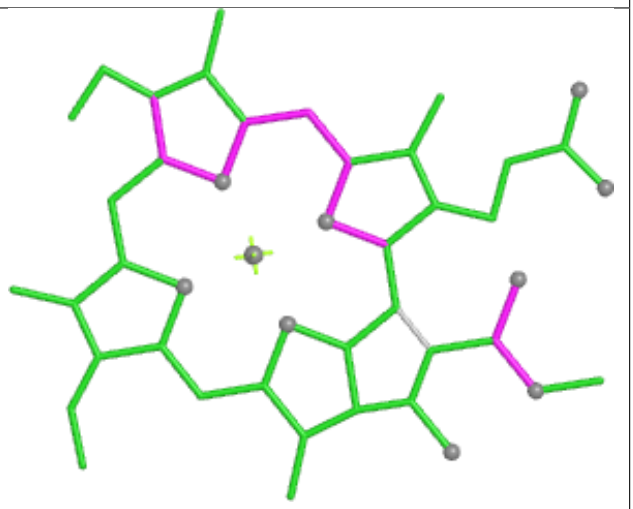


Rings

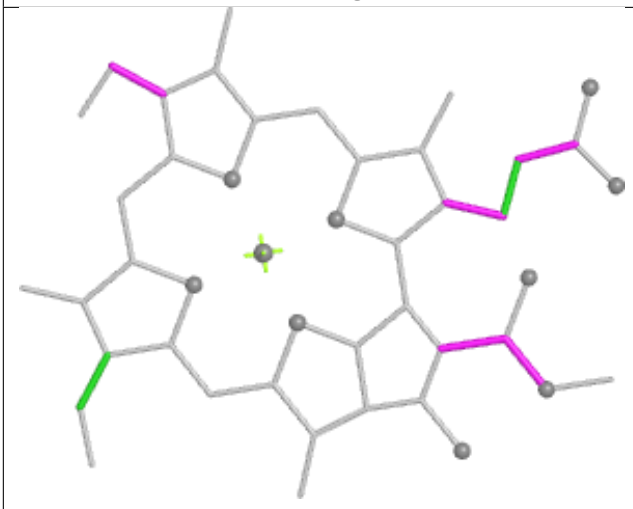
Ligand CLA 1 519



Bond lengths



Bond angles

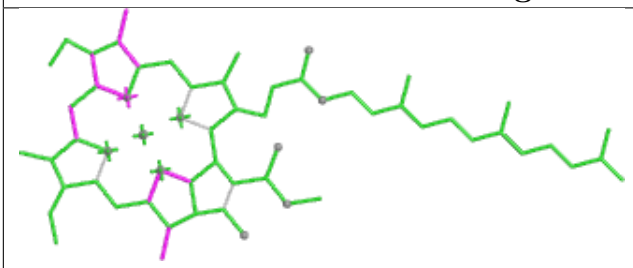


Torsions

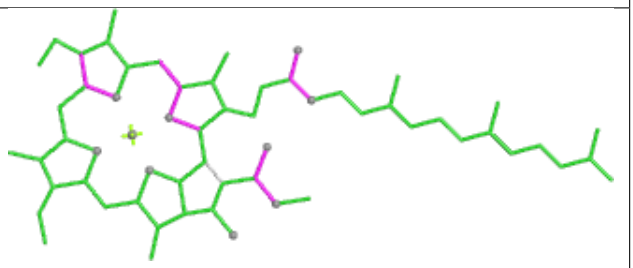


Rings

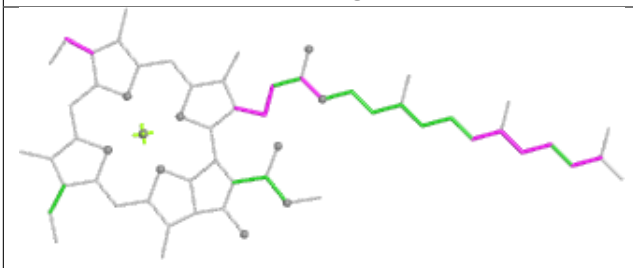
Ligand CLA H 1217



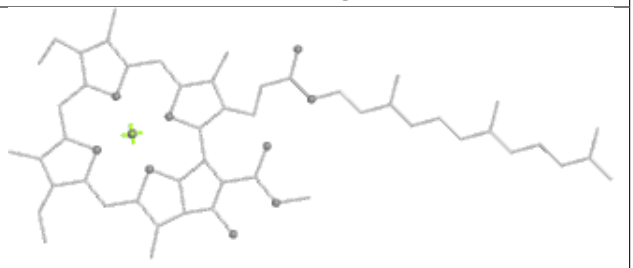
Bond lengths



Bond angles

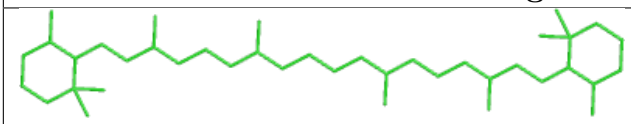


Torsions

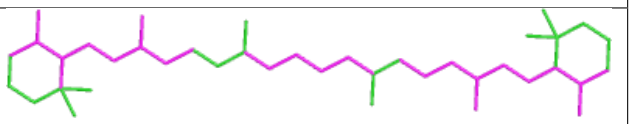


Rings

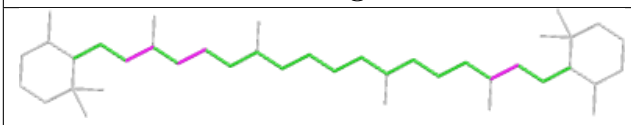
Ligand BCR 3 524



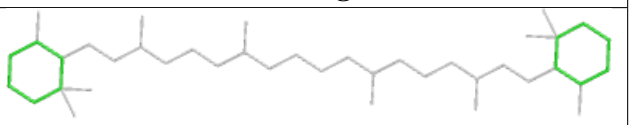
Bond lengths



Bond angles

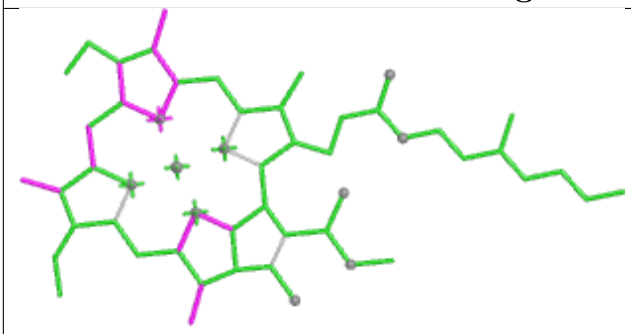


Torsions

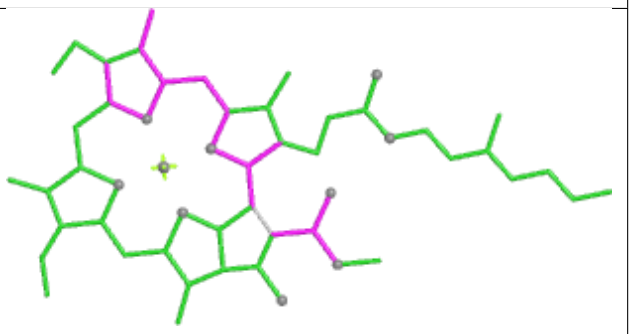


Rings

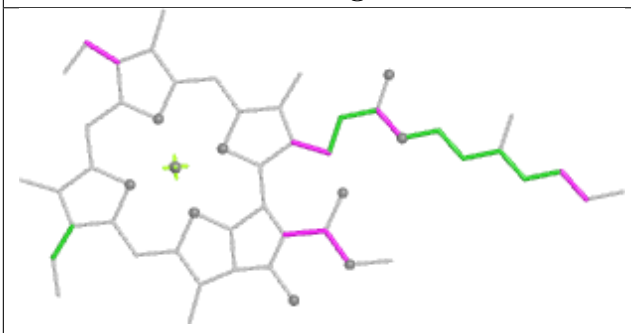
Ligand CLA B 1209



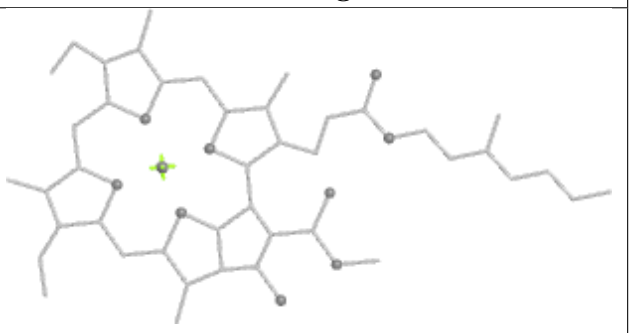
Bond lengths



Bond angles

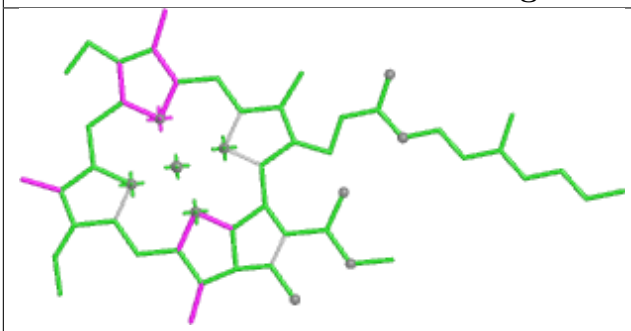


Torsions

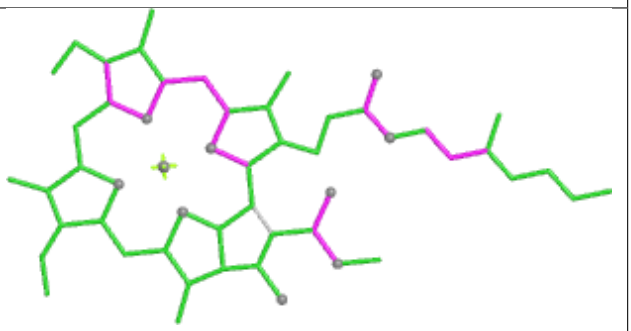


Rings

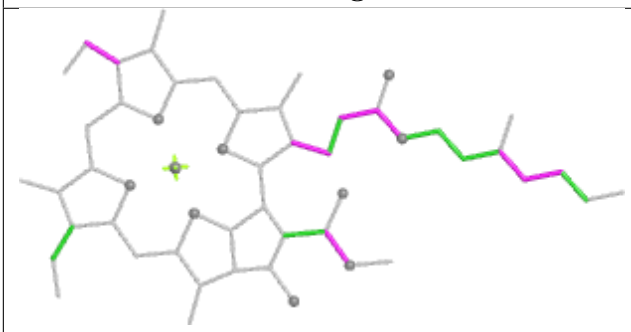
Ligand CLA e 1110



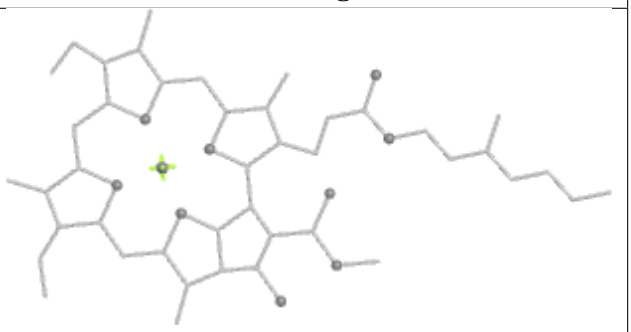
Bond lengths



Bond angles

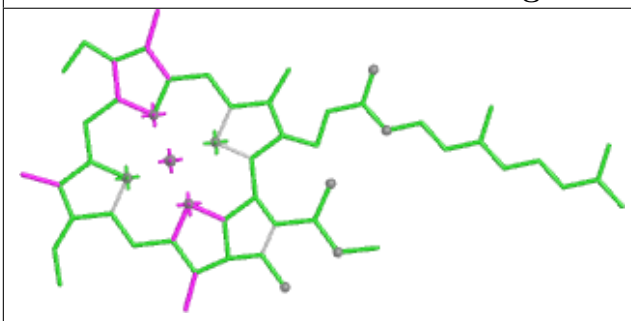


Torsions

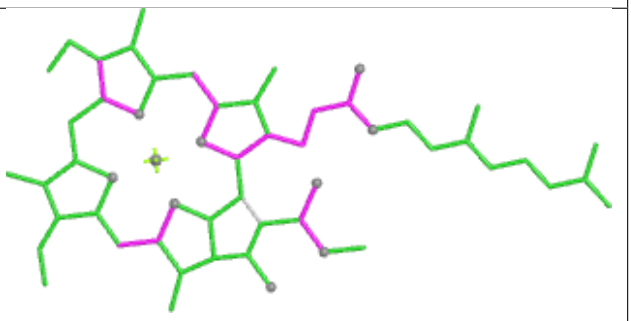


Rings

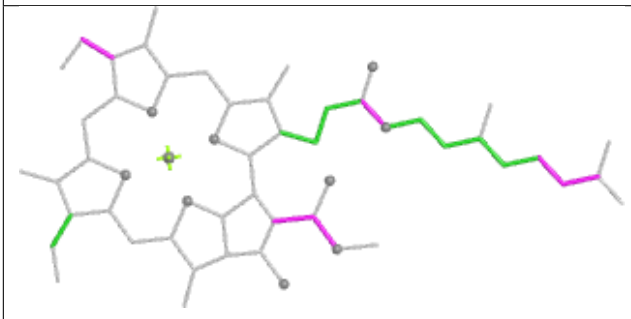
Ligand CLA f 1220



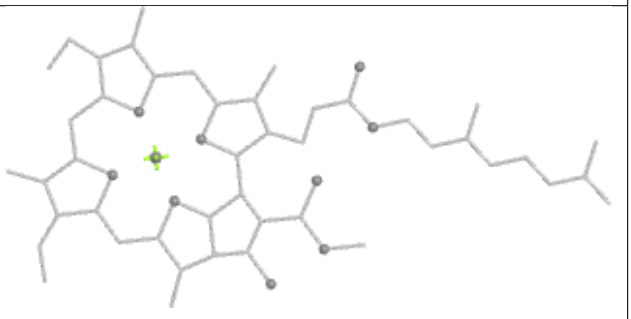
Bond lengths



Bond angles

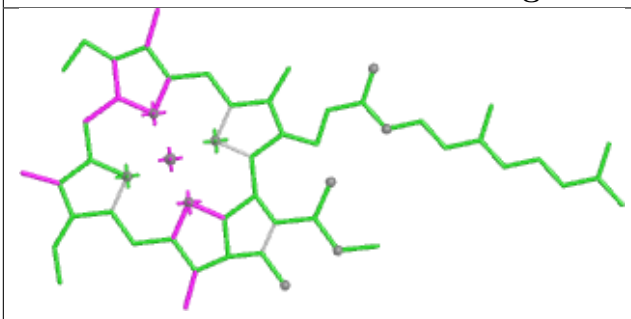


Torsions

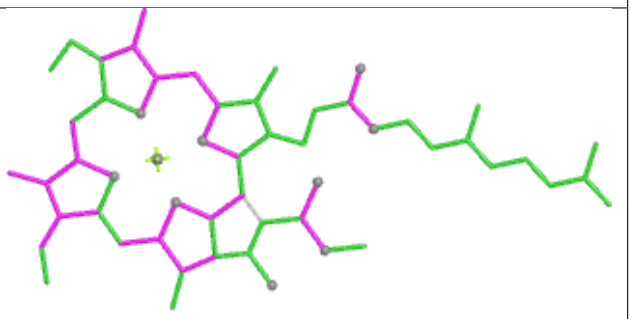


Rings

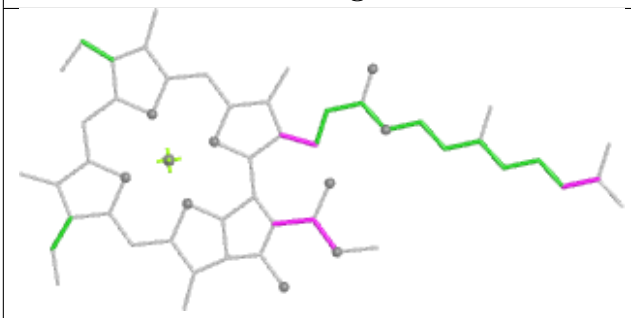
Ligand CLA f 1226



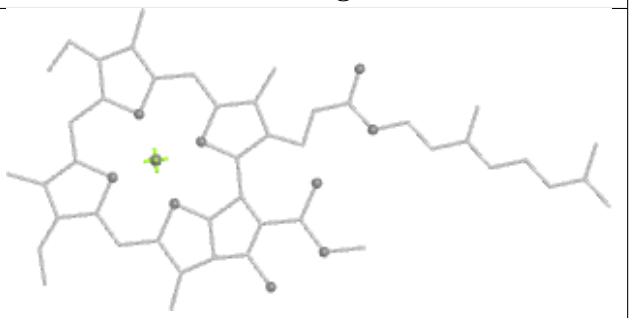
Bond lengths



Bond angles

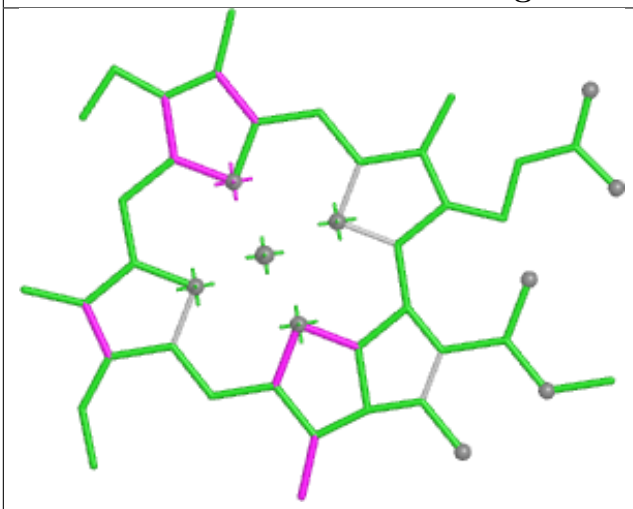


Torsions

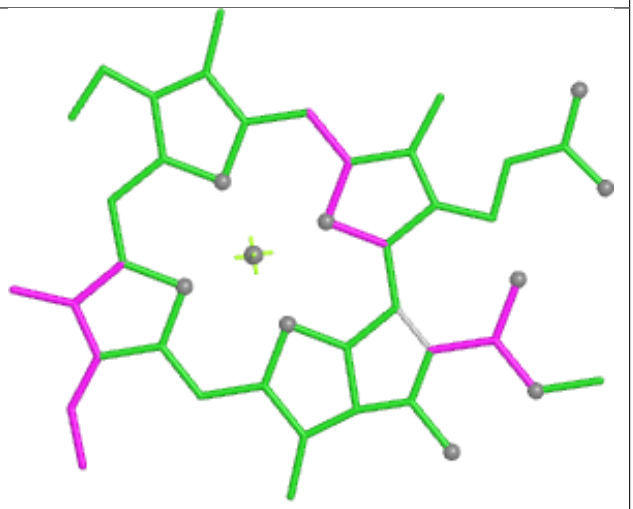


Rings

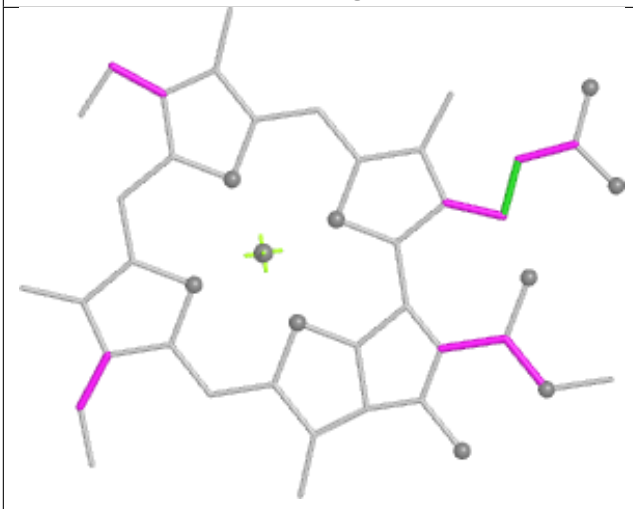
Ligand CLA K 1105



Bond lengths



Bond angles

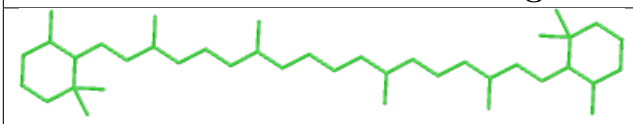


Torsions

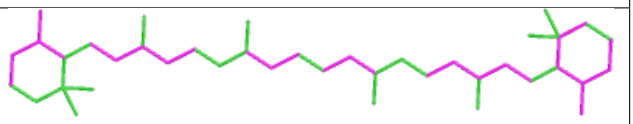


Rings

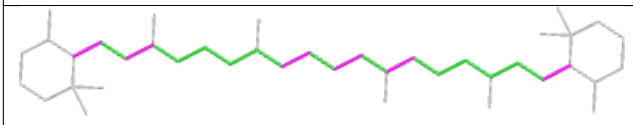
Ligand BCR b 521



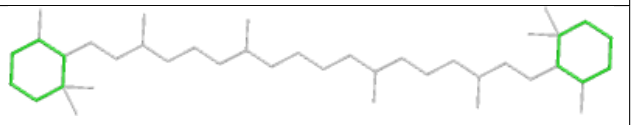
Bond lengths



Bond angles

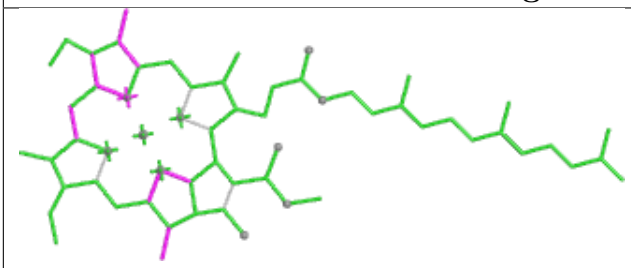


Torsions

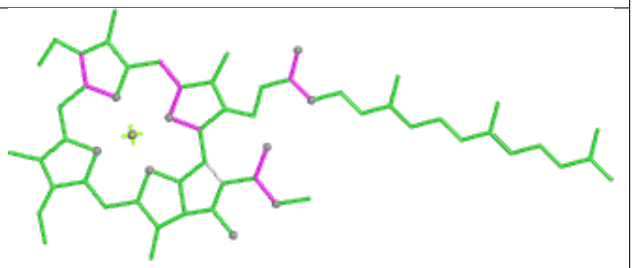


Rings

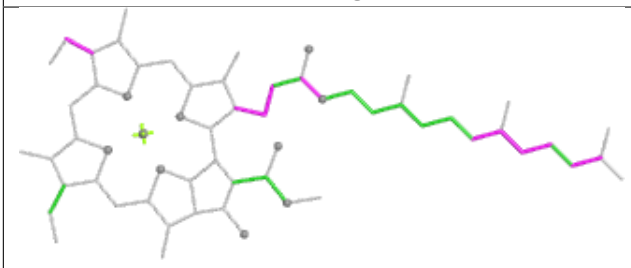
Ligand CLA f 1217



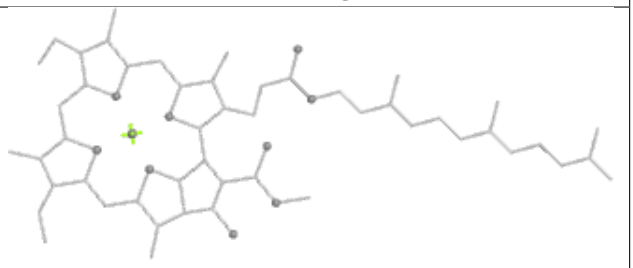
Bond lengths



Bond angles

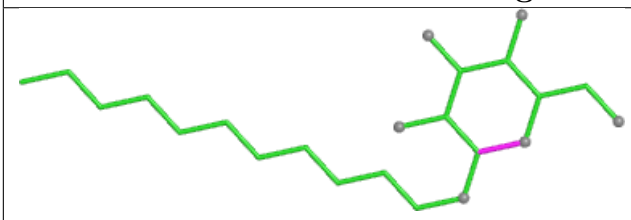


Torsions

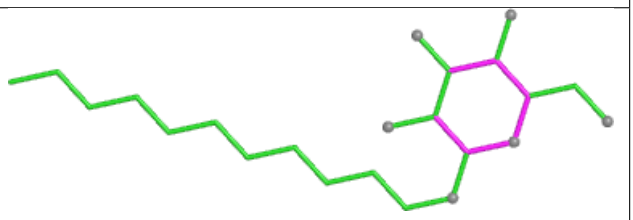


Rings

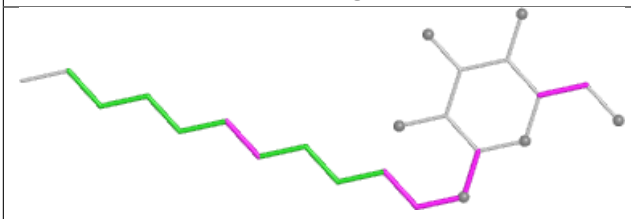
Ligand LMU e 1849



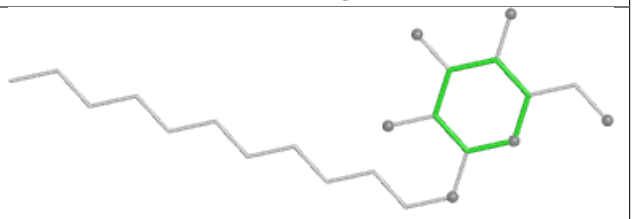
Bond lengths



Bond angles

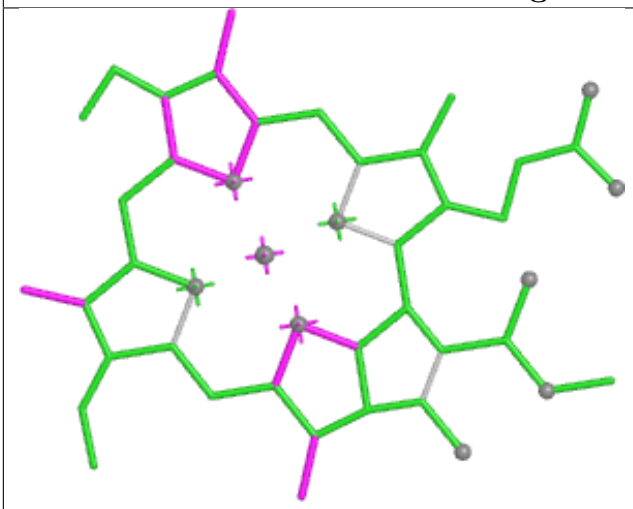


Torsions

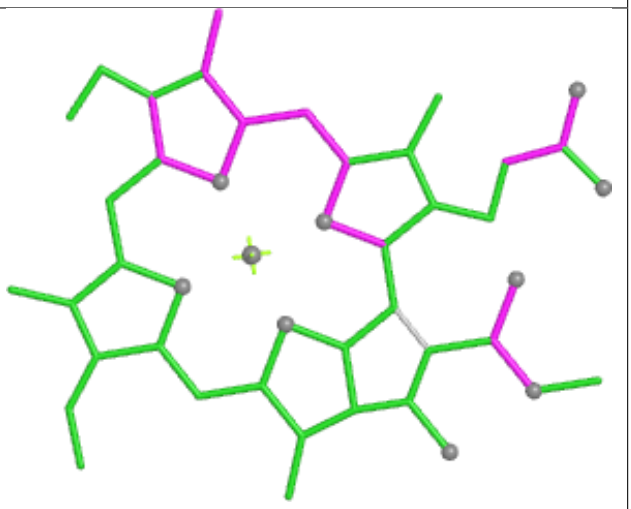


Rings

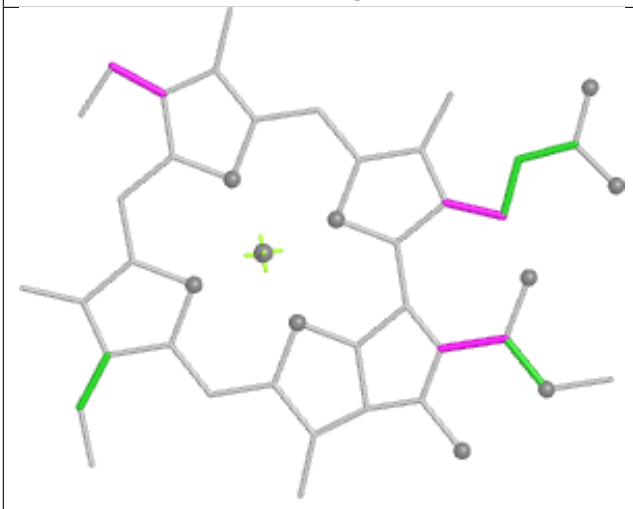
Ligand CLA s 508



Bond lengths



Bond angles

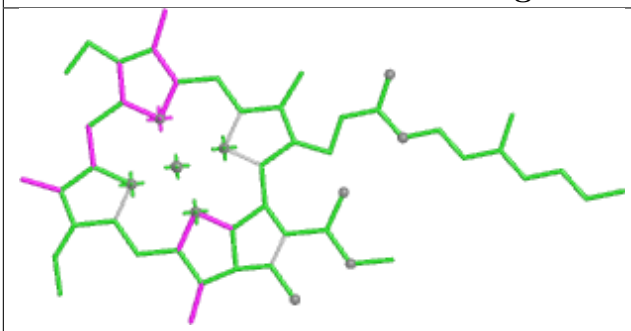


Torsions

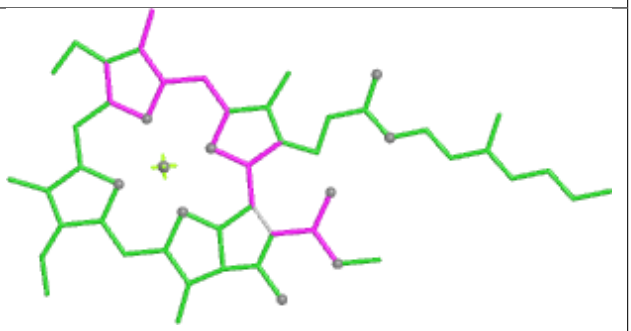


Rings

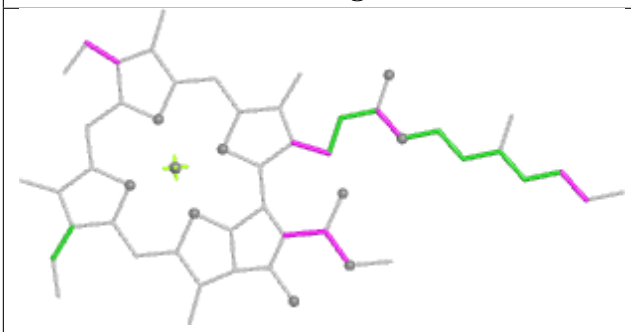
Ligand CLA H 1209



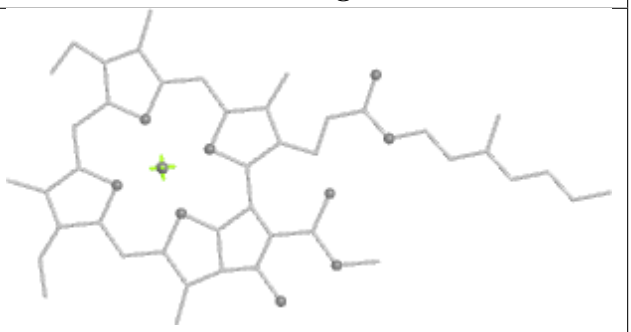
Bond lengths



Bond angles

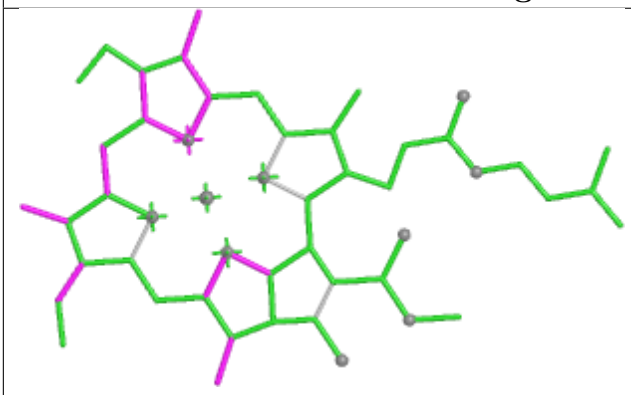


Torsions

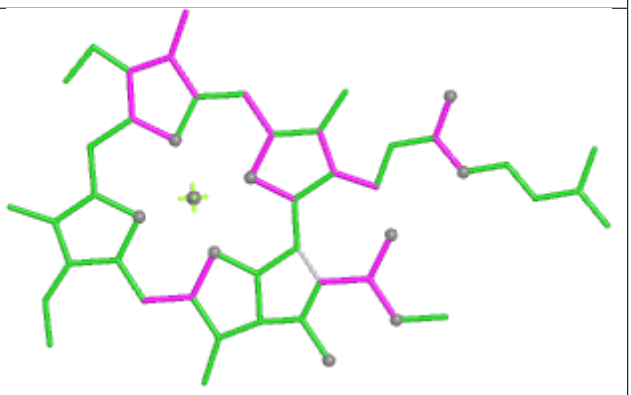


Rings

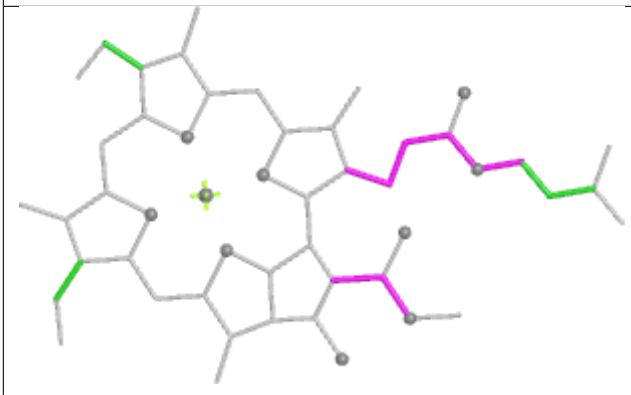
Ligand CLA A 1120



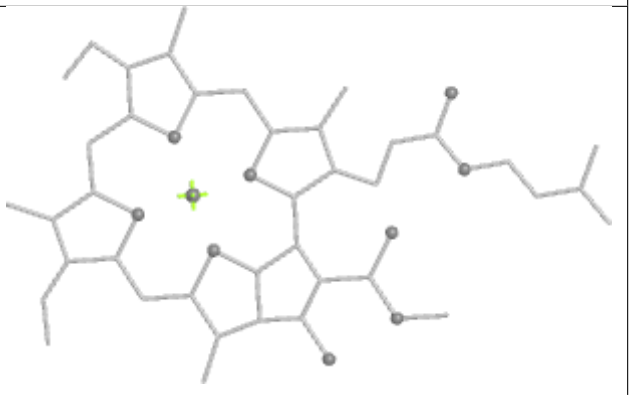
Bond lengths



Bond angles

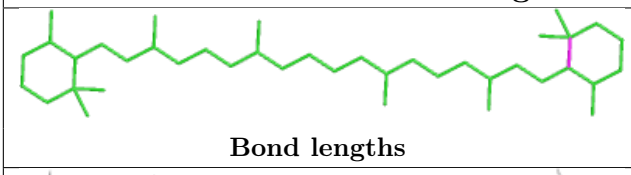


Torsions

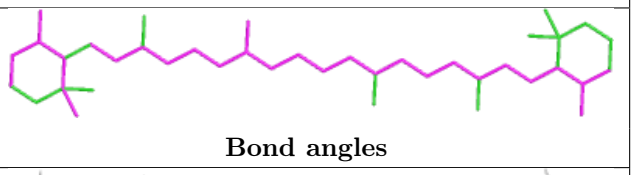


Rings

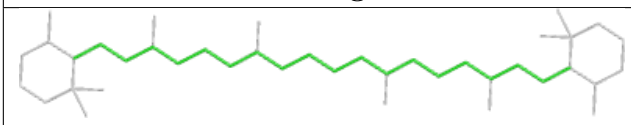
Ligand BCR G 4002



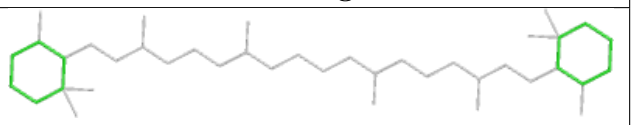
Bond lengths



Bond angles



Torsions



Rings

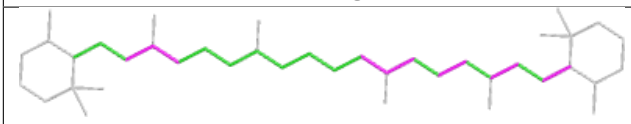
Ligand BCR G 4011



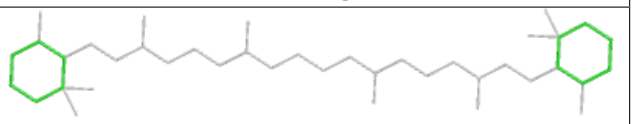
Bond lengths



Bond angles

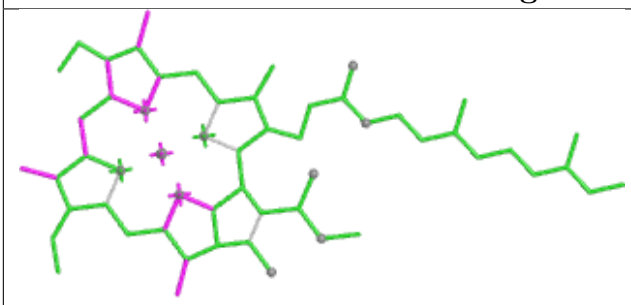


Torsions

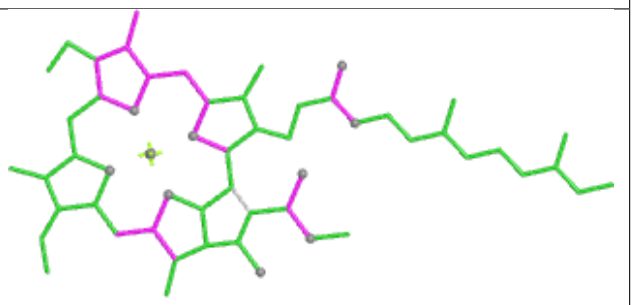


Rings

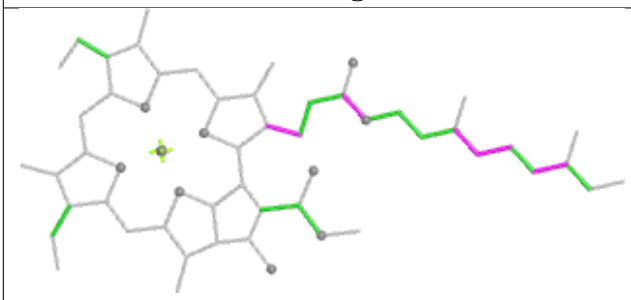
Ligand CLA e 1130



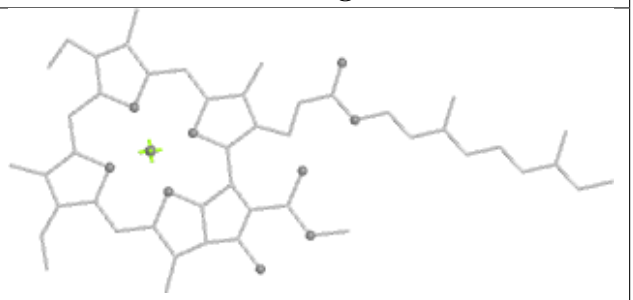
Bond lengths



Bond angles

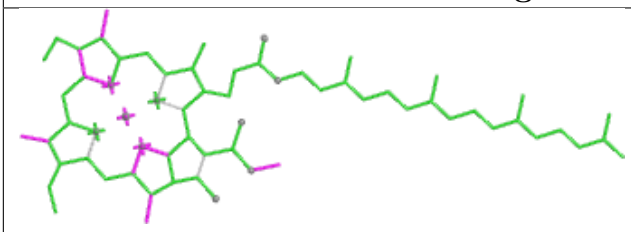


Torsions

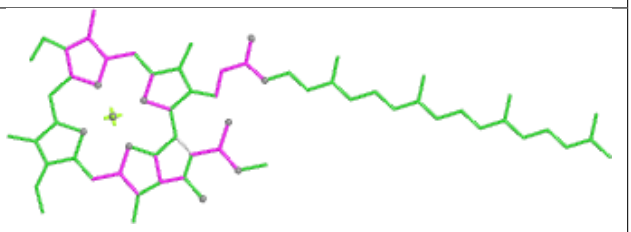


Rings

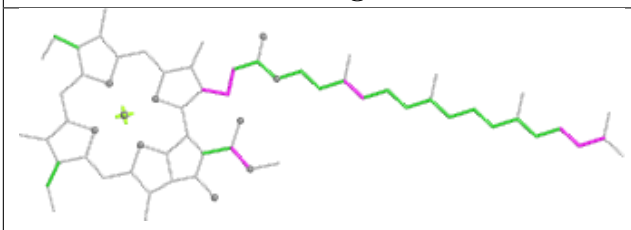
Ligand CLA A 1022



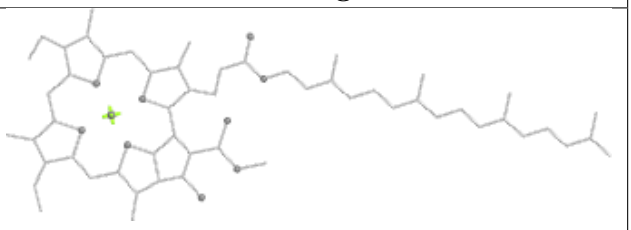
Bond lengths



Bond angles

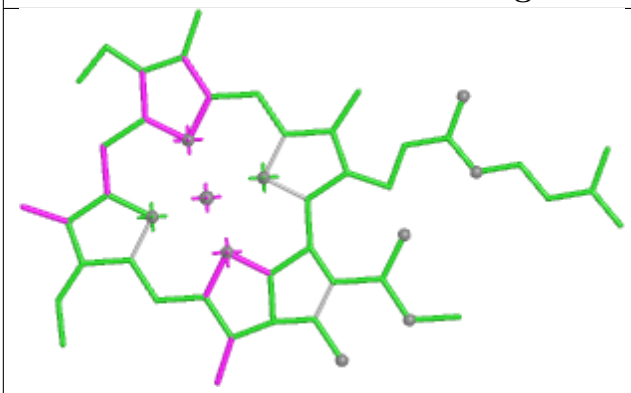


Torsions

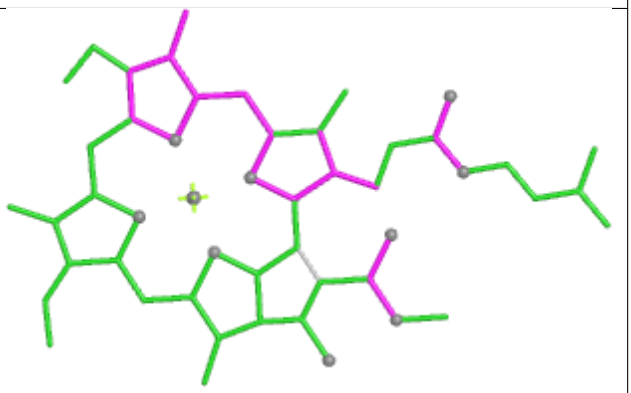


Rings

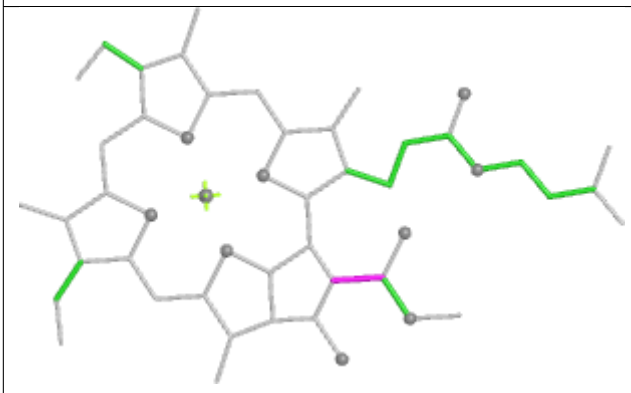
Ligand CLA H 1222



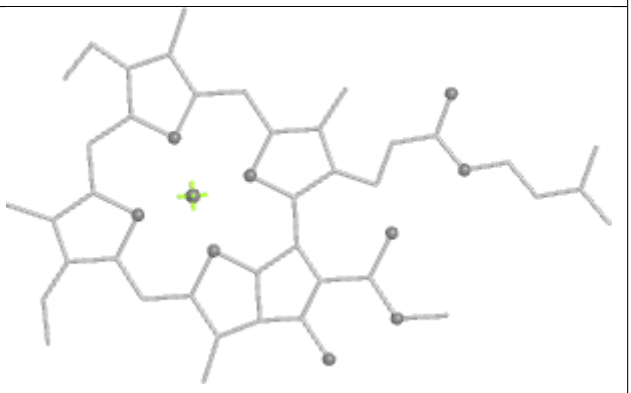
Bond lengths



Bond angles

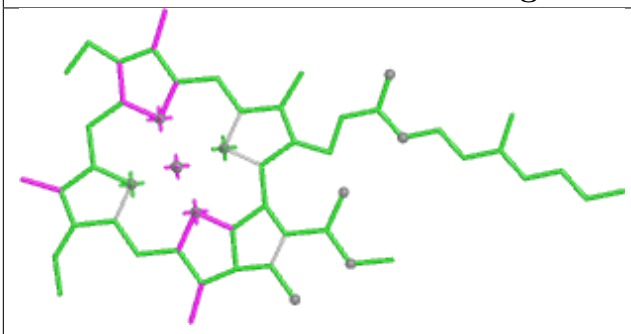


Torsions

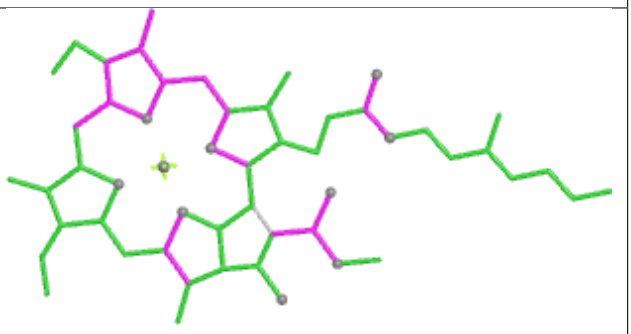


Rings

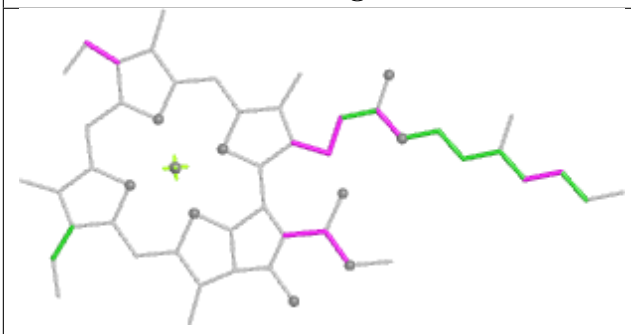
Ligand CLA e 1129



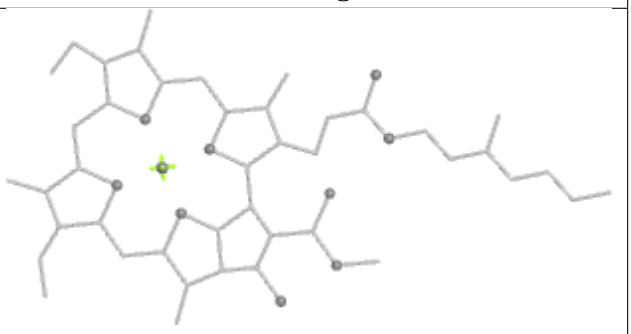
Bond lengths



Bond angles

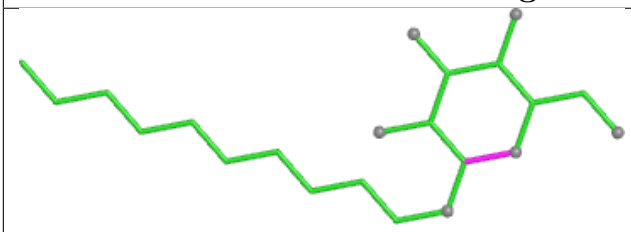


Torsions

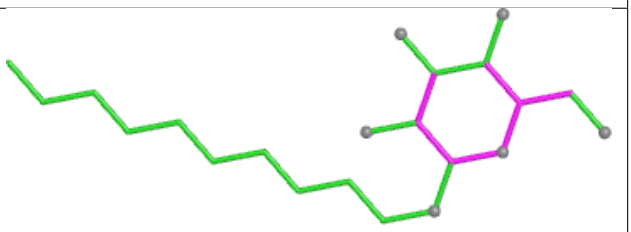


Rings

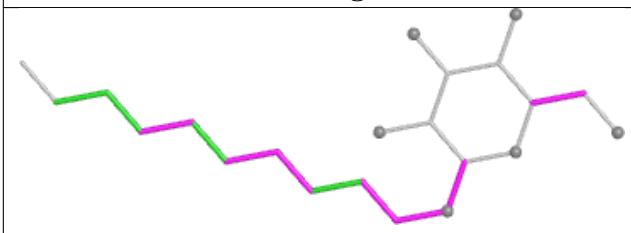
Ligand LMU l 5105



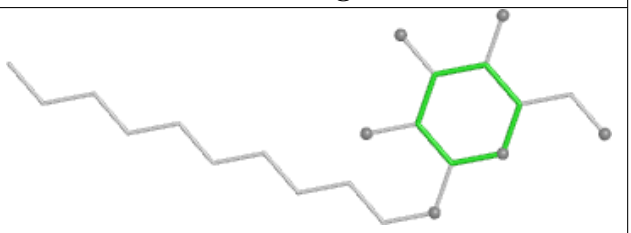
Bond lengths



Bond angles

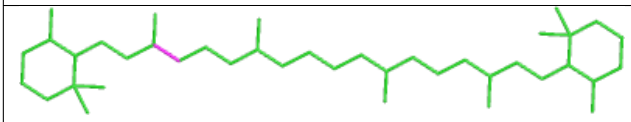


Torsions

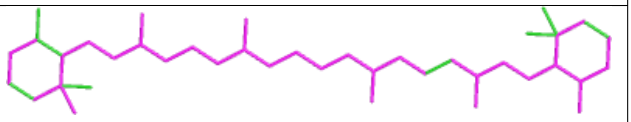


Rings

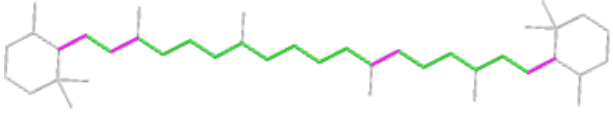
Ligand BCR B 4014



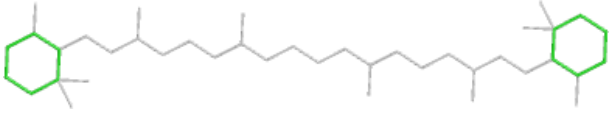
Bond lengths



Bond angles

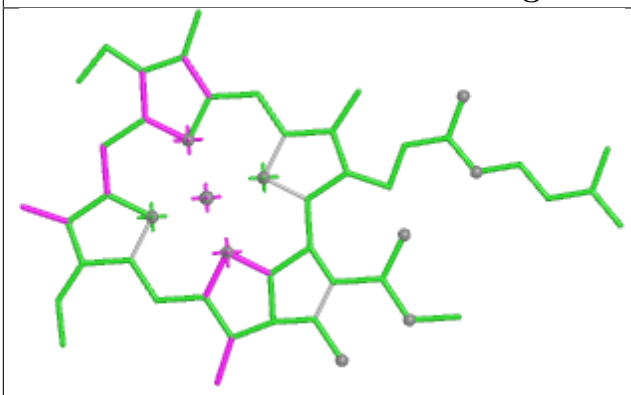


Torsions

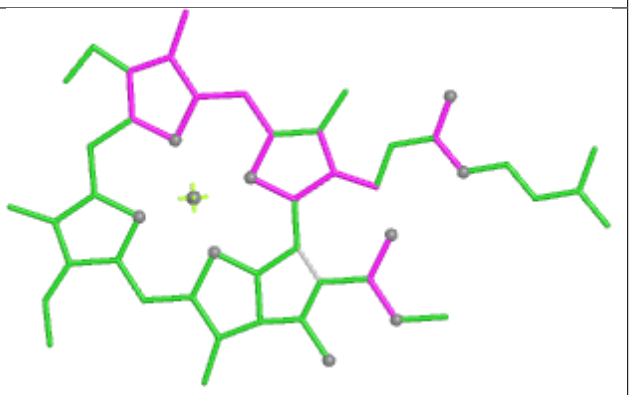


Rings

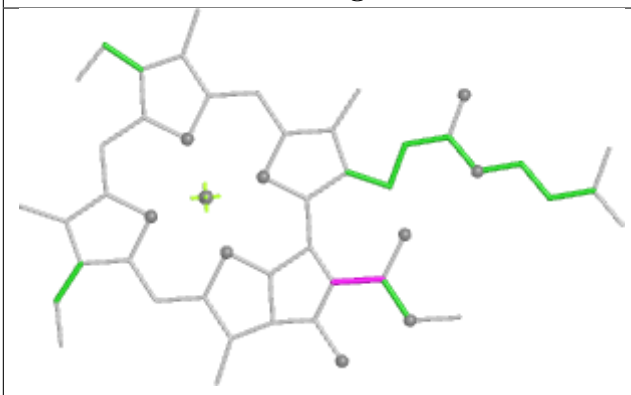
Ligand CLA f 1222



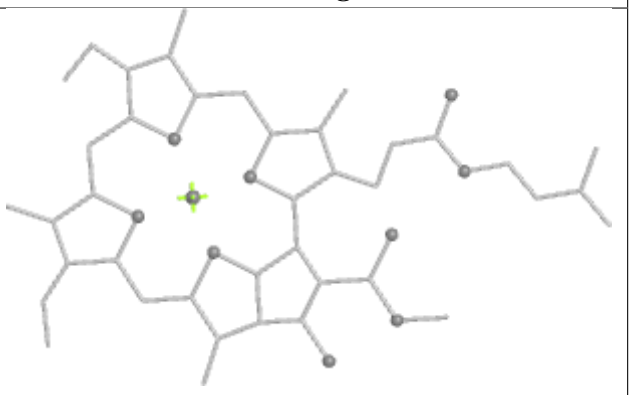
Bond lengths



Bond angles

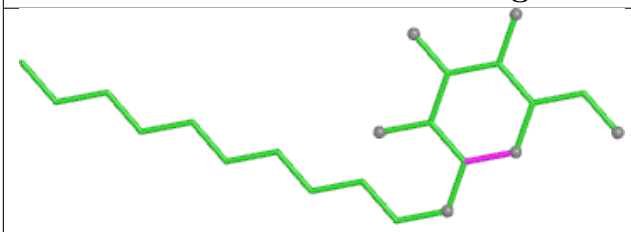


Torsions

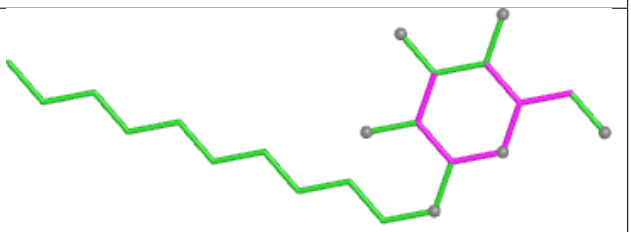


Rings

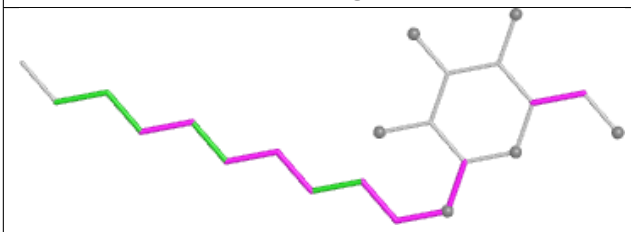
Ligand LMU T 5105



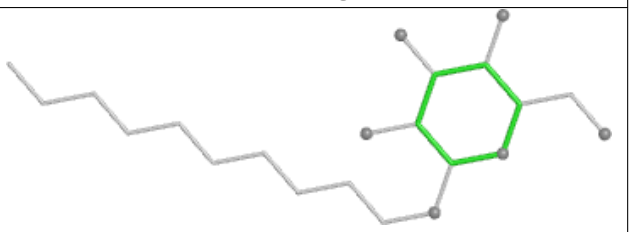
Bond lengths



Bond angles

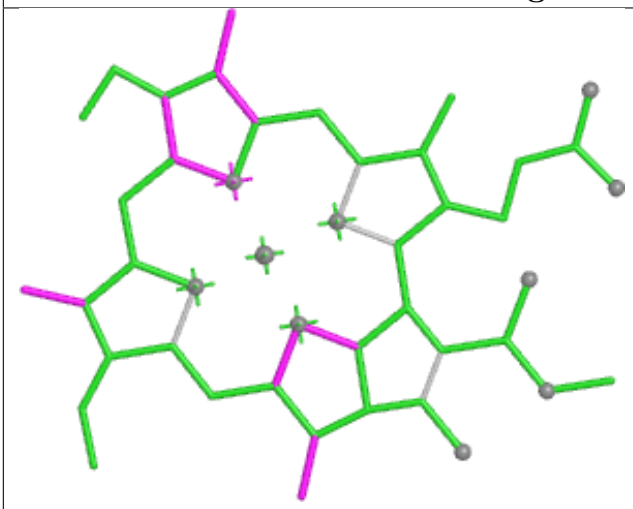


Torsions

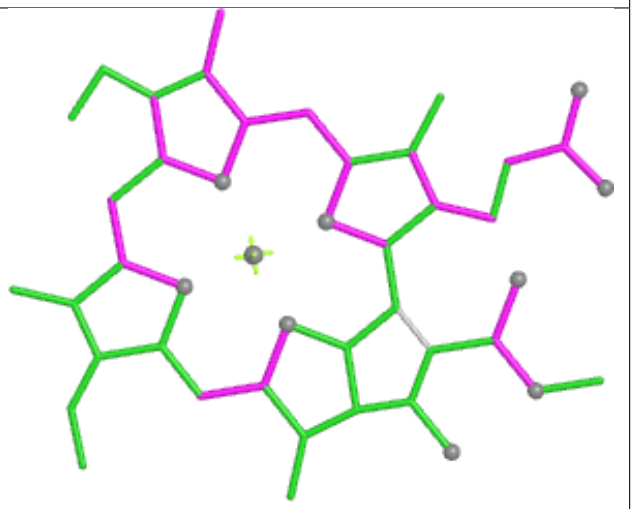


Rings

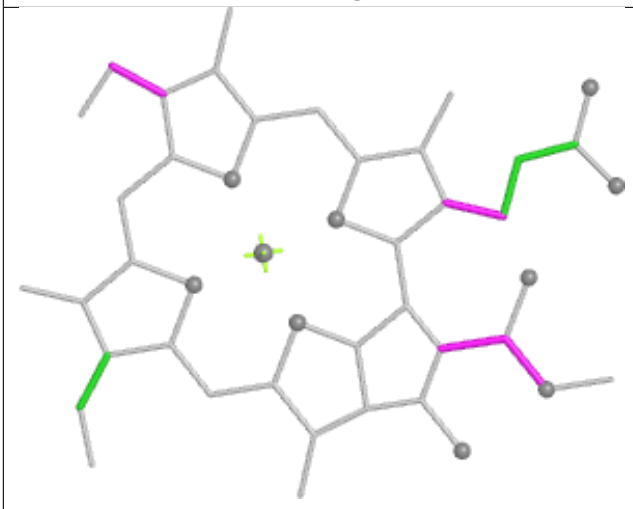
Ligand CLA v 508



Bond lengths



Bond angles

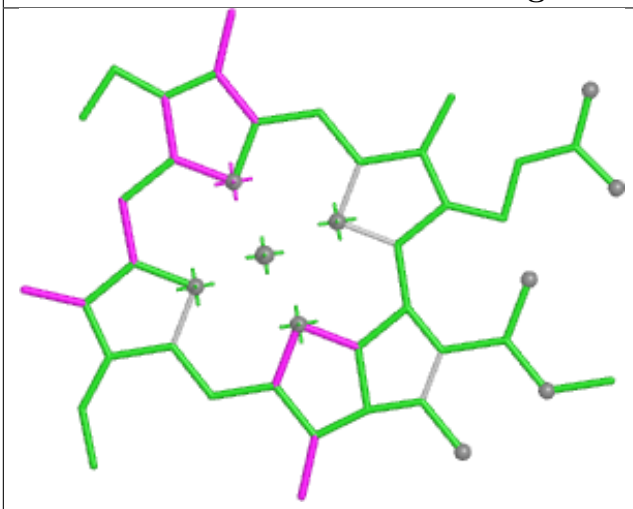


Torsions

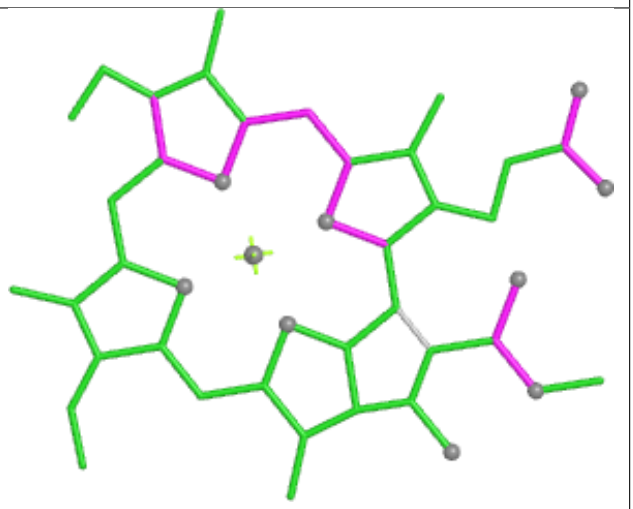


Rings

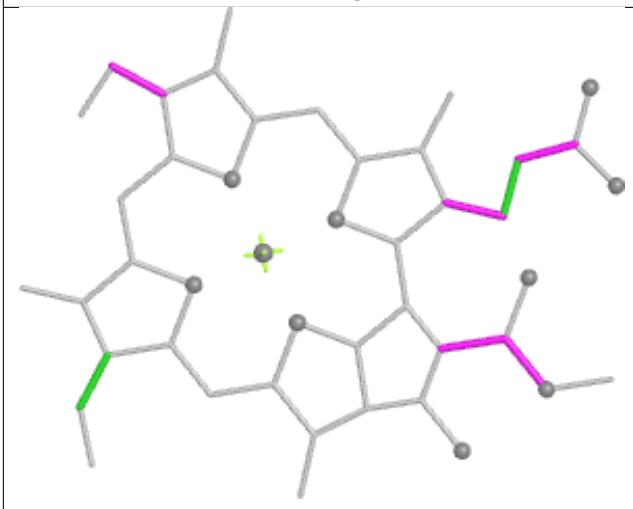
Ligand CLA v 519



Bond lengths



Bond angles

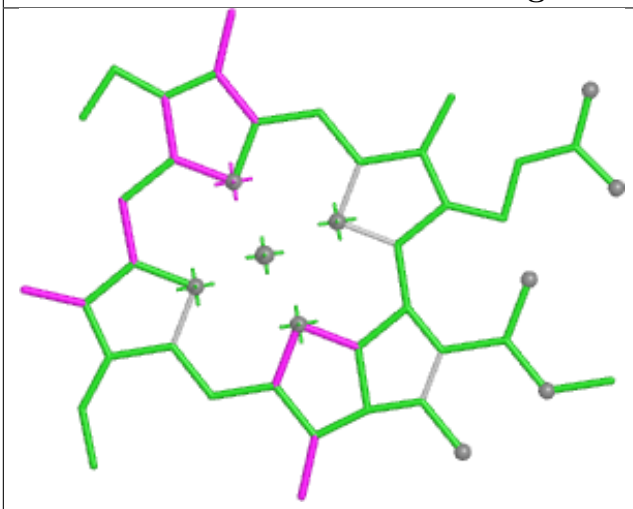


Torsions

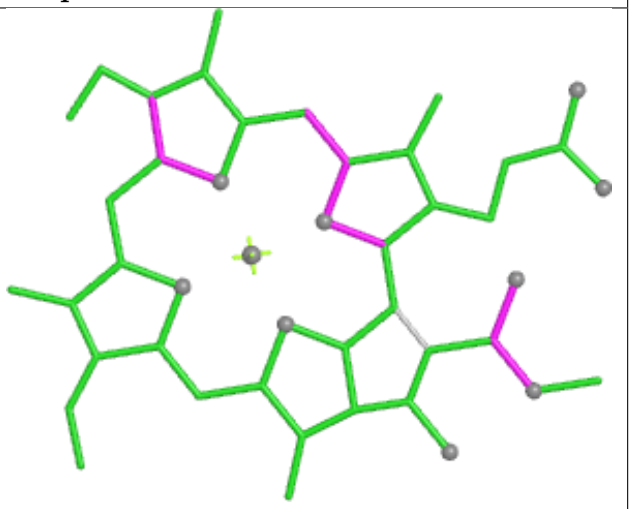


Rings

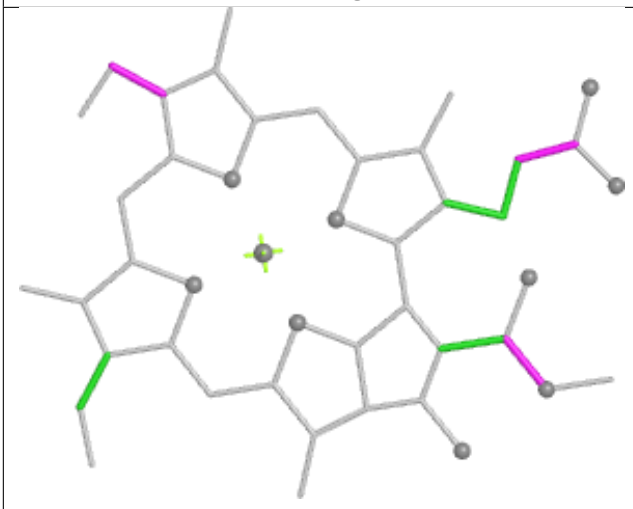
Ligand CLA q 510



Bond lengths



Bond angles

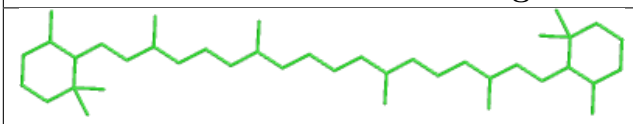


Torsions

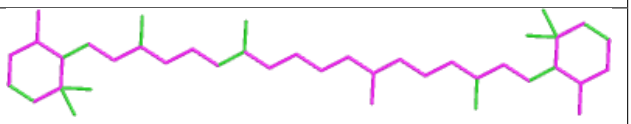


Rings

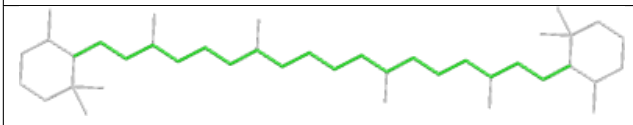
Ligand BCR G 4007



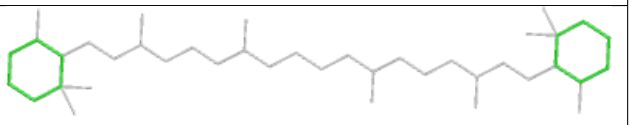
Bond lengths



Bond angles

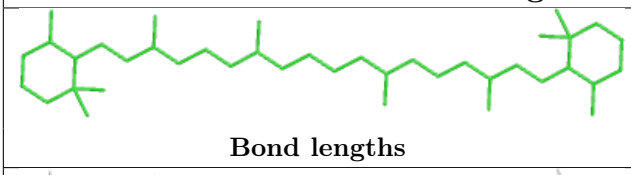


Torsions

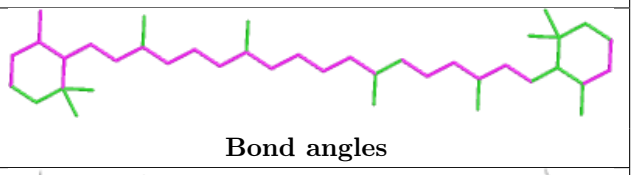


Rings

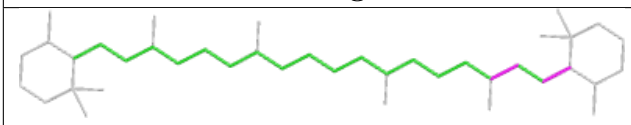
Ligand BCR a 523



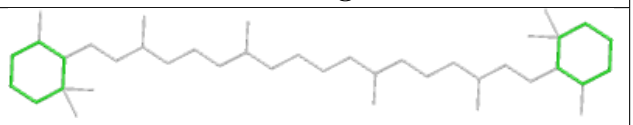
Bond lengths



Bond angles

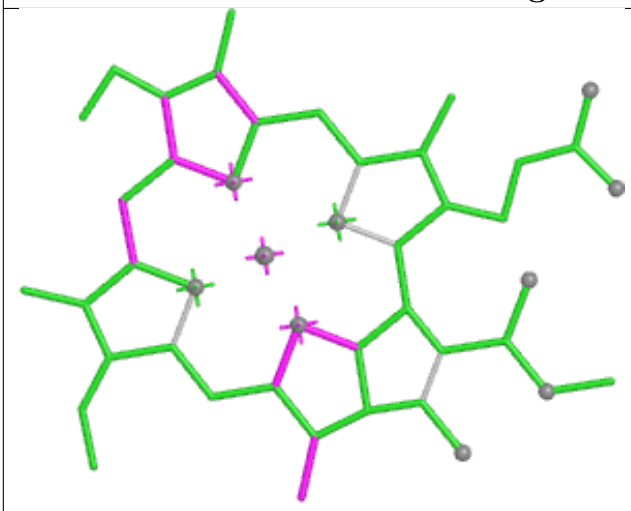


Torsions

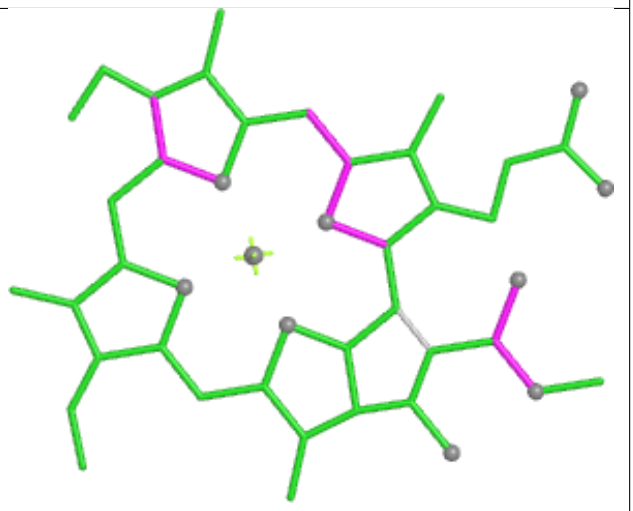


Rings

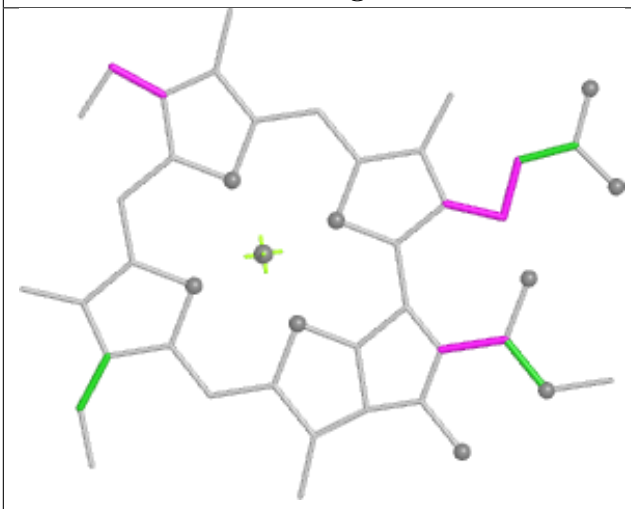
Ligand CLA 5 505



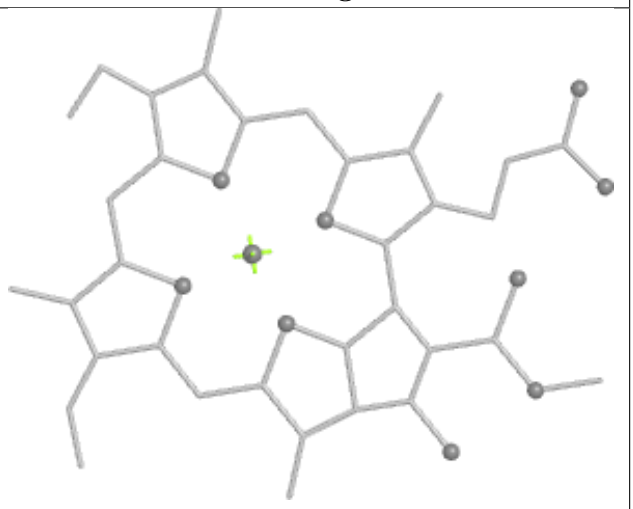
Bond lengths



Bond angles

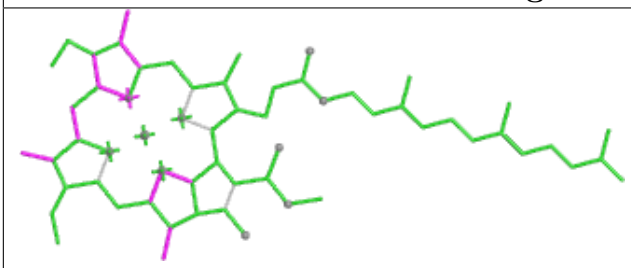


Torsions

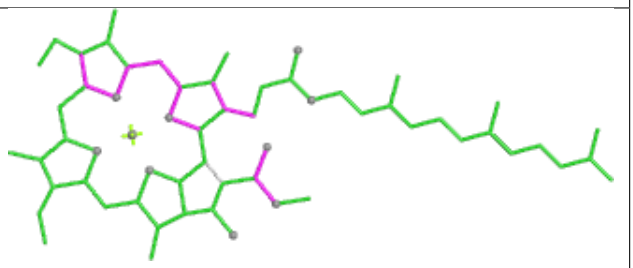


Rings

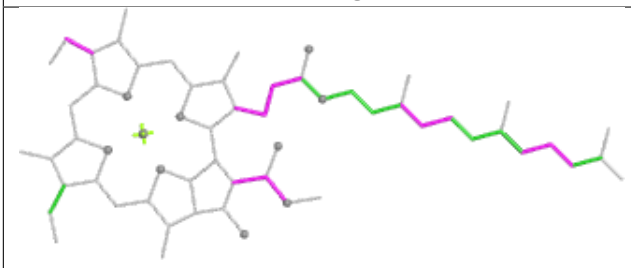
Ligand CLA Z 501



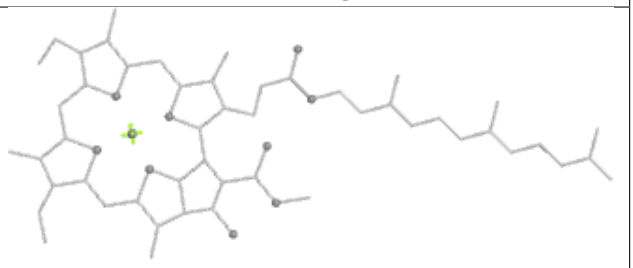
Bond lengths



Bond angles

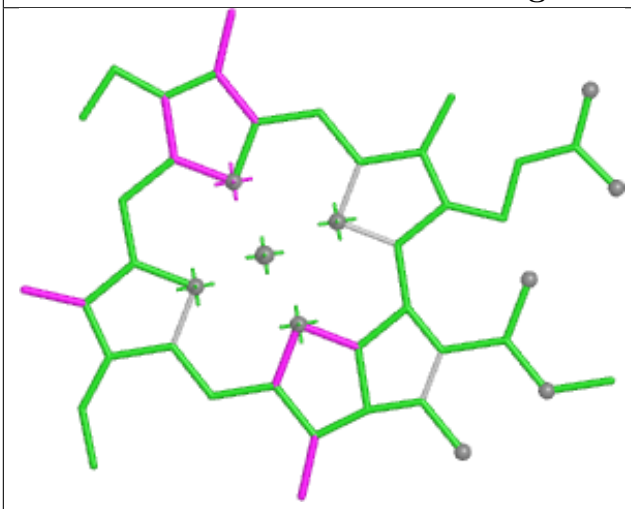


Torsions

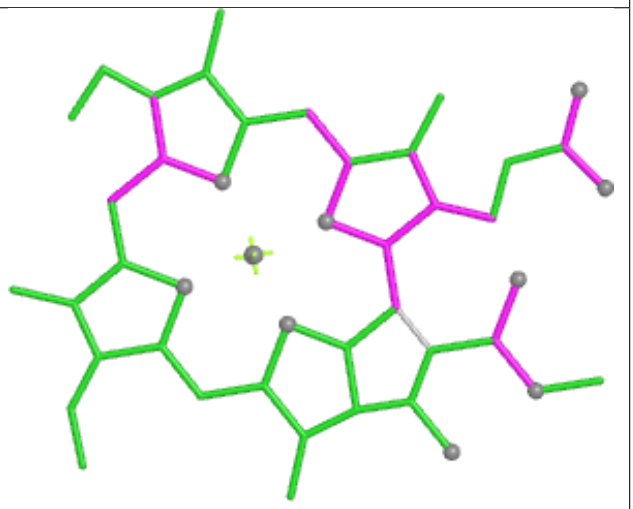


Rings

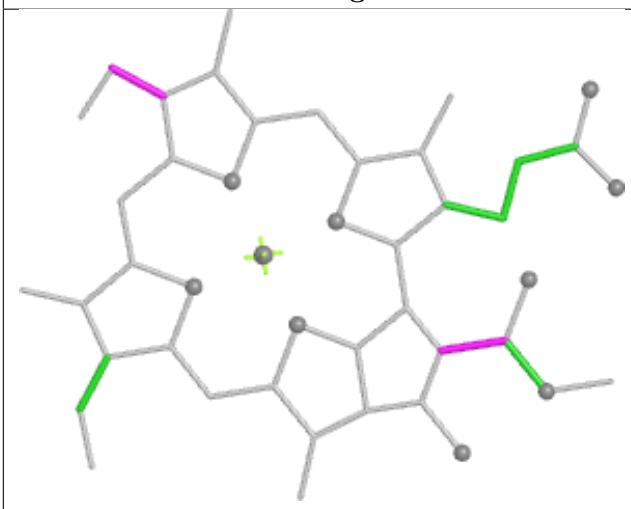
Ligand CLA a 502



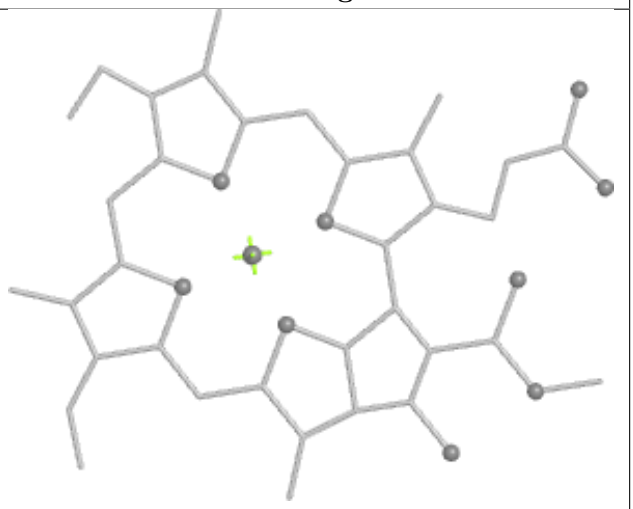
Bond lengths



Bond angles

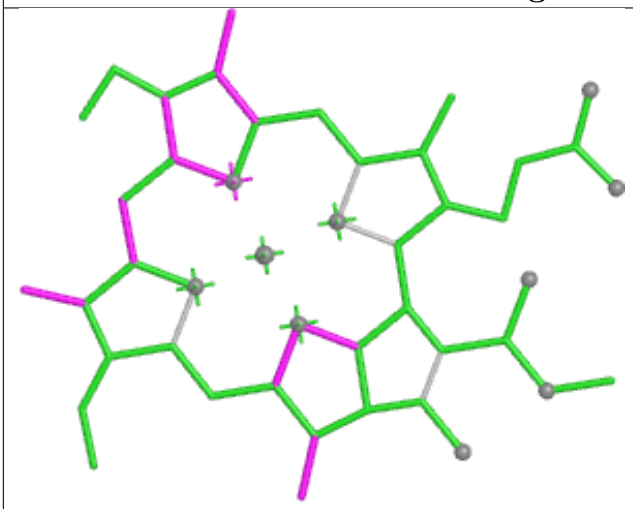


Torsions

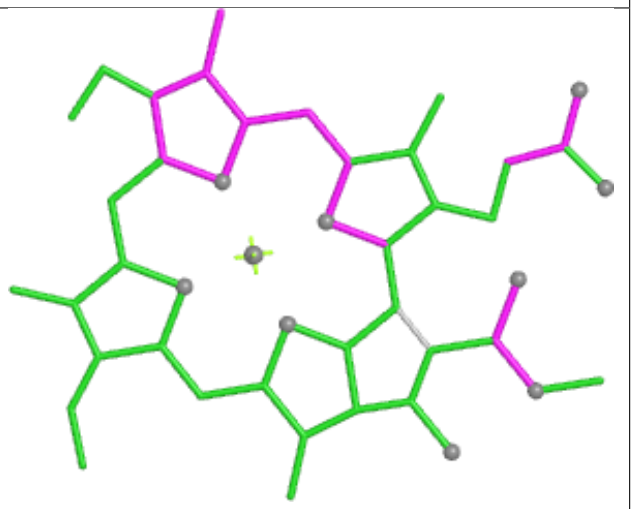


Rings

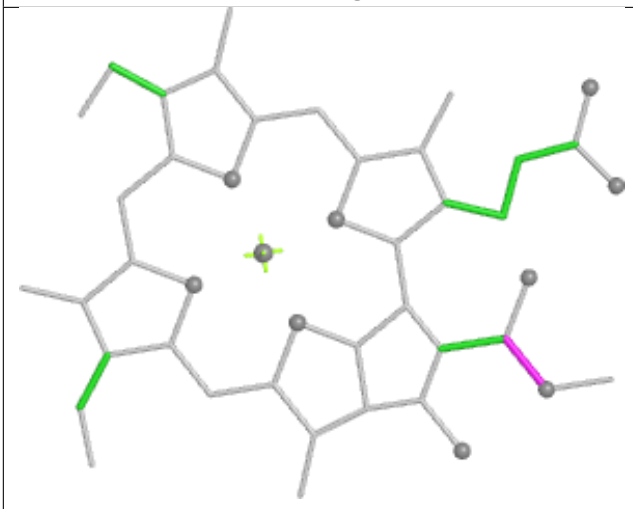
Ligand CLA 3 509



Bond lengths



Bond angles

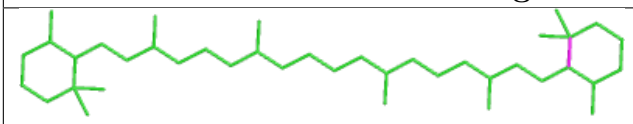


Torsions

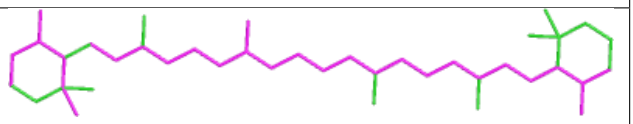


Rings

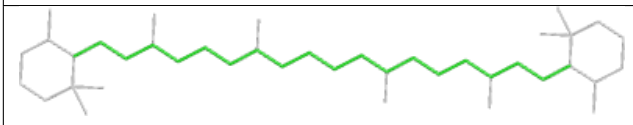
Ligand BCR A 4002



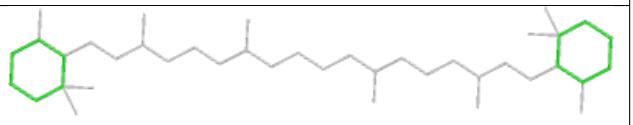
Bond lengths



Bond angles

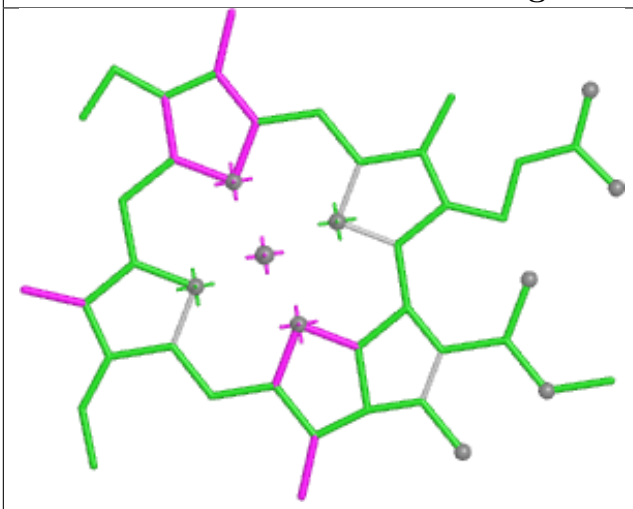


Torsions

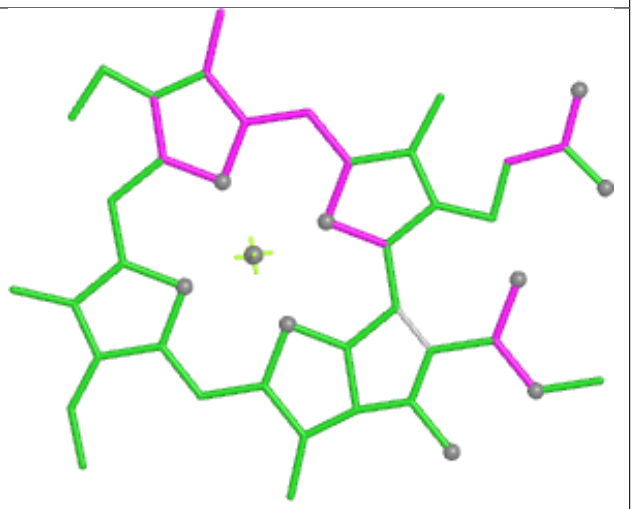


Rings

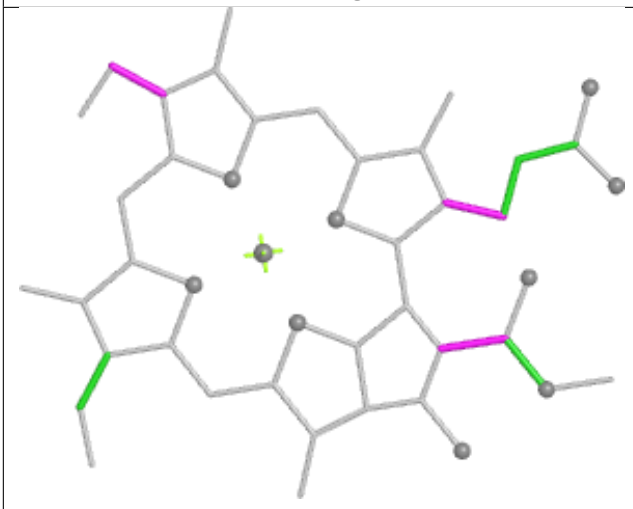
Ligand CLA a 508



Bond lengths



Bond angles

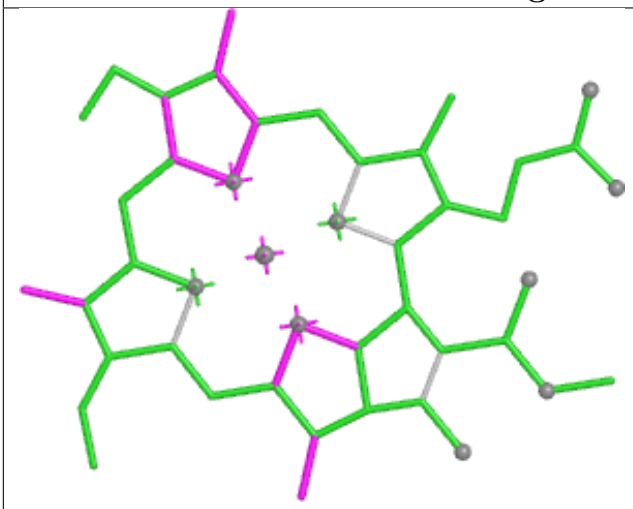


Torsions

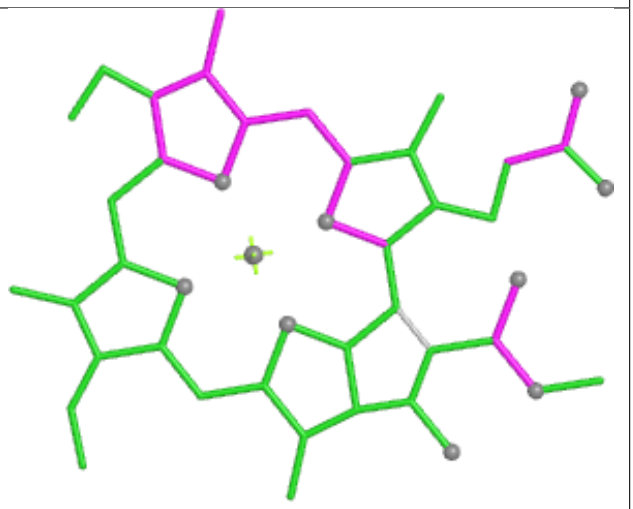


Rings

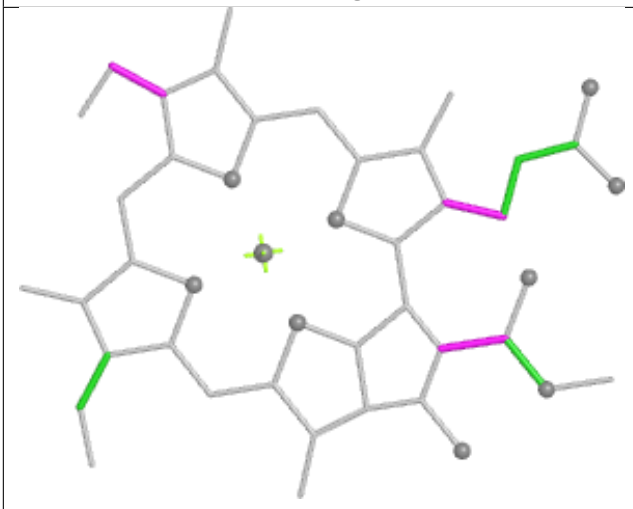
Ligand CLA 3 508



Bond lengths



Bond angles

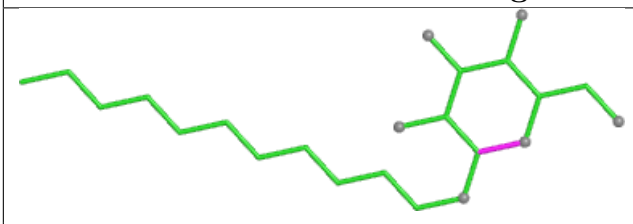


Torsions

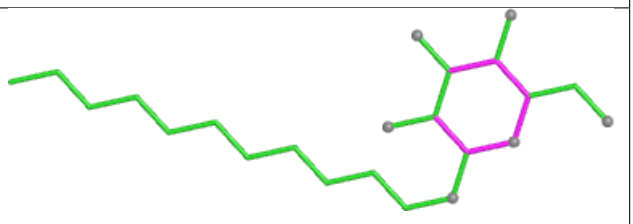


Rings

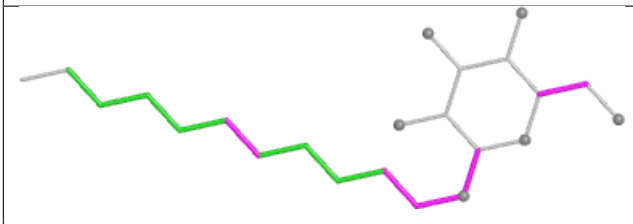
Ligand LMU A 1849



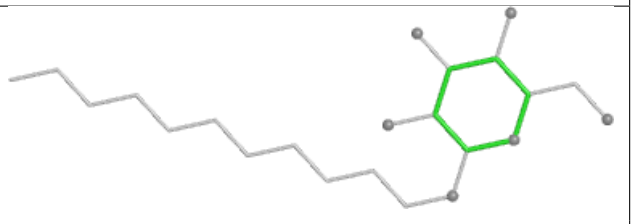
Bond lengths



Bond angles

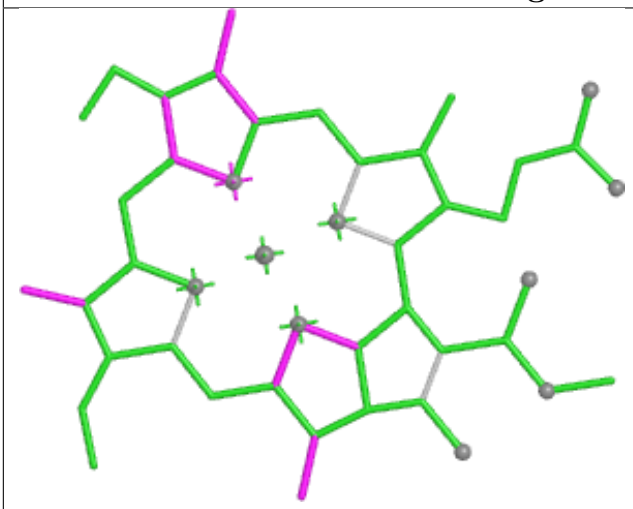


Torsions

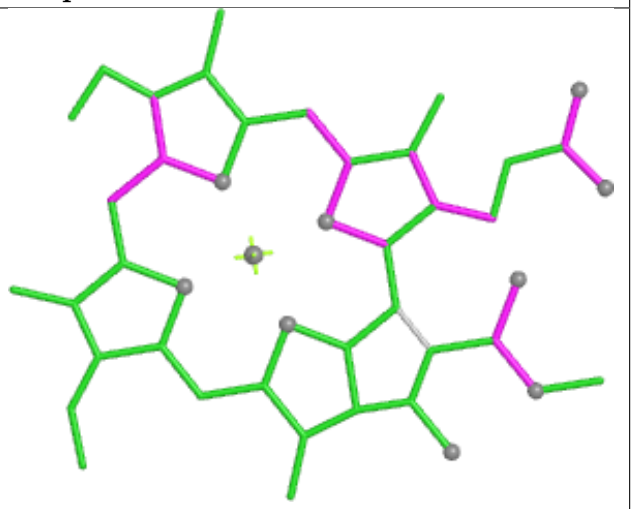


Rings

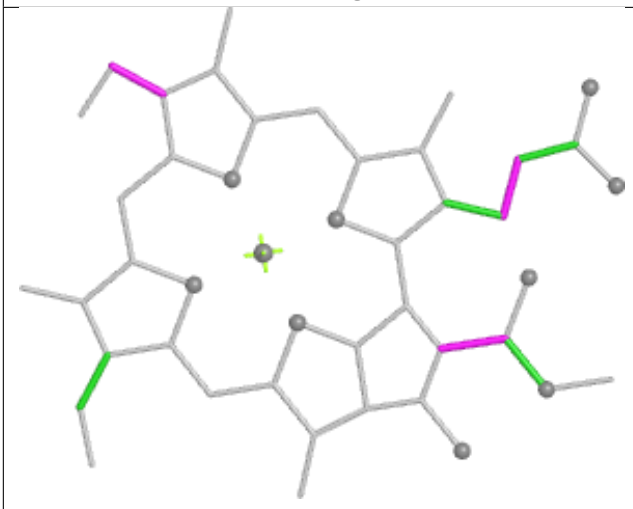
Ligand CLA q 502



Bond lengths



Bond angles

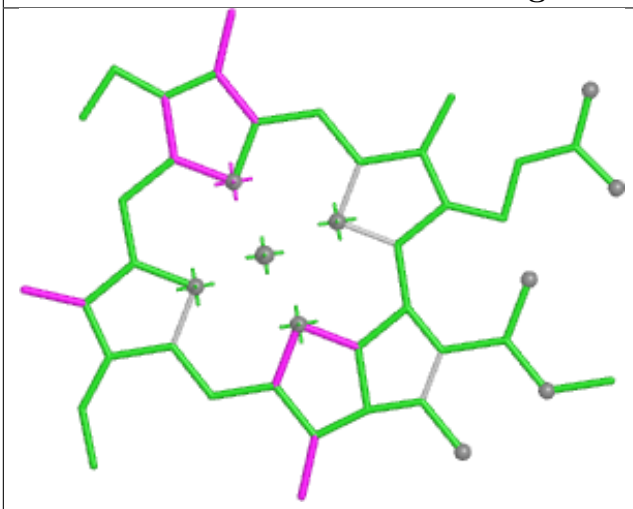


Torsions

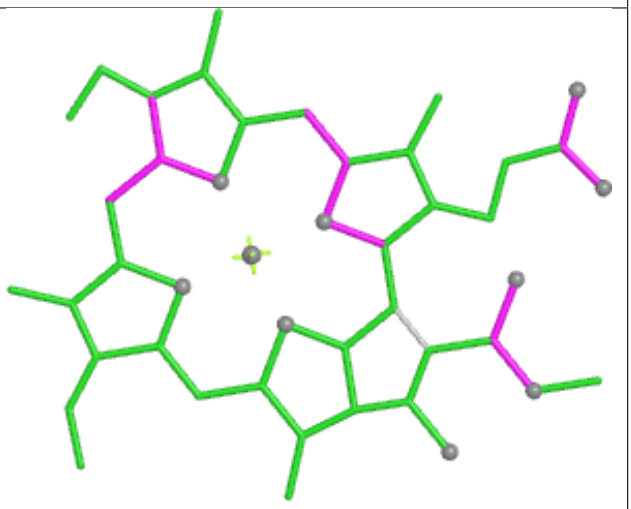


Rings

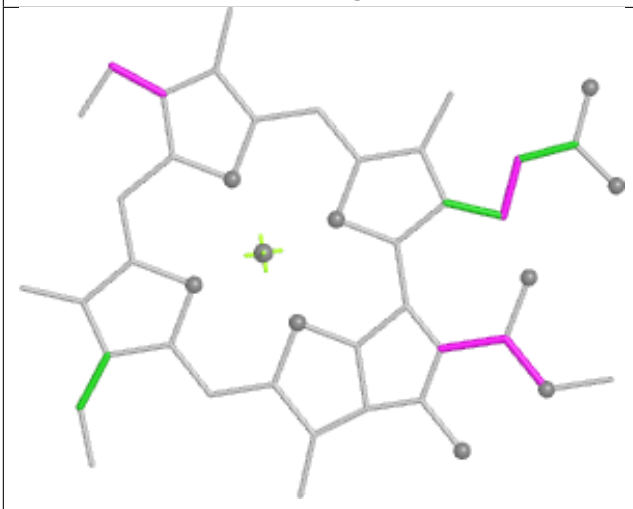
Ligand CLA 2 517



Bond lengths



Bond angles

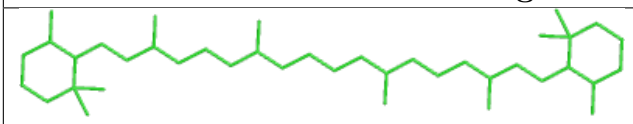


Torsions

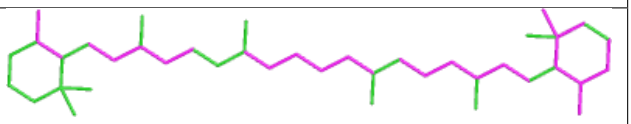


Rings

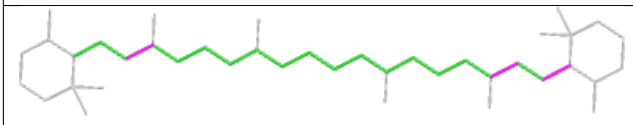
Ligand BCR n 4019



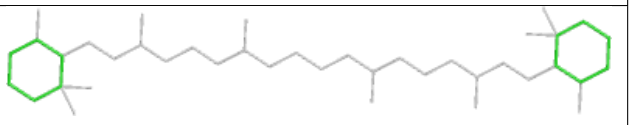
Bond lengths



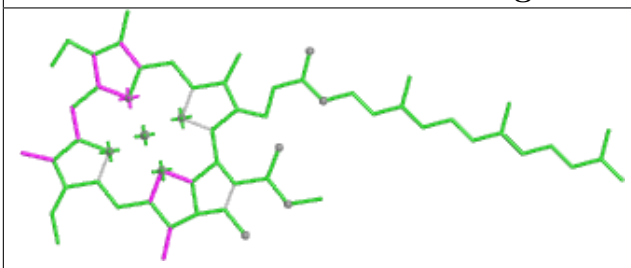
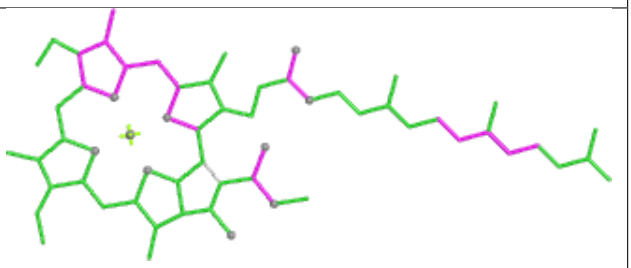
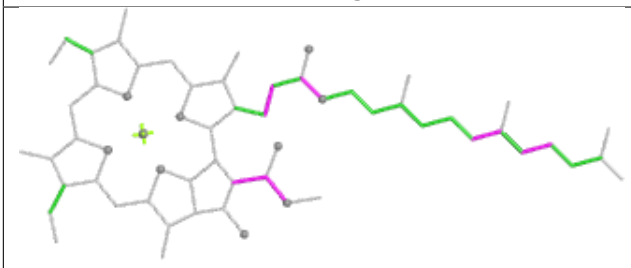
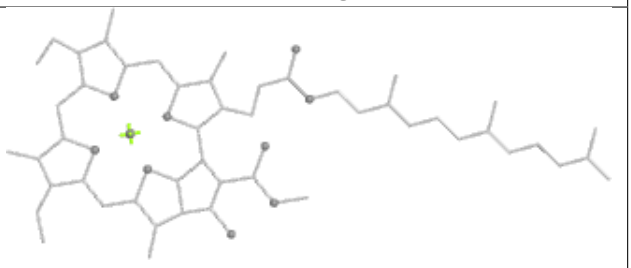
Bond angles

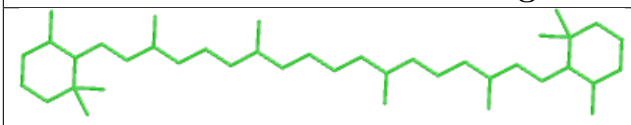
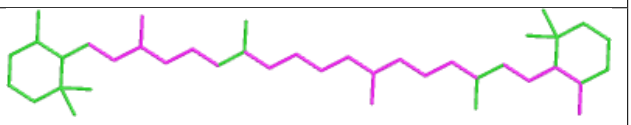
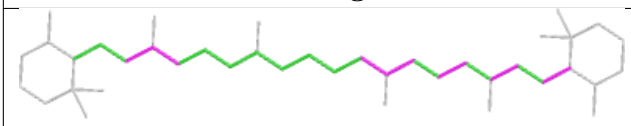
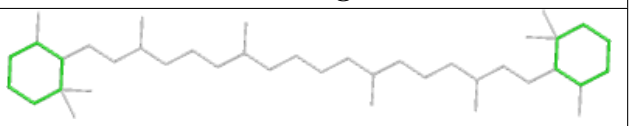


Torsions

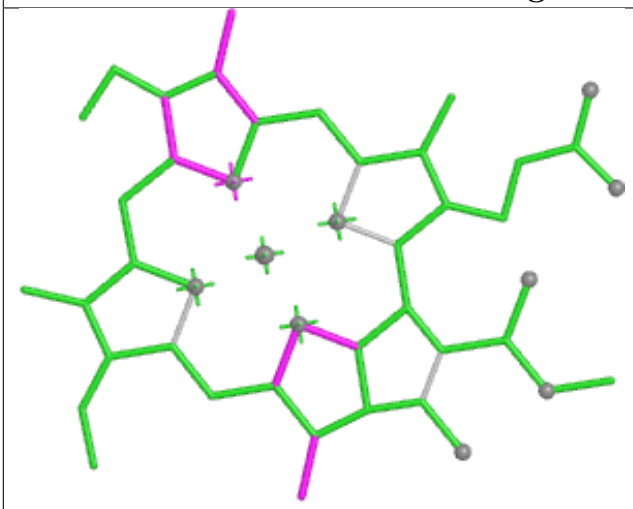


Rings

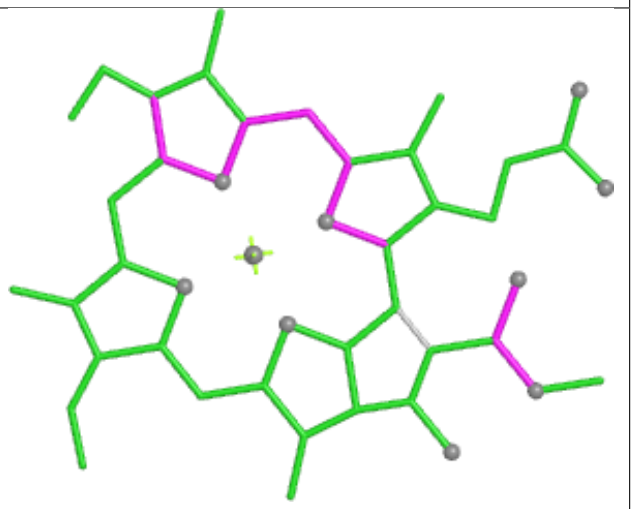
Ligand CLA H 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR e 4011	
	
Bond lengths	Bond angles
	
Torsions	Rings

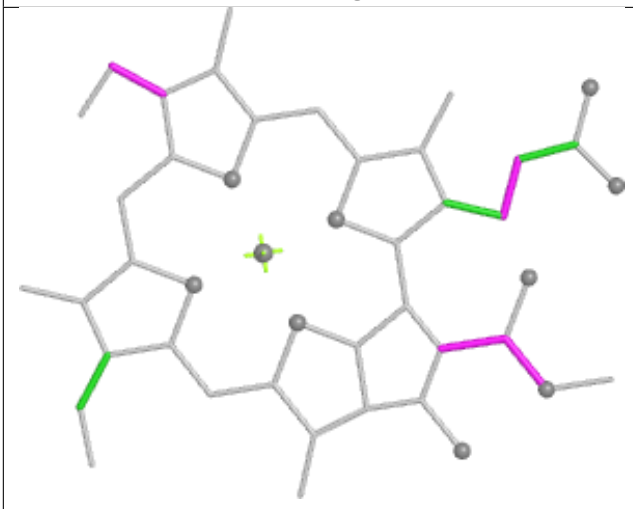
Ligand CLA v 503



Bond lengths



Bond angles

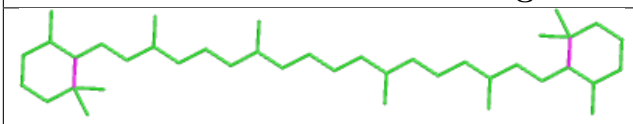


Torsions

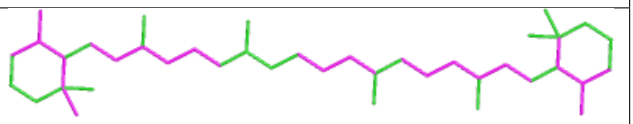


Rings

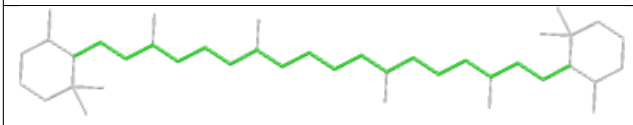
Ligand BCR S 4018



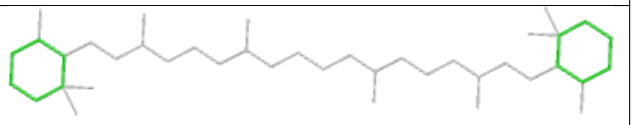
Bond lengths



Bond angles

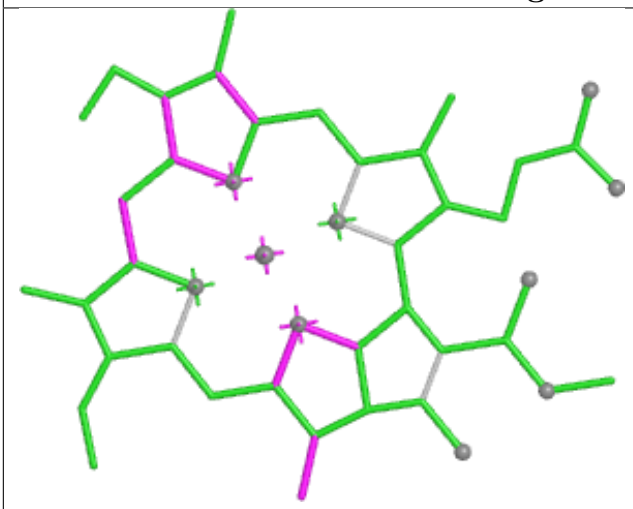


Torsions

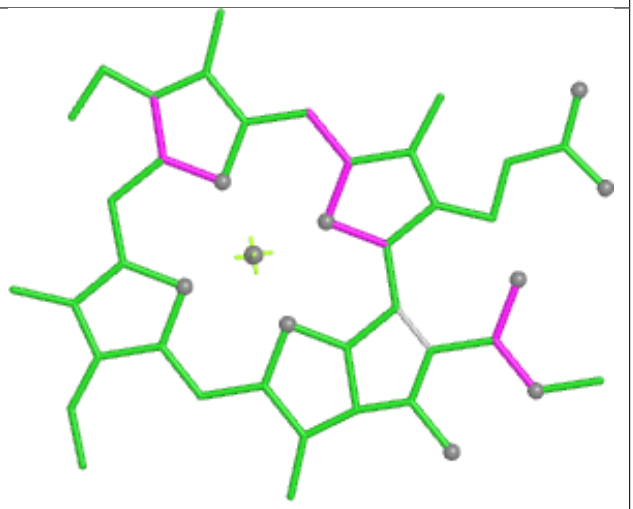


Rings

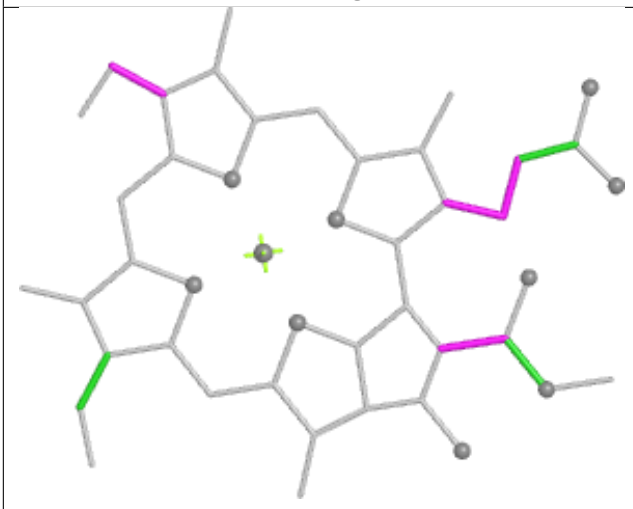
Ligand CLA u 505



Bond lengths



Bond angles

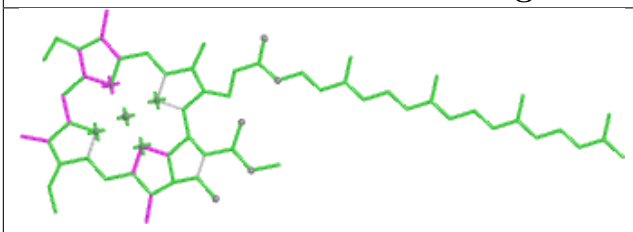


Torsions

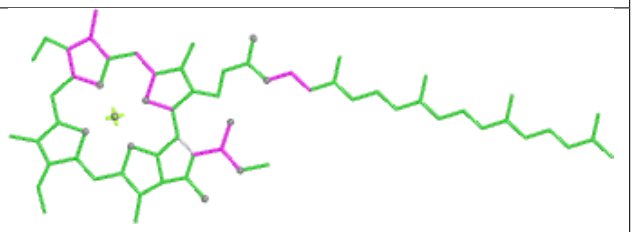


Rings

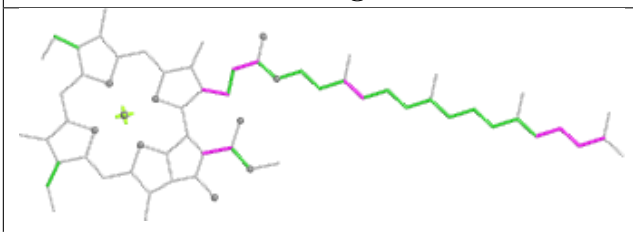
Ligand CLA B 1202



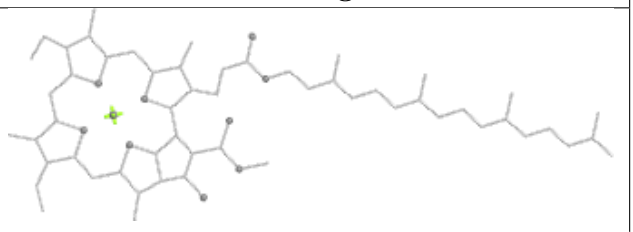
Bond lengths



Bond angles

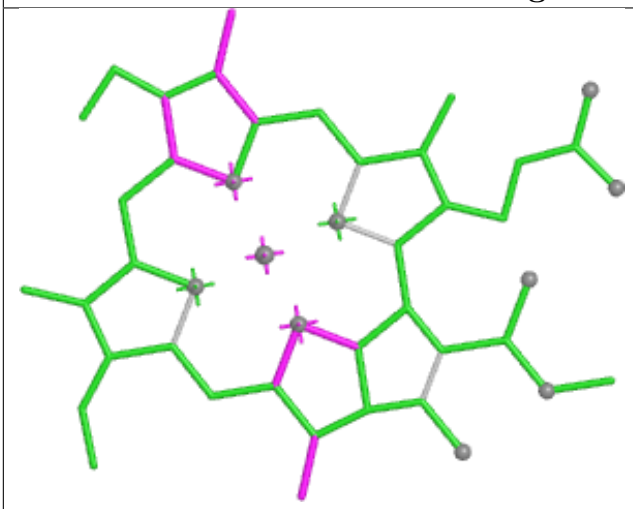


Torsions

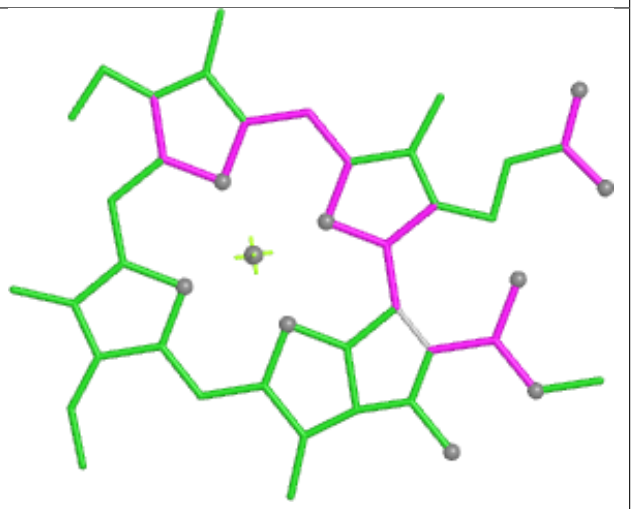


Rings

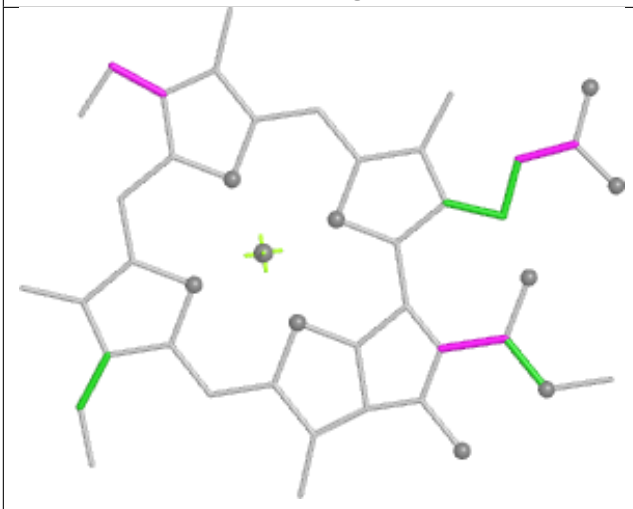
Ligand CLA 1 509



Bond lengths



Bond angles

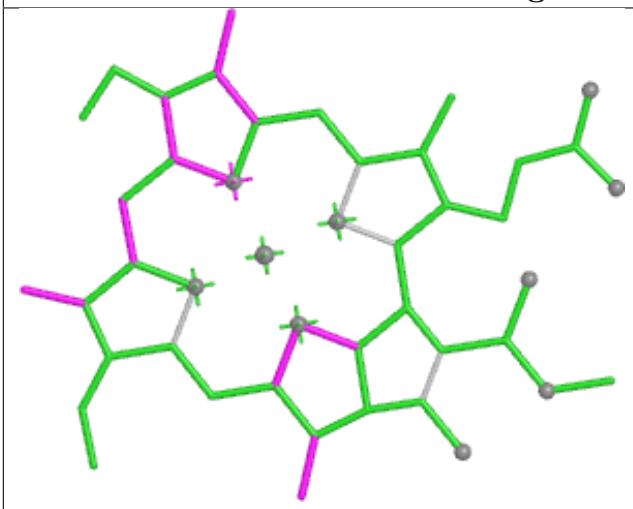


Torsions

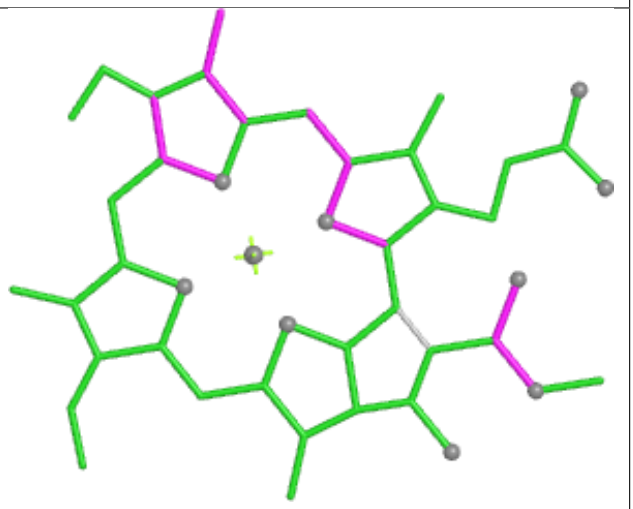


Rings

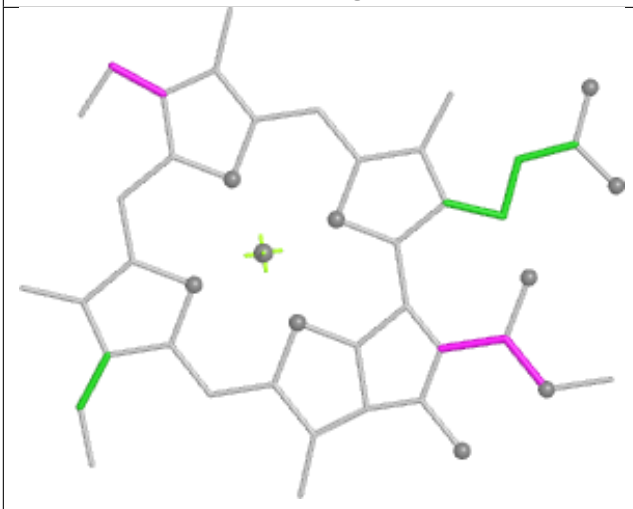
Ligand CLA v 506



Bond lengths



Bond angles

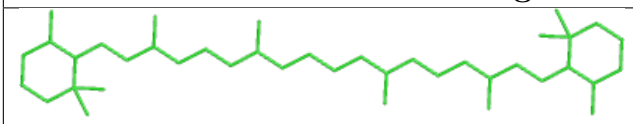


Torsions

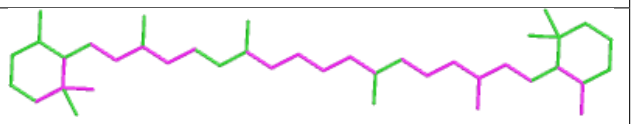


Rings

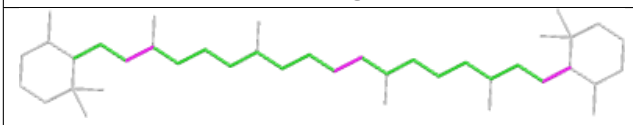
Ligand BCR T 4015



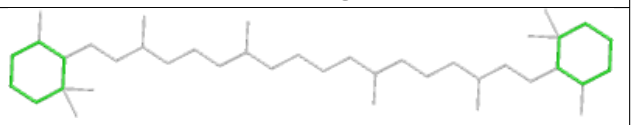
Bond lengths



Bond angles

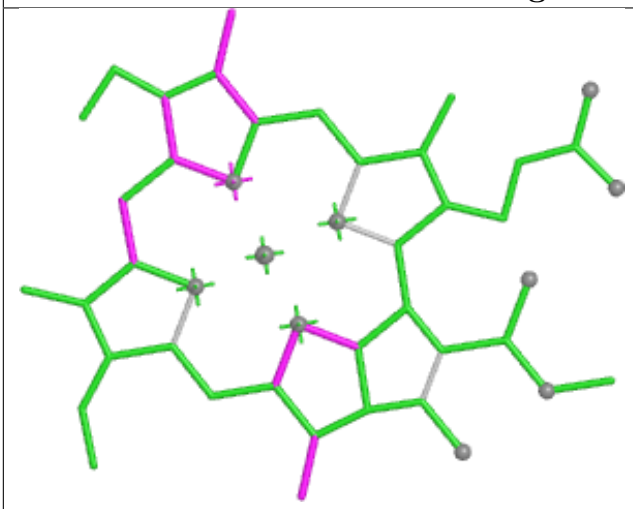


Torsions

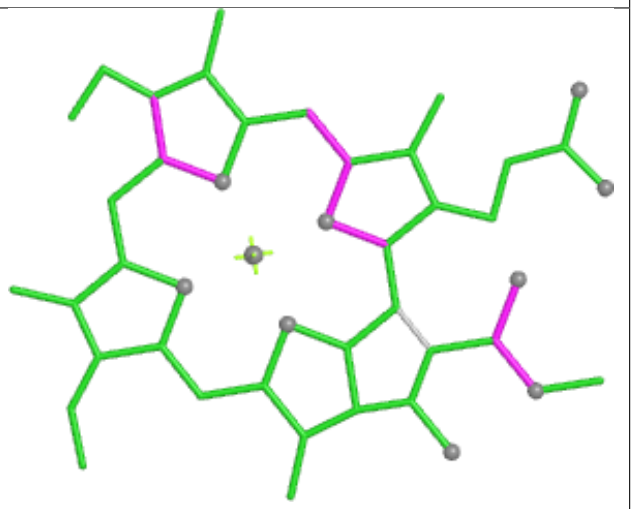


Rings

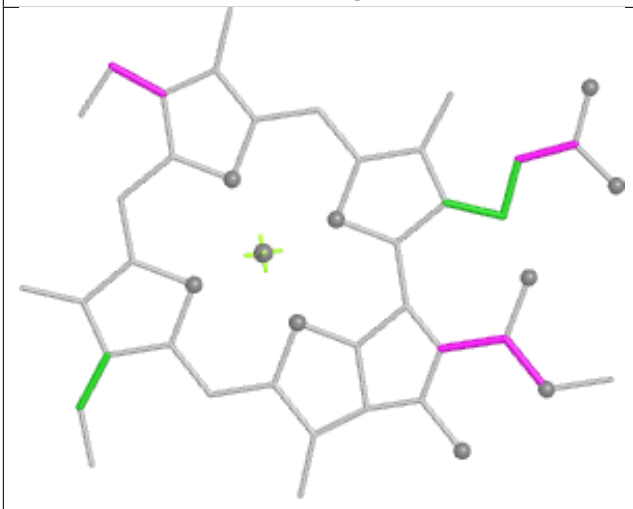
Ligand CLA 4 510



Bond lengths



Bond angles

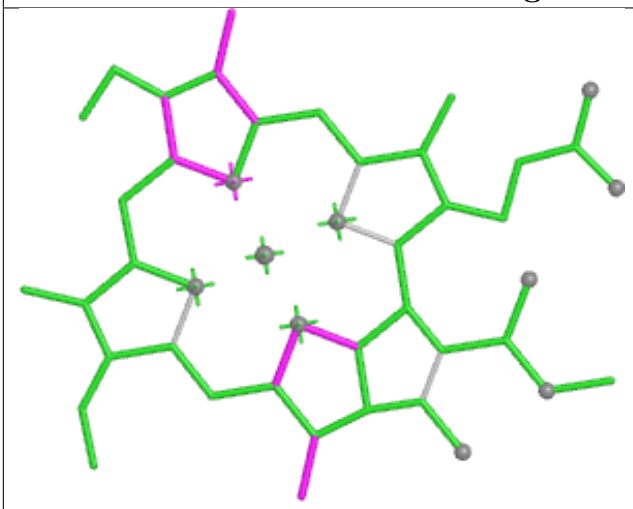


Torsions

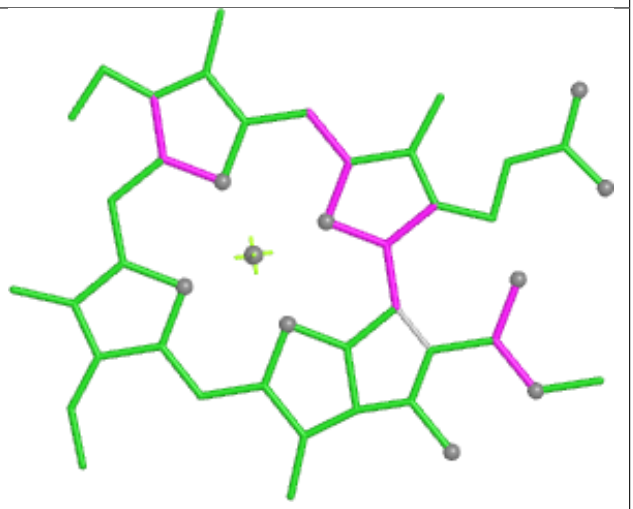


Rings

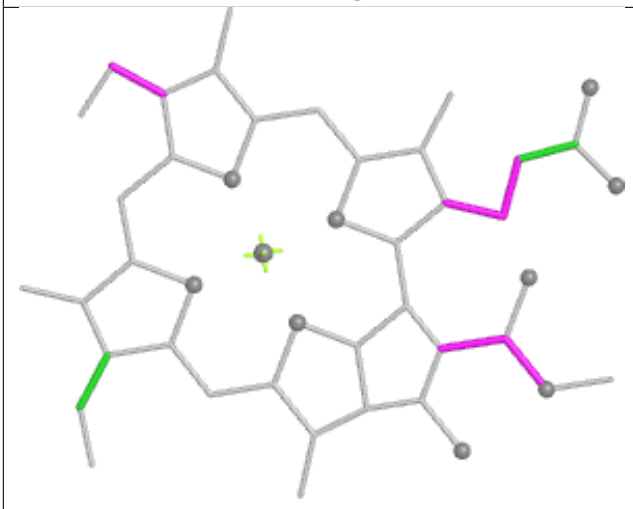
Ligand CLA Y 503



Bond lengths



Bond angles

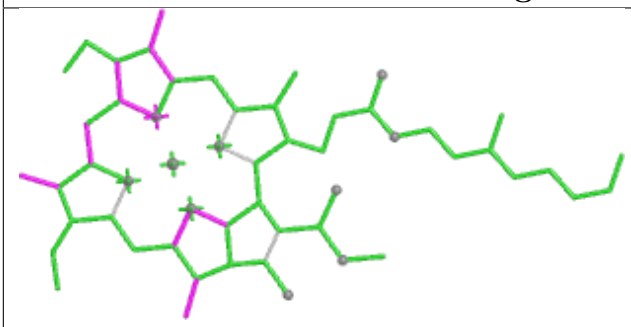


Torsions

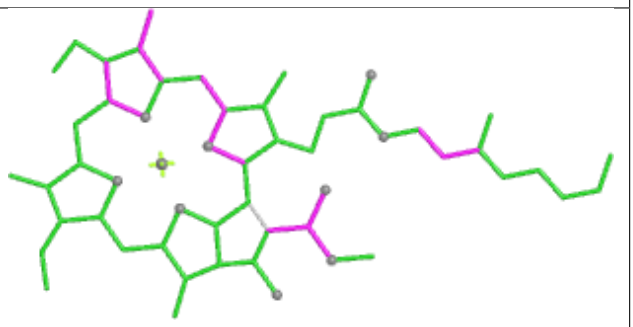


Rings

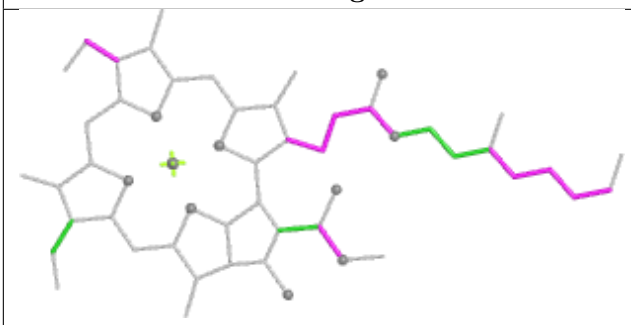
Ligand CLA A 1108



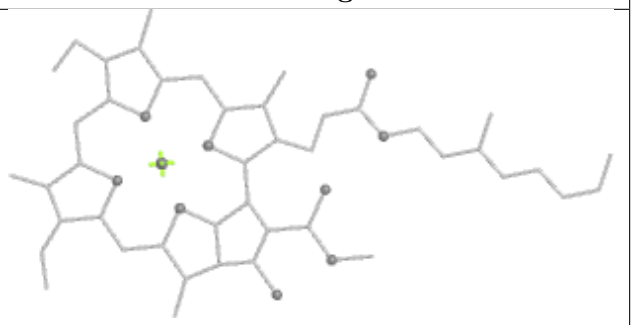
Bond lengths



Bond angles

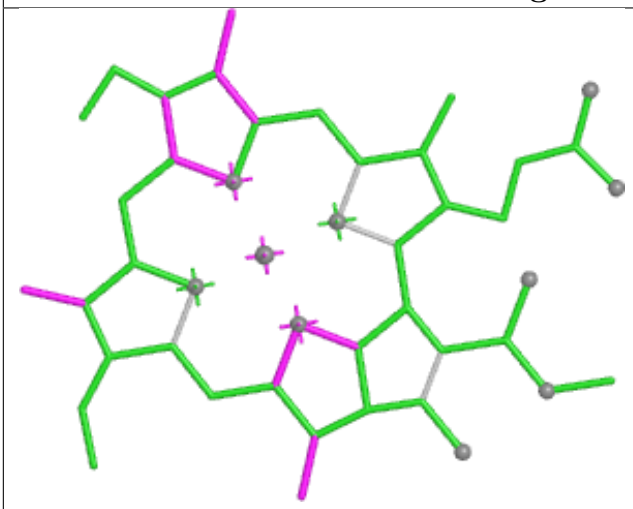


Torsions

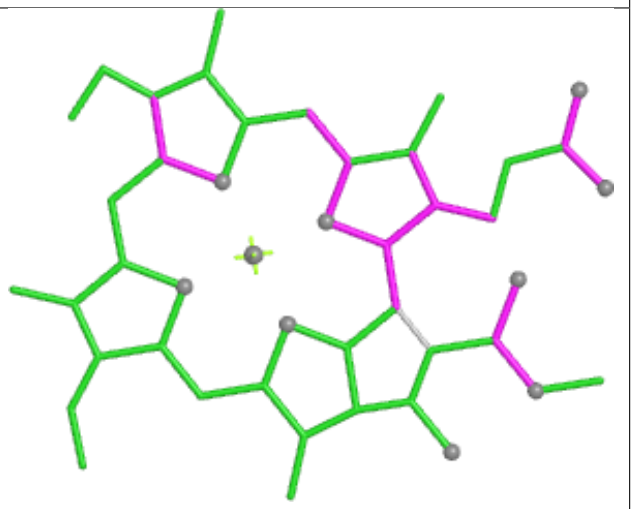


Rings

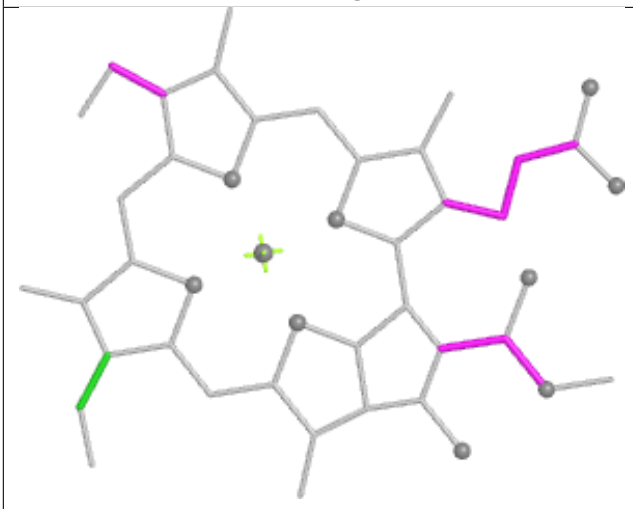
Ligand CLA r 507



Bond lengths



Bond angles

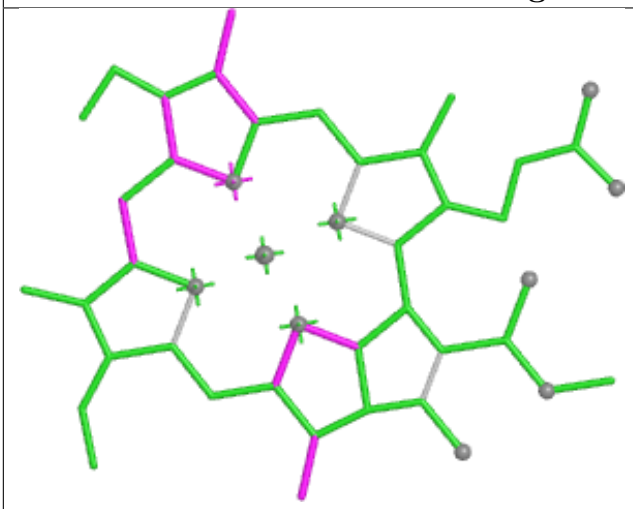


Torsions

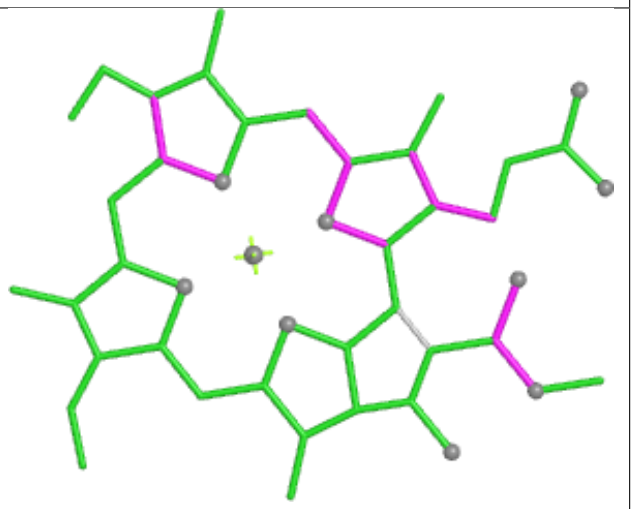


Rings

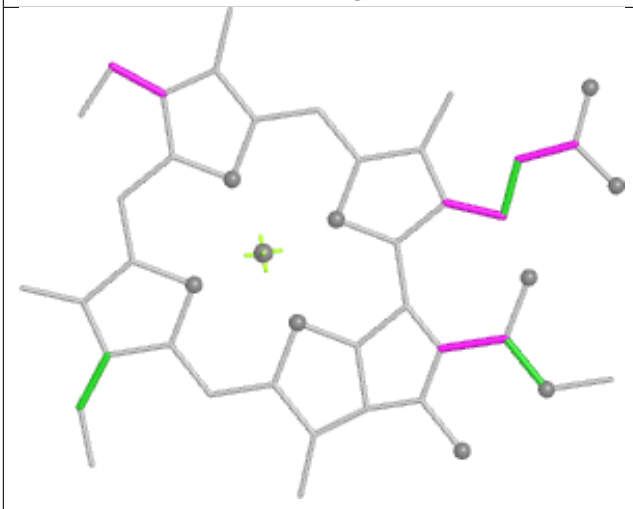
Ligand CLA 4 516



Bond lengths



Bond angles

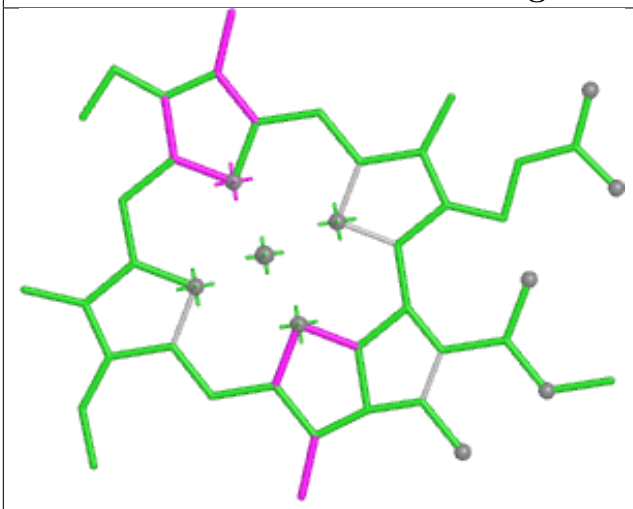


Torsions

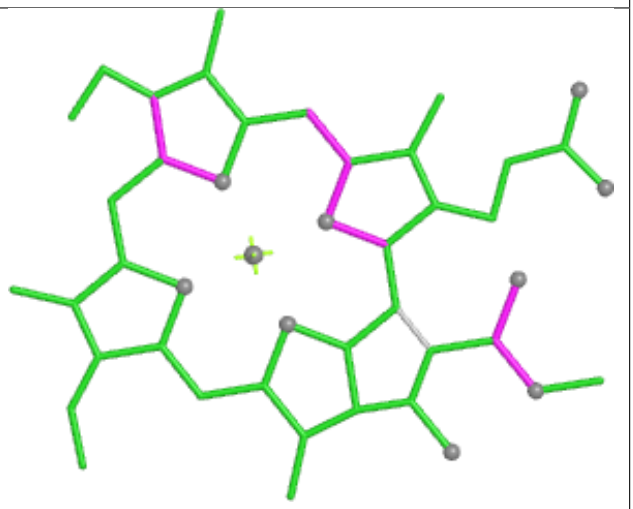


Rings

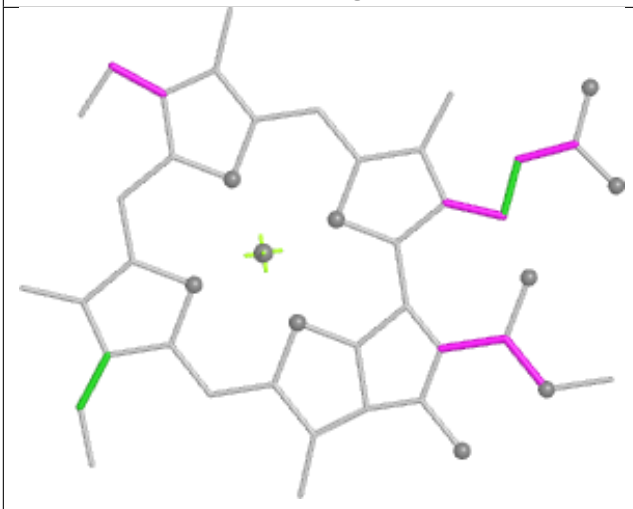
Ligand CLA 6 518



Bond lengths



Bond angles

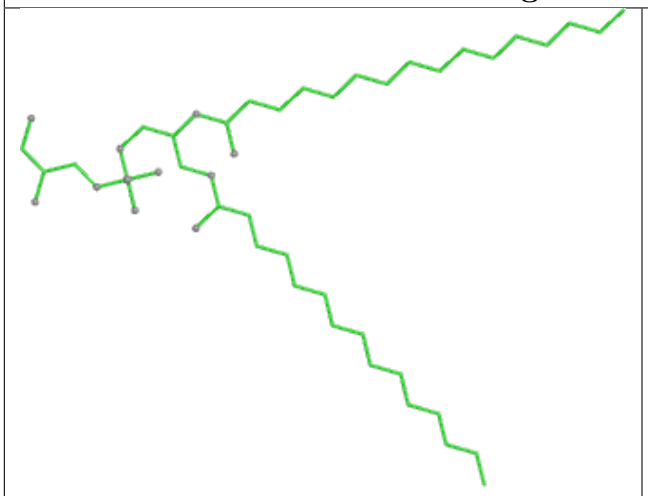


Torsions

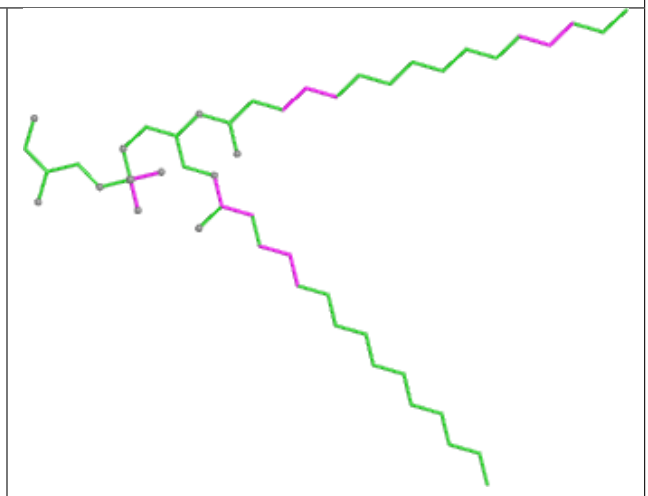


Rings

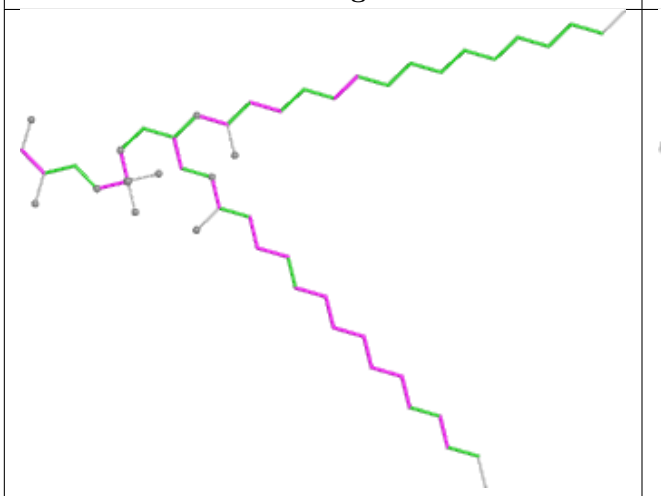
Ligand LHG I 5001



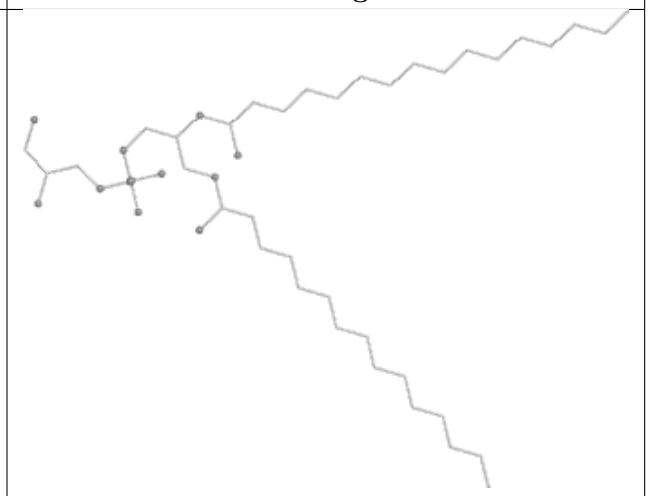
Bond lengths



Bond angles

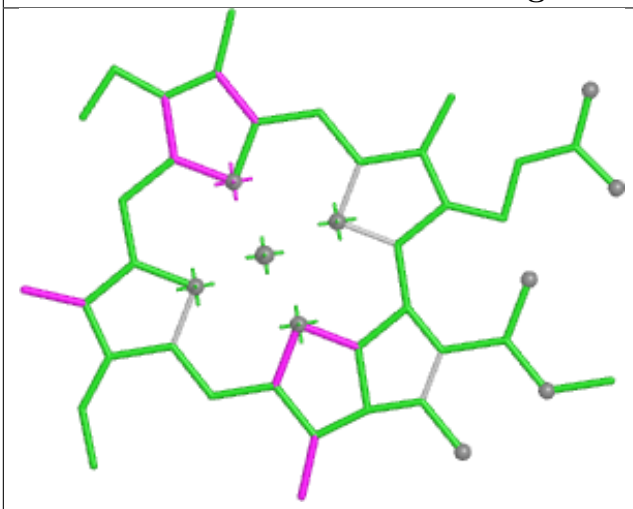


Torsions

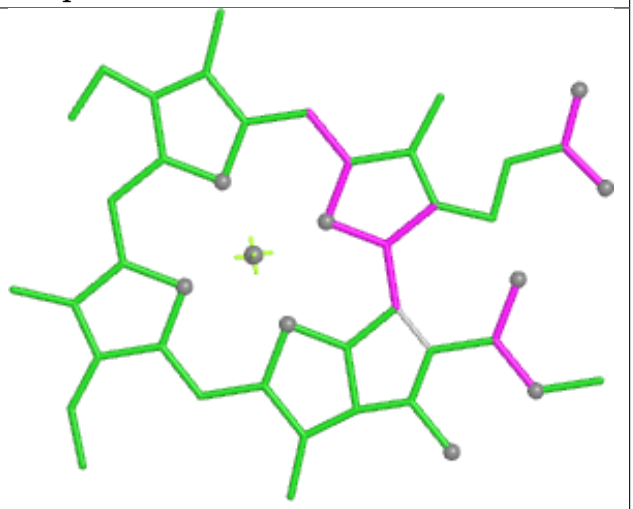


Rings

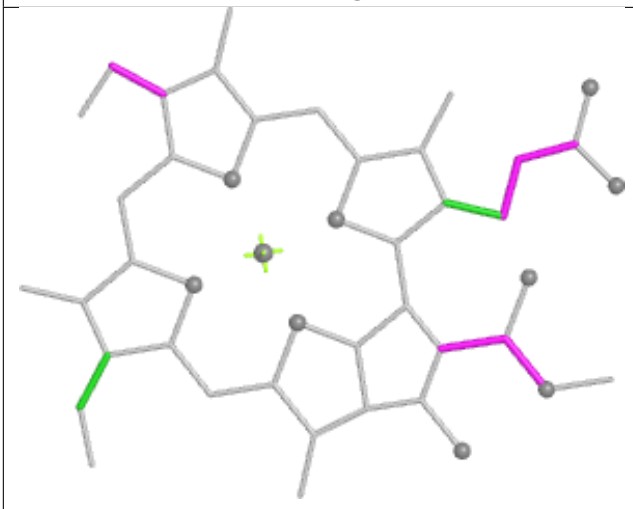
Ligand CLA q 507



Bond lengths



Bond angles

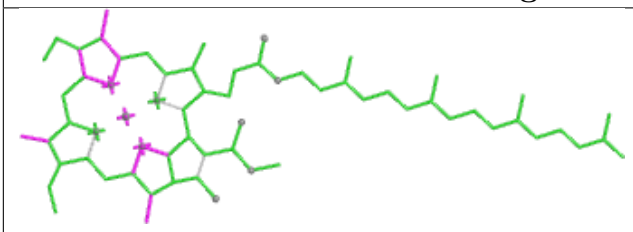


Torsions

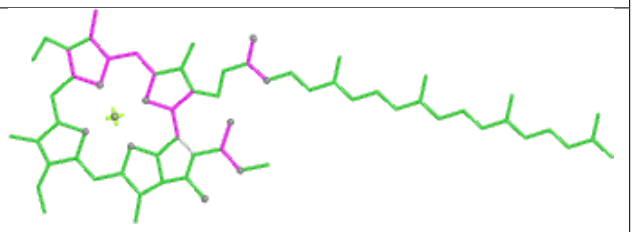


Rings

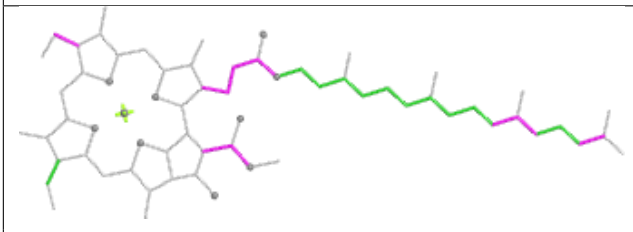
Ligand CLA e 1111



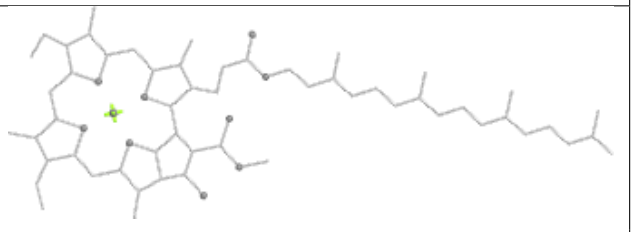
Bond lengths



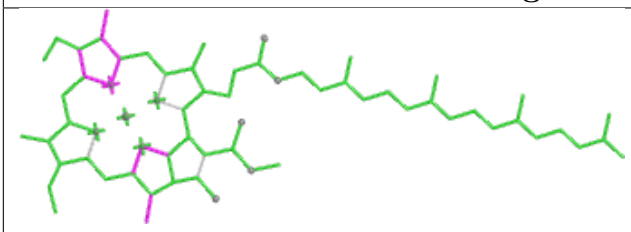
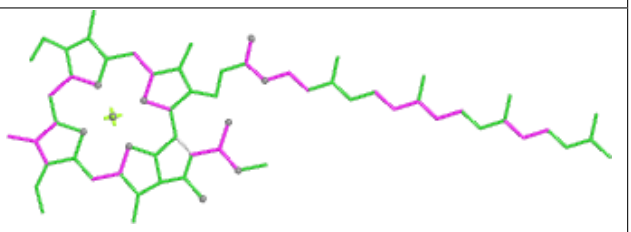
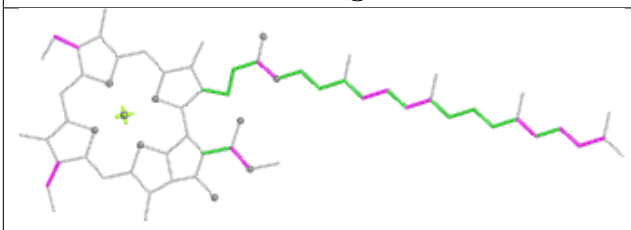
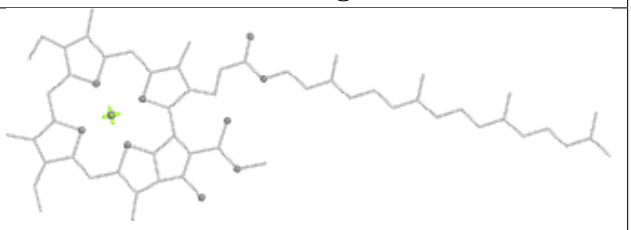
Bond angles

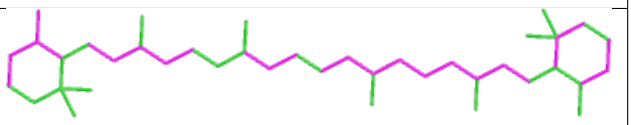
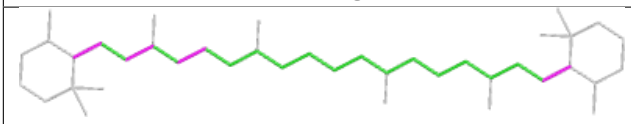
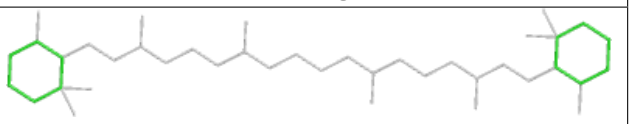


Torsions

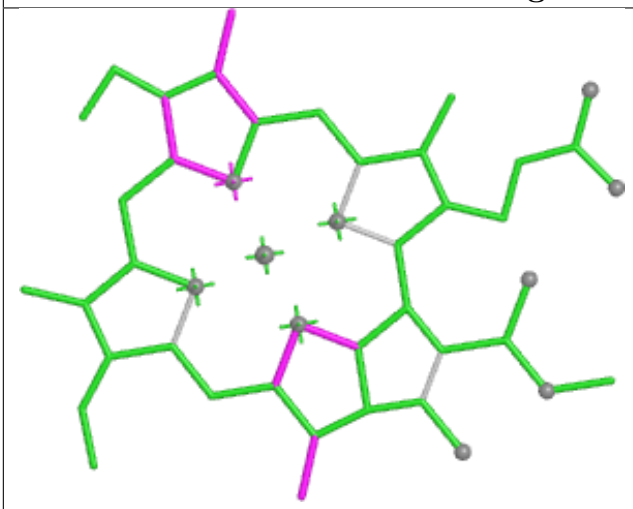


Rings

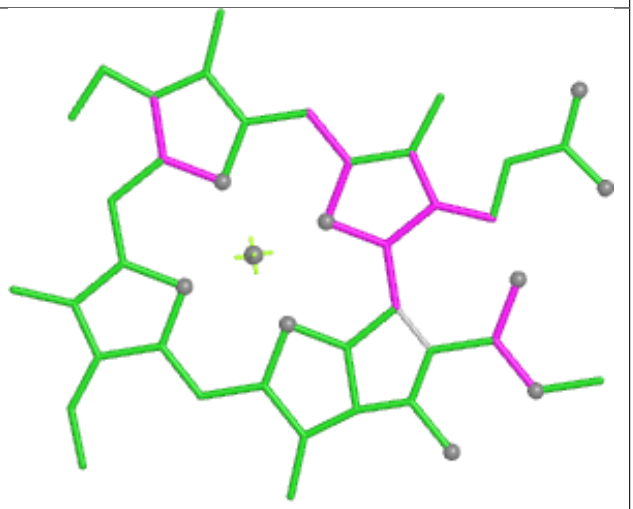
Ligand CLA f 1239	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR s 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

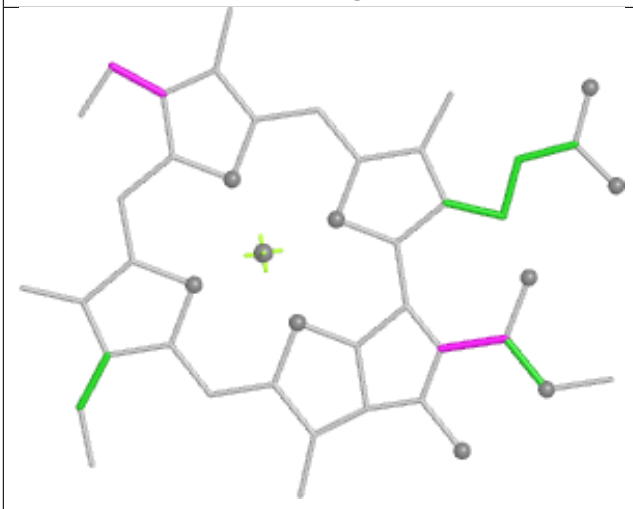
Ligand CLA v 502



Bond lengths



Bond angles

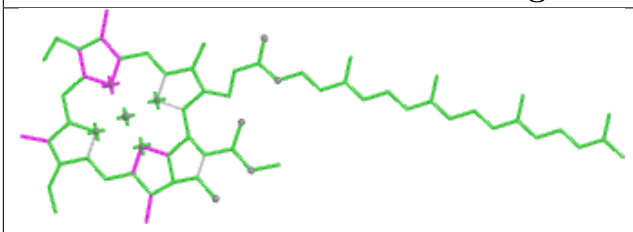


Torsions

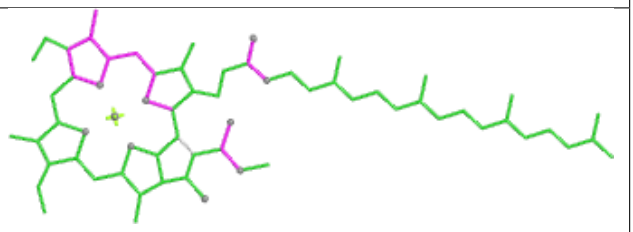


Rings

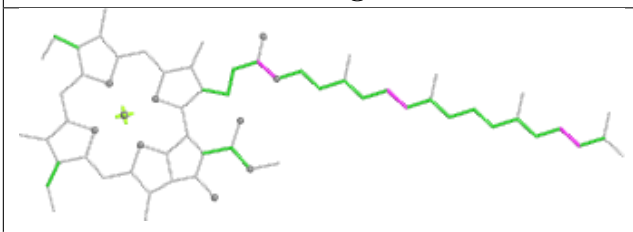
Ligand CLA 2 509



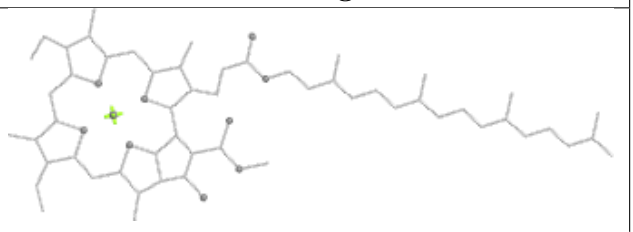
Bond lengths



Bond angles

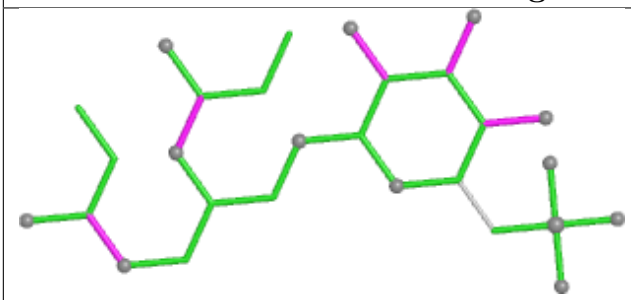


Torsions

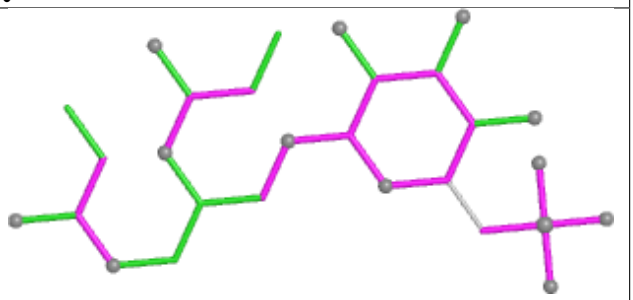


Rings

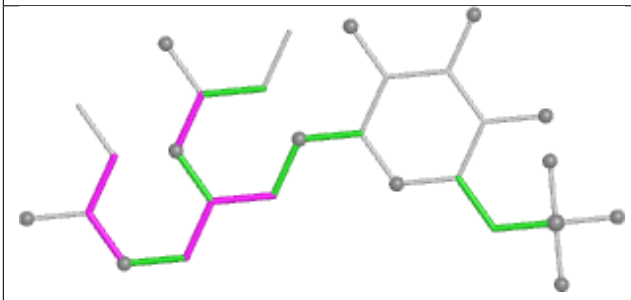
Ligand SQD 3 822



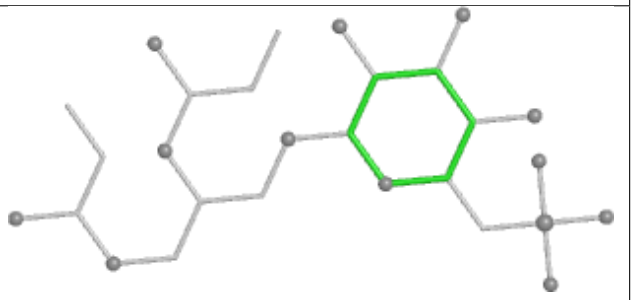
Bond lengths



Bond angles

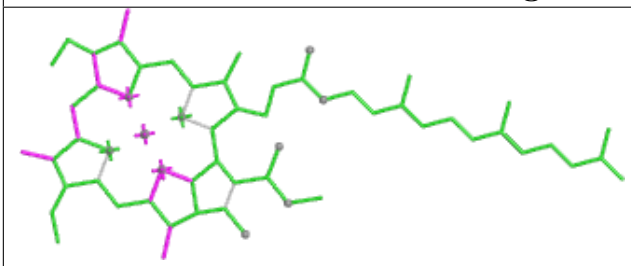


Torsions

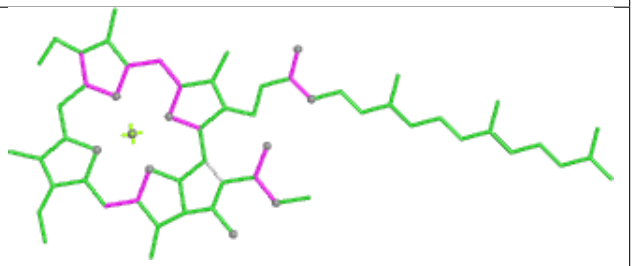


Rings

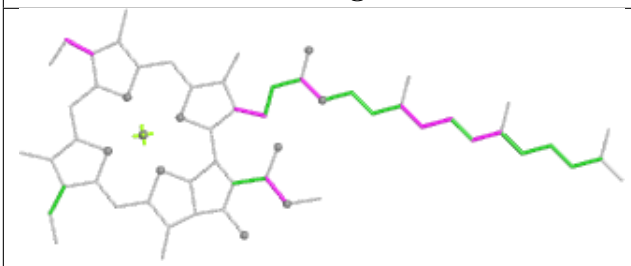
Ligand CLA f 1227



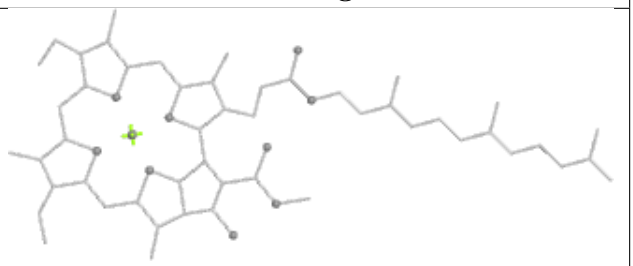
Bond lengths



Bond angles

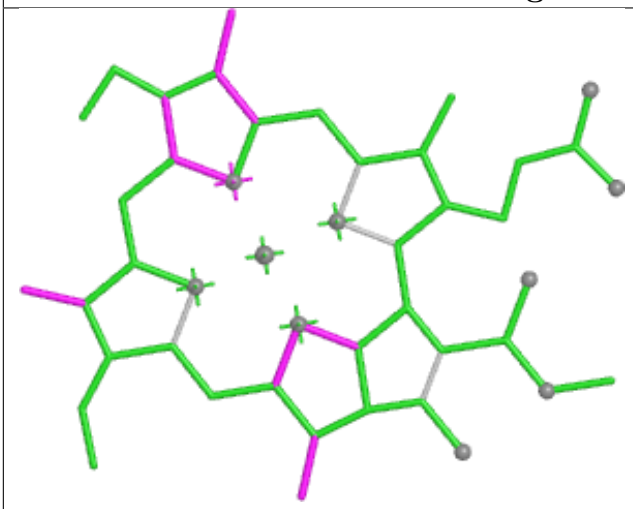


Torsions

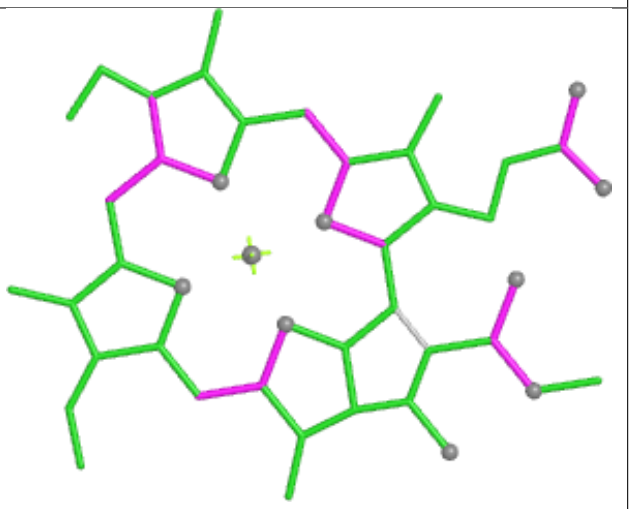


Rings

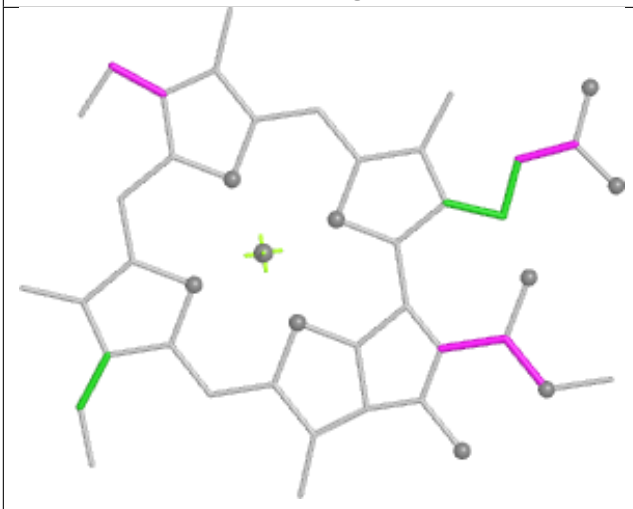
Ligand CLA Z 519



Bond lengths



Bond angles

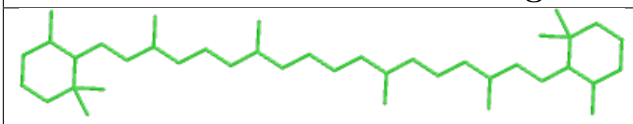


Torsions

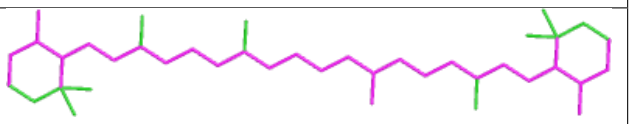


Rings

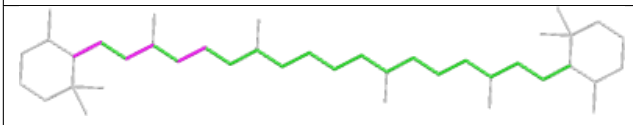
Ligand BCR u 522



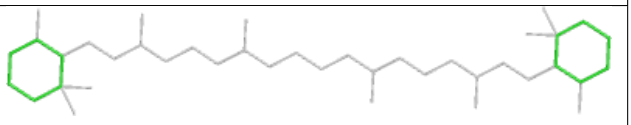
Bond lengths



Bond angles

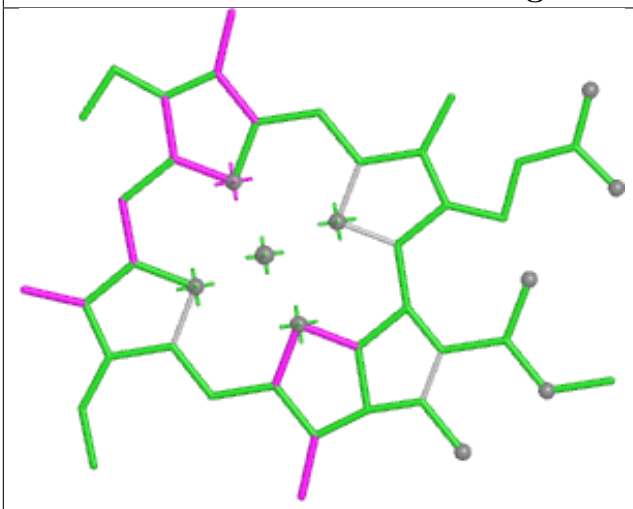


Torsions

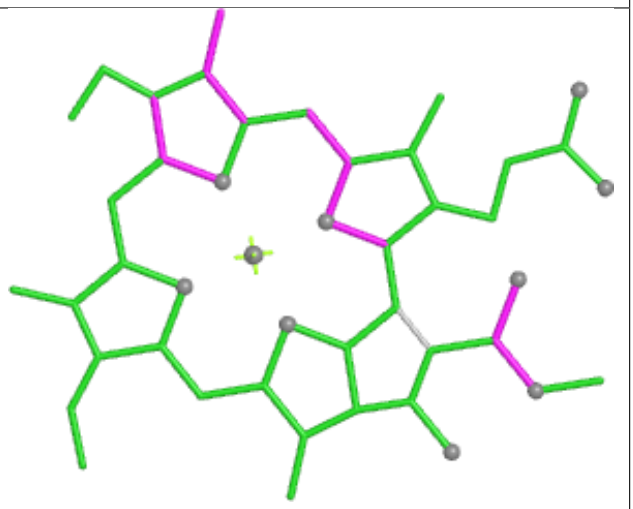


Rings

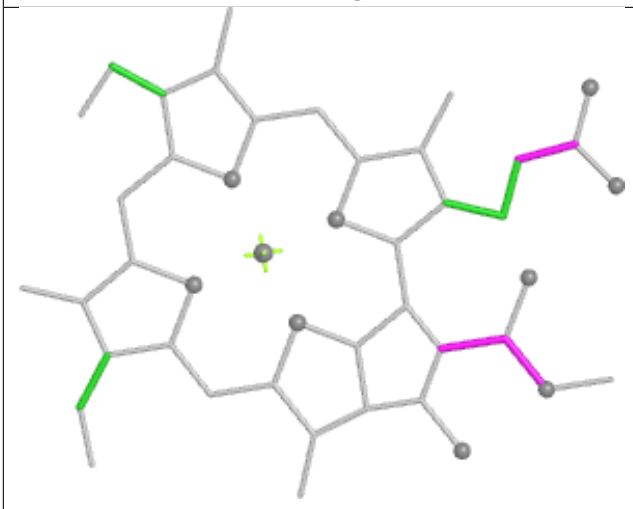
Ligand CLA Z 510



Bond lengths



Bond angles

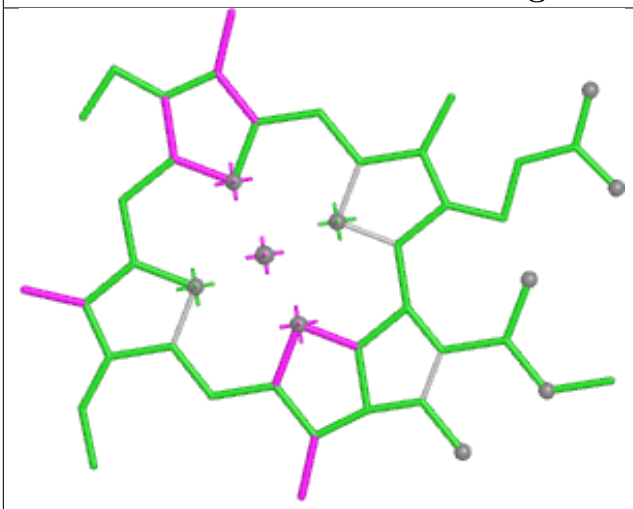


Torsions

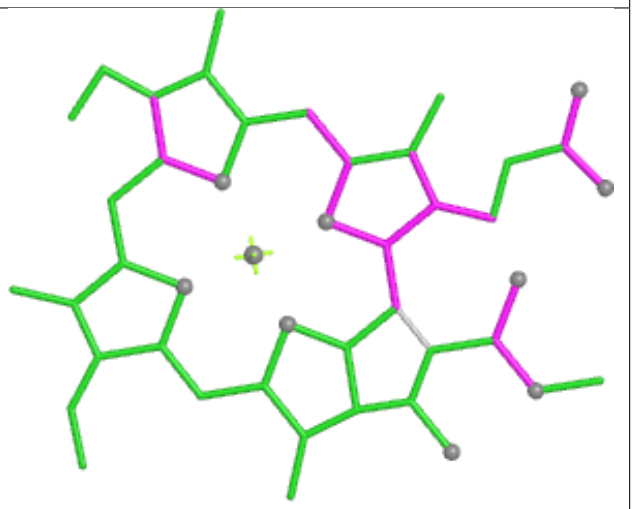


Rings

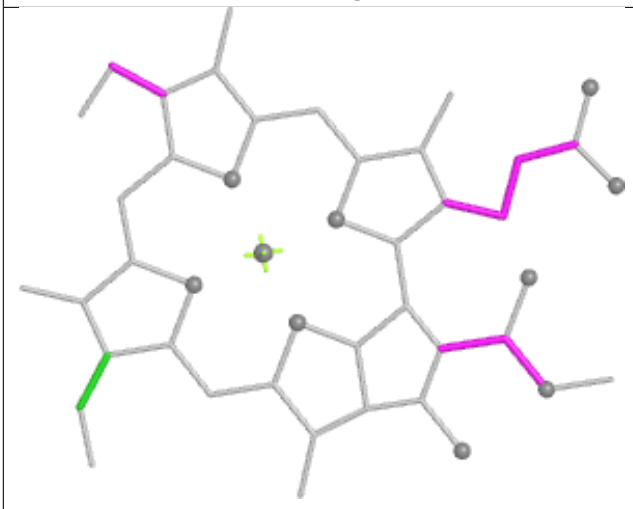
Ligand CLA 2 507



Bond lengths



Bond angles

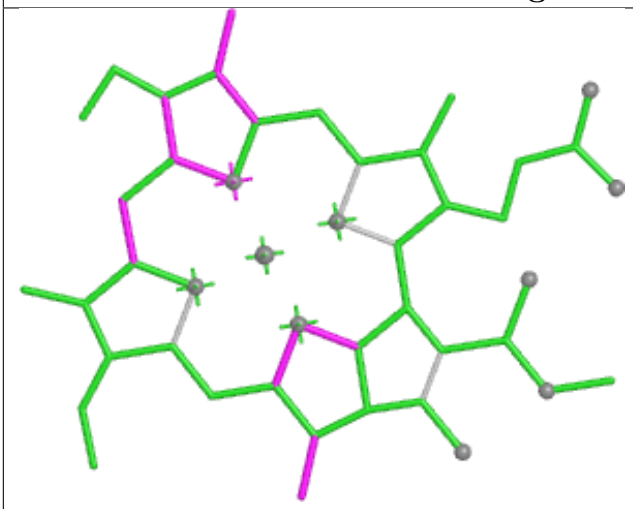


Torsions

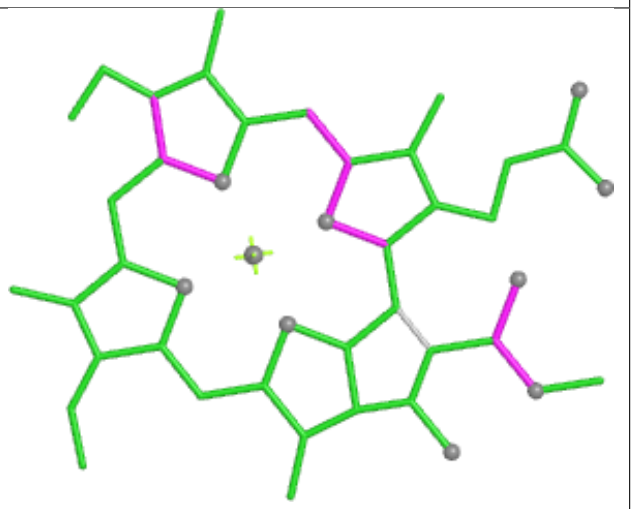


Rings

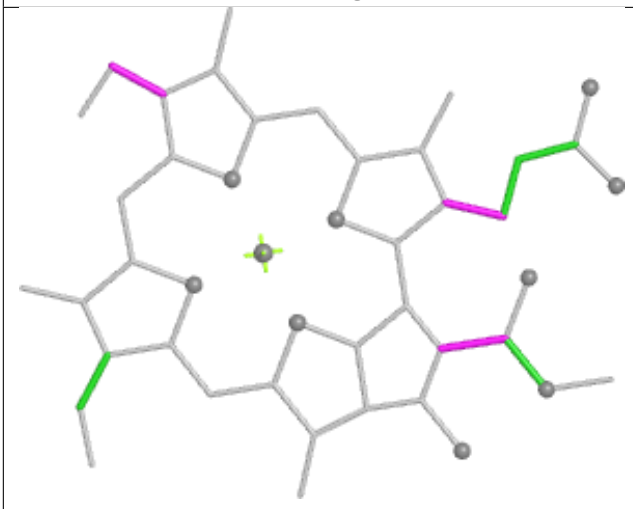
Ligand CLA 5 516



Bond lengths



Bond angles

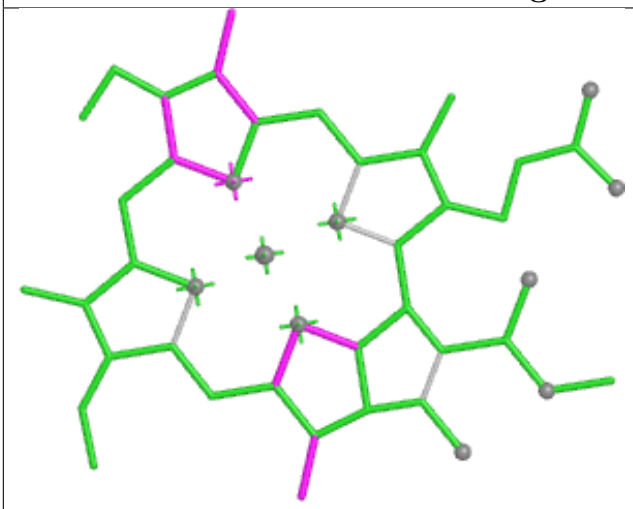


Torsions

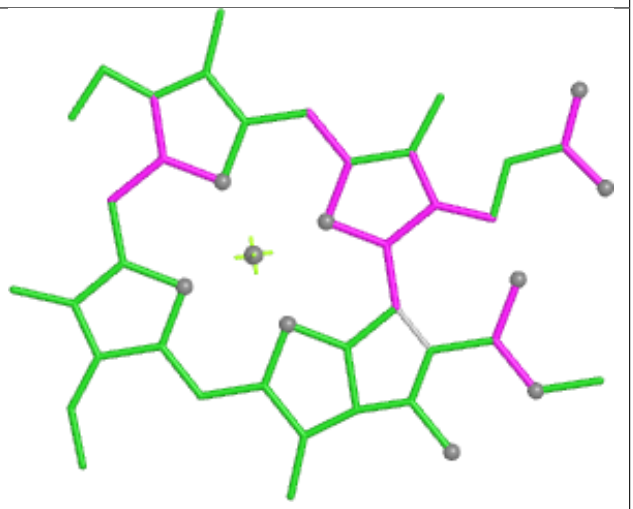


Rings

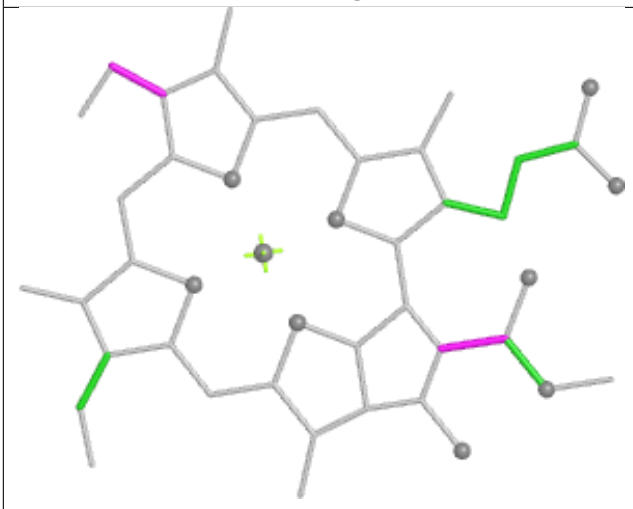
Ligand CLA r 502



Bond lengths



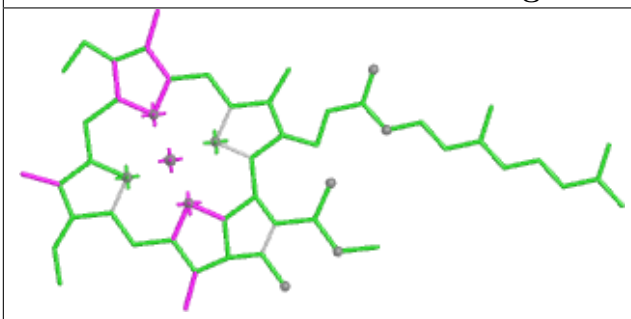
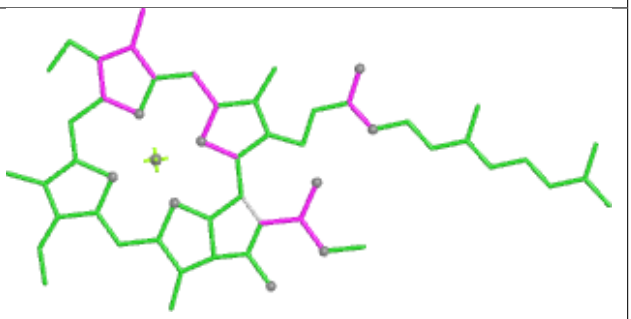
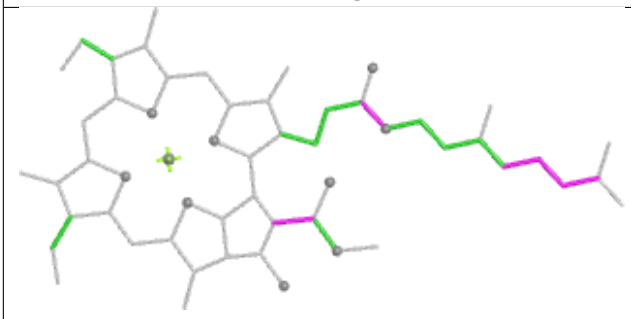
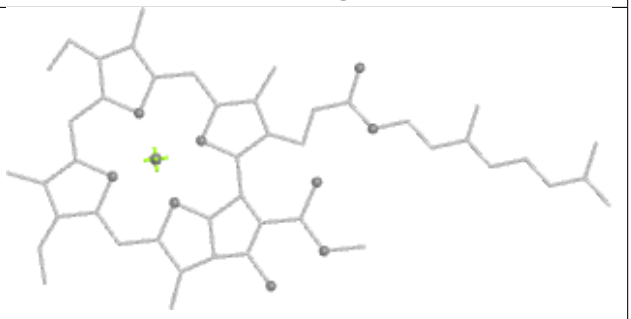
Bond angles

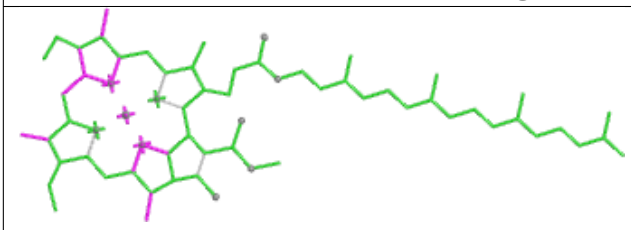
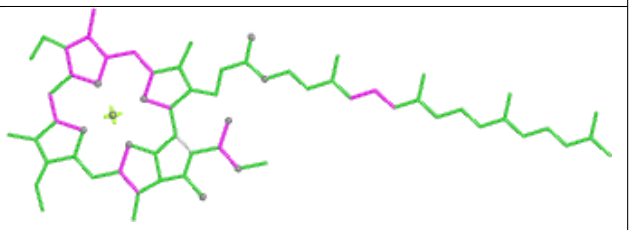
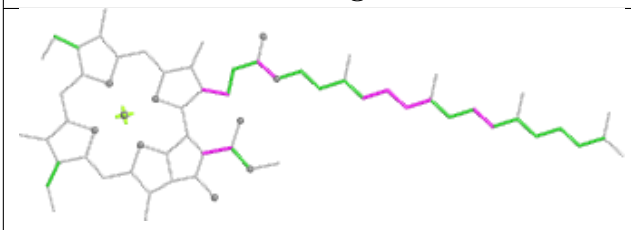
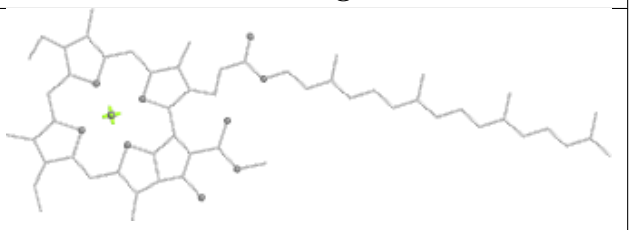


Torsions

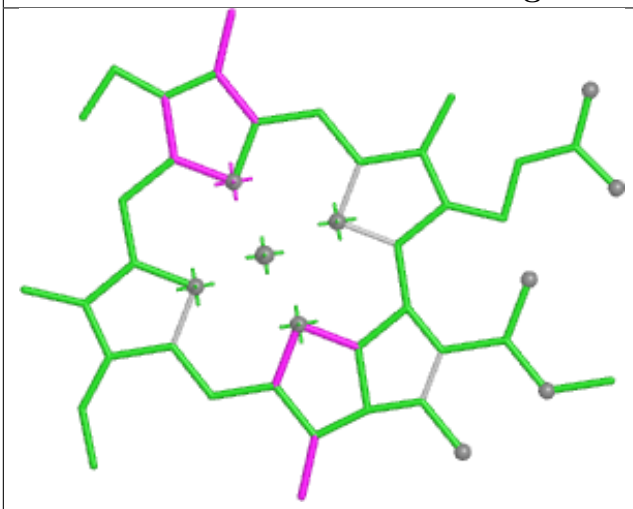


Rings

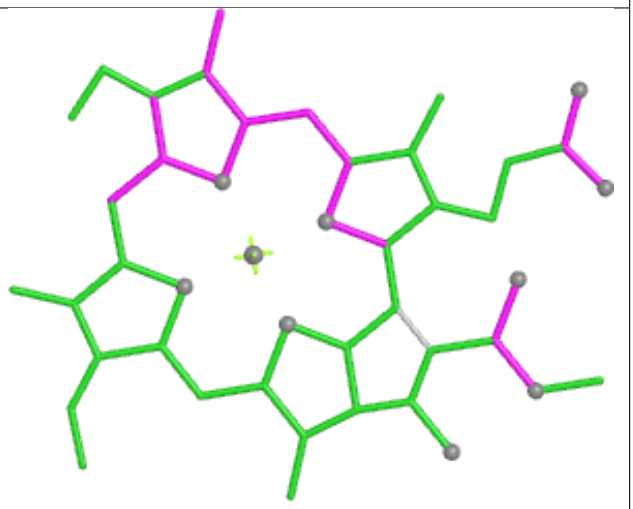
Ligand CLA f 1211	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

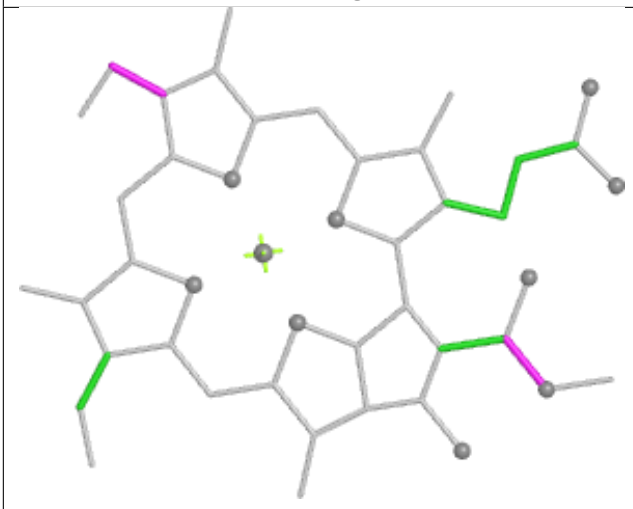
Ligand CLA Y 511



Bond lengths



Bond angles

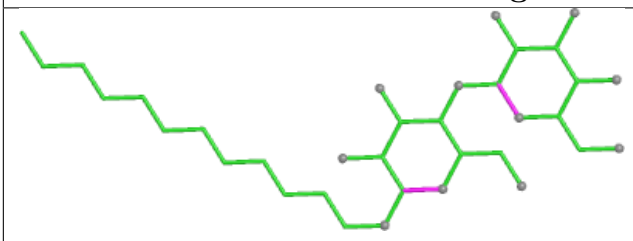


Torsions

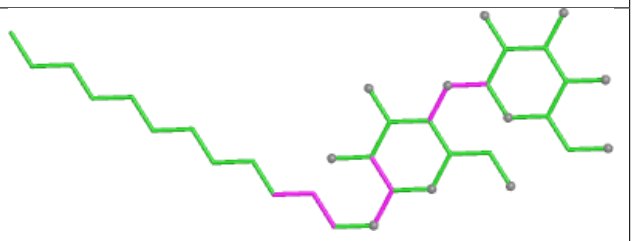


Rings

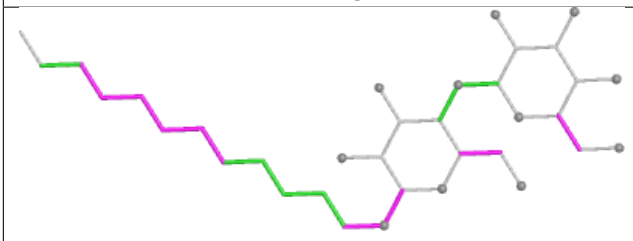
Ligand LMU H 1843



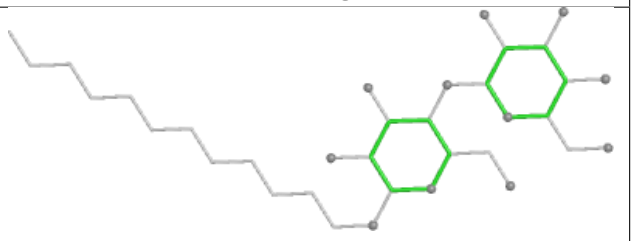
Bond lengths



Bond angles

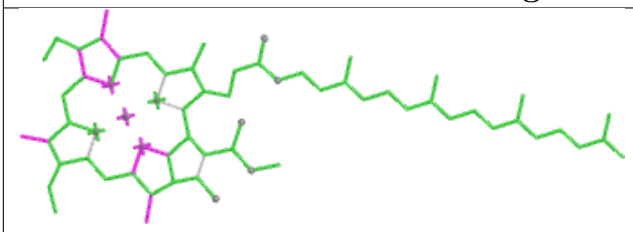


Torsions

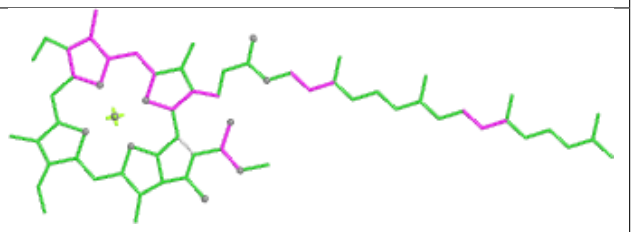


Rings

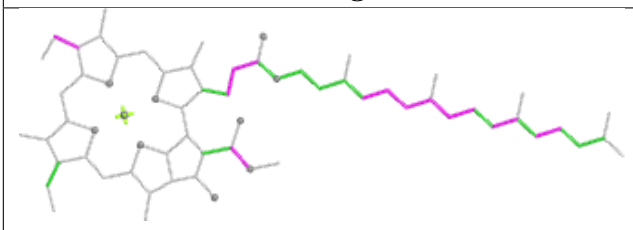
Ligand CLA f 1203



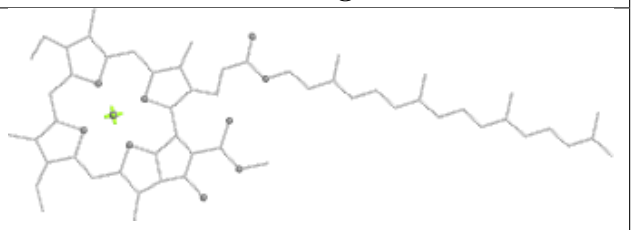
Bond lengths



Bond angles

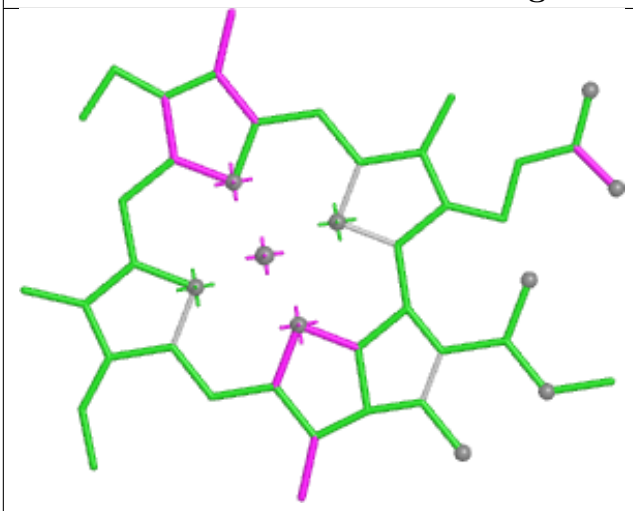


Torsions

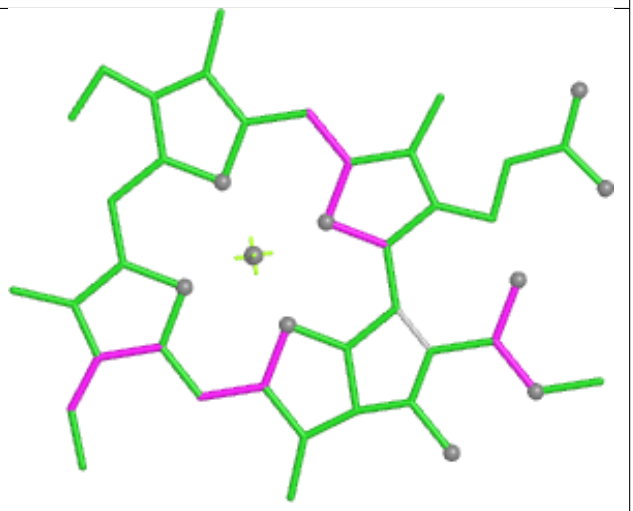


Rings

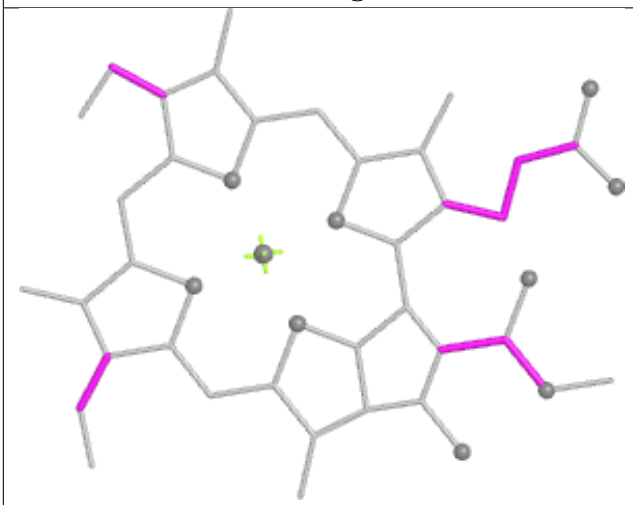
Ligand CLA 1 516



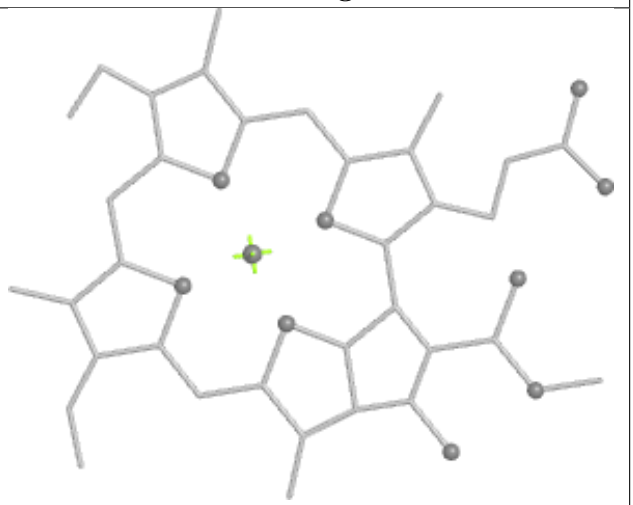
Bond lengths



Bond angles

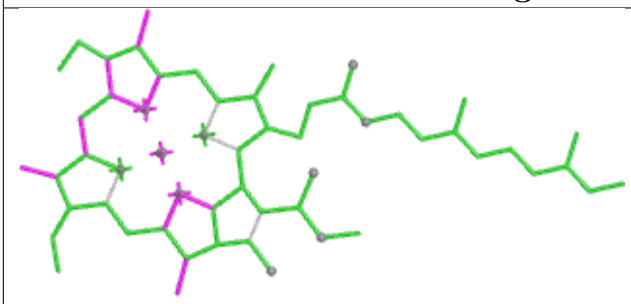


Torsions

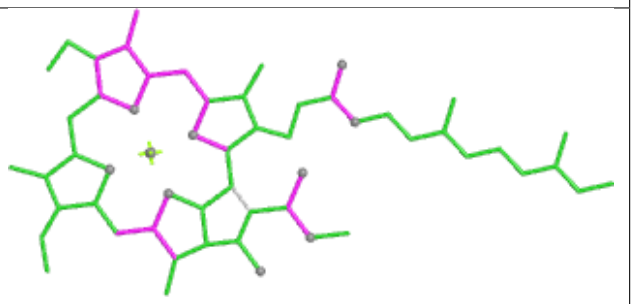


Rings

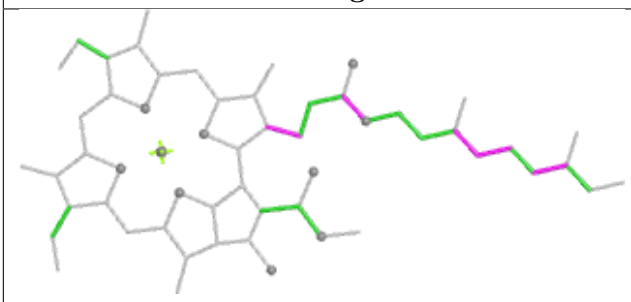
Ligand CLA G 1130



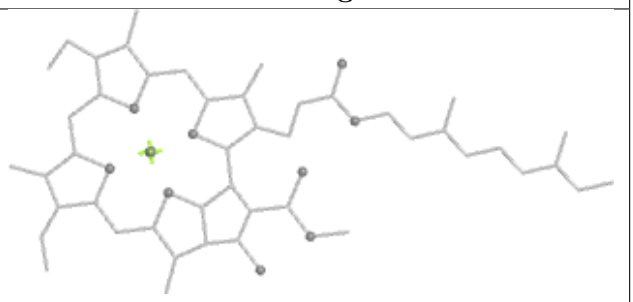
Bond lengths



Bond angles

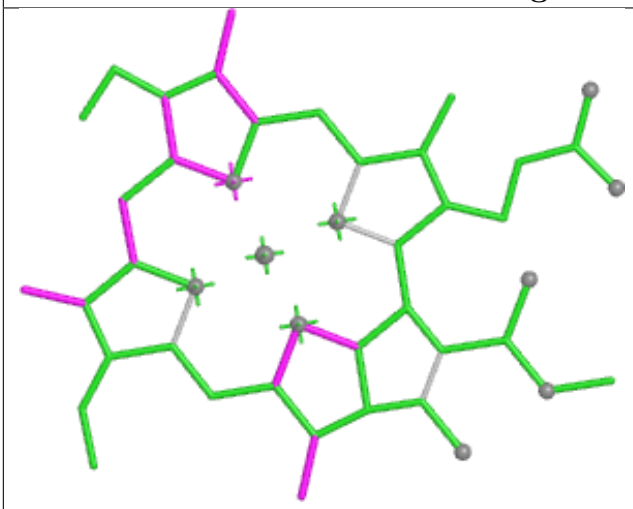


Torsions

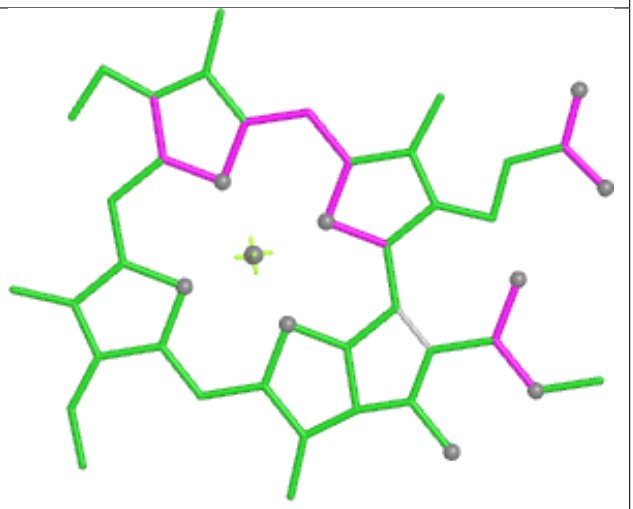


Rings

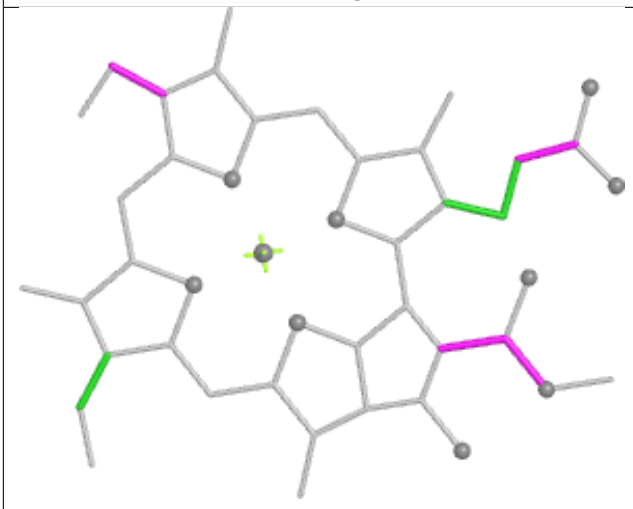
Ligand CLA t 519



Bond lengths



Bond angles

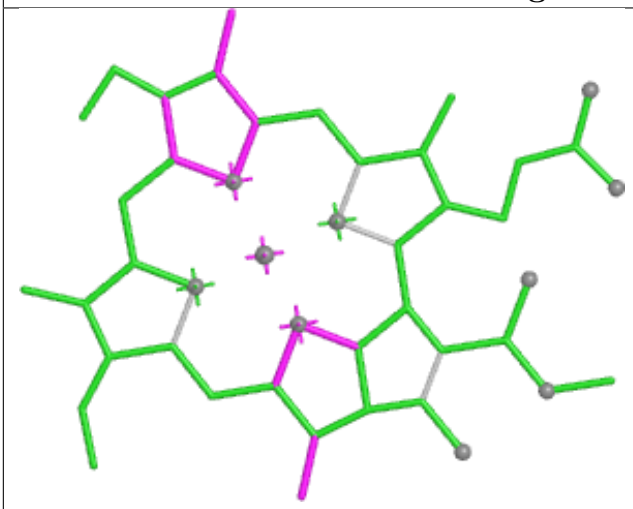


Torsions

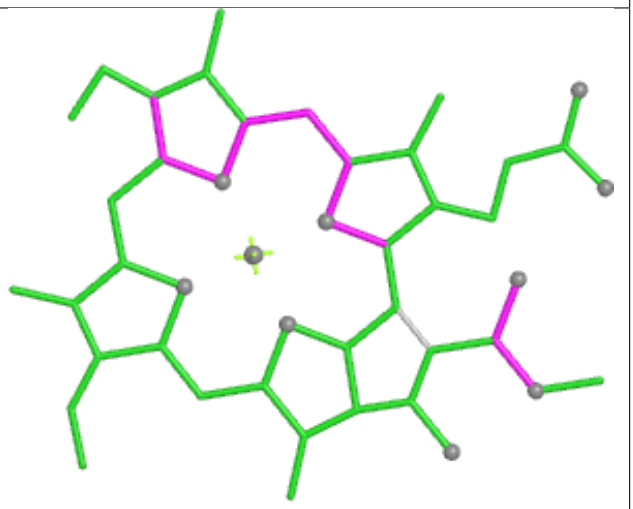


Rings

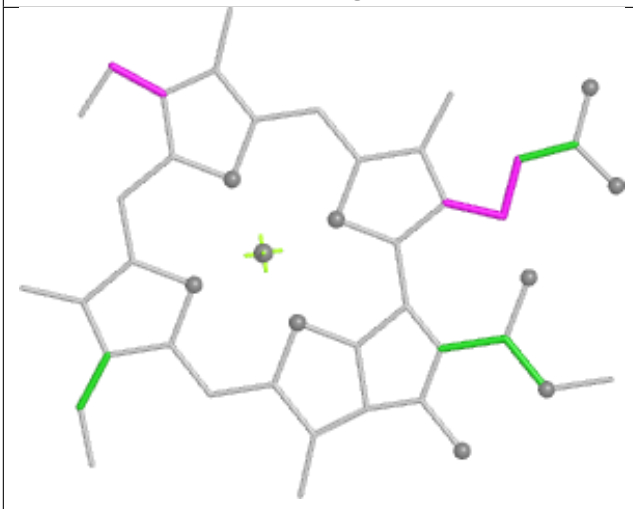
Ligand CLA a 512



Bond lengths



Bond angles

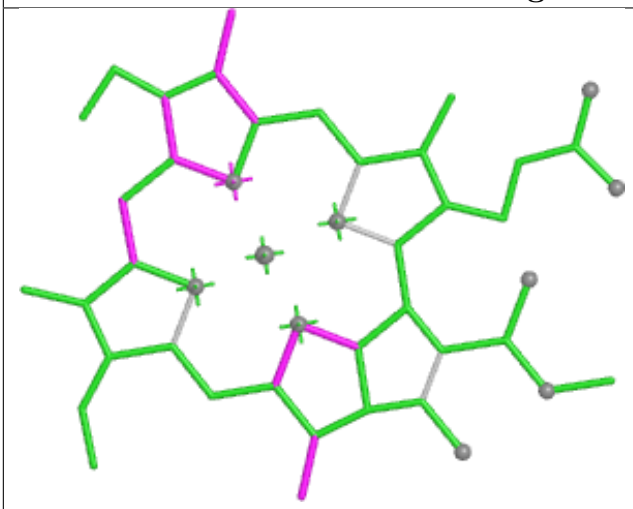


Torsions

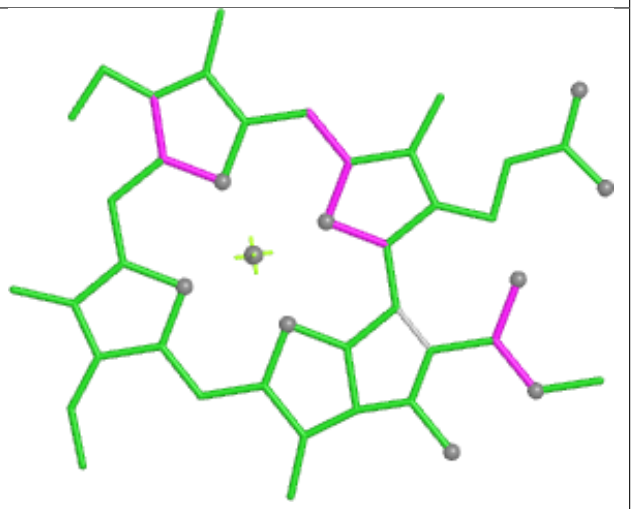


Rings

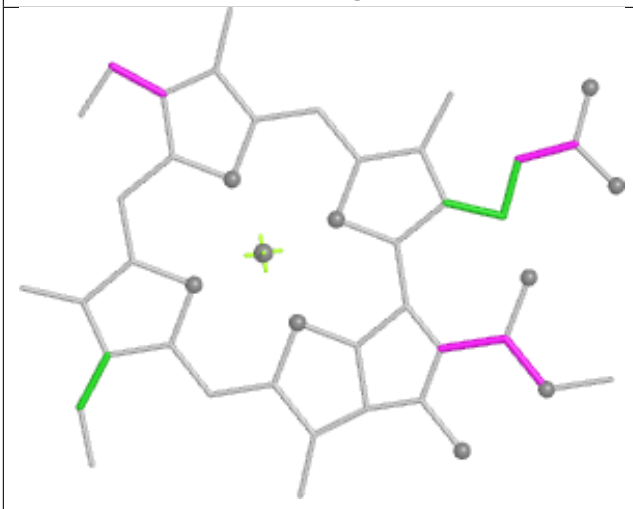
Ligand CLA b 510



Bond lengths



Bond angles

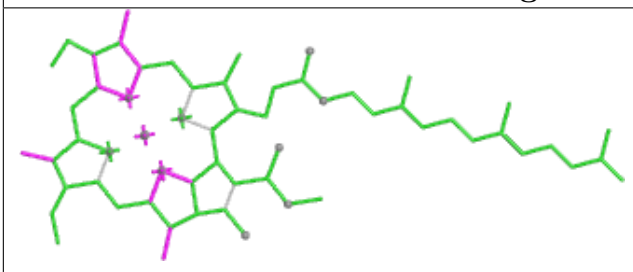


Torsions

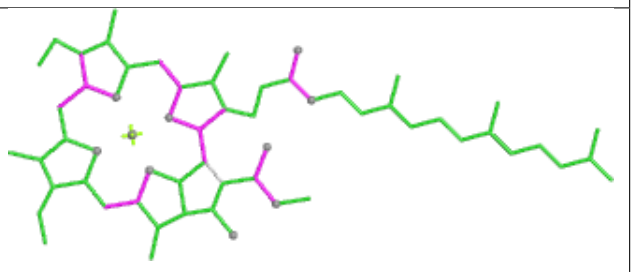


Rings

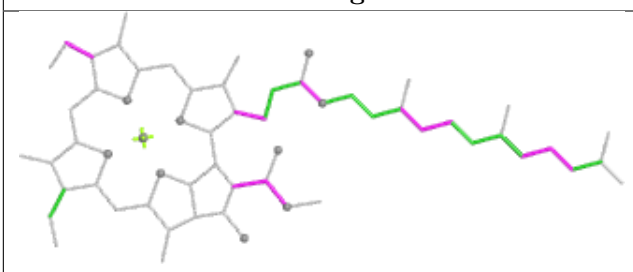
Ligand CLA e 1122



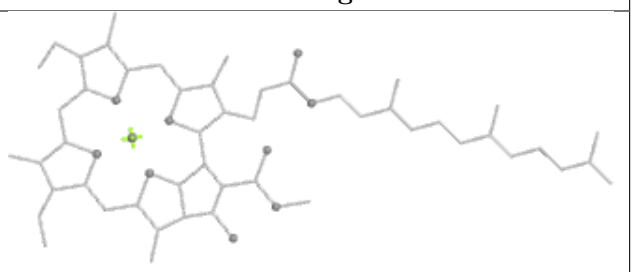
Bond lengths



Bond angles

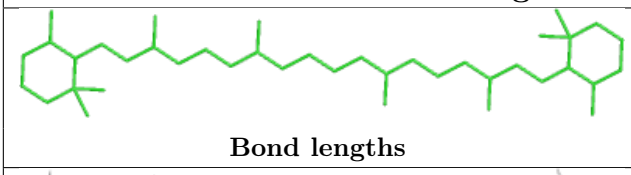


Torsions

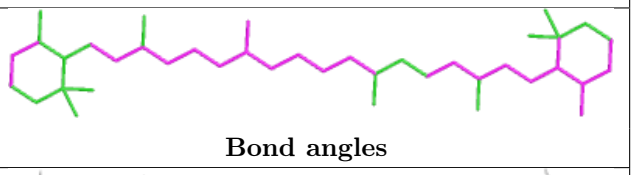


Rings

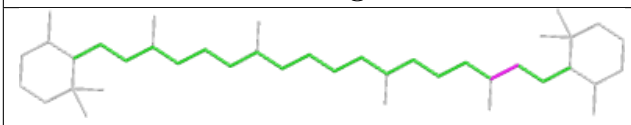
Ligand BCR K 4104



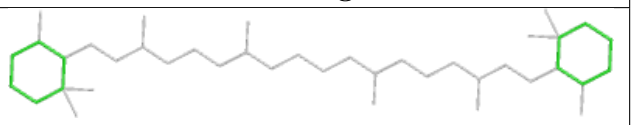
Bond lengths



Bond angles

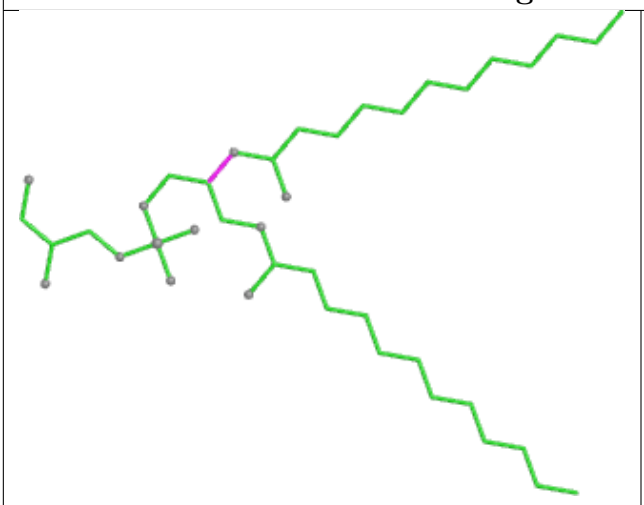


Torsions

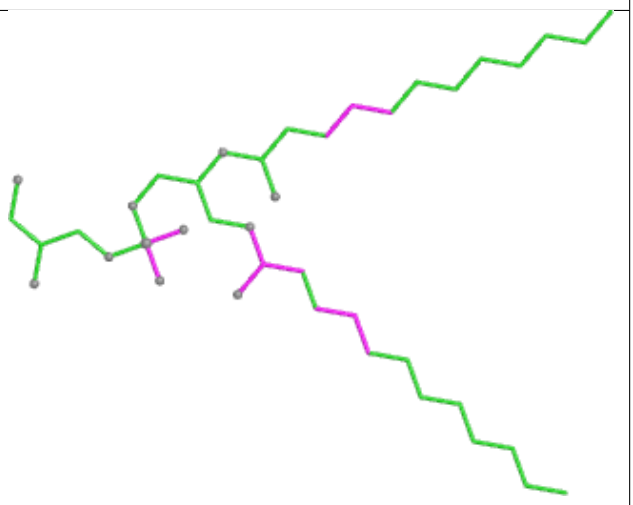


Rings

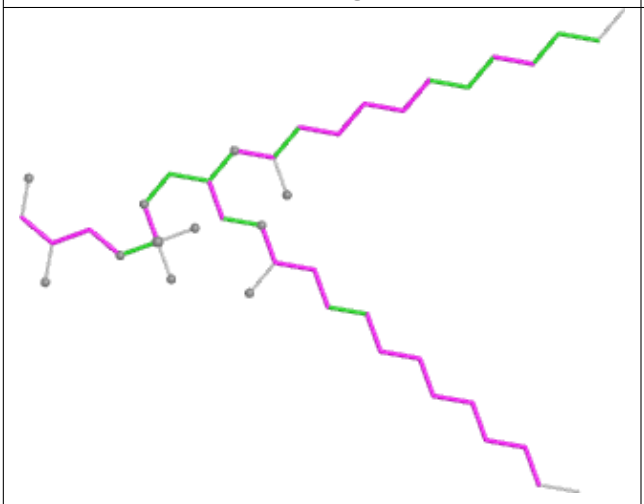
Ligand LHG L 5220



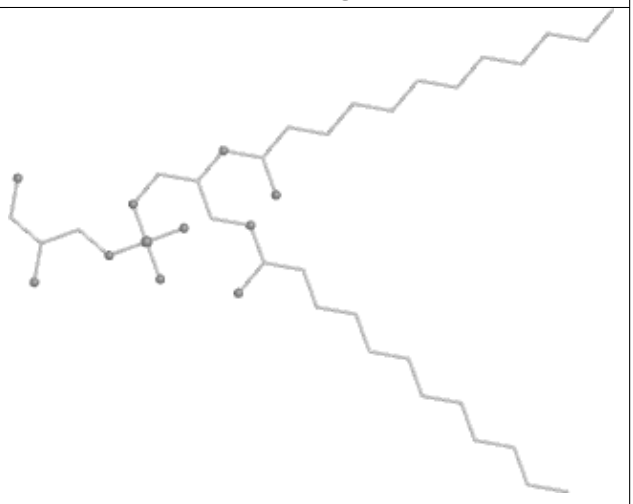
Bond lengths



Bond angles

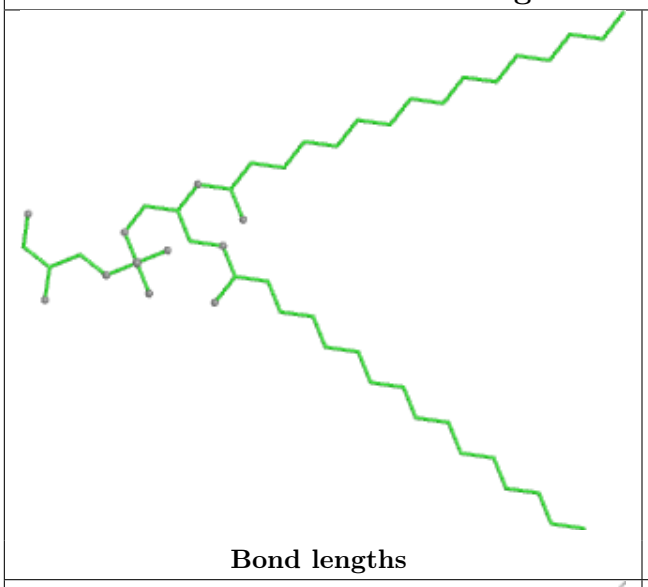


Torsions

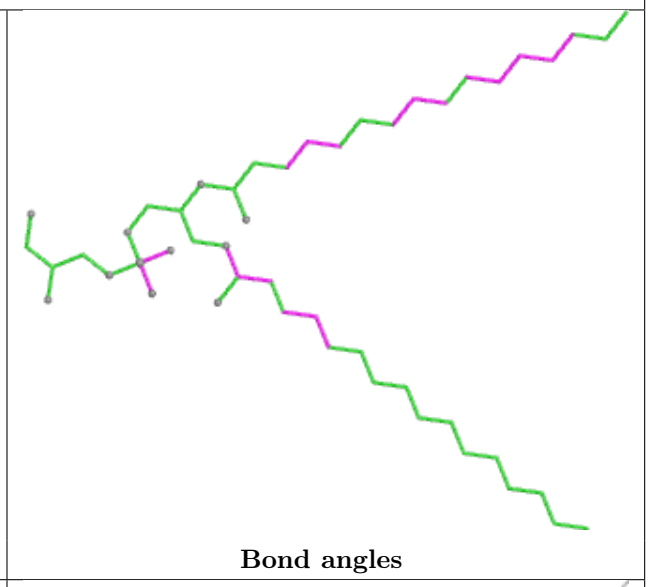


Rings

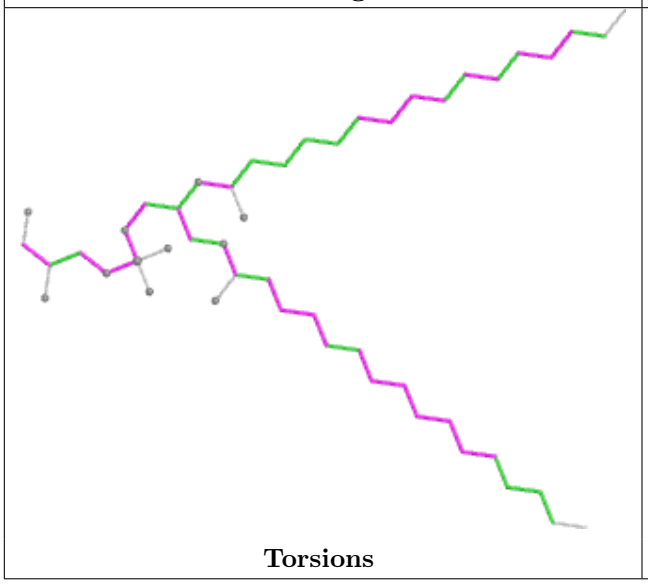
Ligand LHG V 5221



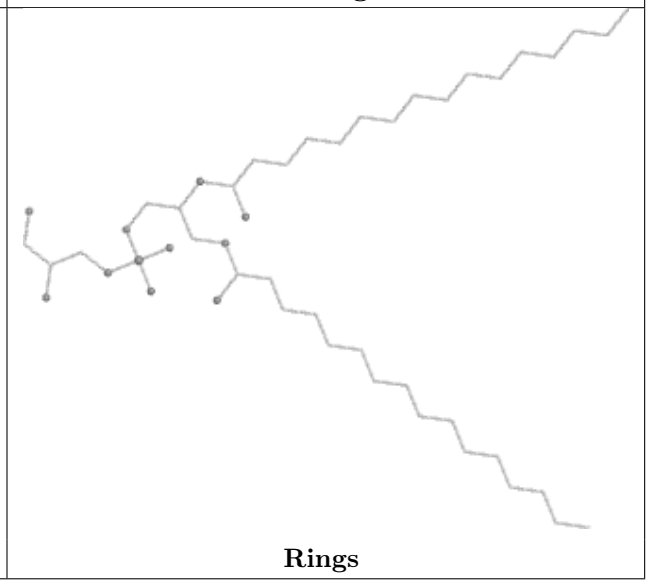
Bond lengths



Bond angles

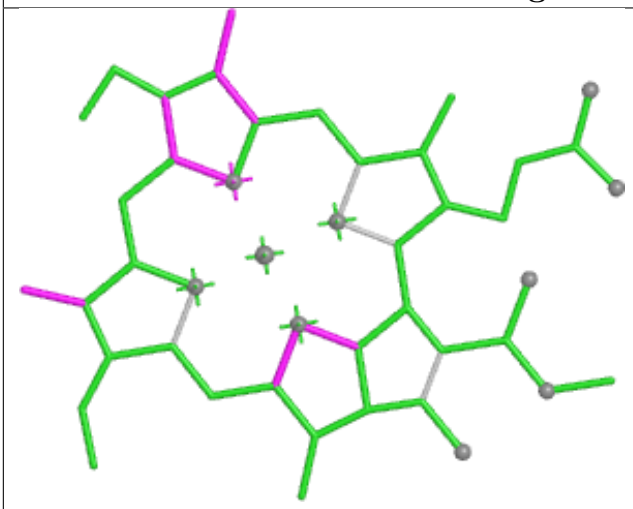


Torsions

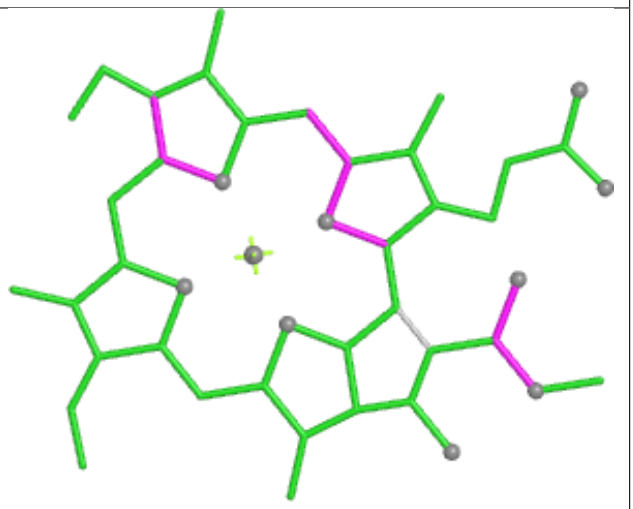


Rings

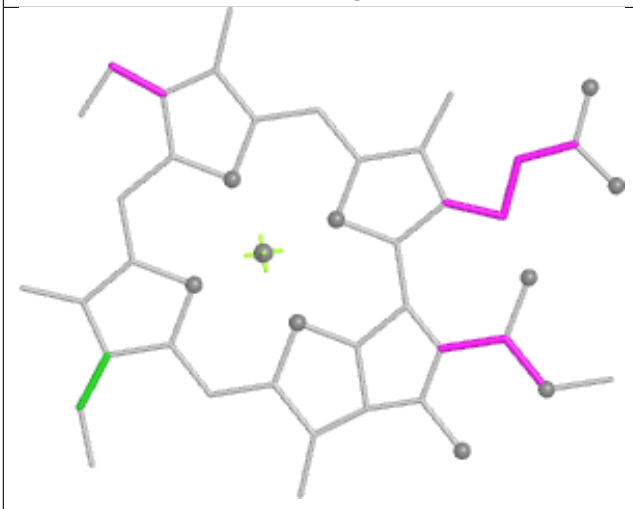
Ligand CLA 1 501



Bond lengths



Bond angles

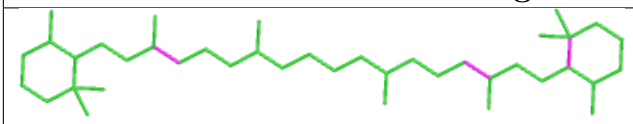


Torsions

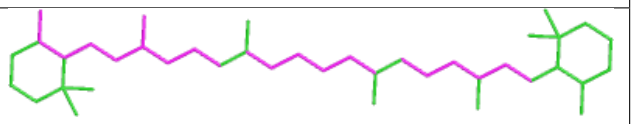


Rings

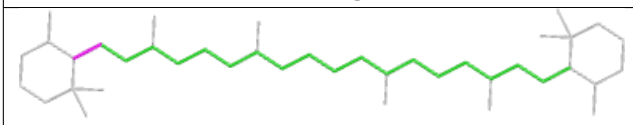
Ligand BCR B 4017



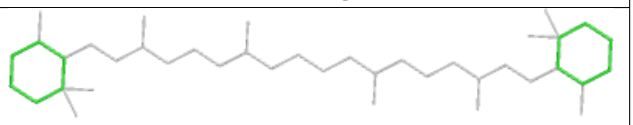
Bond lengths



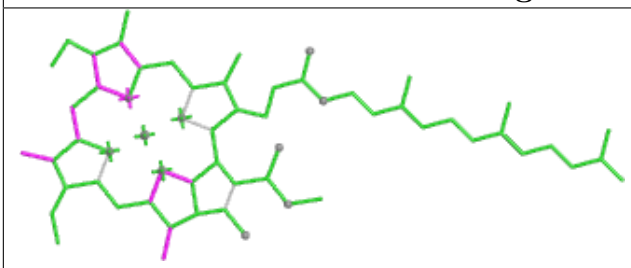
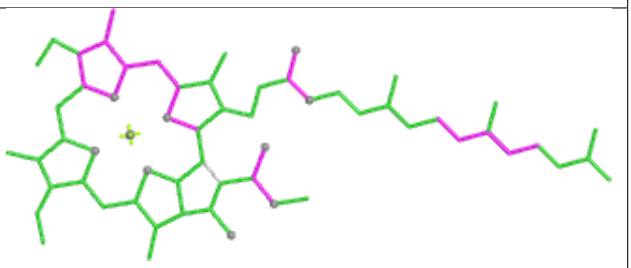
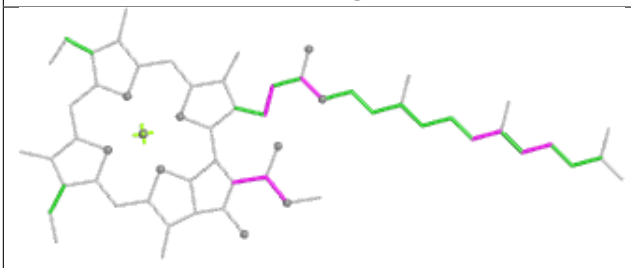
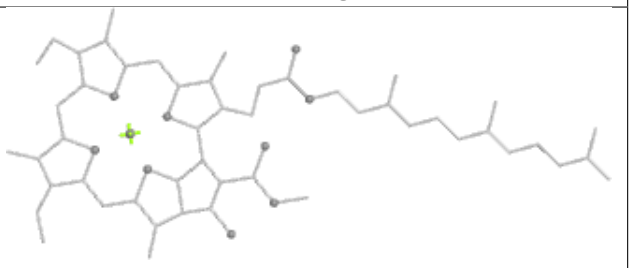
Bond angles

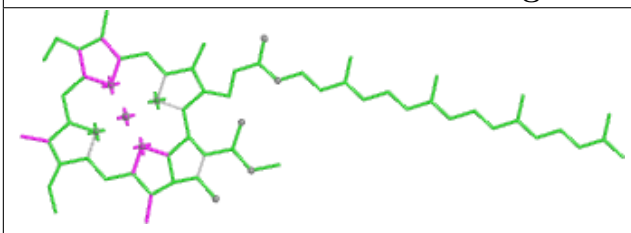
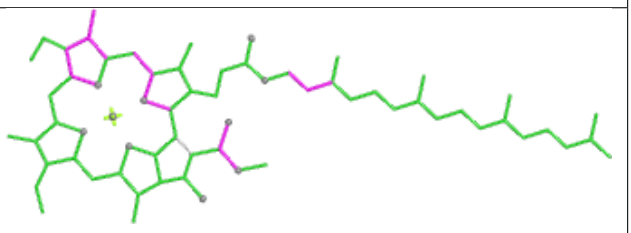
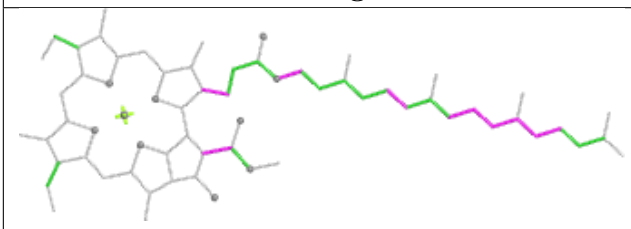
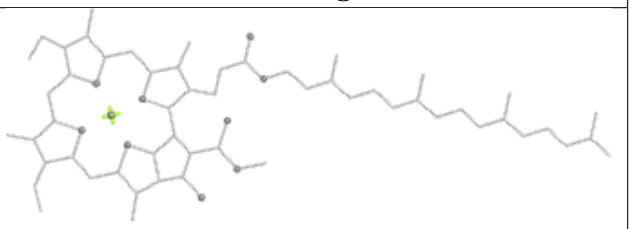


Torsions

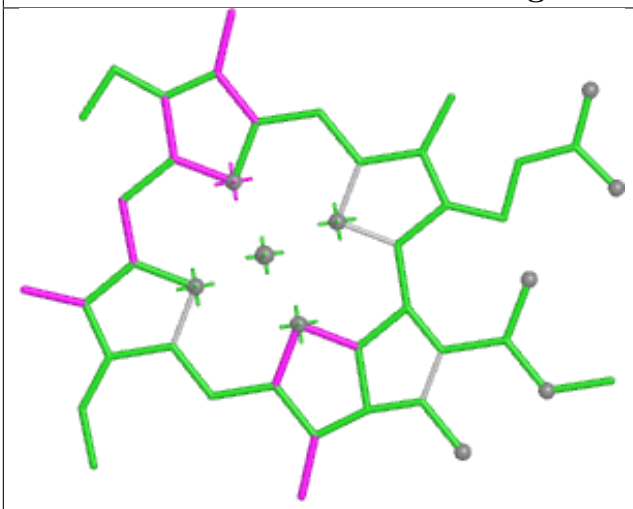


Rings

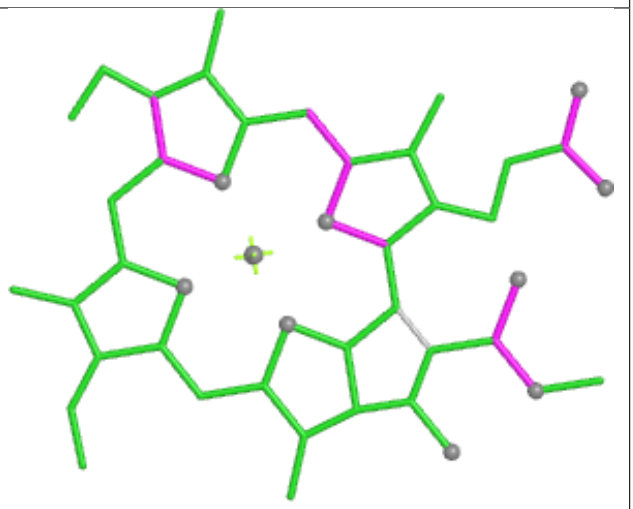
Ligand CLA B 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

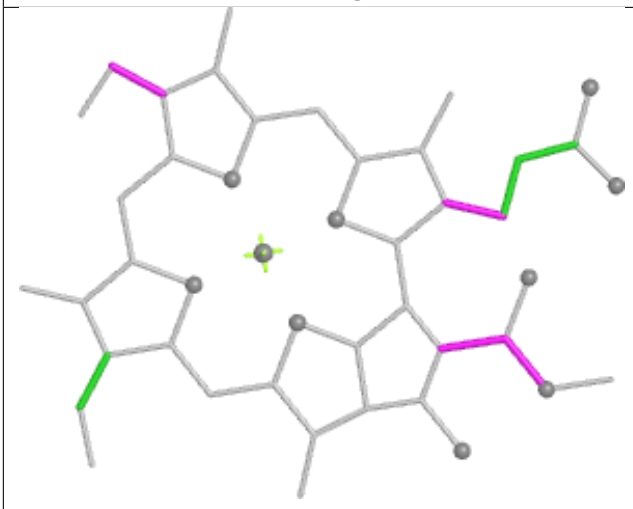
Ligand CLA u 506



Bond lengths



Bond angles

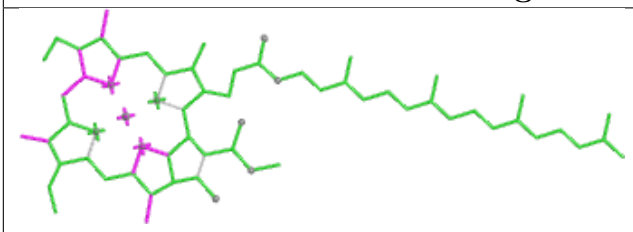


Torsions

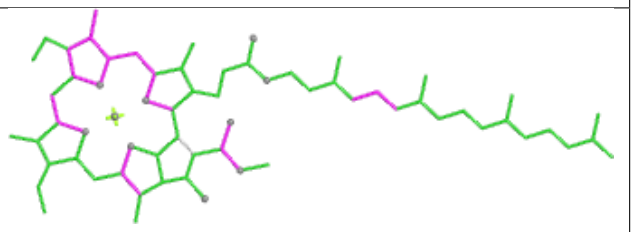


Rings

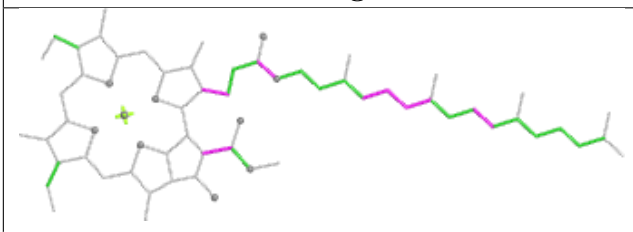
Ligand CLA A 1128



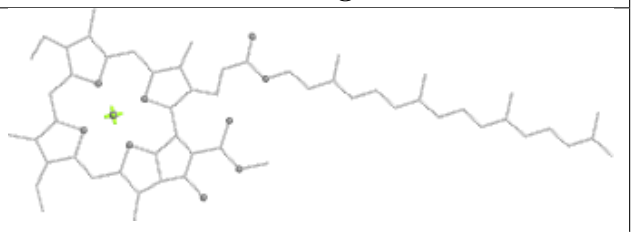
Bond lengths



Bond angles

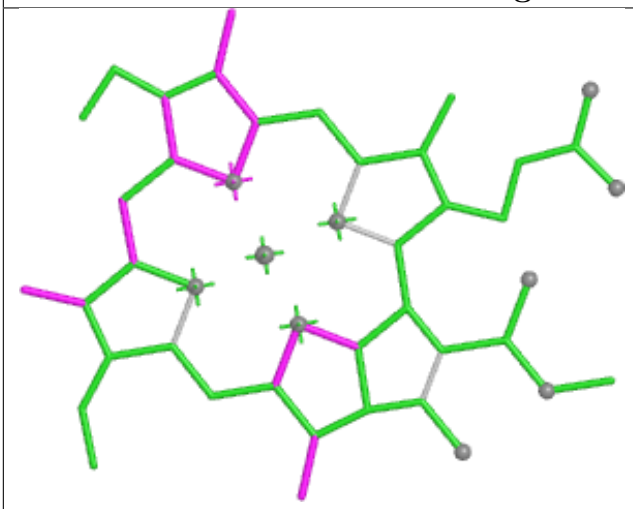


Torsions

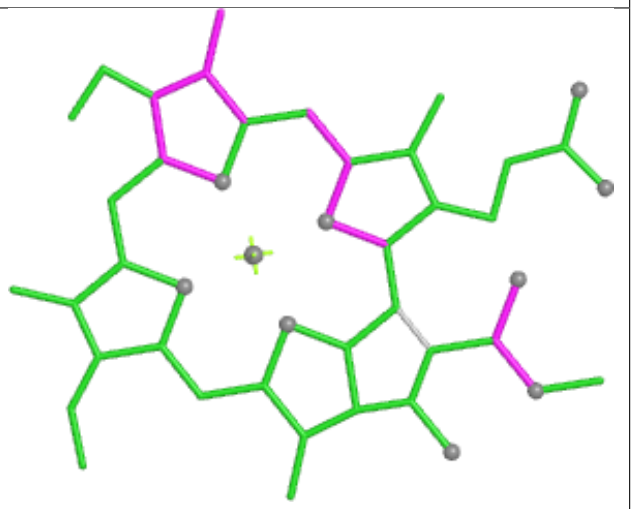


Rings

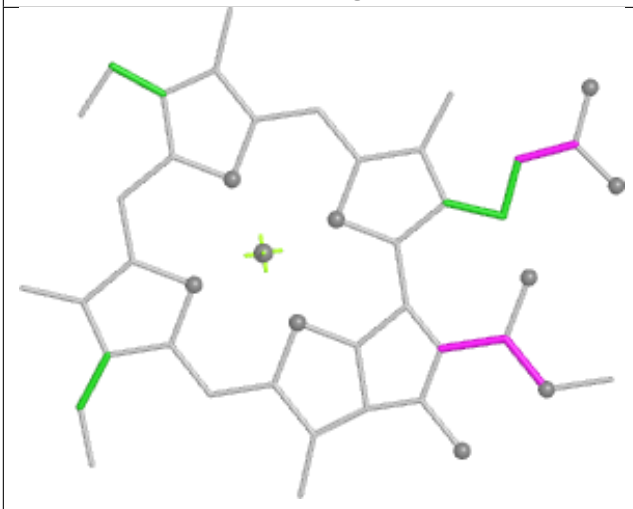
Ligand CLA G 1801



Bond lengths



Bond angles

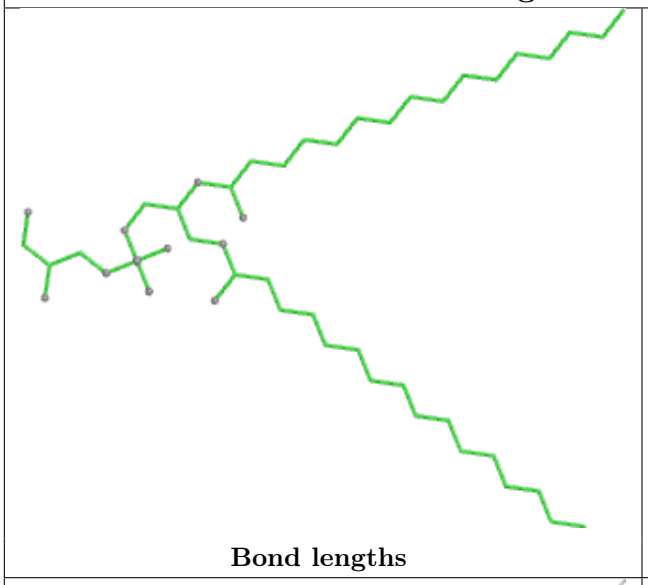


Torsions

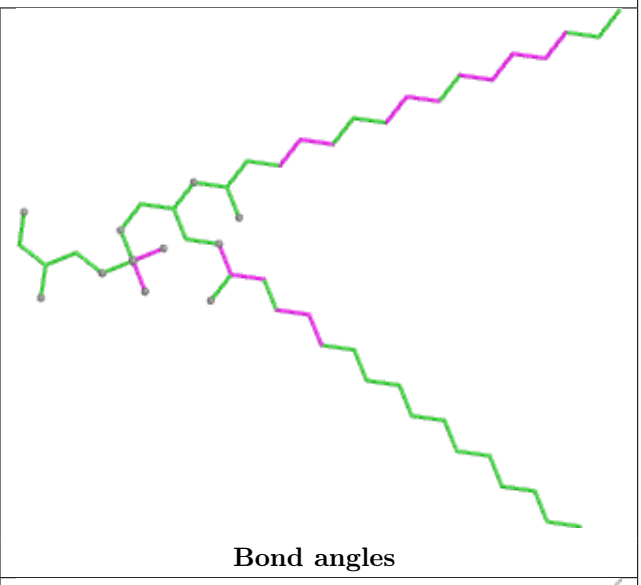


Rings

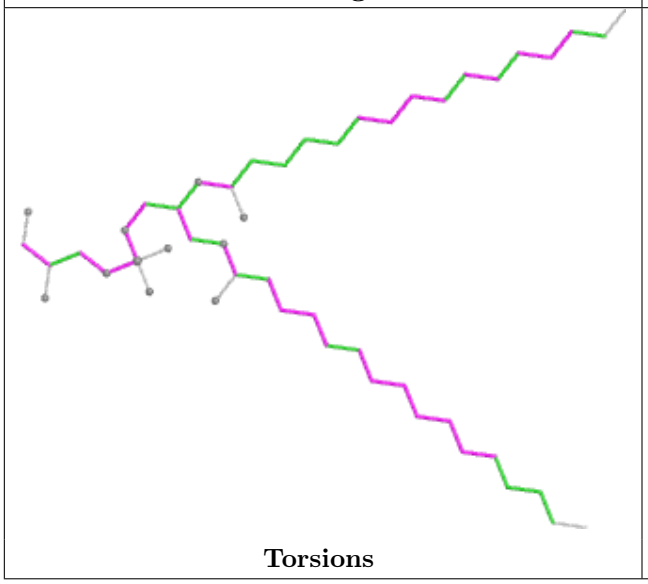
Ligand LHG n 5221



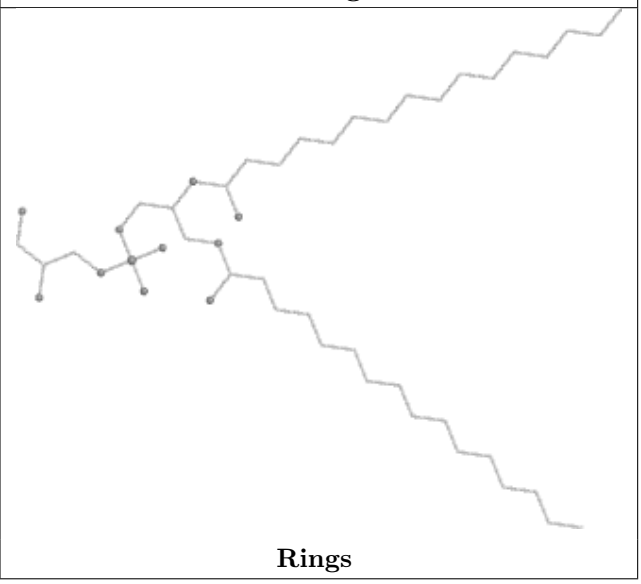
Bond lengths



Bond angles



Torsions

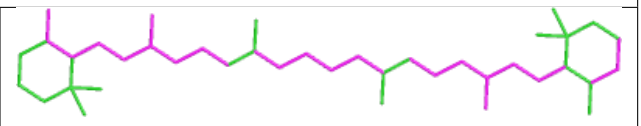


Rings

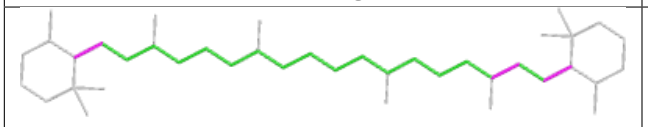
Ligand BCR Y 523



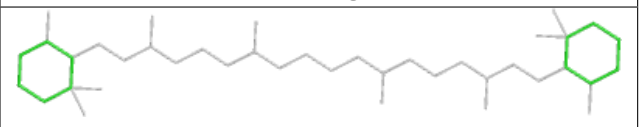
Bond lengths



Bond angles

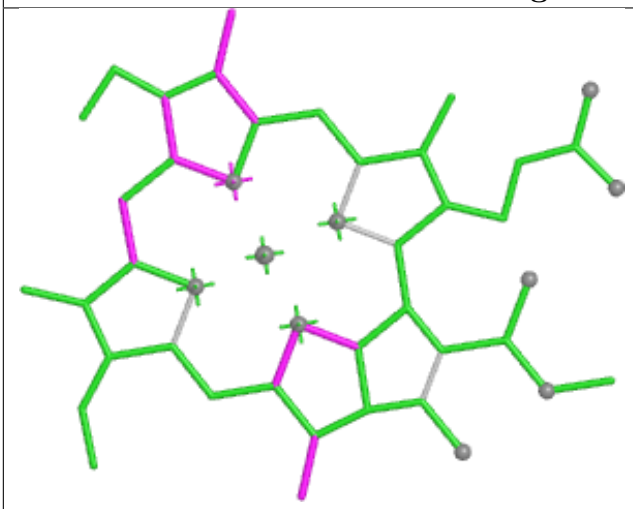


Torsions

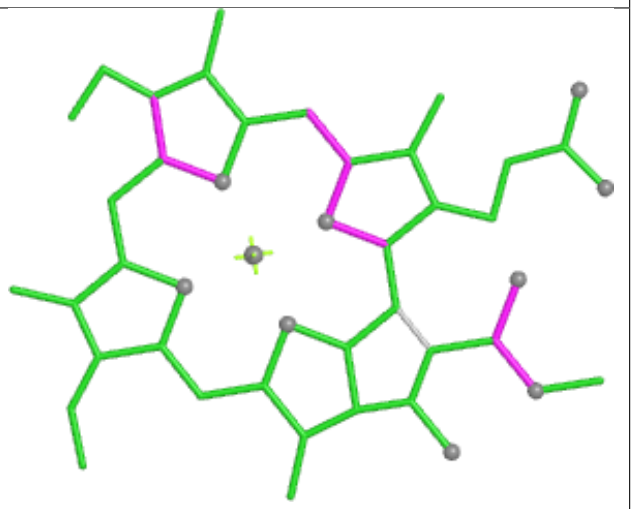


Rings

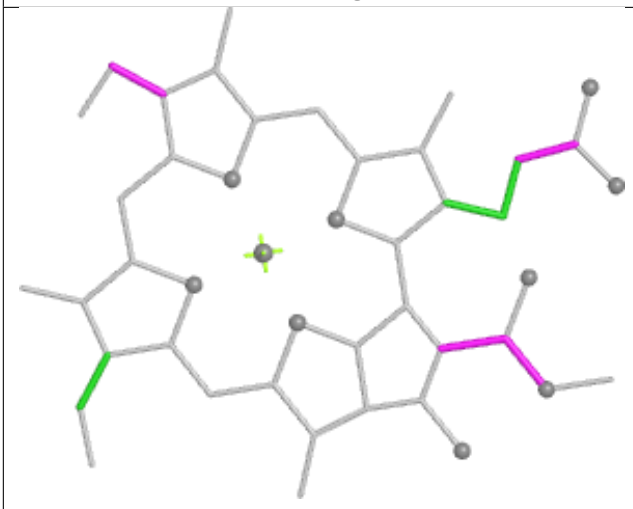
Ligand CLA t 510



Bond lengths



Bond angles

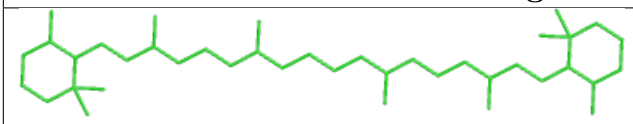


Torsions

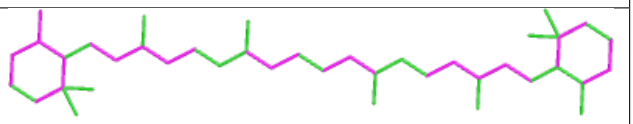


Rings

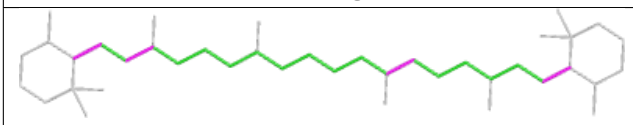
Ligand BCR 1 521



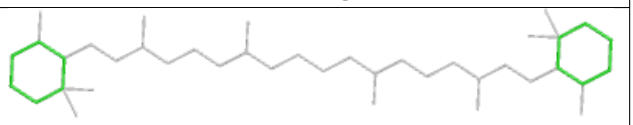
Bond lengths



Bond angles

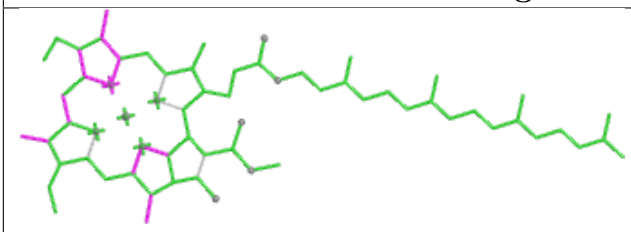


Torsions

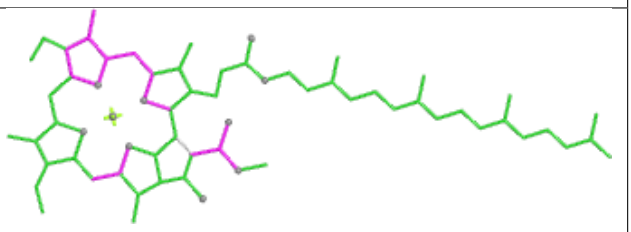


Rings

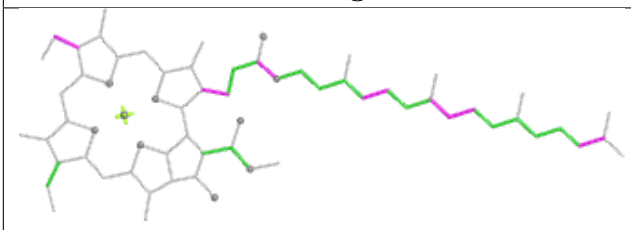
Ligand CLA V 1502



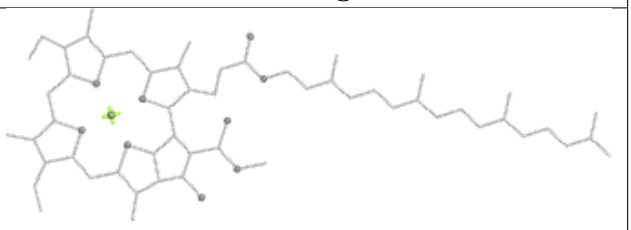
Bond lengths



Bond angles

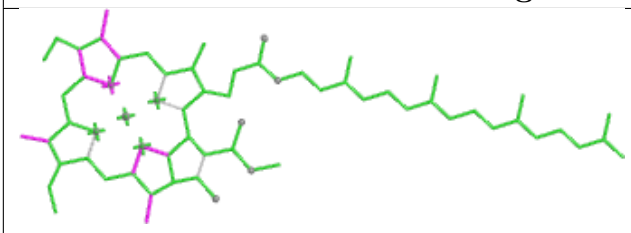


Torsions

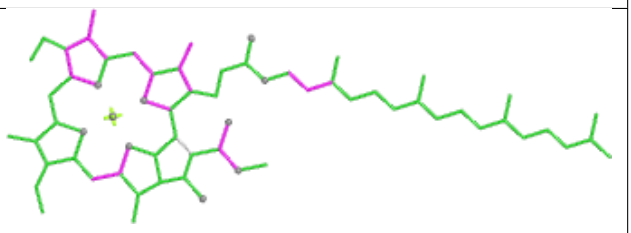


Rings

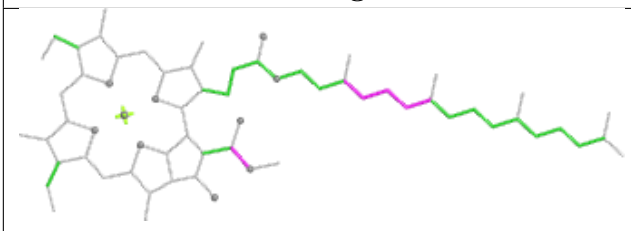
Ligand CLA B 1231



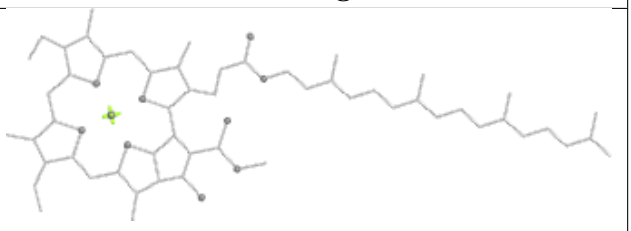
Bond lengths



Bond angles

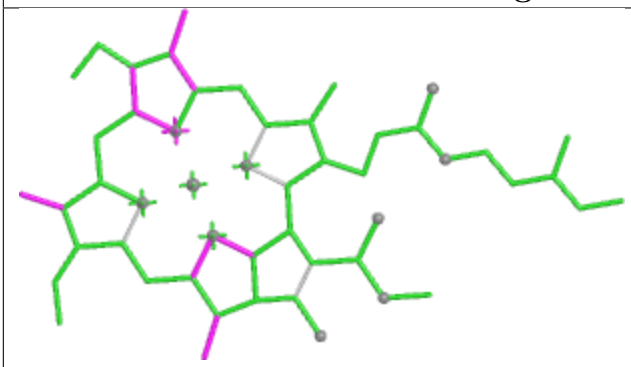


Torsions

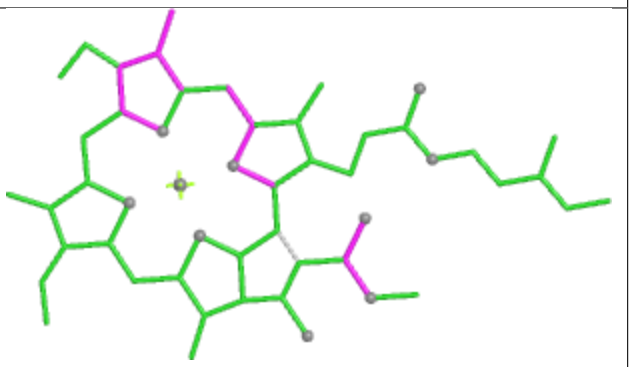


Rings

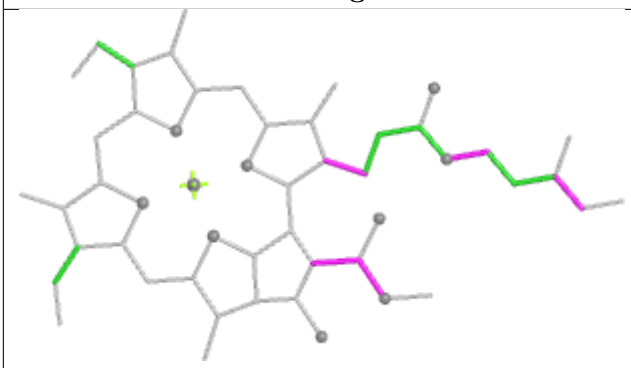
Ligand CLA H 1212



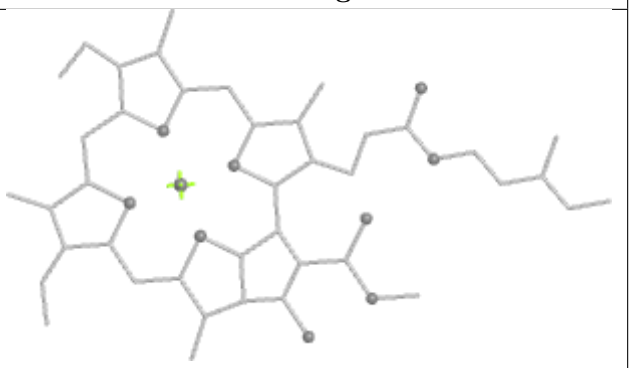
Bond lengths



Bond angles

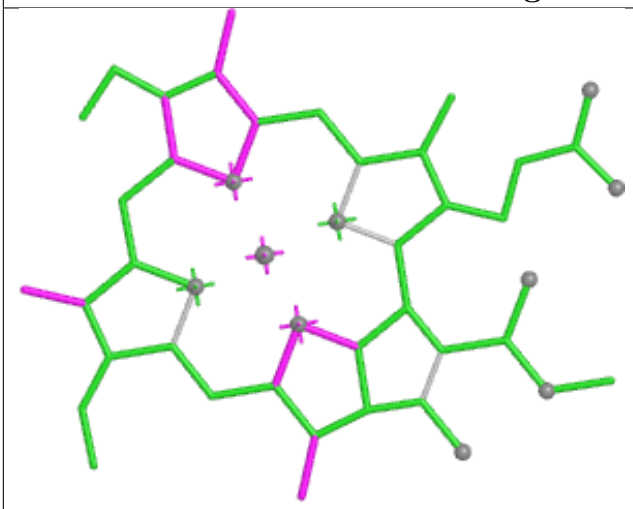


Torsions

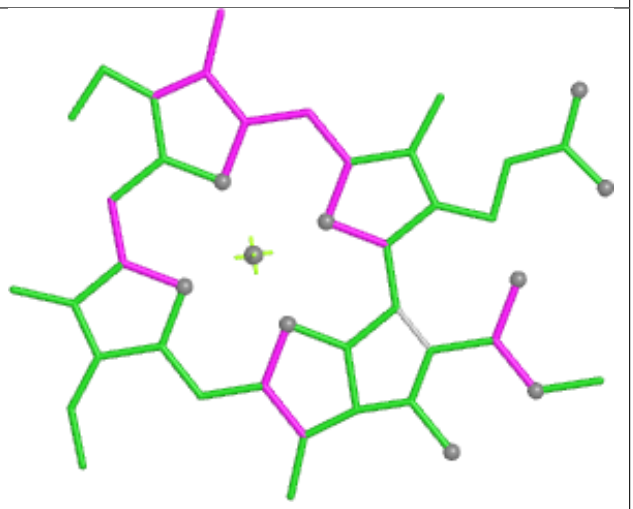


Rings

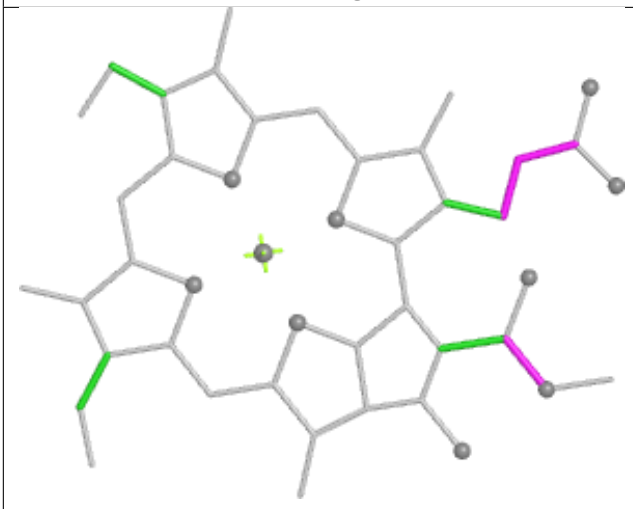
Ligand CLA Y 508



Bond lengths



Bond angles

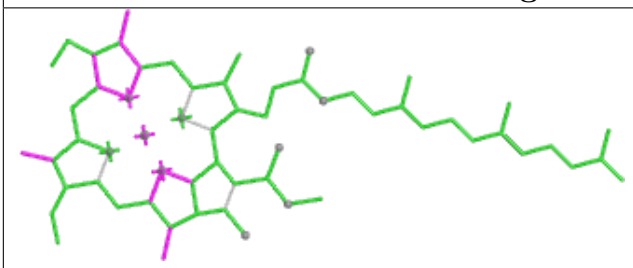


Torsions

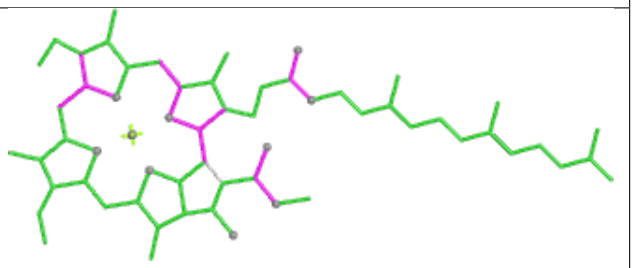


Rings

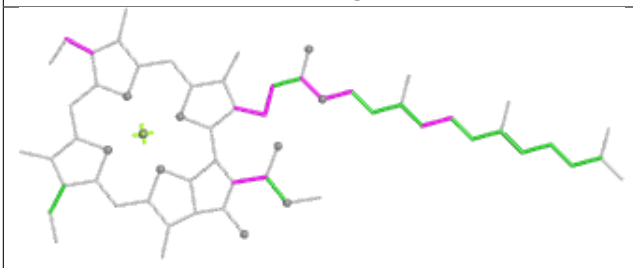
Ligand CLA e 1118



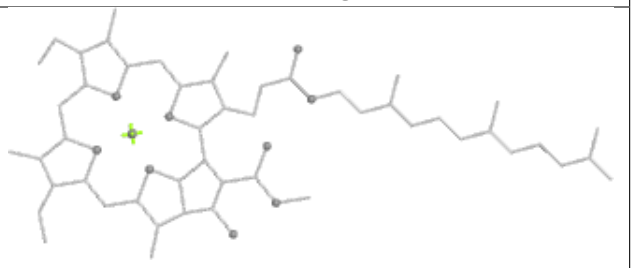
Bond lengths



Bond angles

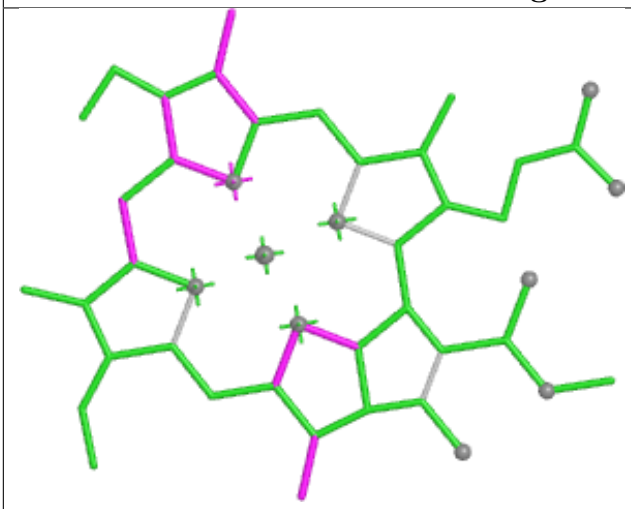


Torsions

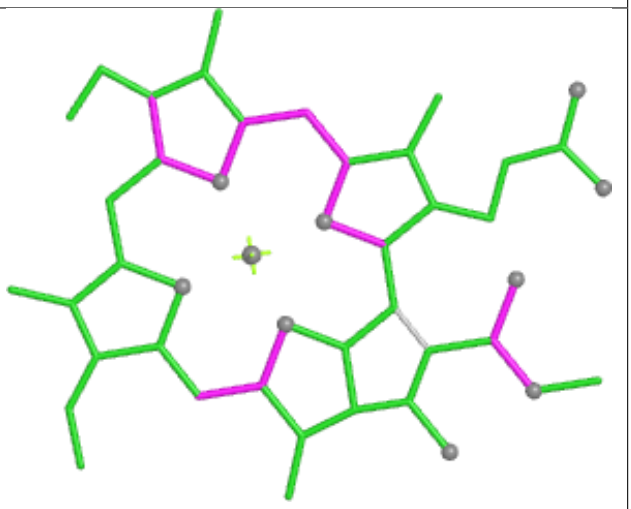


Rings

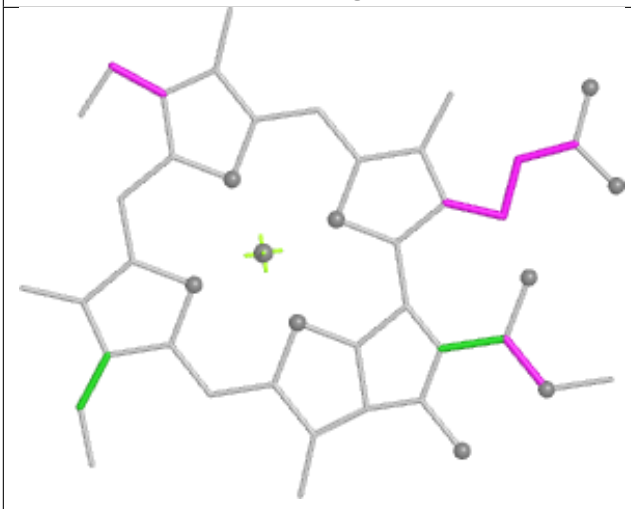
Ligand CLA t 501



Bond lengths



Bond angles

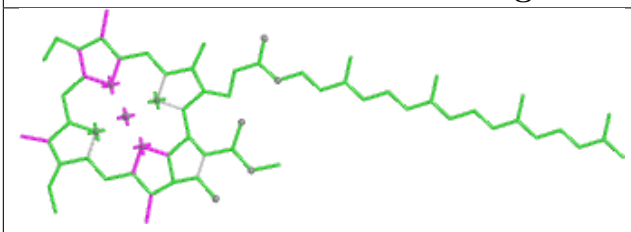


Torsions

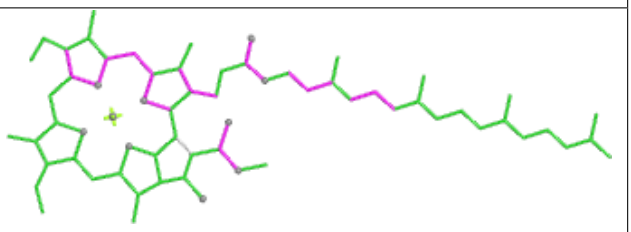


Rings

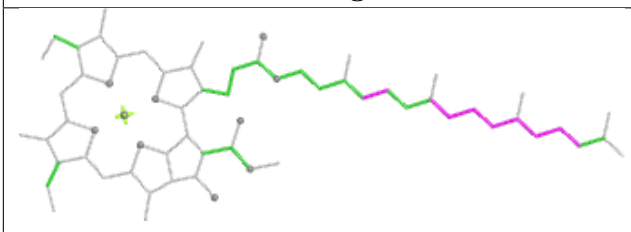
Ligand CLA A 1136



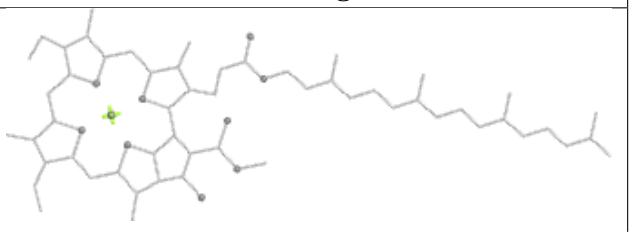
Bond lengths



Bond angles

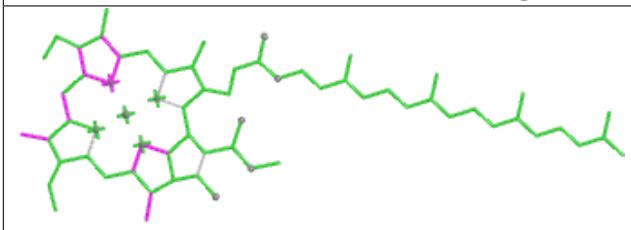


Torsions

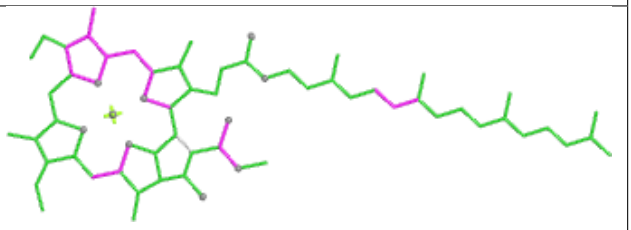


Rings

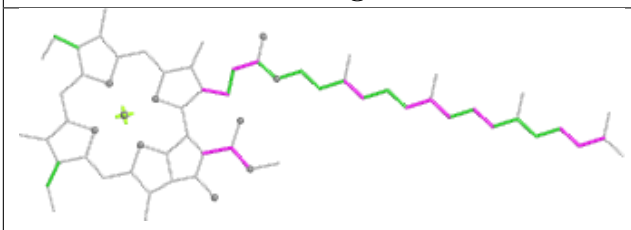
Ligand CLA B 1229



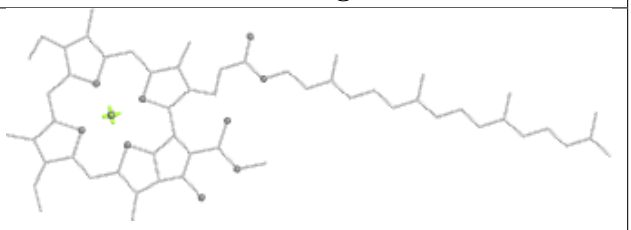
Bond lengths



Bond angles

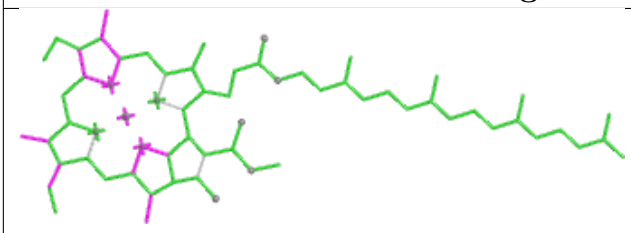


Torsions

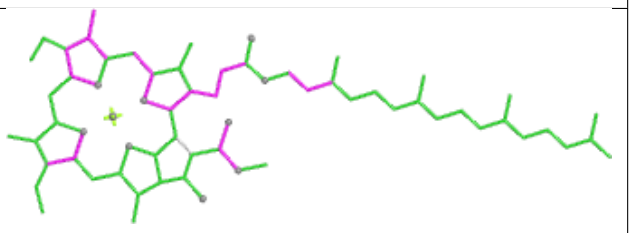


Rings

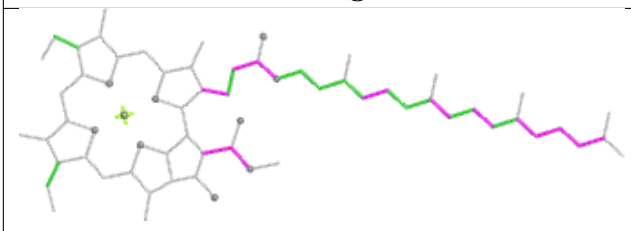
Ligand CLA e 1103



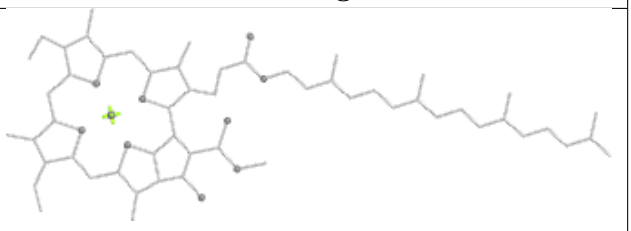
Bond lengths



Bond angles

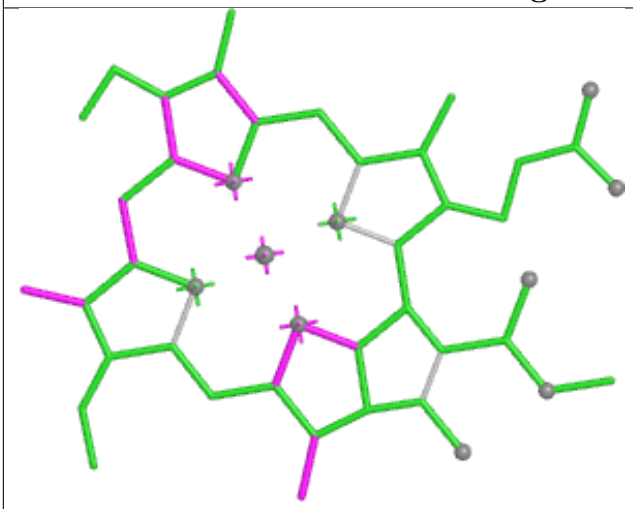


Torsions

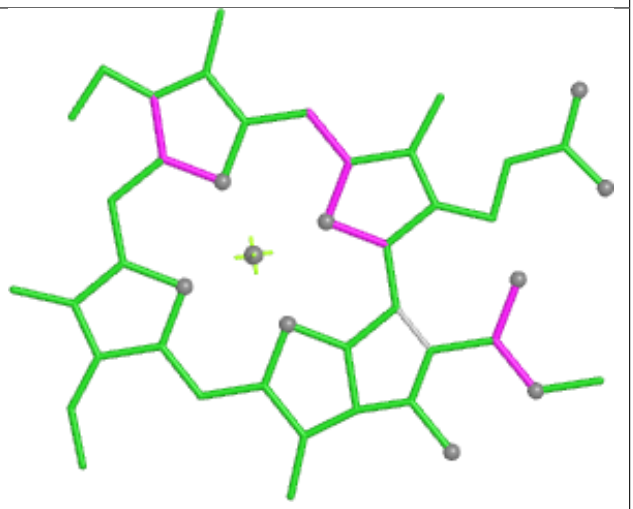


Rings

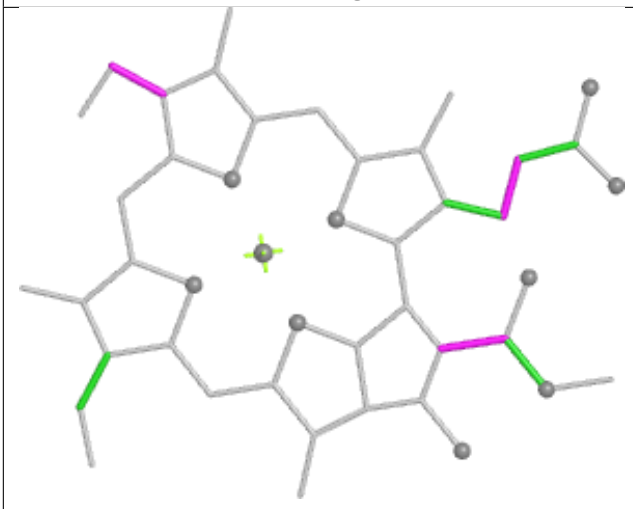
Ligand CLA t 505



Bond lengths



Bond angles

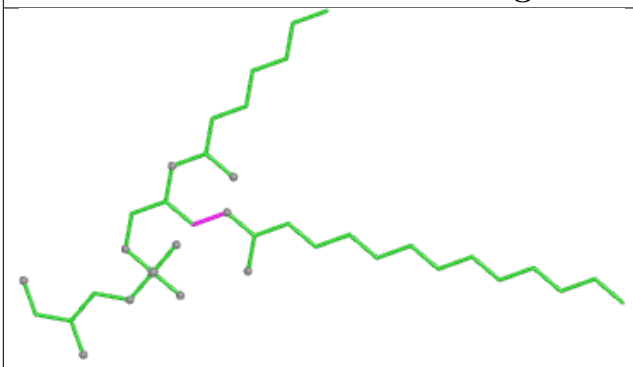


Torsions

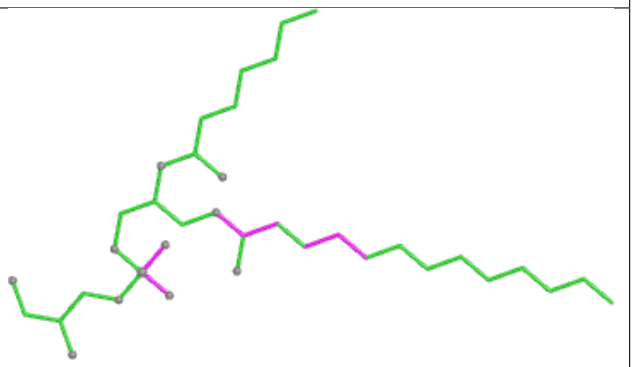


Rings

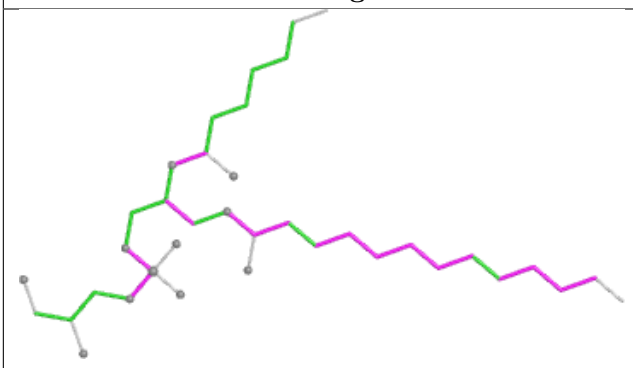
Ligand LHG B 1842



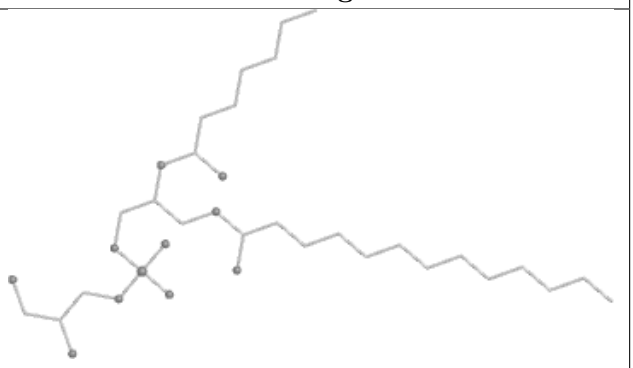
Bond lengths



Bond angles

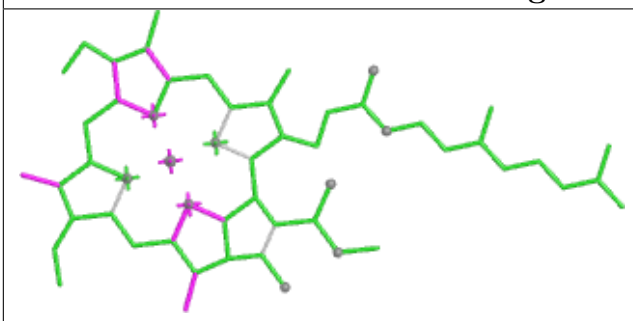


Torsions

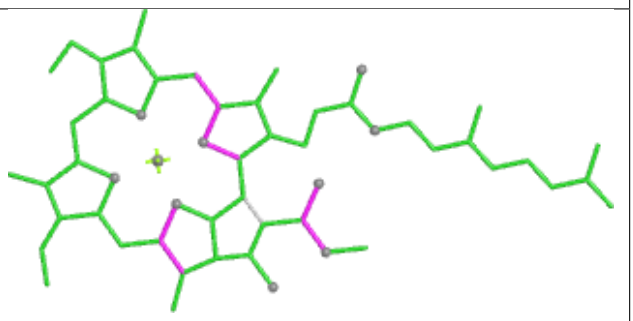


Rings

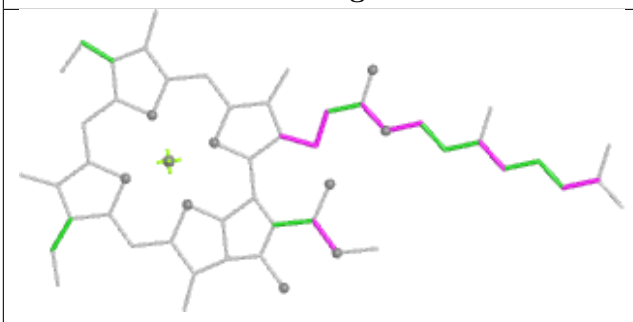
Ligand CLA 3 505



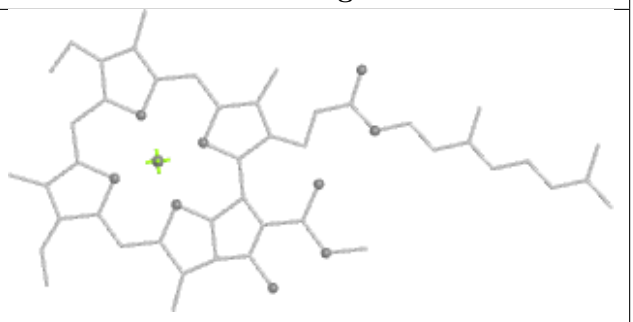
Bond lengths



Bond angles

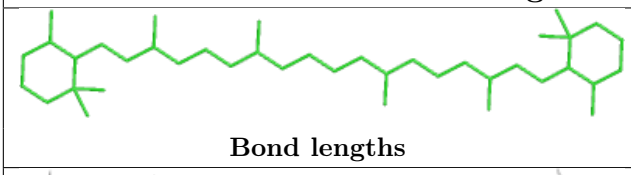


Torsions

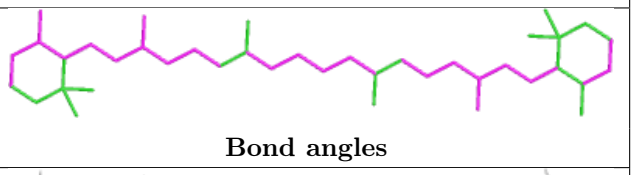


Rings

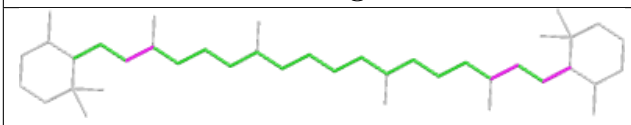
Ligand BCR 2 523



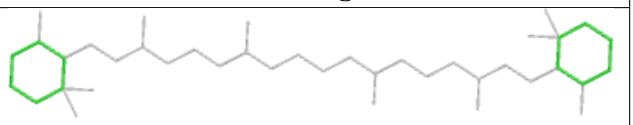
Bond lengths



Bond angles

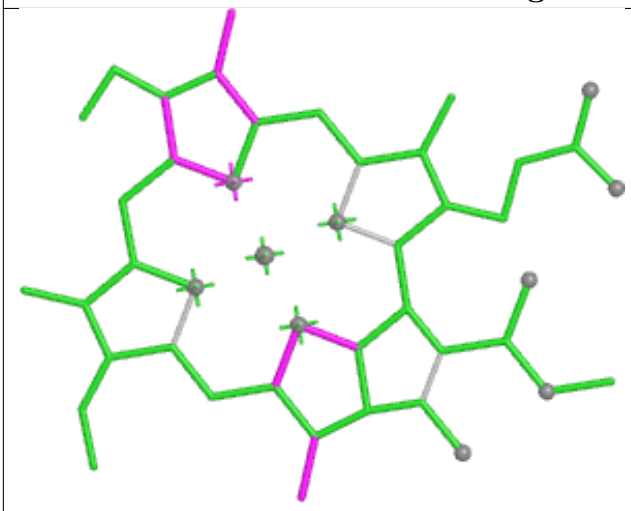


Torsions

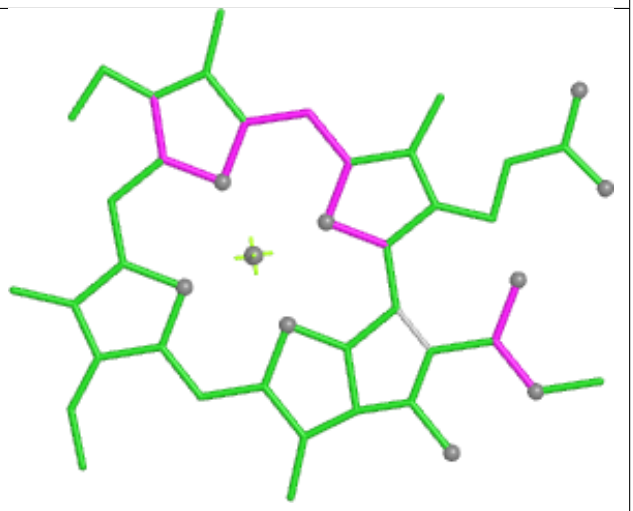


Rings

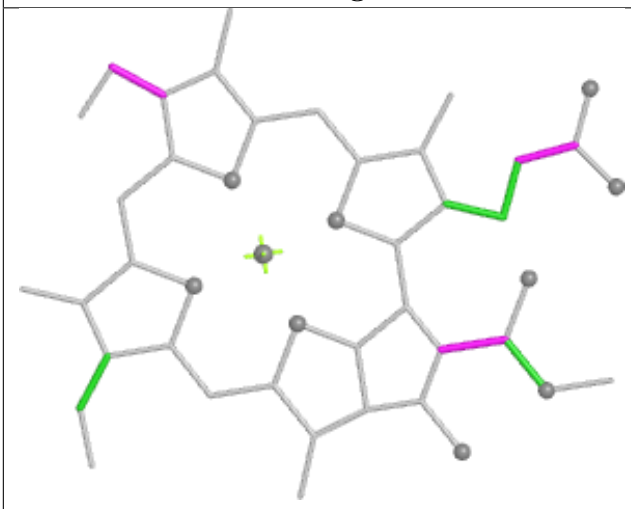
Ligand CLA b 512



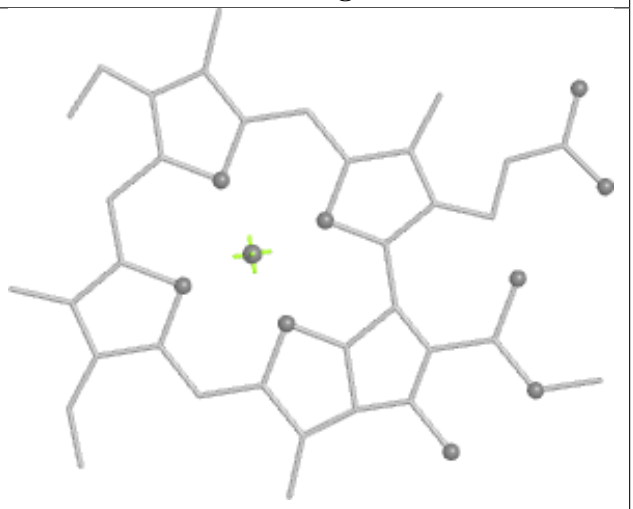
Bond lengths



Bond angles

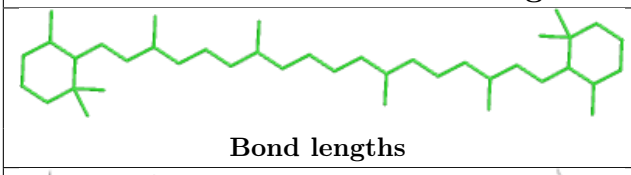


Torsions

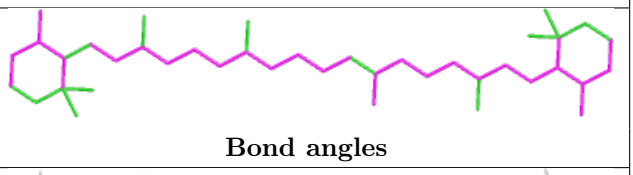


Rings

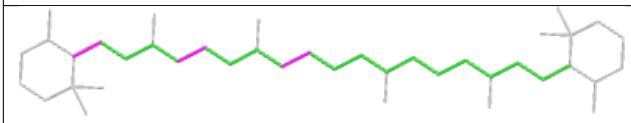
Ligand BCR b 522



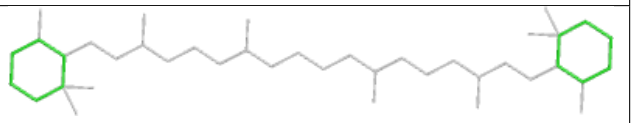
Bond lengths



Bond angles

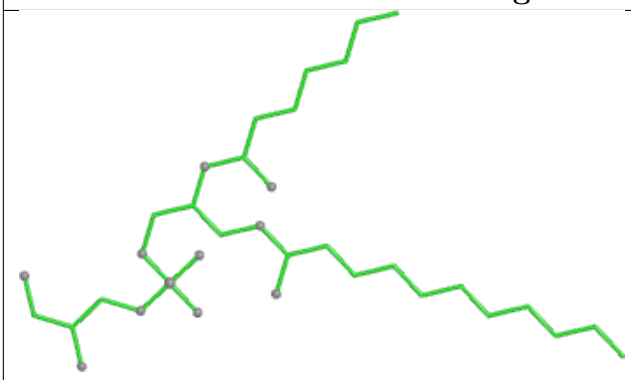


Torsions

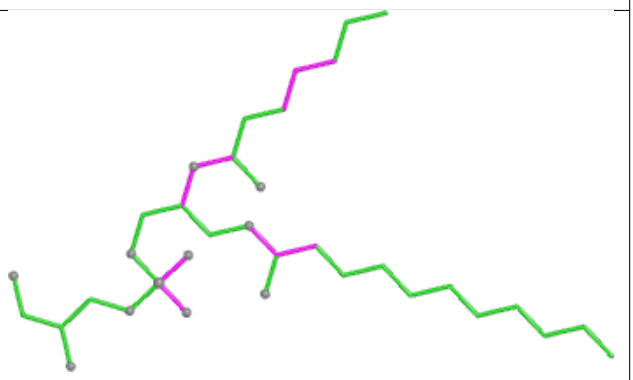


Rings

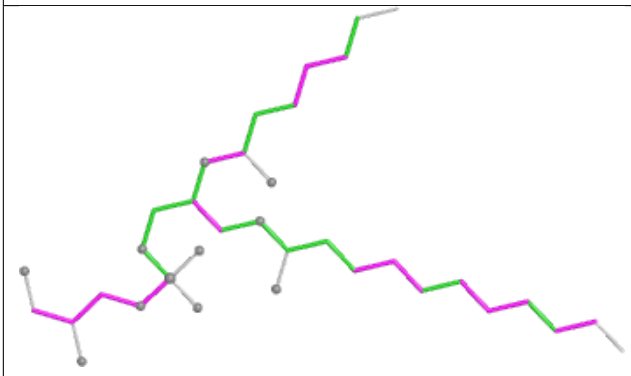
Ligand LHG A 5004



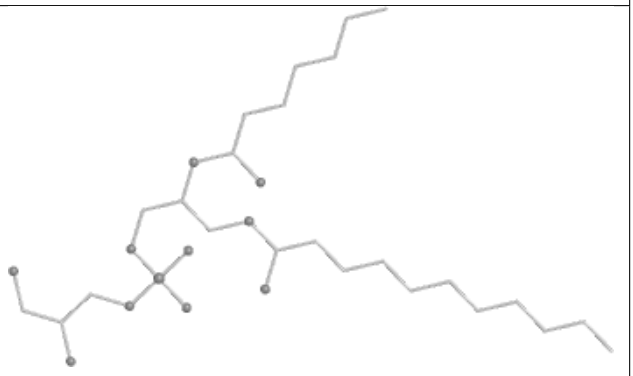
Bond lengths



Bond angles

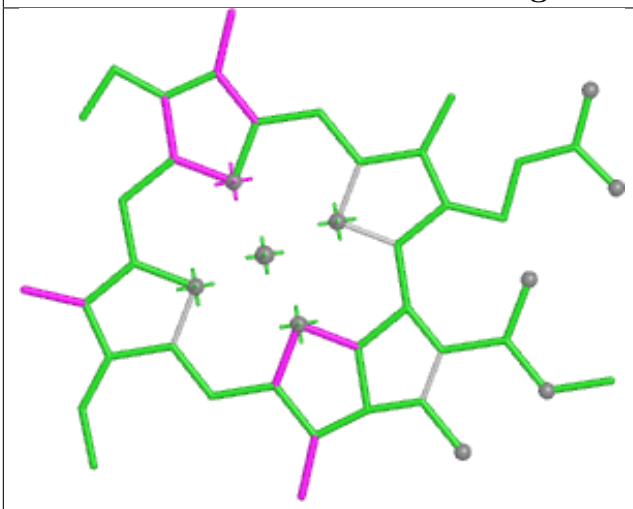


Torsions

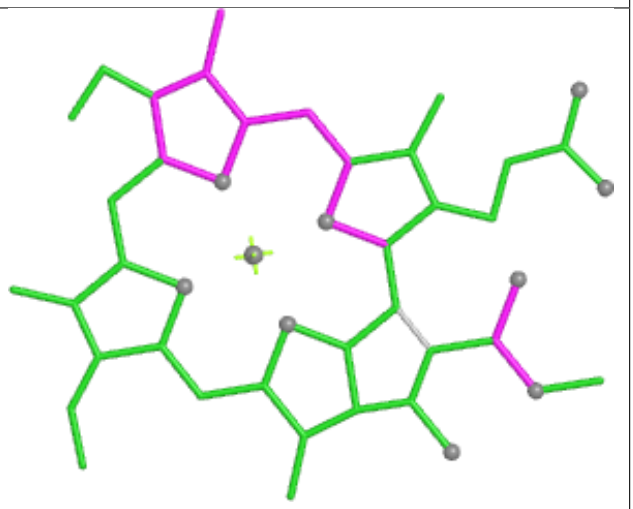


Rings

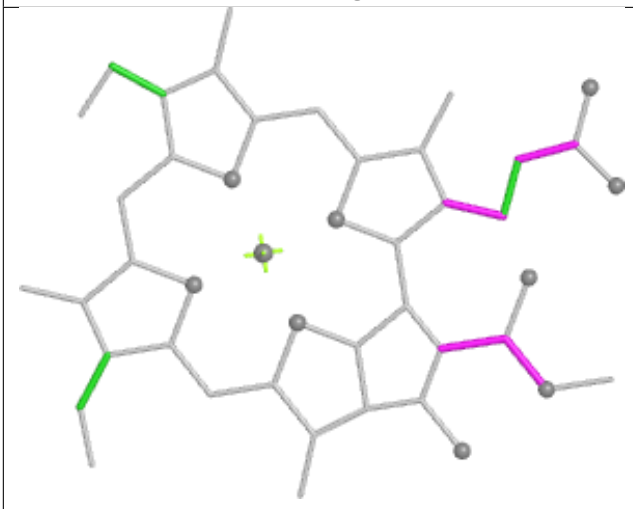
Ligand CLA s 506



Bond lengths



Bond angles

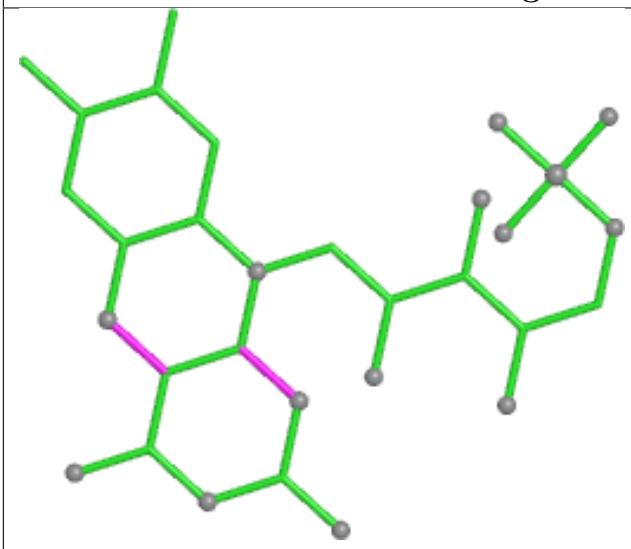


Torsions

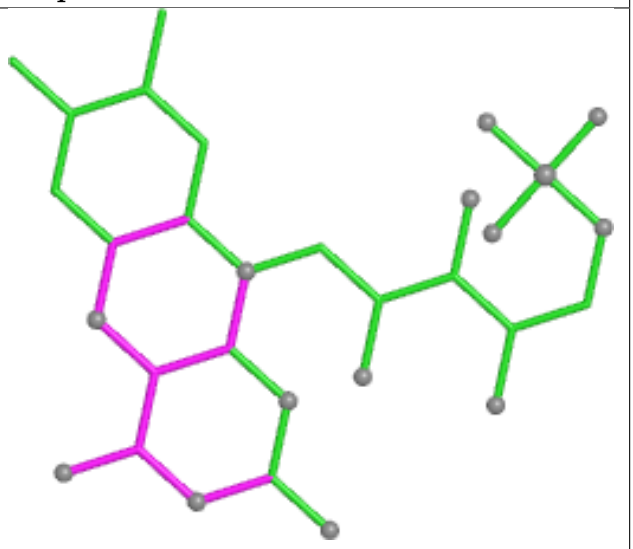


Rings

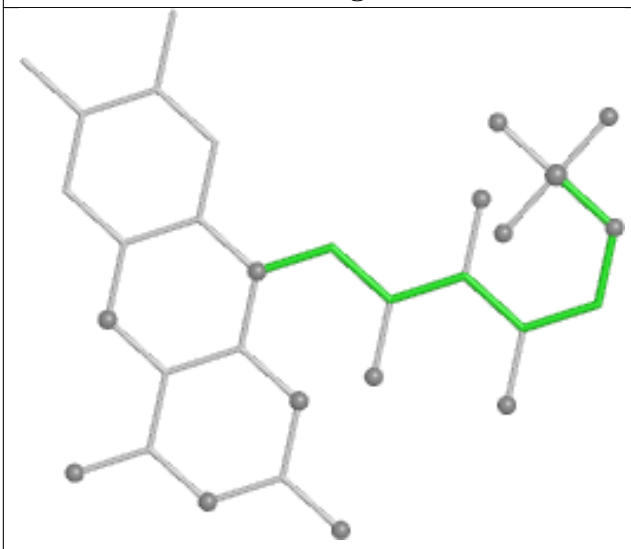
Ligand FMN p 170



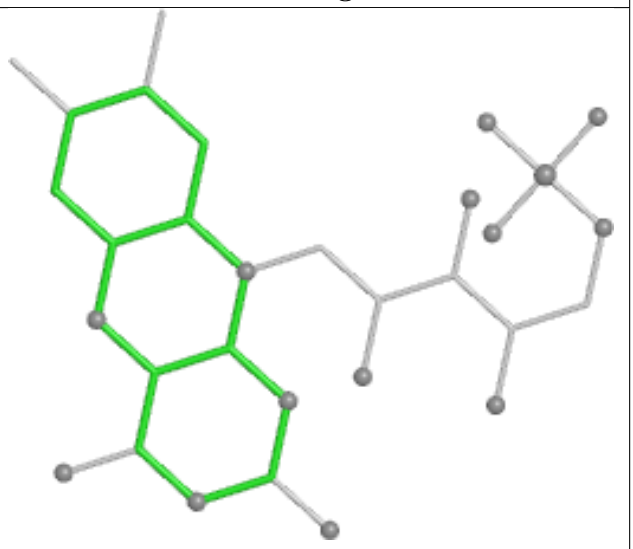
Bond lengths



Bond angles

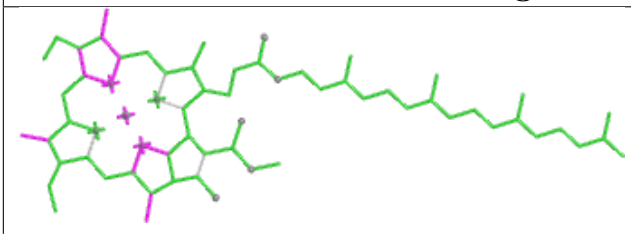


Torsions

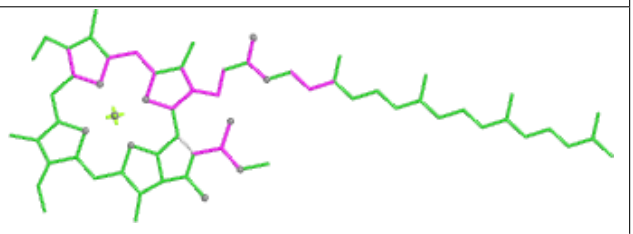


Rings

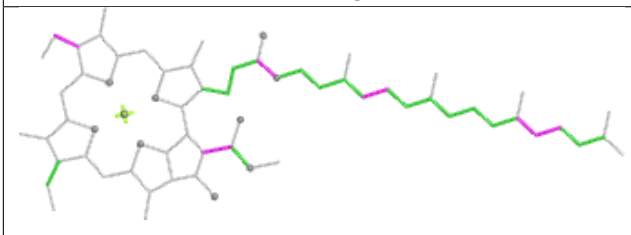
Ligand CLA H 1205



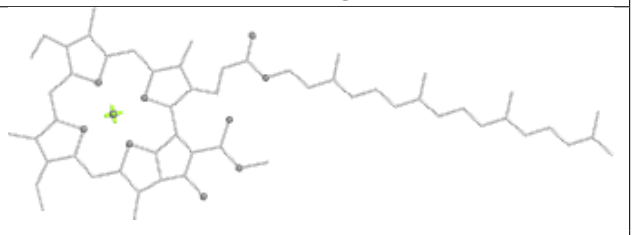
Bond lengths



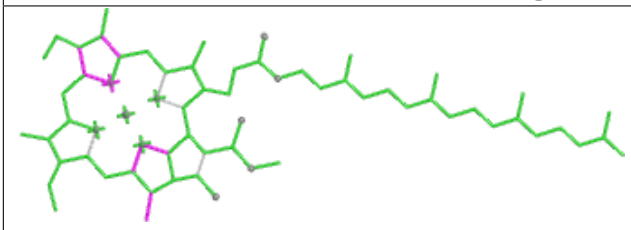
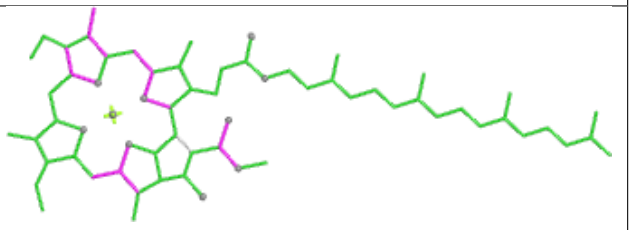
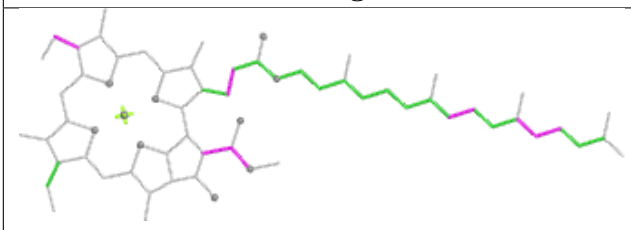
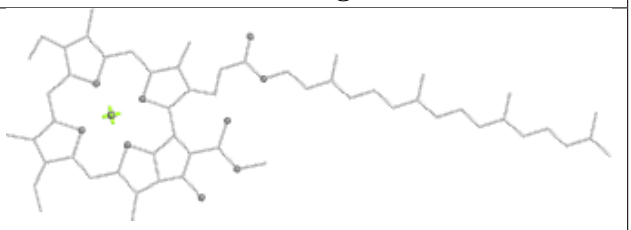
Bond angles

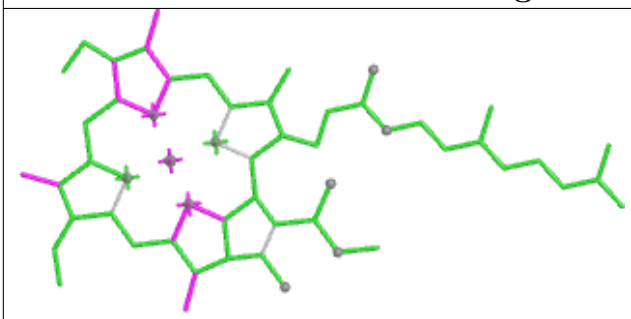
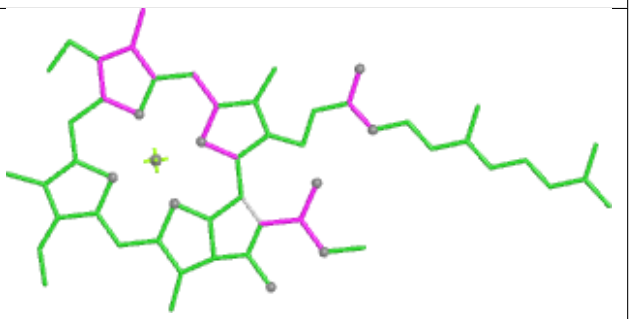
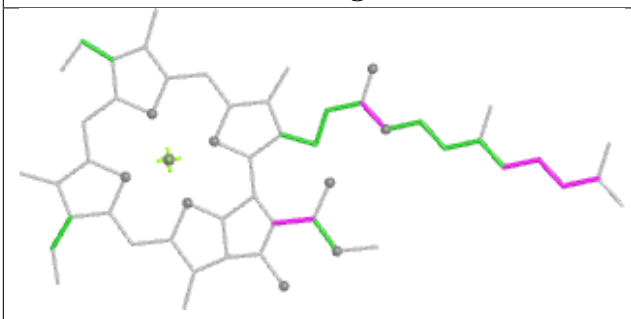
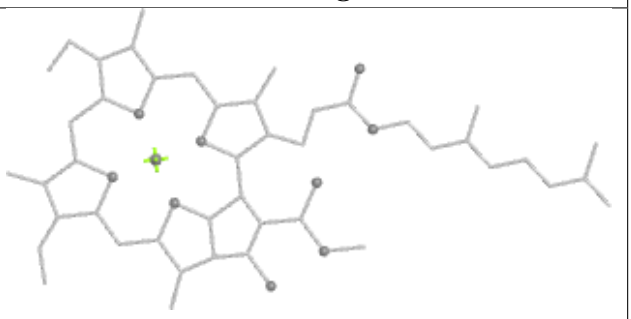


Torsions

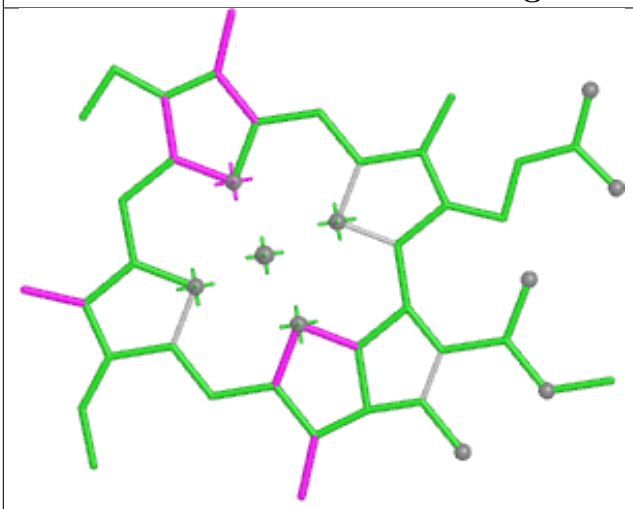


Rings

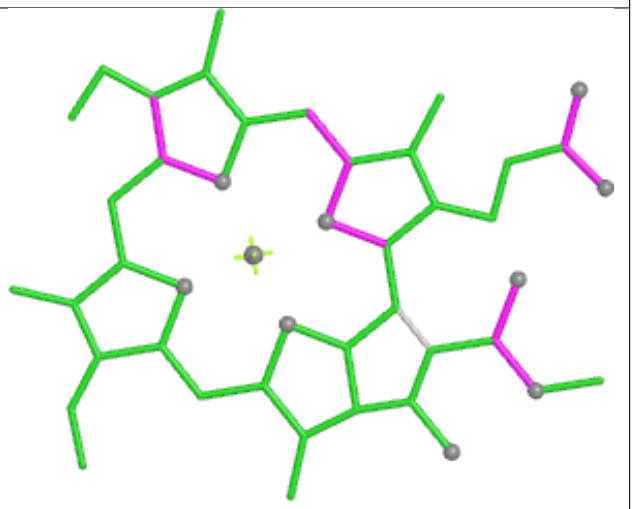
Ligand CLA r 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1211	
 Bond lengths	 Bond angles
 Torsions	 Rings

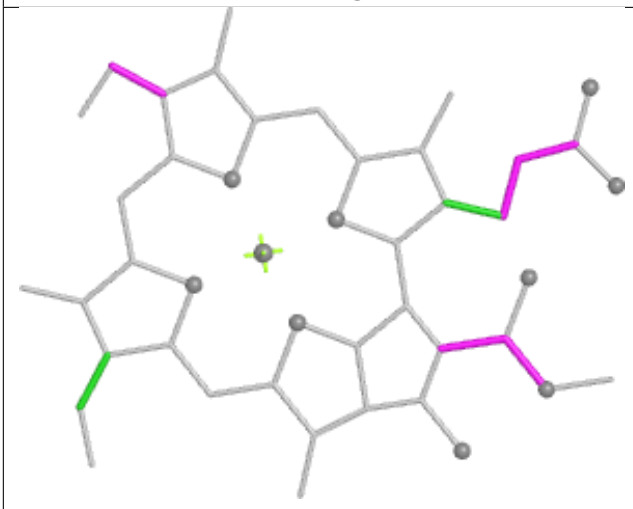
Ligand CLA Y 517



Bond lengths



Bond angles

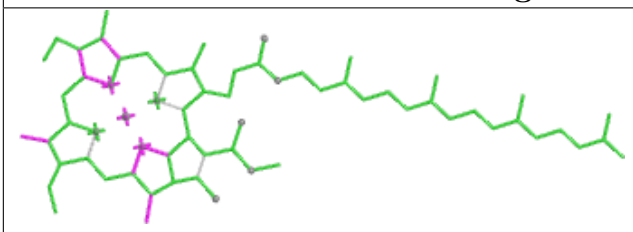


Torsions

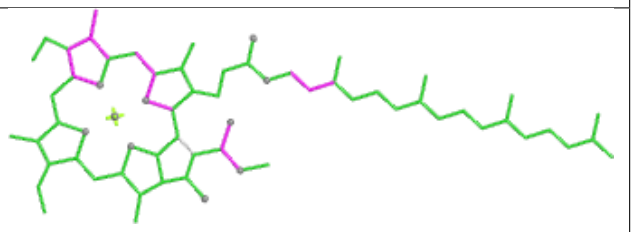


Rings

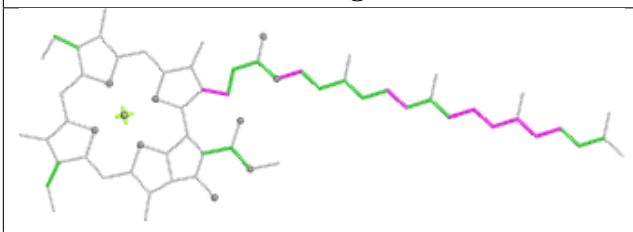
Ligand CLA H 1223



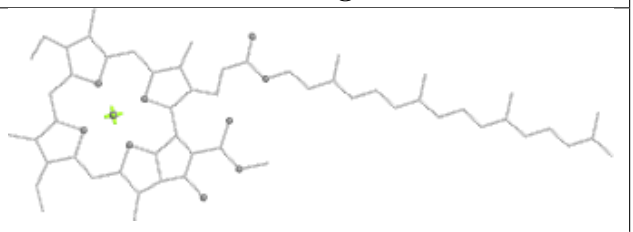
Bond lengths



Bond angles

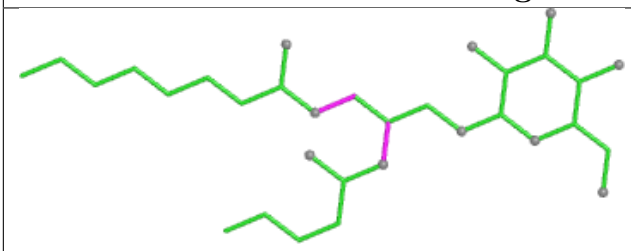


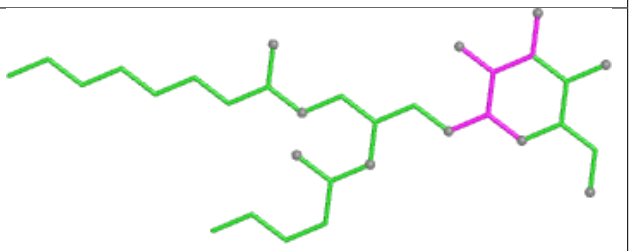
Torsions

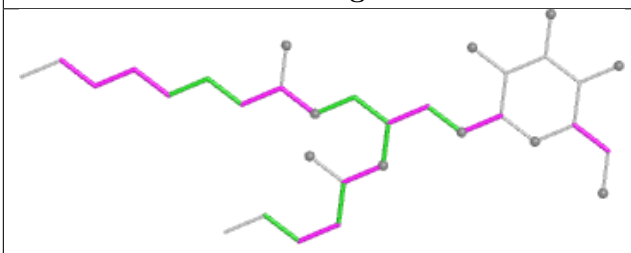


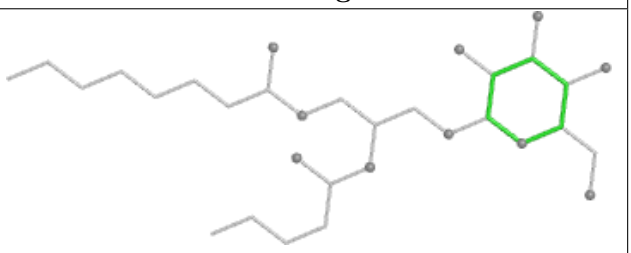
Rings

Ligand LMG J 5104


Bond lengths

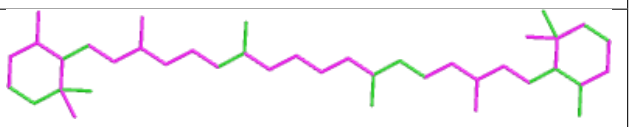

Bond angles

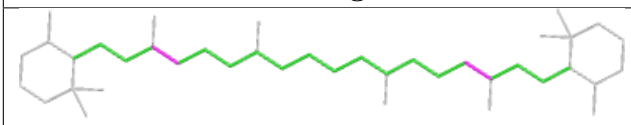

Torsions

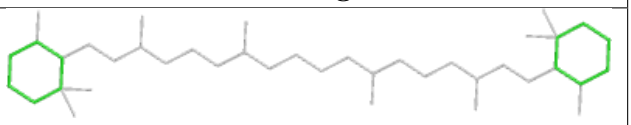

Rings

Ligand BCR f 4006

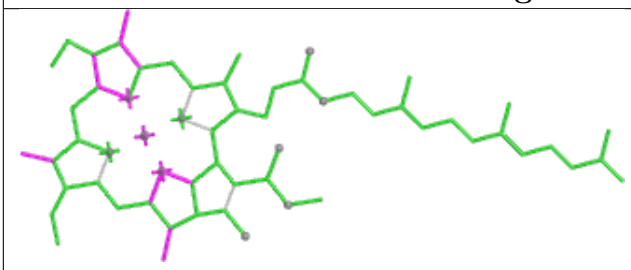

Bond lengths

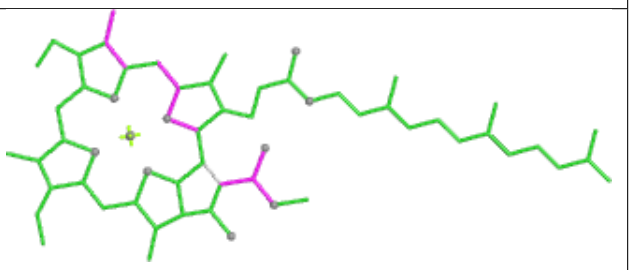

Bond angles

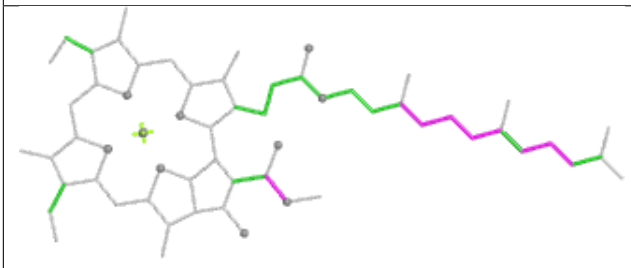

Torsions

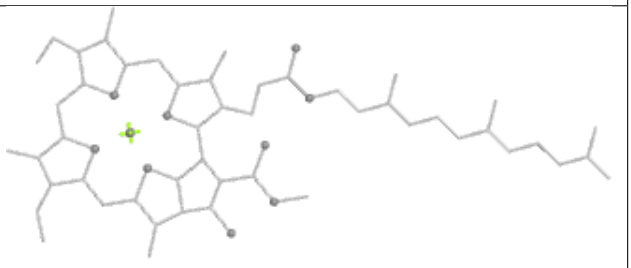

Rings

Ligand CLA V 1503

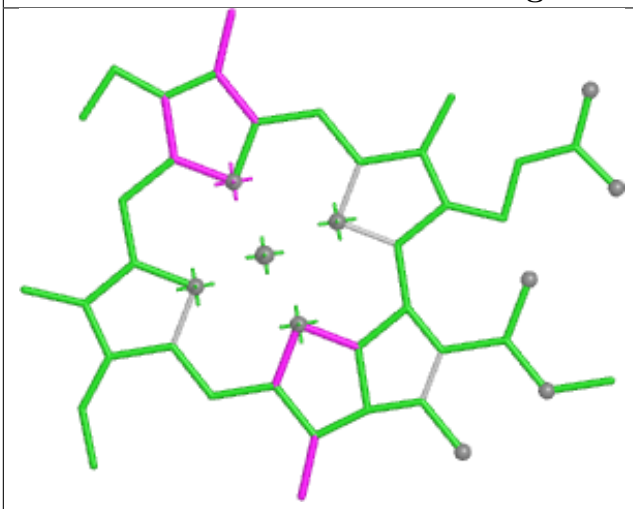

Bond lengths


Bond angles

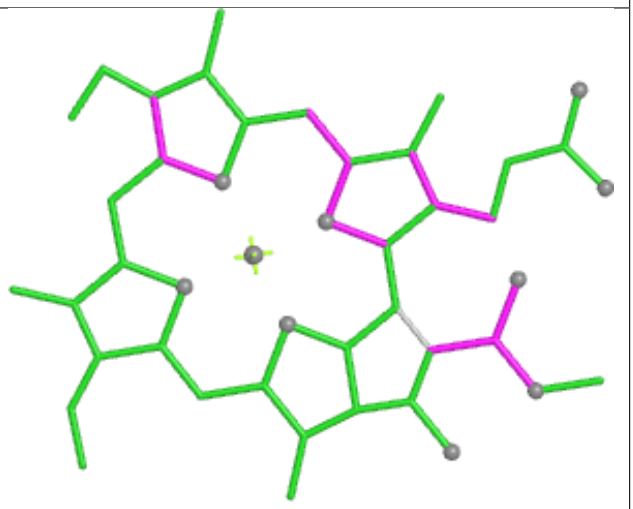

Torsions


Rings

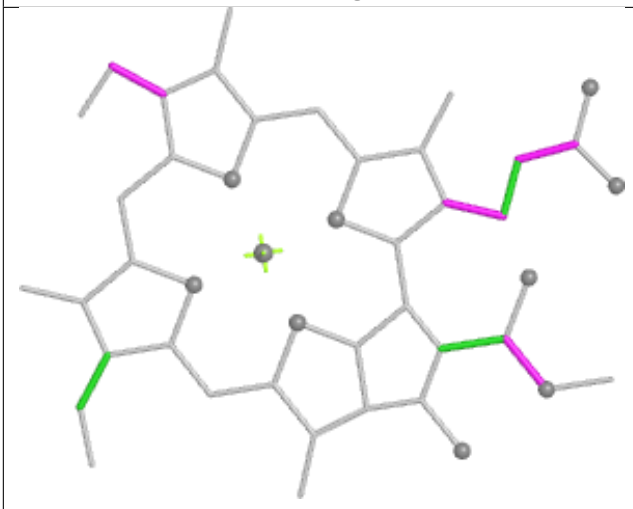
Ligand CLA Z 516



Bond lengths



Bond angles

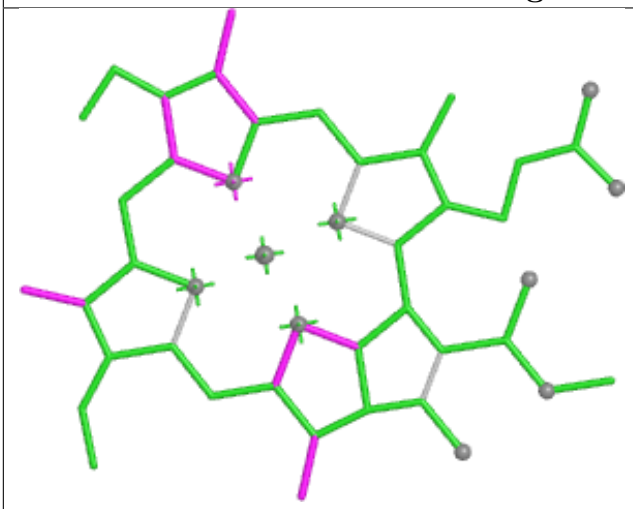


Torsions

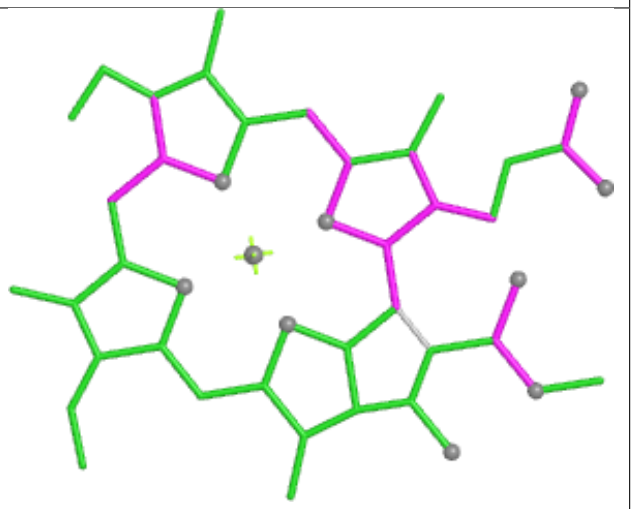


Rings

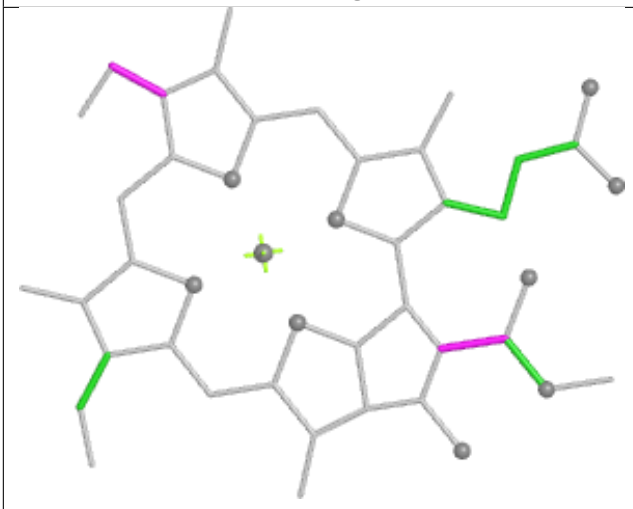
Ligand CLA Z 502



Bond lengths



Bond angles

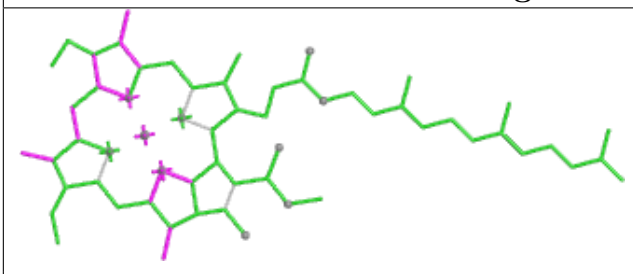


Torsions

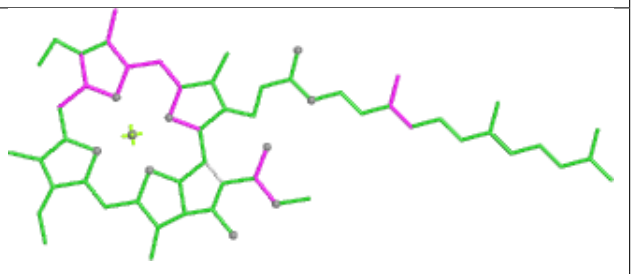


Rings

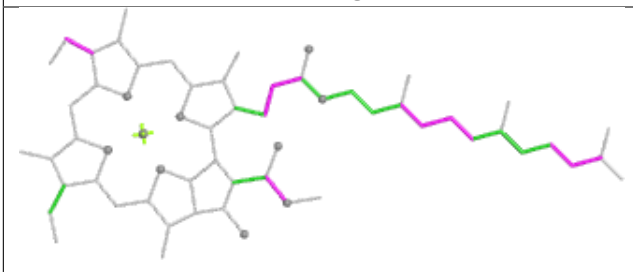
Ligand CLA G 1115



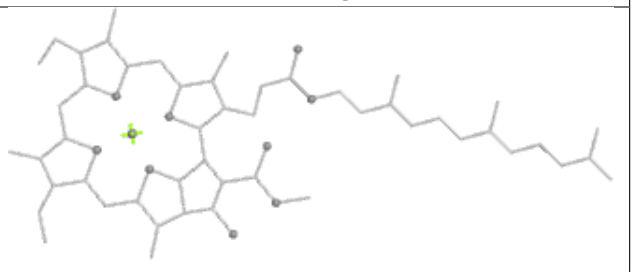
Bond lengths



Bond angles

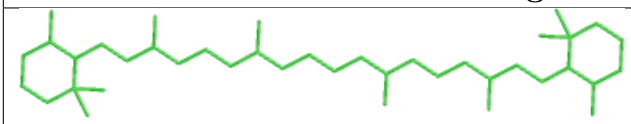


Torsions

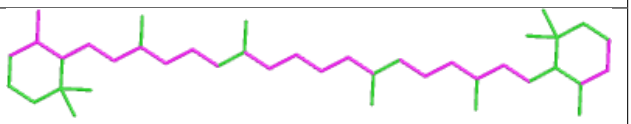


Rings

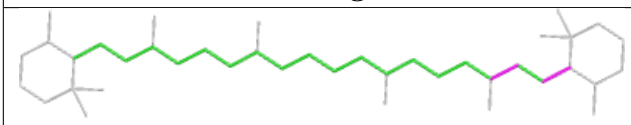
Ligand BCR 6 523



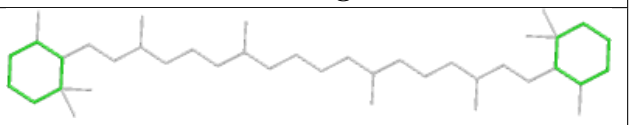
Bond lengths



Bond angles

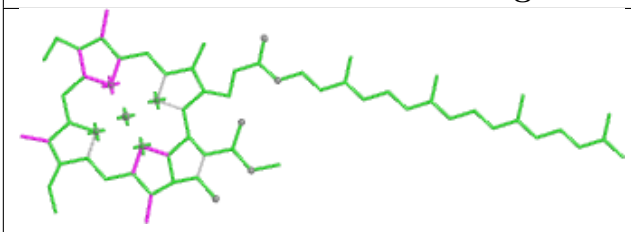


Torsions

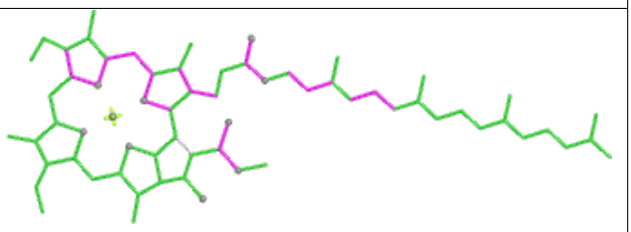


Rings

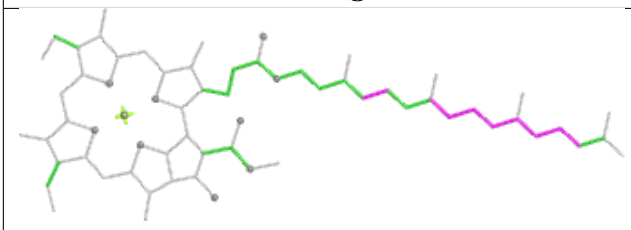
Ligand CLA G 1136



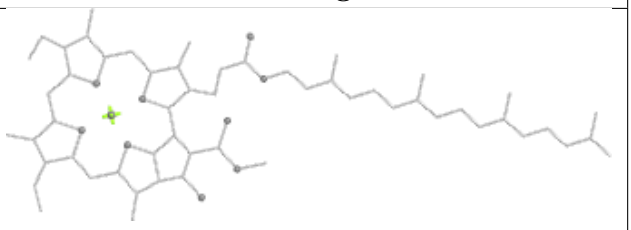
Bond lengths



Bond angles

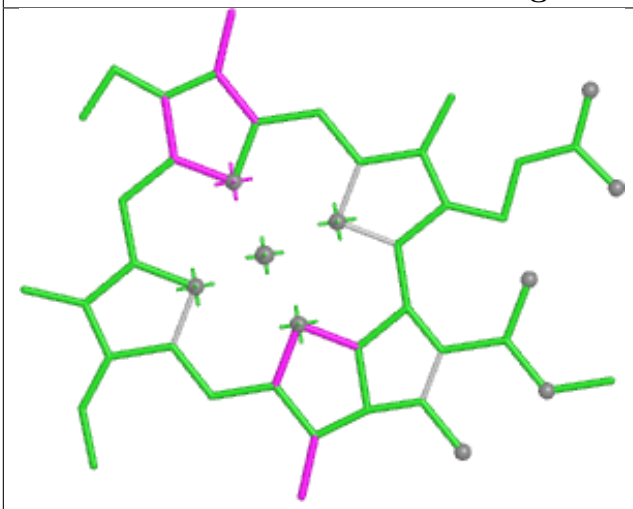


Torsions

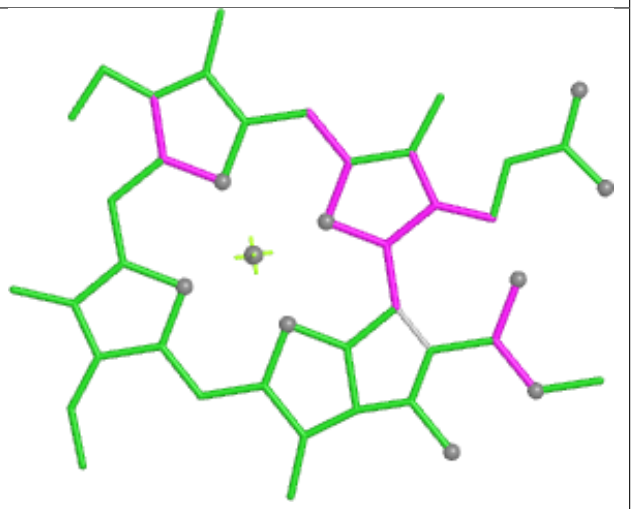


Rings

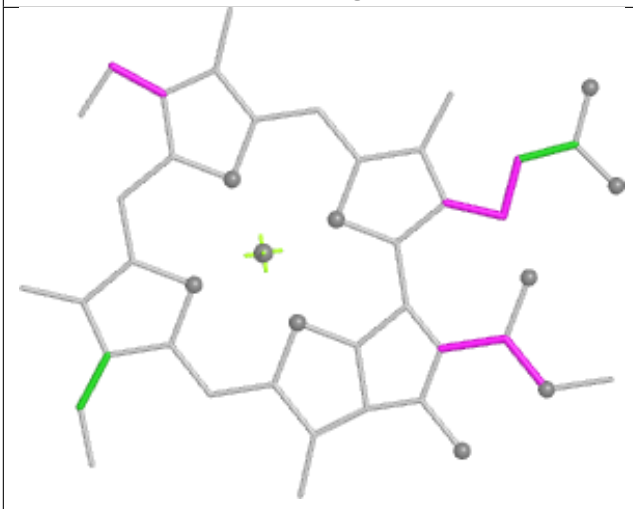
Ligand CLA r 504



Bond lengths



Bond angles

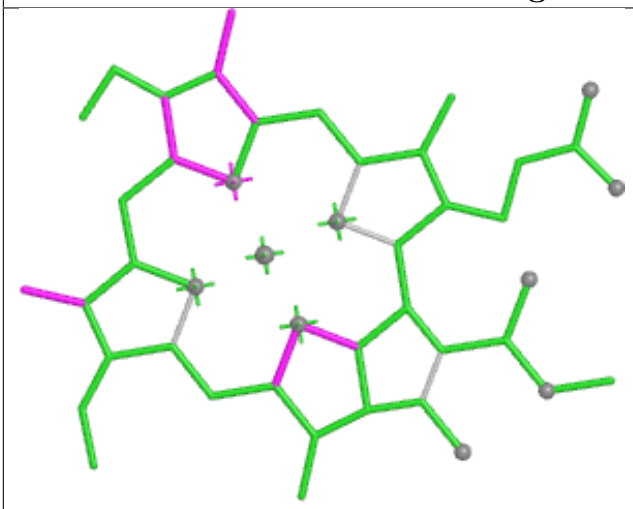


Torsions

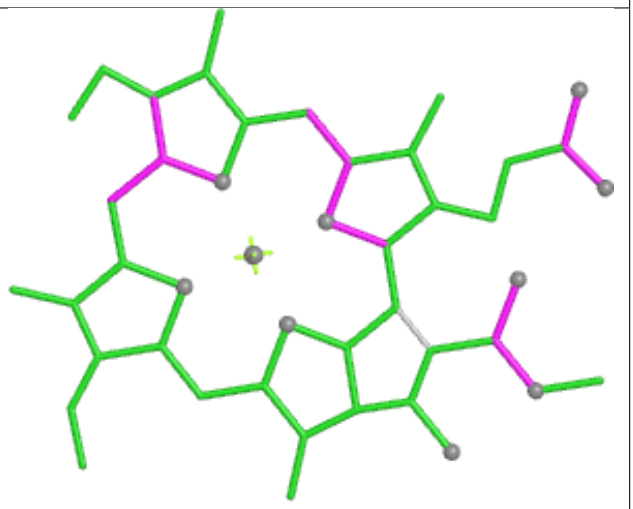


Rings

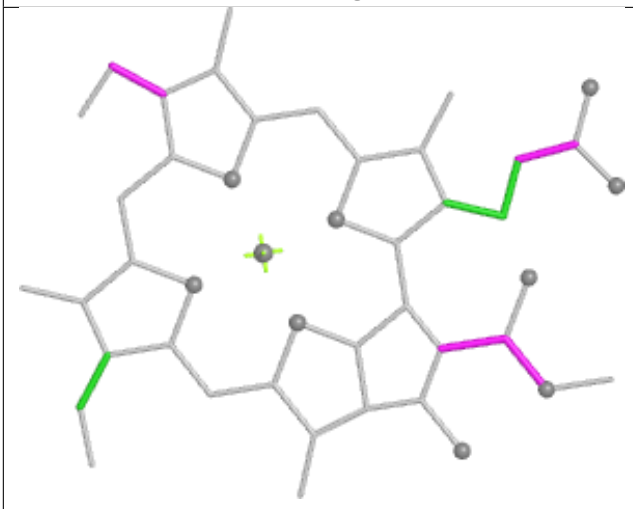
Ligand CLA a 519



Bond lengths



Bond angles

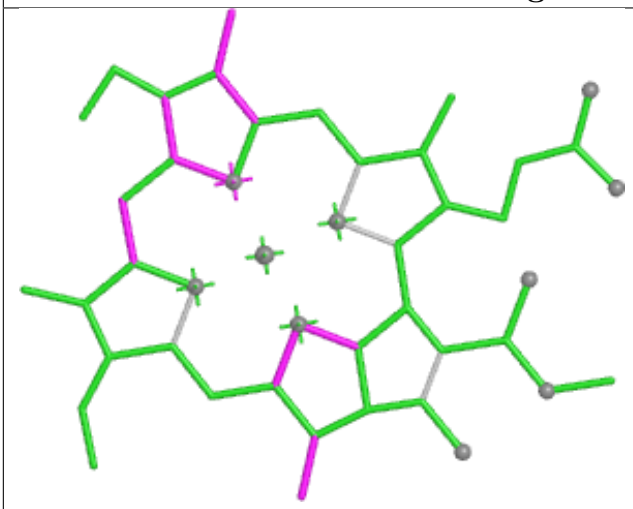


Torsions

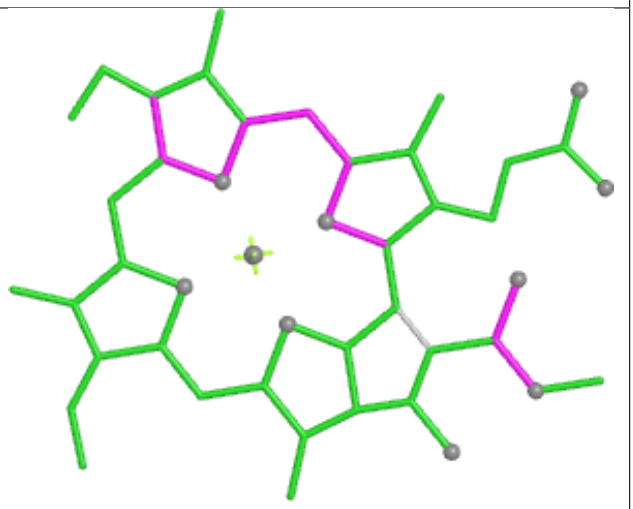


Rings

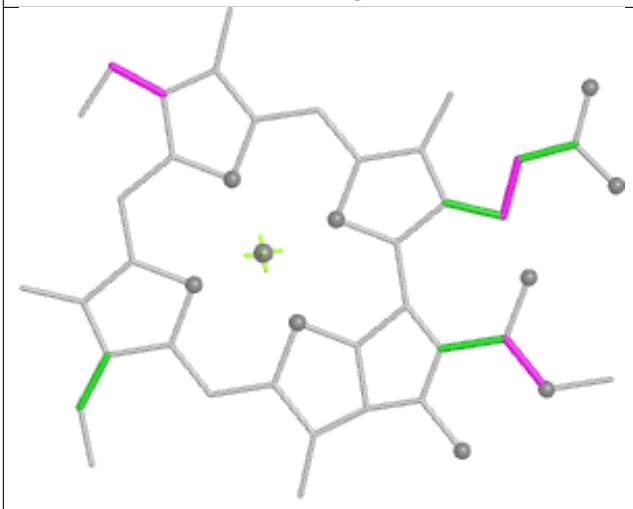
Ligand CLA d 513



Bond lengths



Bond angles

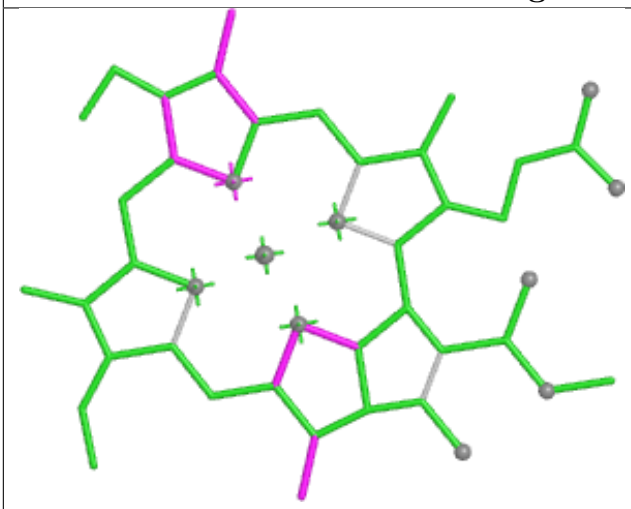


Torsions

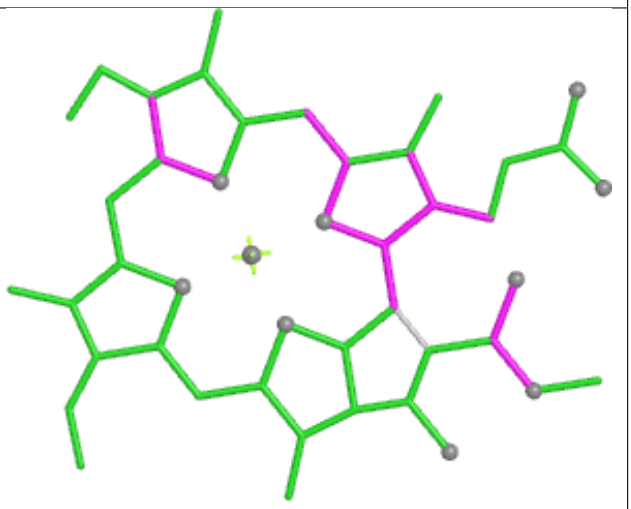


Rings

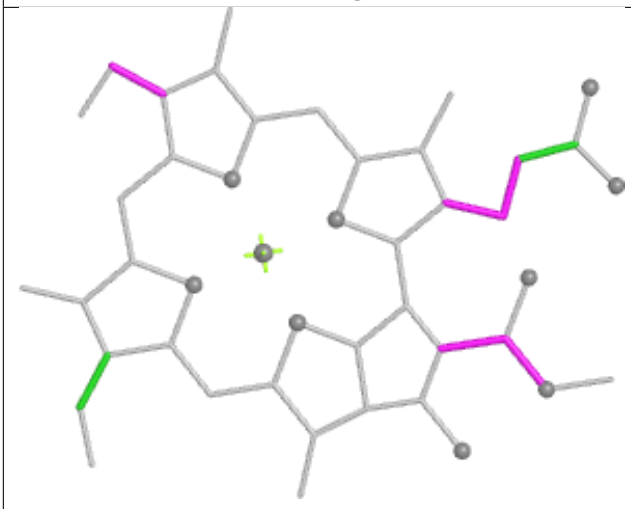
Ligand CLA 2 504



Bond lengths



Bond angles

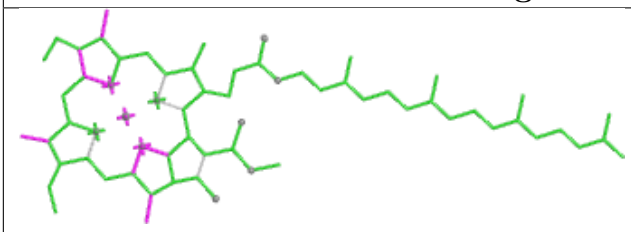


Torsions

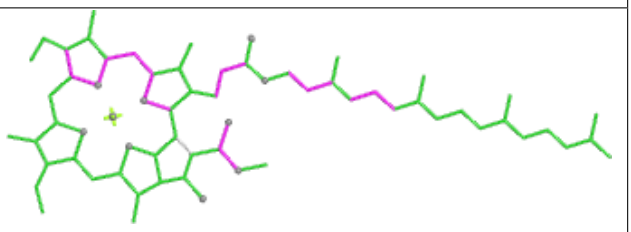


Rings

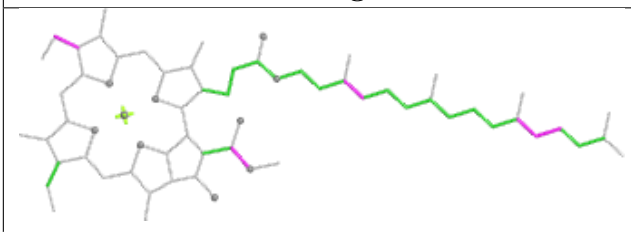
Ligand CLA A 1131



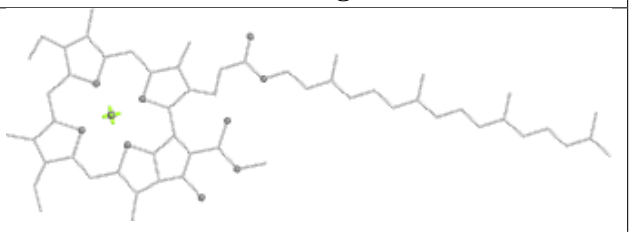
Bond lengths



Bond angles

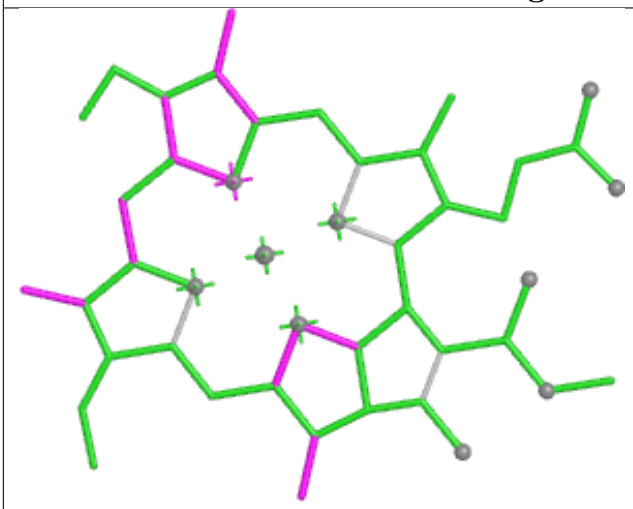


Torsions

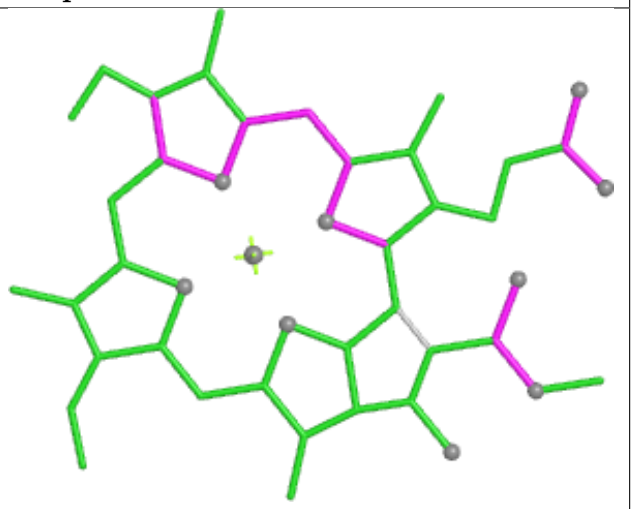


Rings

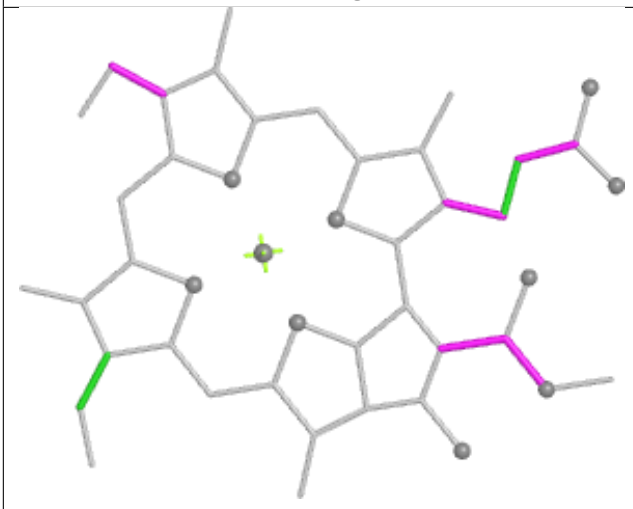
Ligand CLA q 519



Bond lengths



Bond angles

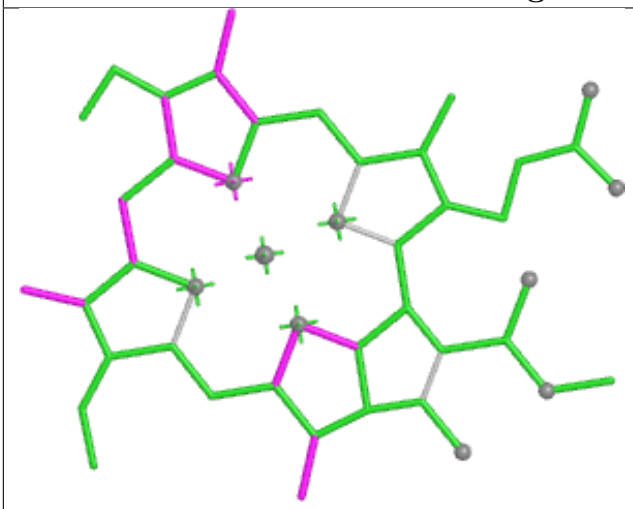


Torsions

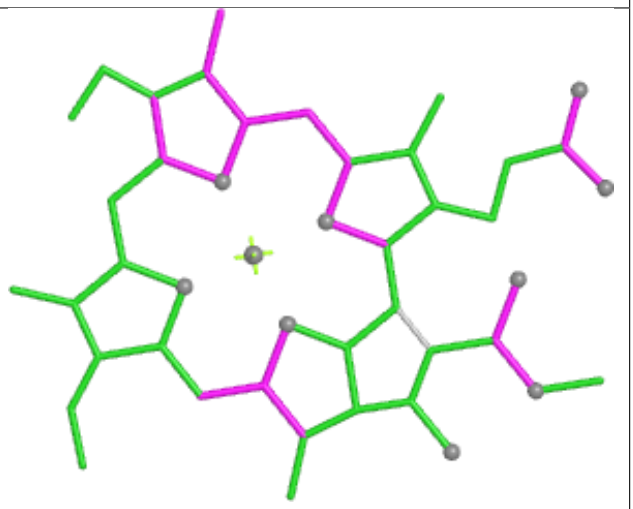


Rings

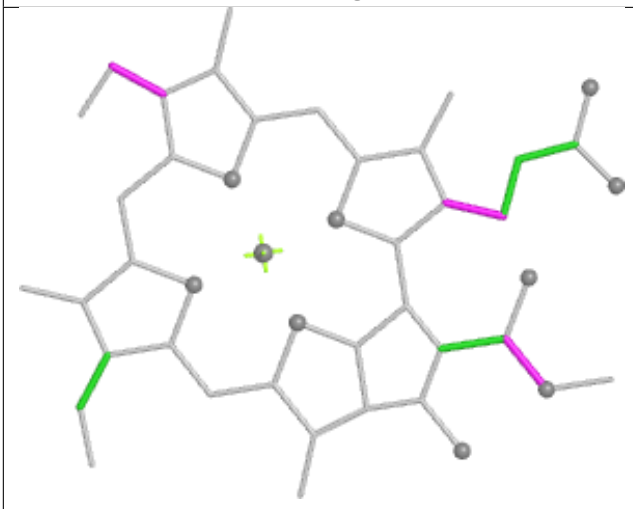
Ligand CLA b 511



Bond lengths



Bond angles

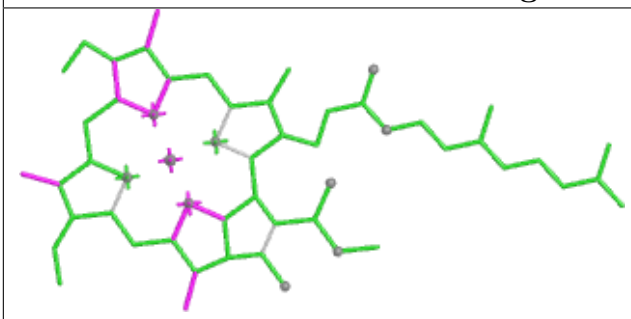


Torsions

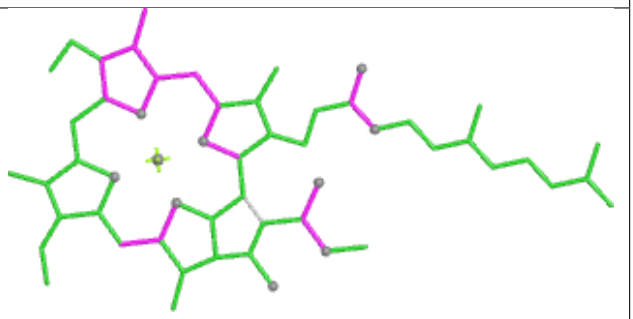


Rings

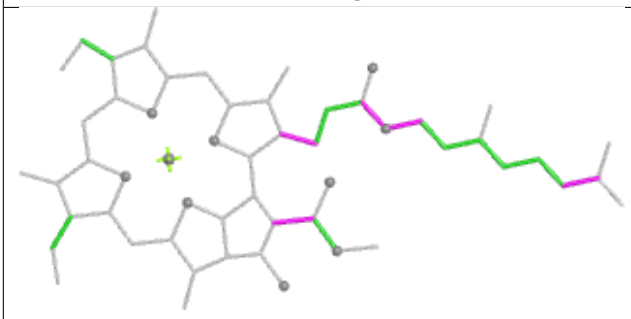
Ligand CLA e 1105



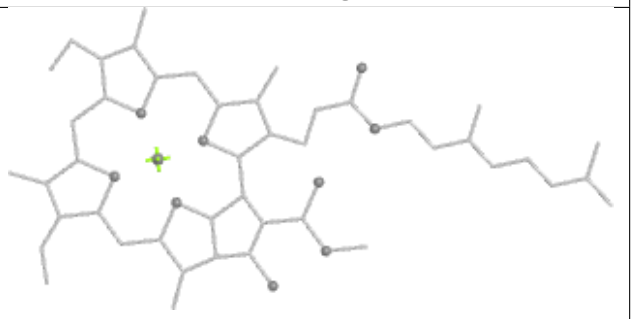
Bond lengths



Bond angles

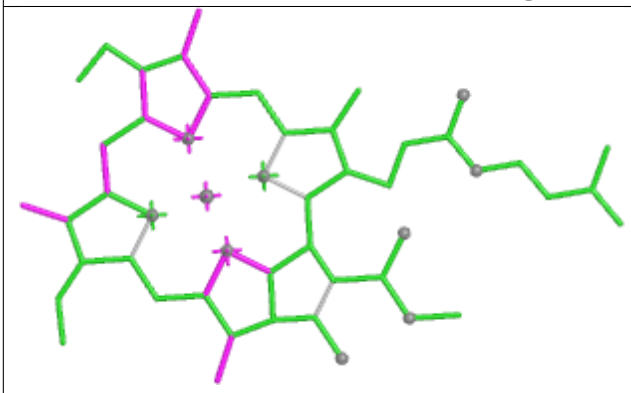


Torsions

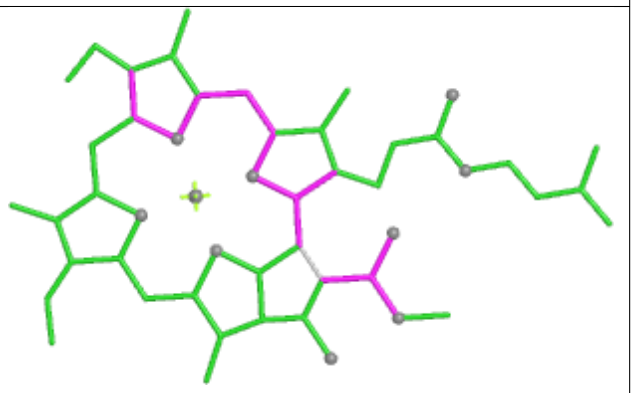


Rings

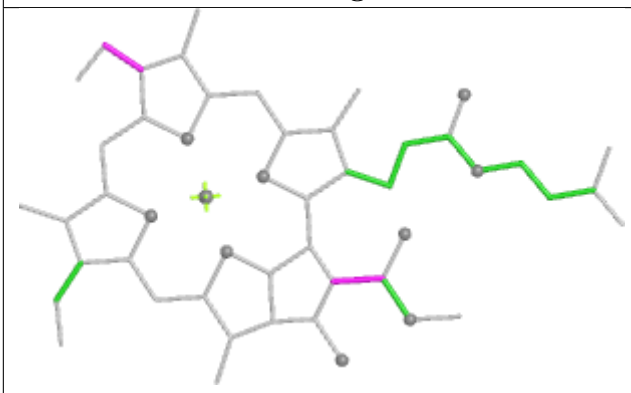
Ligand CLA e 1112



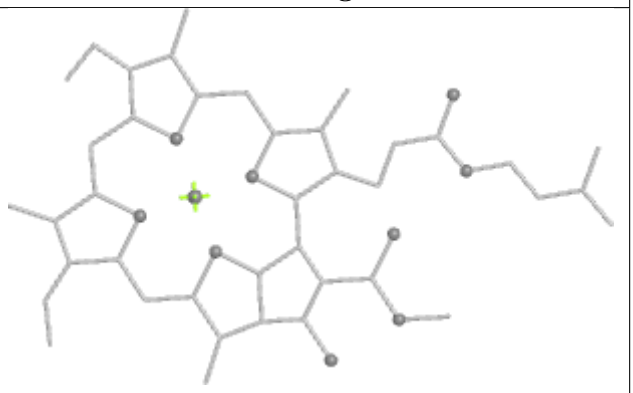
Bond lengths



Bond angles

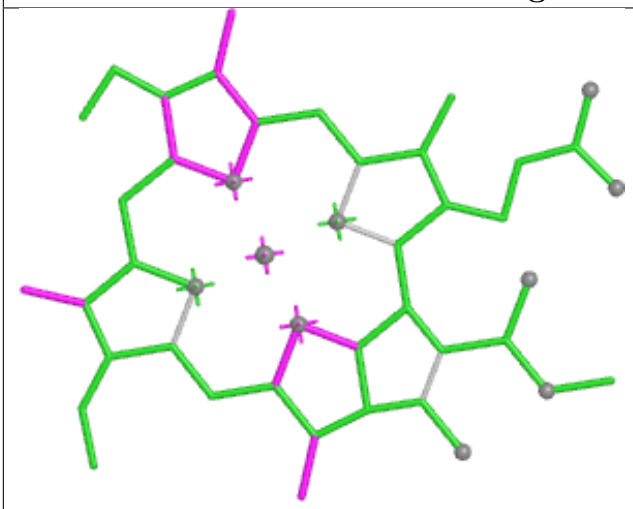


Torsions

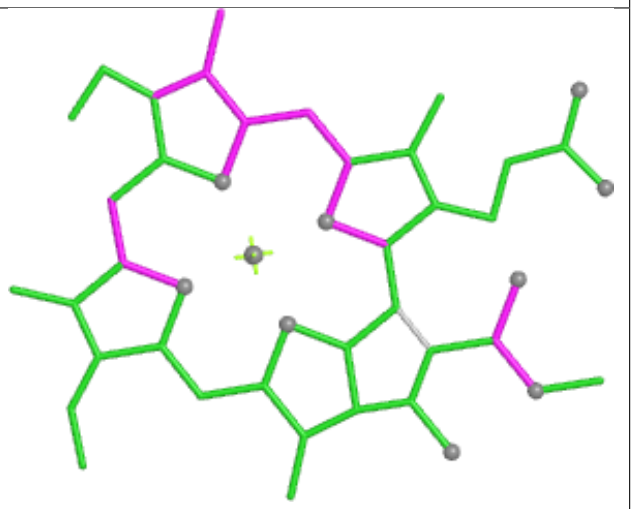


Rings

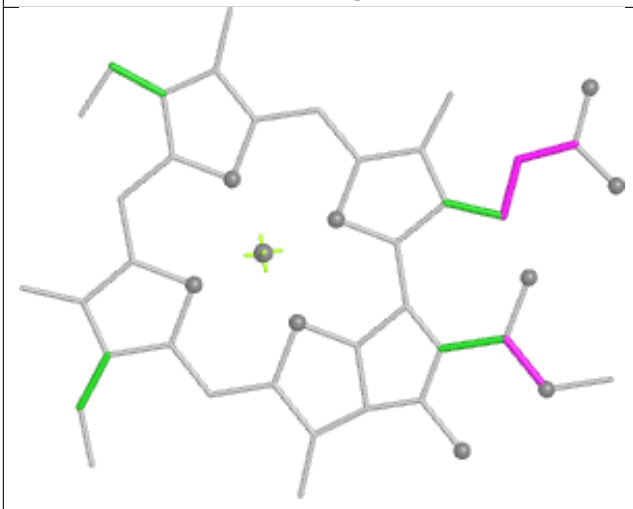
Ligand CLA 1 508



Bond lengths



Bond angles

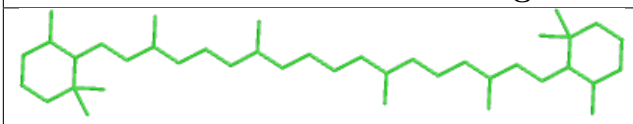


Torsions

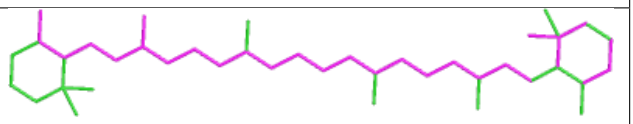


Rings

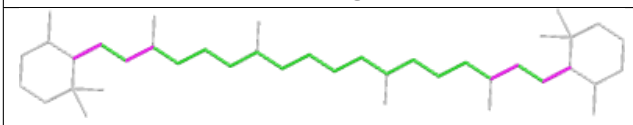
Ligand BCR B 4004



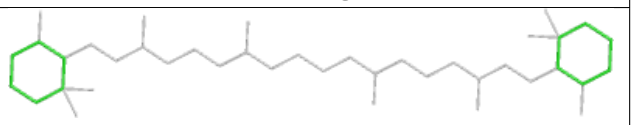
Bond lengths



Bond angles

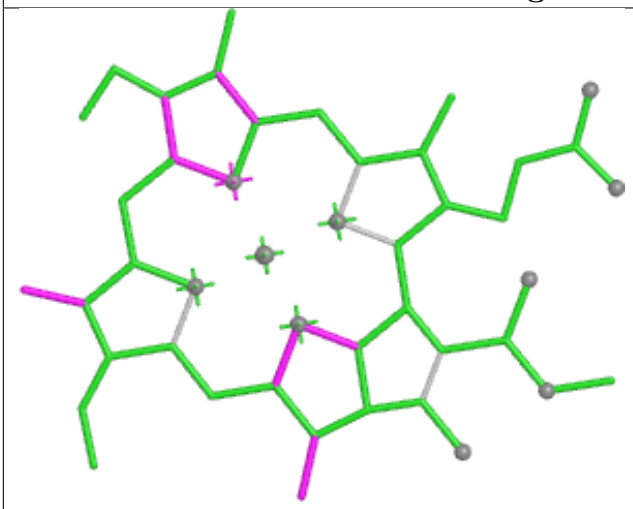


Torsions

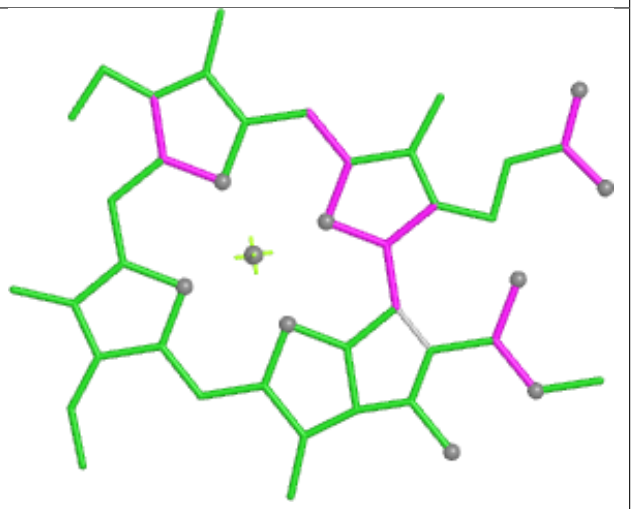


Rings

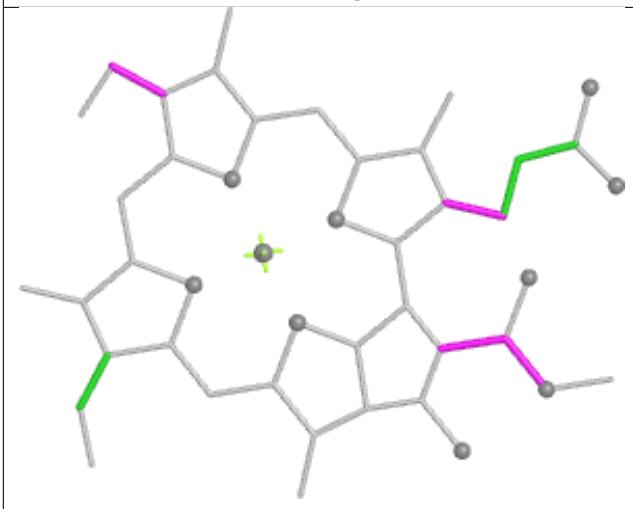
Ligand CLA b 517



Bond lengths



Bond angles

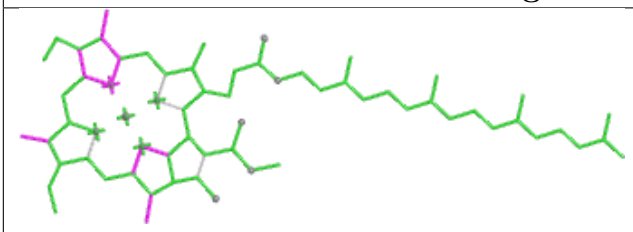


Torsions

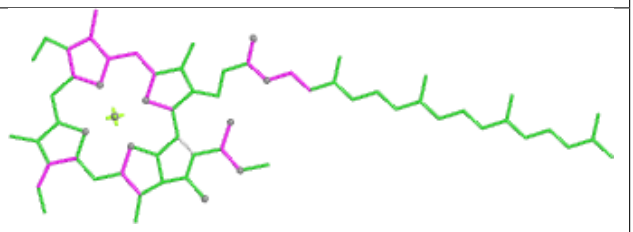


Rings

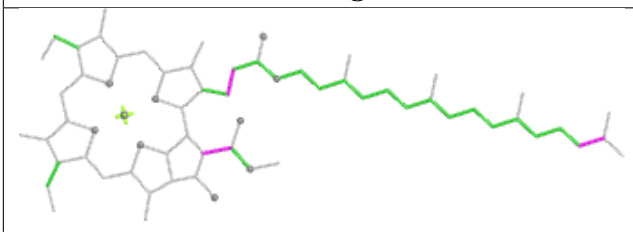
Ligand CLA f 1238



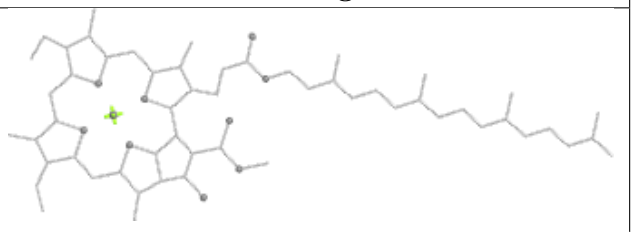
Bond lengths



Bond angles

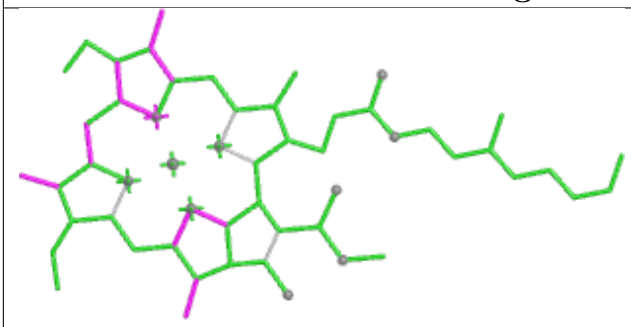


Torsions

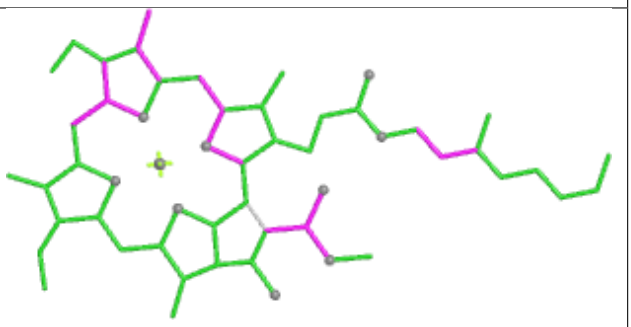


Rings

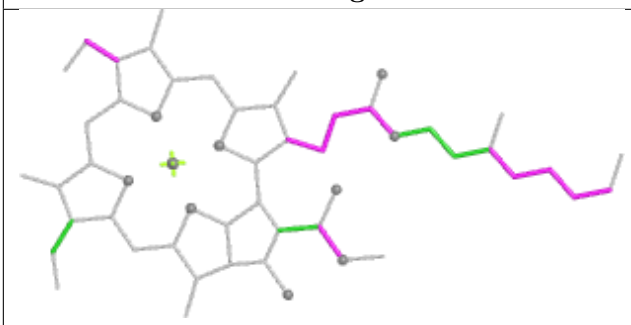
Ligand CLA G 1108



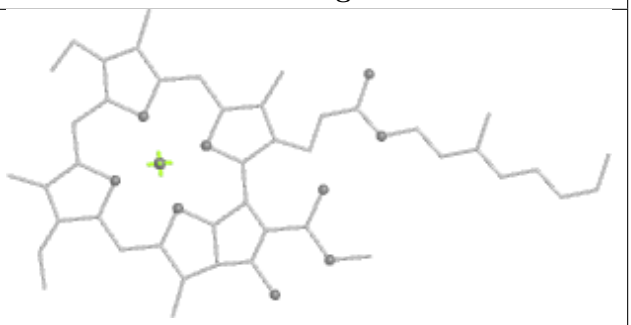
Bond lengths



Bond angles

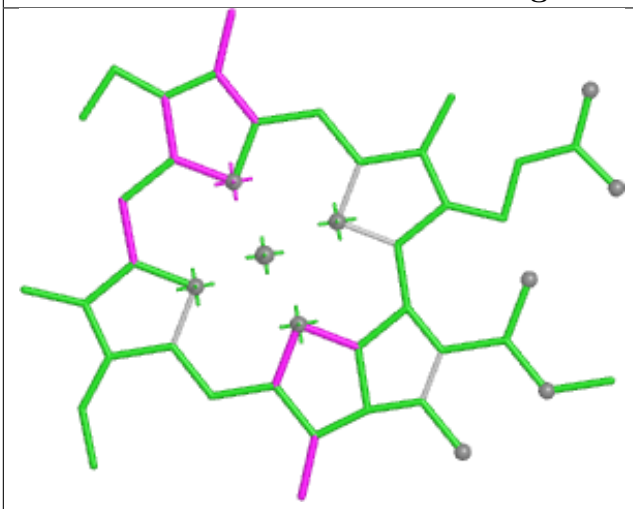


Torsions

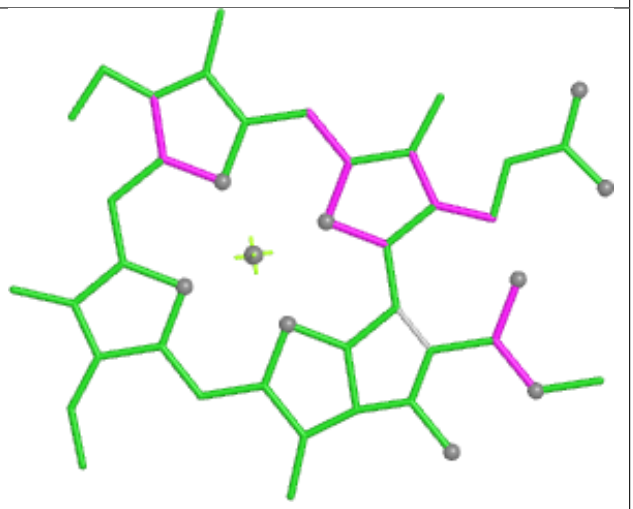


Rings

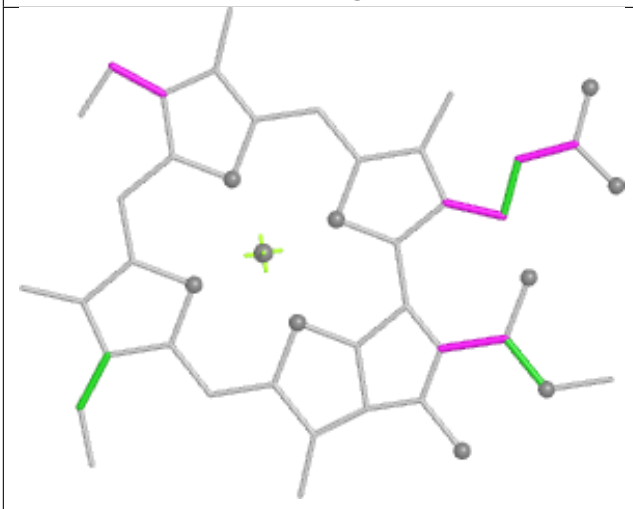
Ligand CLA t 516



Bond lengths



Bond angles

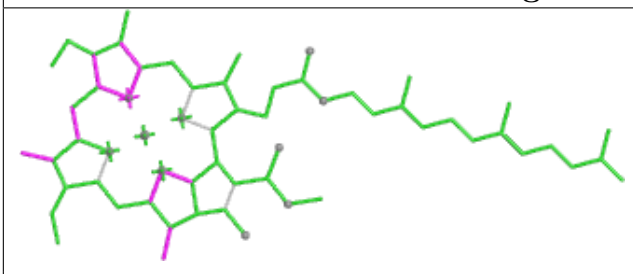


Torsions

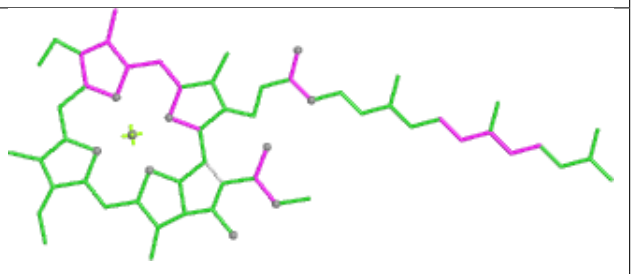


Rings

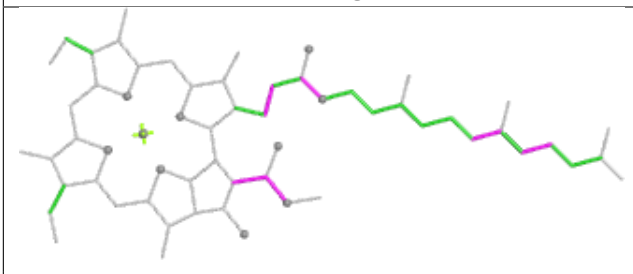
Ligand CLA f 1201



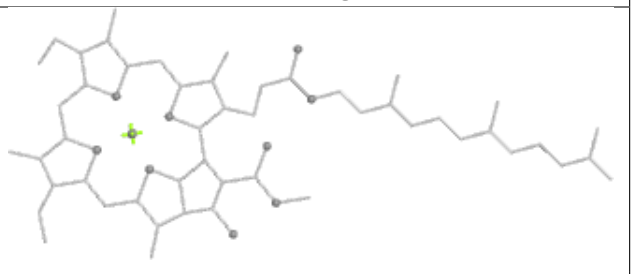
Bond lengths



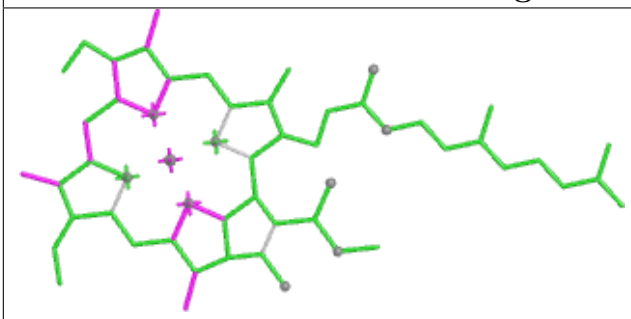
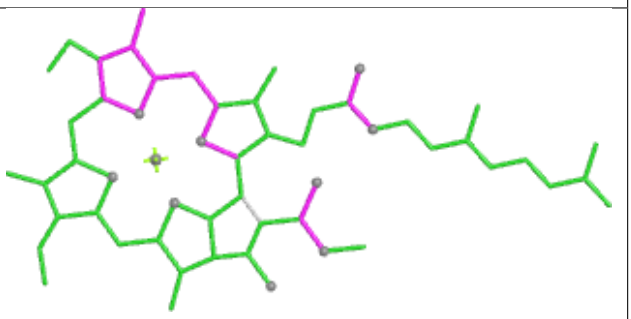
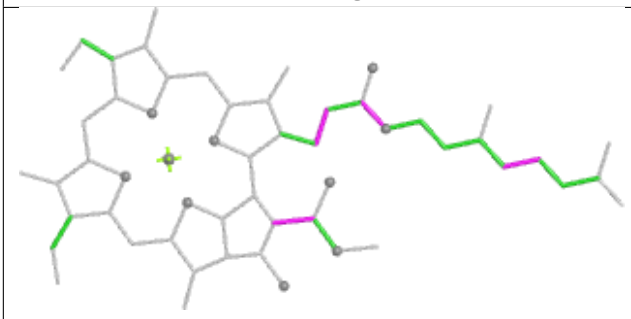
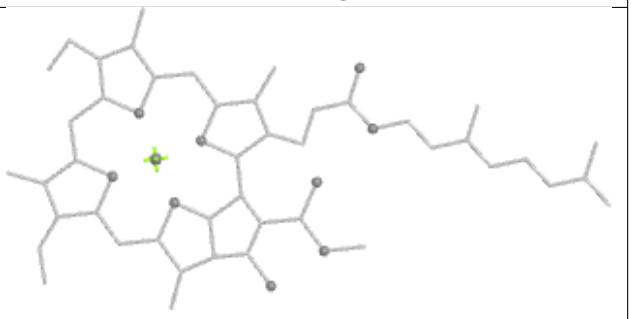
Bond angles

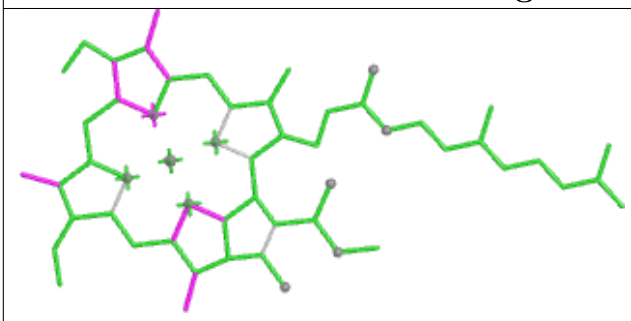
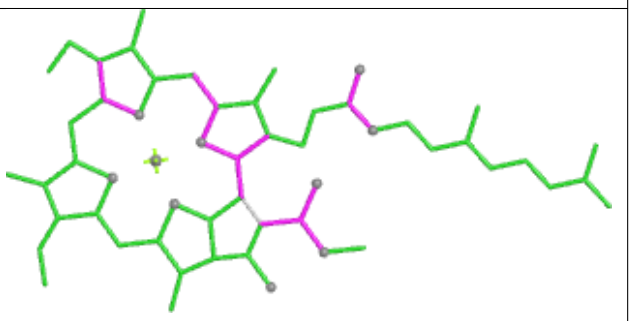
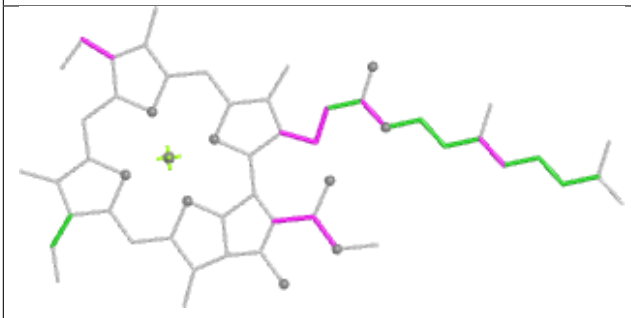
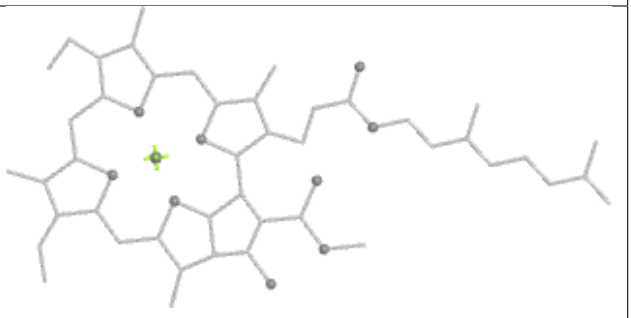


Torsions

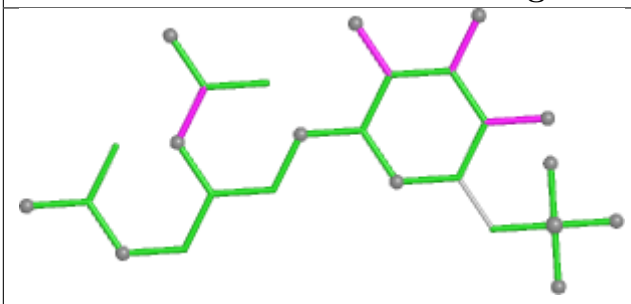


Rings

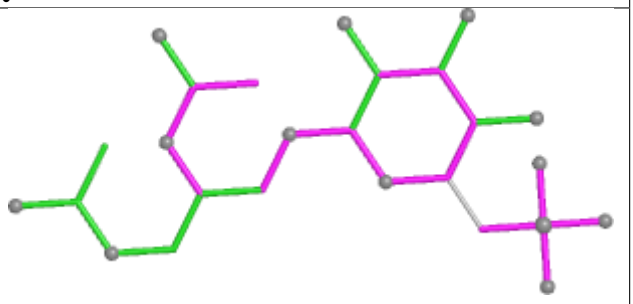
Ligand CLA H 1232	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA T 1302	
	
Bond lengths	Bond angles
	
Torsions	Rings

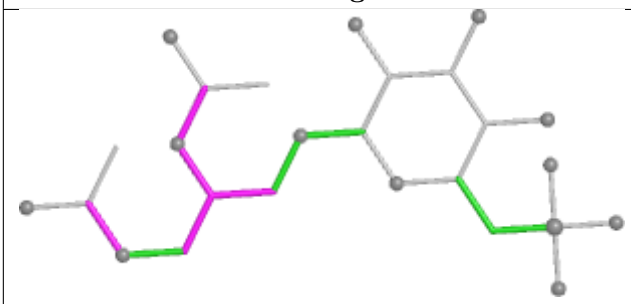
Ligand SQD v 822



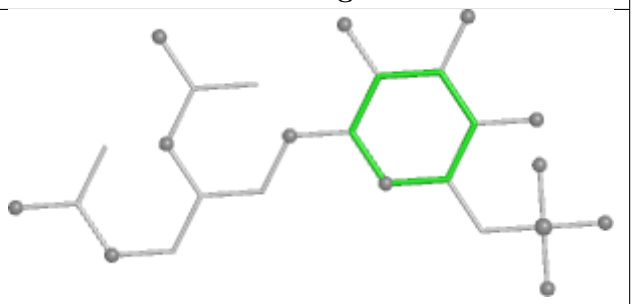
Bond lengths



Bond angles

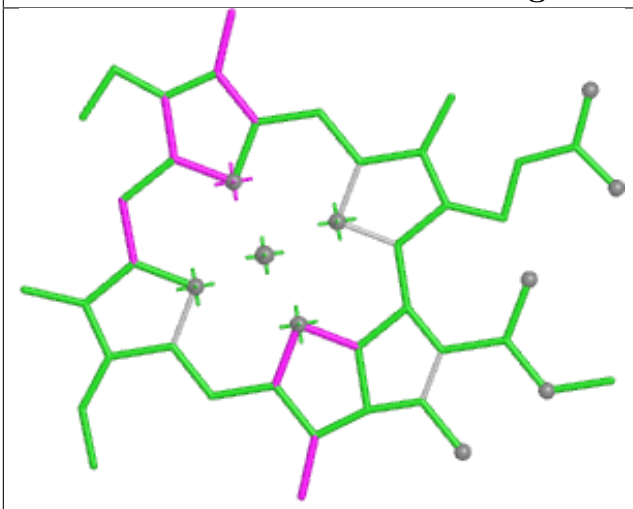


Torsions

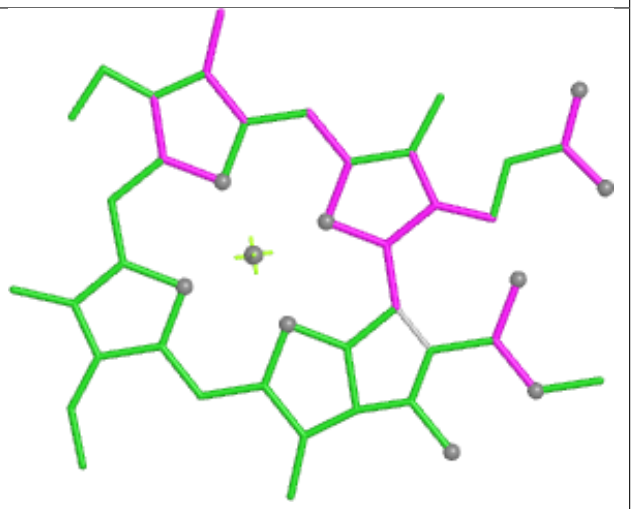


Rings

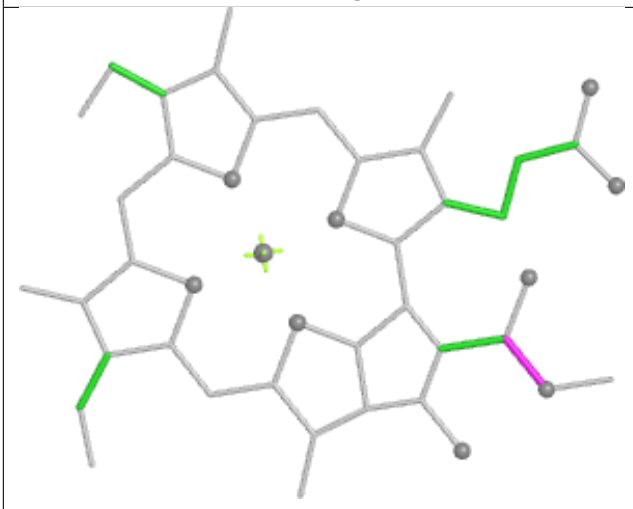
Ligand CLA a 511



Bond lengths



Bond angles

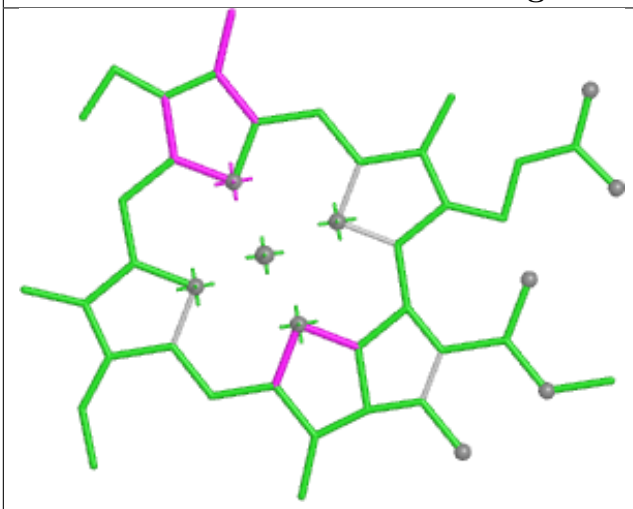


Torsions

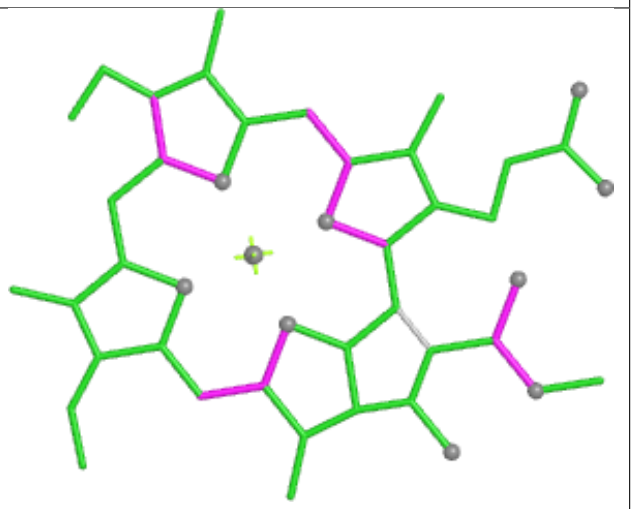


Rings

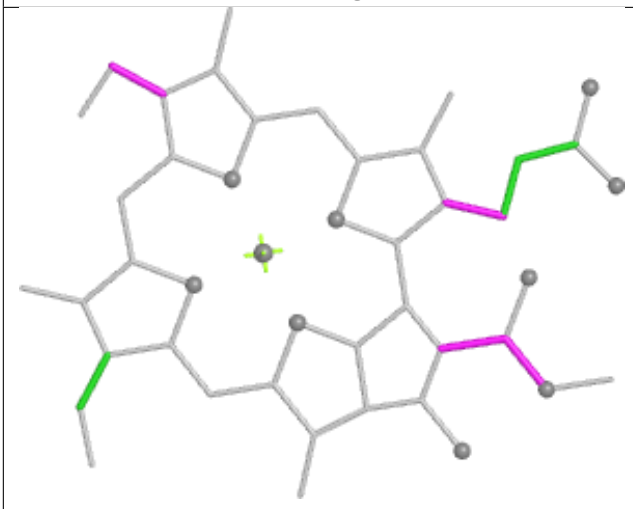
Ligand CLA b 504



Bond lengths



Bond angles

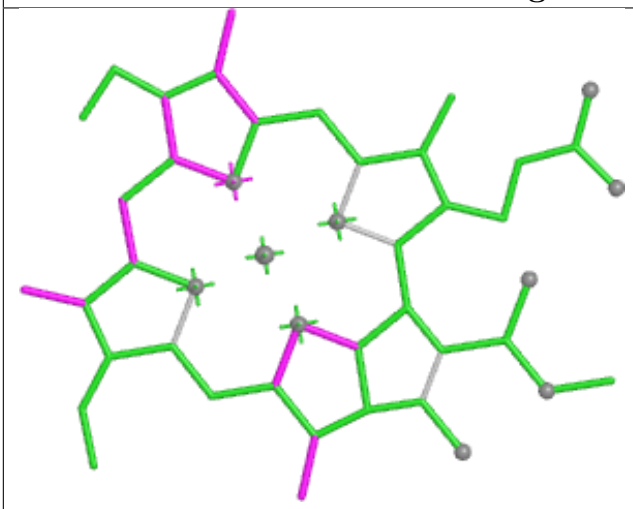


Torsions

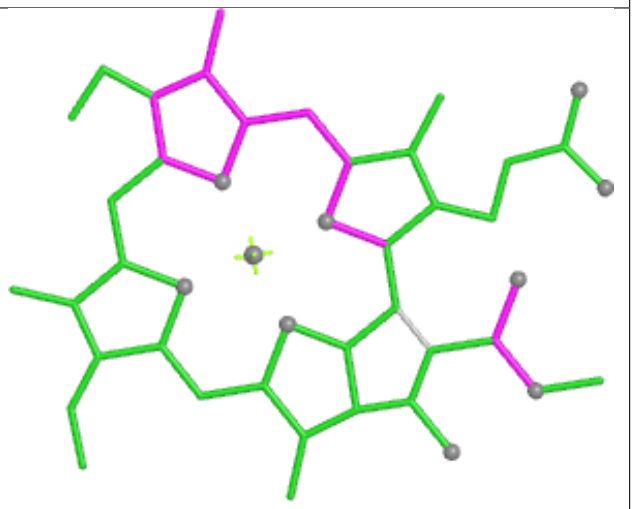


Rings

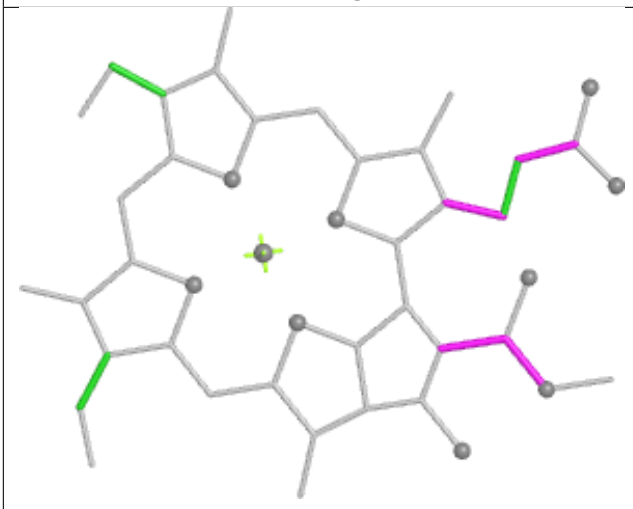
Ligand CLA 3 506



Bond lengths



Bond angles

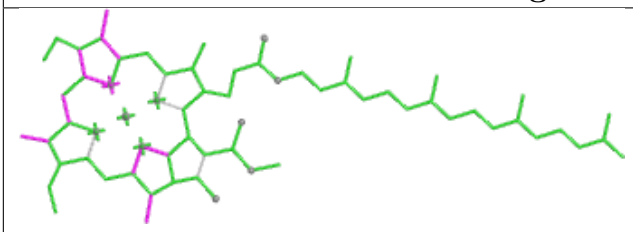


Torsions

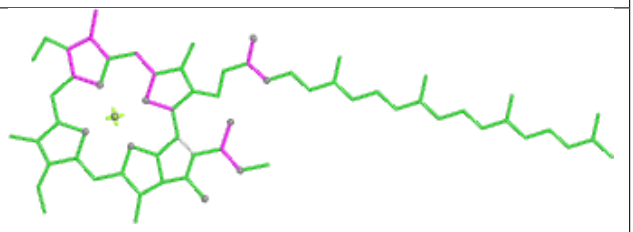


Rings

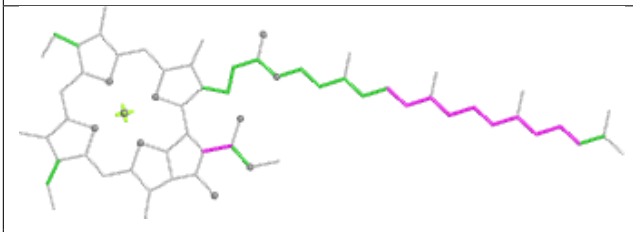
Ligand CLA c 509



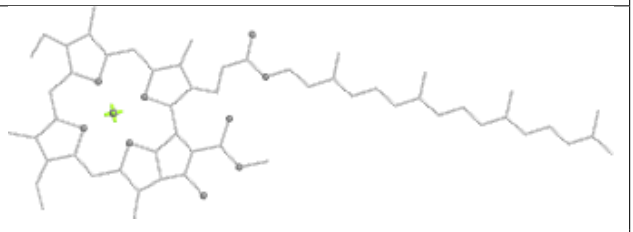
Bond lengths



Bond angles

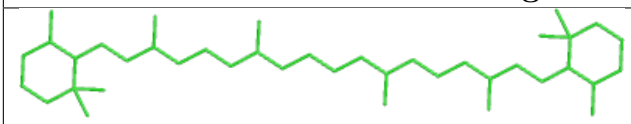


Torsions

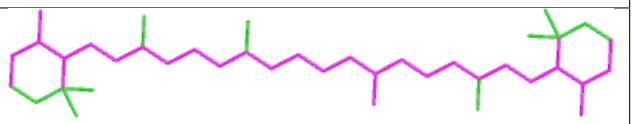


Rings

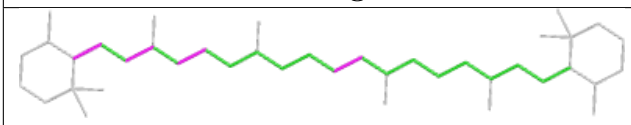
Ligand BCR Y 522



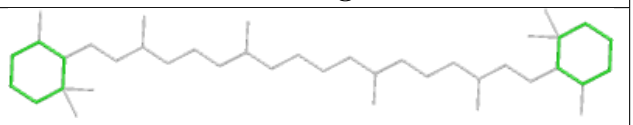
Bond lengths



Bond angles

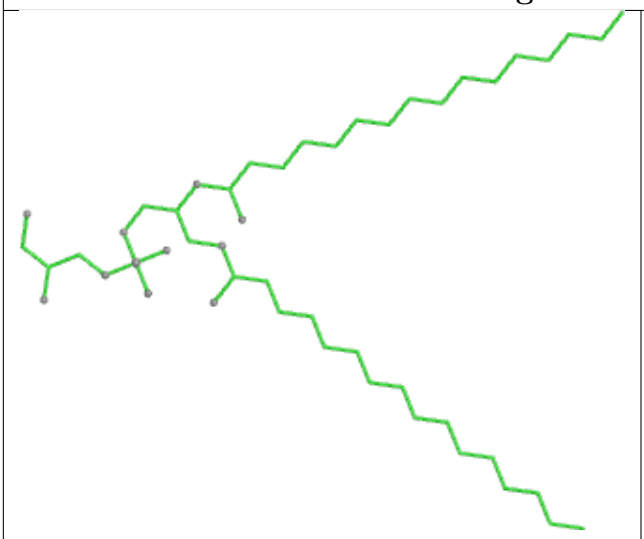


Torsions

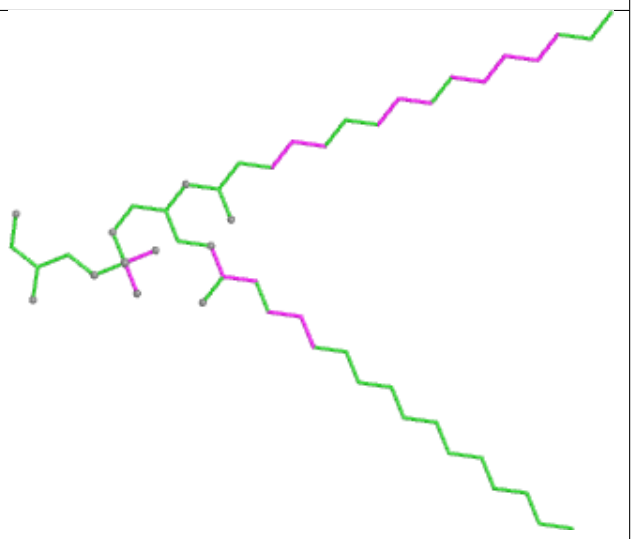


Rings

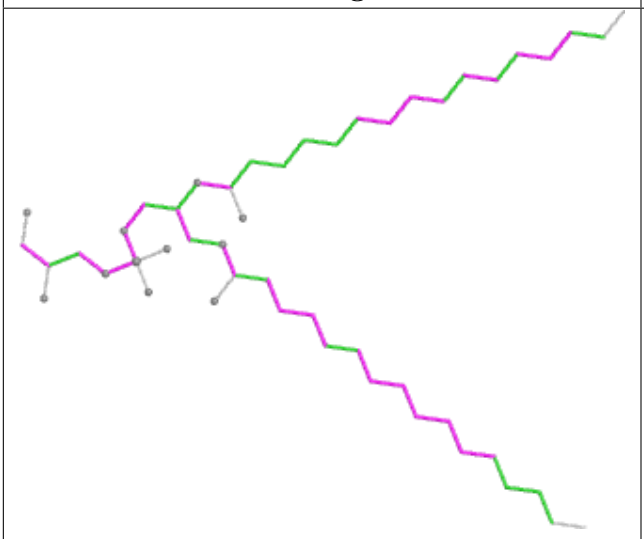
Ligand LHG L 5221



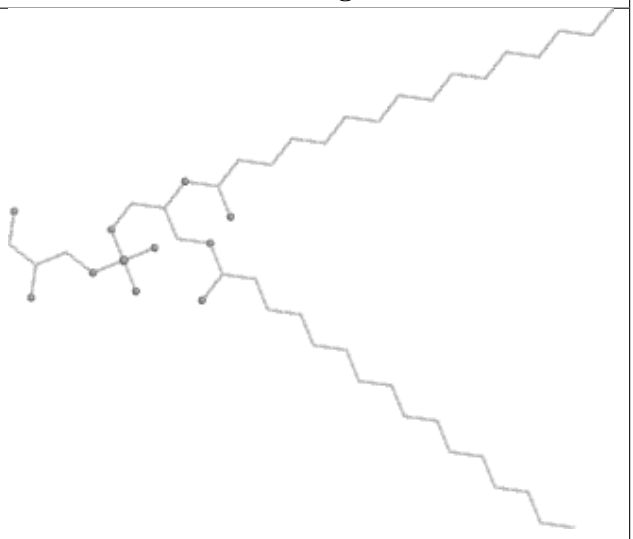
Bond lengths



Bond angles

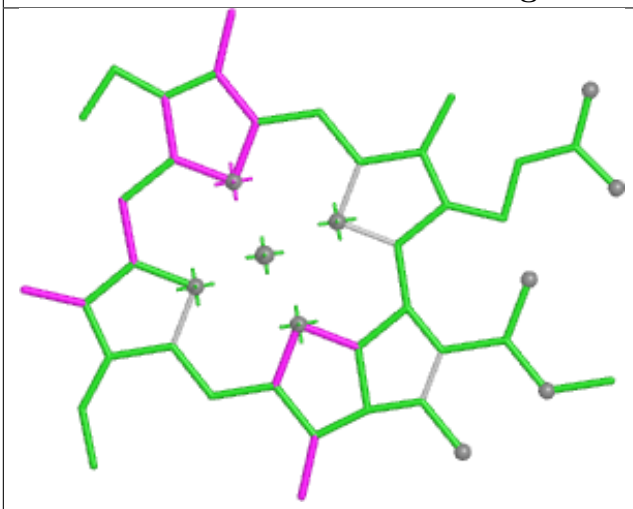


Torsions

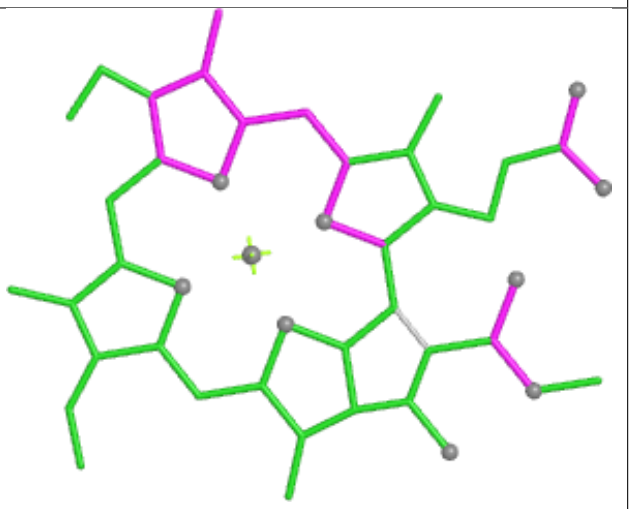


Rings

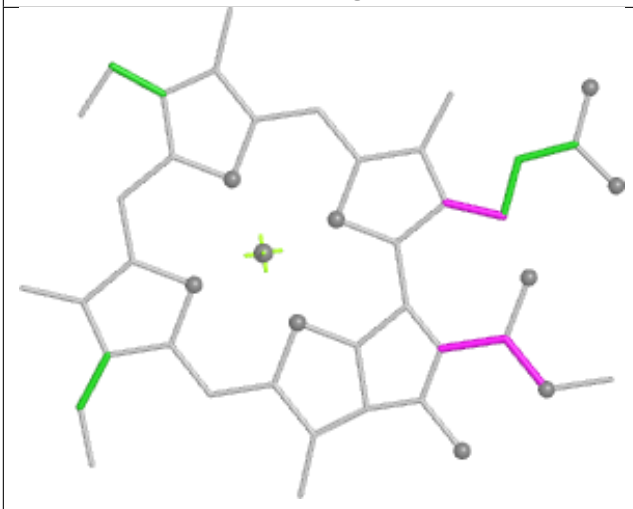
Ligand CLA e 1113



Bond lengths



Bond angles

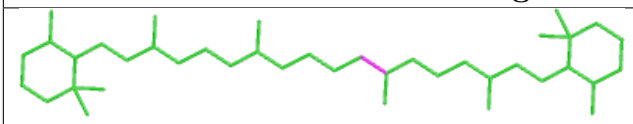


Torsions

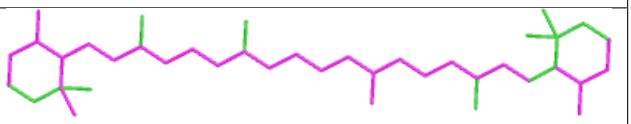


Rings

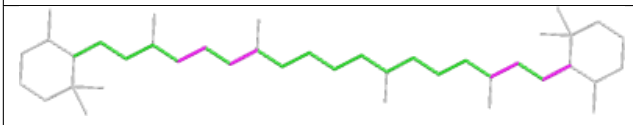
Ligand BCR H 4010



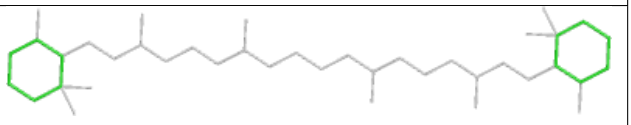
Bond lengths



Bond angles

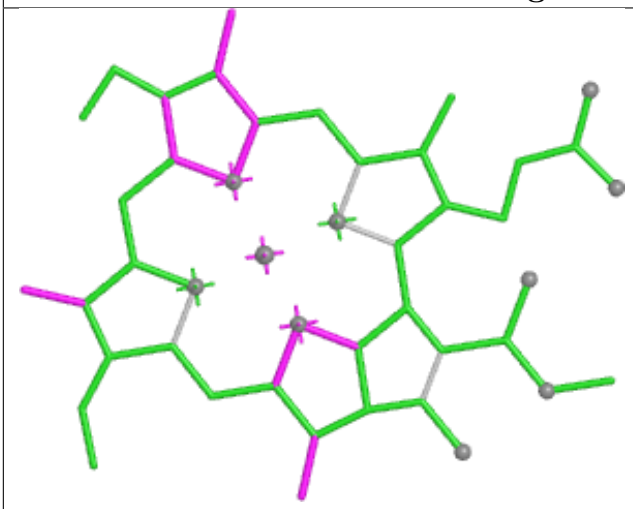


Torsions

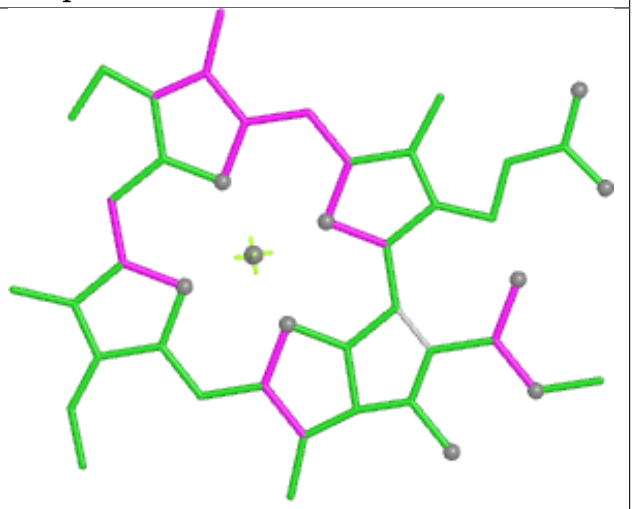


Rings

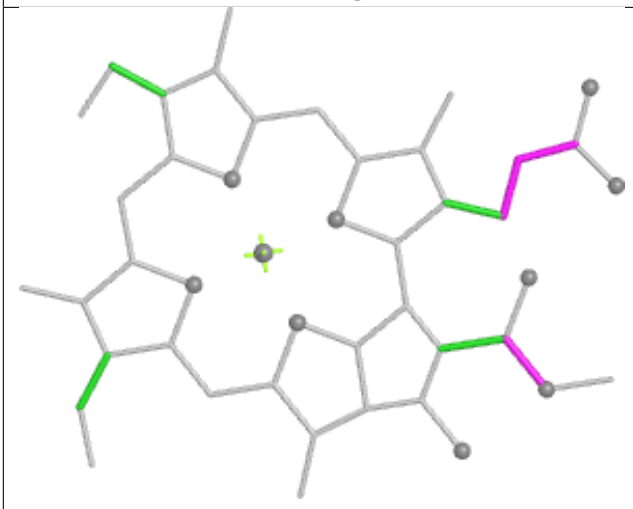
Ligand CLA q 508



Bond lengths



Bond angles

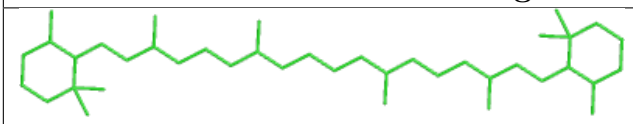


Torsions

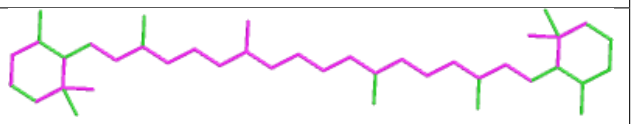


Rings

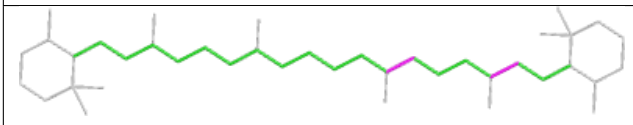
Ligand BCR T 4013



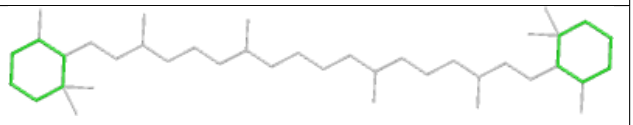
Bond lengths



Bond angles

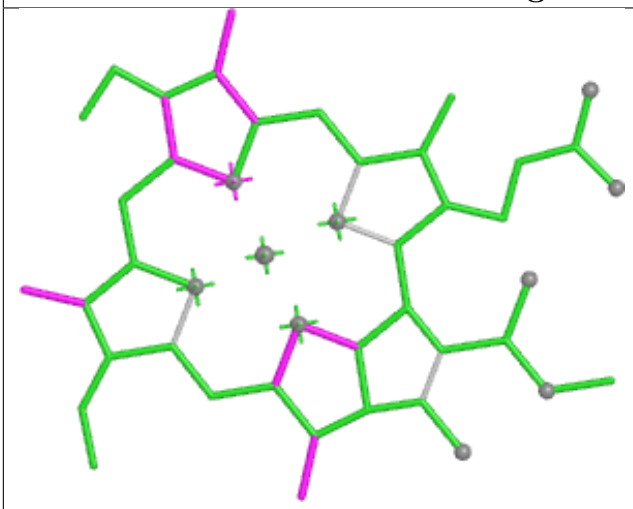


Torsions

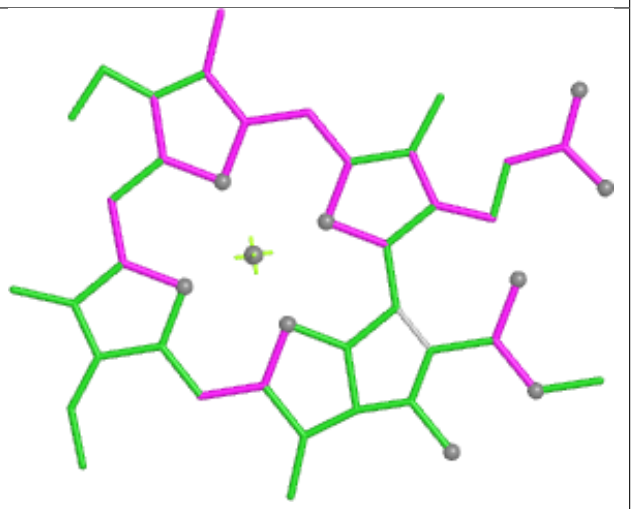


Rings

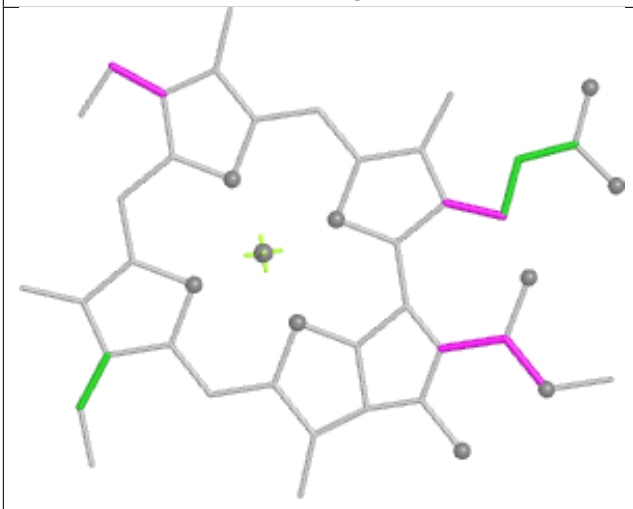
Ligand CLA d 508



Bond lengths



Bond angles

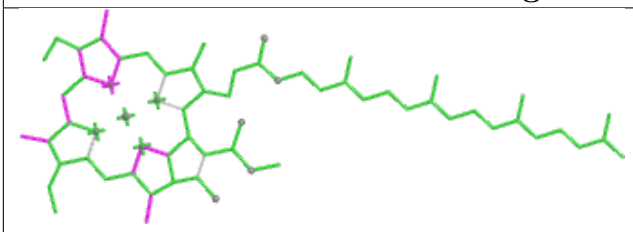


Torsions

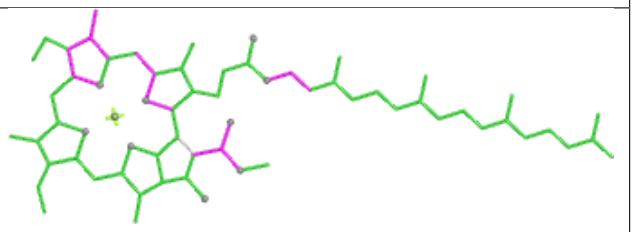


Rings

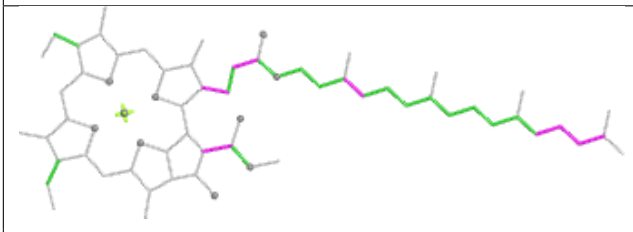
Ligand CLA f 1202



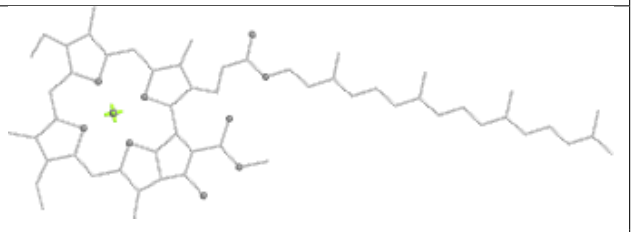
Bond lengths



Bond angles

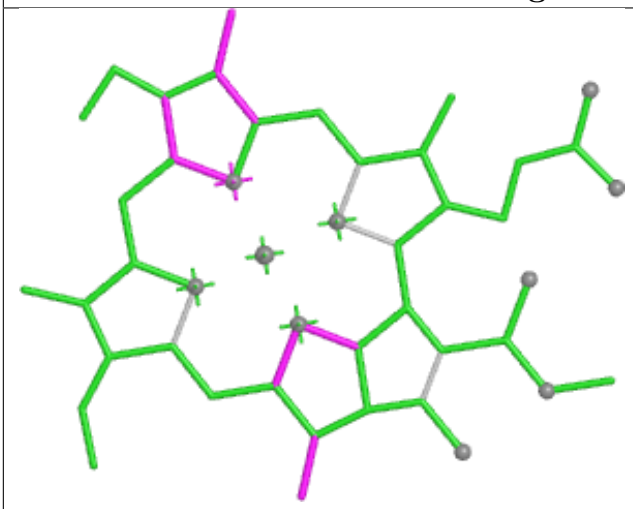


Torsions

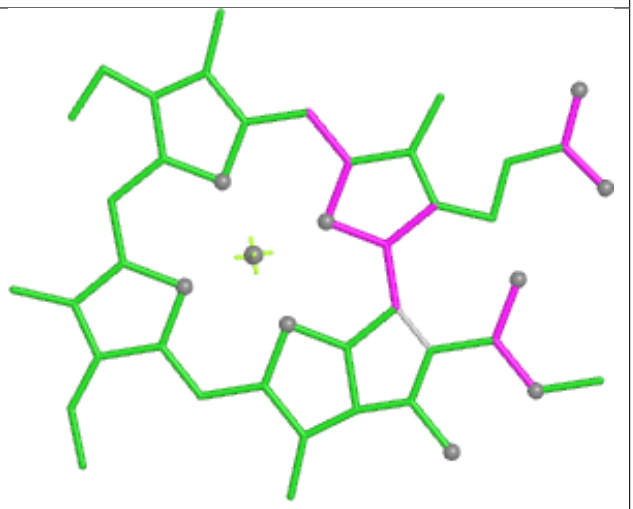


Rings

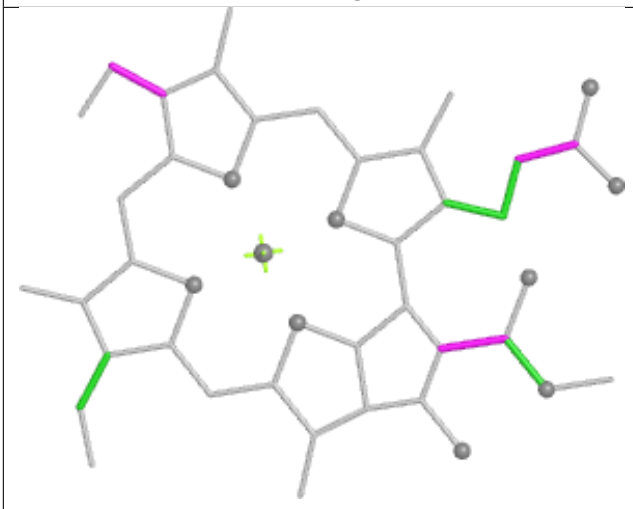
Ligand CLA a 507



Bond lengths



Bond angles

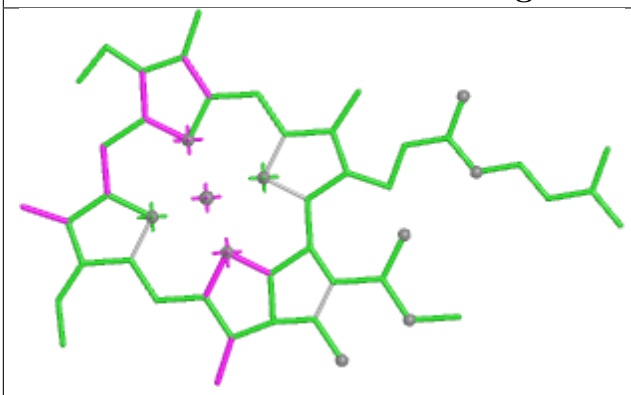


Torsions

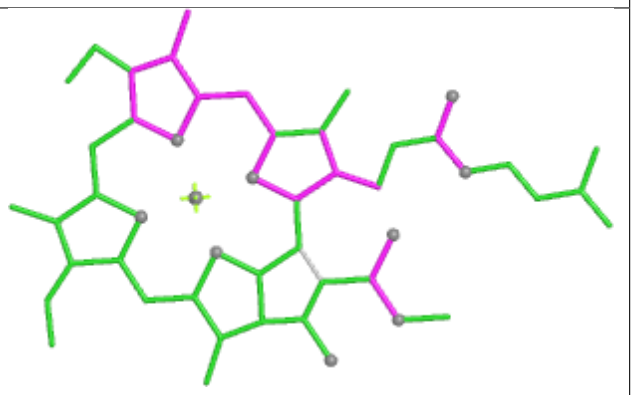


Rings

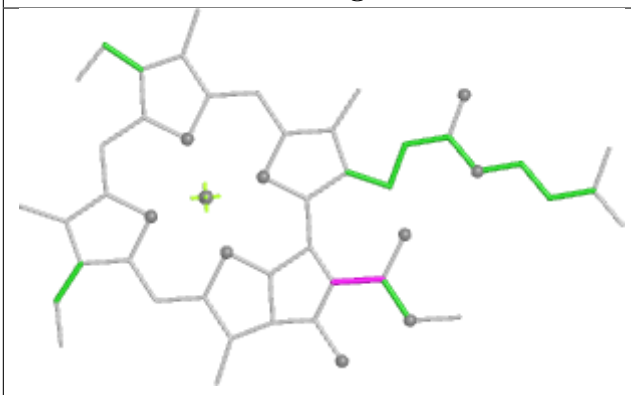
Ligand CLA B 1222



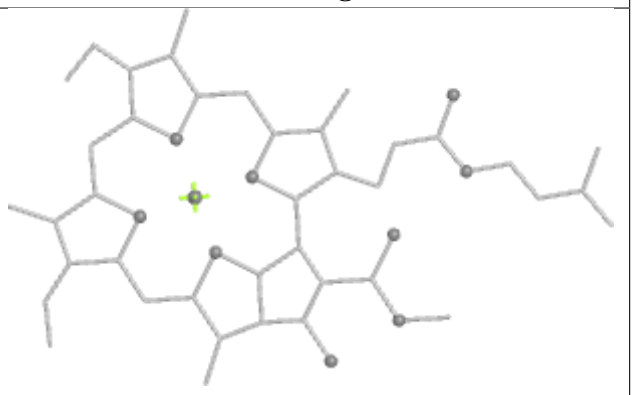
Bond lengths



Bond angles

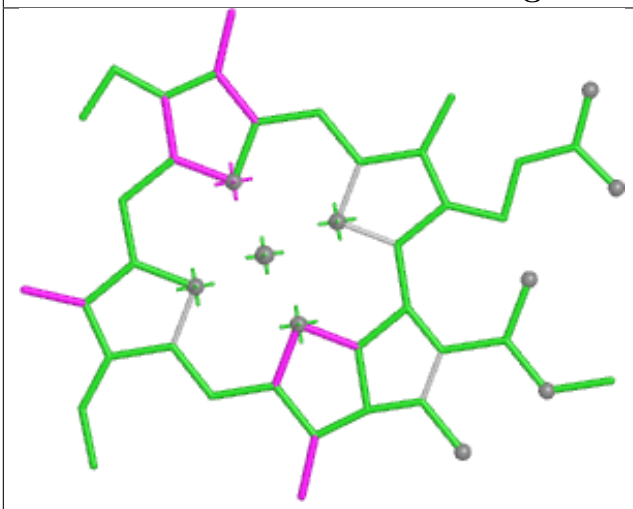


Torsions

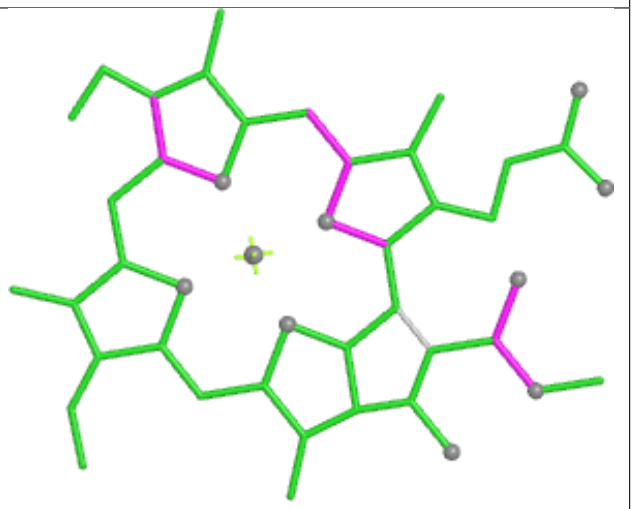


Rings

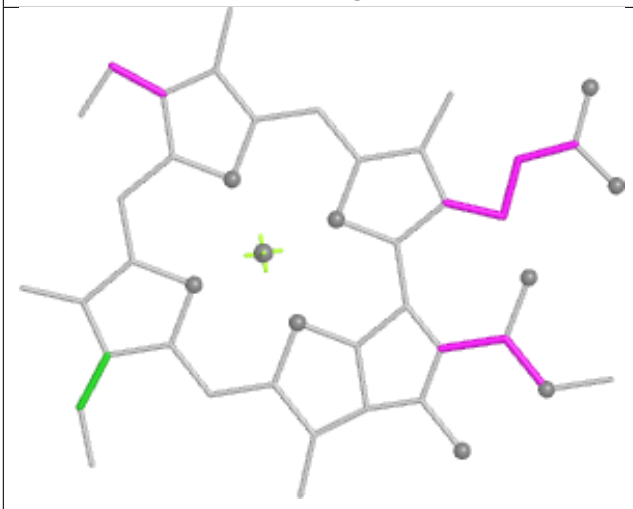
Ligand CLA Y 501



Bond lengths



Bond angles

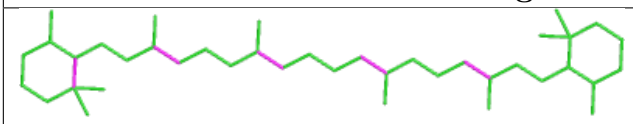


Torsions

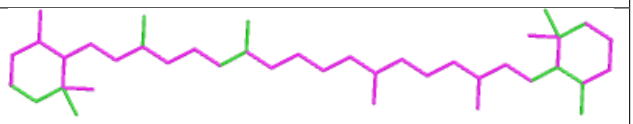


Rings

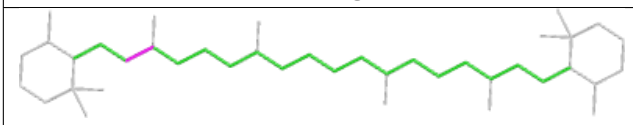
Ligand BCR L 4219



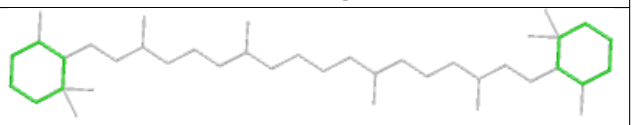
Bond lengths



Bond angles

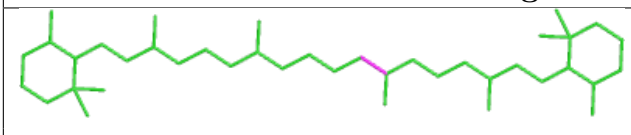


Torsions

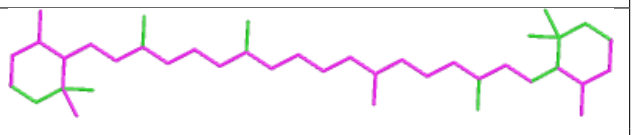


Rings

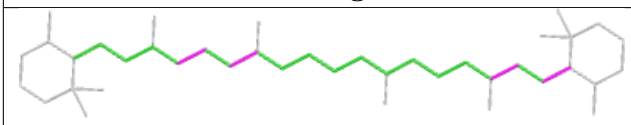
Ligand BCR f 4010



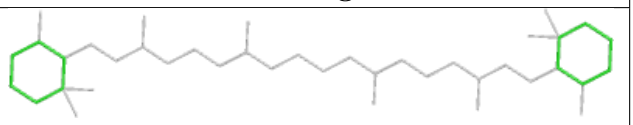
Bond lengths



Bond angles

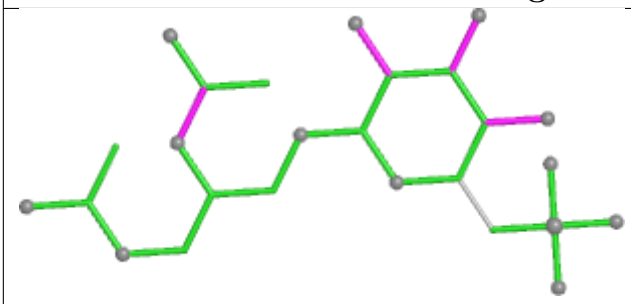


Torsions

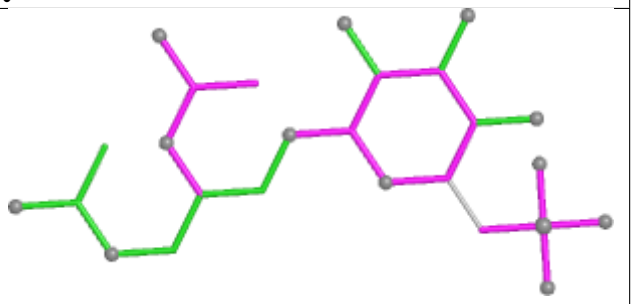


Rings

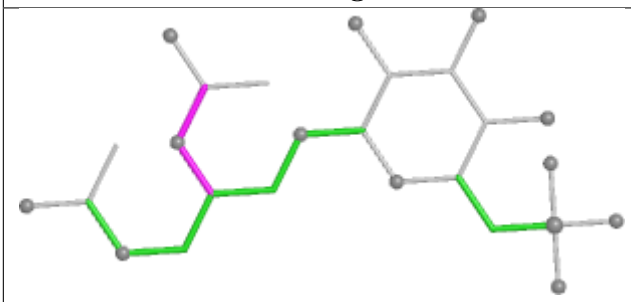
Ligand SQD 5 822



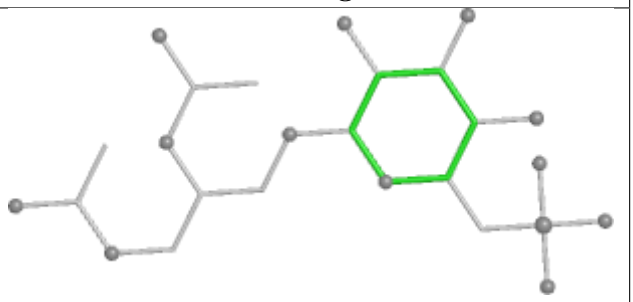
Bond lengths



Bond angles

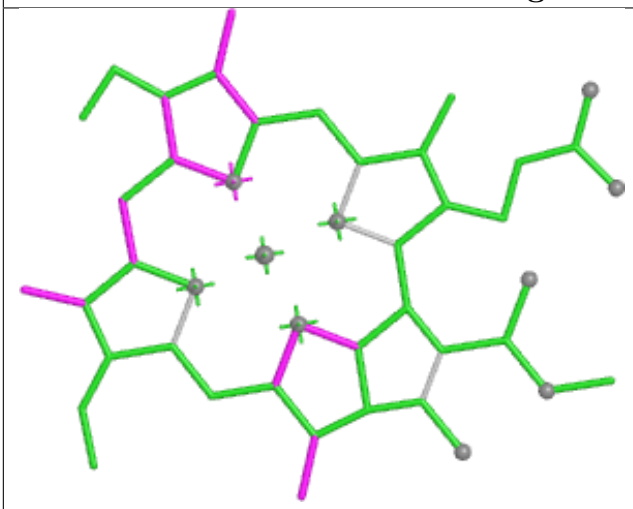


Torsions

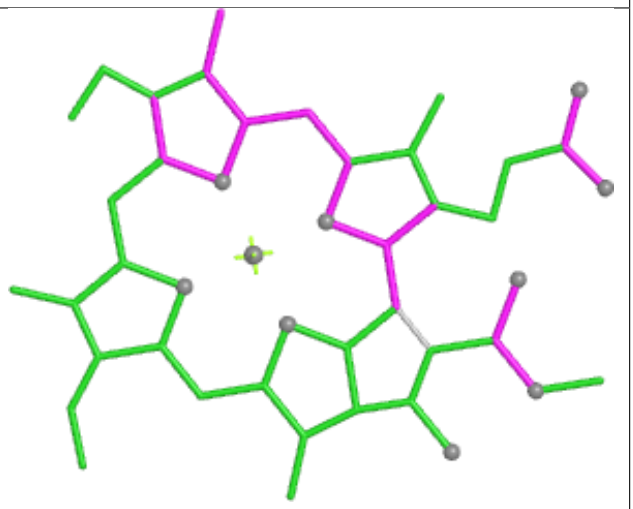


Rings

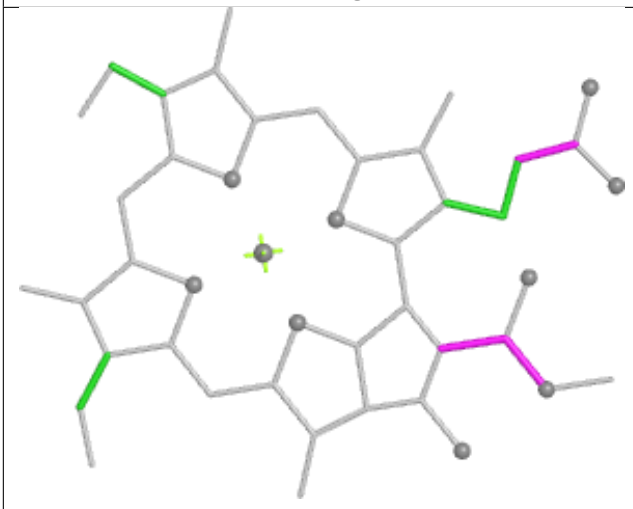
Ligand CLA b 509



Bond lengths



Bond angles

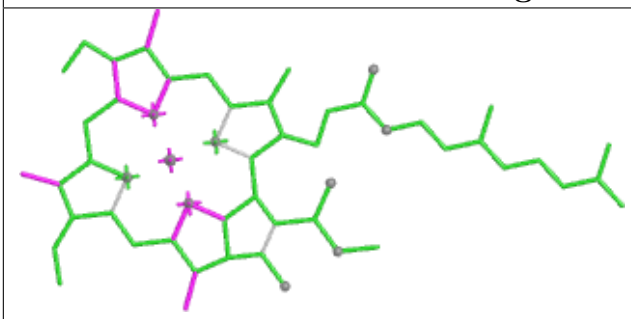


Torsions

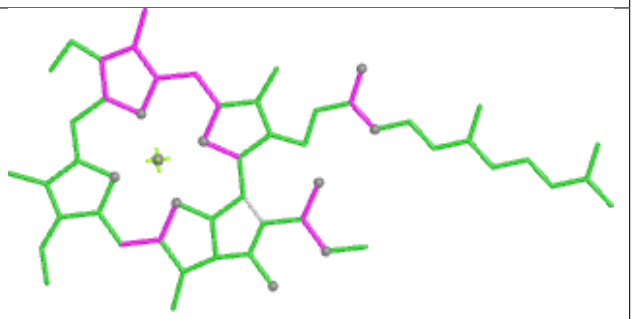


Rings

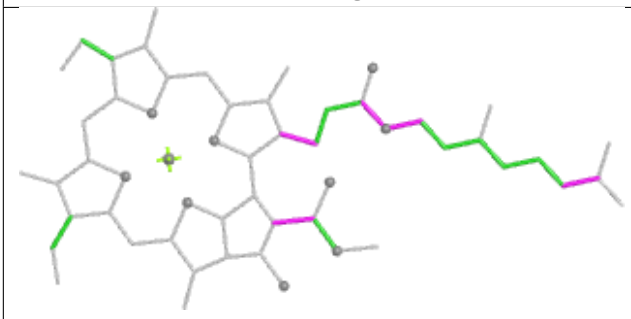
Ligand CLA A 1105



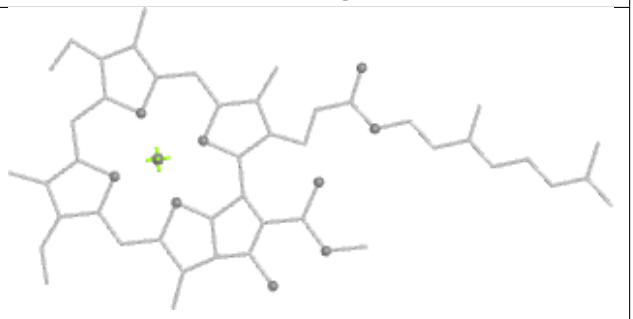
Bond lengths



Bond angles

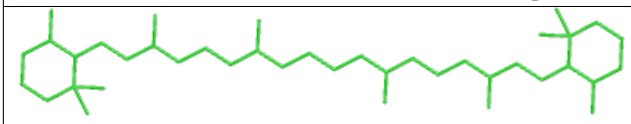


Torsions

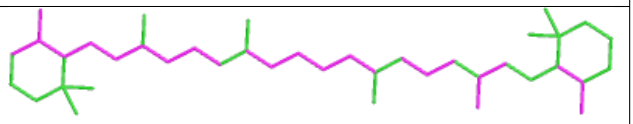


Rings

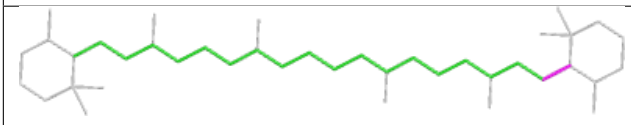
Ligand BCR 5 524



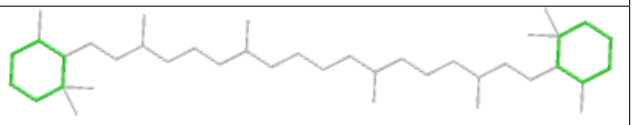
Bond lengths



Bond angles

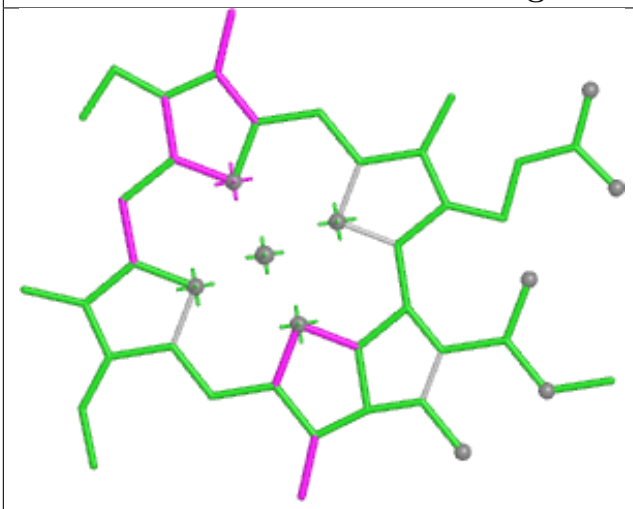


Torsions

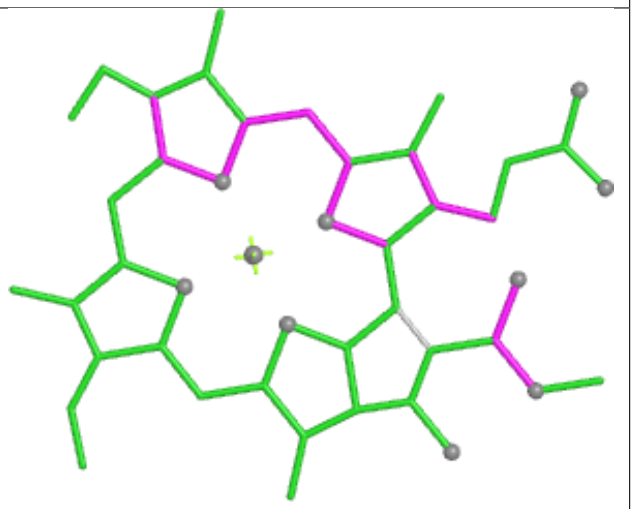


Rings

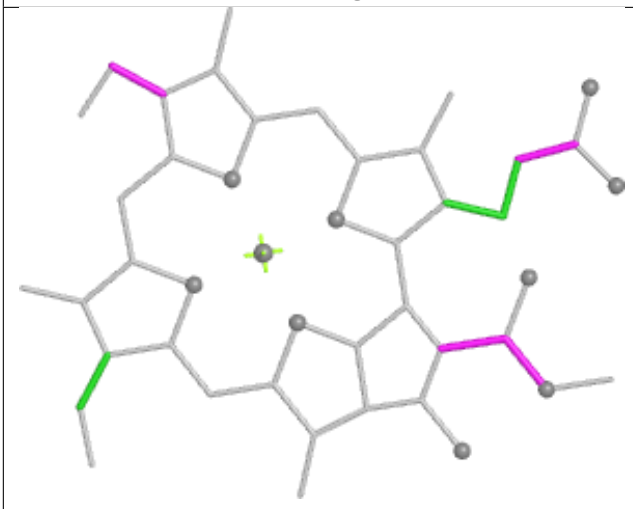
Ligand CLA u 512



Bond lengths



Bond angles

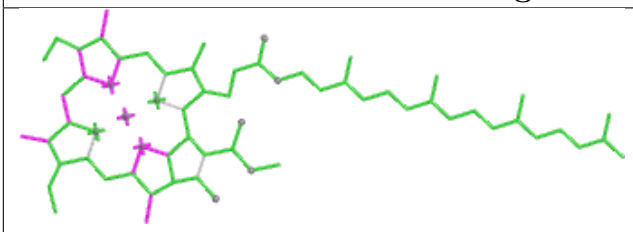


Torsions

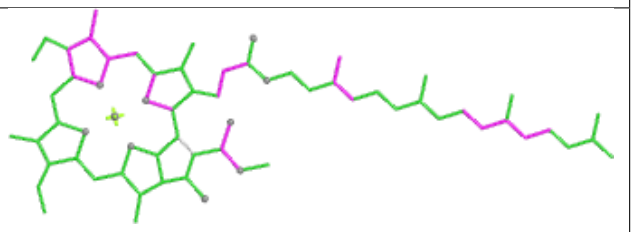


Rings

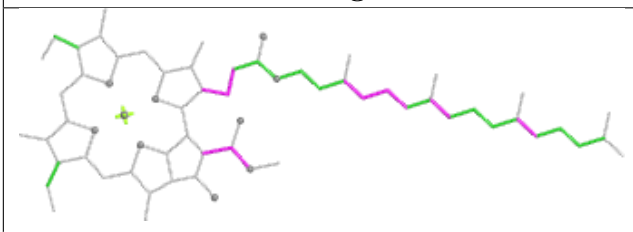
Ligand CLA H 1012



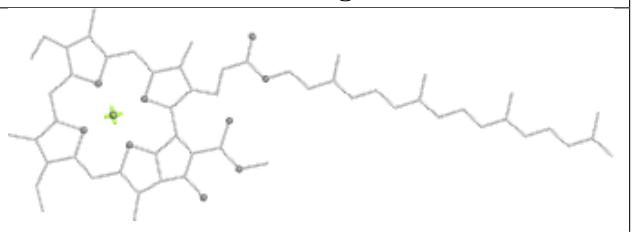
Bond lengths



Bond angles

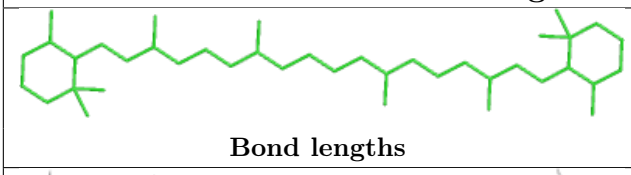


Torsions

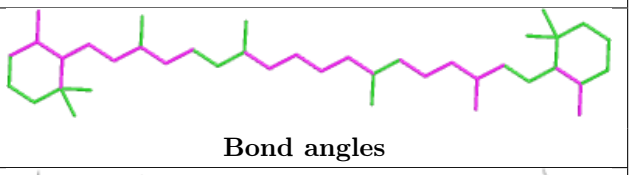


Rings

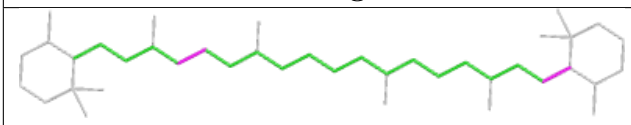
Ligand BCR r 524



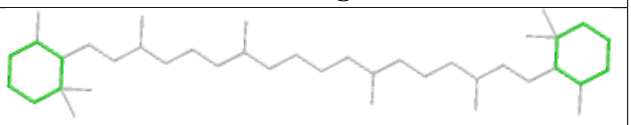
Bond lengths



Bond angles

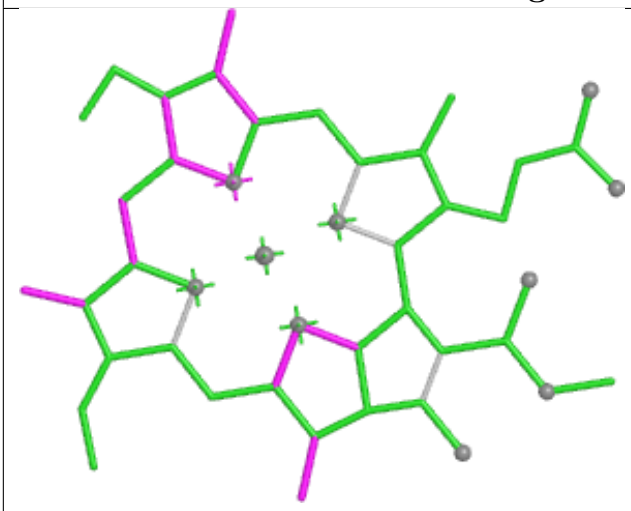


Torsions

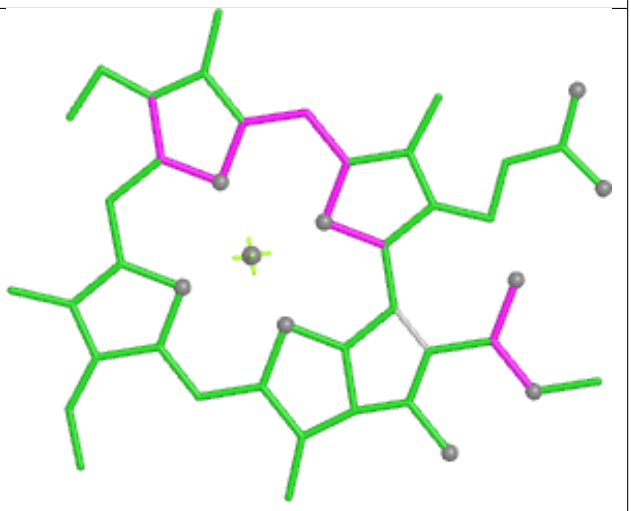


Rings

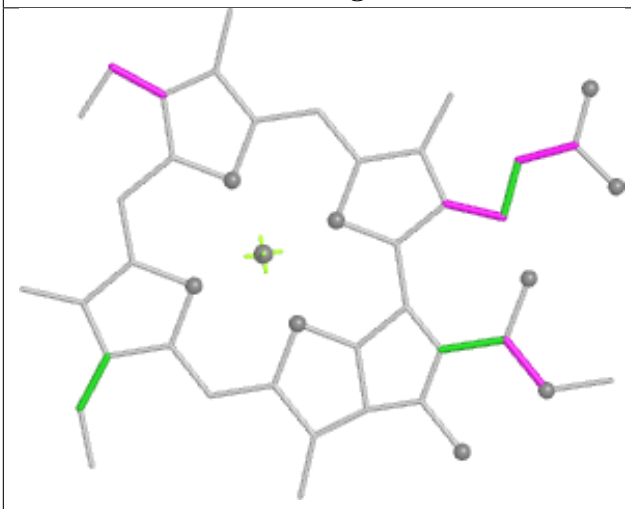
Ligand CLA 5 513



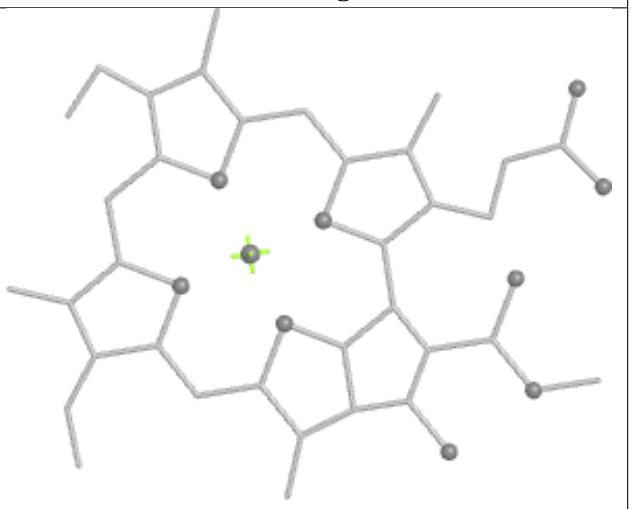
Bond lengths



Bond angles

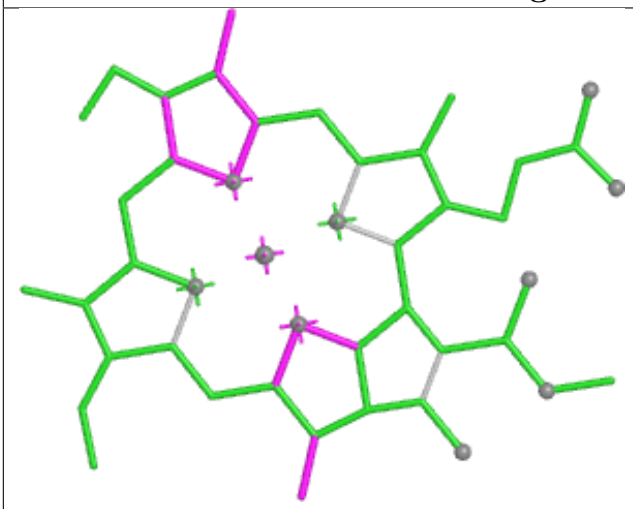


Torsions

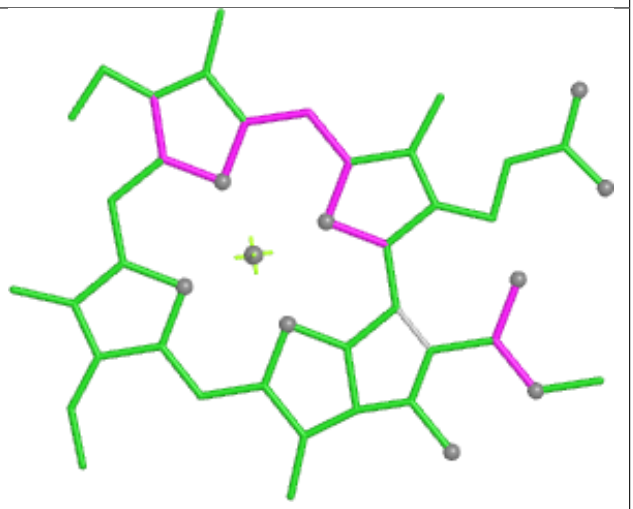


Rings

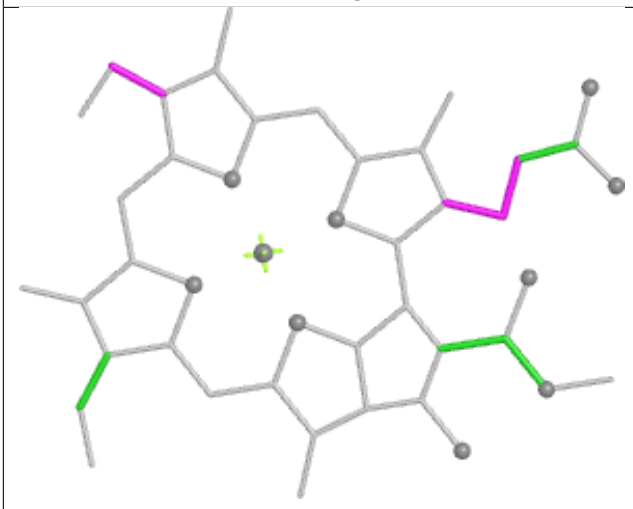
Ligand CLA s 512



Bond lengths



Bond angles

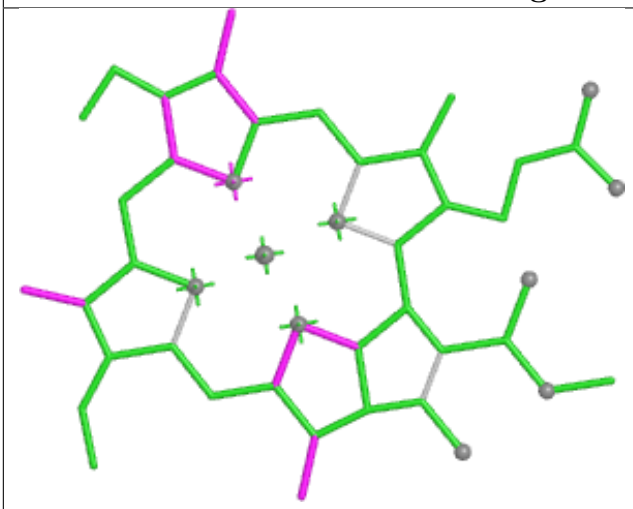


Torsions

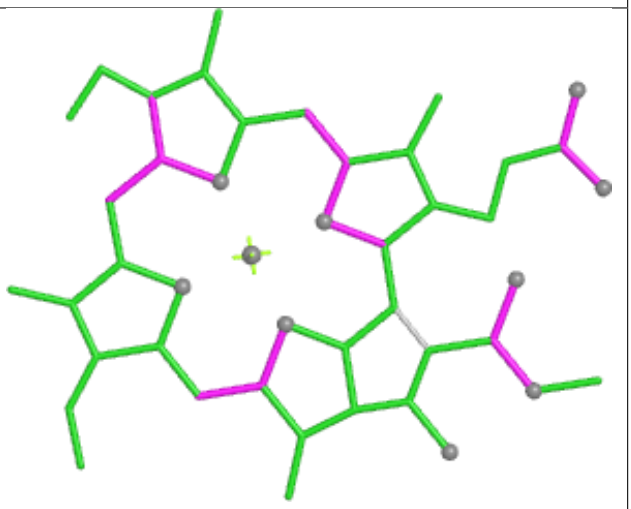


Rings

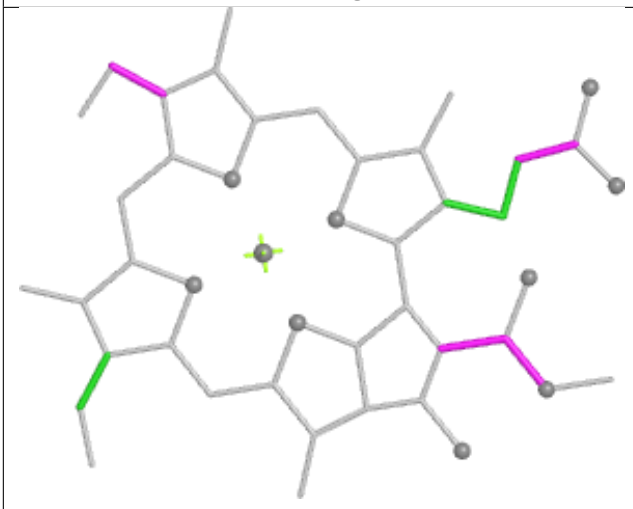
Ligand CLA r 519



Bond lengths



Bond angles

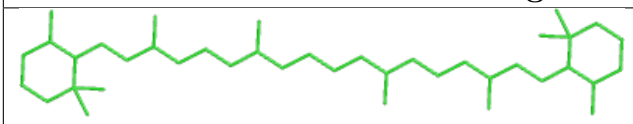


Torsions

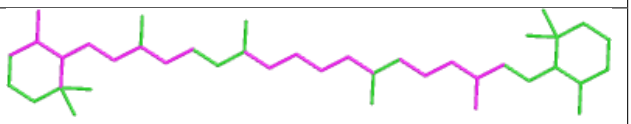


Rings

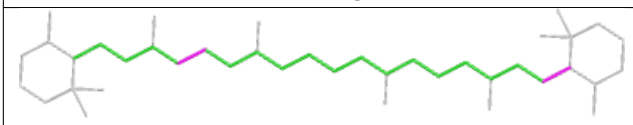
Ligand BCR 2 524



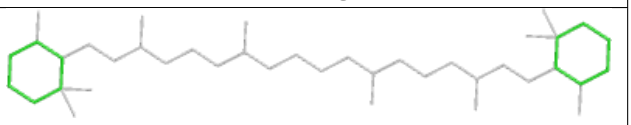
Bond lengths



Bond angles

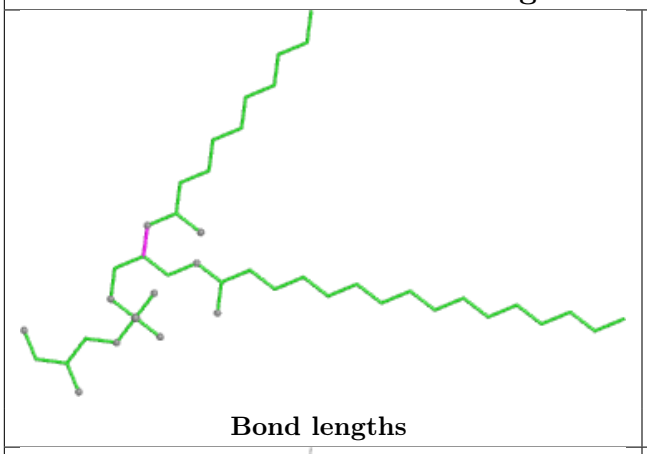


Torsions

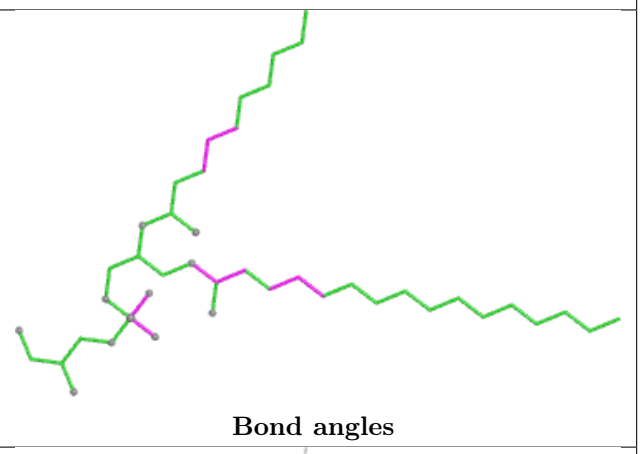


Rings

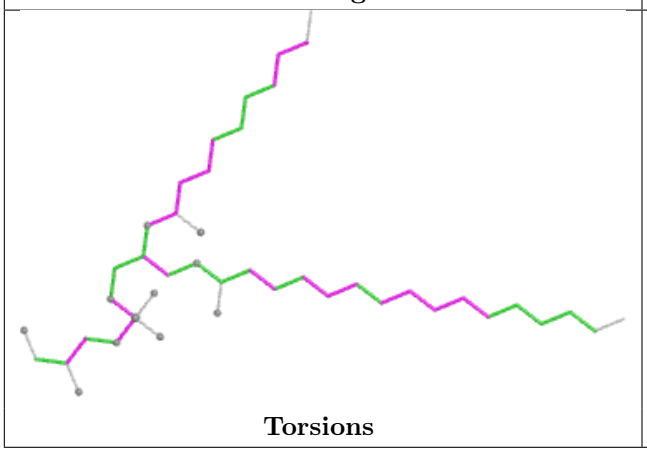
Ligand LHG e 5002



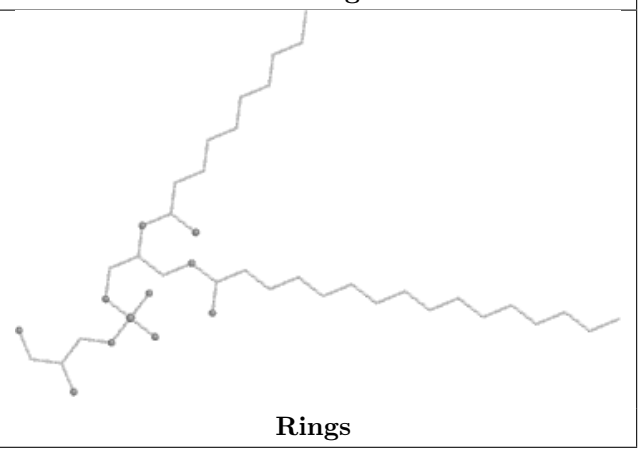
Bond lengths



Bond angles

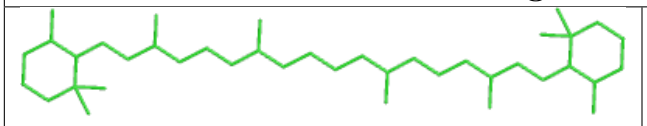


Torsions

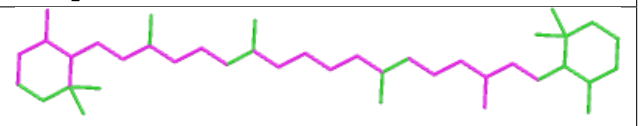


Rings

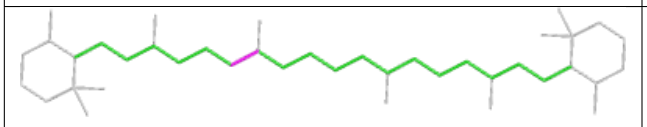
Ligand BCR q 524



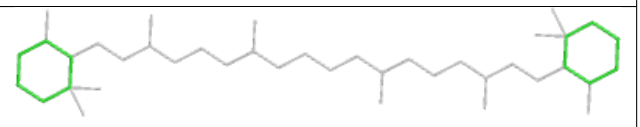
Bond lengths



Bond angles

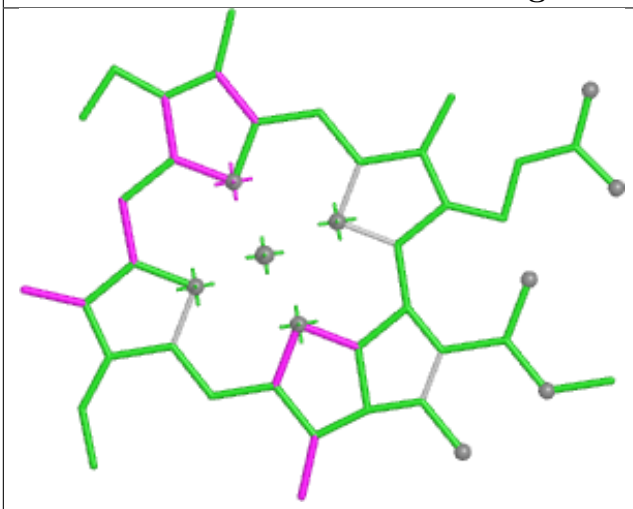


Torsions

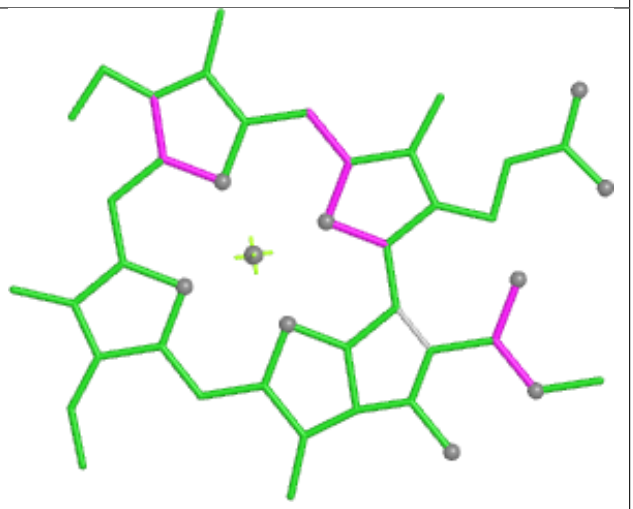


Rings

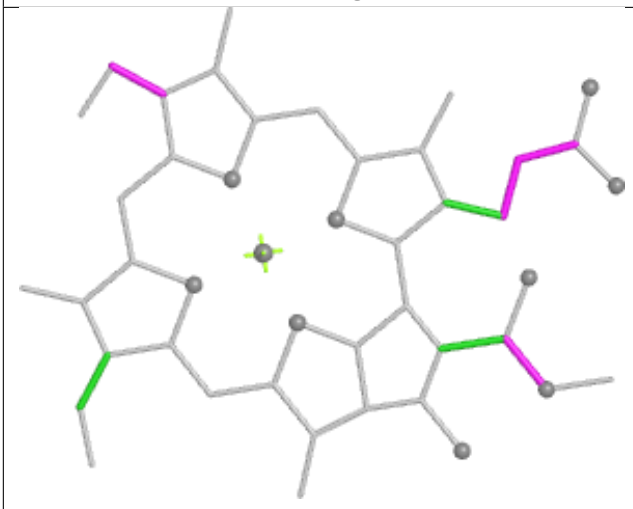
Ligand CLA 4 513



Bond lengths



Bond angles

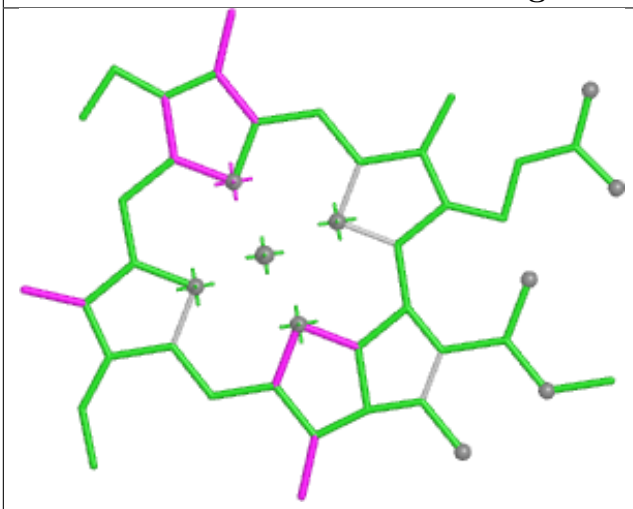


Torsions

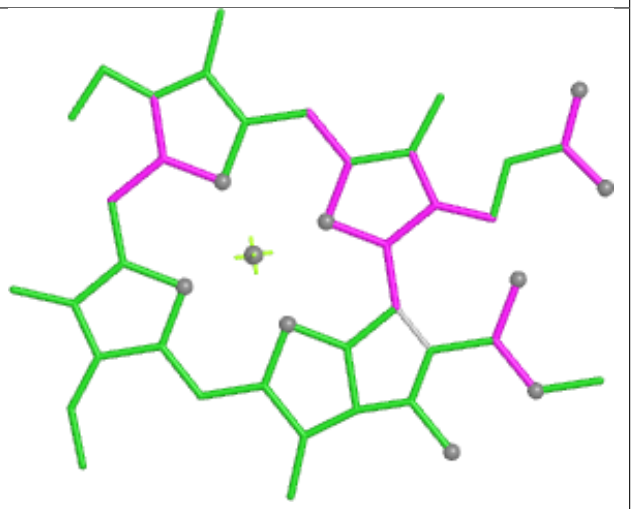


Rings

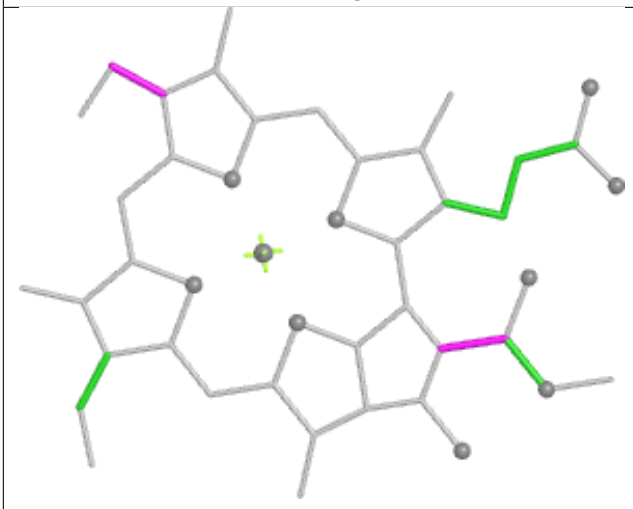
Ligand CLA 2 502



Bond lengths



Bond angles

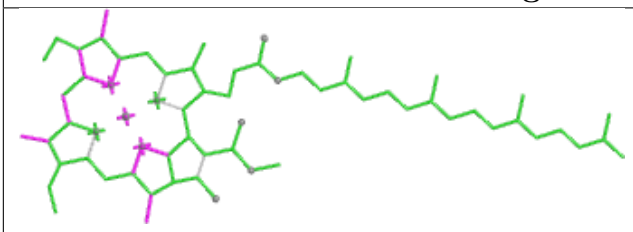


Torsions

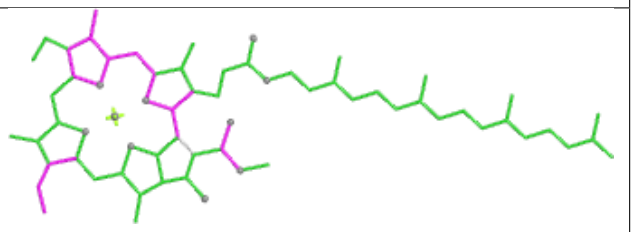


Rings

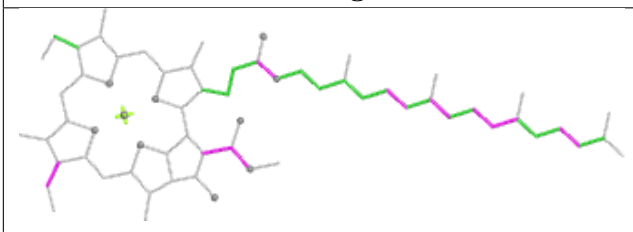
Ligand CLA f 1234



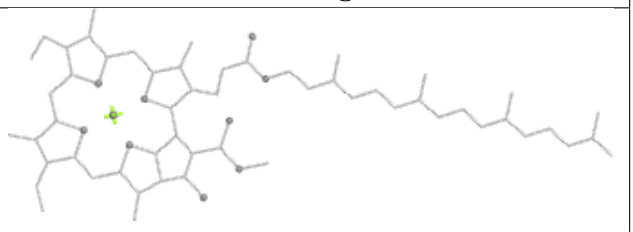
Bond lengths



Bond angles

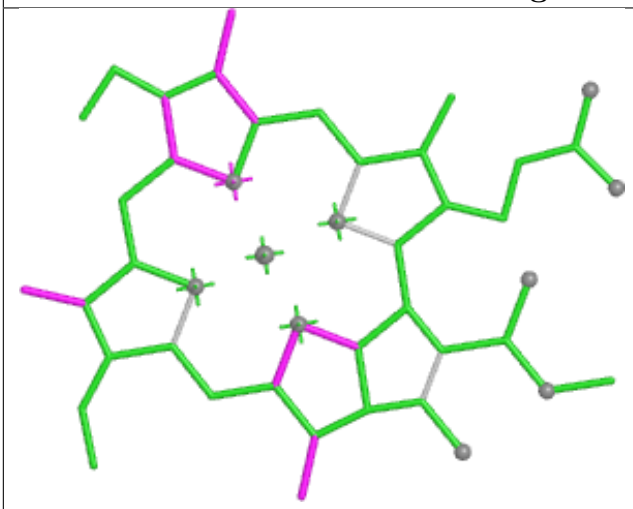


Torsions

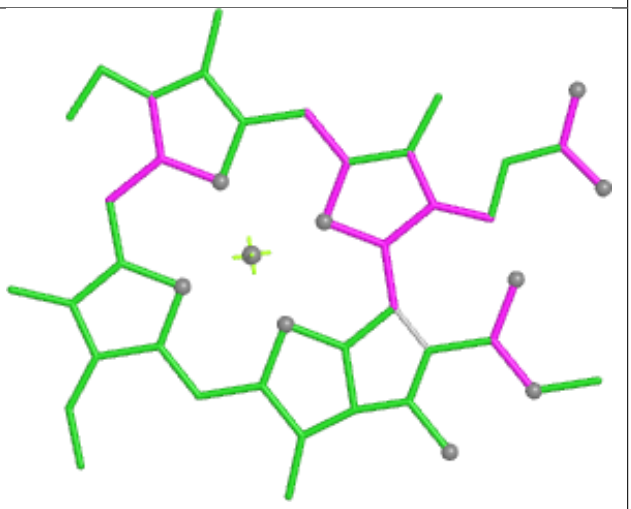


Rings

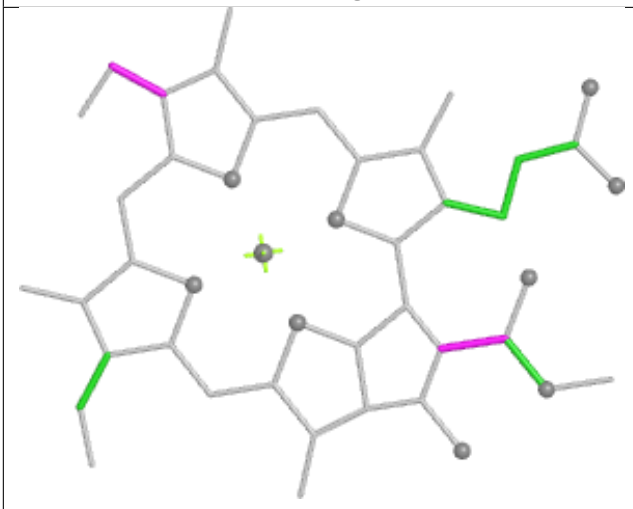
Ligand CLA s 502



Bond lengths



Bond angles

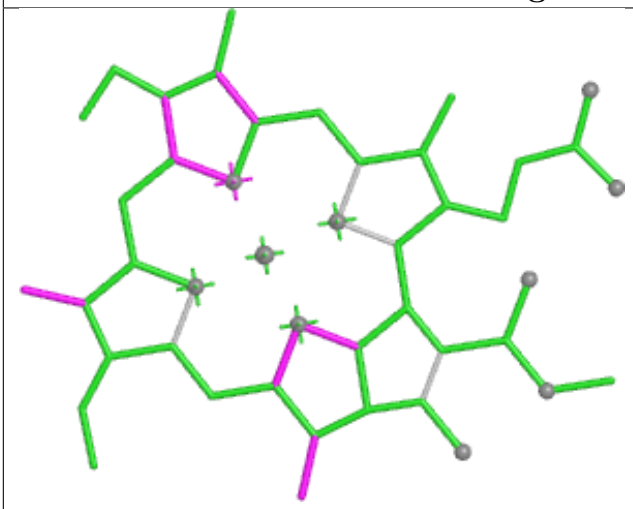


Torsions

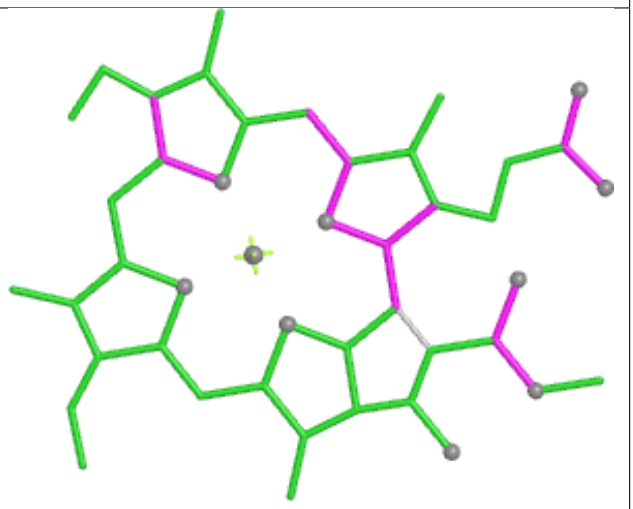


Rings

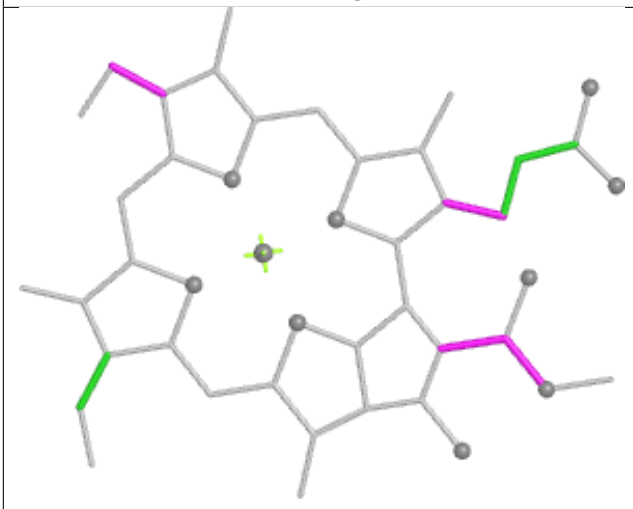
Ligand CLA 4 517



Bond lengths



Bond angles

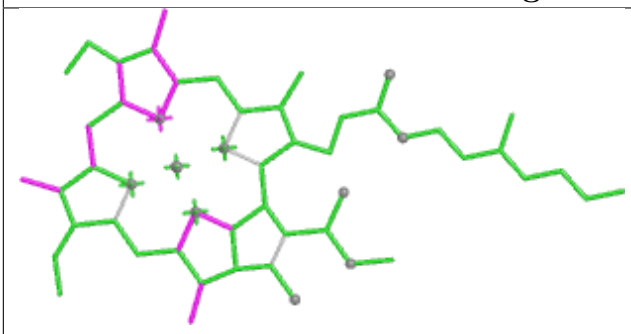


Torsions

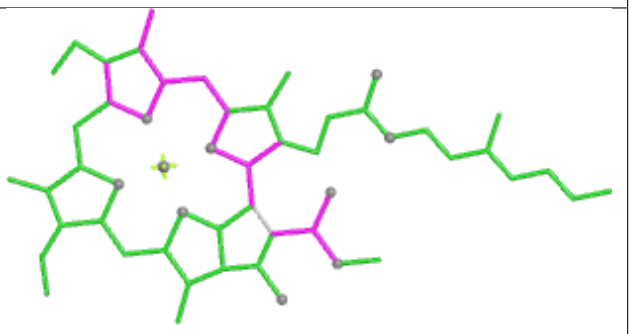


Rings

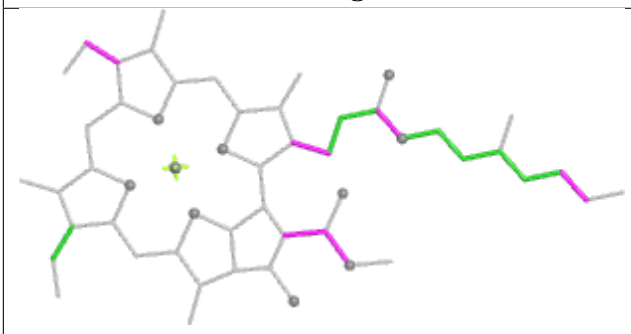
Ligand CLA f 1209



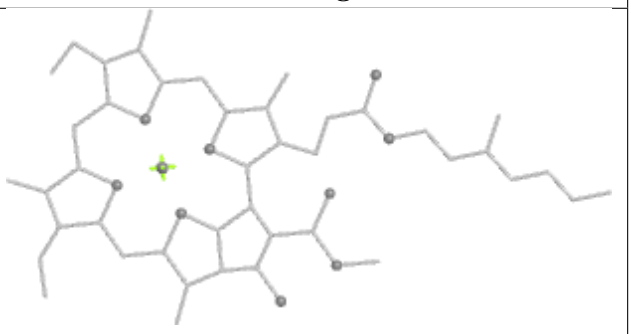
Bond lengths



Bond angles

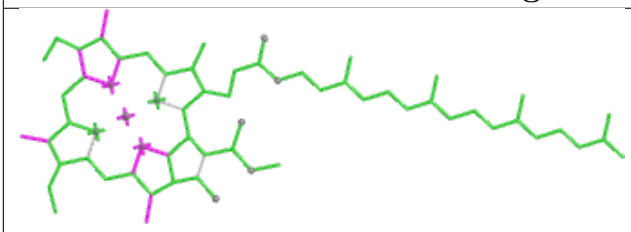


Torsions

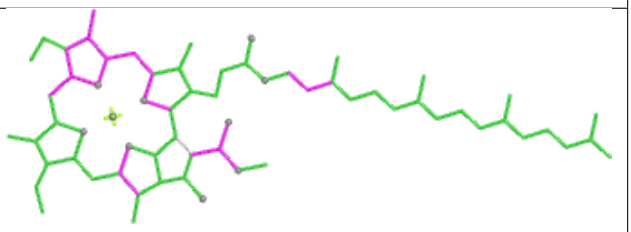


Rings

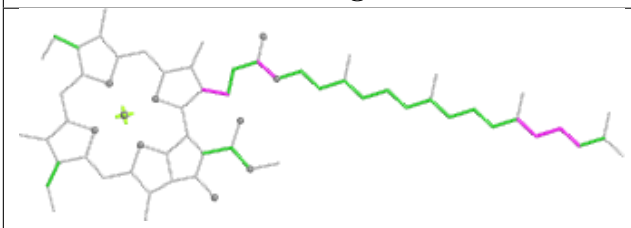
Ligand CLA f 1225



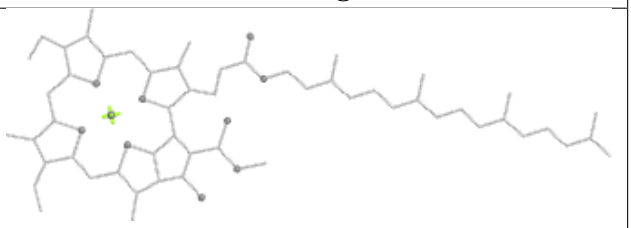
Bond lengths



Bond angles

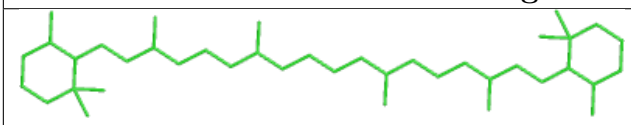


Torsions

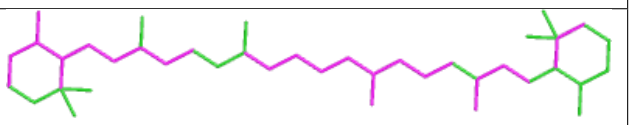


Rings

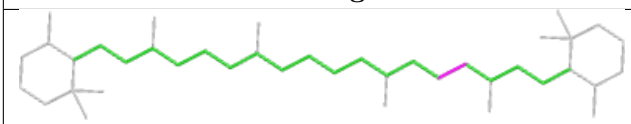
Ligand BCR f 4009



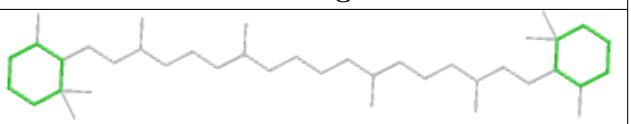
Bond lengths



Bond angles

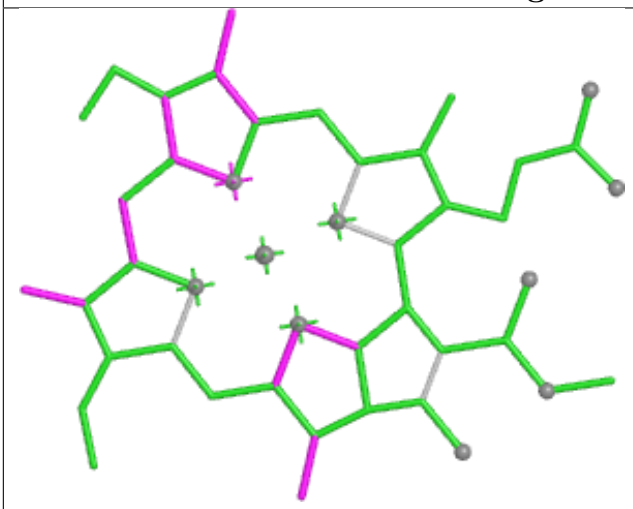


Torsions

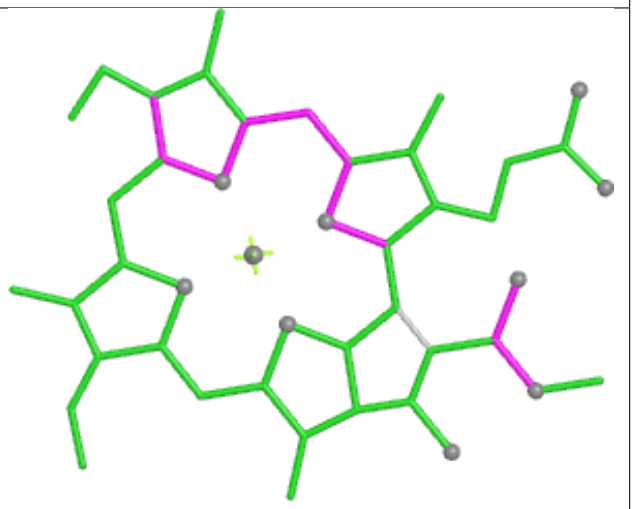


Rings

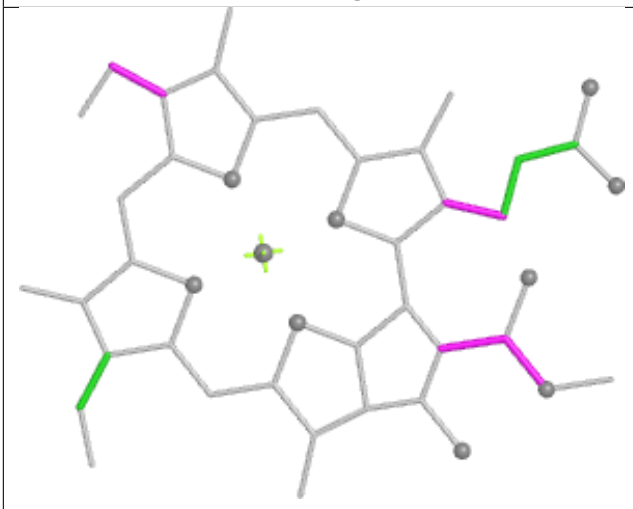
Ligand CLA b 506



Bond lengths



Bond angles

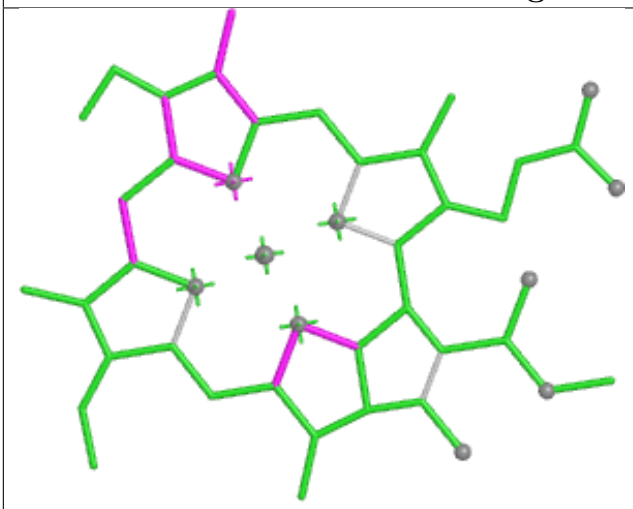


Torsions

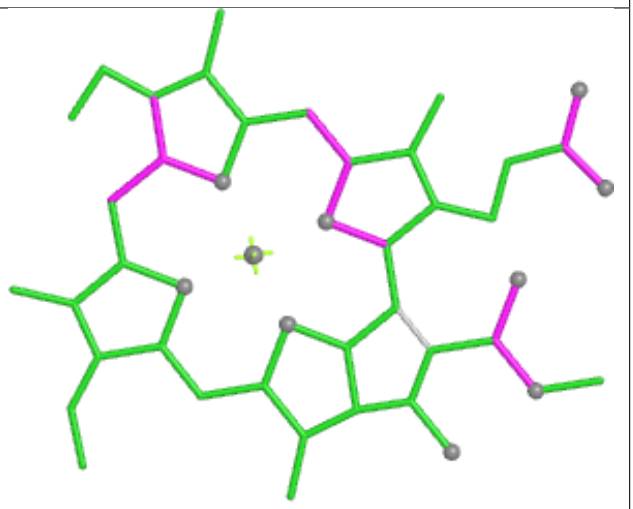


Rings

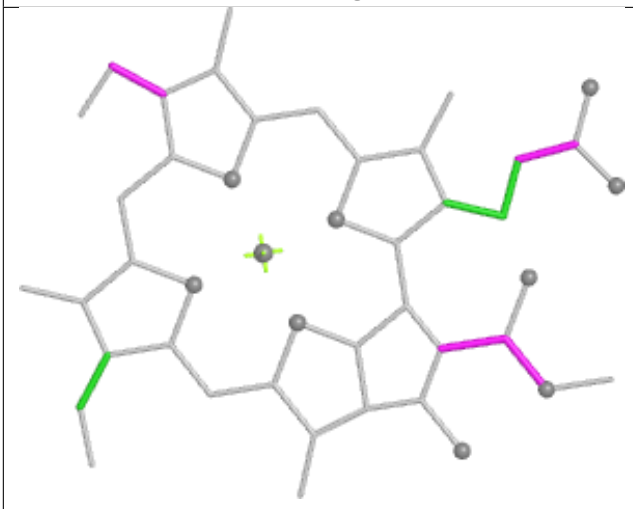
Ligand CLA u 519



Bond lengths



Bond angles

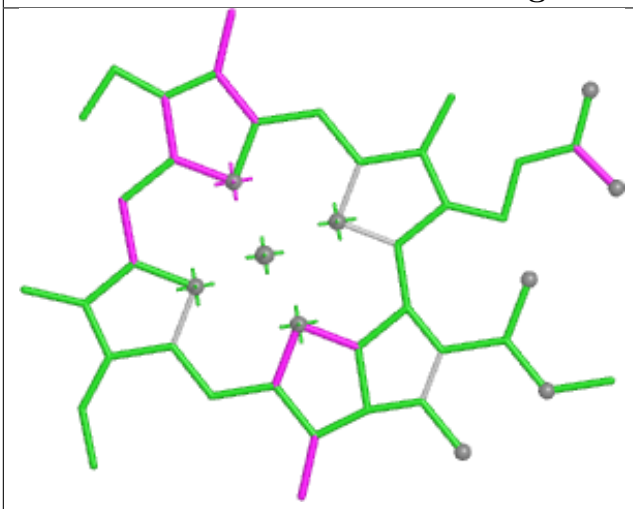


Torsions

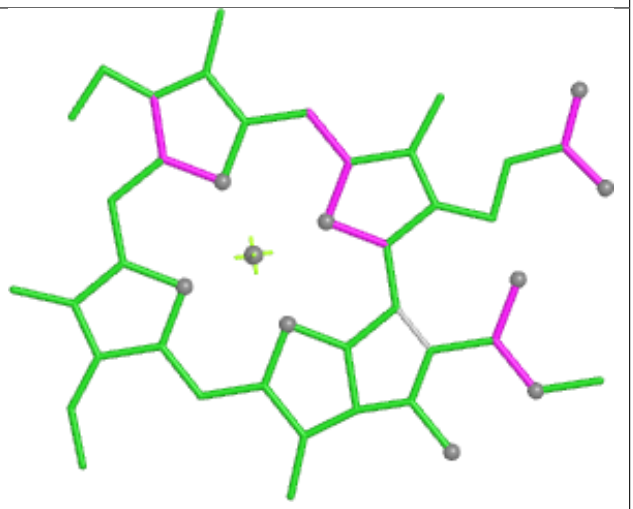


Rings

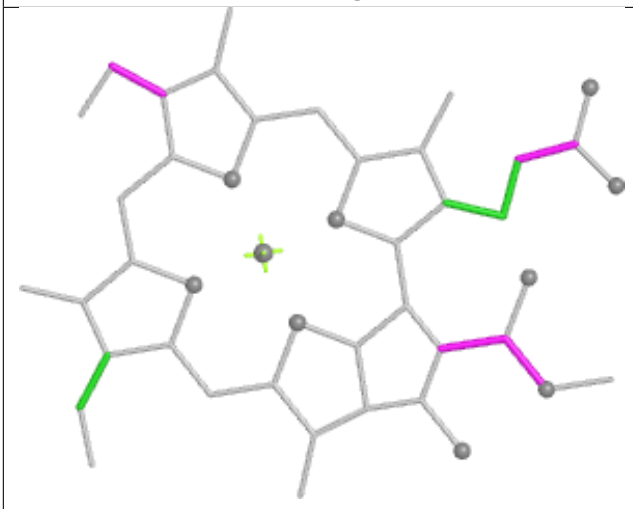
Ligand CLA 3 510



Bond lengths



Bond angles

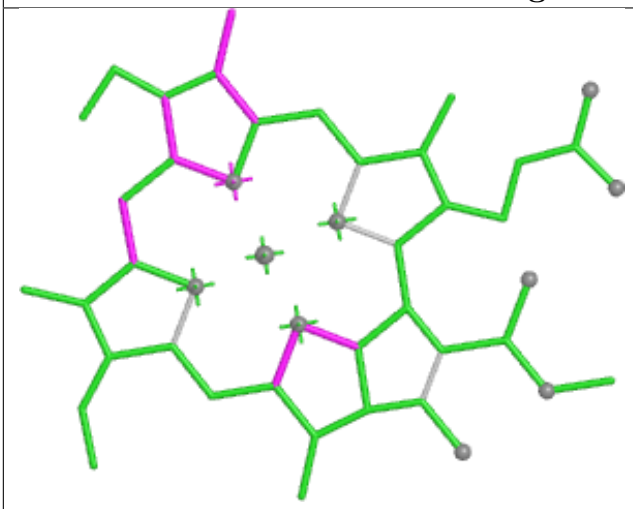


Torsions

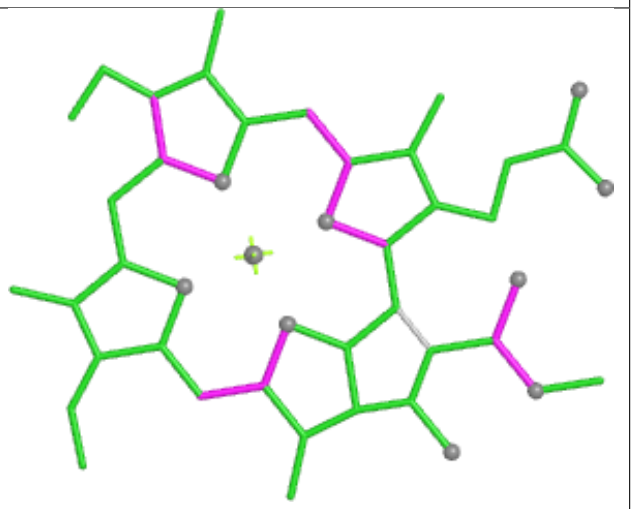


Rings

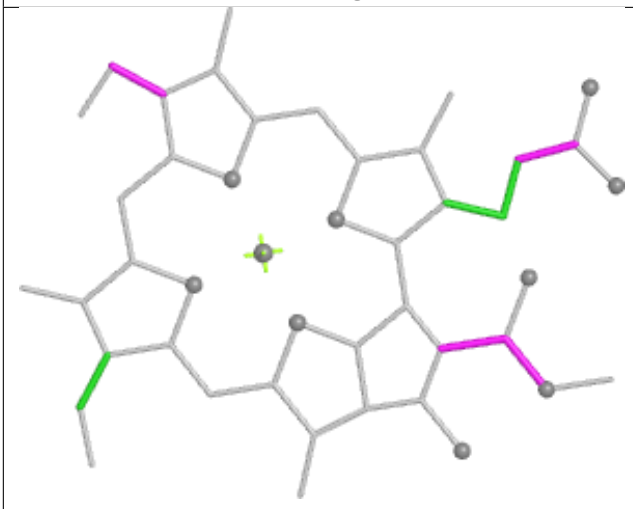
Ligand CLA 6 511



Bond lengths



Bond angles

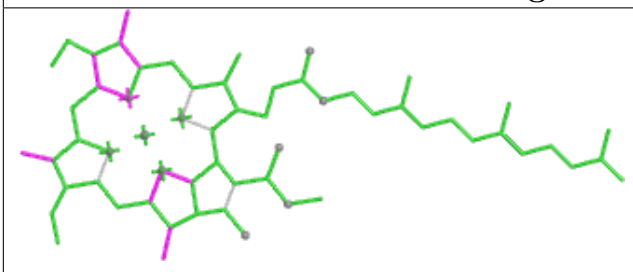


Torsions

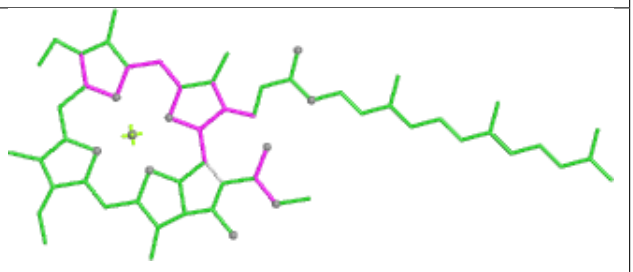


Rings

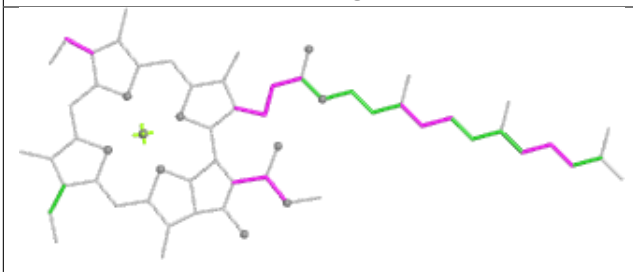
Ligand CLA 2 501



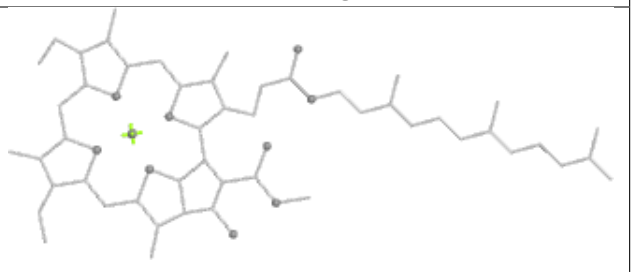
Bond lengths



Bond angles

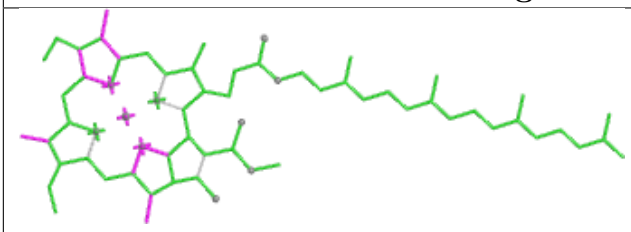


Torsions

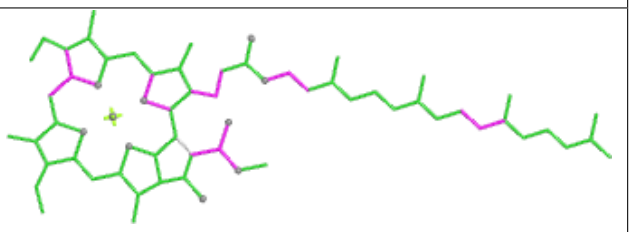


Rings

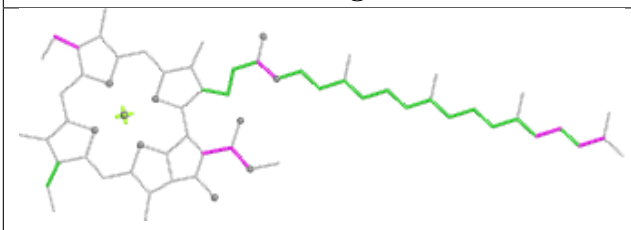
Ligand CLA B 1021



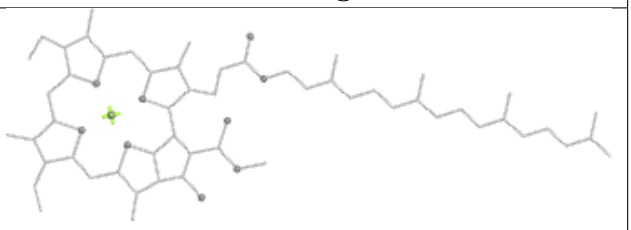
Bond lengths



Bond angles

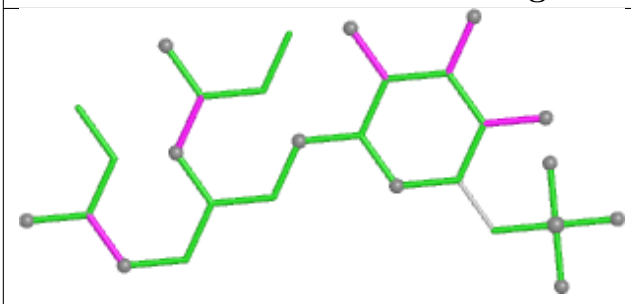


Torsions

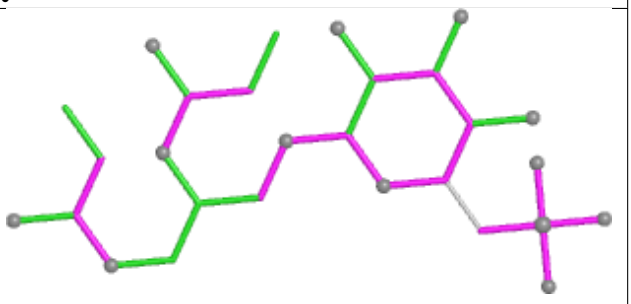


Rings

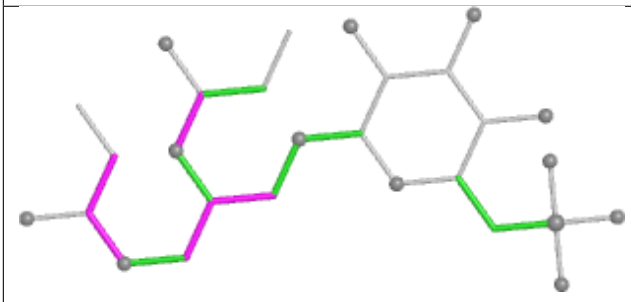
Ligand SQD a 822



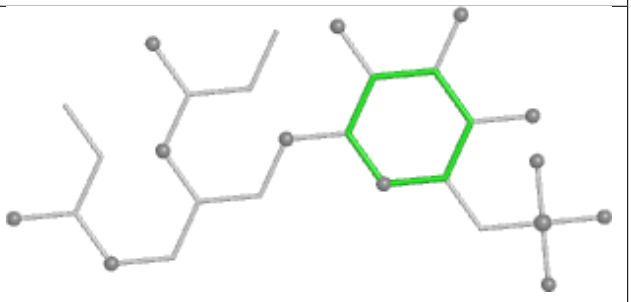
Bond lengths



Bond angles

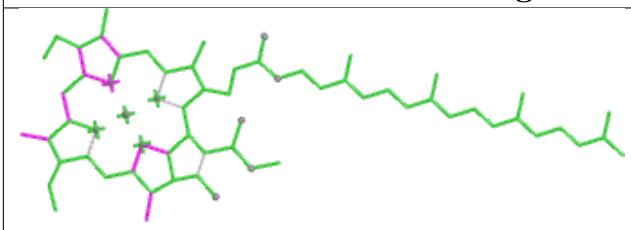


Torsions

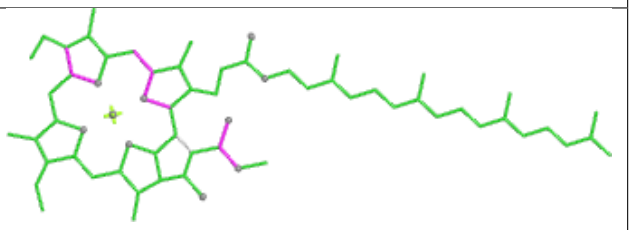


Rings

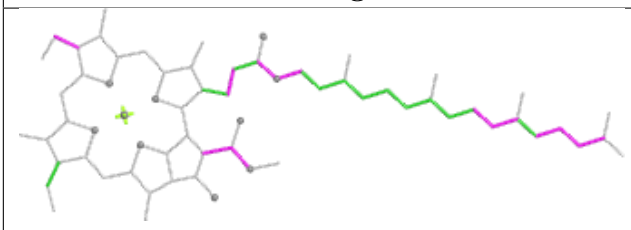
Ligand CLA B 1207



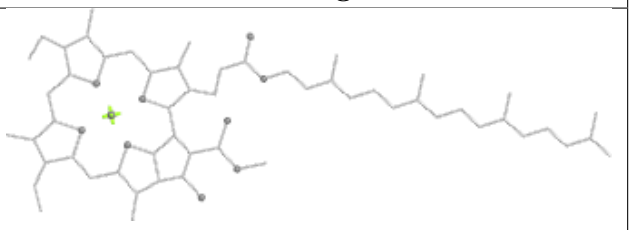
Bond lengths



Bond angles

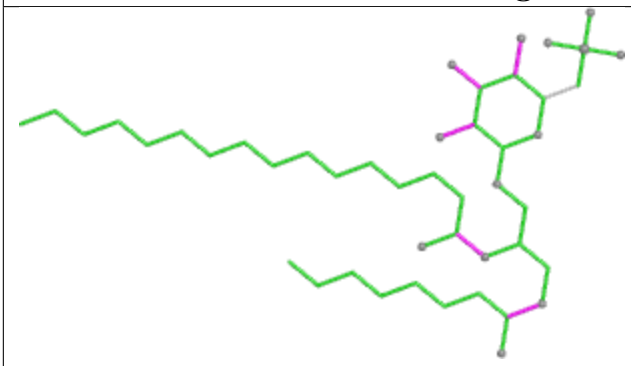


Torsions

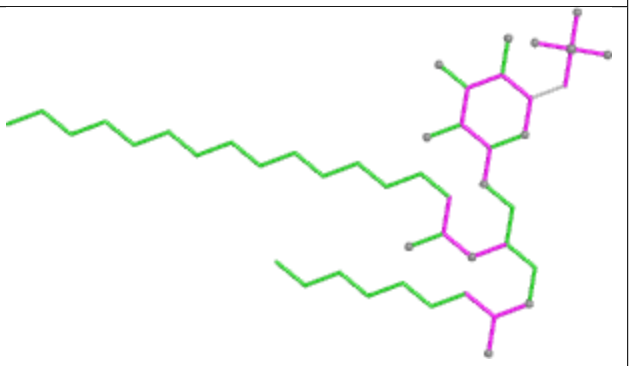


Rings

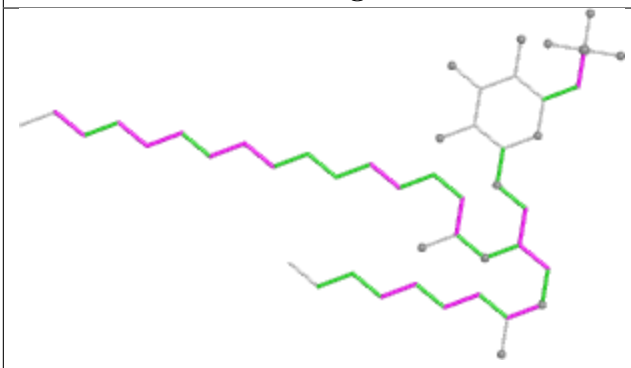
Ligand SQD V 5216



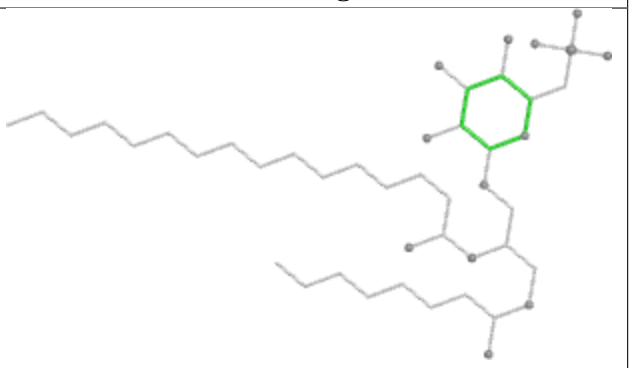
Bond lengths



Bond angles

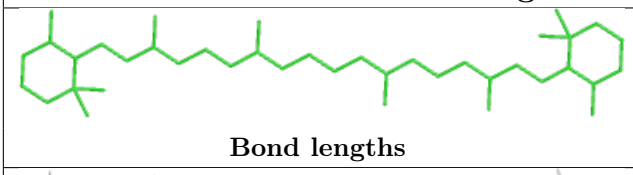


Torsions

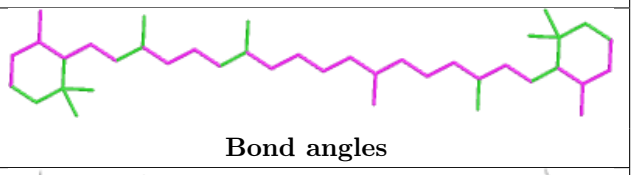


Rings

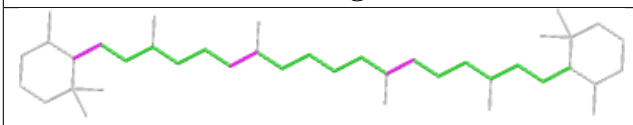
Ligand BCR o 4021



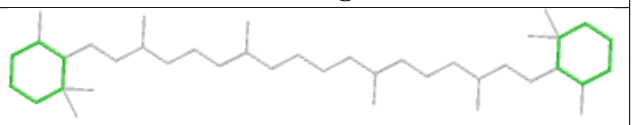
Bond lengths



Bond angles

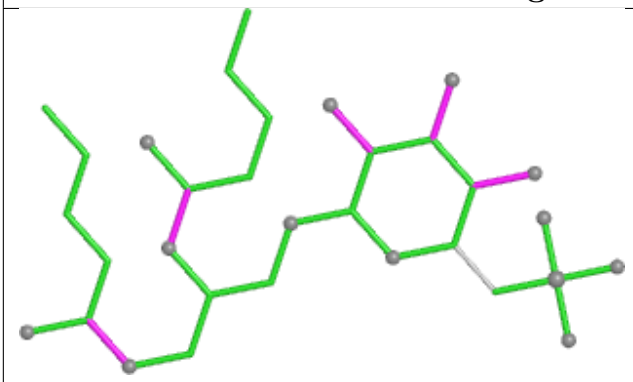


Torsions

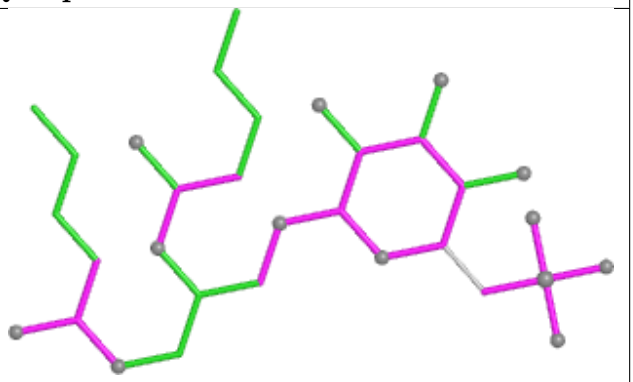


Rings

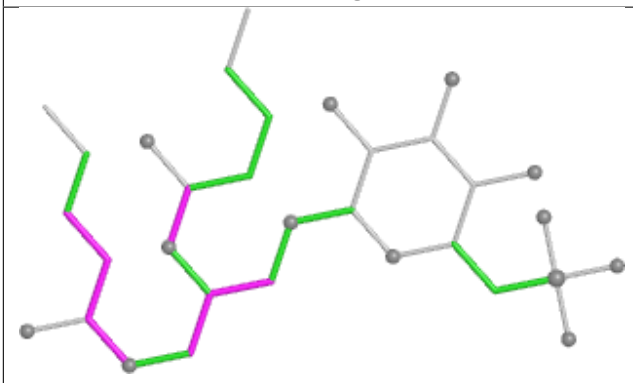
Ligand SQD q 822



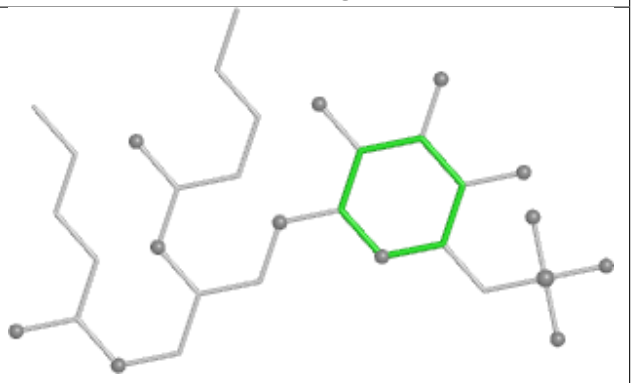
Bond lengths



Bond angles



Torsions

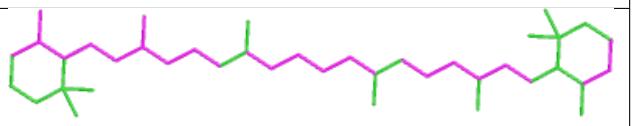


Rings

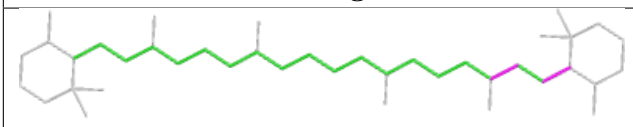
Ligand BCR v 523



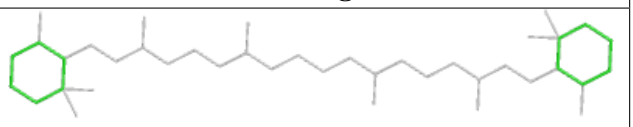
Bond lengths



Bond angles

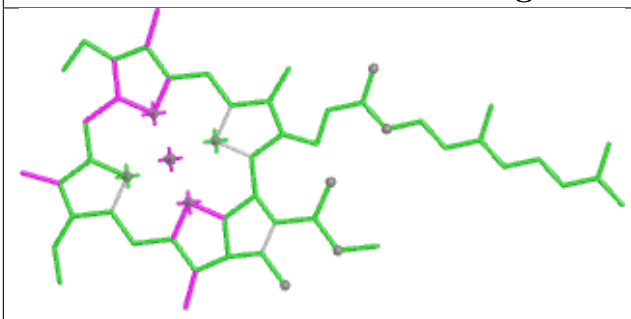


Torsions

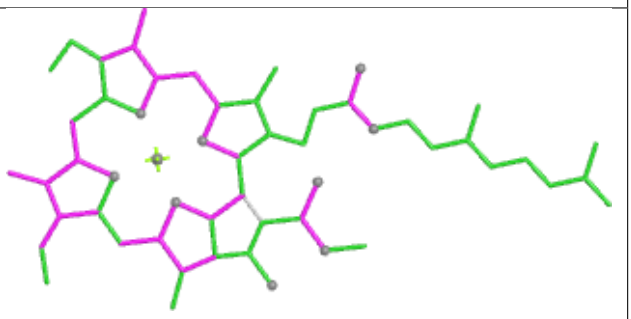


Rings

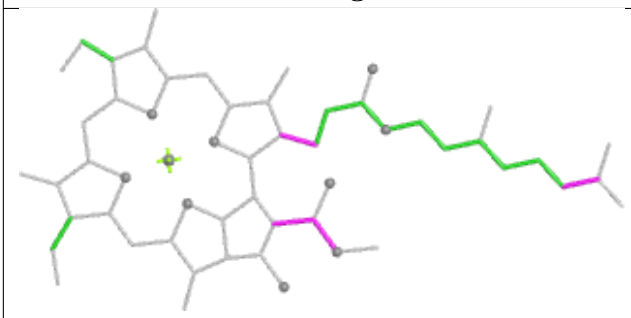
Ligand CLA B 1226



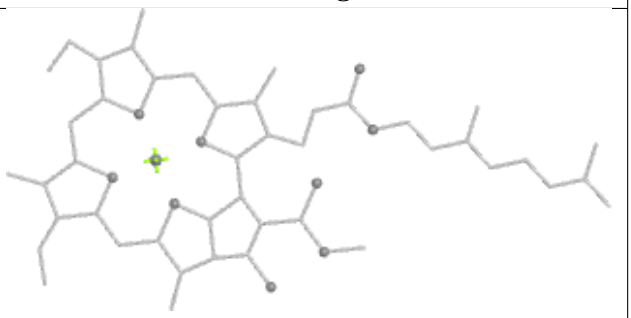
Bond lengths



Bond angles

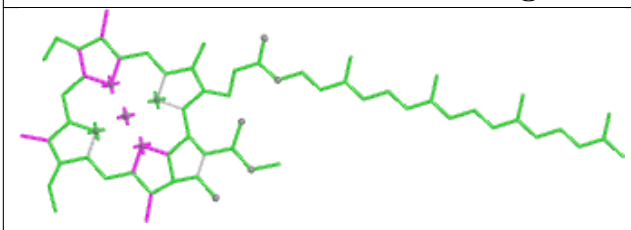


Torsions

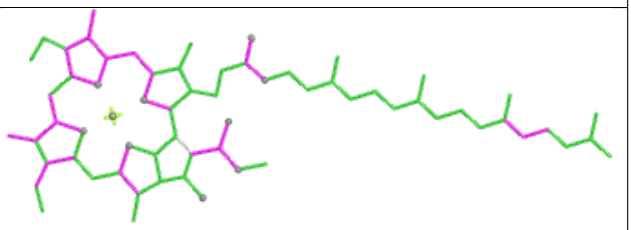


Rings

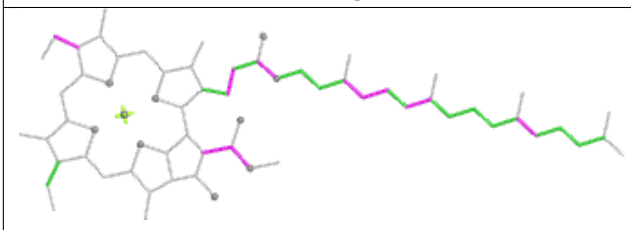
Ligand CLA e 1119



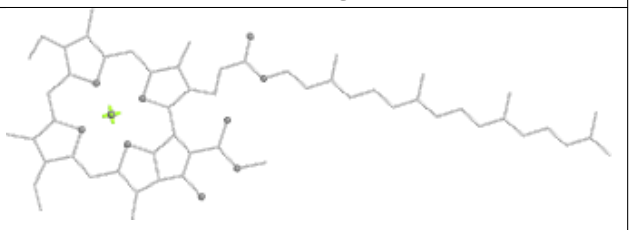
Bond lengths



Bond angles

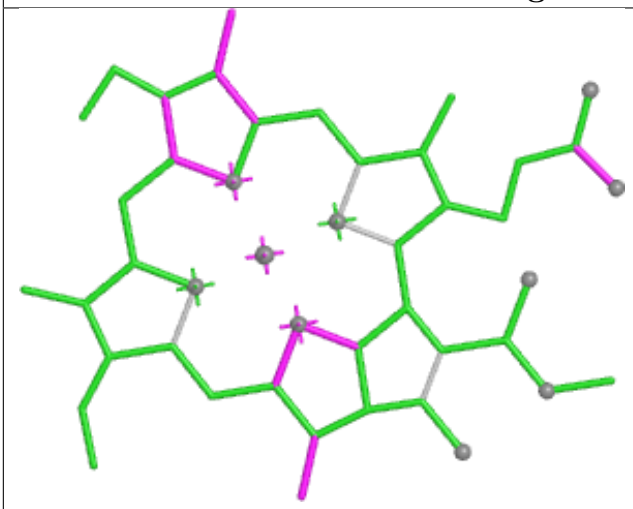


Torsions

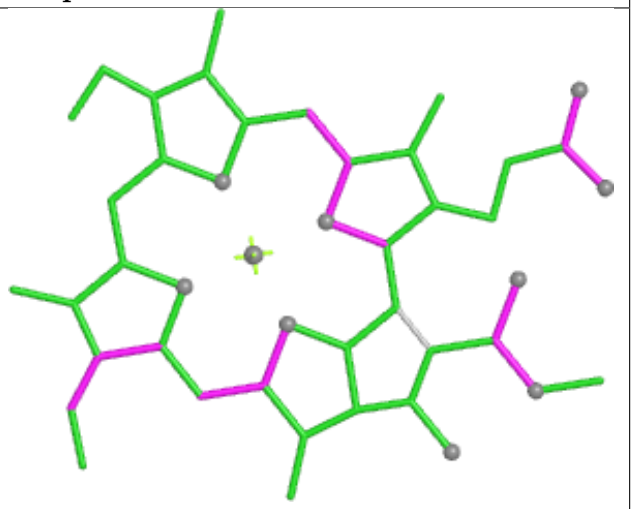


Rings

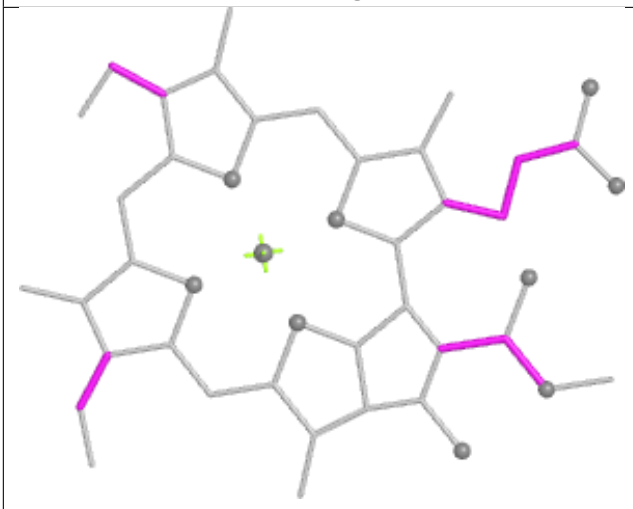
Ligand CLA q 516



Bond lengths



Bond angles

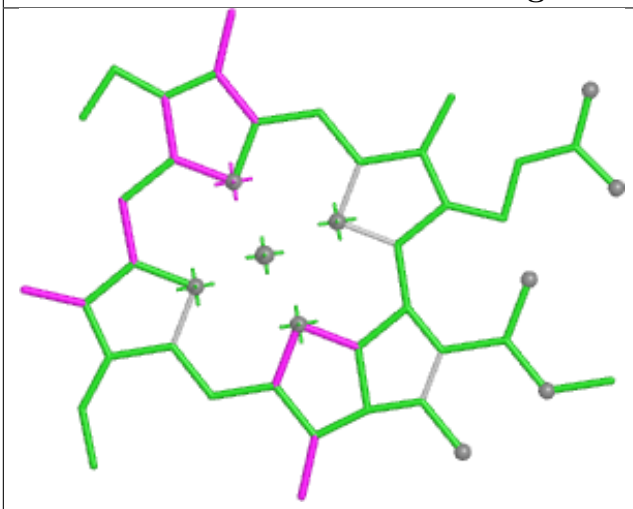


Torsions

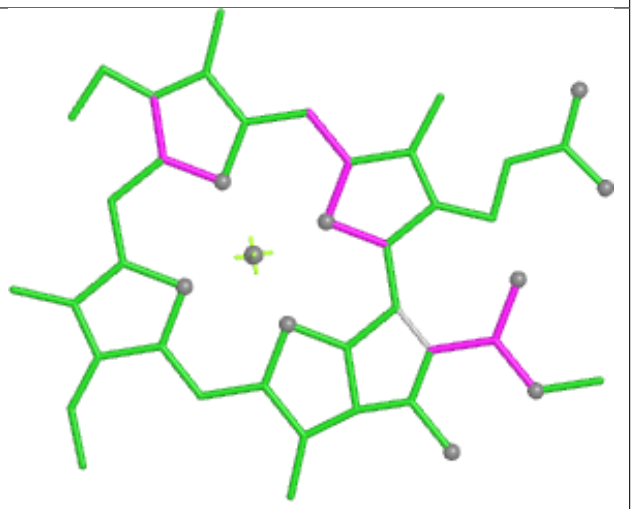


Rings

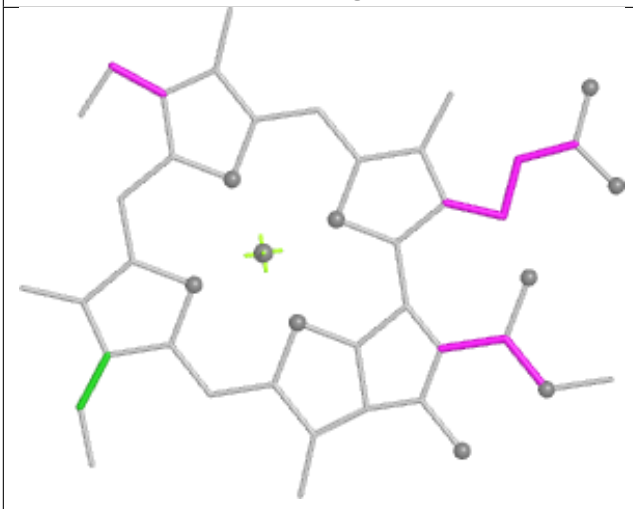
Ligand CLA d 501



Bond lengths



Bond angles

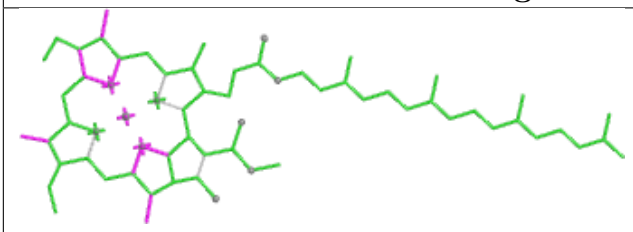


Torsions

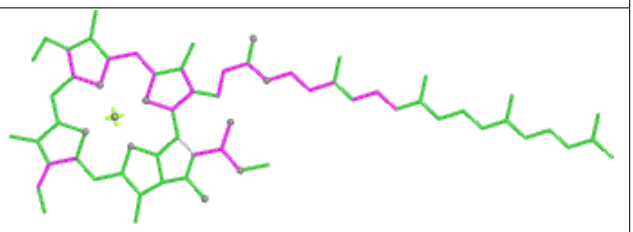


Rings

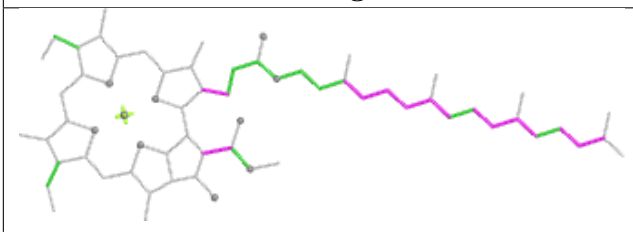
Ligand CLA G 1101



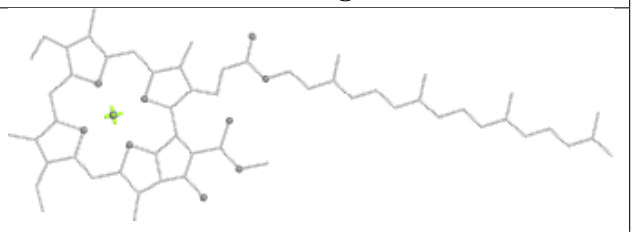
Bond lengths



Bond angles

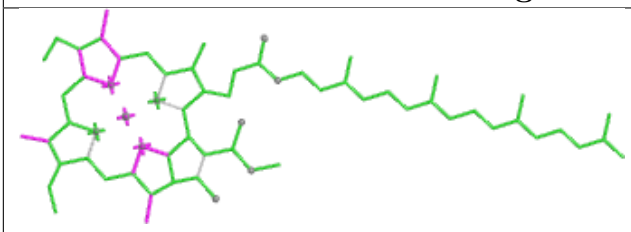


Torsions

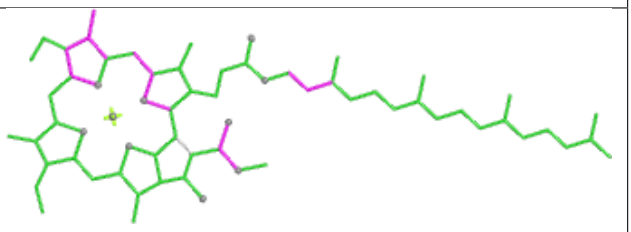


Rings

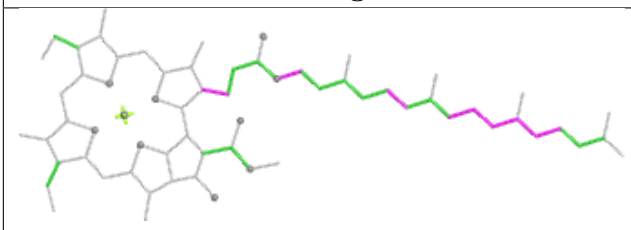
Ligand CLA B 1223



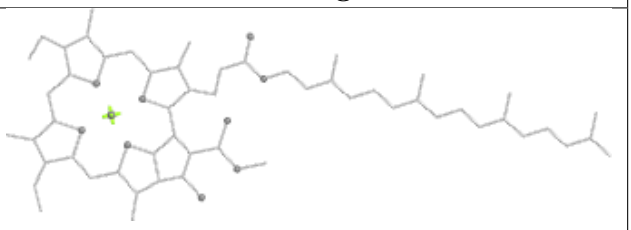
Bond lengths



Bond angles

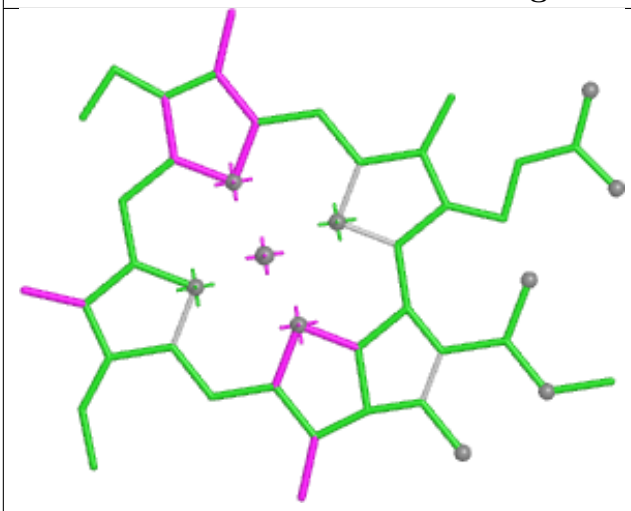


Torsions

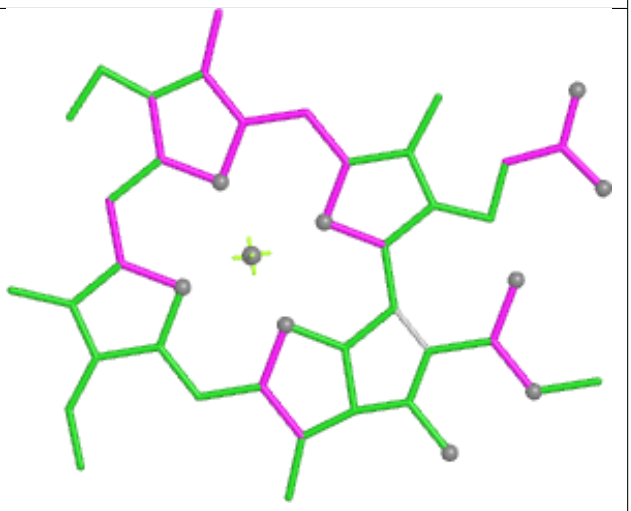


Rings

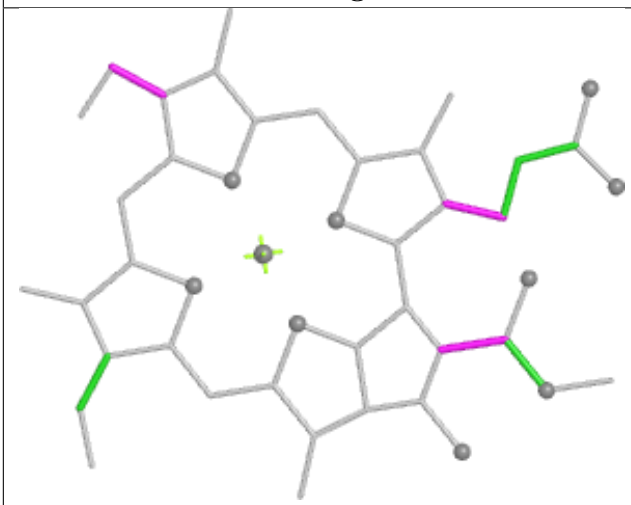
Ligand CLA r 508



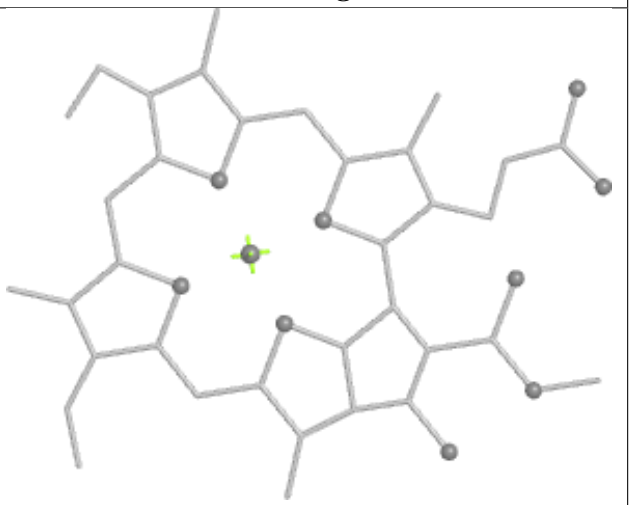
Bond lengths



Bond angles

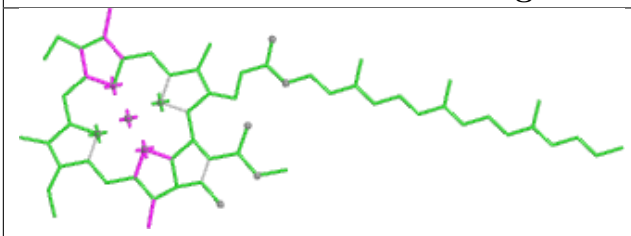


Torsions

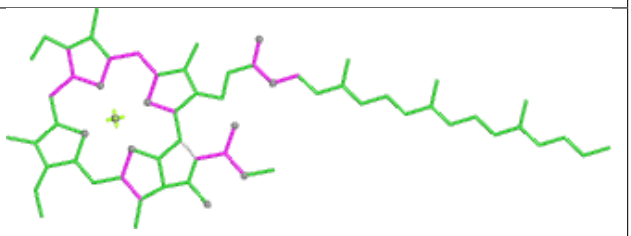


Rings

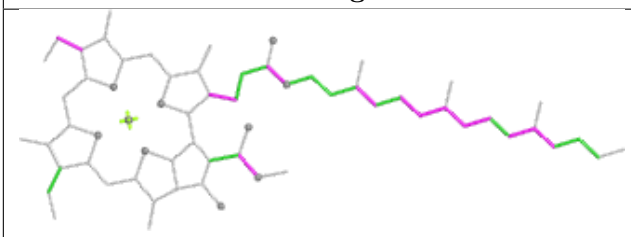
Ligand CLA B 1219



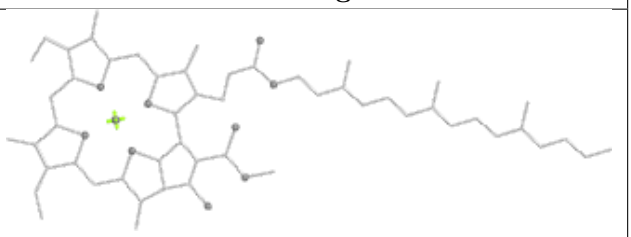
Bond lengths



Bond angles

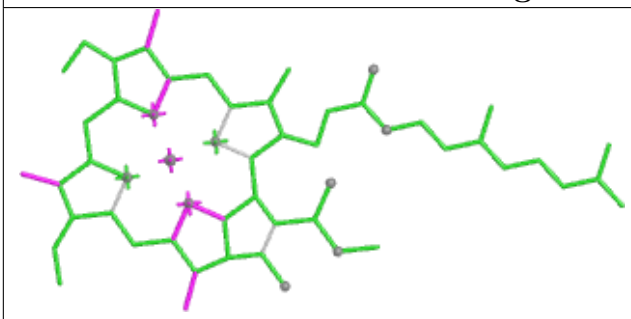


Torsions

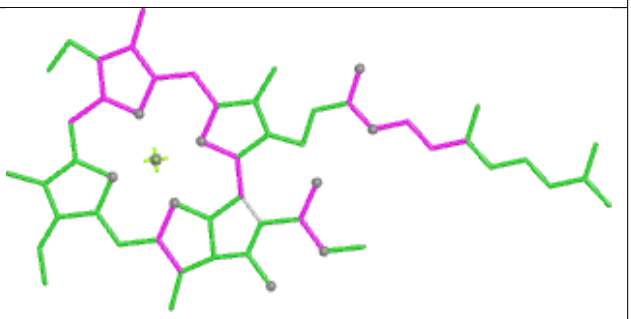


Rings

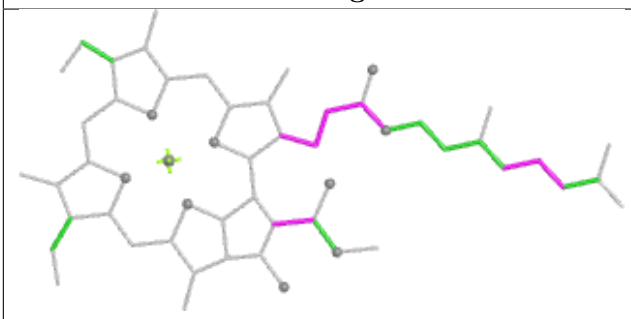
Ligand CLA G 1135



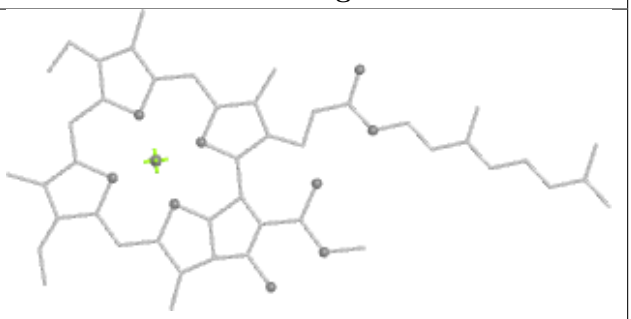
Bond lengths



Bond angles

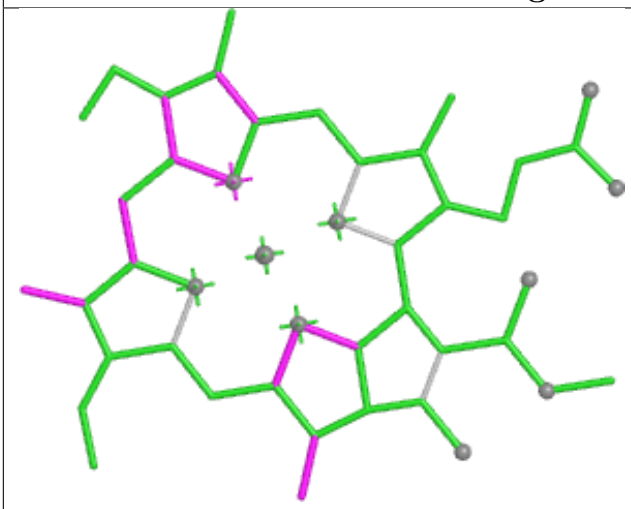


Torsions

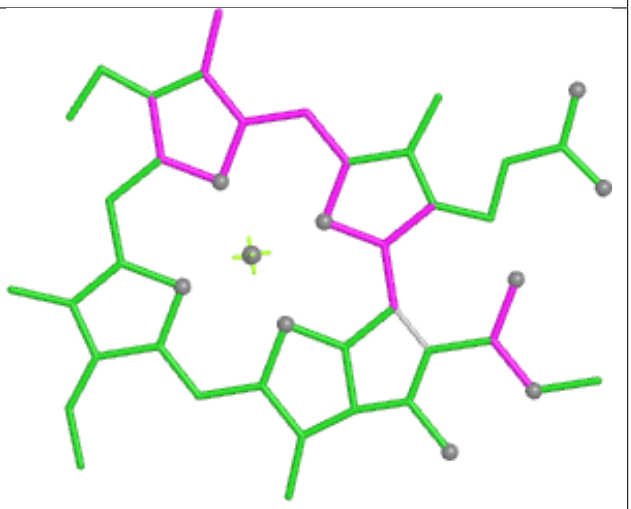


Rings

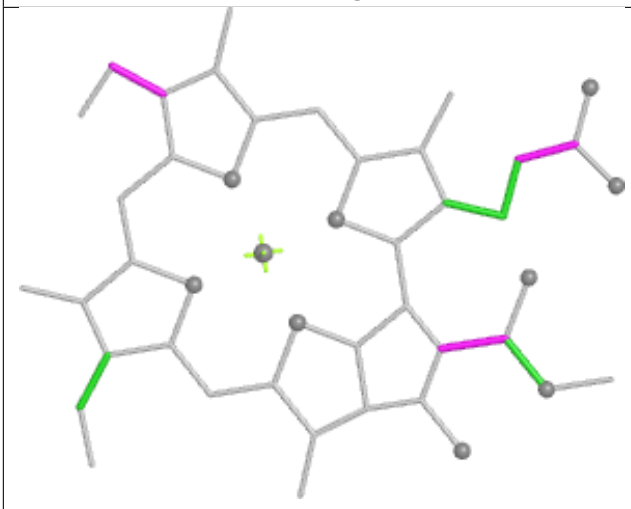
Ligand CLA 6 504



Bond lengths



Bond angles

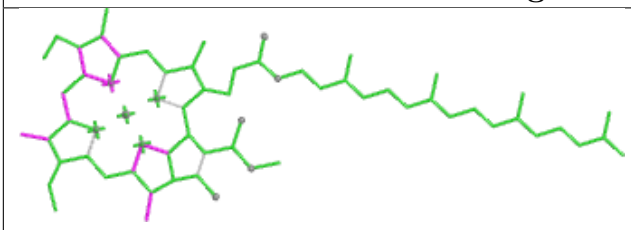


Torsions

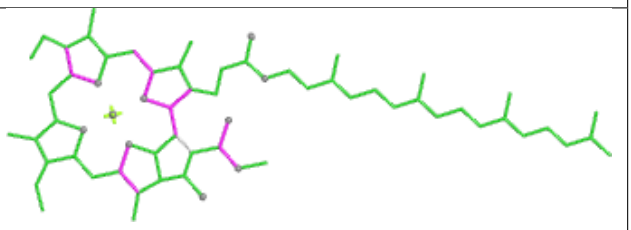


Rings

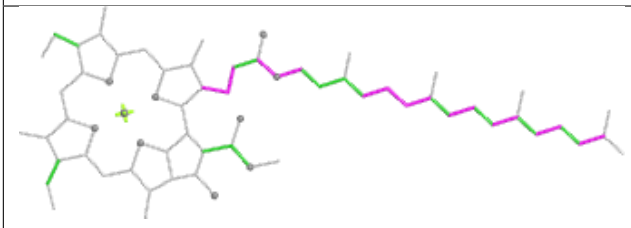
Ligand CLA d 505



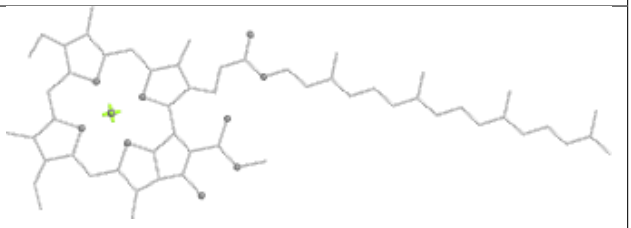
Bond lengths



Bond angles

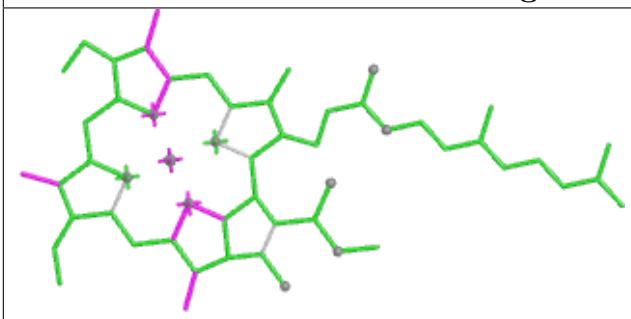


Torsions

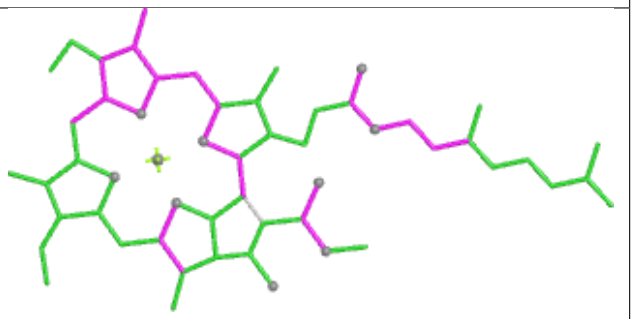


Rings

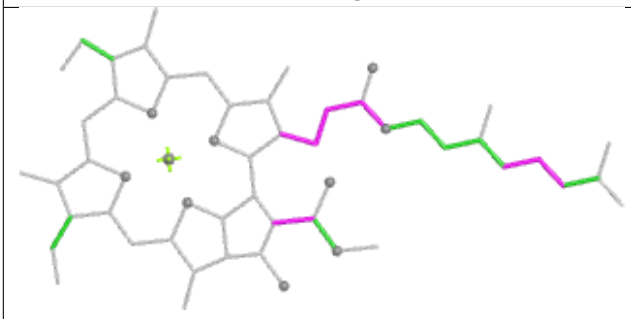
Ligand CLA e 1135



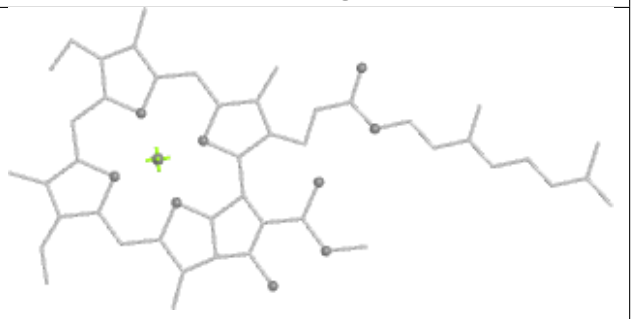
Bond lengths



Bond angles

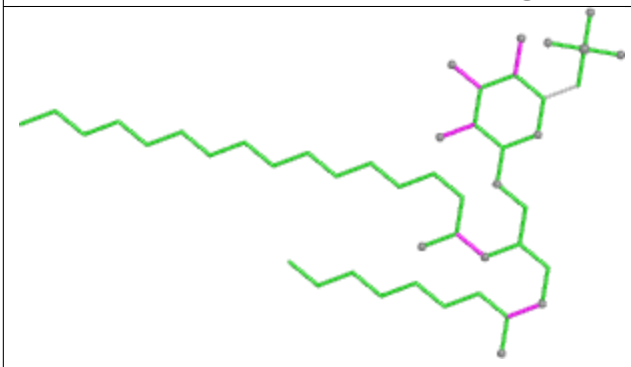


Torsions

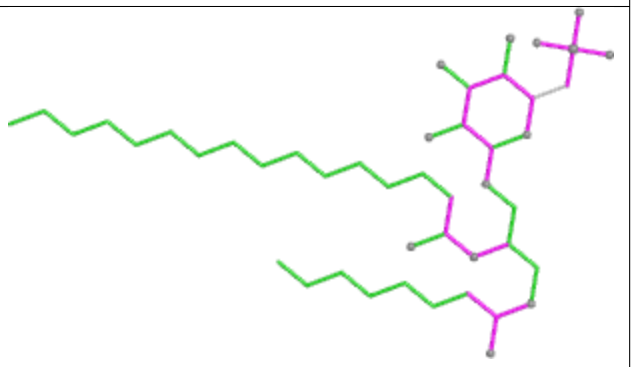


Rings

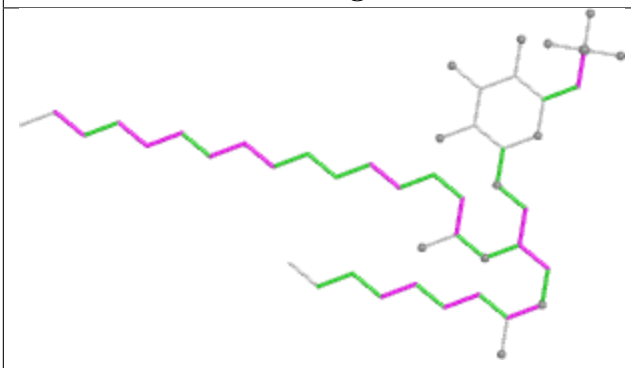
Ligand SQD n 5216



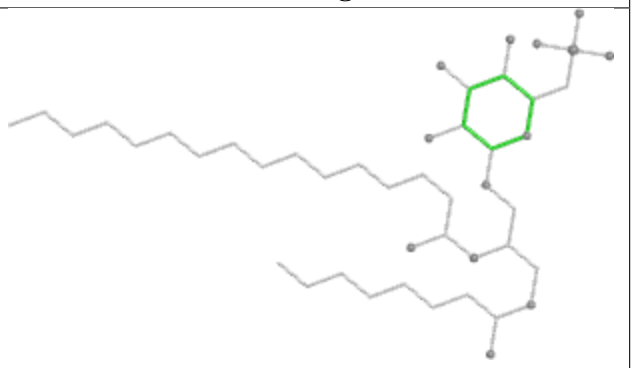
Bond lengths



Bond angles

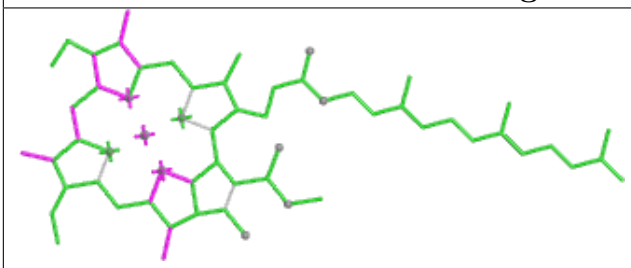


Torsions

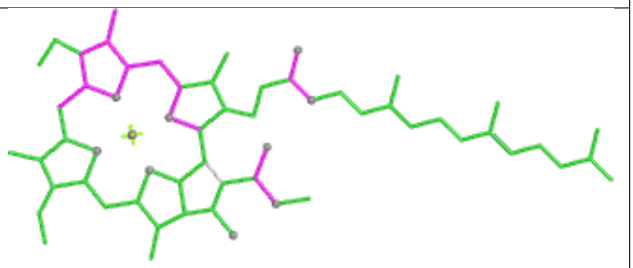


Rings

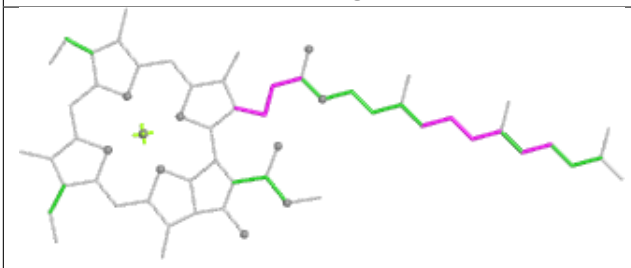
Ligand CLA e 1116



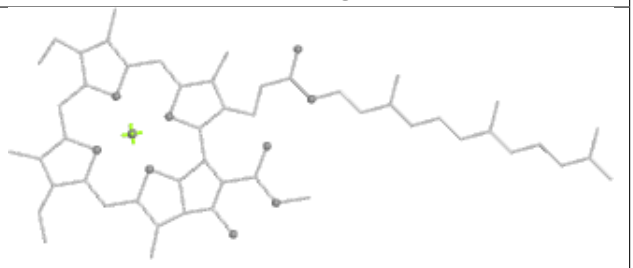
Bond lengths



Bond angles

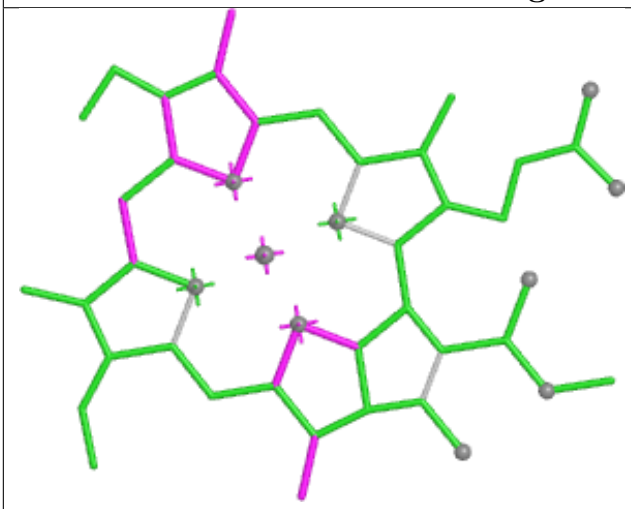


Torsions

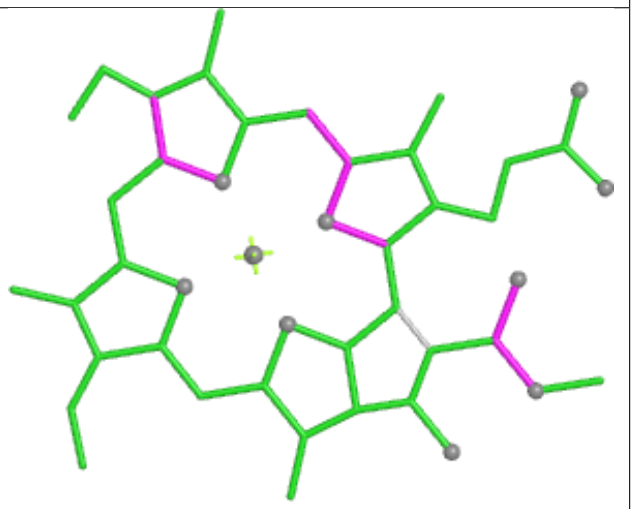


Rings

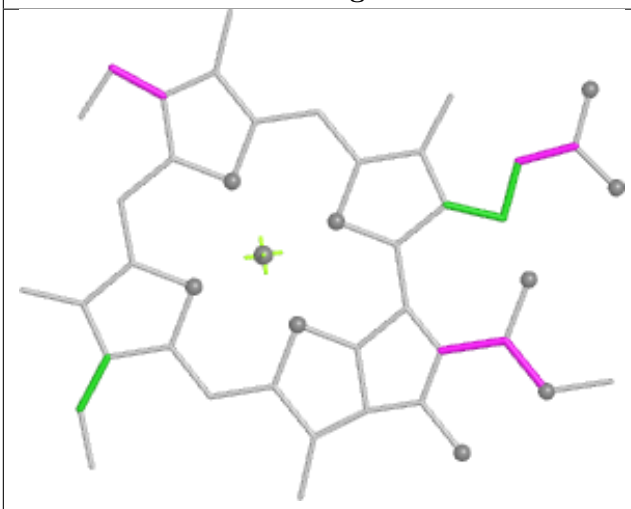
Ligand CLA 1 512



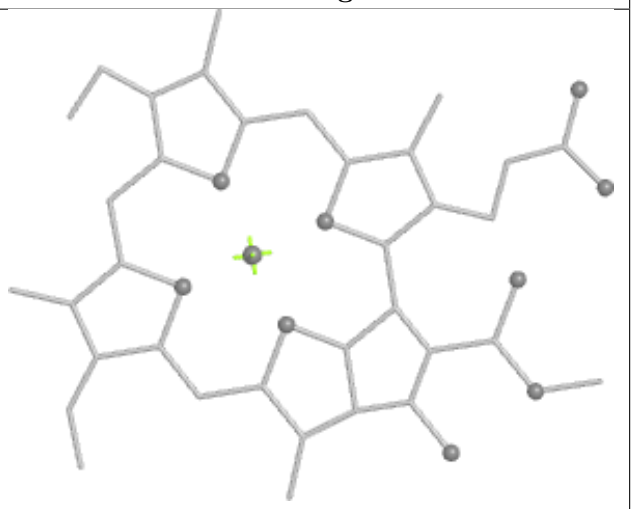
Bond lengths



Bond angles

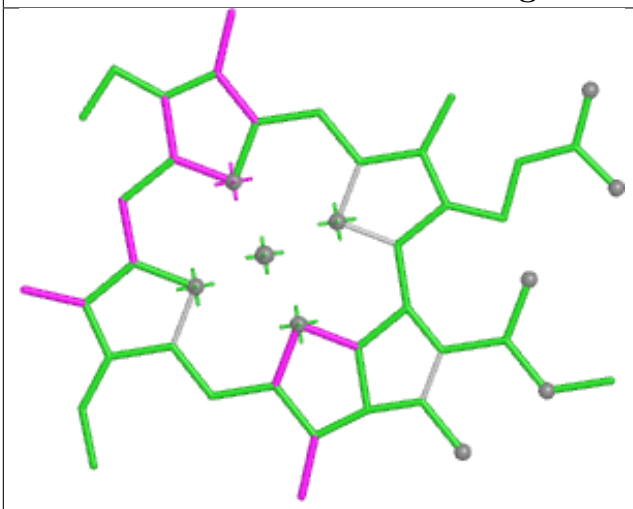


Torsions

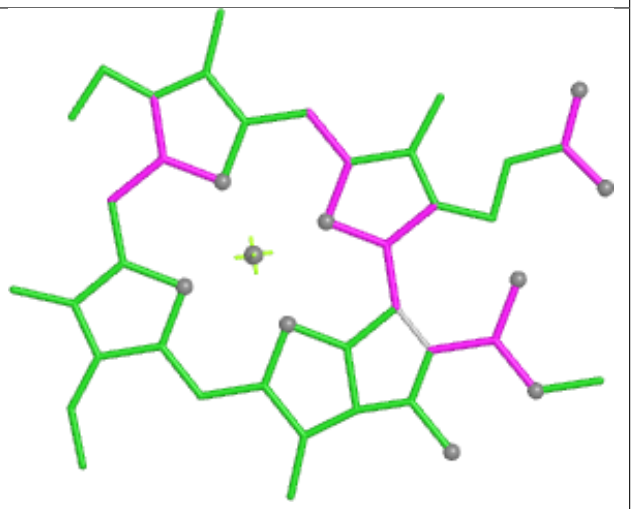


Rings

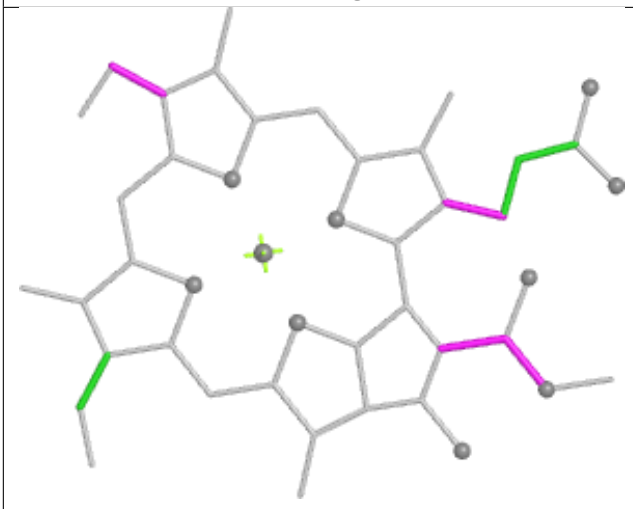
Ligand CLA J 1303



Bond lengths



Bond angles

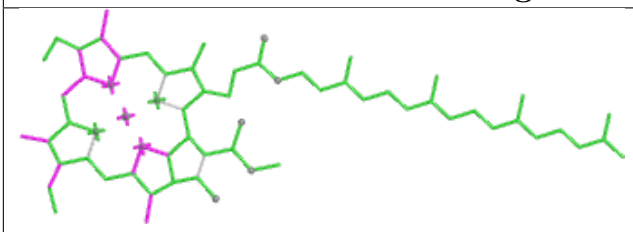


Torsions

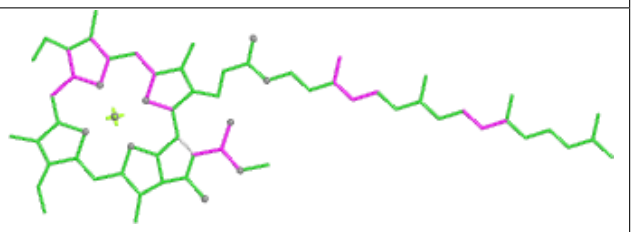


Rings

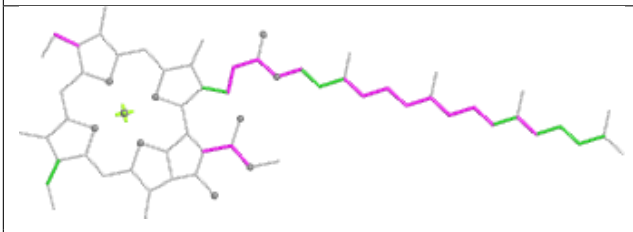
Ligand CLA A 1237



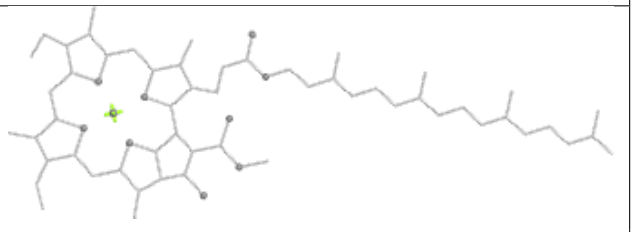
Bond lengths



Bond angles

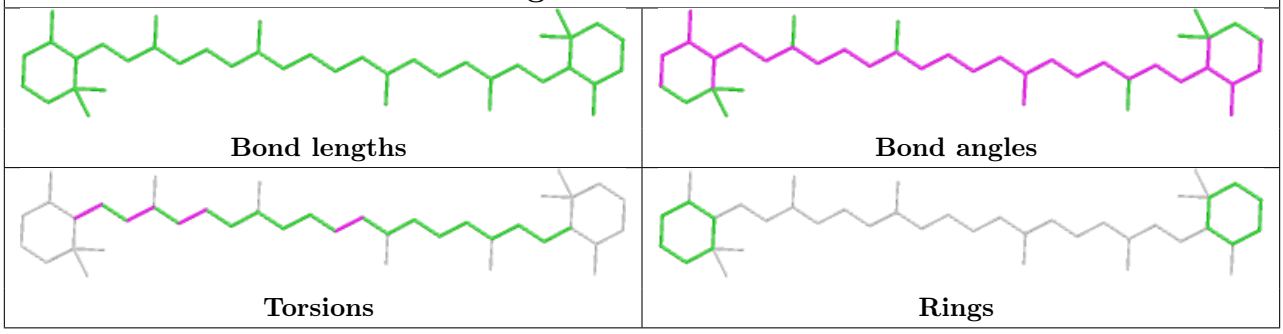


Torsions

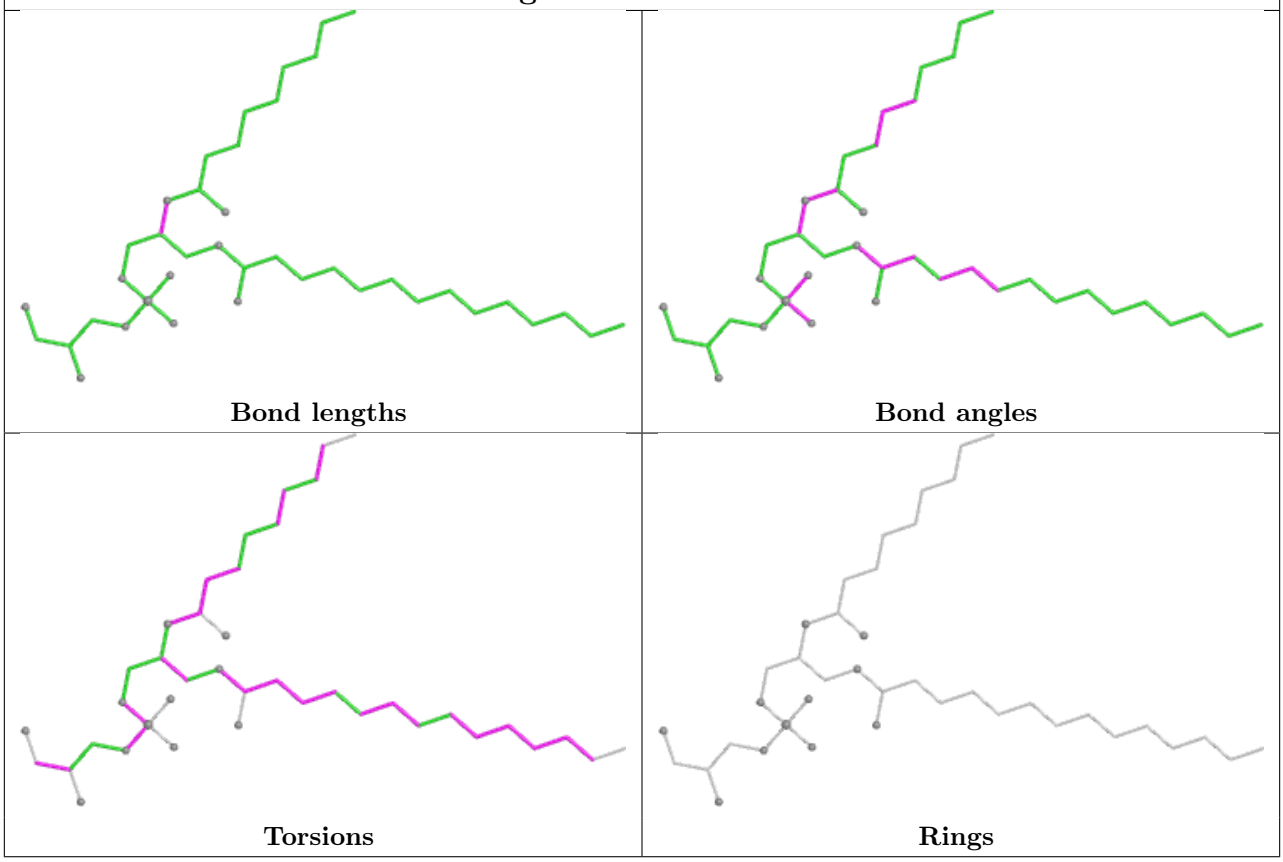


Rings

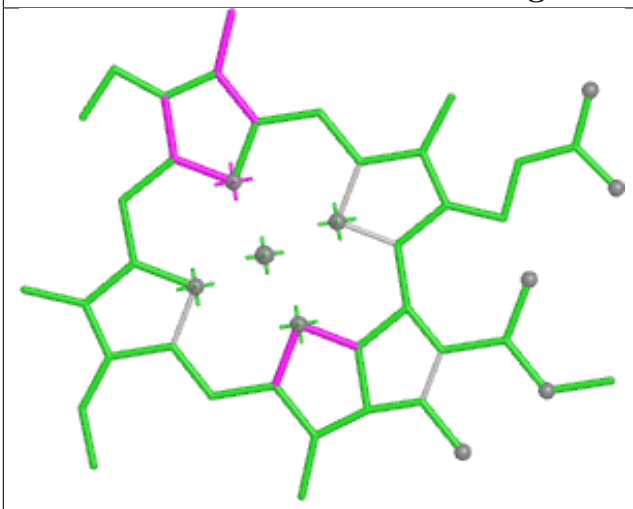
Ligand BCR 1 522



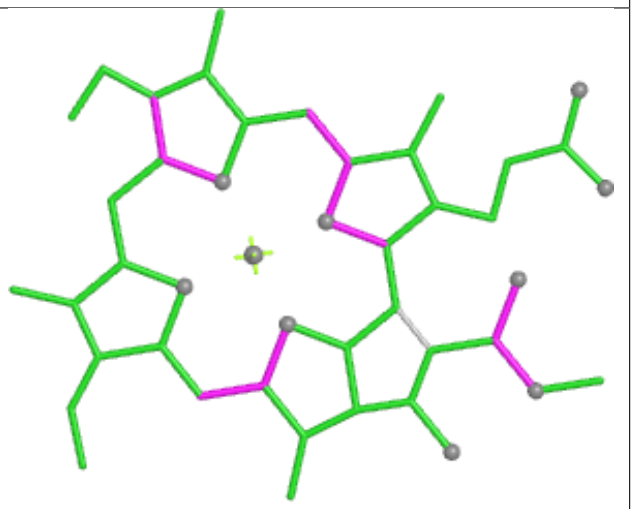
Ligand LHG e 5006



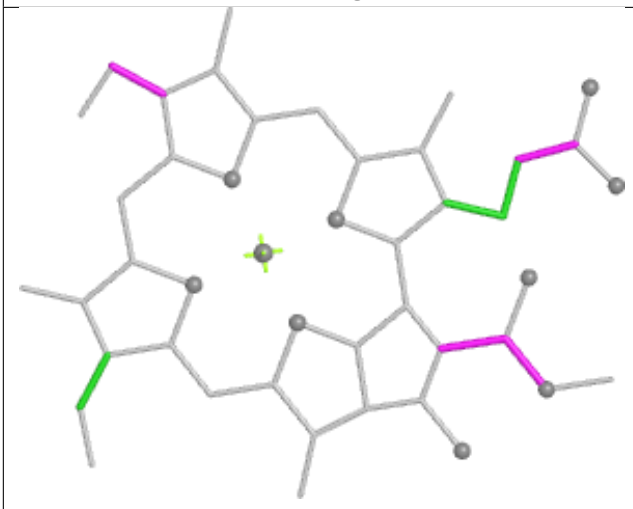
Ligand CLA v 511



Bond lengths



Bond angles

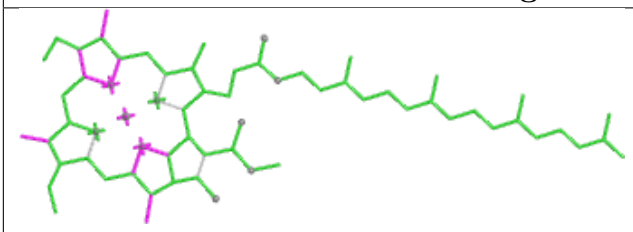


Torsions

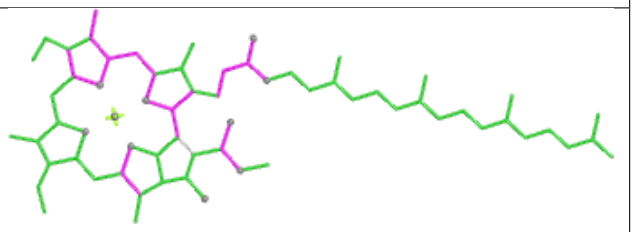


Rings

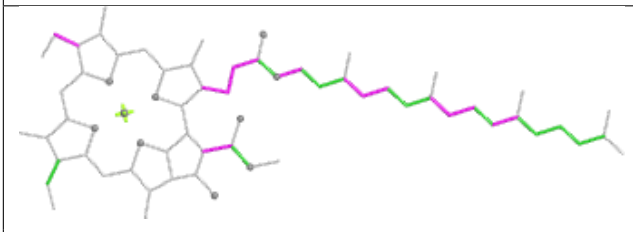
Ligand CLA e 1107



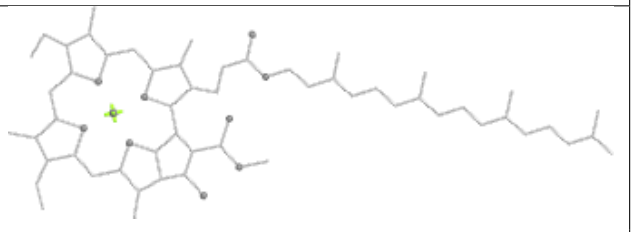
Bond lengths



Bond angles

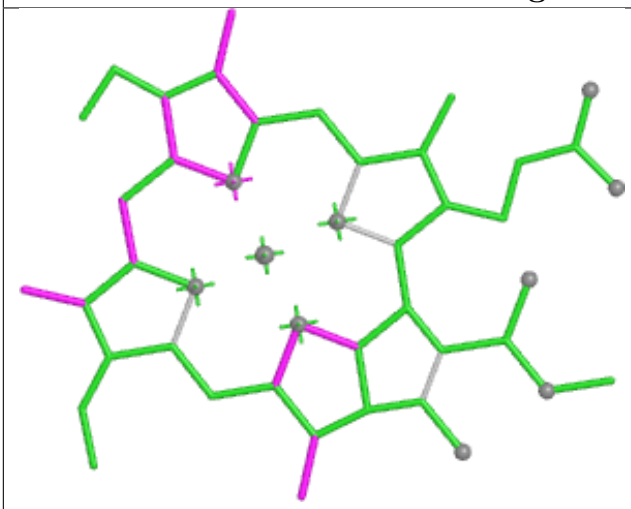


Torsions

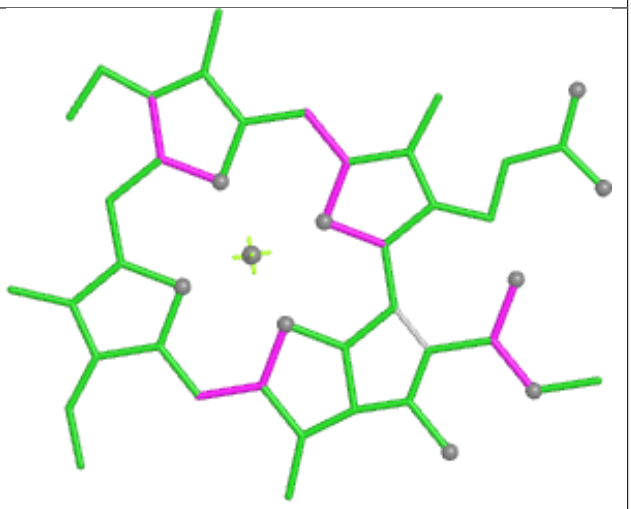


Rings

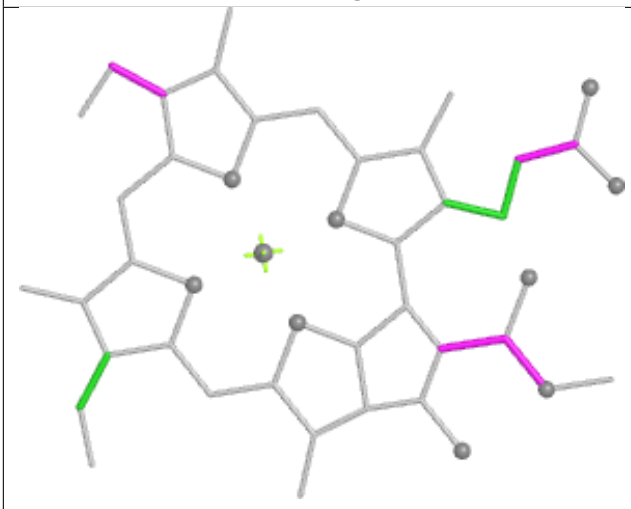
Ligand CLA 5 510



Bond lengths



Bond angles

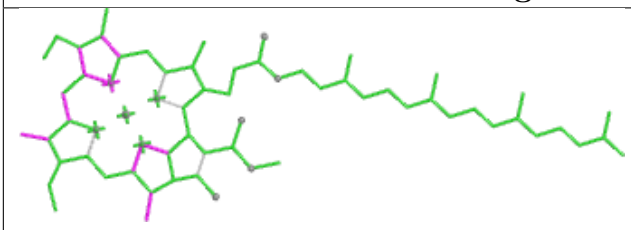


Torsions

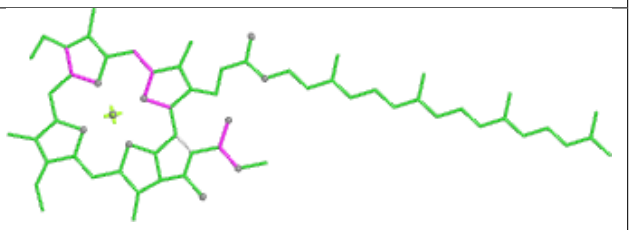


Rings

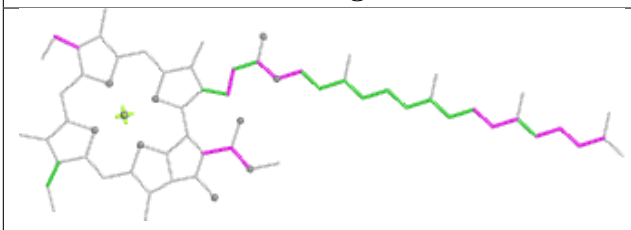
Ligand CLA H 1207



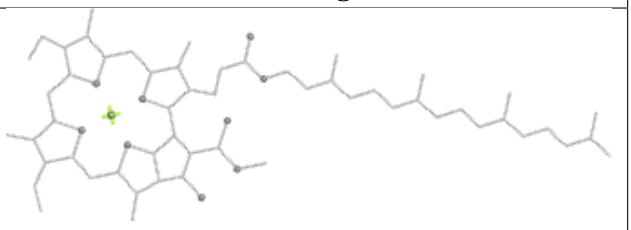
Bond lengths



Bond angles

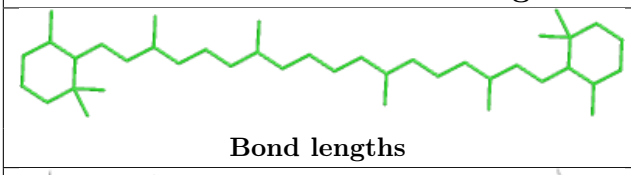


Torsions

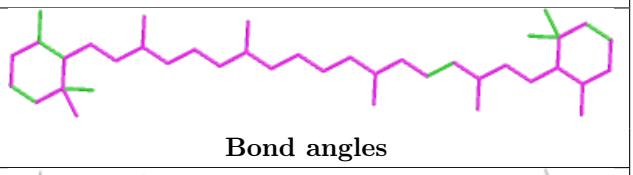


Rings

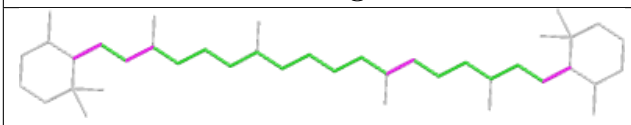
Ligand BCR H 4014



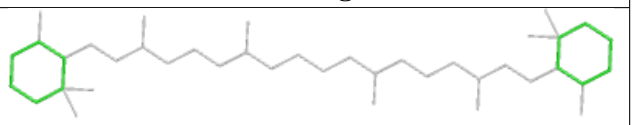
Bond lengths



Bond angles

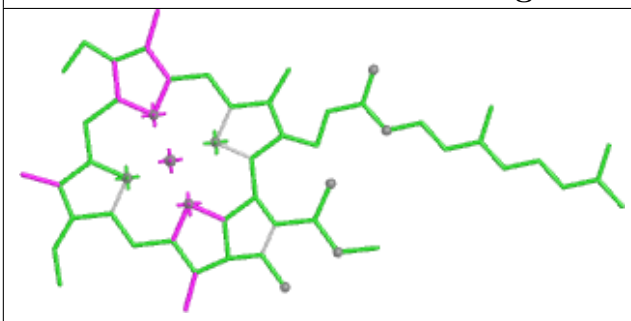


Torsions

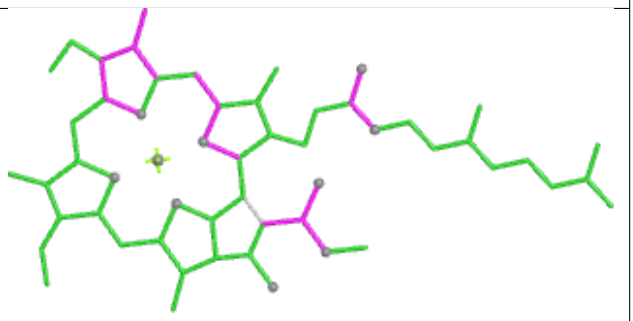


Rings

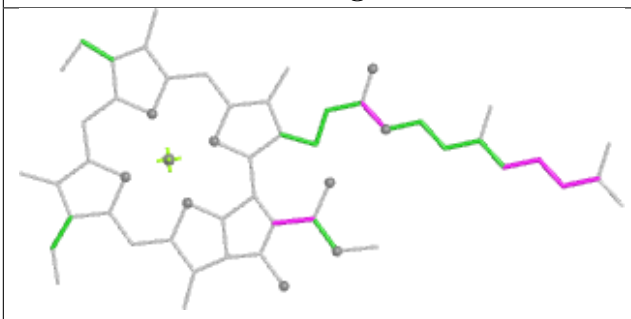
Ligand CLA B 1211



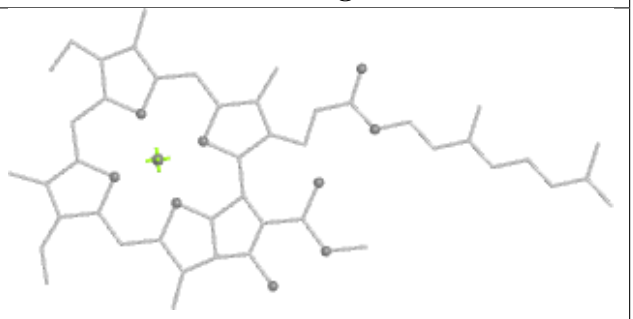
Bond lengths



Bond angles

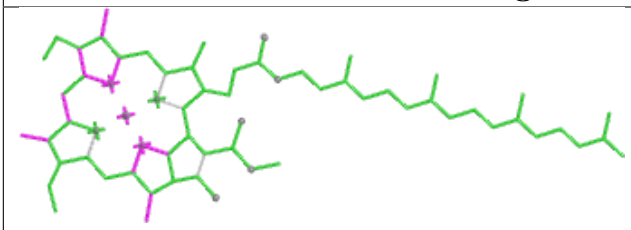


Torsions

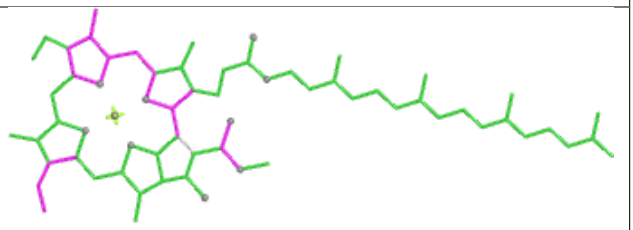


Rings

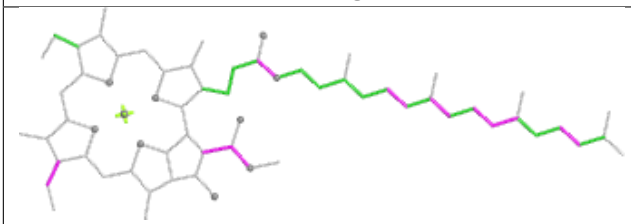
Ligand CLA H 1234



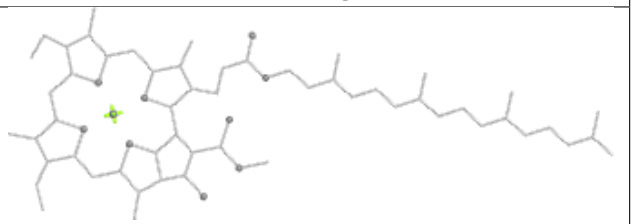
Bond lengths



Bond angles

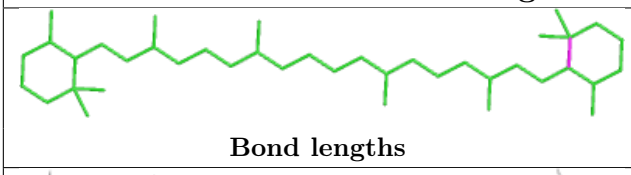


Torsions

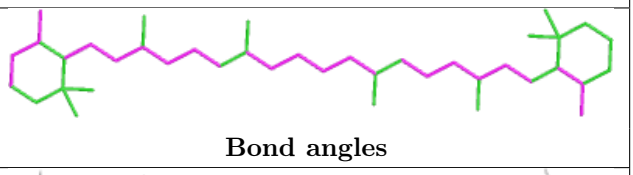


Rings

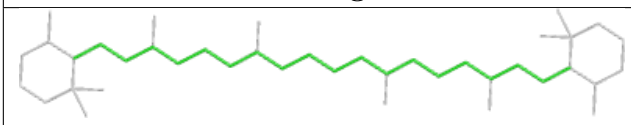
Ligand BCR e 4003



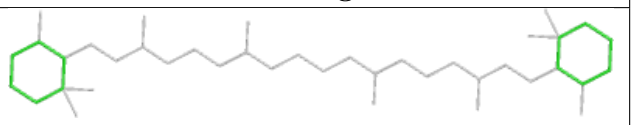
Bond lengths



Bond angles

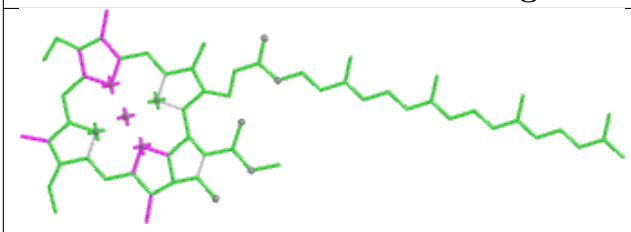


Torsions

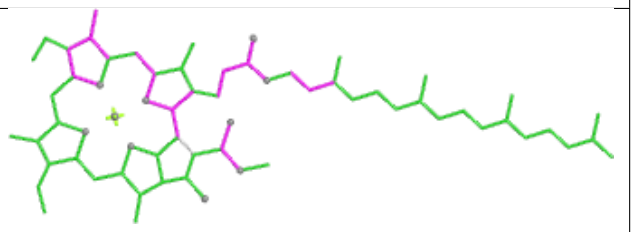


Rings

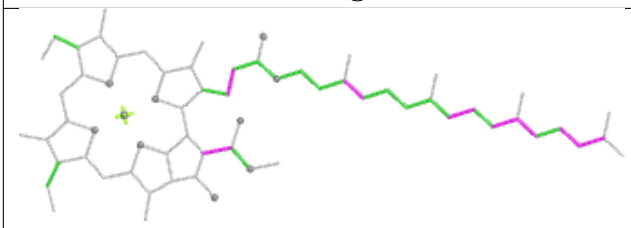
Ligand CLA e 1127



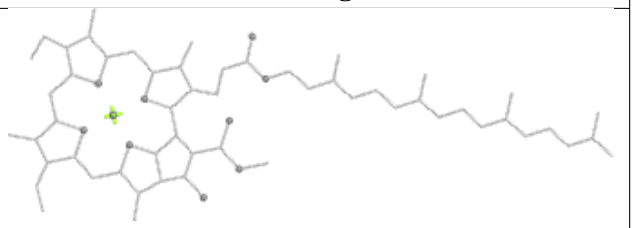
Bond lengths



Bond angles

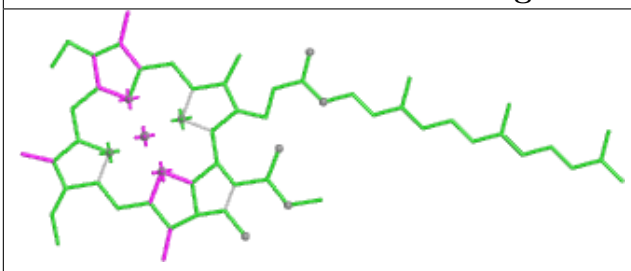


Torsions

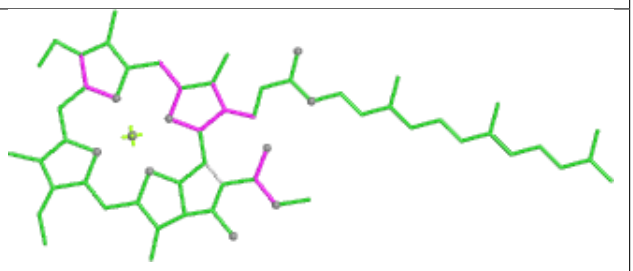


Rings

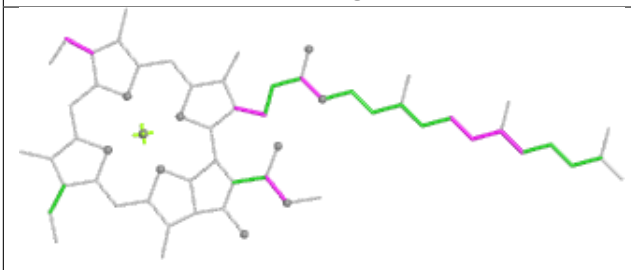
Ligand CLA H 1230



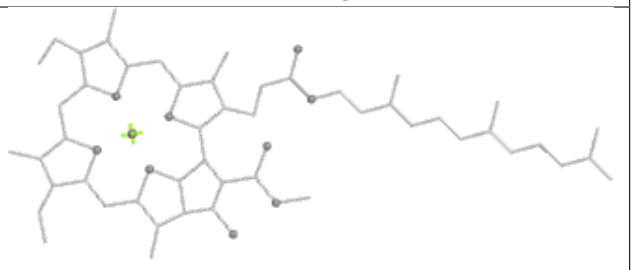
Bond lengths



Bond angles

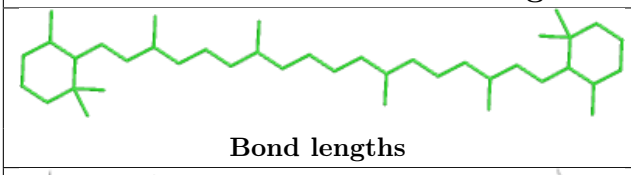


Torsions

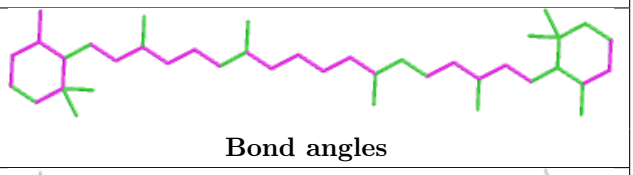


Rings

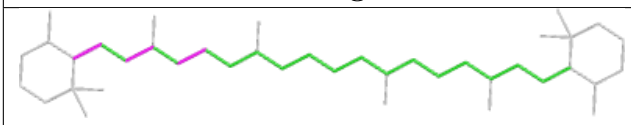
Ligand BCR 6 521



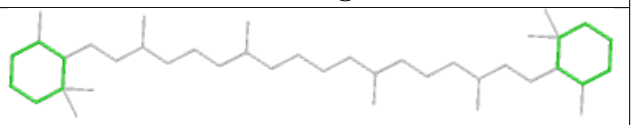
Bond lengths



Bond angles

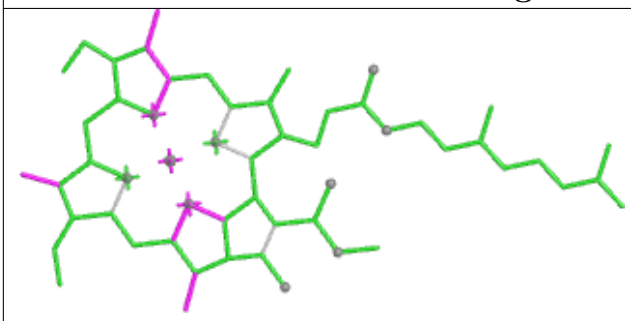


Torsions

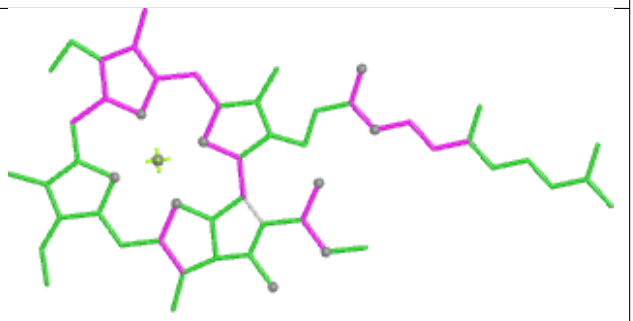


Rings

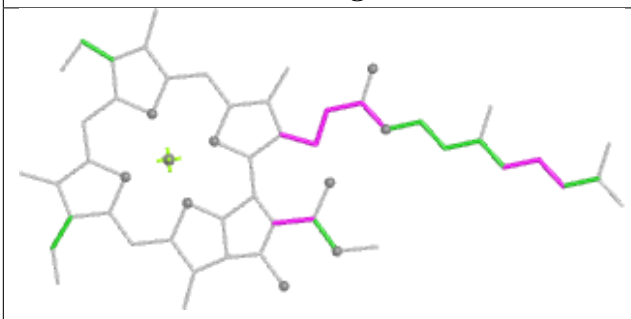
Ligand CLA A 1135



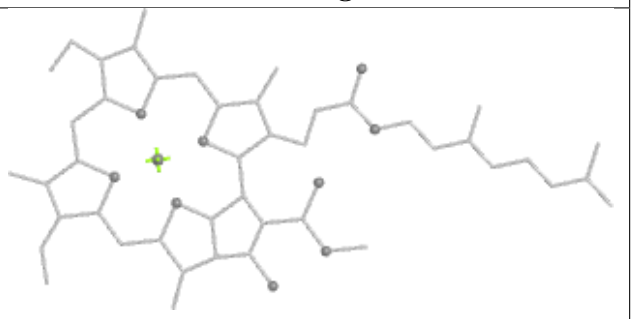
Bond lengths



Bond angles

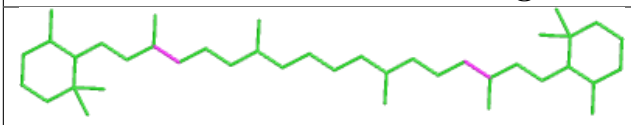


Torsions

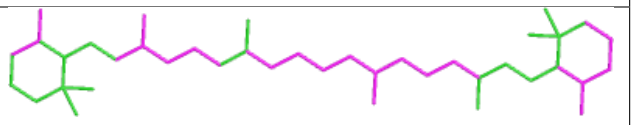


Rings

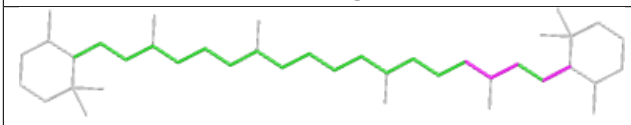
Ligand BCR L 4020



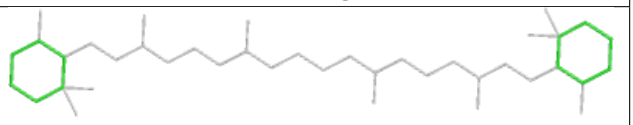
Bond lengths



Bond angles

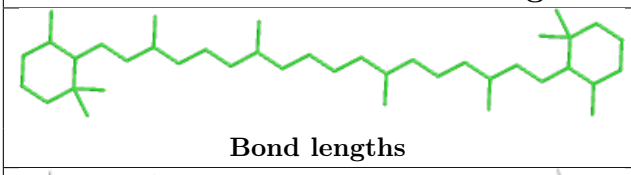


Torsions

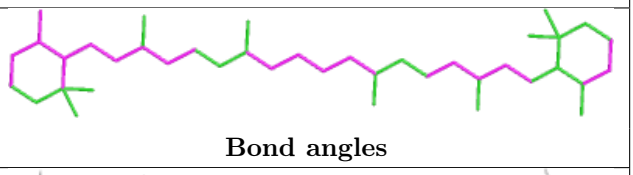


Rings

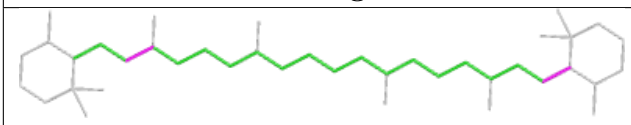
Ligand BCR 4 524



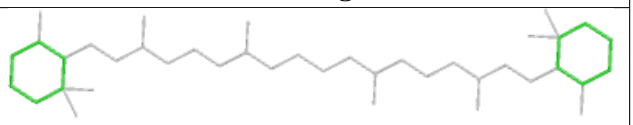
Bond lengths



Bond angles



Torsions

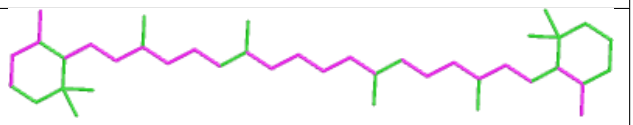


Rings

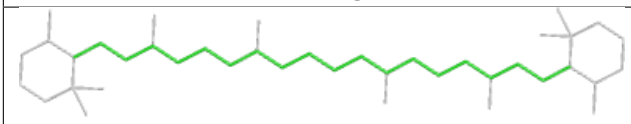
Ligand BCR G 4003



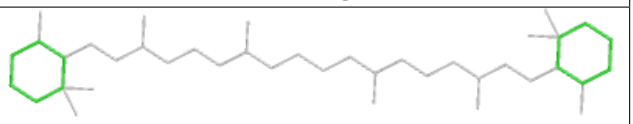
Bond lengths



Bond angles

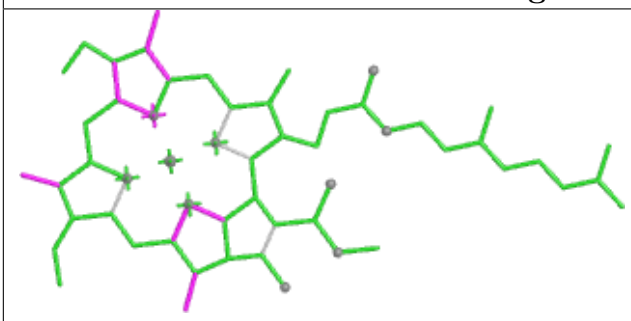


Torsions

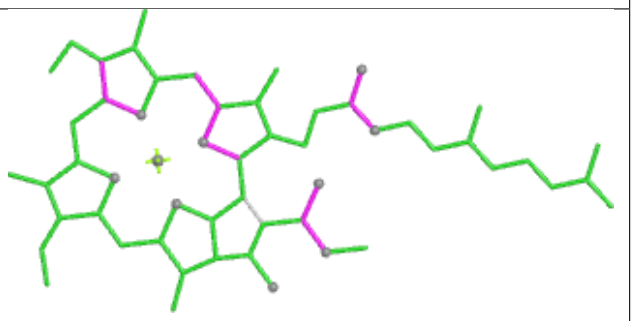


Rings

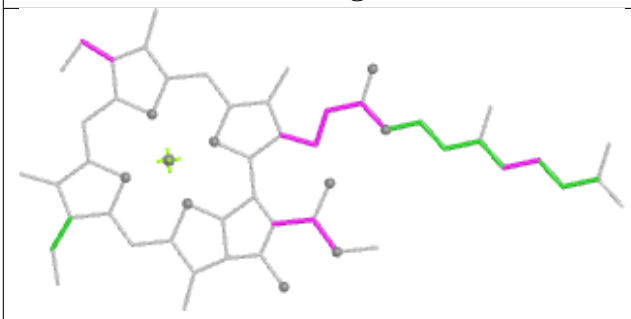
Ligand CLA a 518



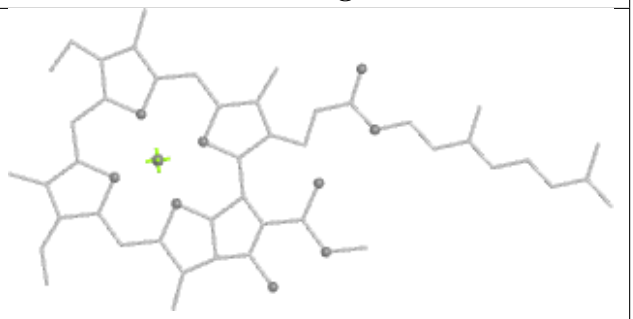
Bond lengths



Bond angles

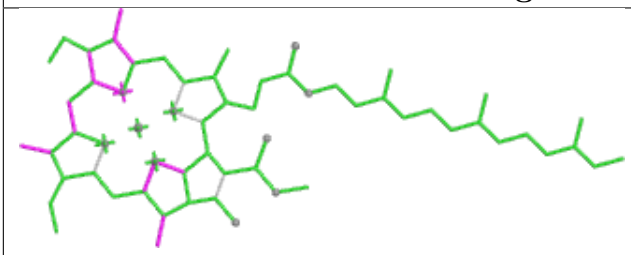


Torsions

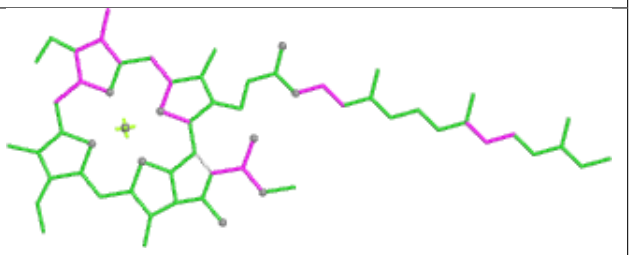


Rings

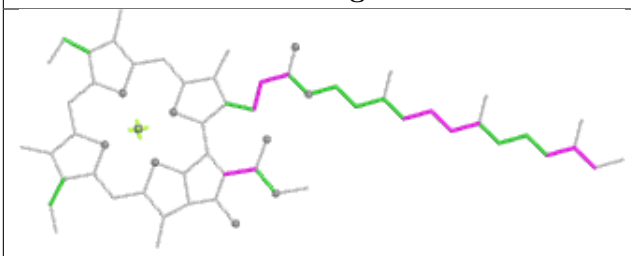
Ligand CLA B 1213



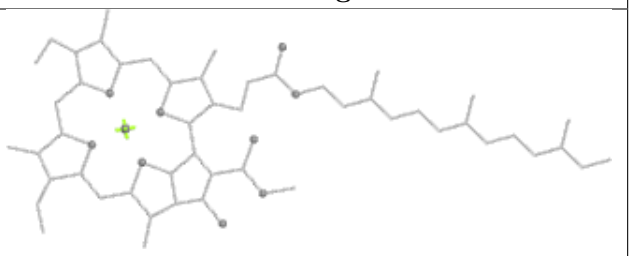
Bond lengths



Bond angles

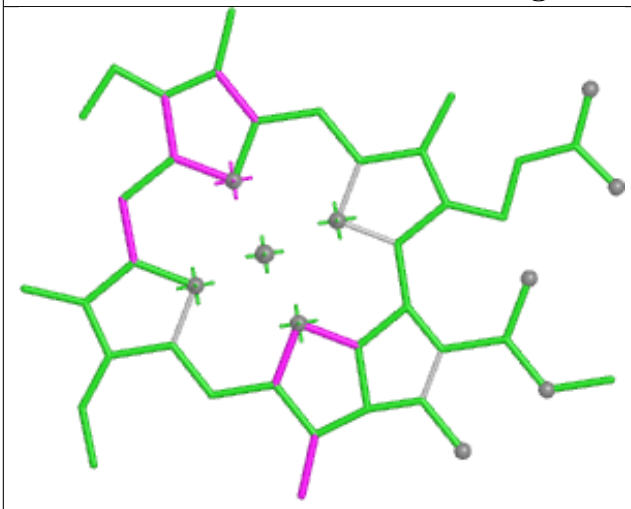


Torsions

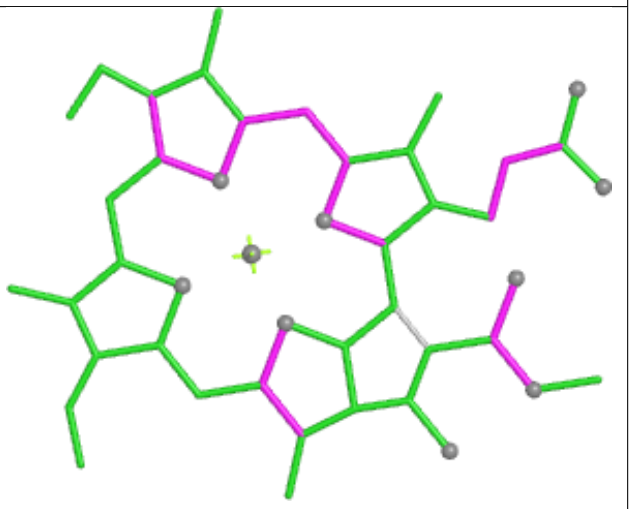


Rings

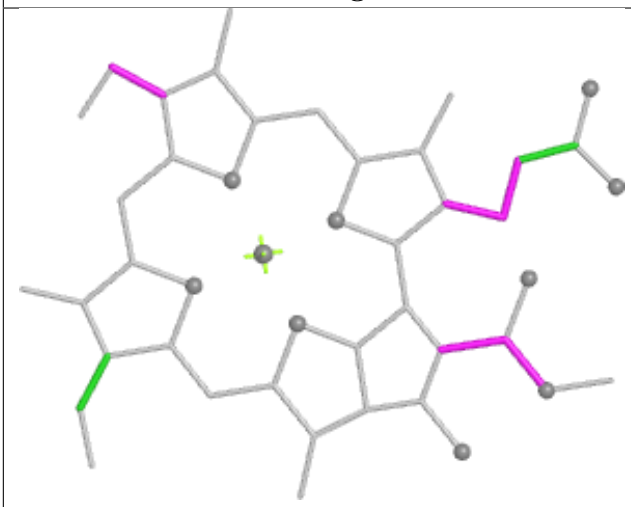
Ligand CLA s 503



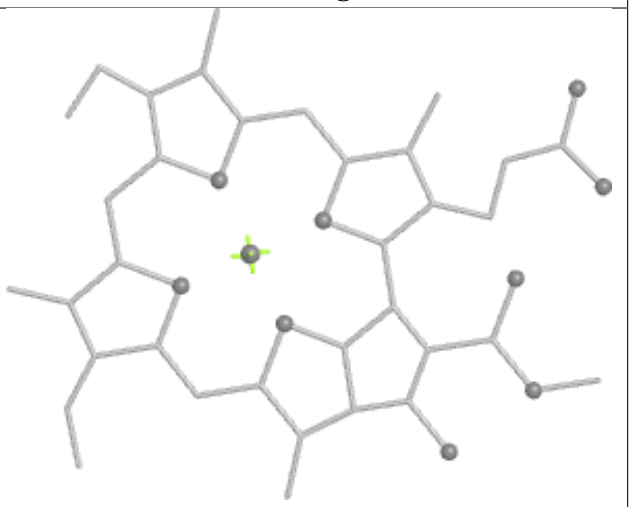
Bond lengths



Bond angles

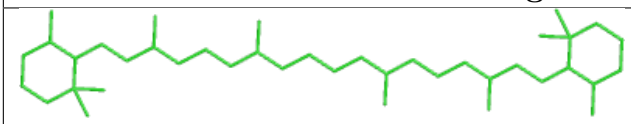


Torsions

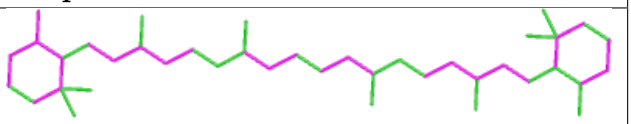


Rings

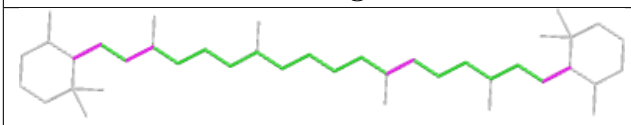
Ligand BCR q 521



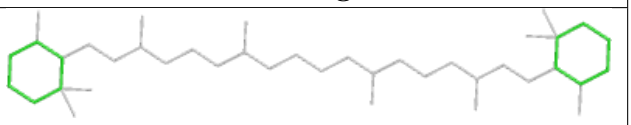
Bond lengths



Bond angles

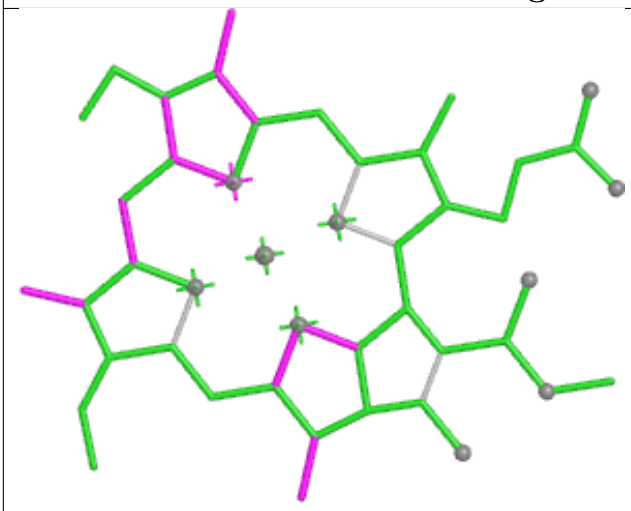


Torsions

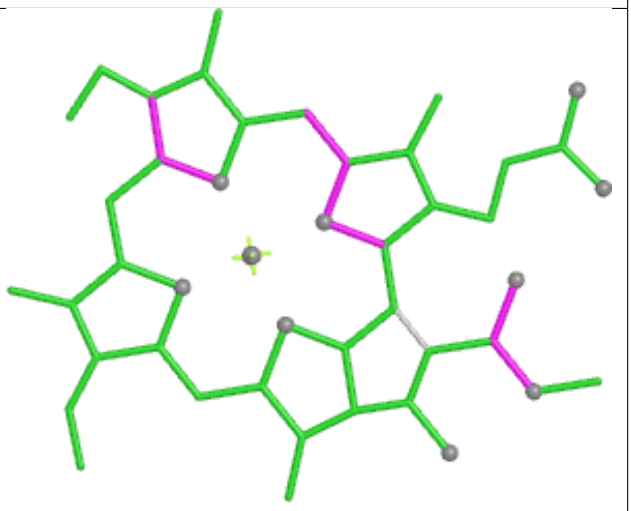


Rings

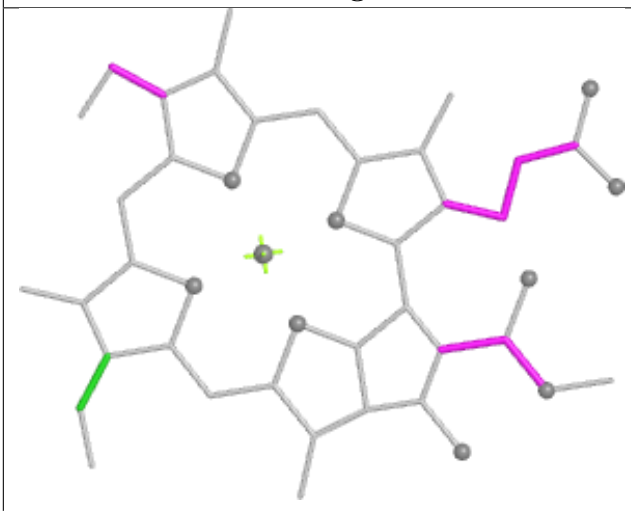
Ligand CLA 5 517



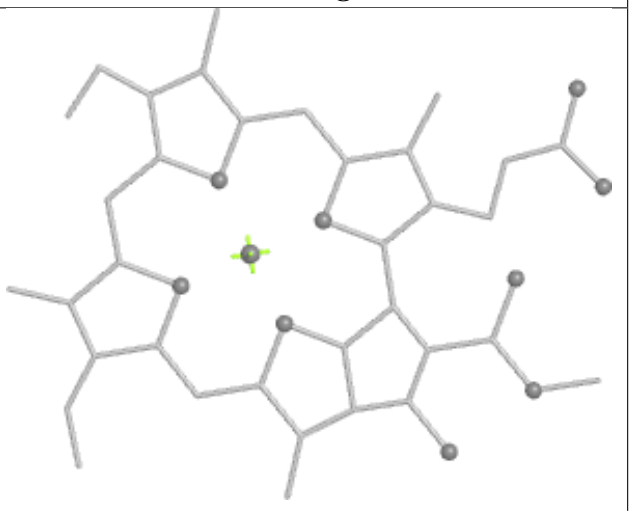
Bond lengths



Bond angles

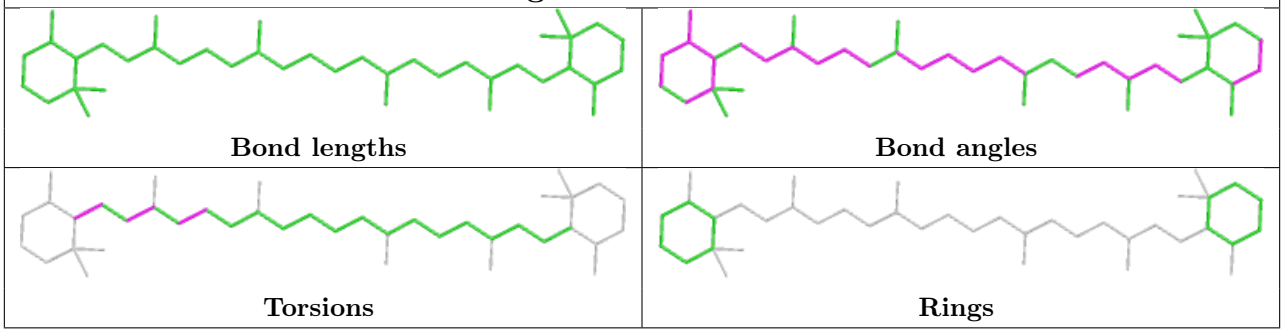


Torsions

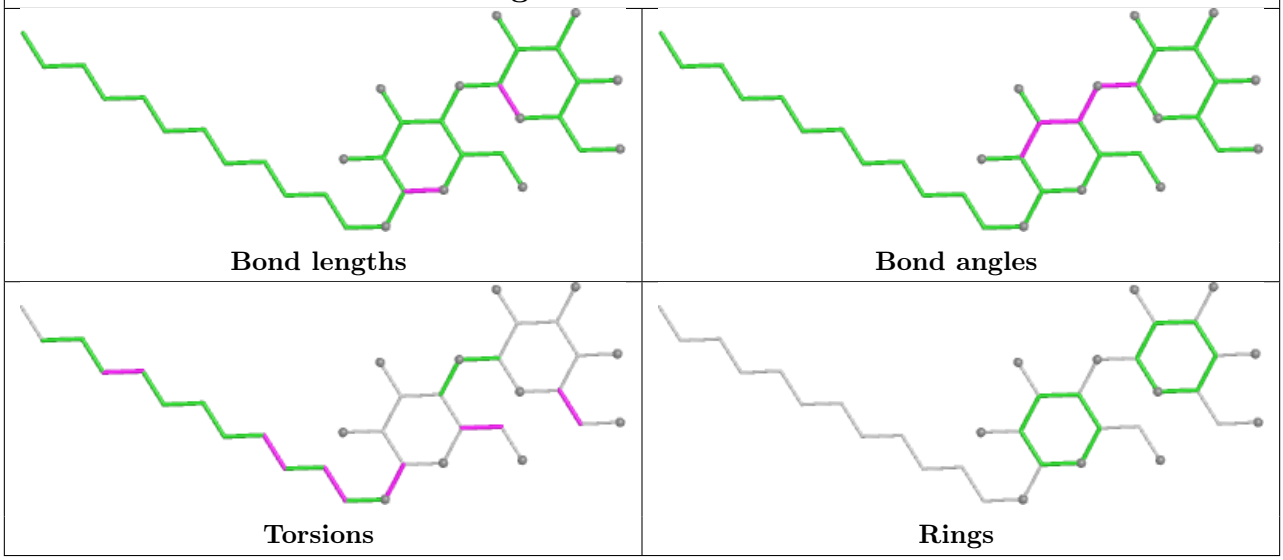


Rings

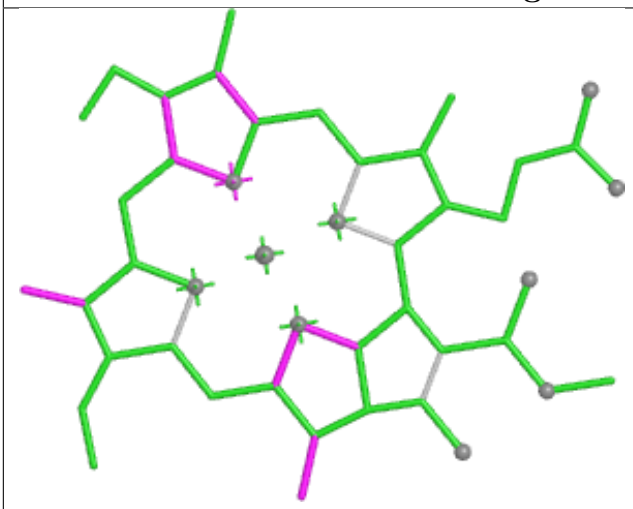
Ligand BCR v 521



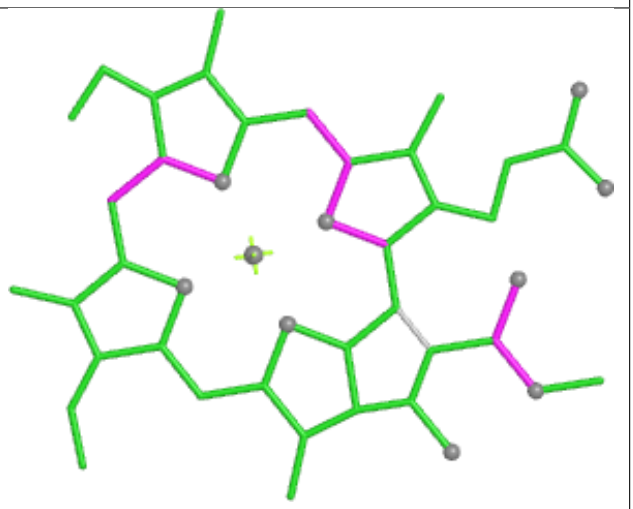
Ligand LMU G 1848



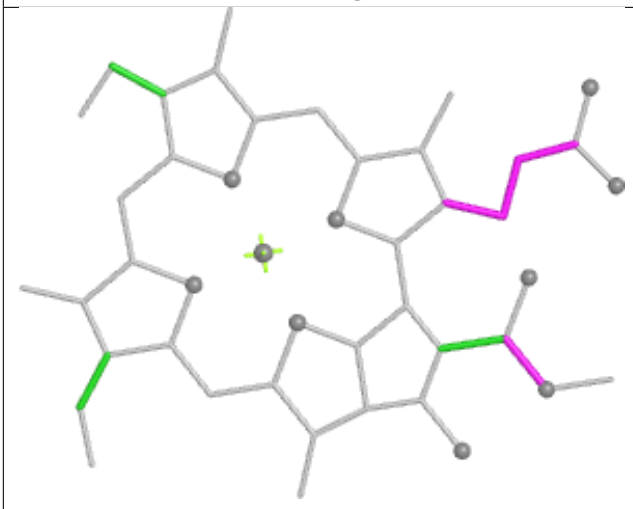
Ligand CLA Y 505



Bond lengths



Bond angles

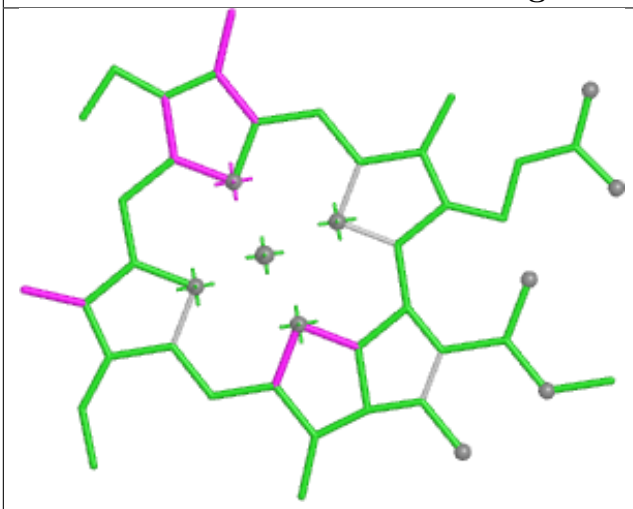


Torsions

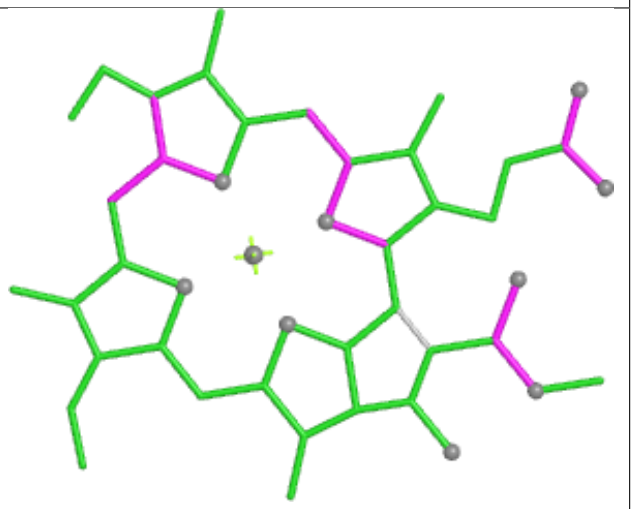


Rings

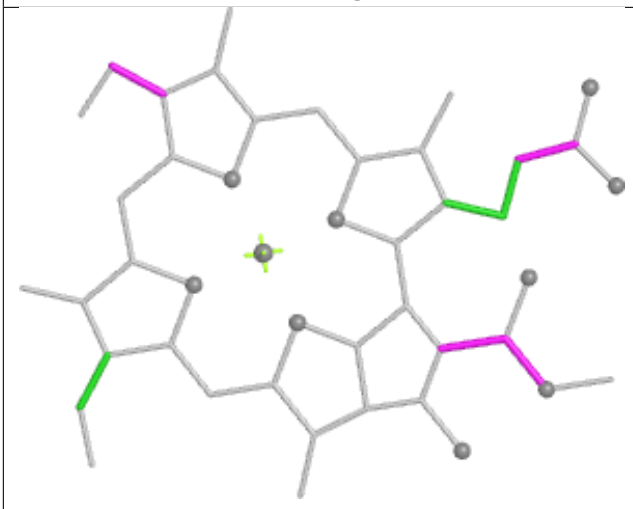
Ligand CLA 3 519



Bond lengths



Bond angles

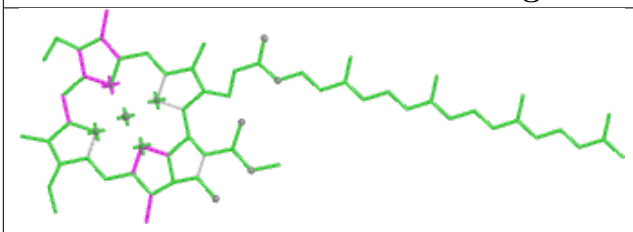


Torsions

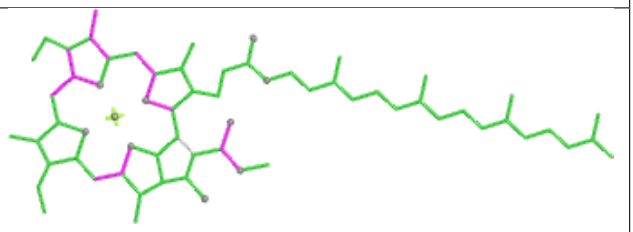


Rings

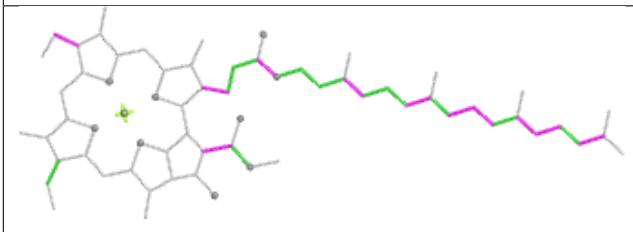
Ligand CLA f 1208



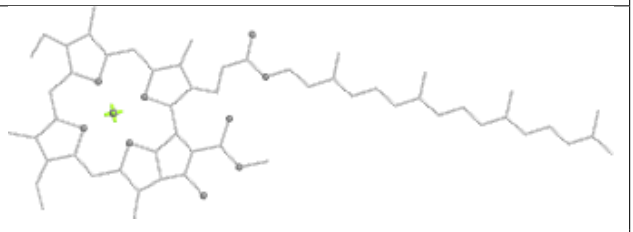
Bond lengths



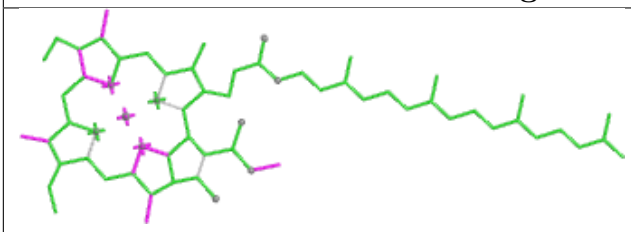
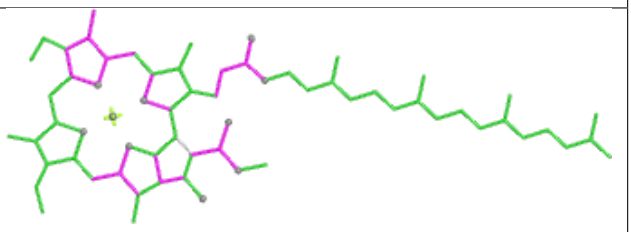
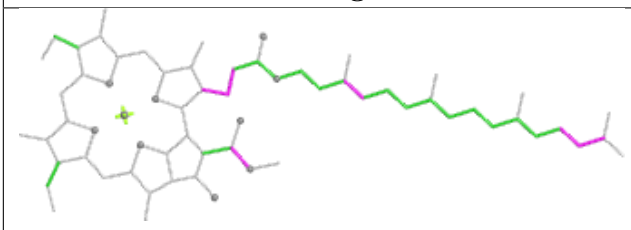
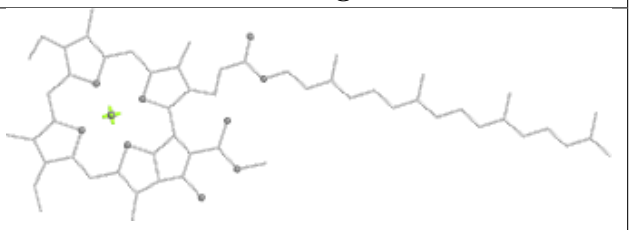
Bond angles

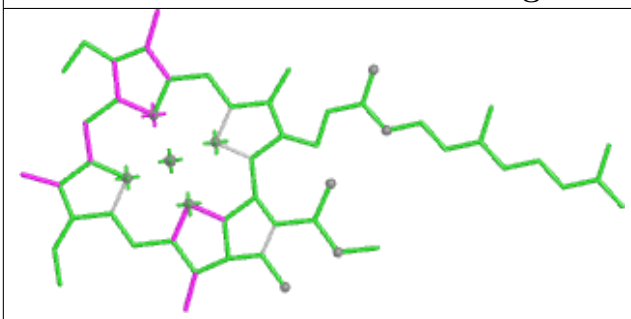
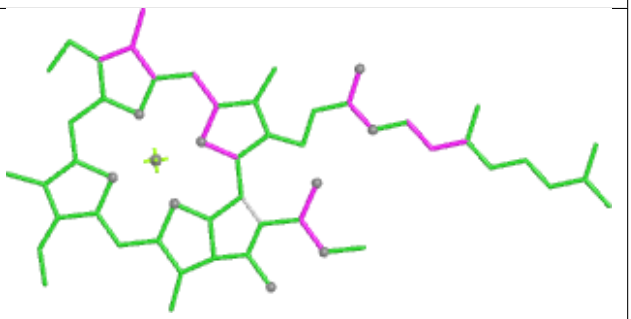
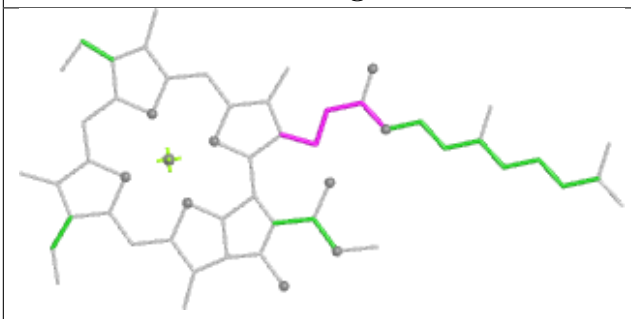
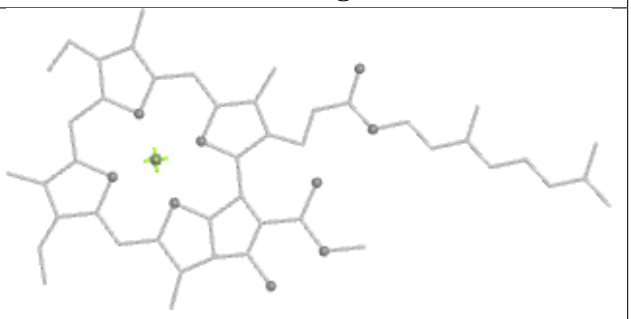


Torsions

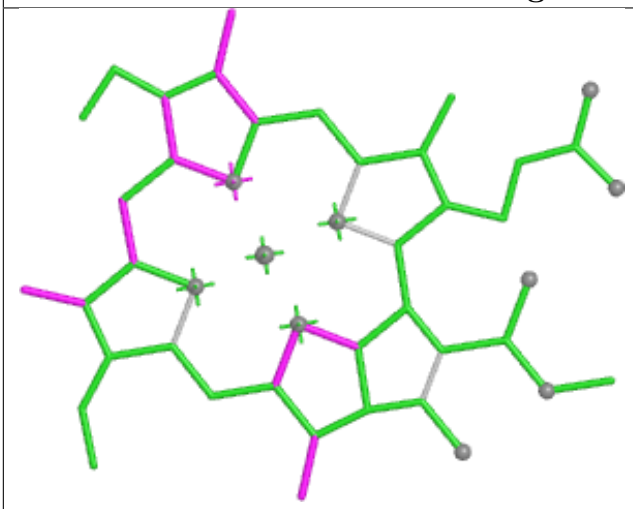


Rings

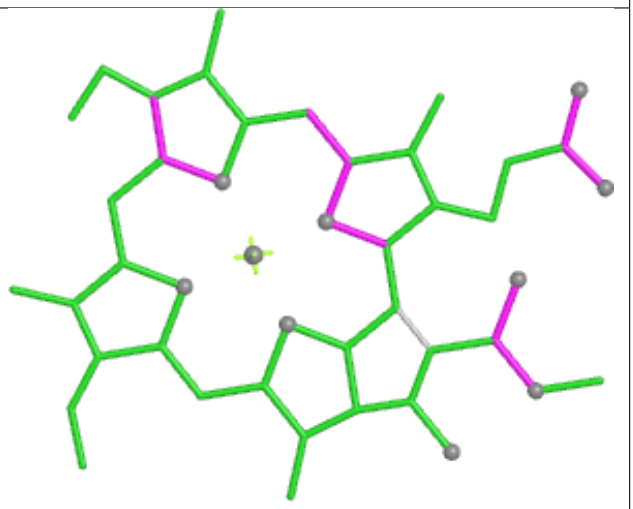
Ligand CLA e 1022	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 1228	
 Bond lengths	 Bond angles
 Torsions	 Rings

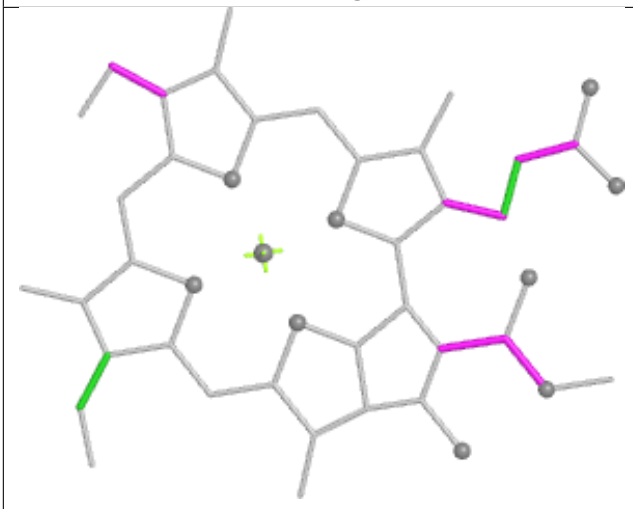
Ligand CLA d 519



Bond lengths



Bond angles

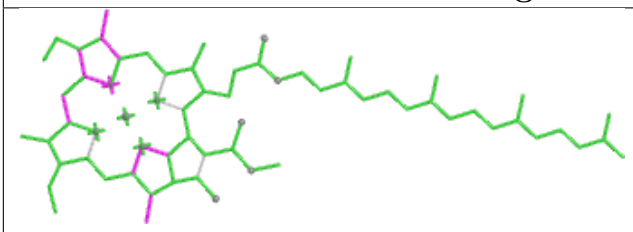


Torsions

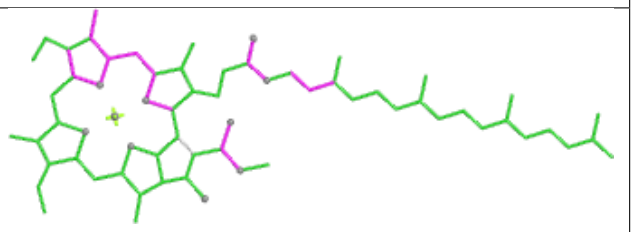


Rings

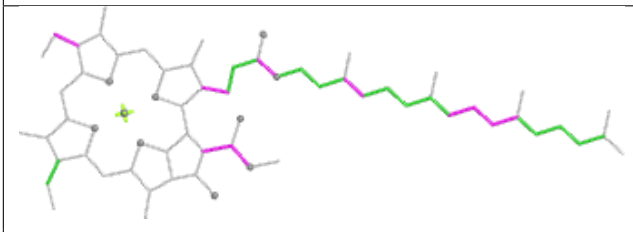
Ligand CLA B 1240



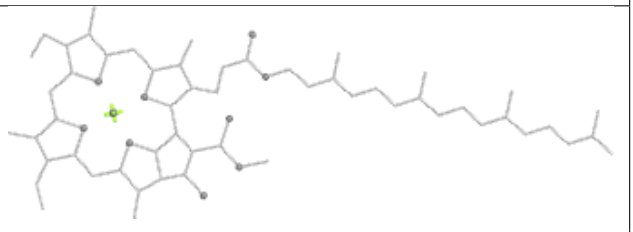
Bond lengths



Bond angles

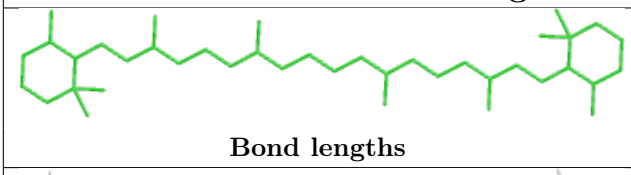


Torsions

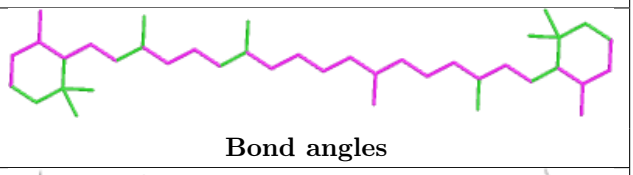


Rings

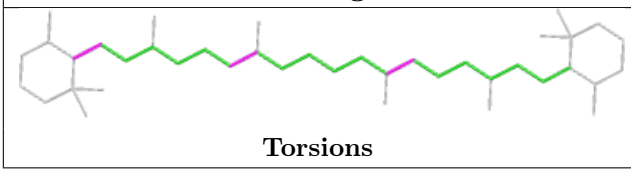
Ligand BCR M 4021



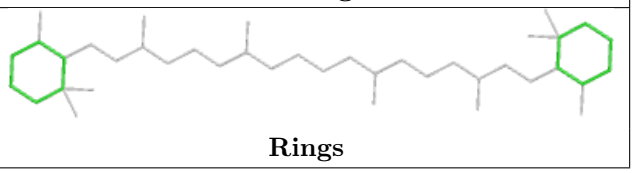
Bond lengths



Bond angles

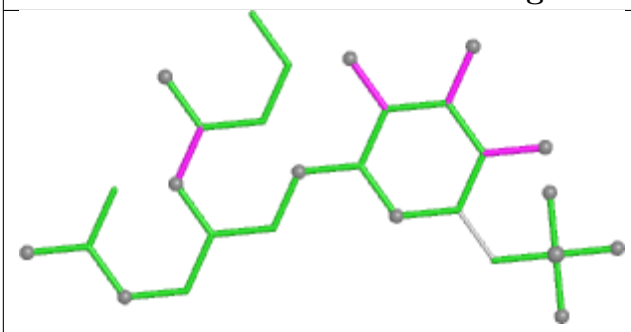


Torsions

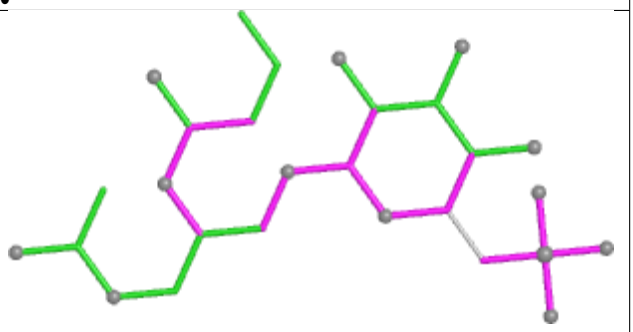


Rings

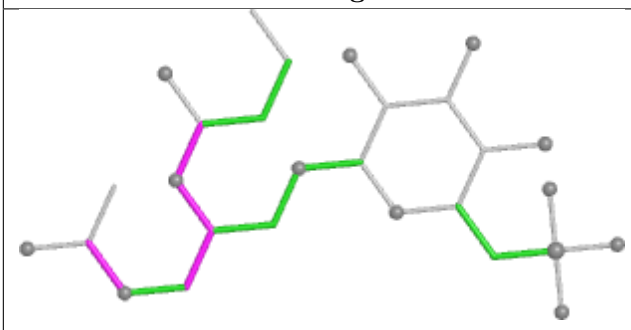
Ligand SQD Z 822



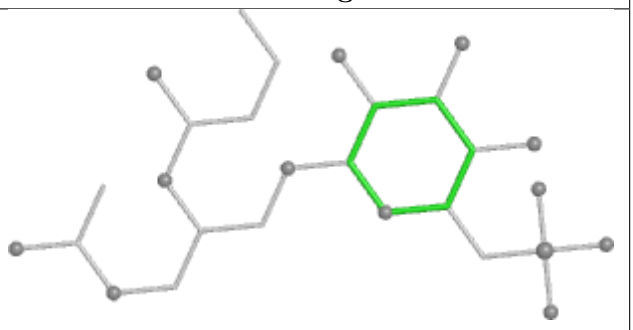
Bond lengths



Bond angles

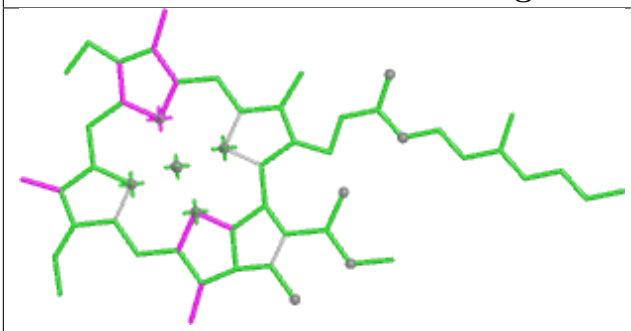


Torsions

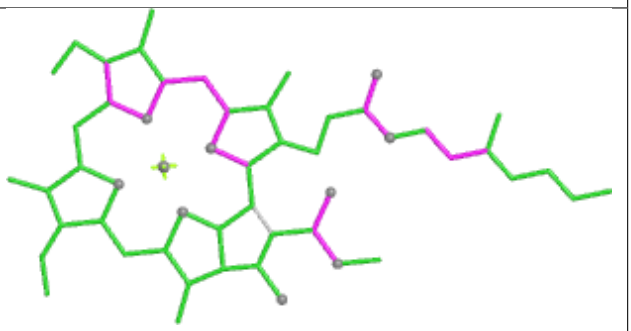


Rings

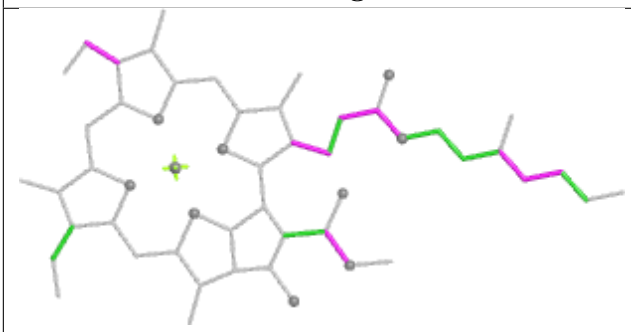
Ligand CLA A 1110



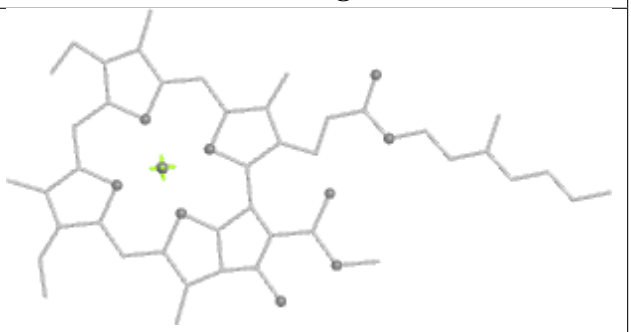
Bond lengths



Bond angles

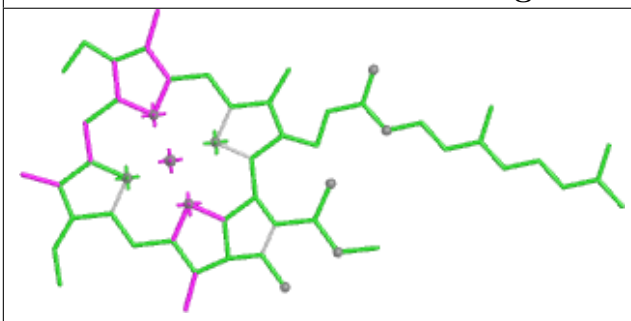


Torsions

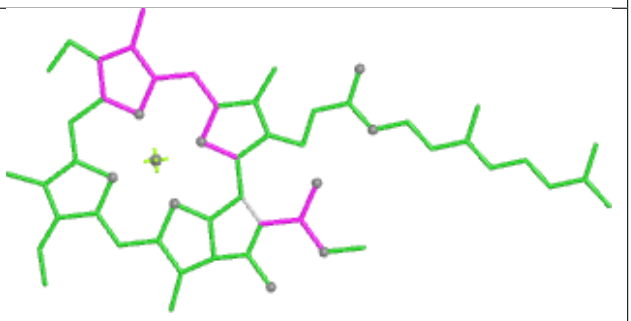


Rings

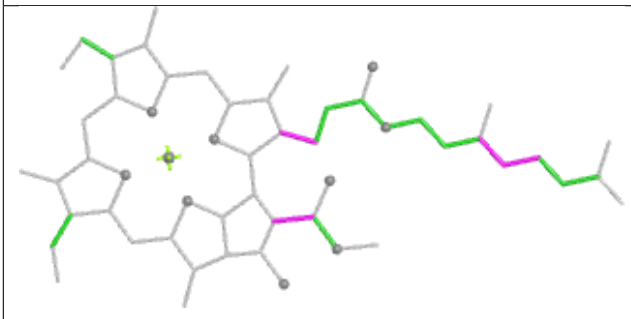
Ligand CLA A 1102



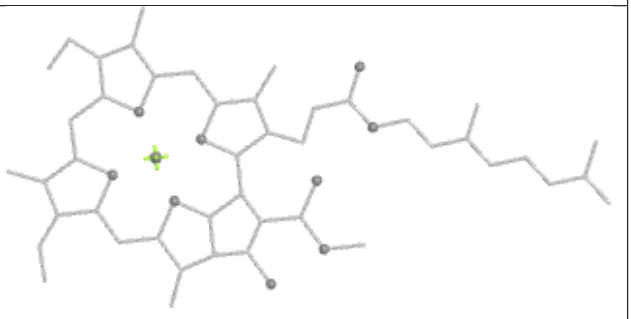
Bond lengths



Bond angles

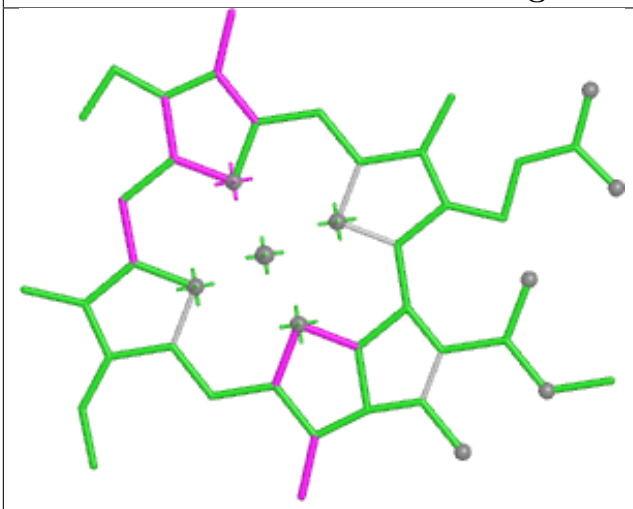


Torsions

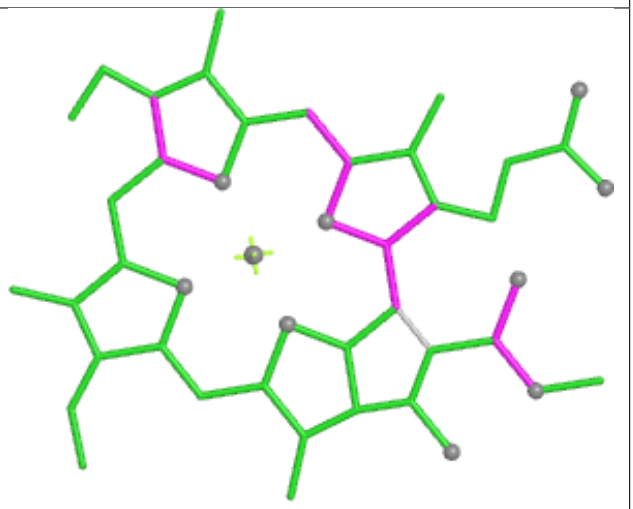


Rings

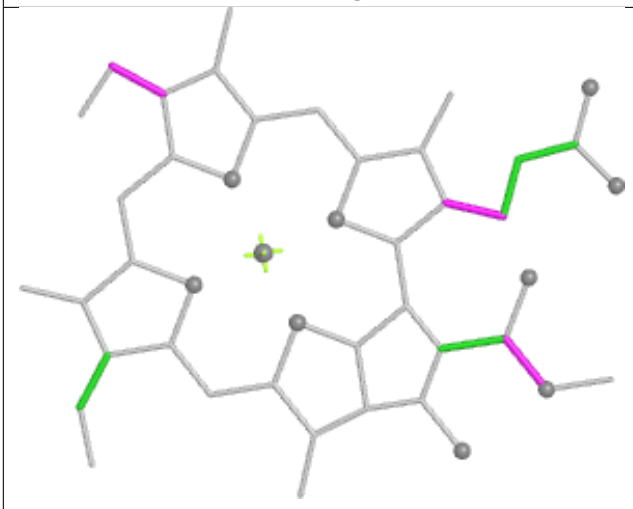
Ligand CLA 5 504



Bond lengths



Bond angles

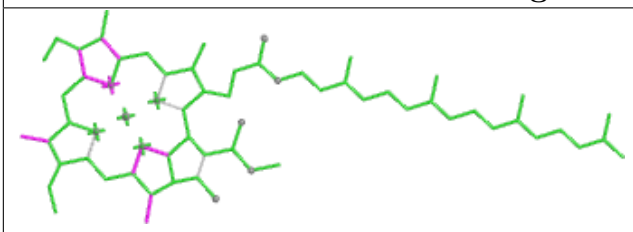


Torsions

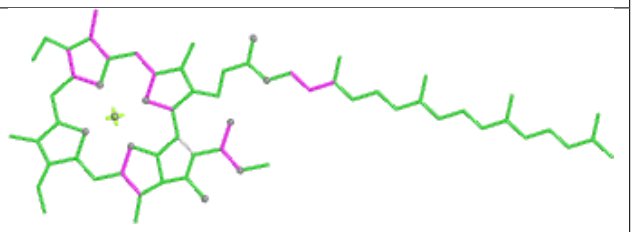


Rings

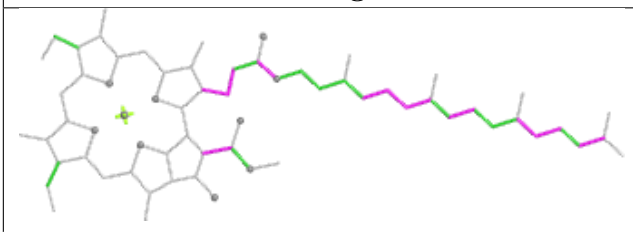
Ligand CLA r 505



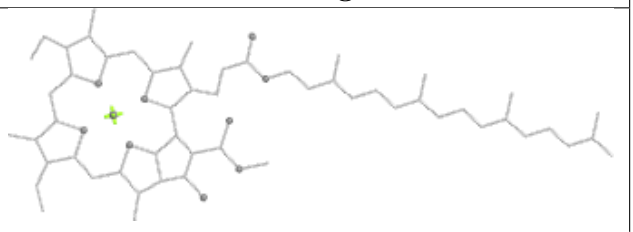
Bond lengths



Bond angles

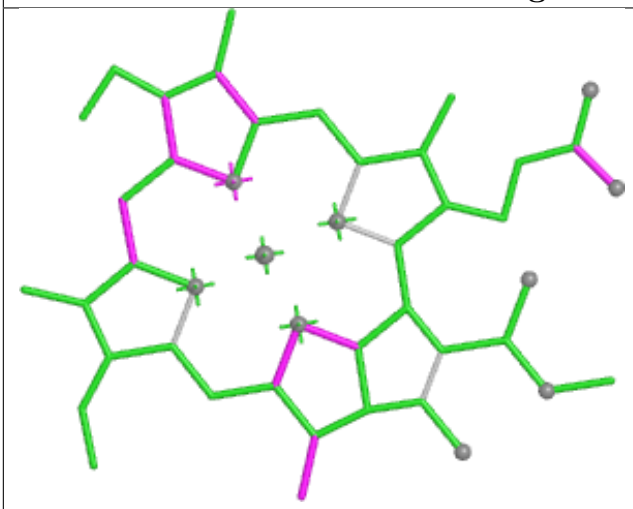


Torsions

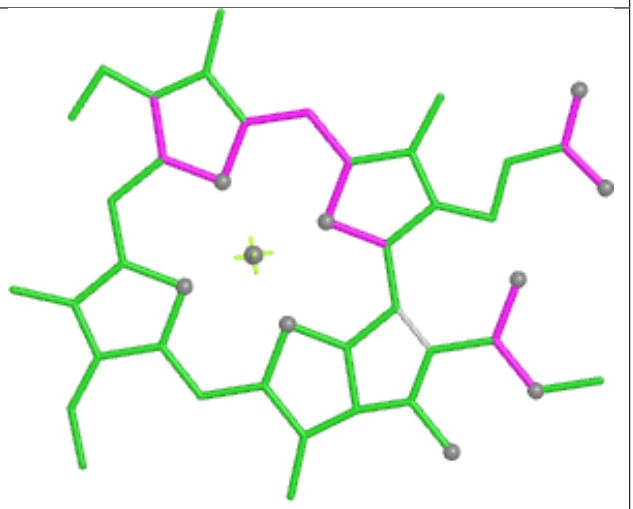


Rings

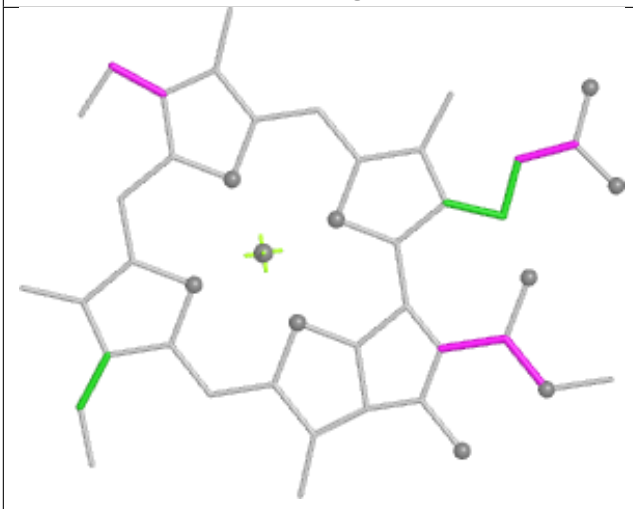
Ligand CLA a 510



Bond lengths



Bond angles

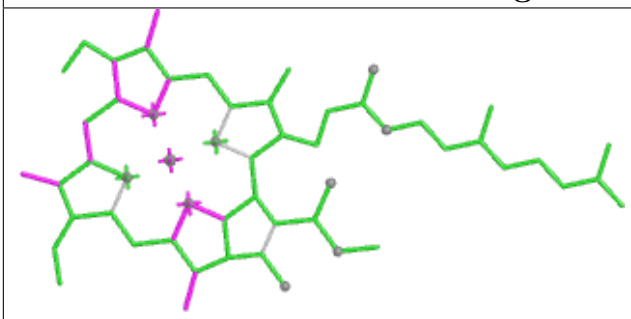


Torsions

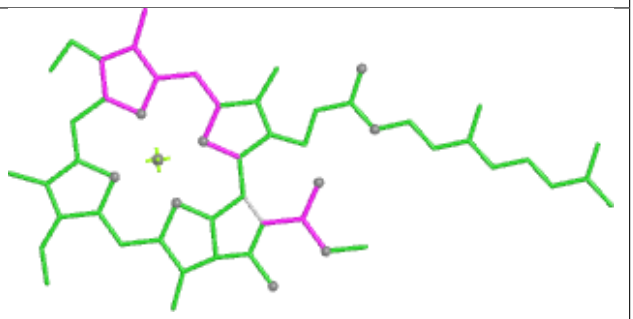


Rings

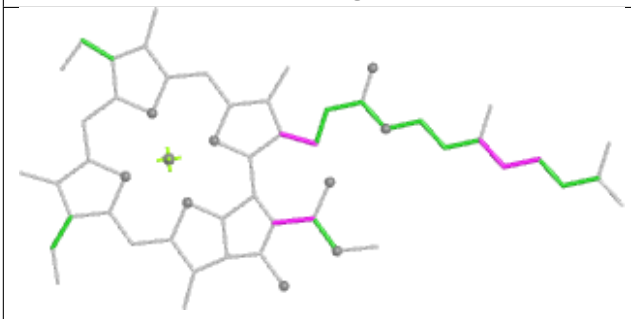
Ligand CLA G 1102



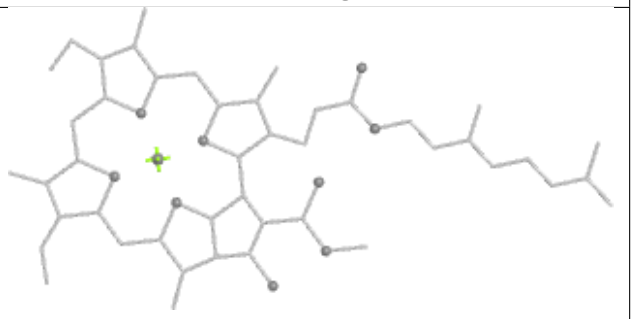
Bond lengths



Bond angles

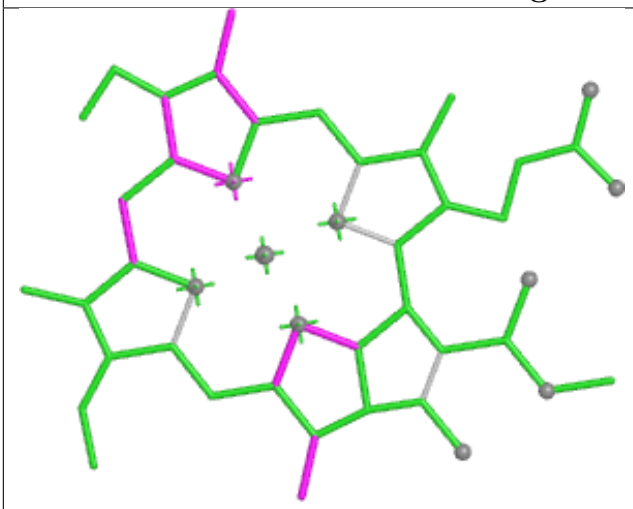


Torsions

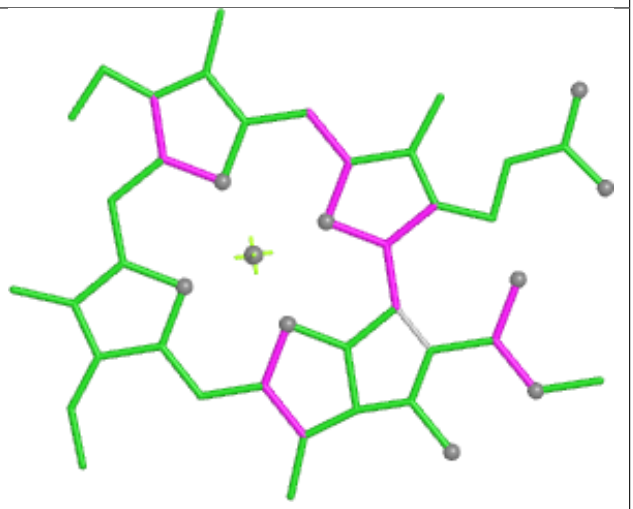


Rings

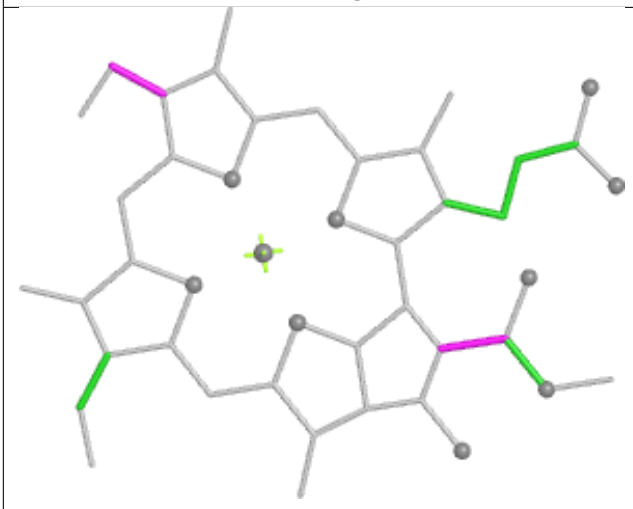
Ligand CLA t 503



Bond lengths



Bond angles

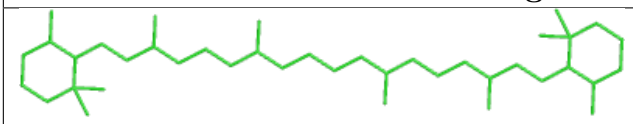


Torsions

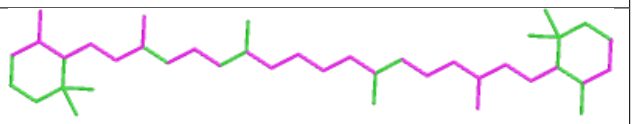


Rings

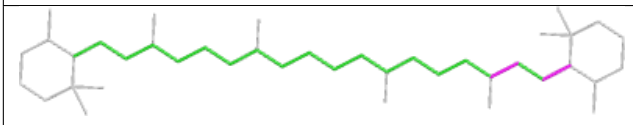
Ligand BCR u 523



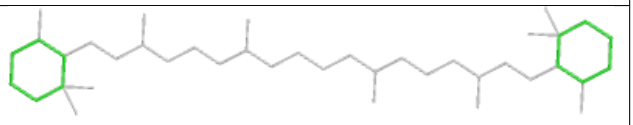
Bond lengths



Bond angles

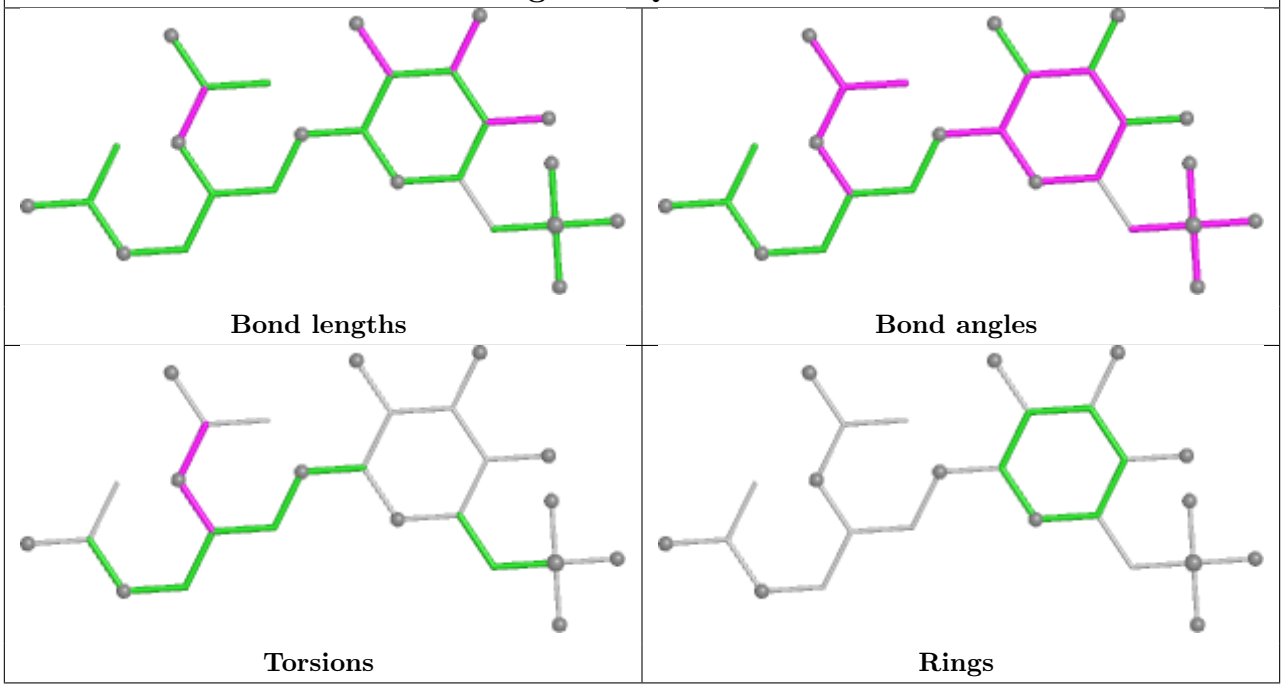


Torsions

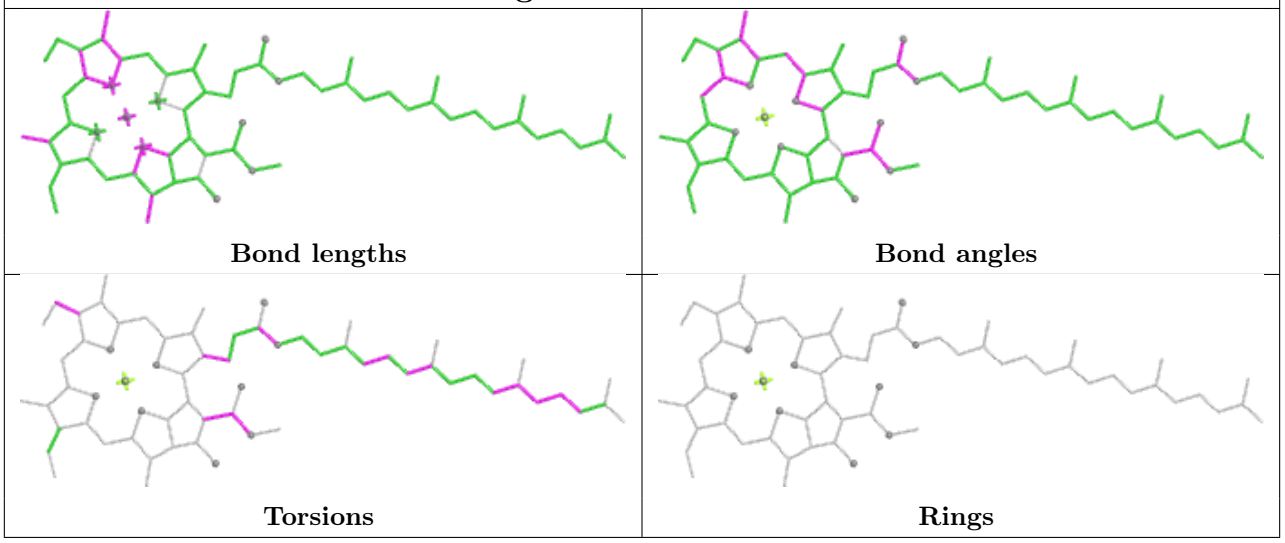


Rings

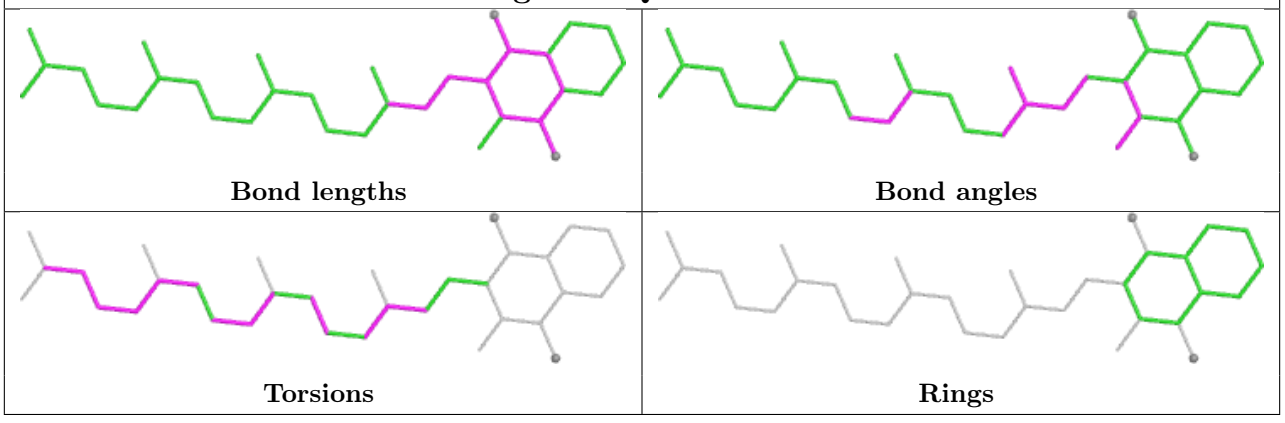
Ligand SQD u 822



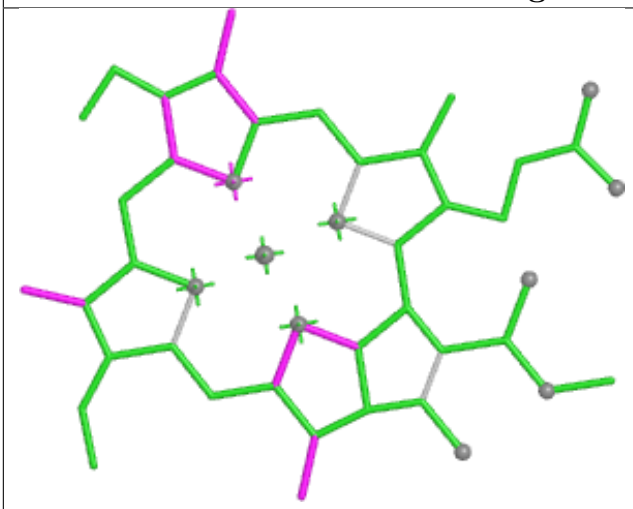
Ligand CLA A 1109



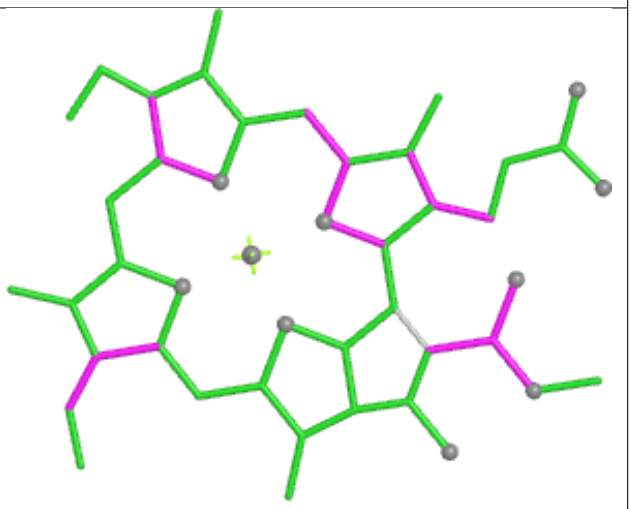
Ligand PQN A 2001



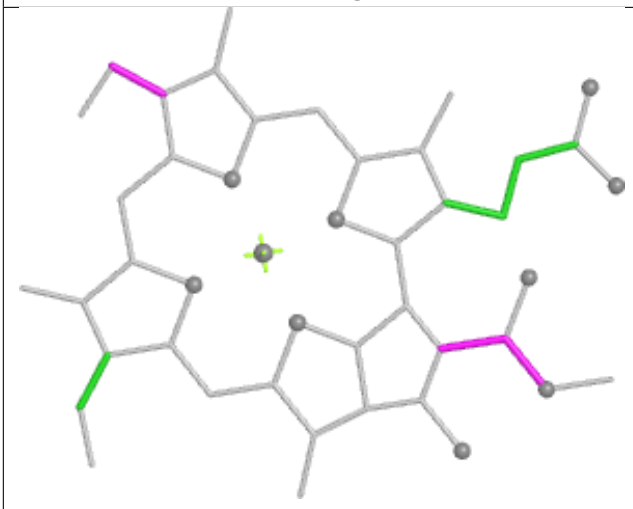
Ligand CLA 1 504



Bond lengths



Bond angles

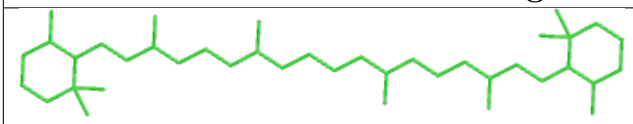


Torsions

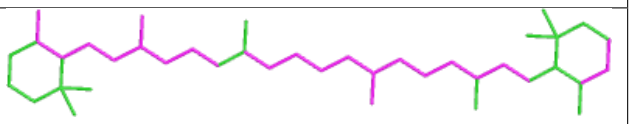


Rings

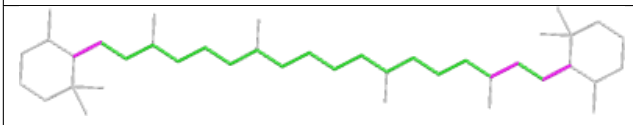
Ligand BCR 4 523



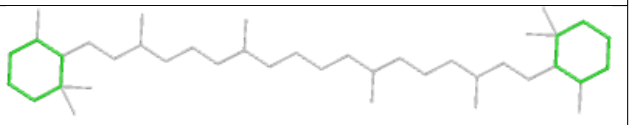
Bond lengths



Bond angles

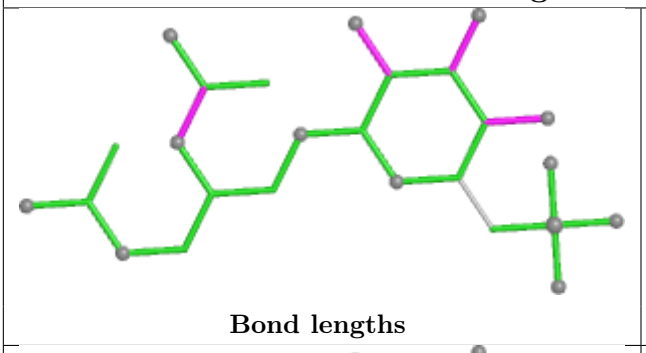


Torsions

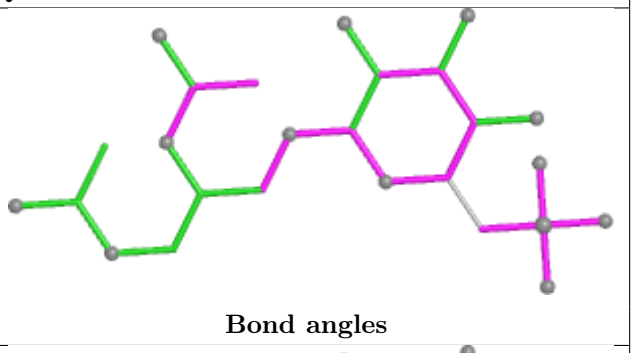


Rings

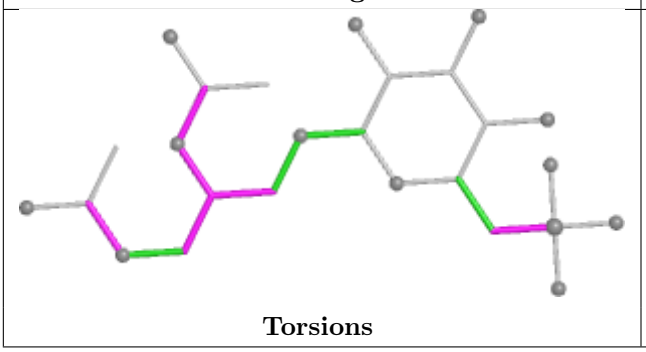
Ligand SQD t 822



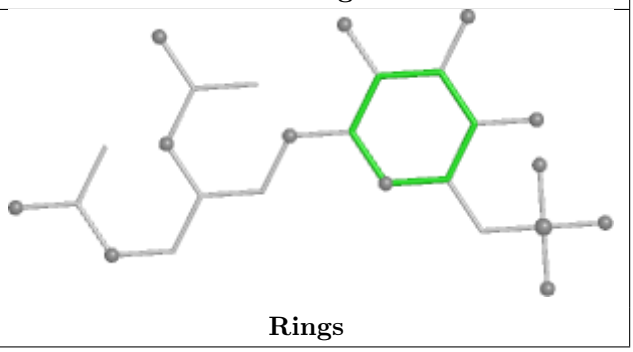
Bond lengths



Bond angles

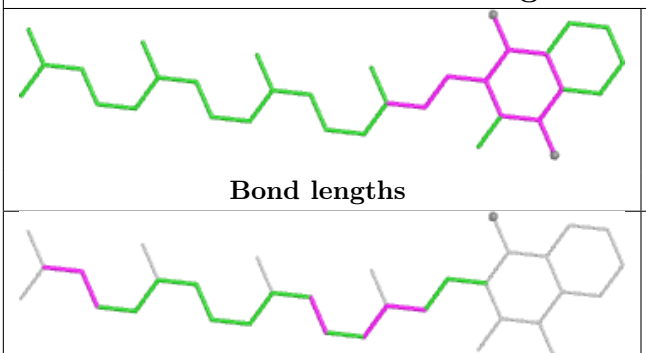


Torsions

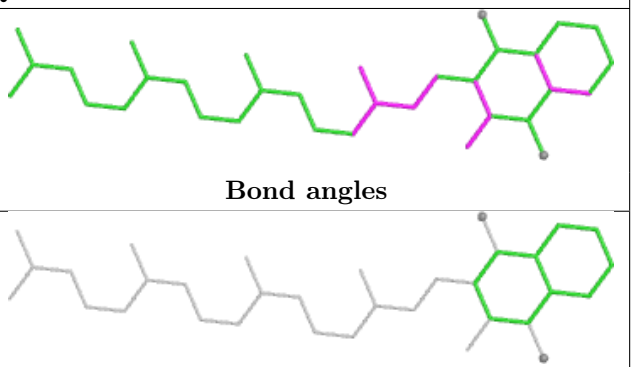


Rings

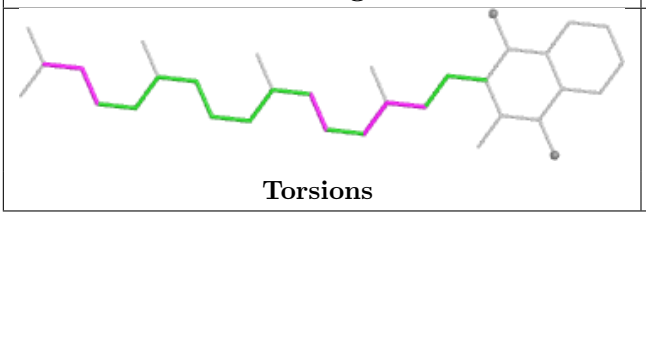
Ligand PQN f 2002



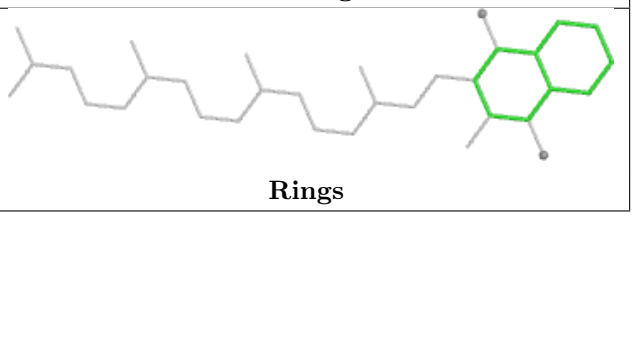
Bond lengths



Bond angles

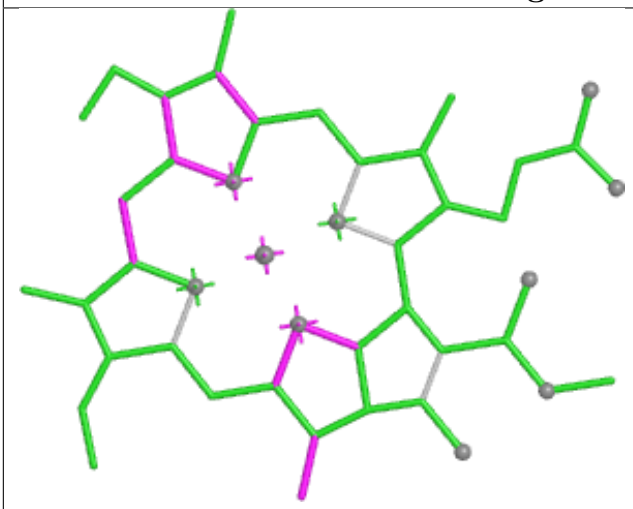


Torsions

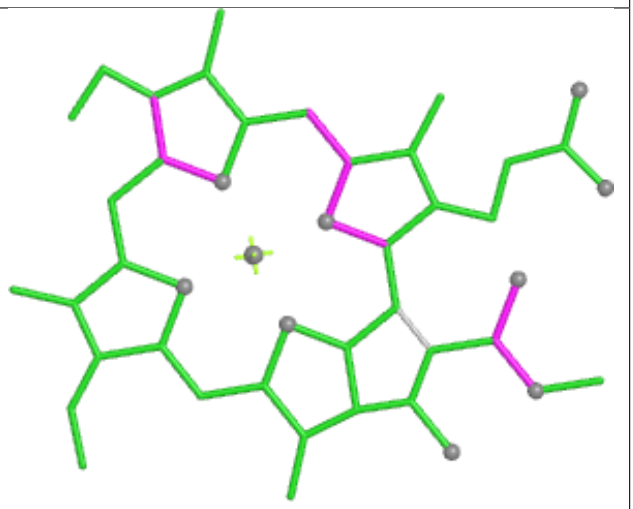


Rings

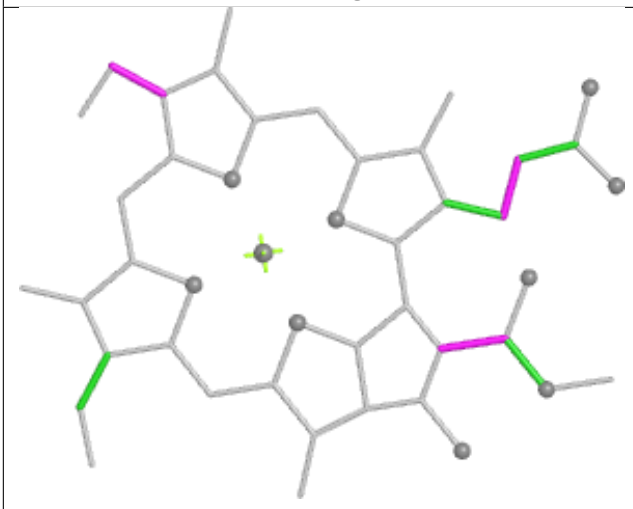
Ligand CLA b 505



Bond lengths



Bond angles

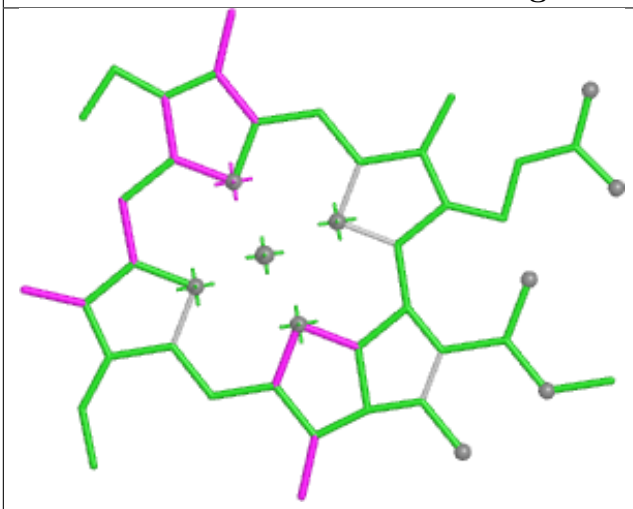


Torsions

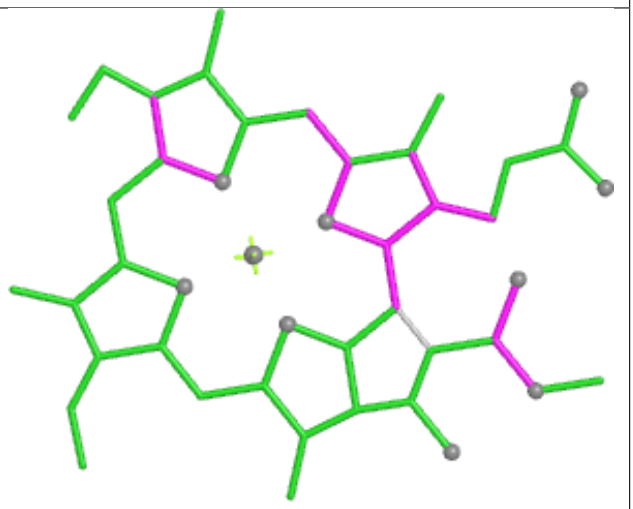


Rings

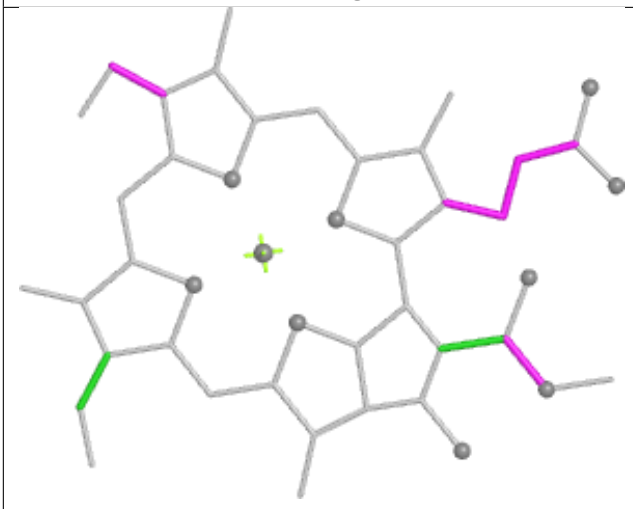
Ligand CLA c 501



Bond lengths



Bond angles

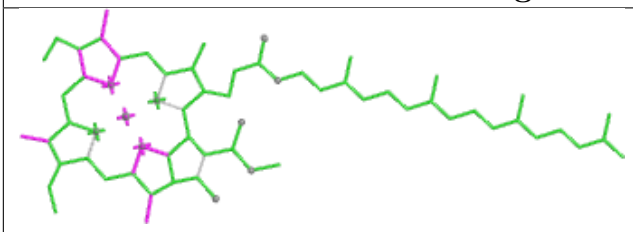


Torsions

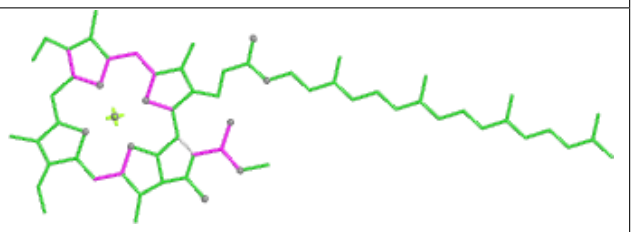


Rings

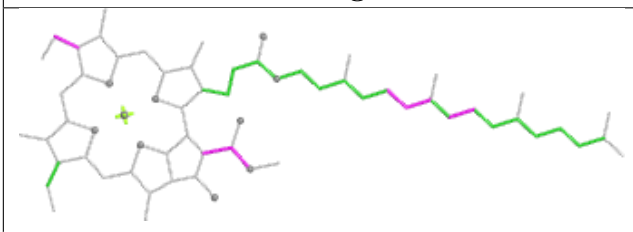
Ligand CLA H 1235



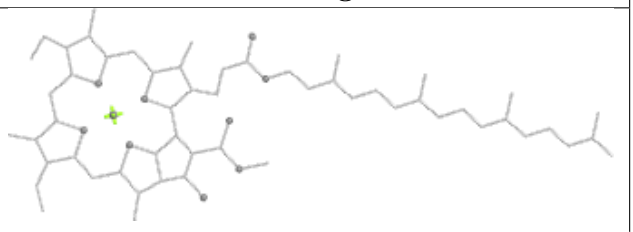
Bond lengths



Bond angles

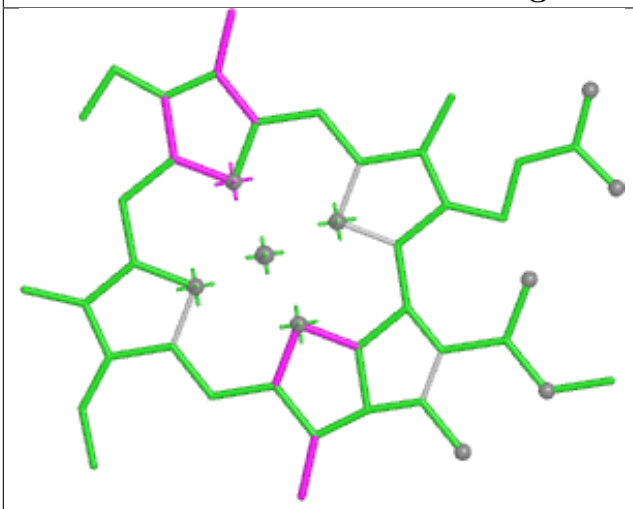


Torsions

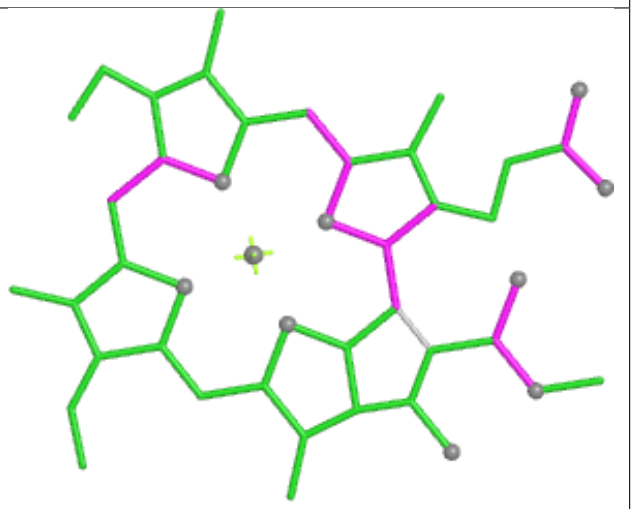


Rings

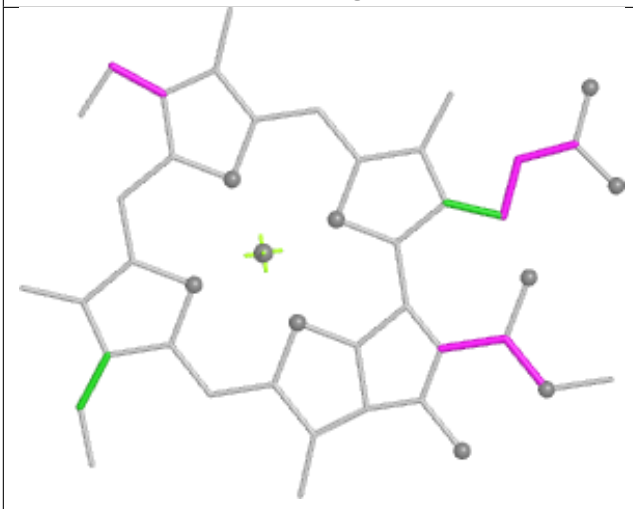
Ligand CLA c 507



Bond lengths



Bond angles

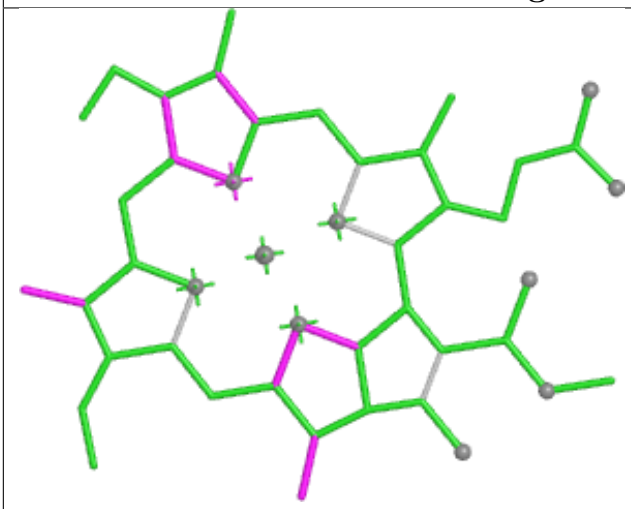


Torsions

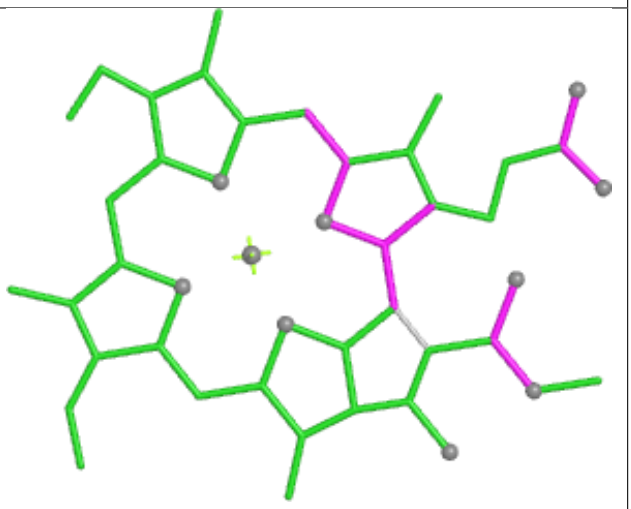


Rings

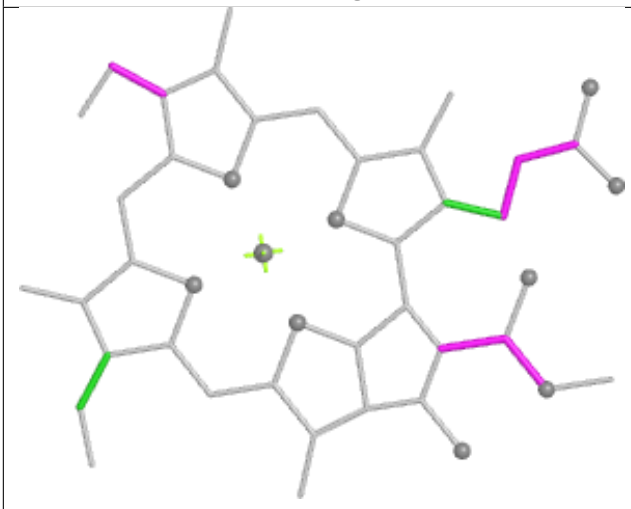
Ligand CLA 1 507



Bond lengths



Bond angles

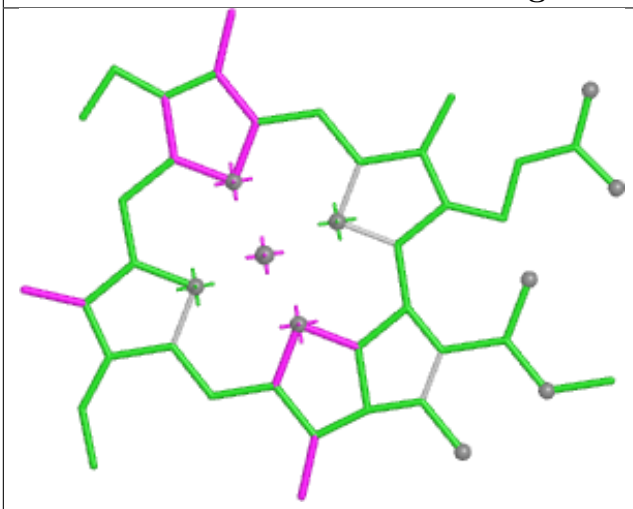


Torsions

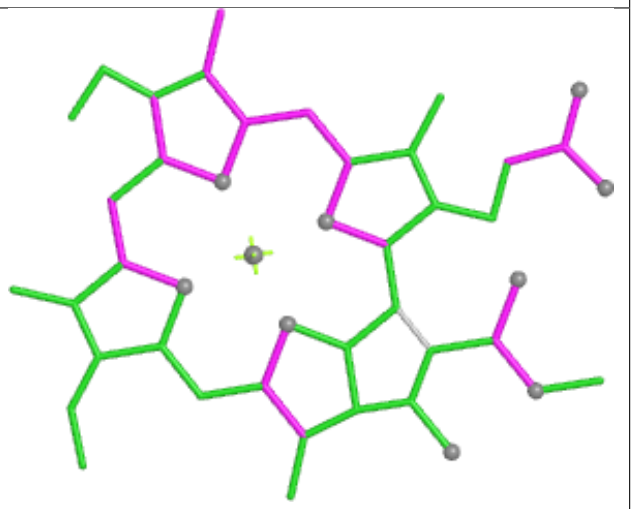


Rings

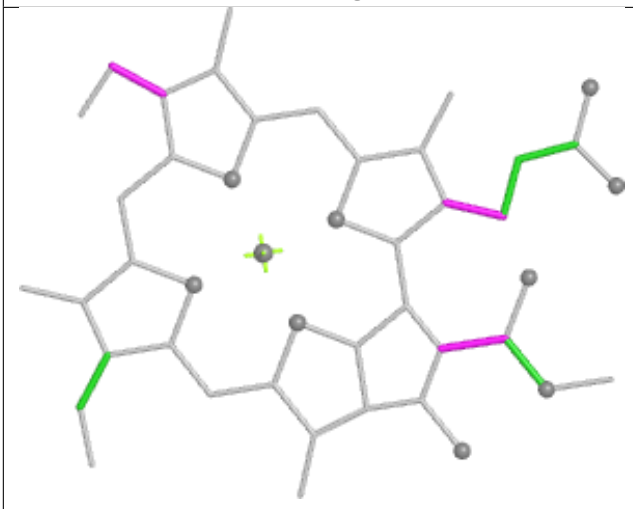
Ligand CLA 2 508



Bond lengths



Bond angles

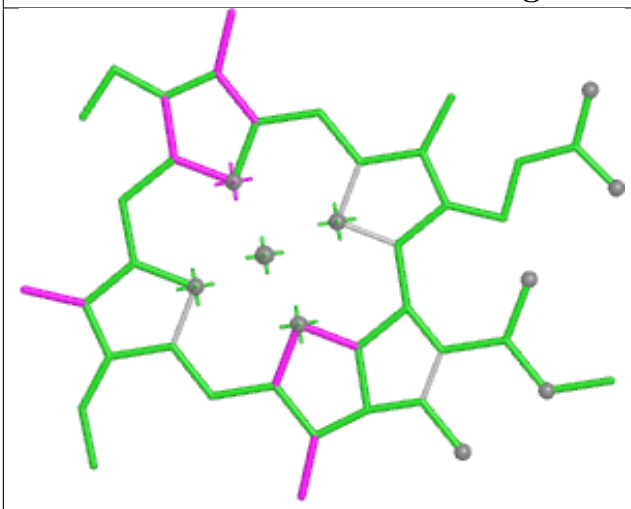


Torsions

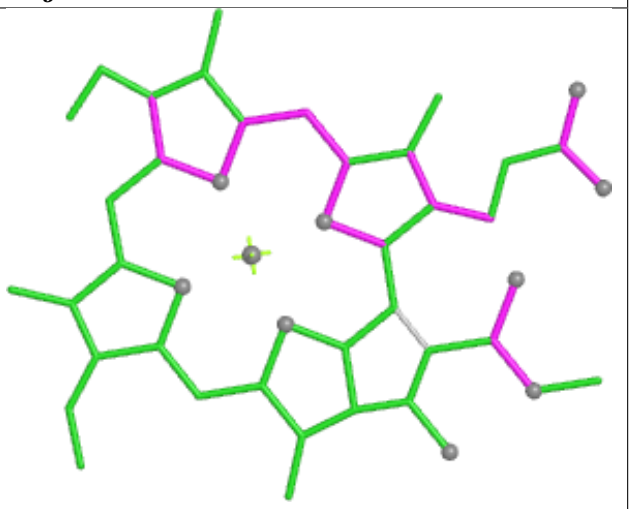


Rings

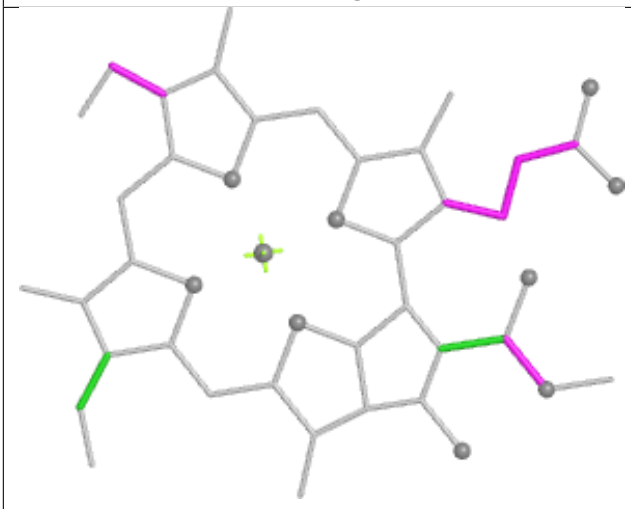
Ligand CLA j 1302



Bond lengths



Bond angles

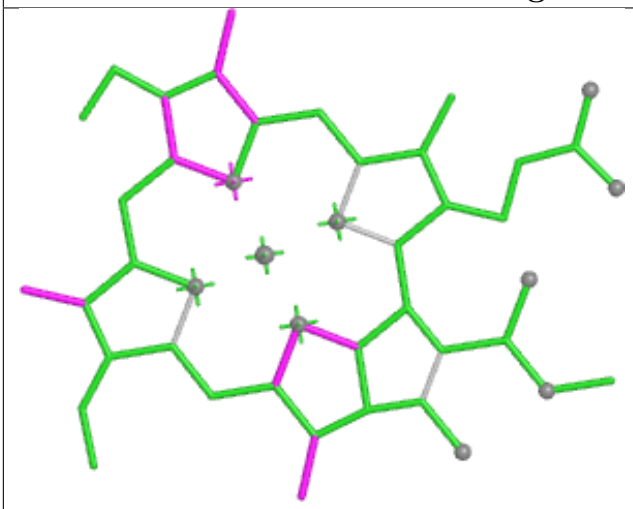


Torsions

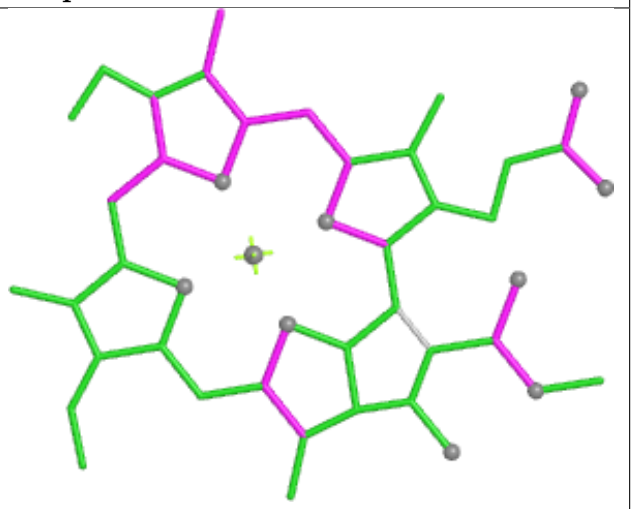


Rings

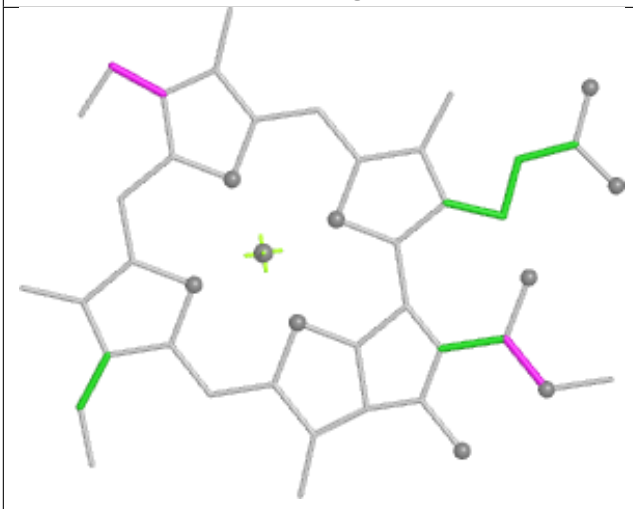
Ligand CLA q 511



Bond lengths



Bond angles

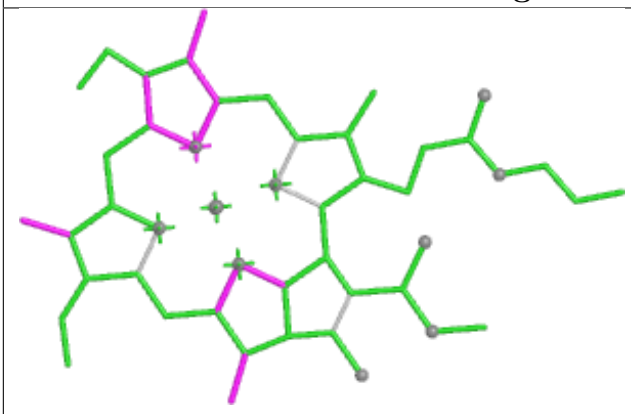


Torsions

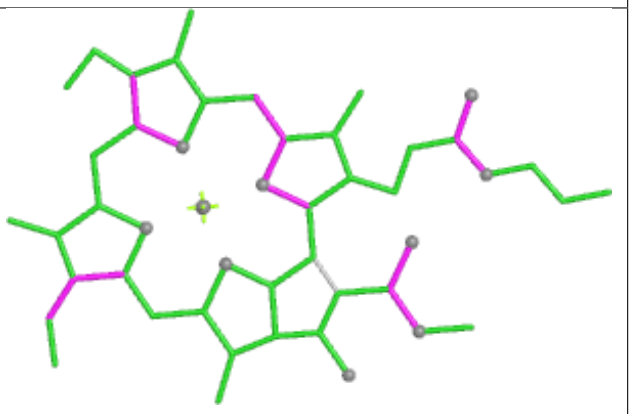


Rings

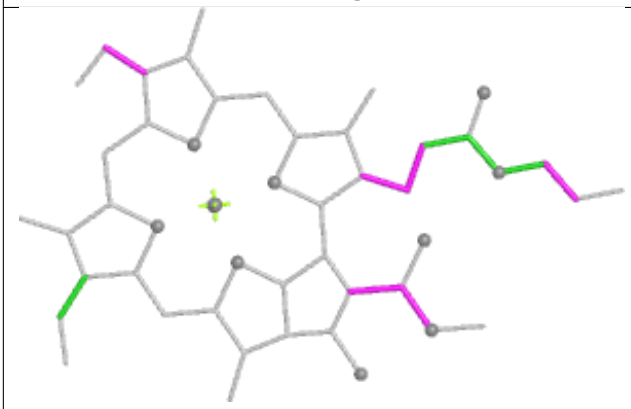
Ligand CLA m 1103



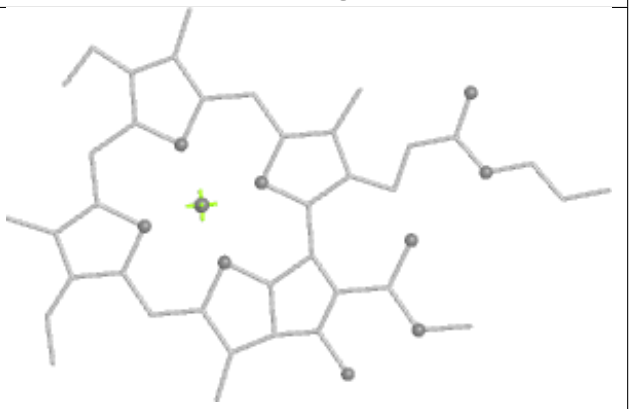
Bond lengths



Bond angles

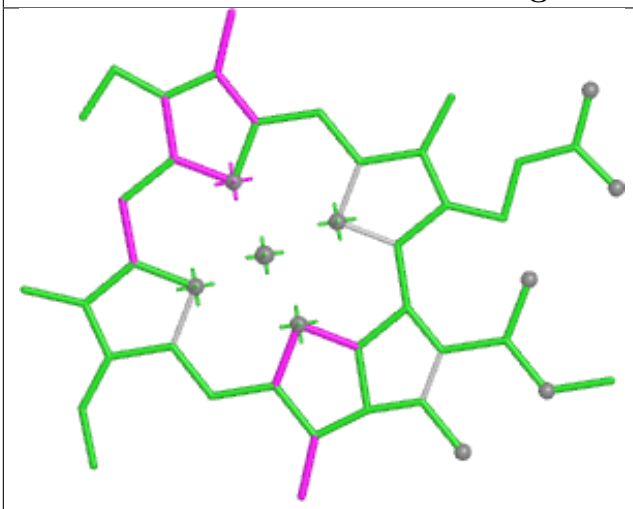


Torsions

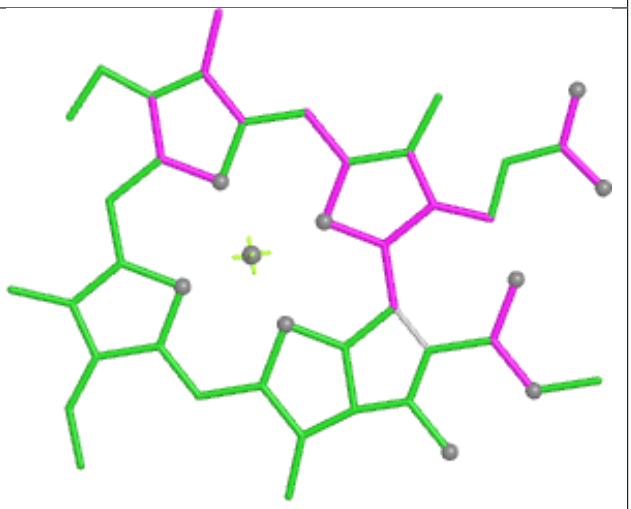


Rings

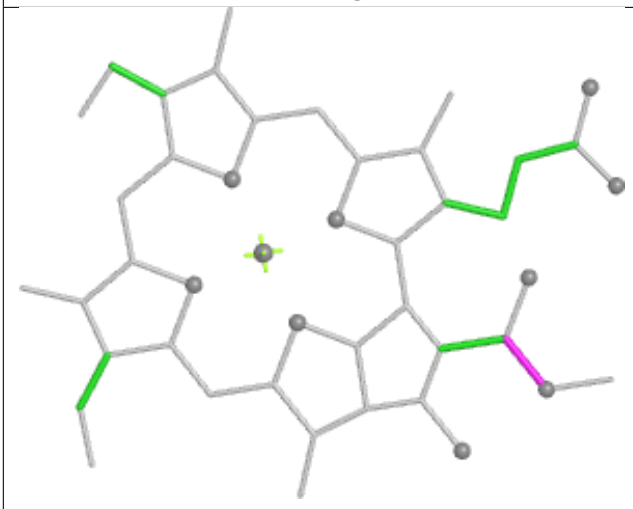
Ligand CLA s 511



Bond lengths



Bond angles

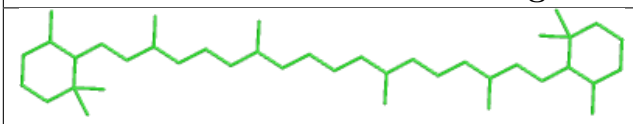


Torsions

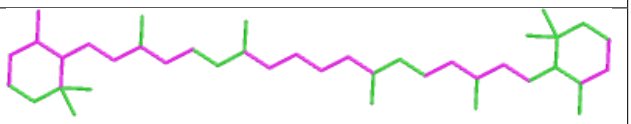


Rings

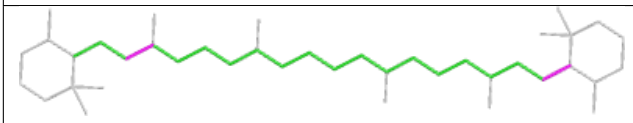
Ligand BCR t 524



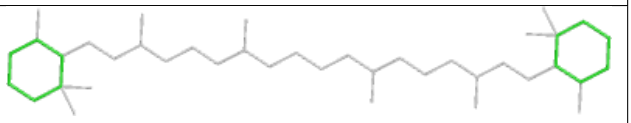
Bond lengths



Bond angles

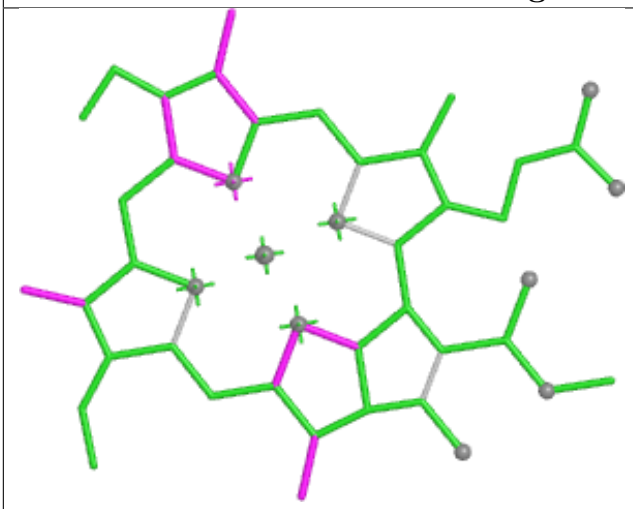


Torsions

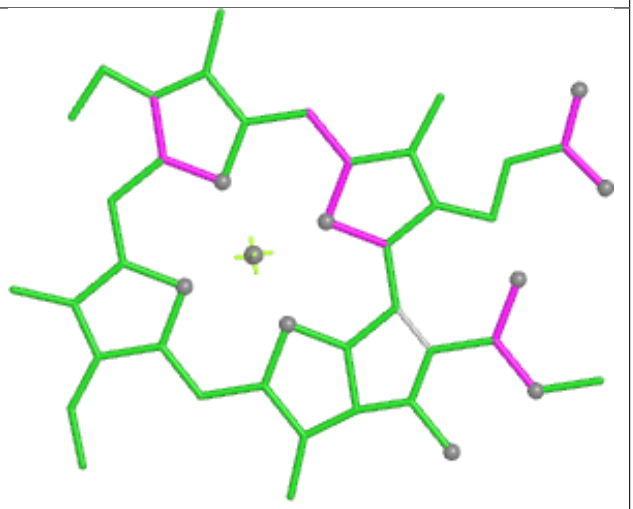


Rings

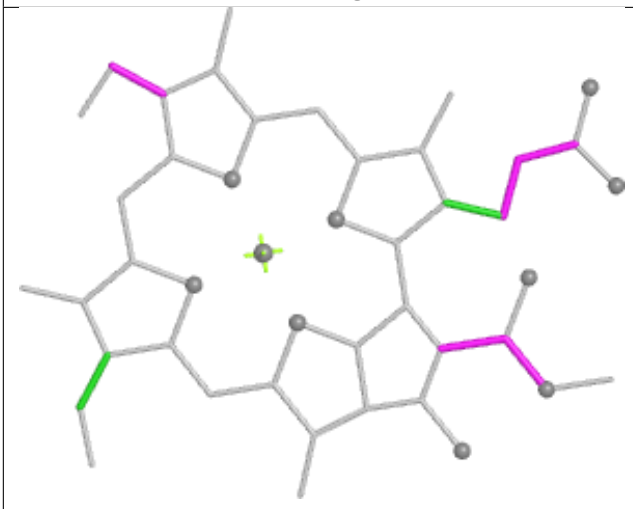
Ligand CLA 1 517



Bond lengths



Bond angles

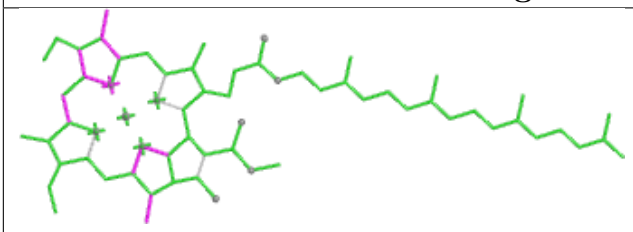


Torsions

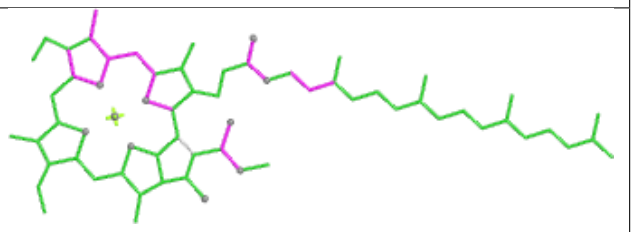


Rings

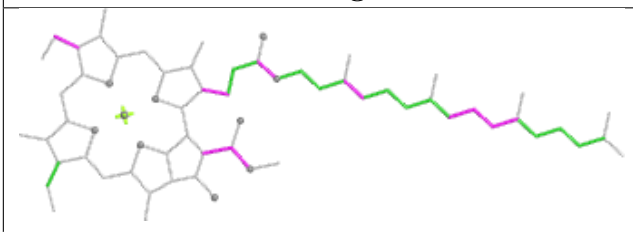
Ligand CLA H 1240



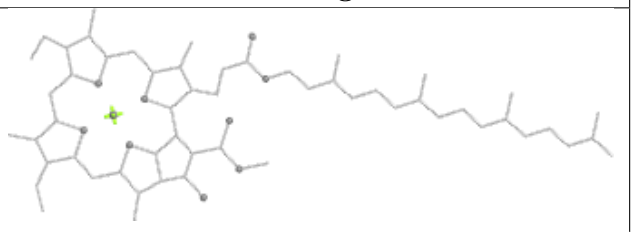
Bond lengths



Bond angles

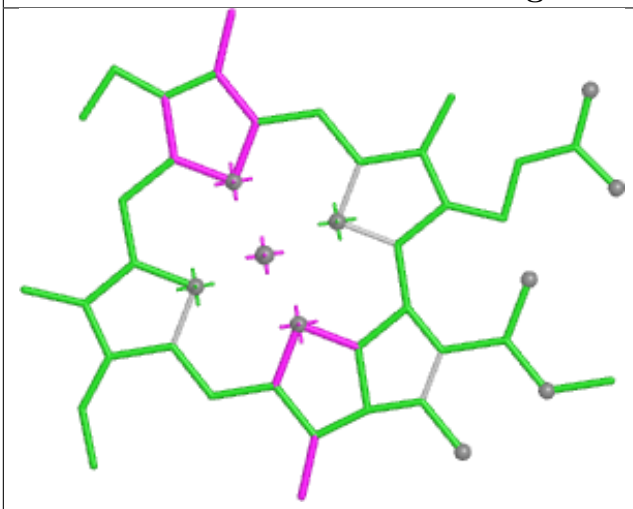


Torsions

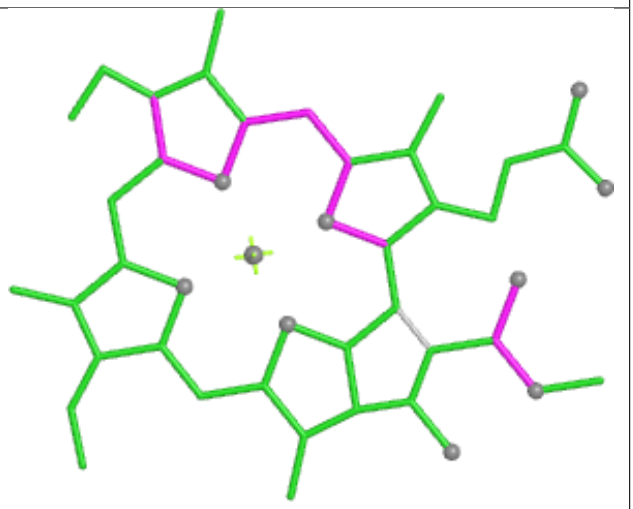


Rings

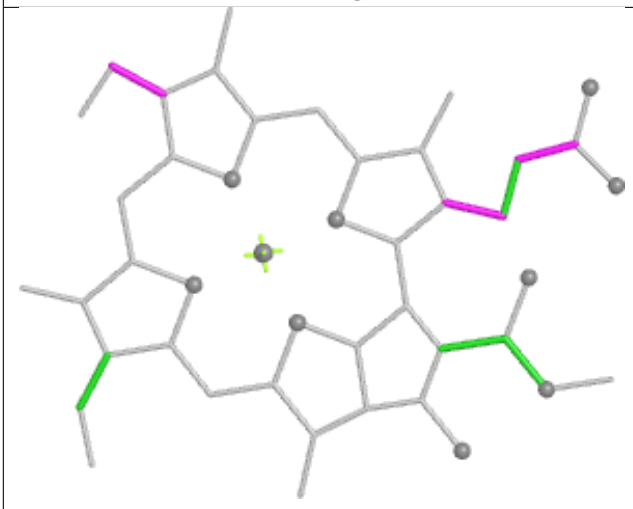
Ligand CLA Z 512



Bond lengths



Bond angles

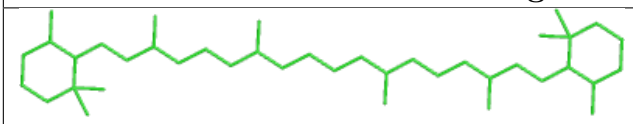


Torsions

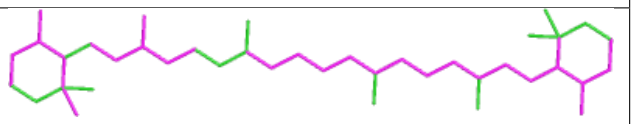


Rings

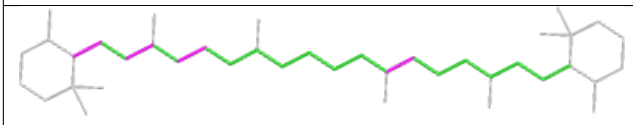
Ligand BCR c 521



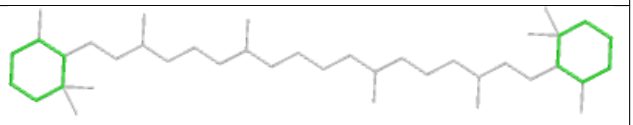
Bond lengths



Bond angles

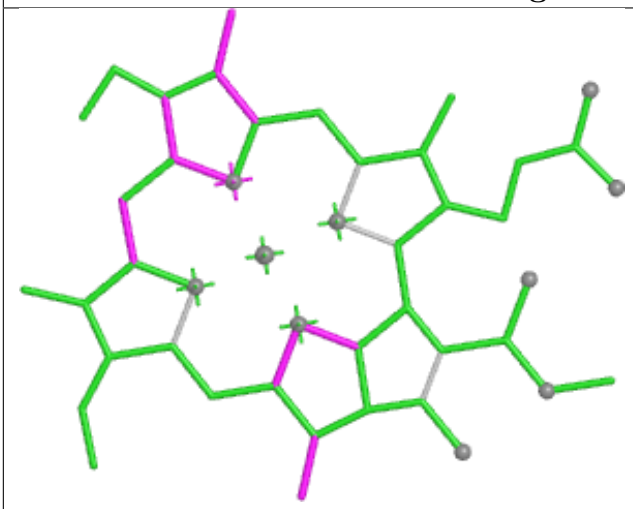


Torsions

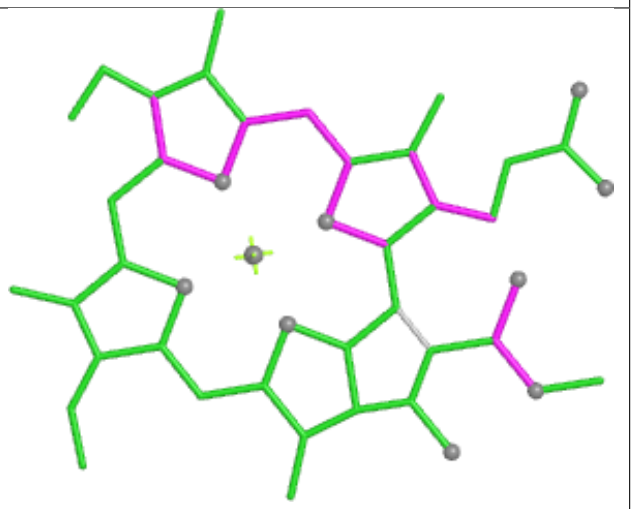


Rings

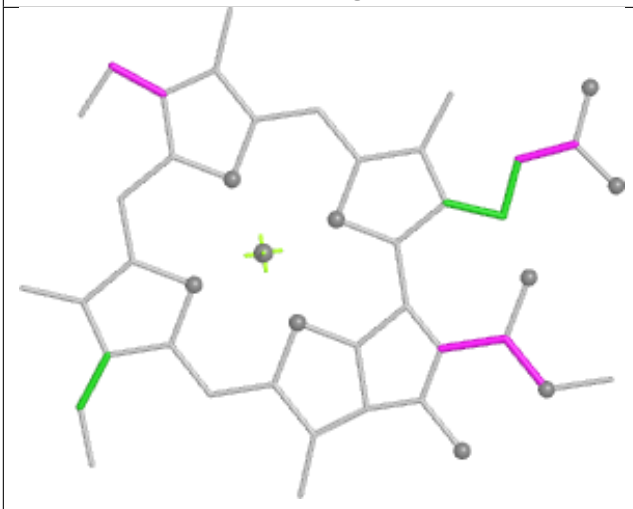
Ligand CLA c 512



Bond lengths



Bond angles

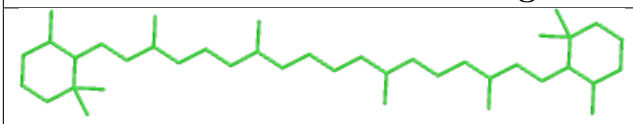


Torsions

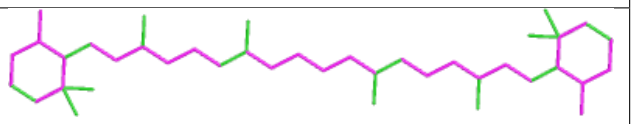


Rings

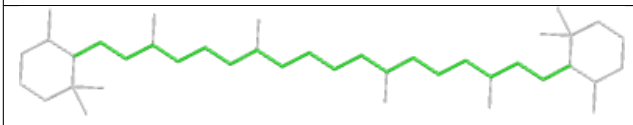
Ligand BCR e 4007



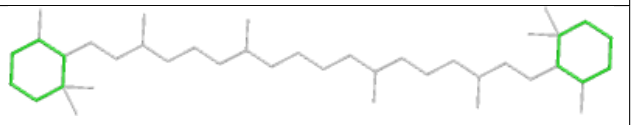
Bond lengths



Bond angles

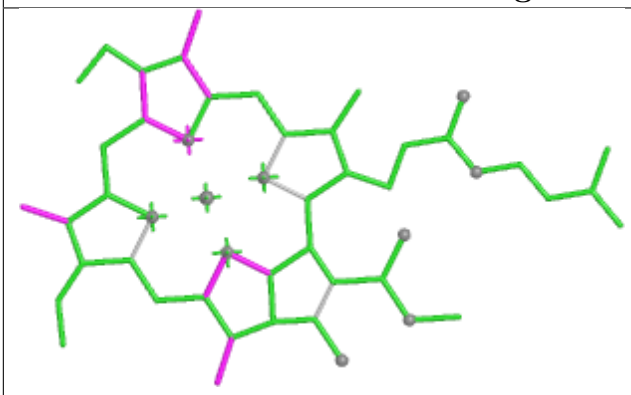


Torsions

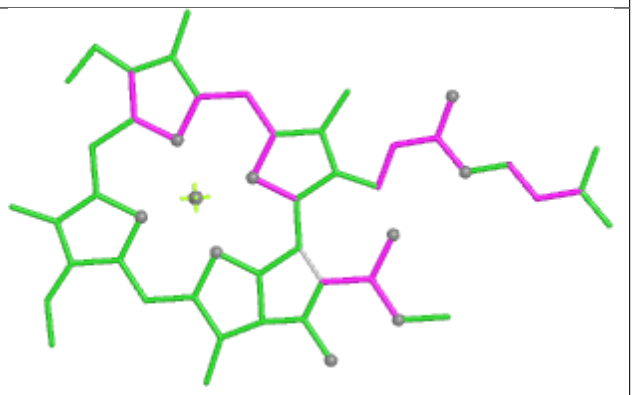


Rings

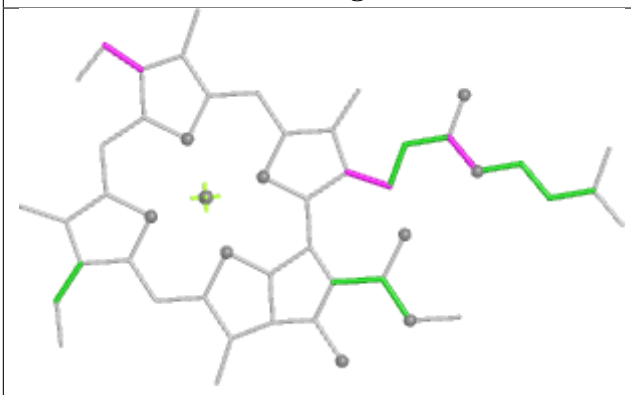
Ligand CLA H 1236



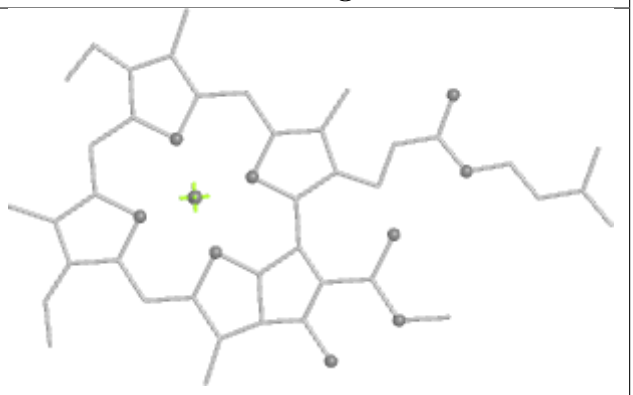
Bond lengths



Bond angles

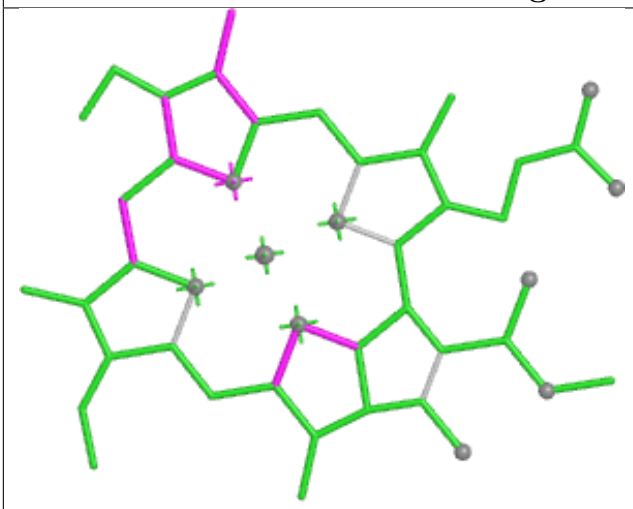


Torsions

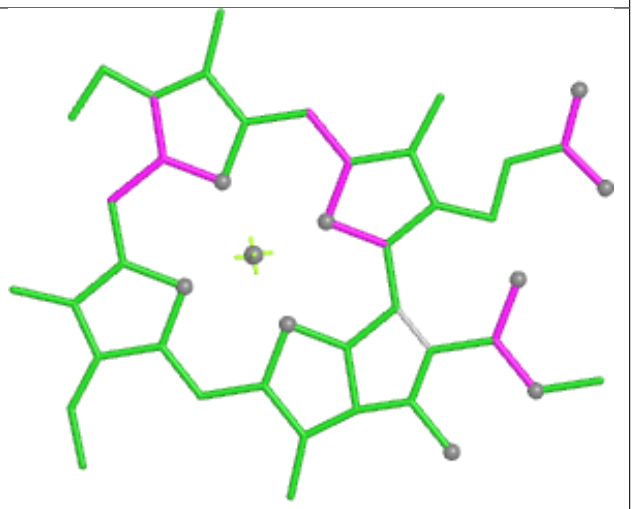


Rings

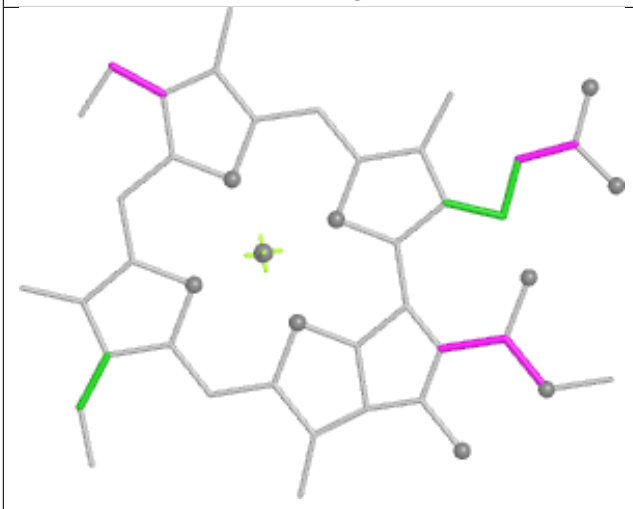
Ligand CLA c 519



Bond lengths



Bond angles

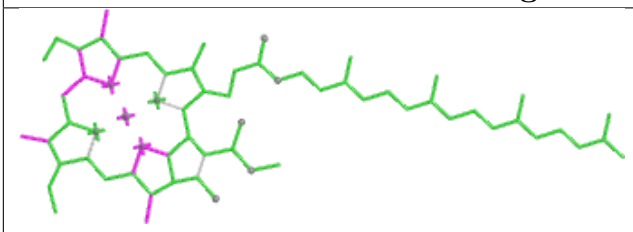


Torsions

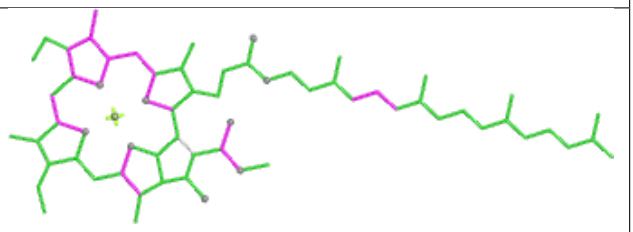


Rings

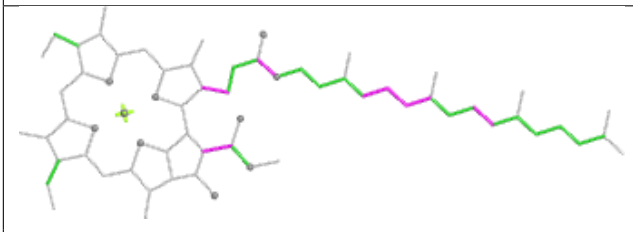
Ligand CLA e 1128



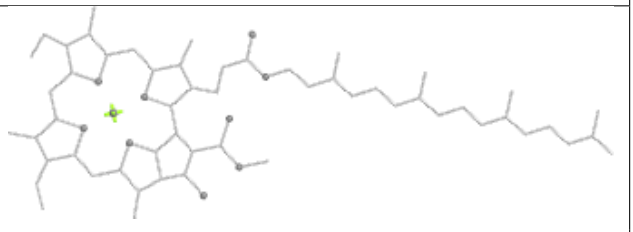
Bond lengths



Bond angles

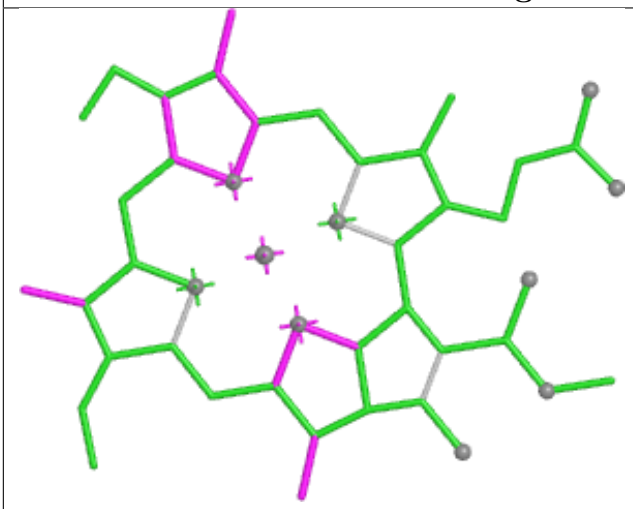


Torsions

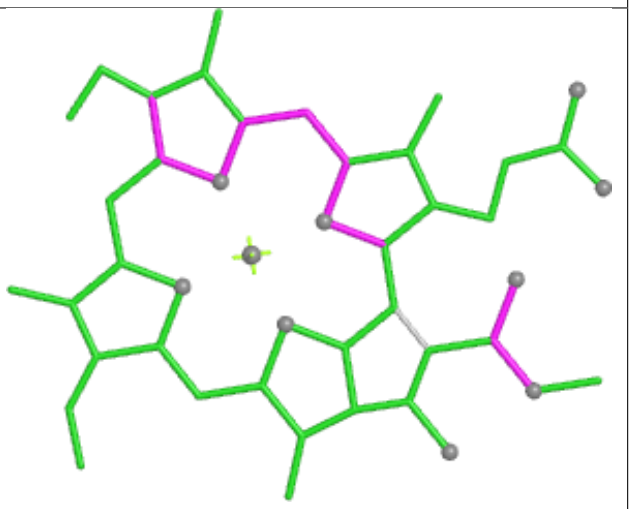


Rings

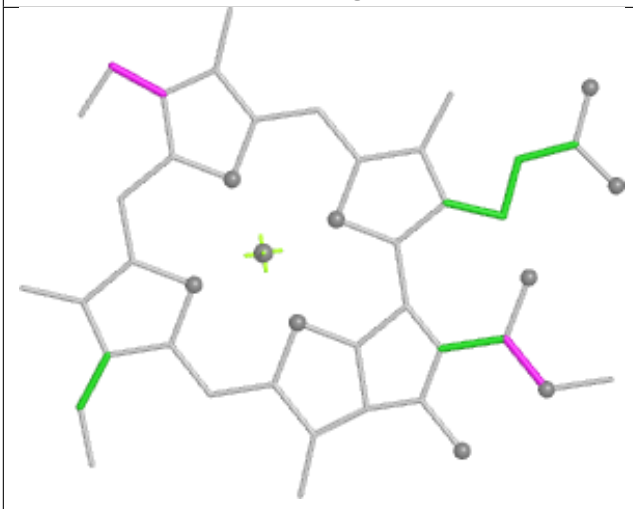
Ligand CLA R 1301



Bond lengths



Bond angles

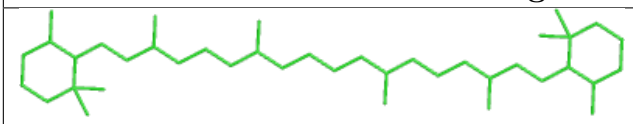


Torsions

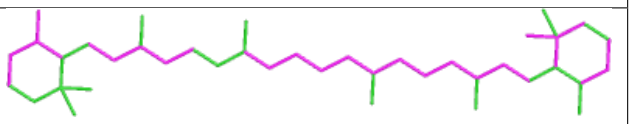


Rings

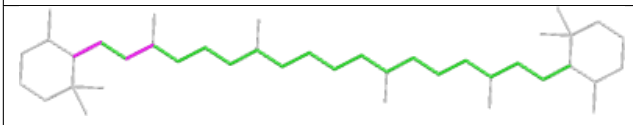
Ligand BCR r 521



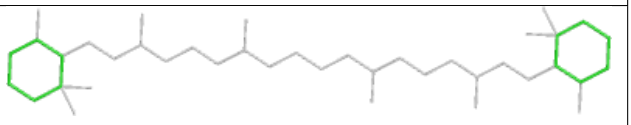
Bond lengths



Bond angles

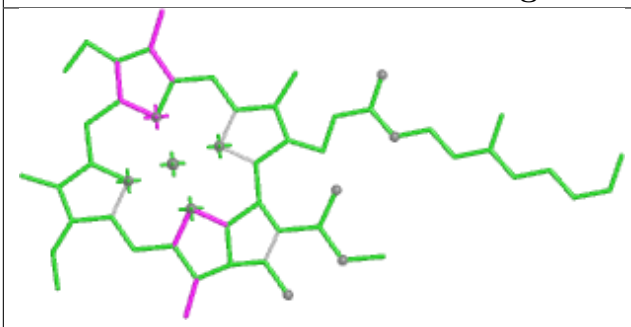


Torsions

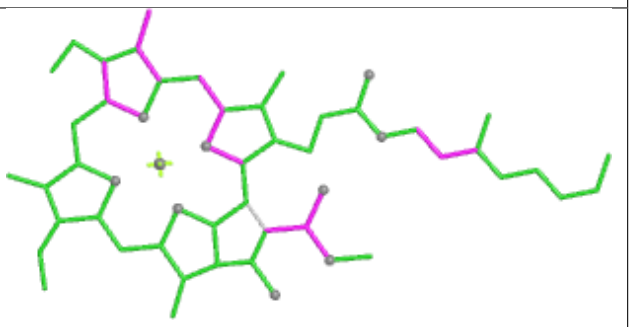


Rings

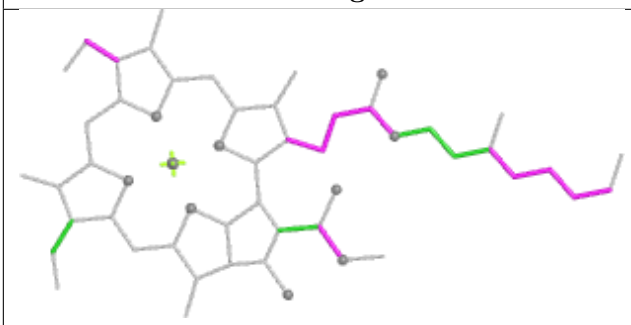
Ligand CLA e 1108



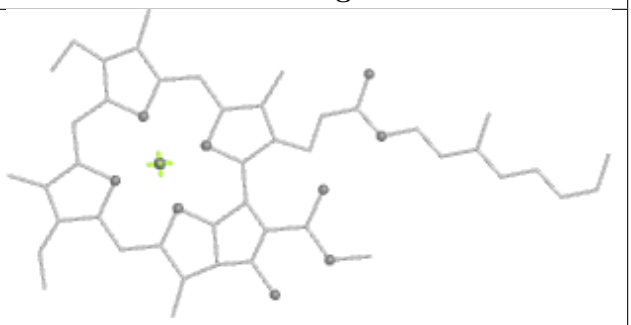
Bond lengths



Bond angles

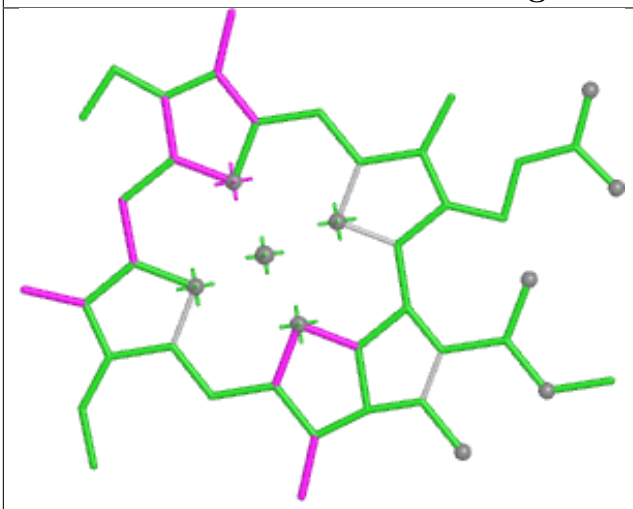


Torsions

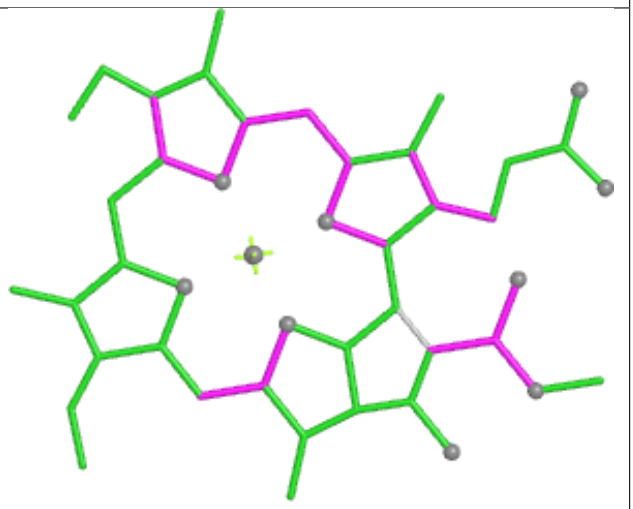


Rings

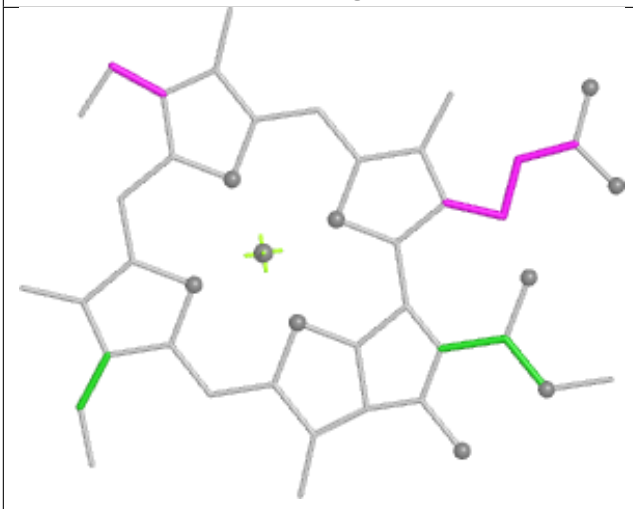
Ligand CLA a 501



Bond lengths



Bond angles

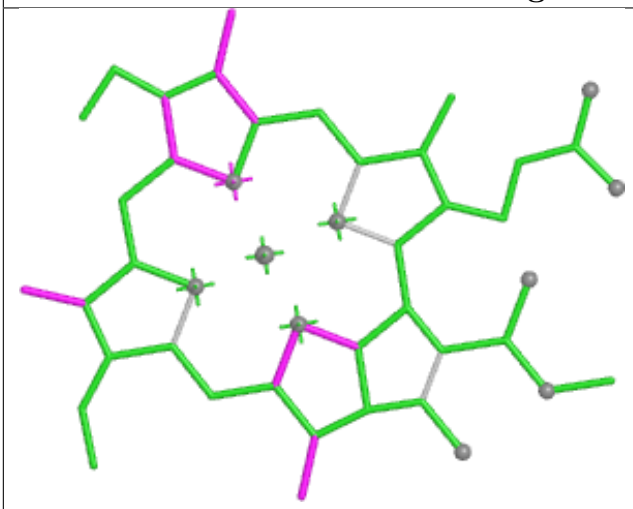


Torsions

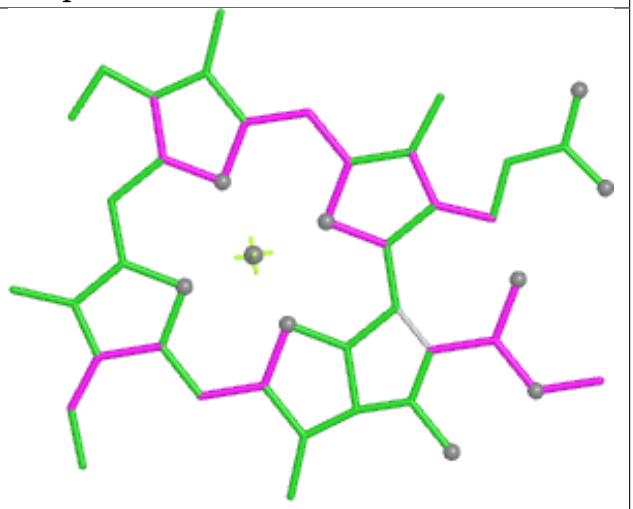


Rings

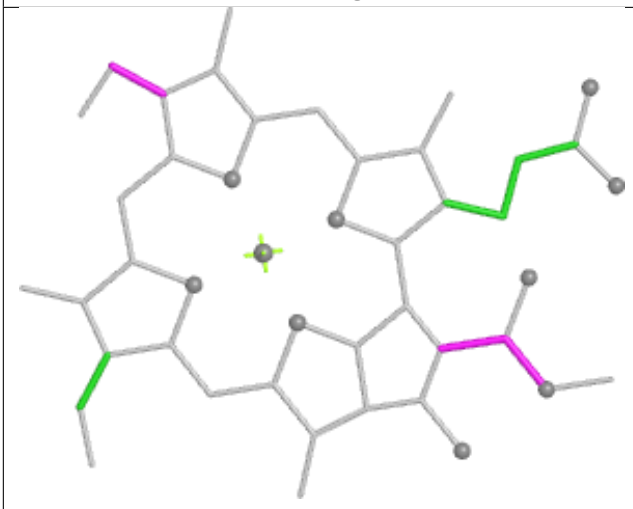
Ligand CLA q 504



Bond lengths



Bond angles

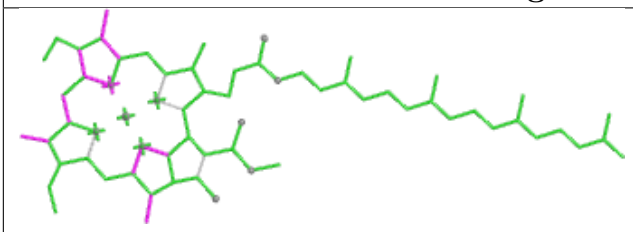


Torsions

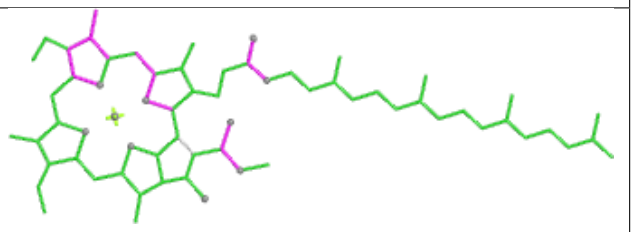


Rings

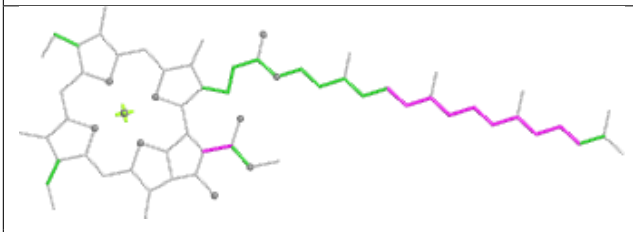
Ligand CLA u 509



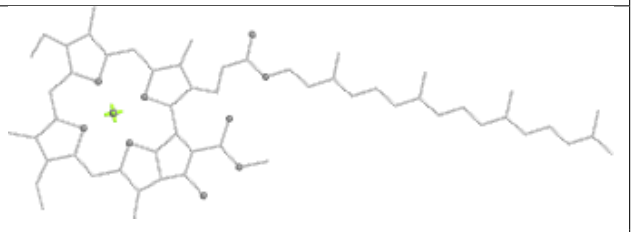
Bond lengths



Bond angles

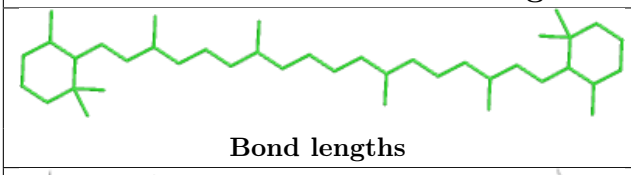


Torsions

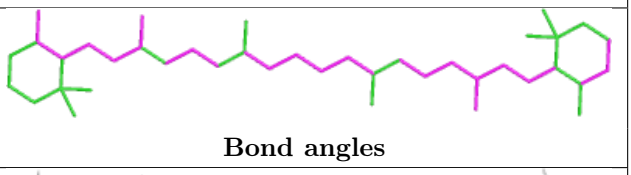


Rings

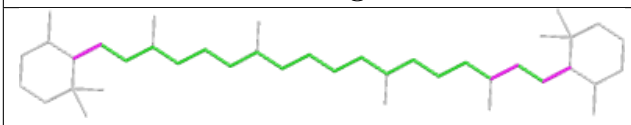
Ligand BCR 1 523



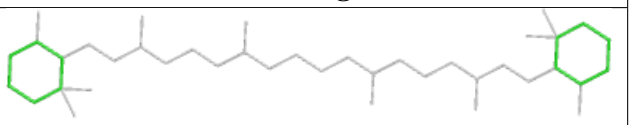
Bond lengths



Bond angles

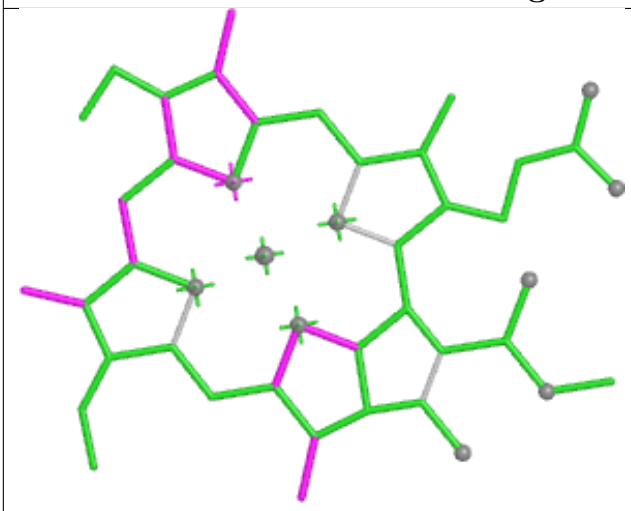


Torsions

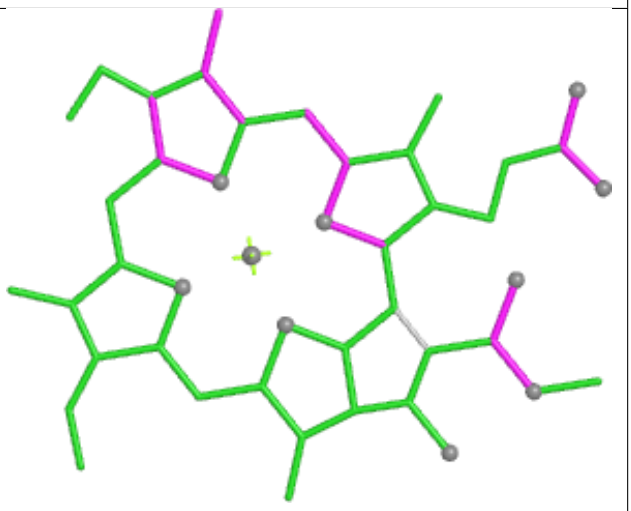


Rings

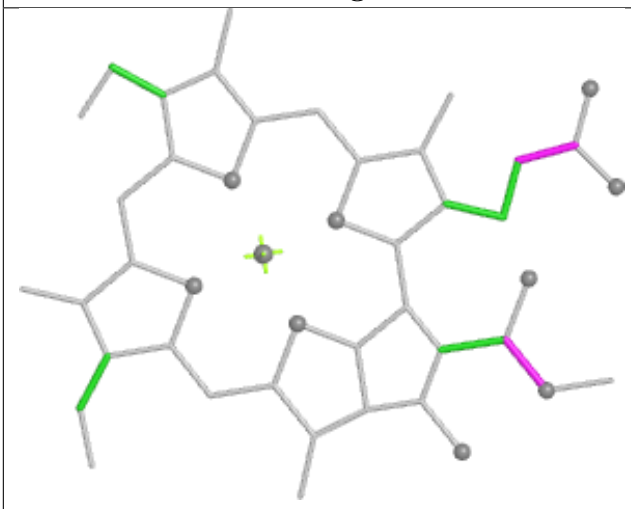
Ligand CLA 6 509



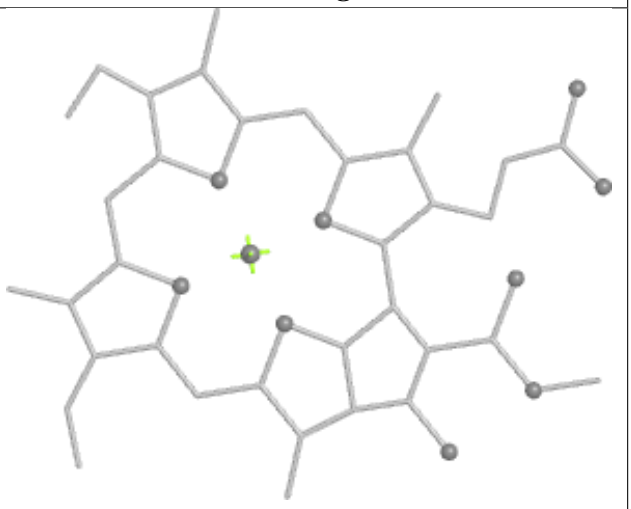
Bond lengths



Bond angles

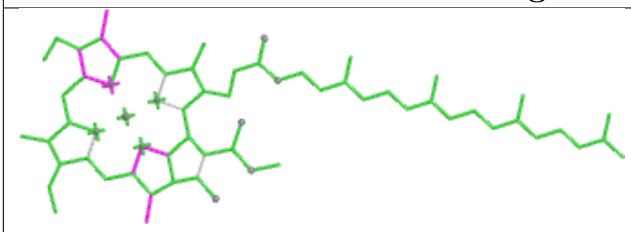


Torsions

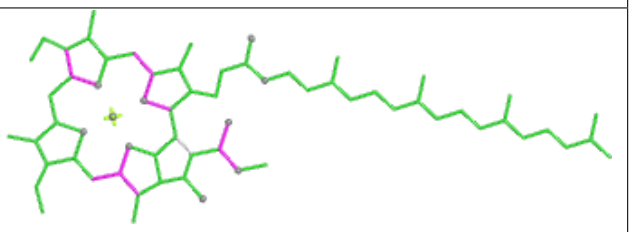


Rings

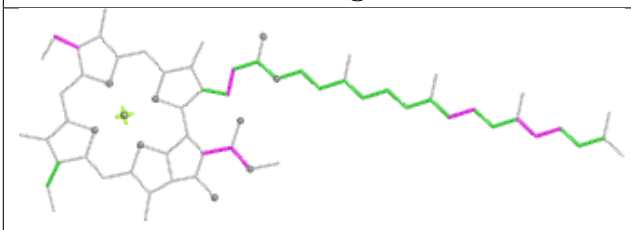
Ligand CLA 2 503



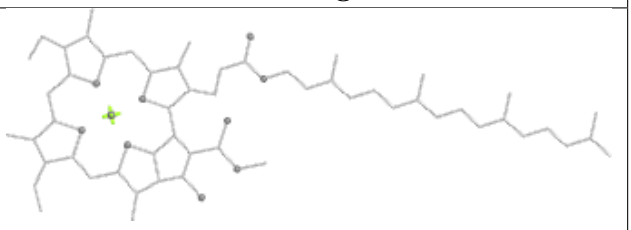
Bond lengths



Bond angles



Torsions

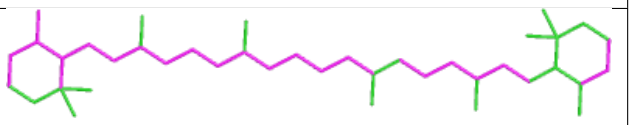


Rings

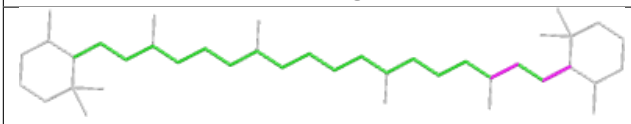
Ligand BCR s 523



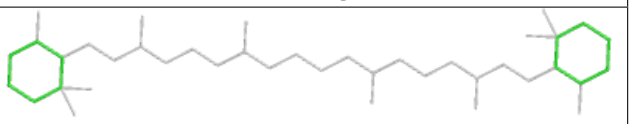
Bond lengths



Bond angles

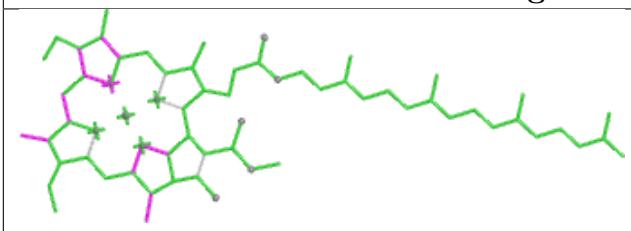


Torsions

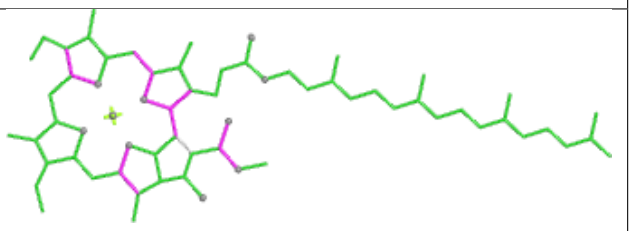


Rings

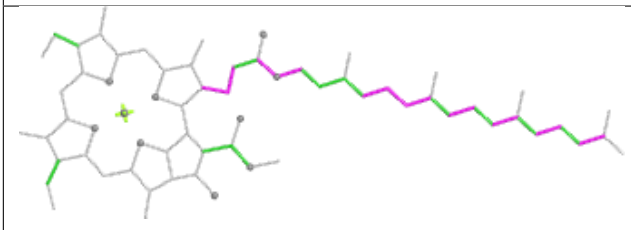
Ligand CLA v 505



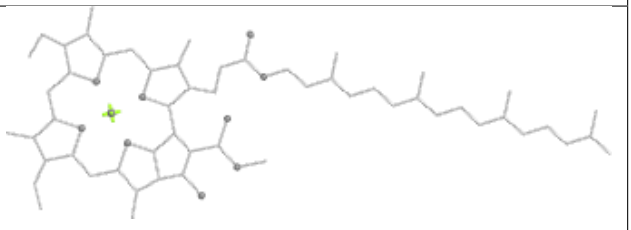
Bond lengths



Bond angles

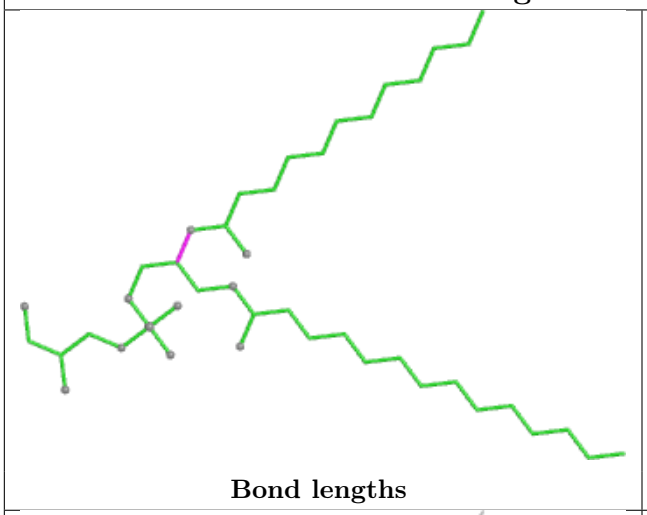


Torsions

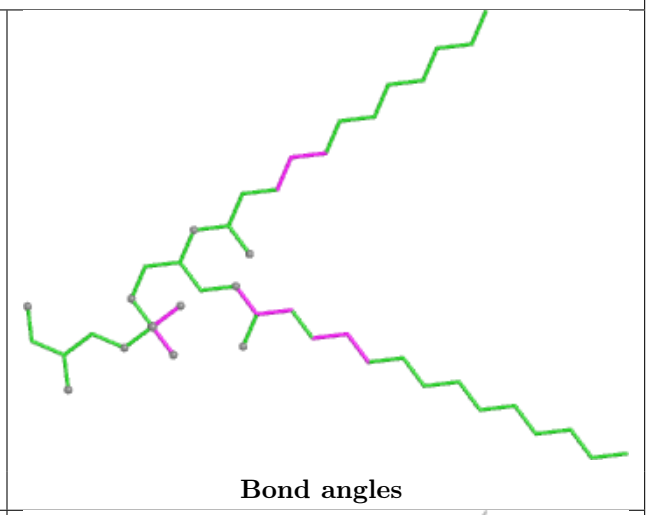


Rings

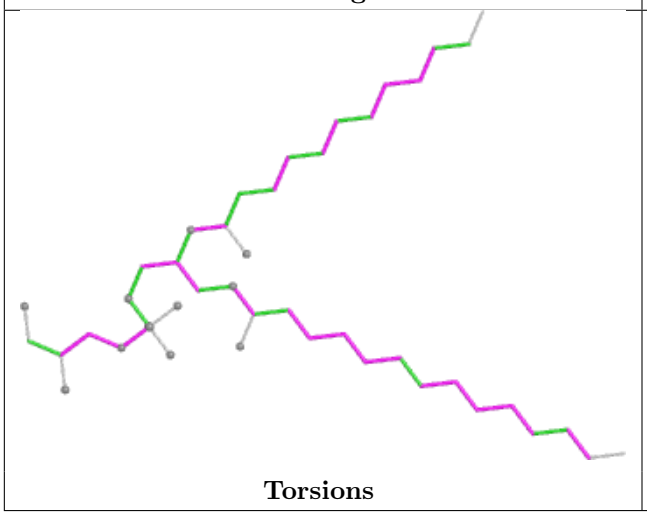
Ligand LHG G 5005



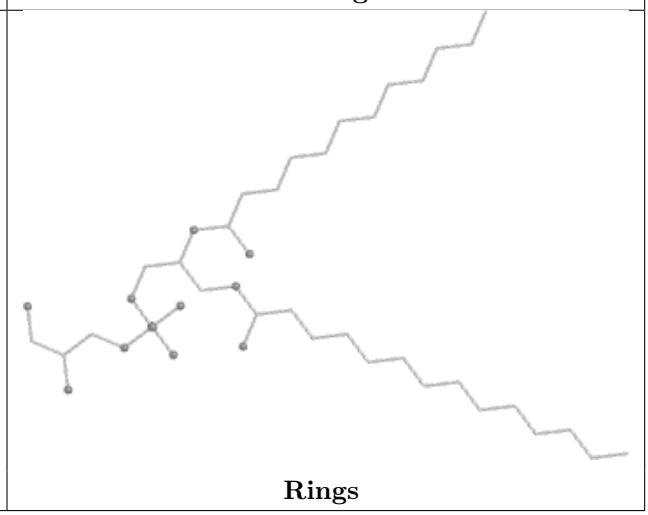
Bond lengths



Bond angles

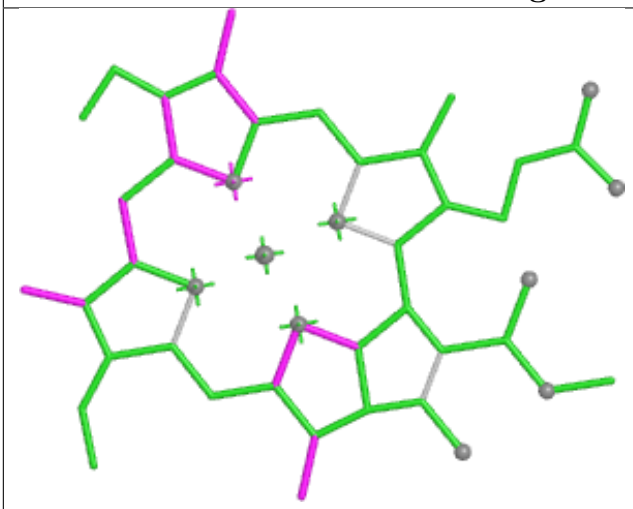


Torsions

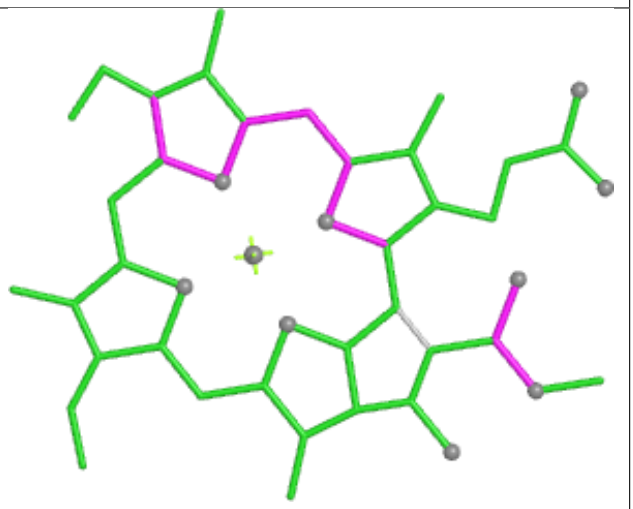


Rings

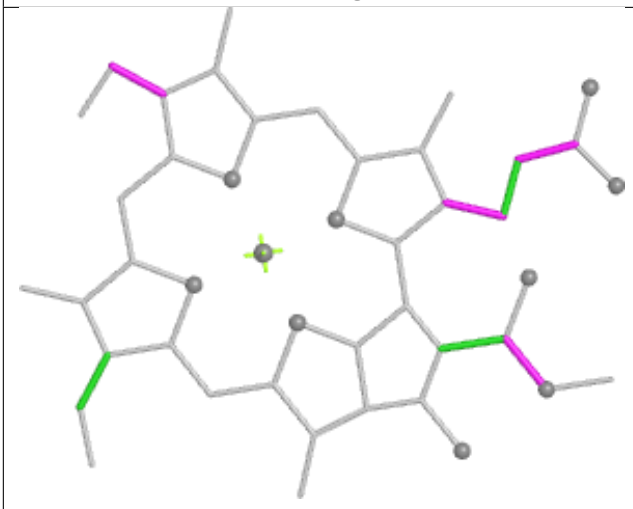
Ligand CLA c 513



Bond lengths



Bond angles

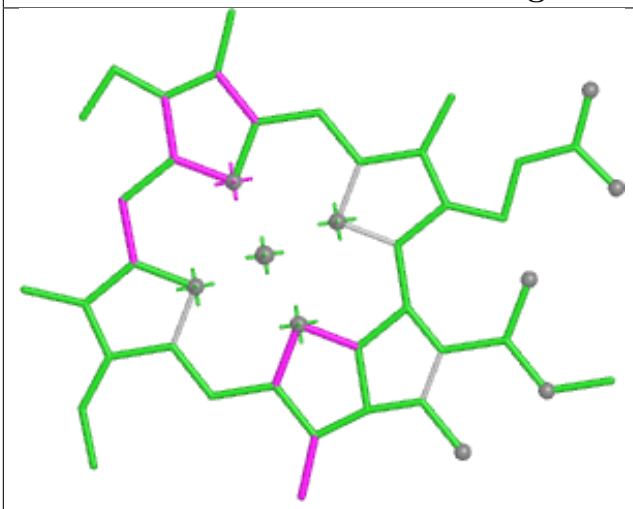


Torsions

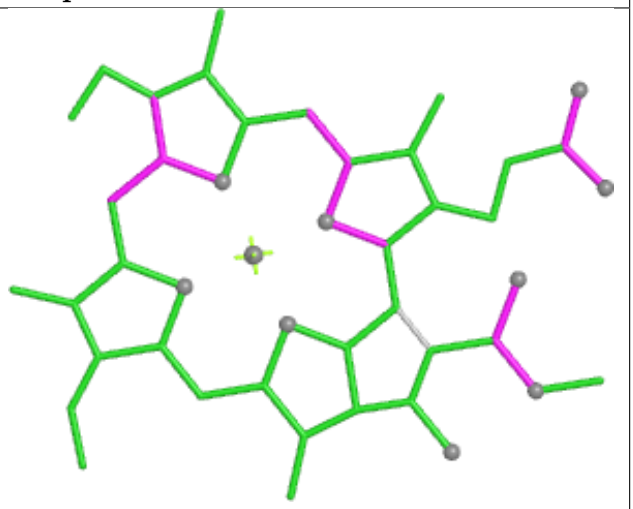


Rings

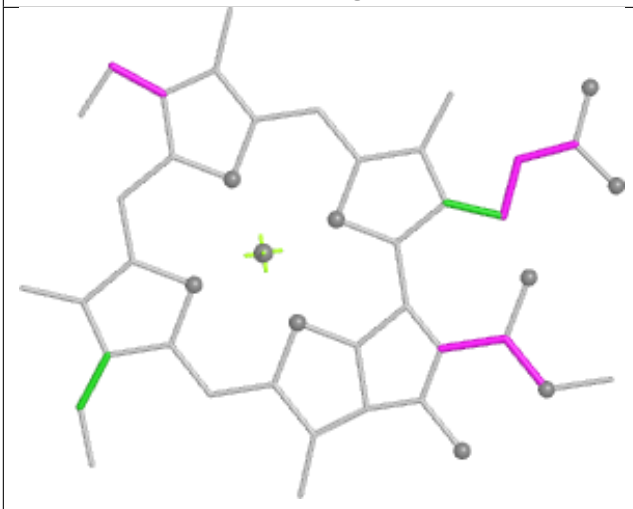
Ligand CLA q 518



Bond lengths



Bond angles

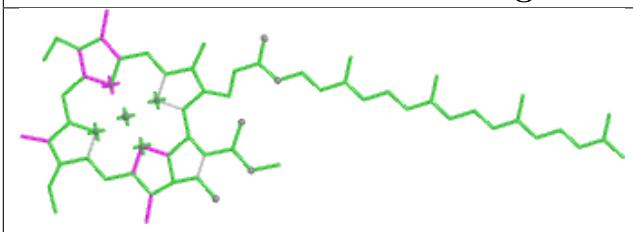


Torsions

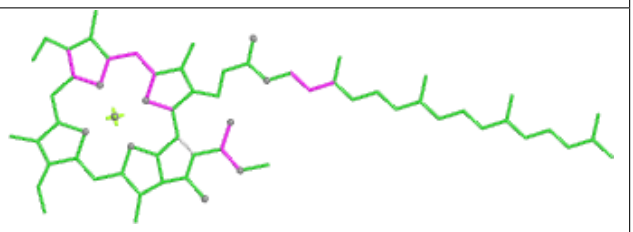


Rings

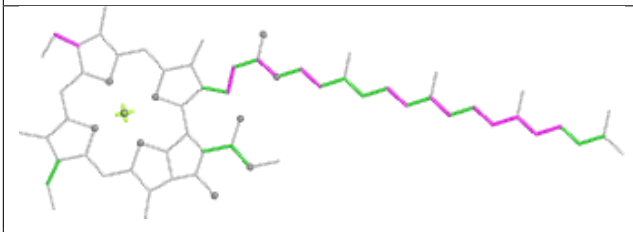
Ligand CLA B 1214



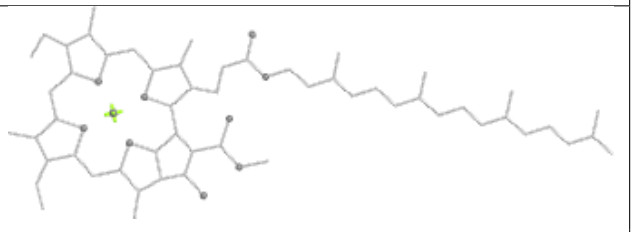
Bond lengths



Bond angles

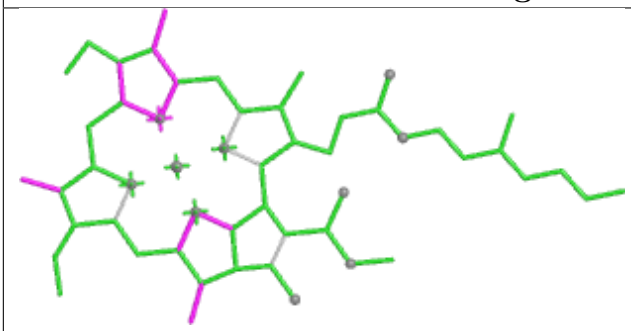


Torsions

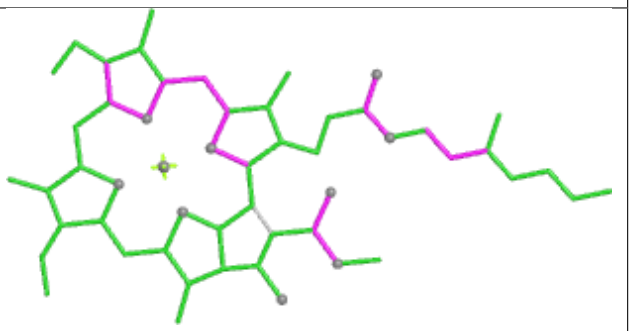


Rings

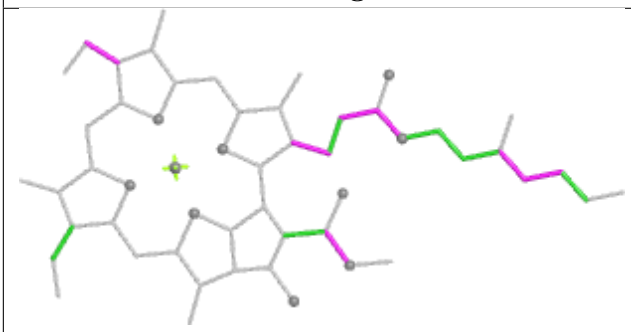
Ligand CLA G 1110



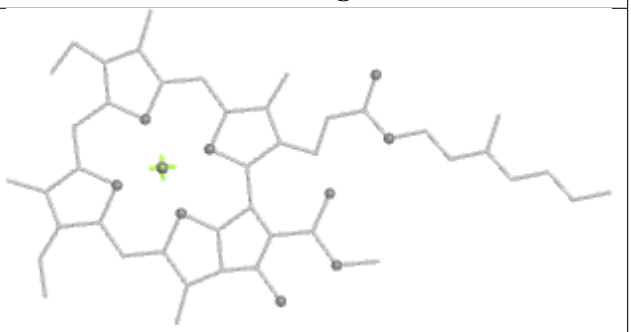
Bond lengths



Bond angles



Torsions

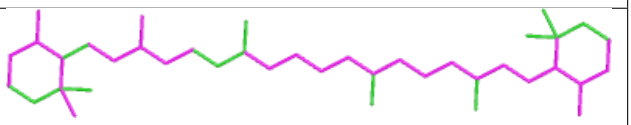


Rings

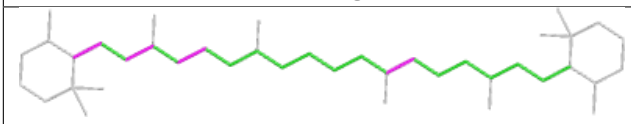
Ligand BCR u 521



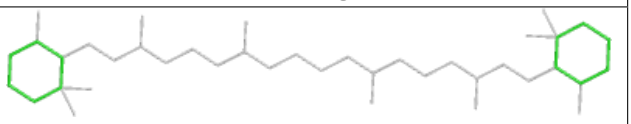
Bond lengths



Bond angles

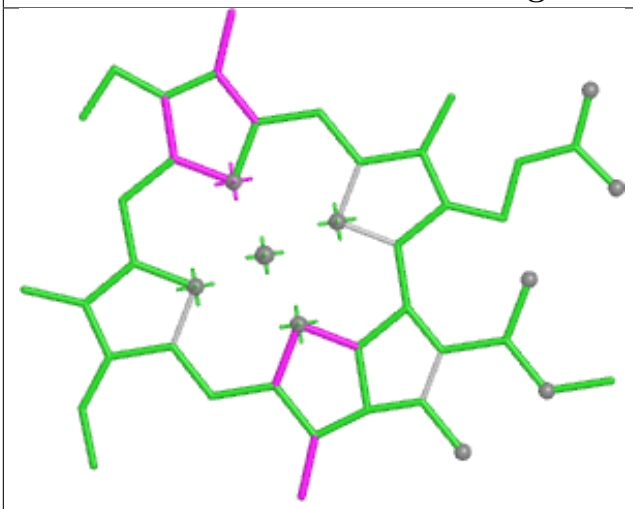


Torsions

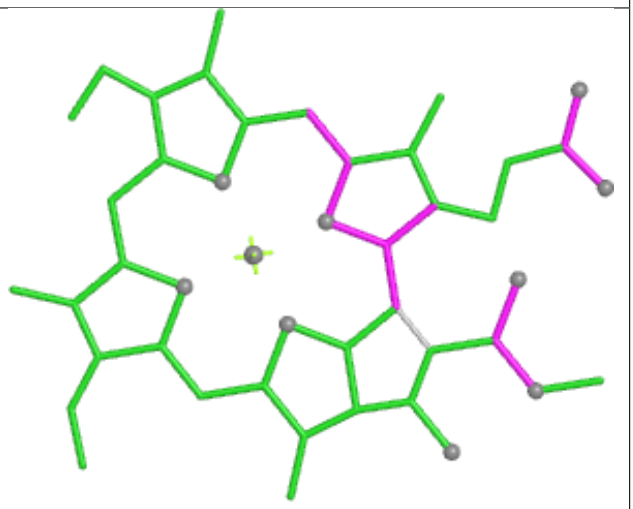


Rings

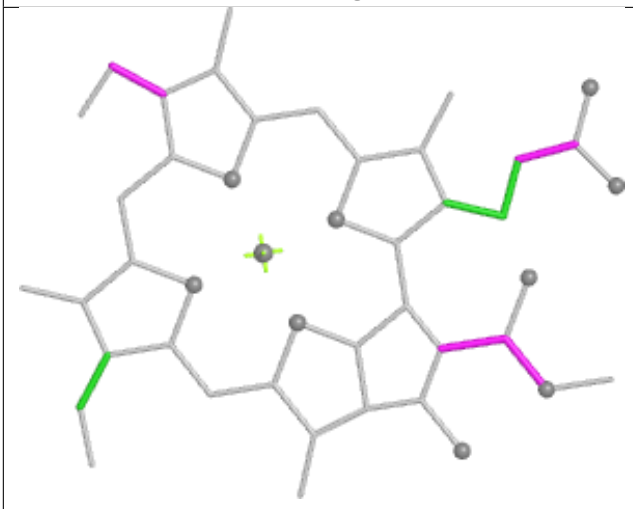
Ligand CLA v 507



Bond lengths



Bond angles

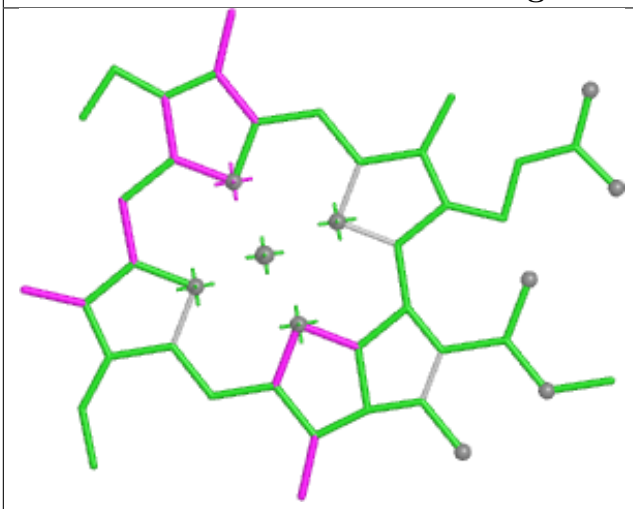


Torsions

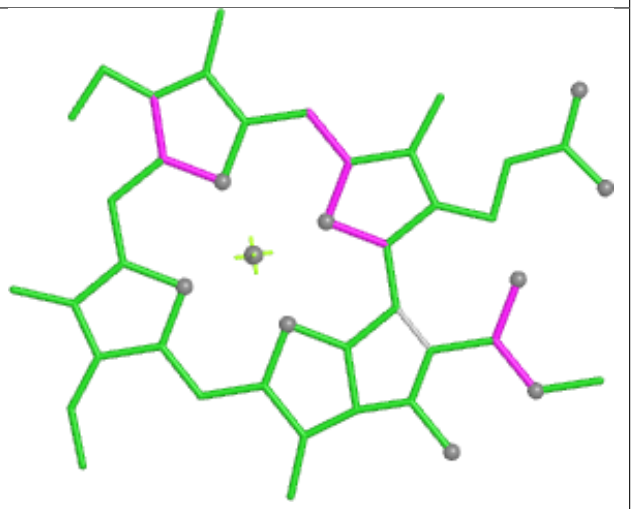


Rings

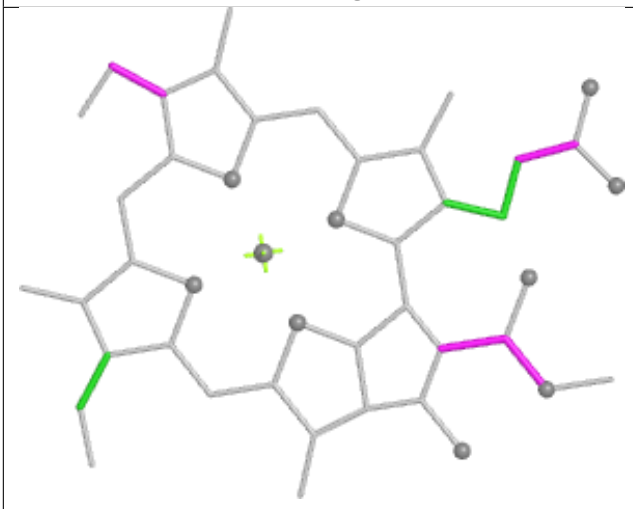
Ligand CLA d 510



Bond lengths



Bond angles

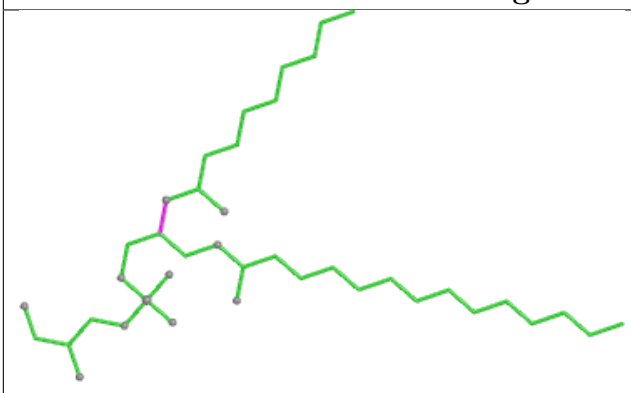


Torsions

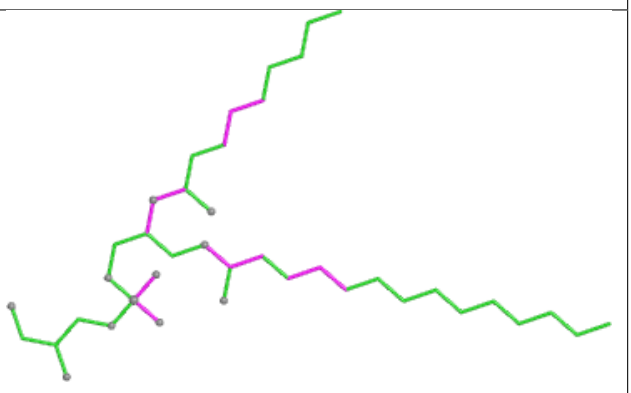


Rings

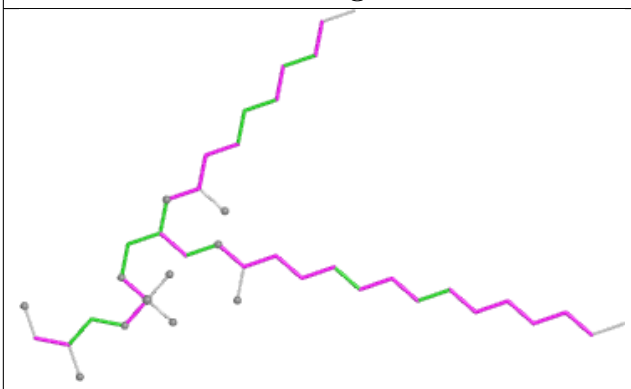
Ligand LHG G 5006



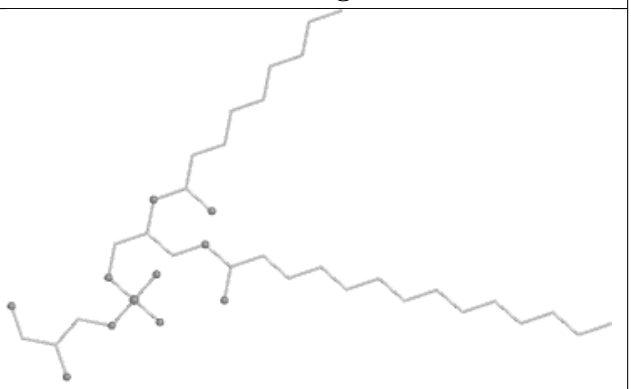
Bond lengths



Bond angles

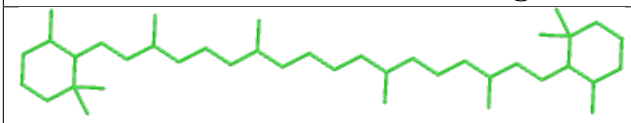


Torsions

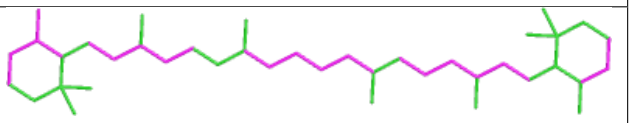


Rings

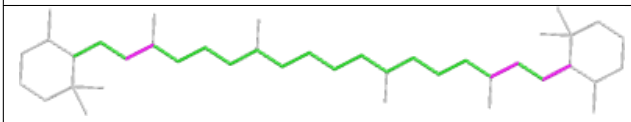
Ligand BCR H 4005



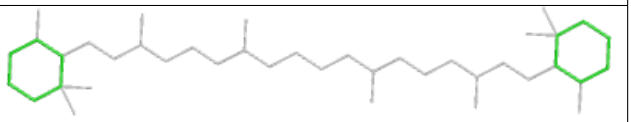
Bond lengths



Bond angles

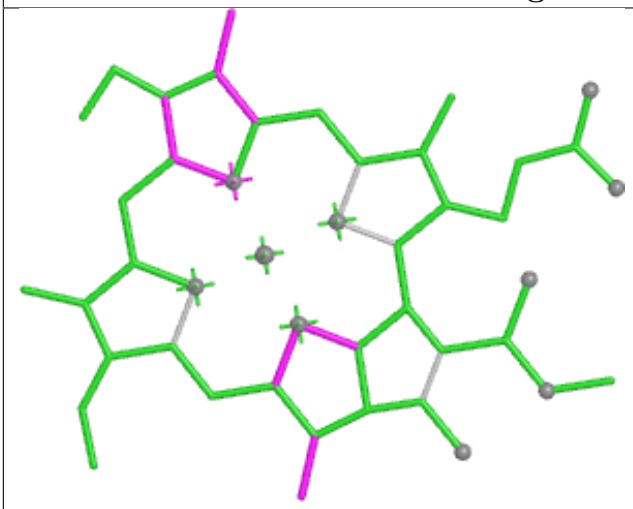


Torsions

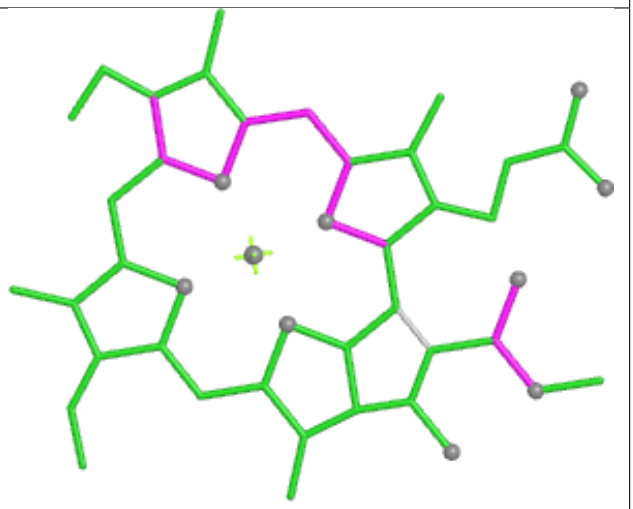


Rings

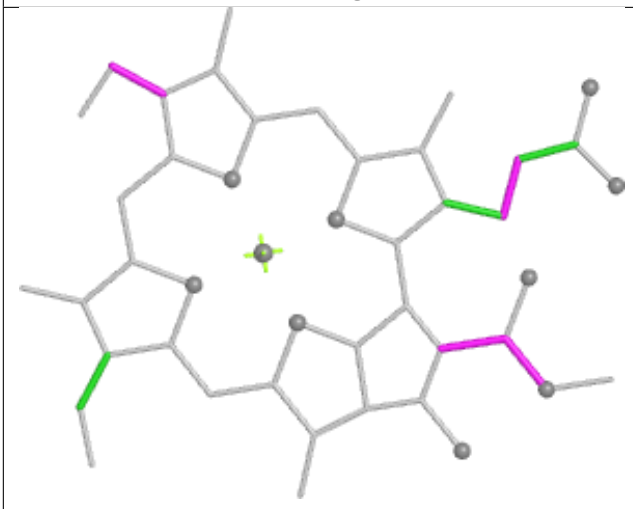
Ligand CLA d 503



Bond lengths



Bond angles

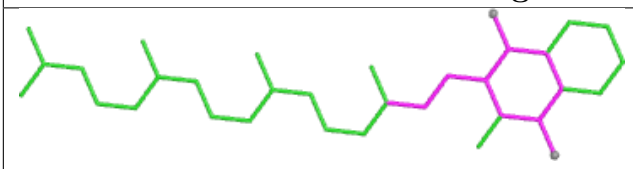


Torsions

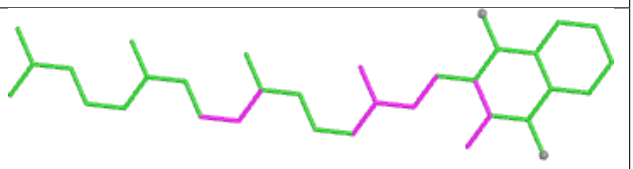


Rings

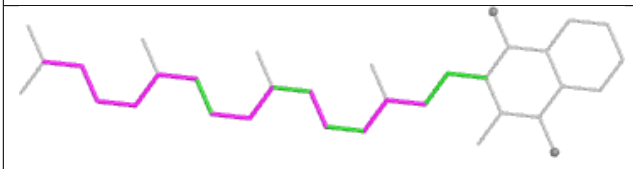
Ligand PQN G 2001



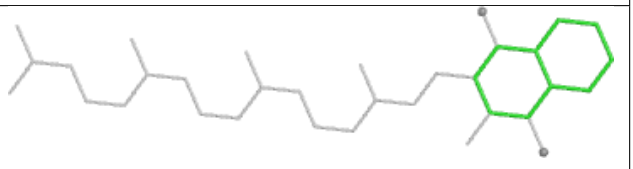
Bond lengths



Bond angles

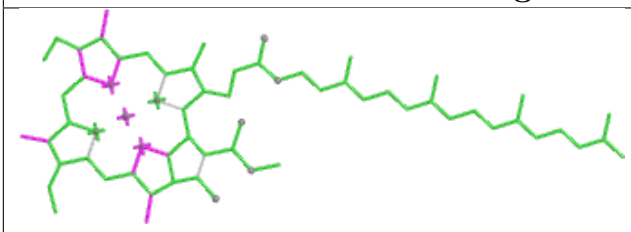


Torsions

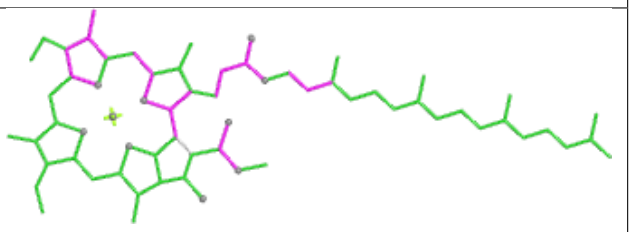


Rings

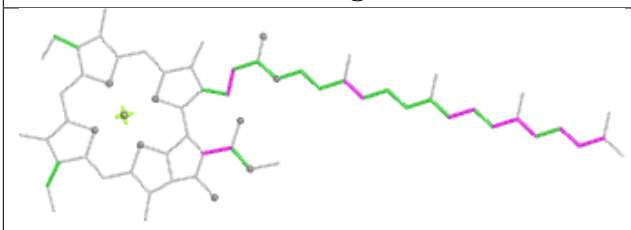
Ligand CLA G 1127



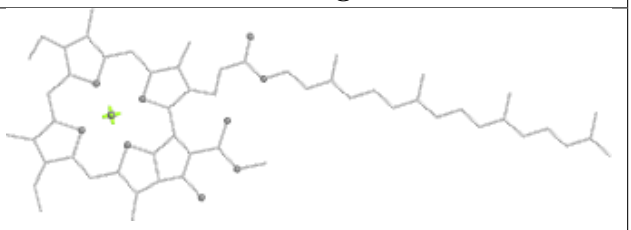
Bond lengths



Bond angles

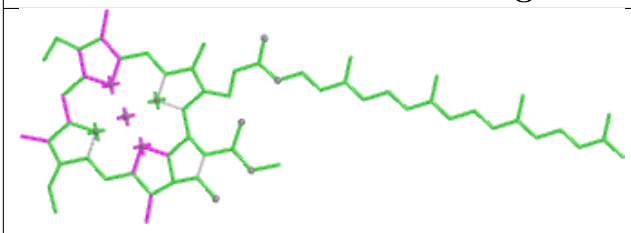


Torsions

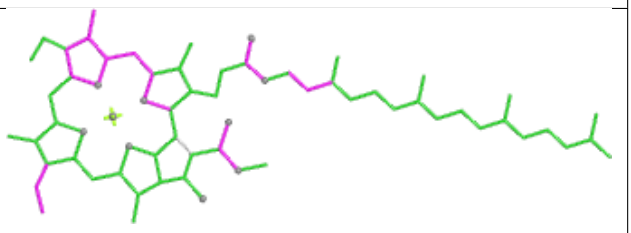


Rings

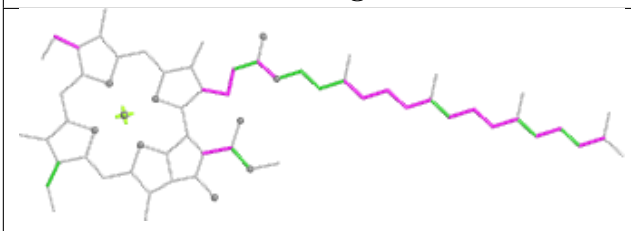
Ligand CLA B 1210



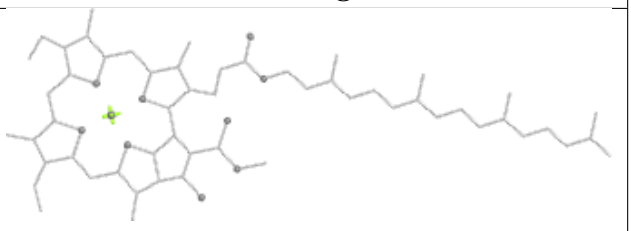
Bond lengths



Bond angles

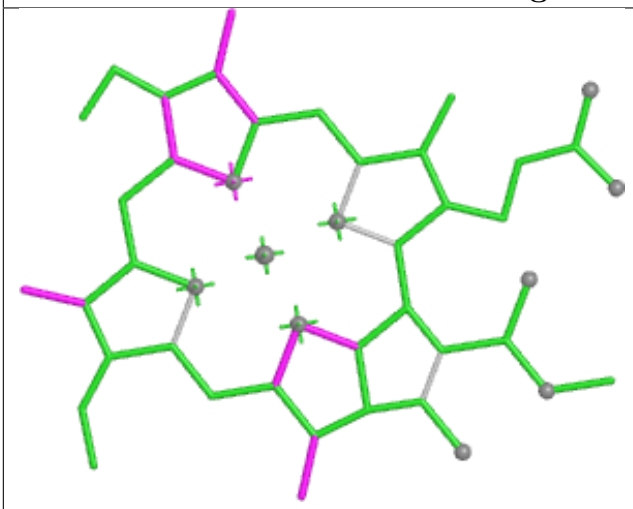


Torsions

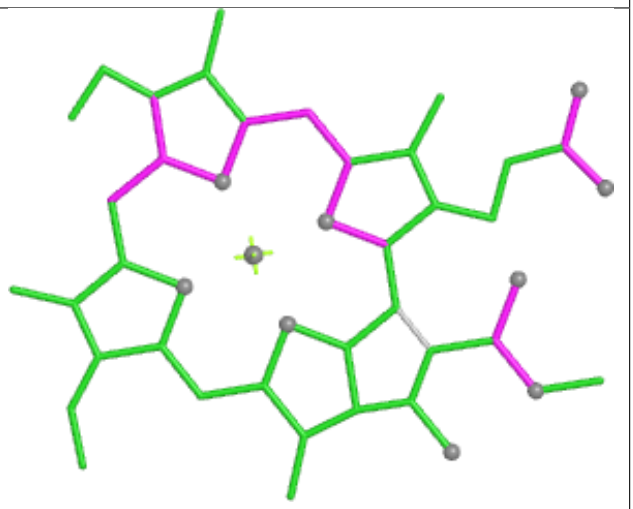


Rings

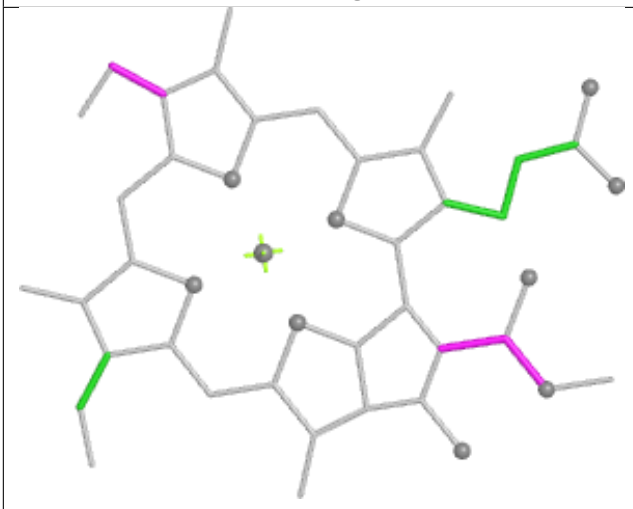
Ligand CLA r 506



Bond lengths



Bond angles

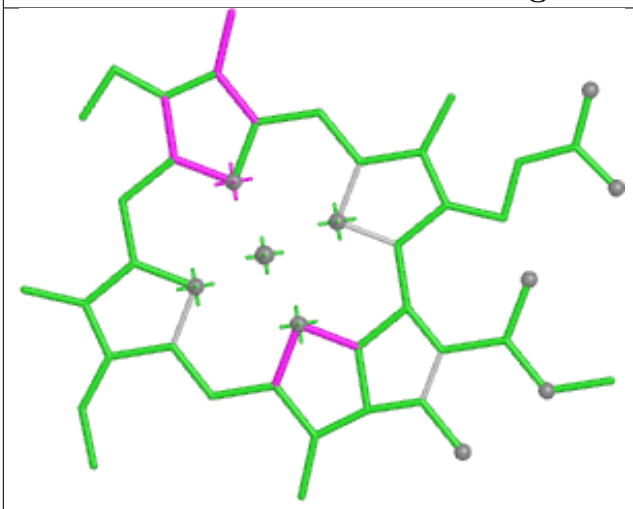


Torsions

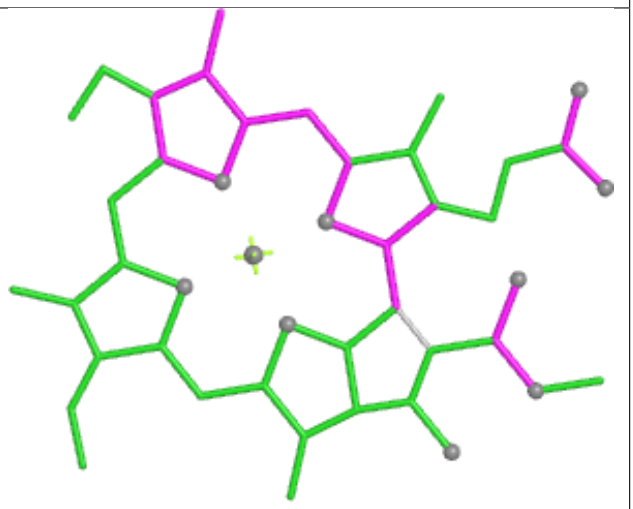


Rings

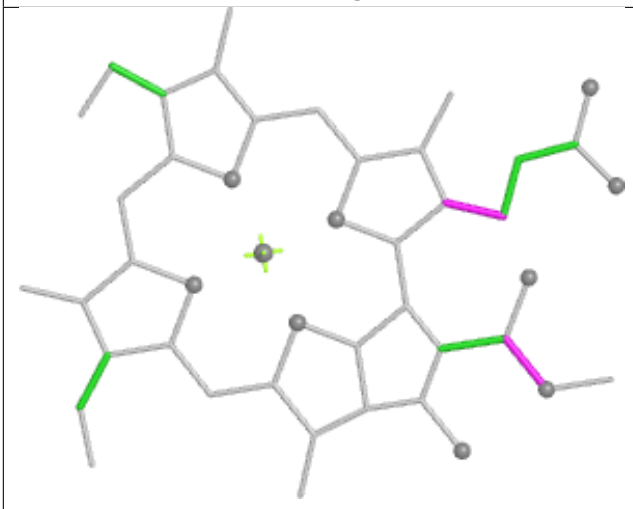
Ligand CLA c 511



Bond lengths



Bond angles

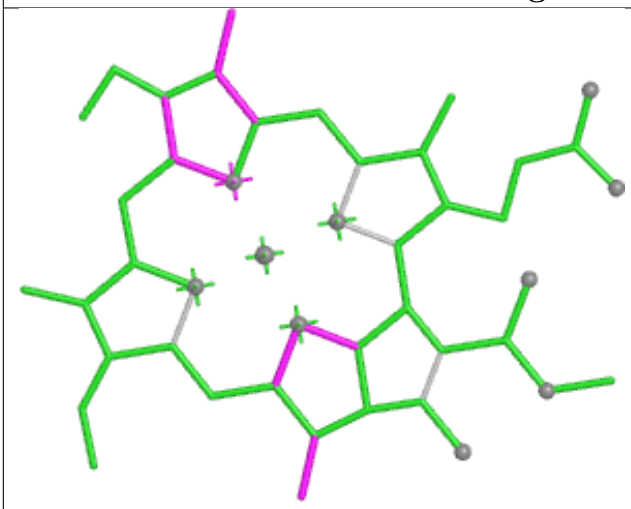


Torsions

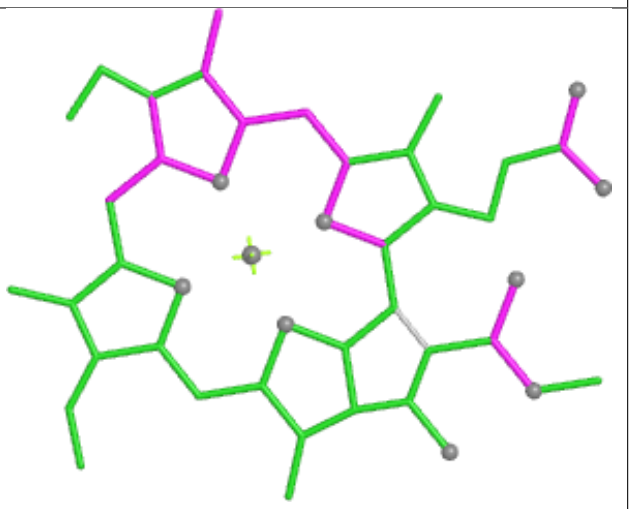


Rings

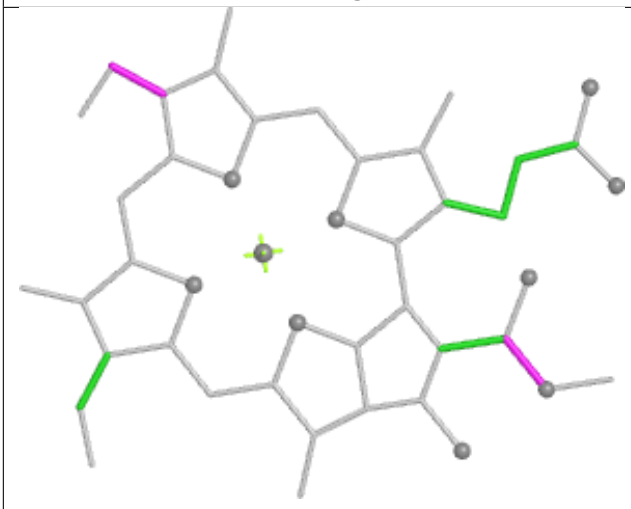
Ligand CLA 1 511



Bond lengths



Bond angles

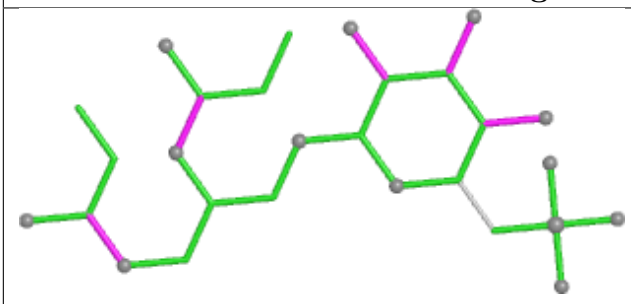


Torsions

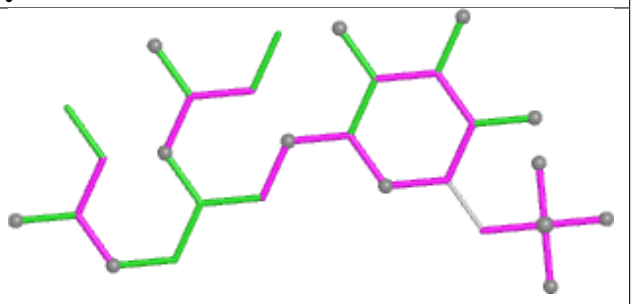


Rings

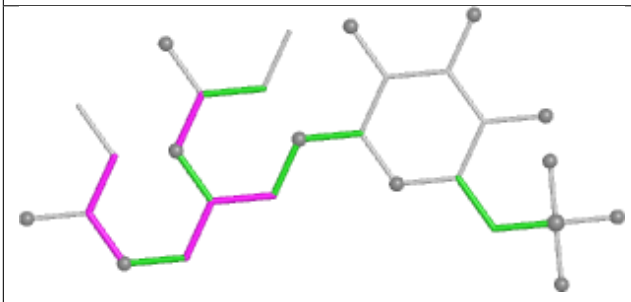
Ligand SQD s 822



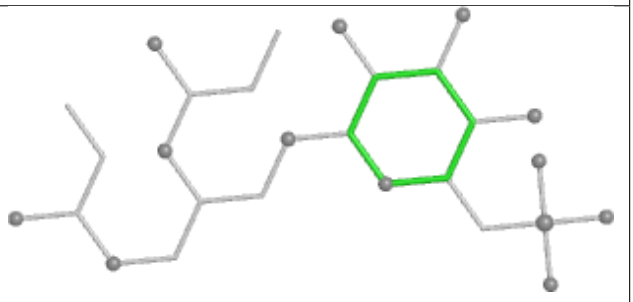
Bond lengths



Bond angles

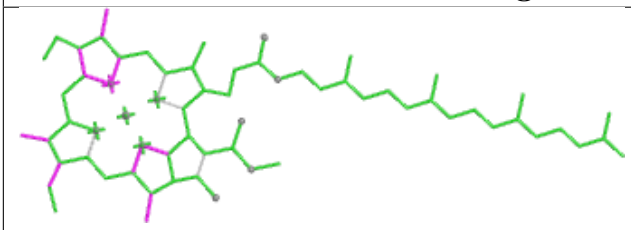


Torsions

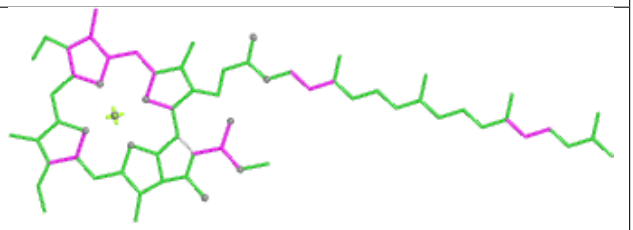


Rings

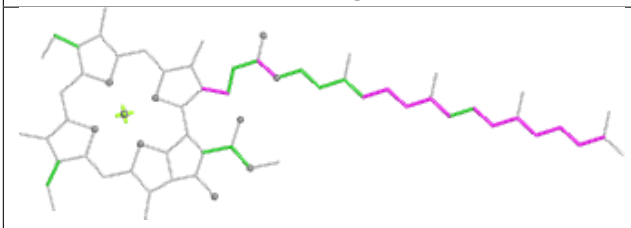
Ligand CLA B 1215



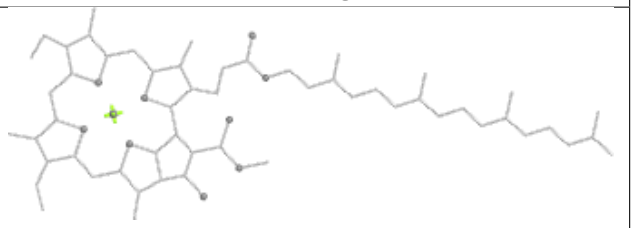
Bond lengths



Bond angles

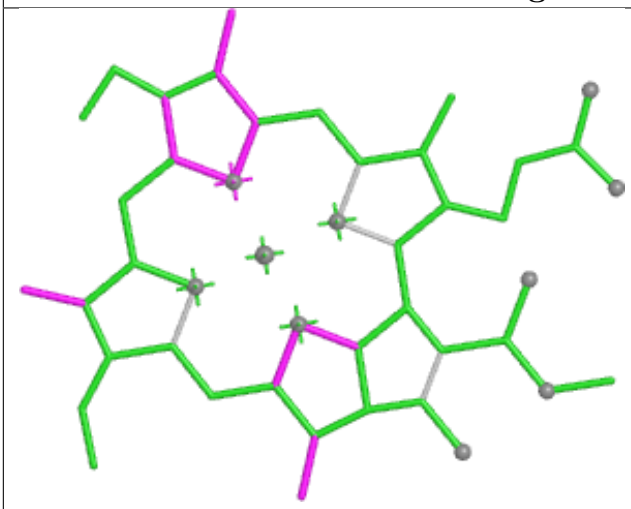


Torsions

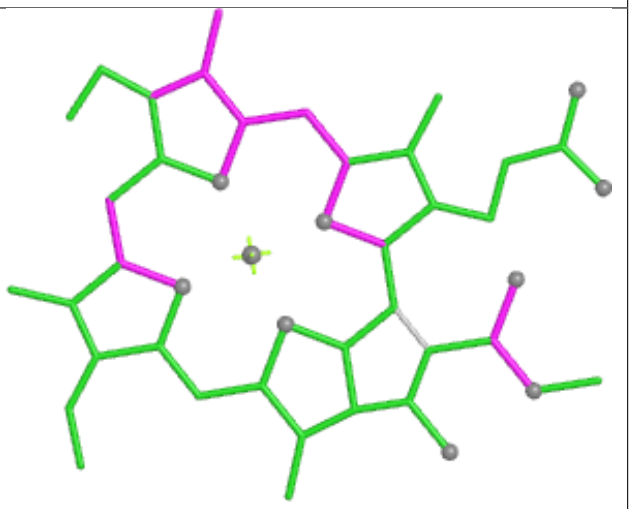


Rings

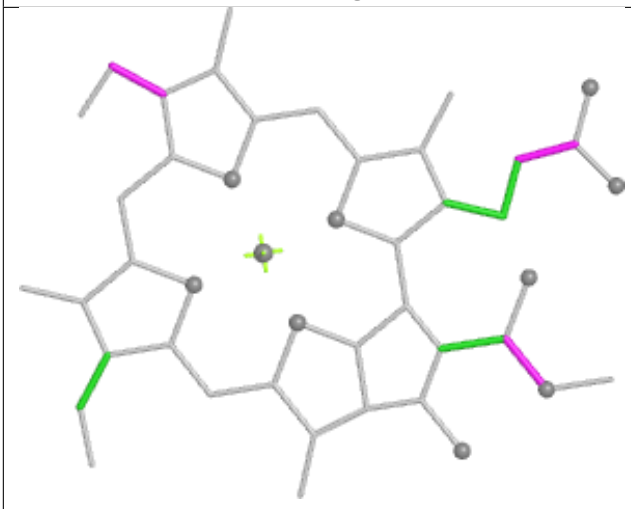
Ligand CLA 5 508



Bond lengths



Bond angles

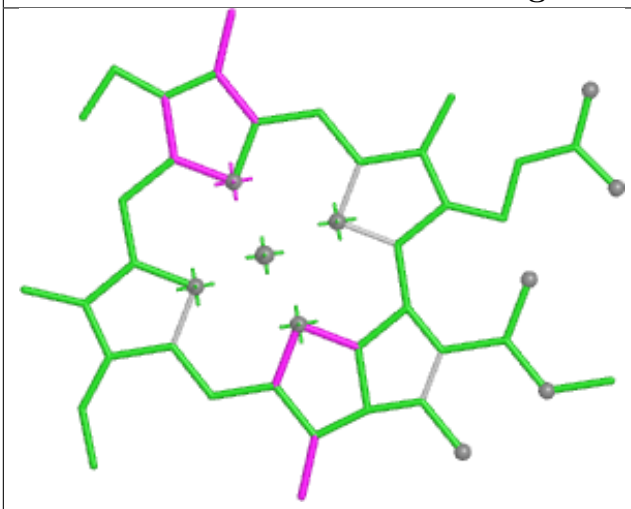


Torsions

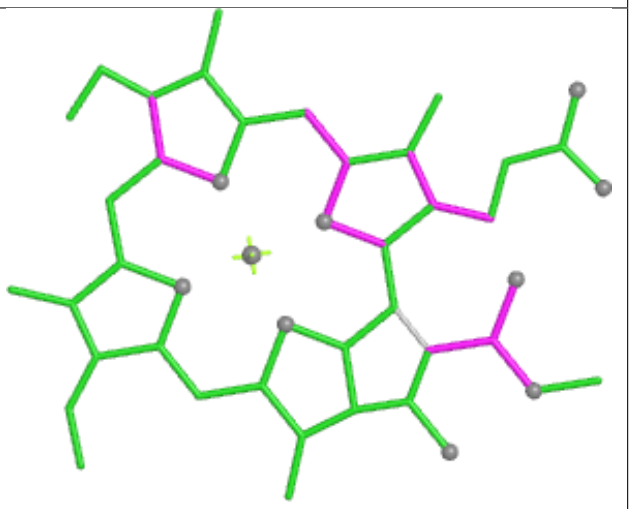


Rings

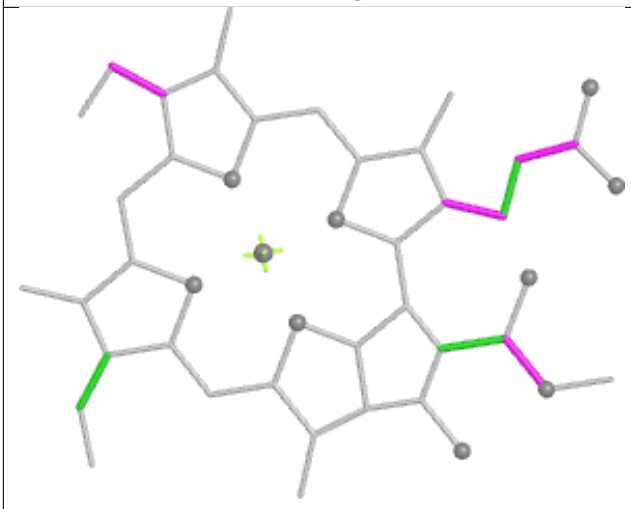
Ligand CLA 2 516



Bond lengths



Bond angles

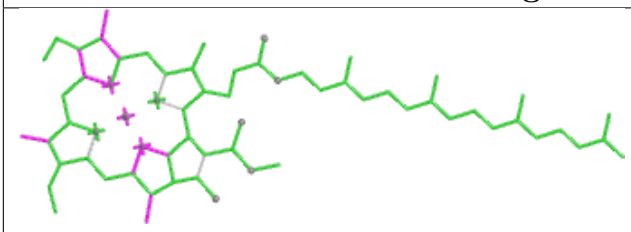


Torsions

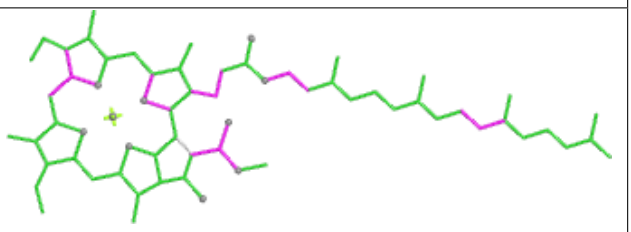


Rings

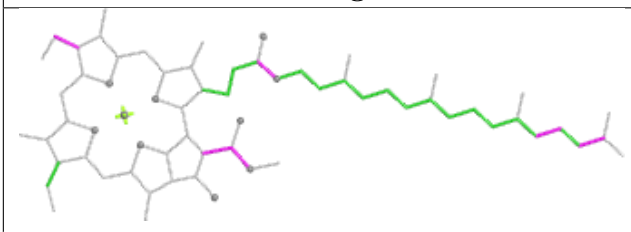
Ligand CLA f 1021



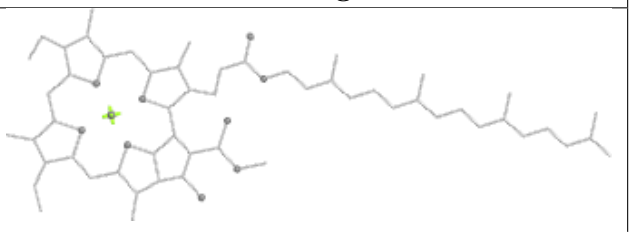
Bond lengths



Bond angles

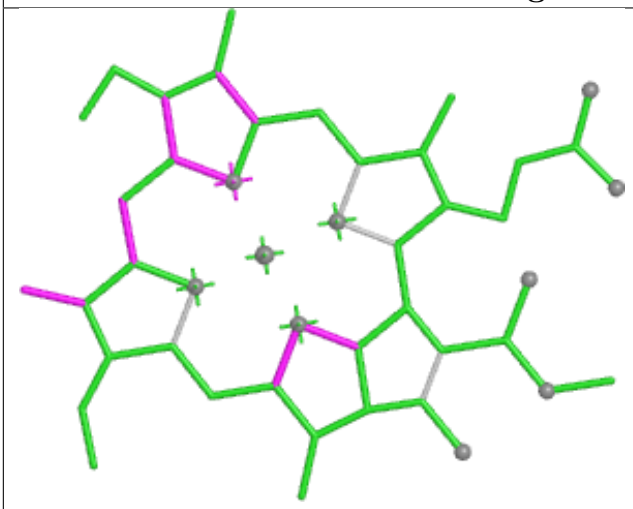


Torsions

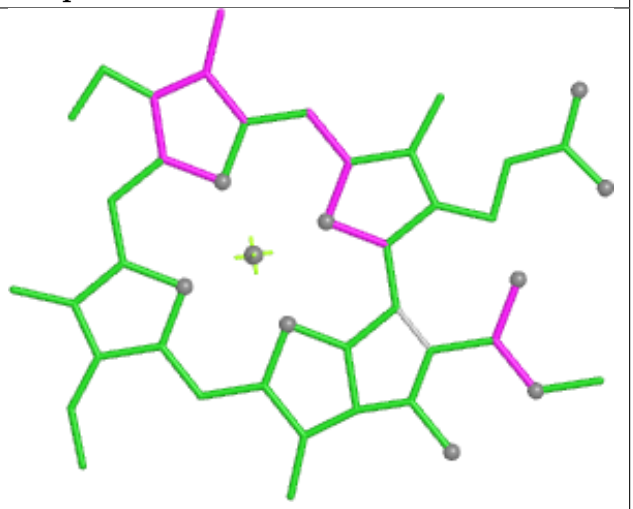


Rings

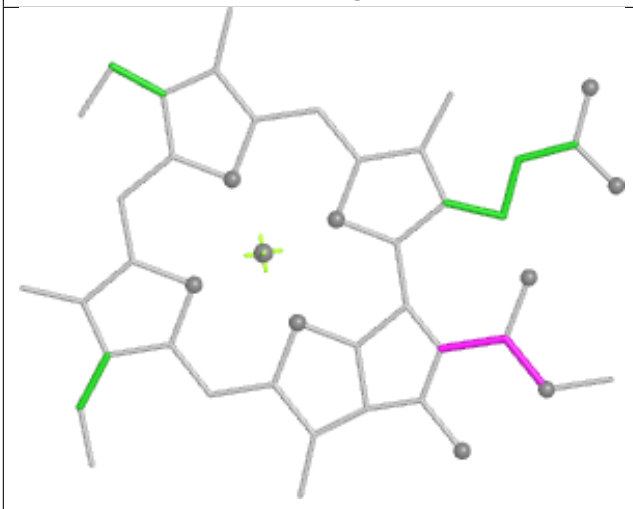
Ligand CLA q 506



Bond lengths



Bond angles

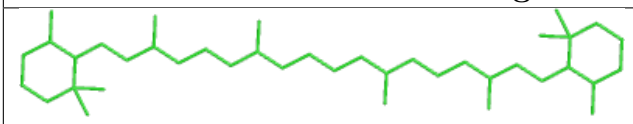


Torsions

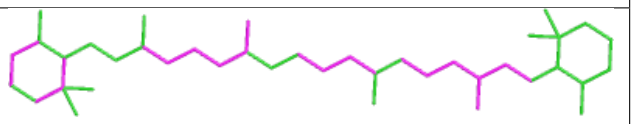


Rings

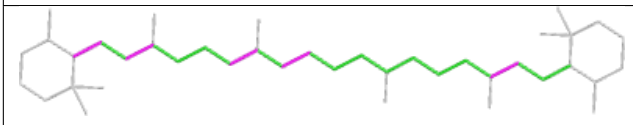
Ligand BCR A 4001



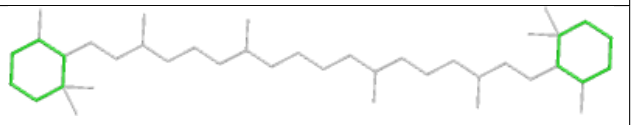
Bond lengths



Bond angles

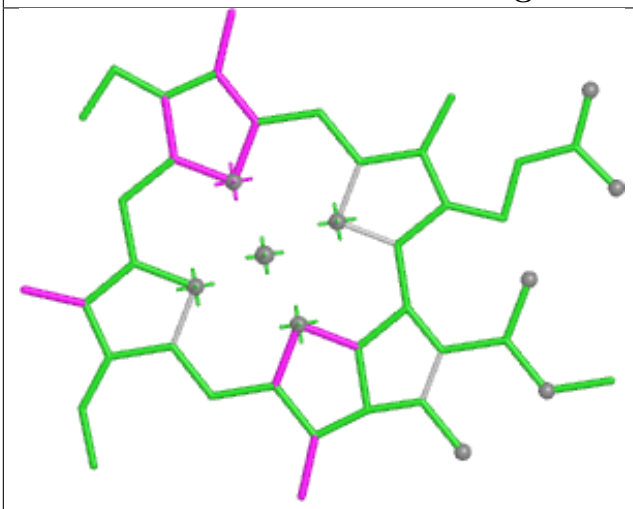


Torsions

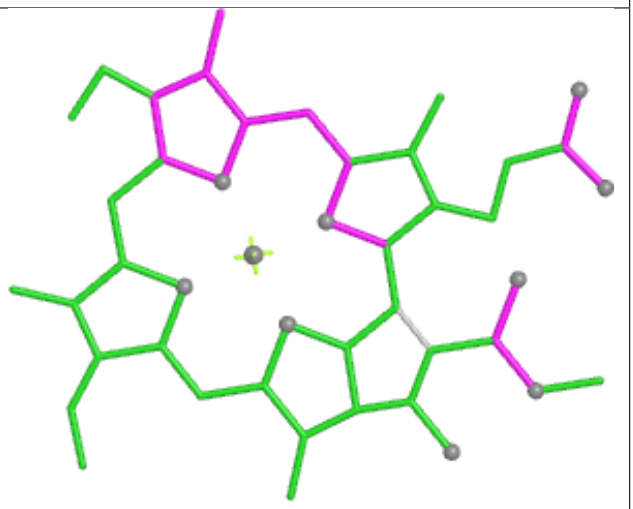


Rings

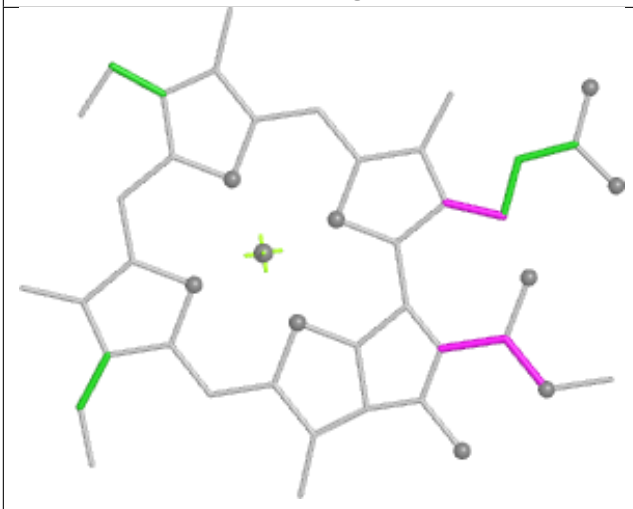
Ligand CLA A 1113



Bond lengths



Bond angles

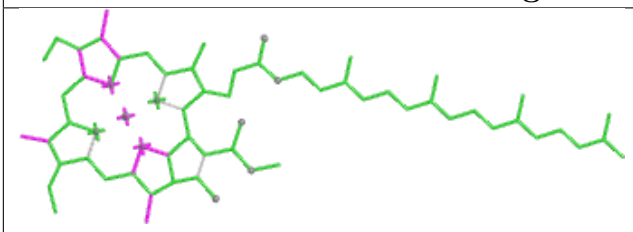


Torsions

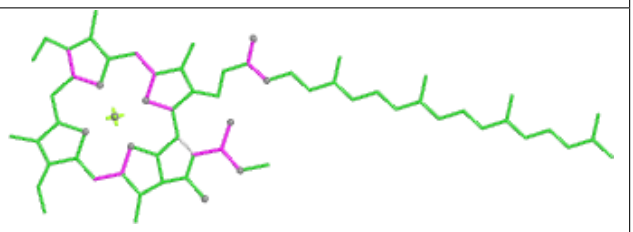


Rings

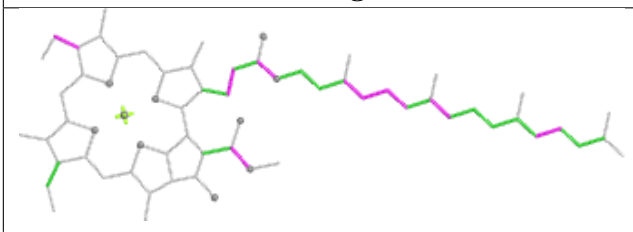
Ligand CLA f 1204



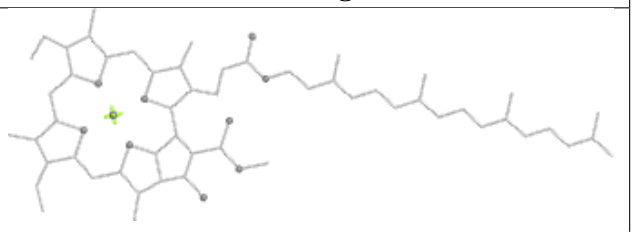
Bond lengths



Bond angles

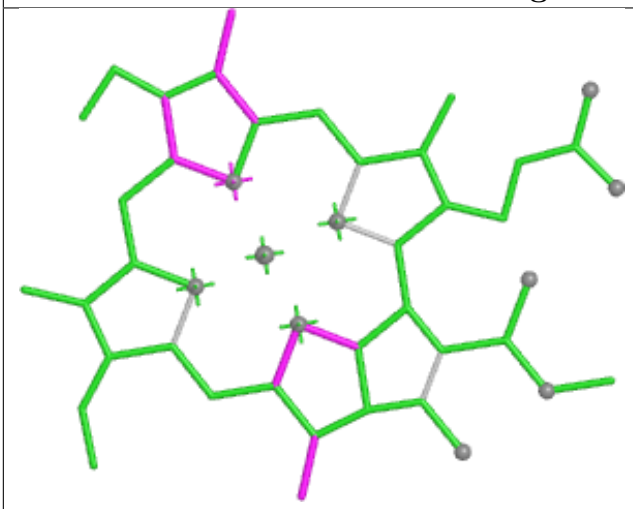


Torsions

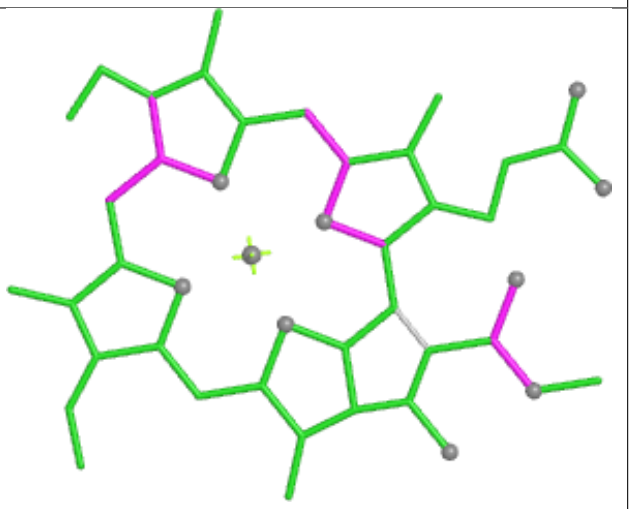


Rings

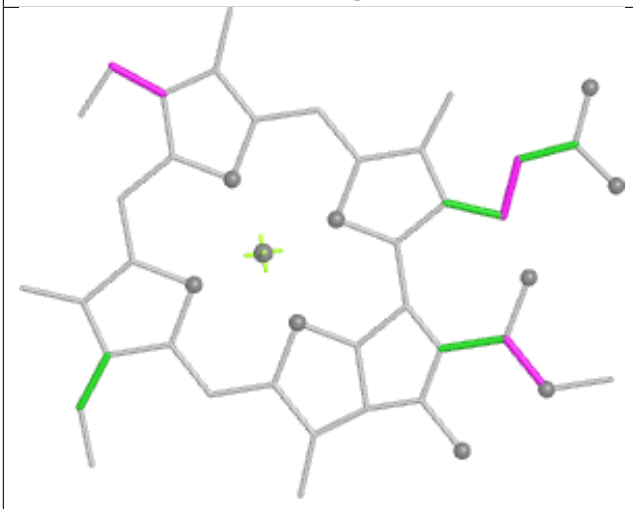
Ligand CLA s 513



Bond lengths



Bond angles

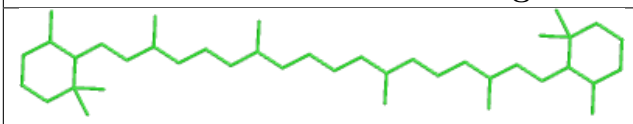


Torsions

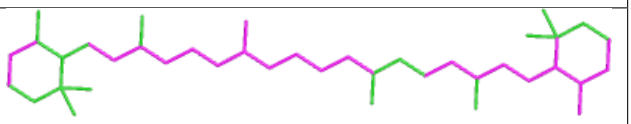


Rings

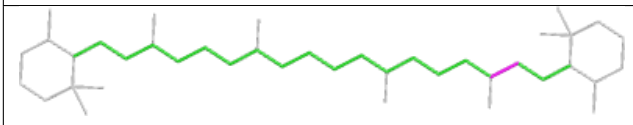
Ligand BCR U 4104



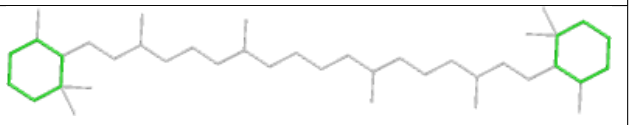
Bond lengths



Bond angles

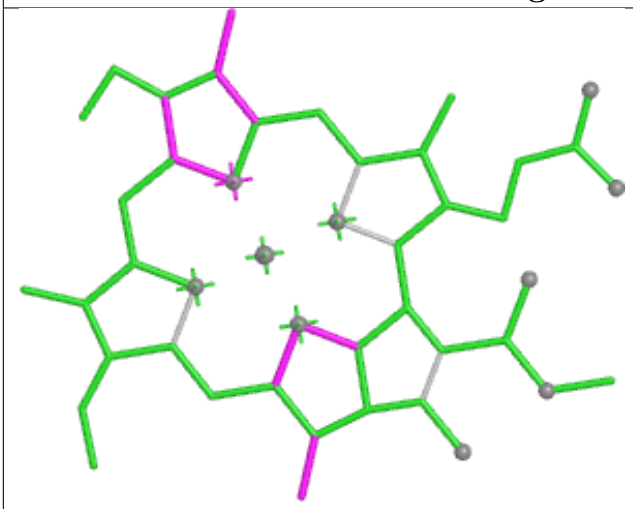


Torsions

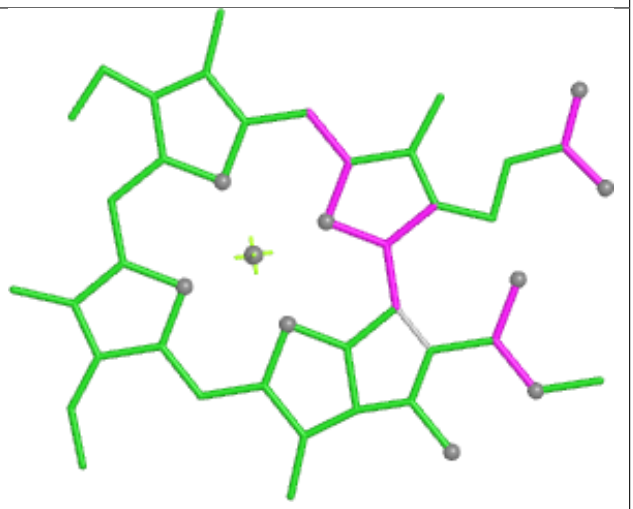


Rings

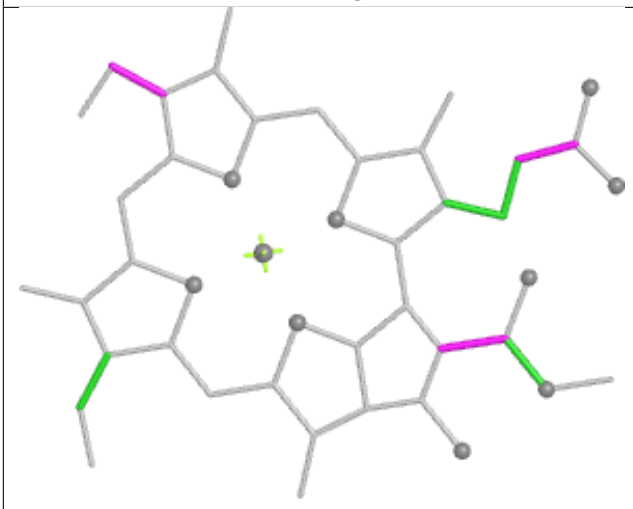
Ligand CLA 3 507



Bond lengths



Bond angles

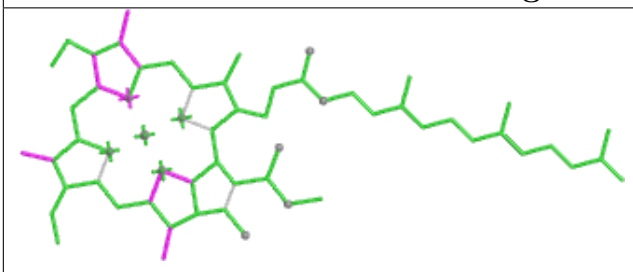


Torsions

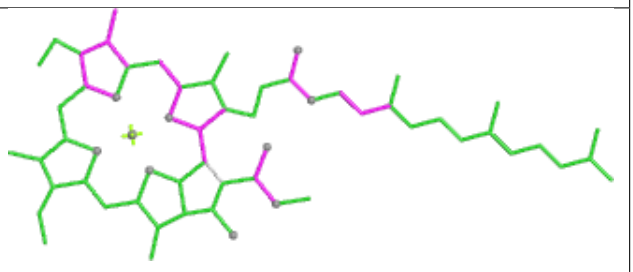


Rings

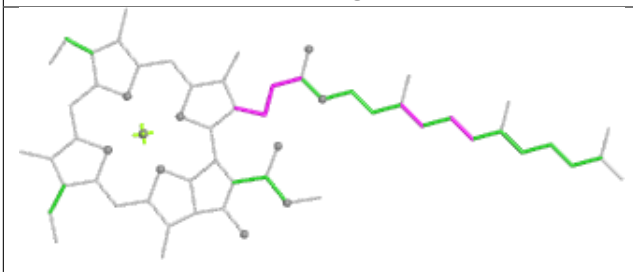
Ligand CLA f 1224



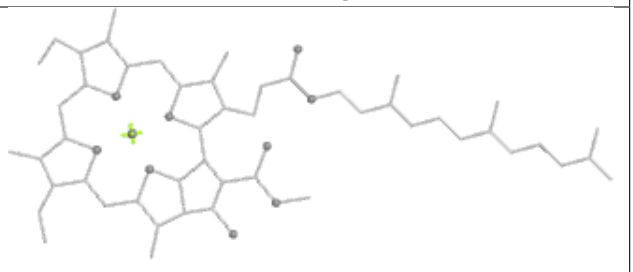
Bond lengths



Bond angles

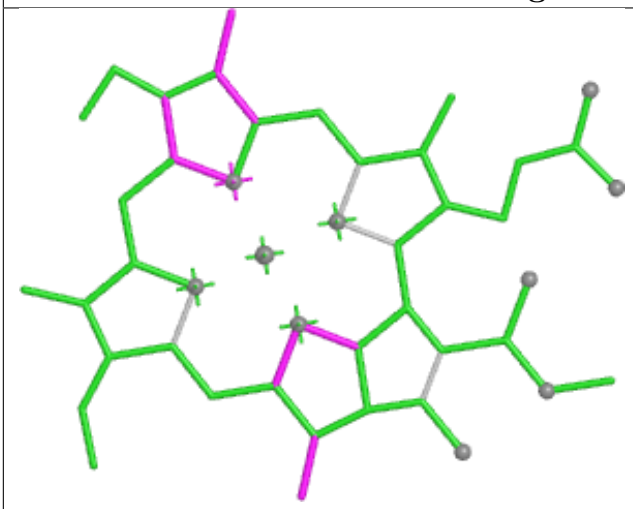


Torsions

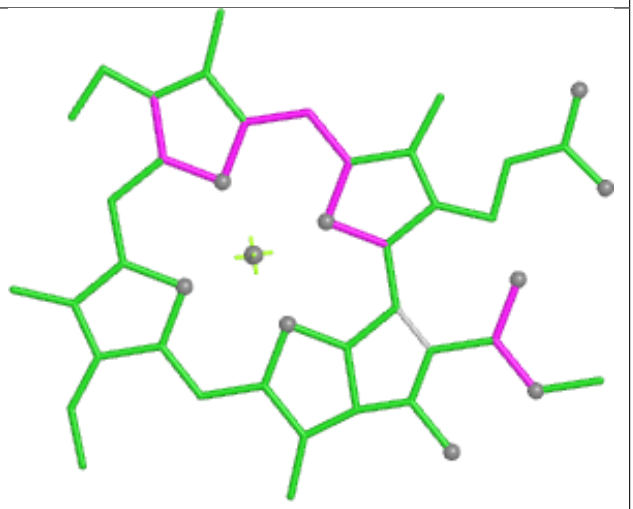


Rings

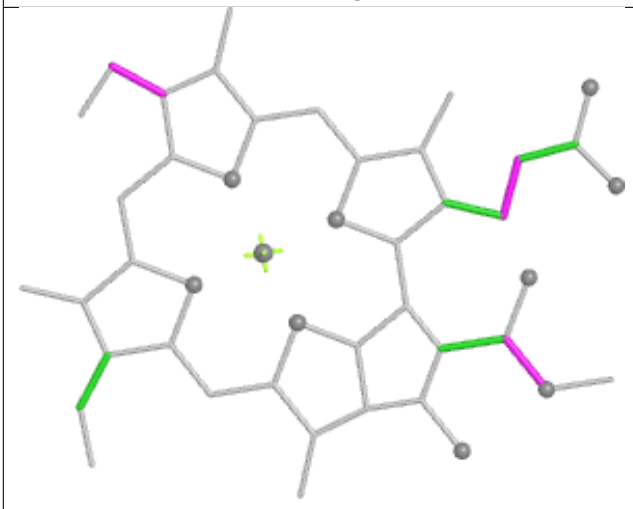
Ligand CLA 6 513



Bond lengths



Bond angles

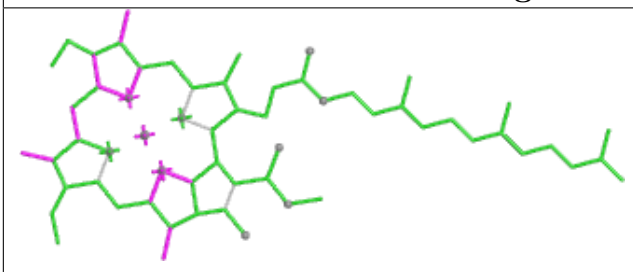


Torsions

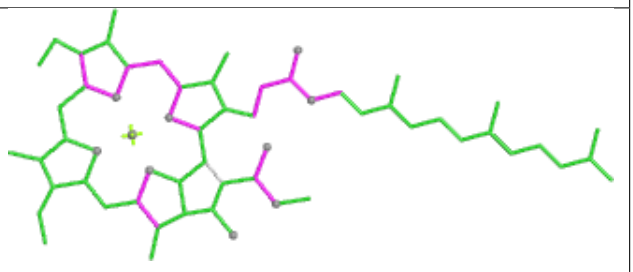


Rings

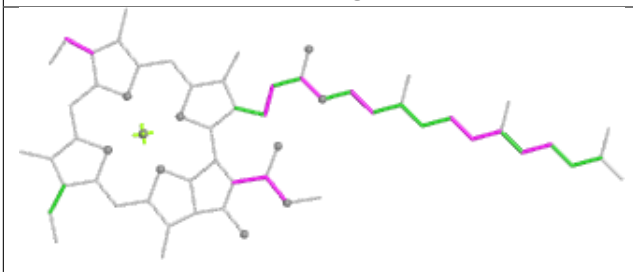
Ligand CLA H 1216



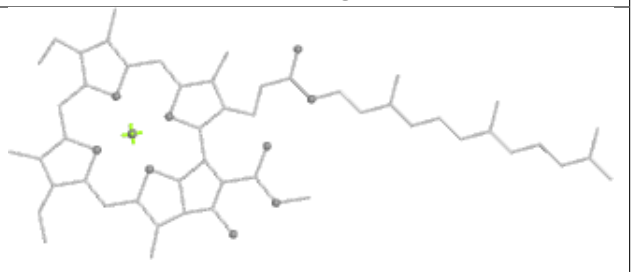
Bond lengths



Bond angles

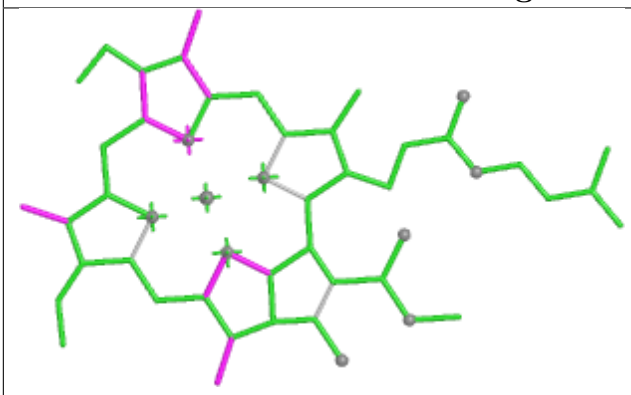


Torsions

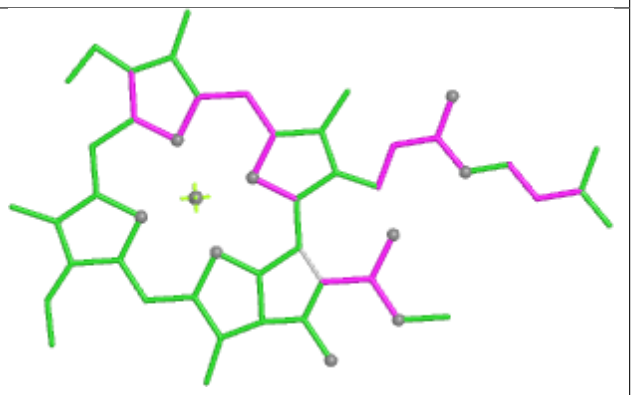


Rings

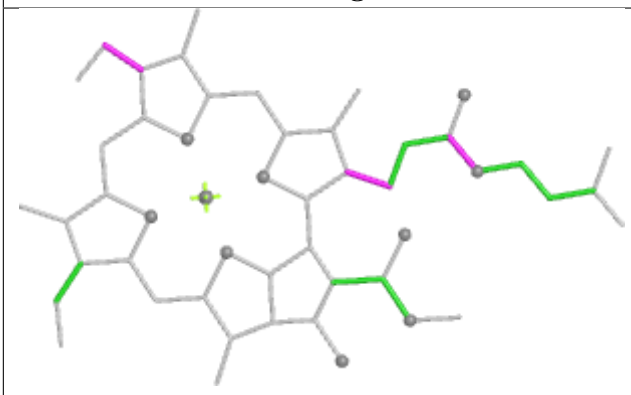
Ligand CLA B 1236



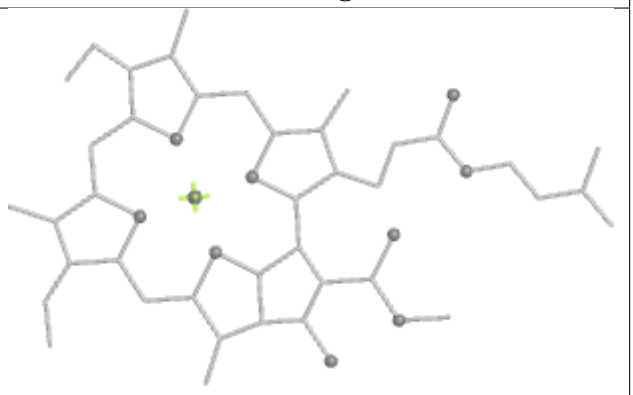
Bond lengths



Bond angles



Torsions

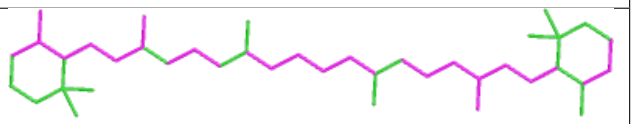


Rings

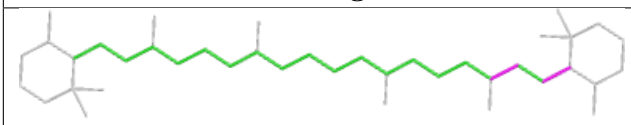
Ligand BCR 5 523



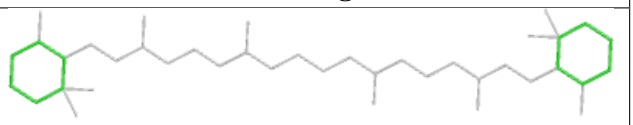
Bond lengths



Bond angles

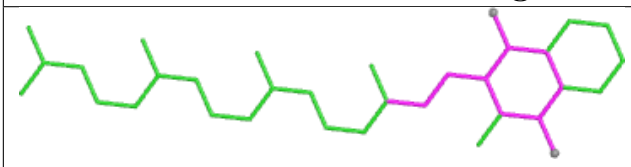


Torsions

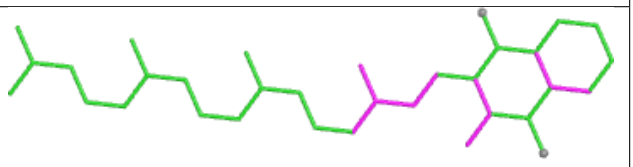


Rings

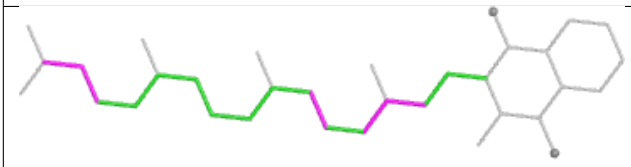
Ligand PQN H 2002



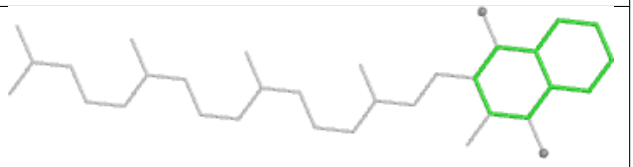
Bond lengths



Bond angles

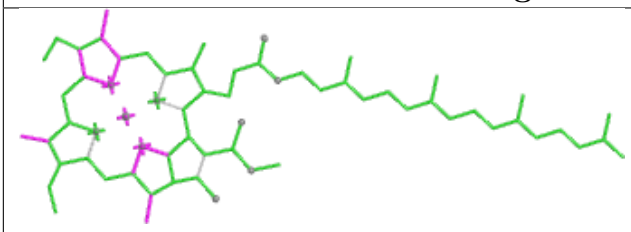


Torsions

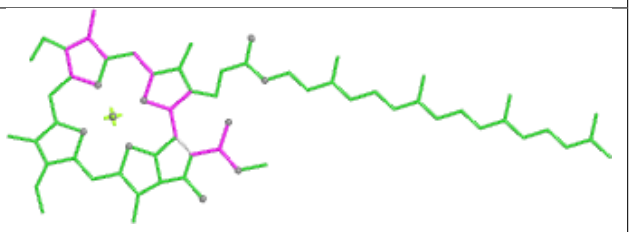


Rings

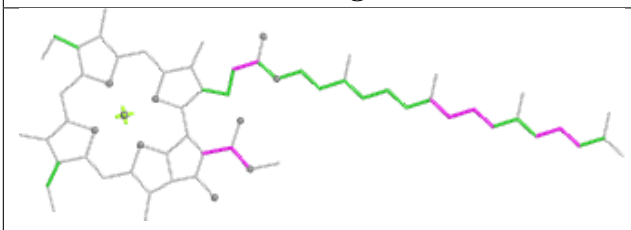
Ligand CLA G 1123



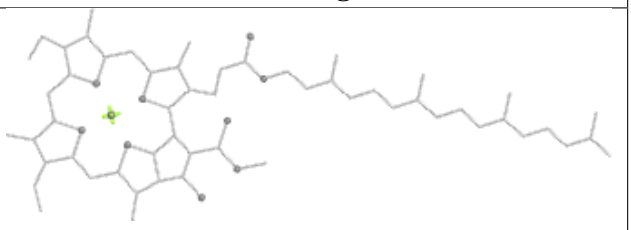
Bond lengths



Bond angles

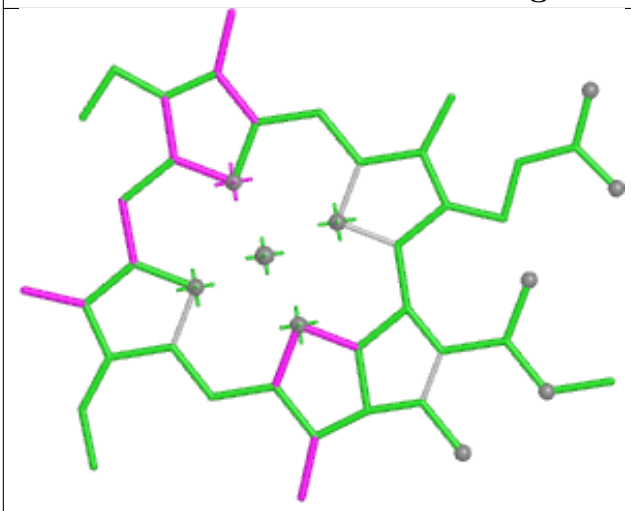


Torsions

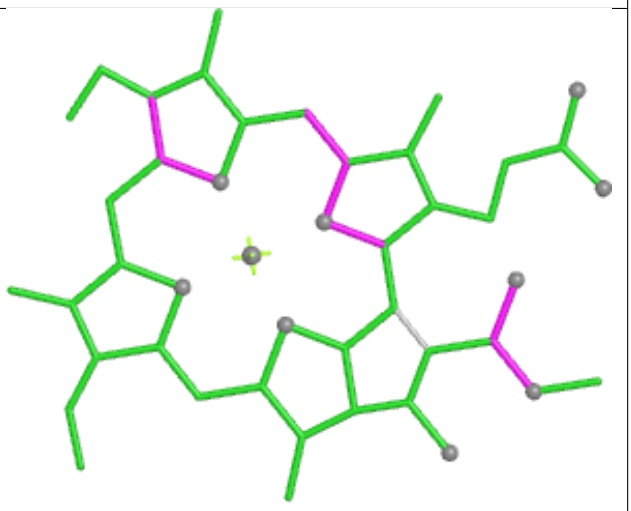


Rings

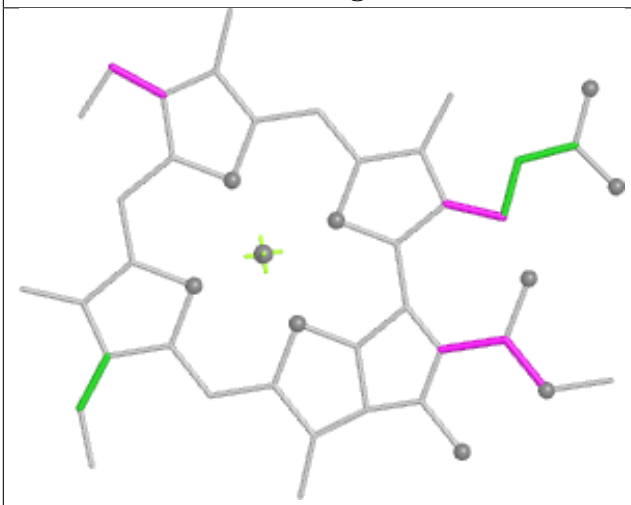
Ligand CLA s 517



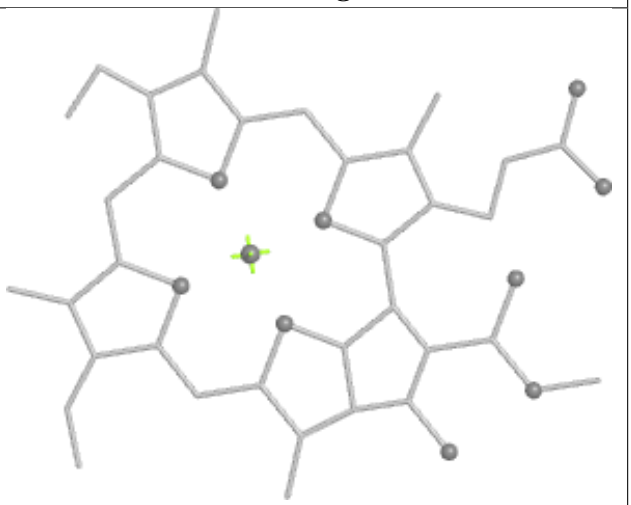
Bond lengths



Bond angles

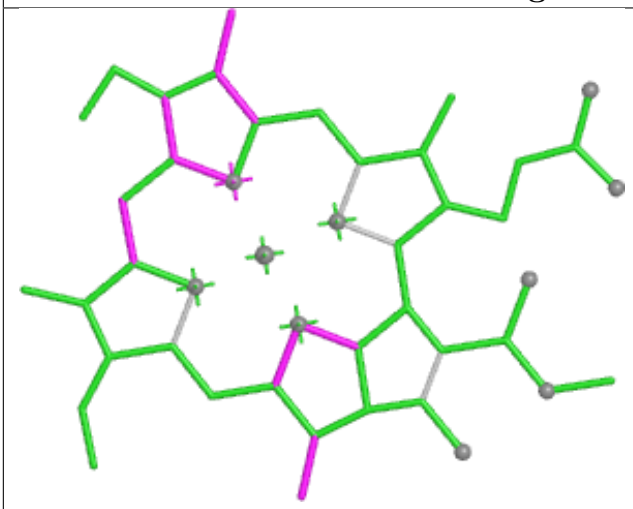


Torsions

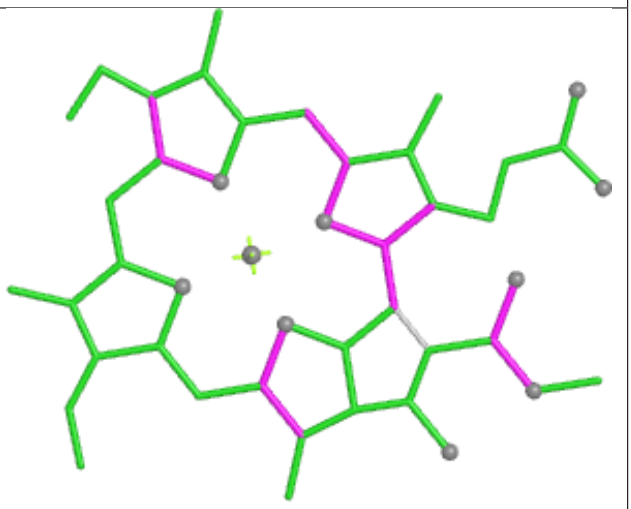


Rings

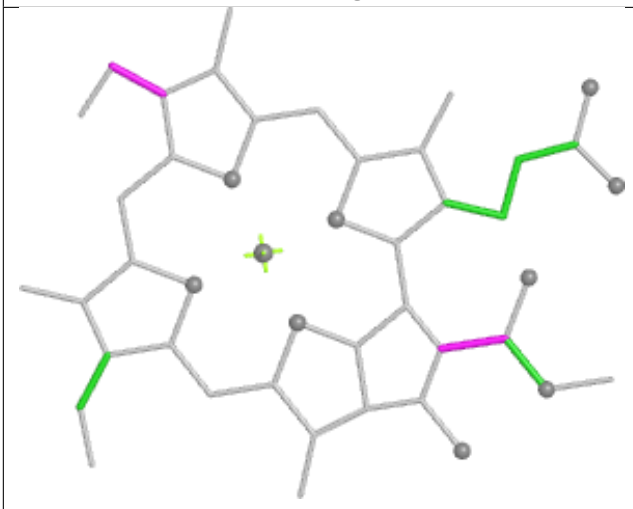
Ligand CLA 4 503



Bond lengths



Bond angles

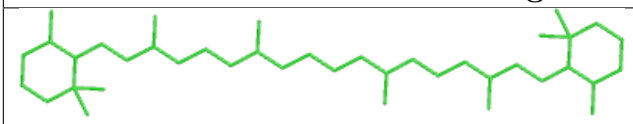


Torsions

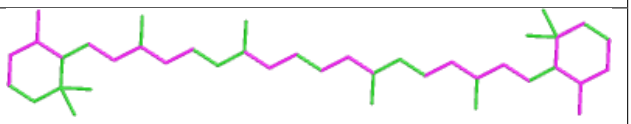


Rings

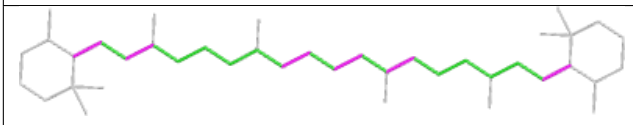
Ligand BCR 4 521



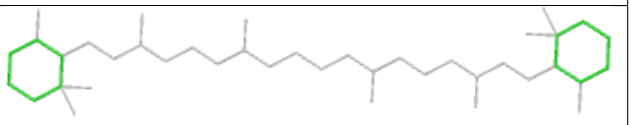
Bond lengths



Bond angles

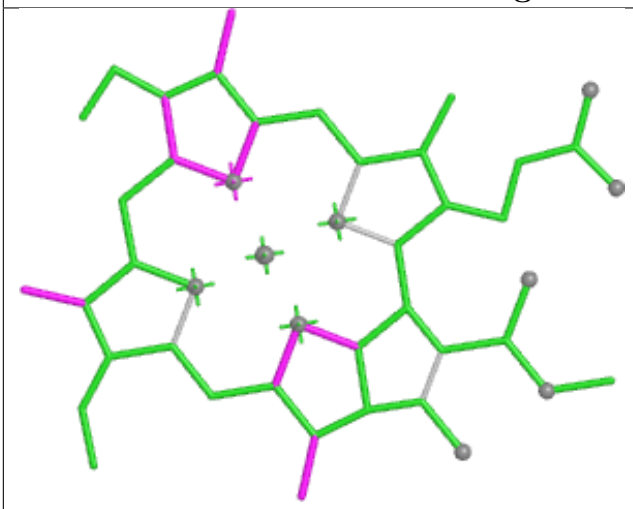


Torsions

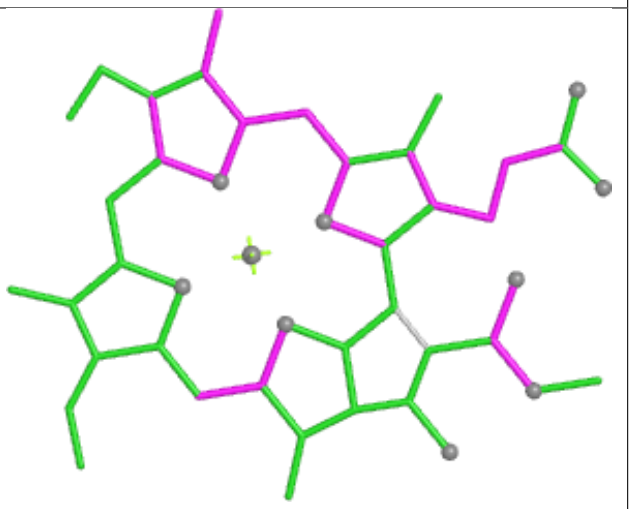


Rings

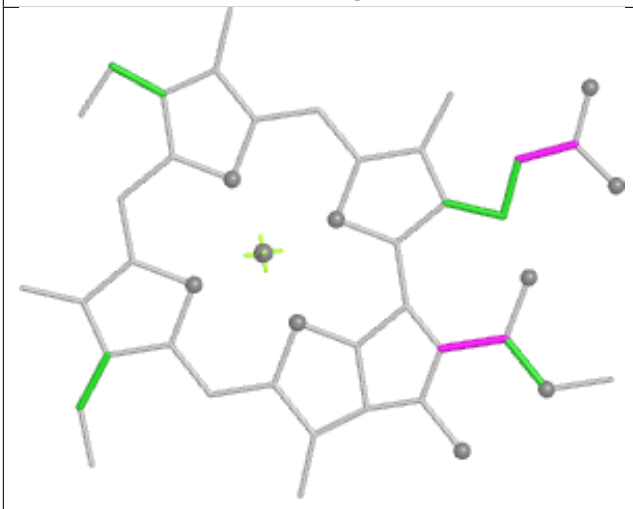
Ligand CLA G 1114



Bond lengths



Bond angles

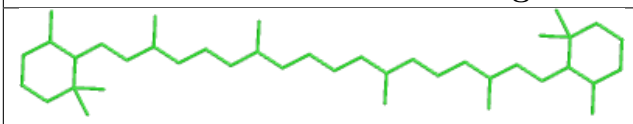


Torsions

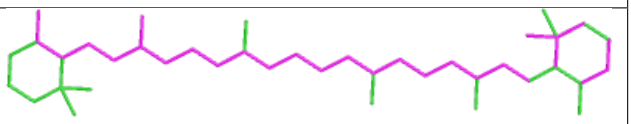


Rings

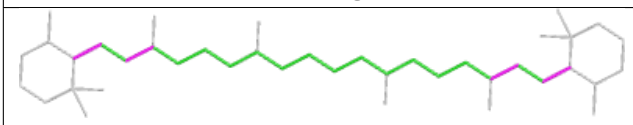
Ligand BCR H 4004



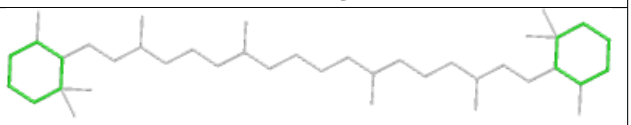
Bond lengths



Bond angles

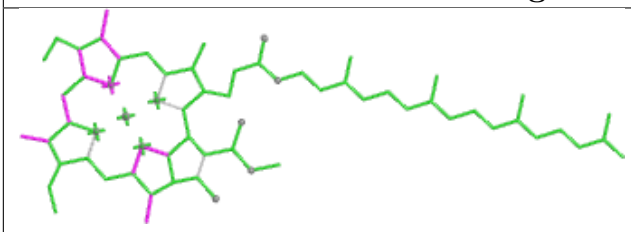


Torsions

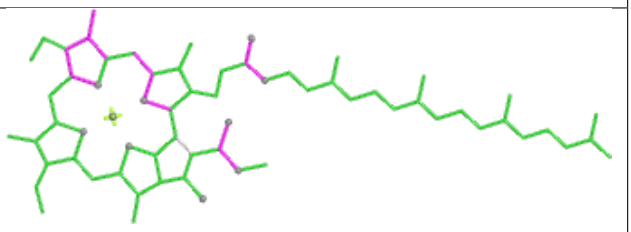


Rings

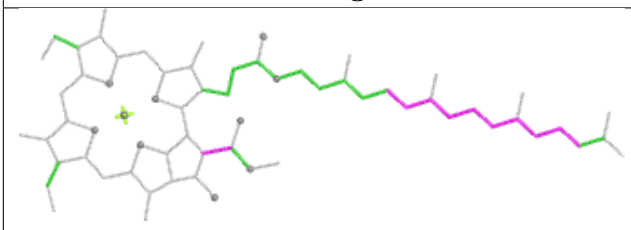
Ligand CLA 5 509



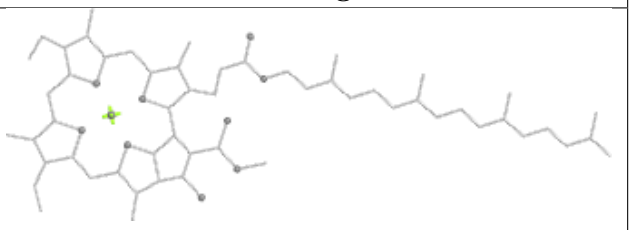
Bond lengths



Bond angles

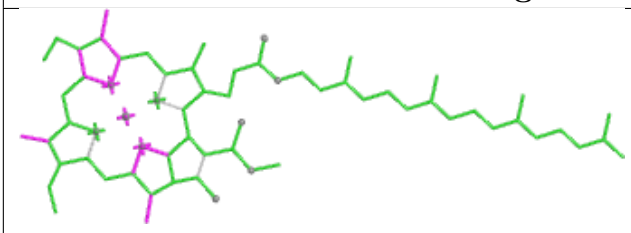


Torsions

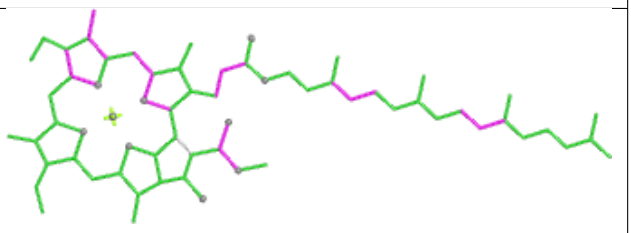


Rings

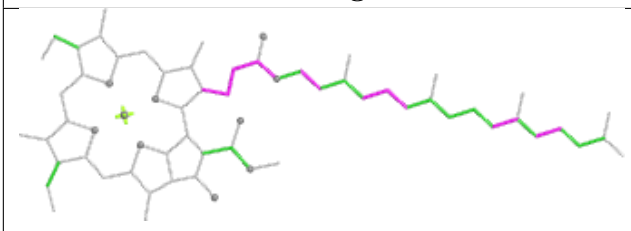
Ligand CLA A 1125



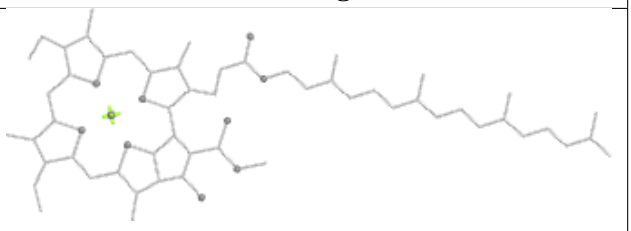
Bond lengths



Bond angles

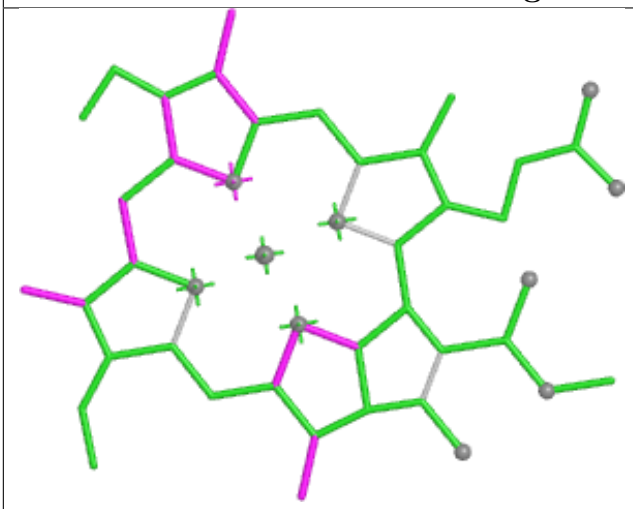


Torsions

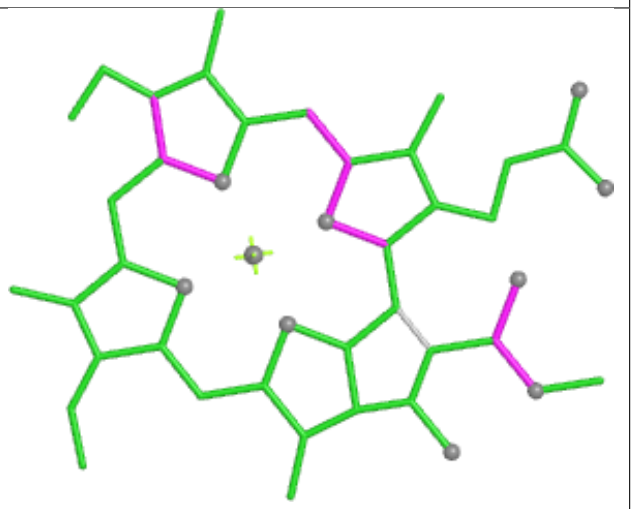


Rings

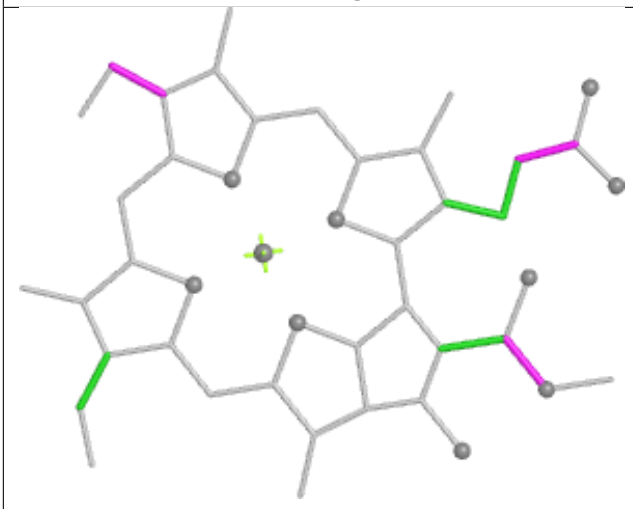
Ligand CLA Y 510



Bond lengths



Bond angles

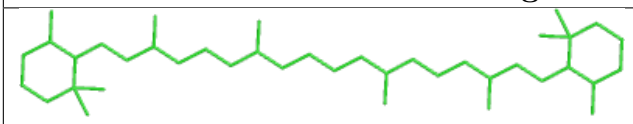


Torsions

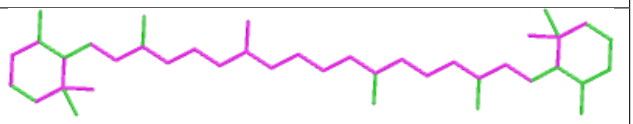


Rings

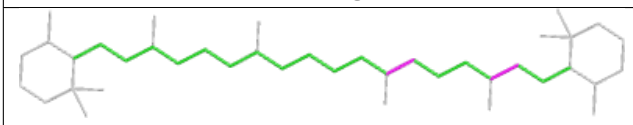
Ligand BCR l 4013



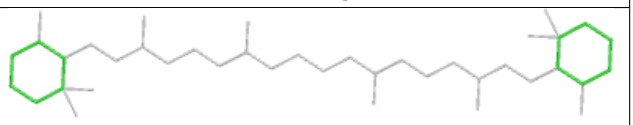
Bond lengths



Bond angles

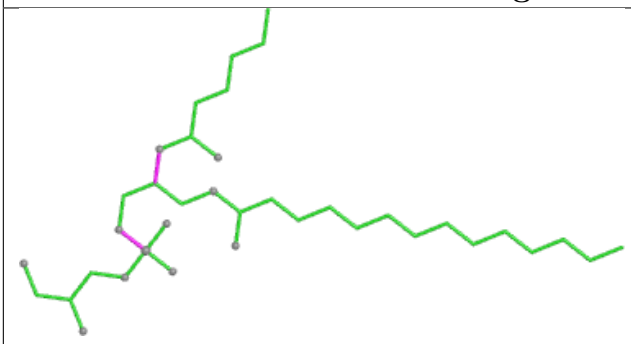


Torsions

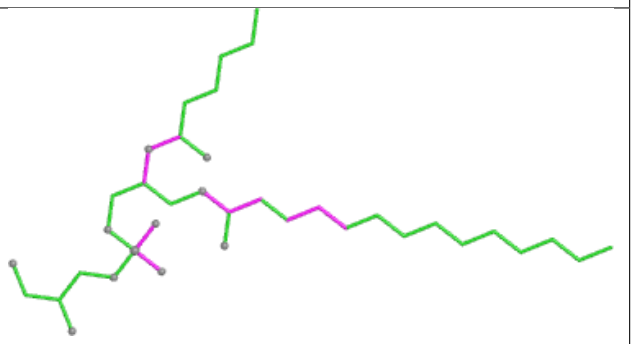


Rings

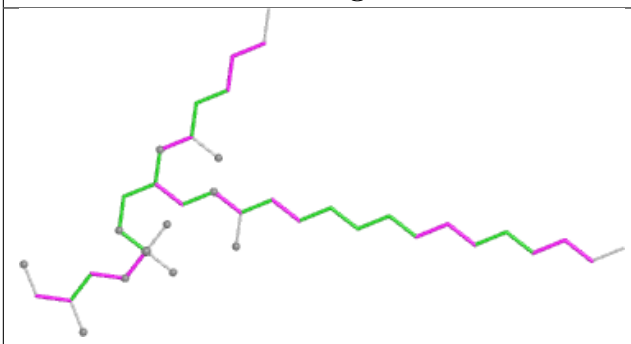
Ligand LHG V 5218



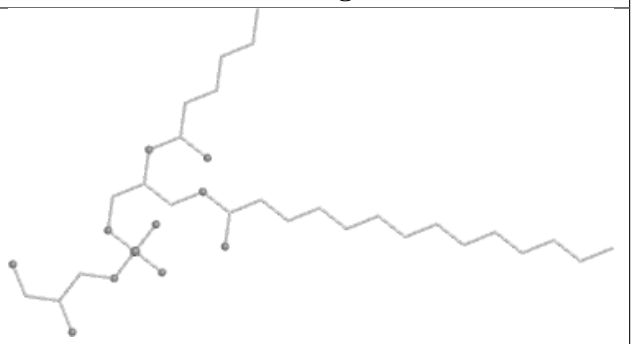
Bond lengths



Bond angles

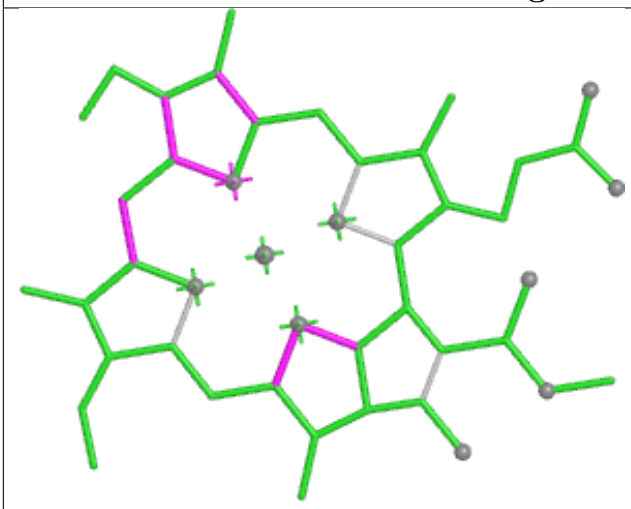


Torsions

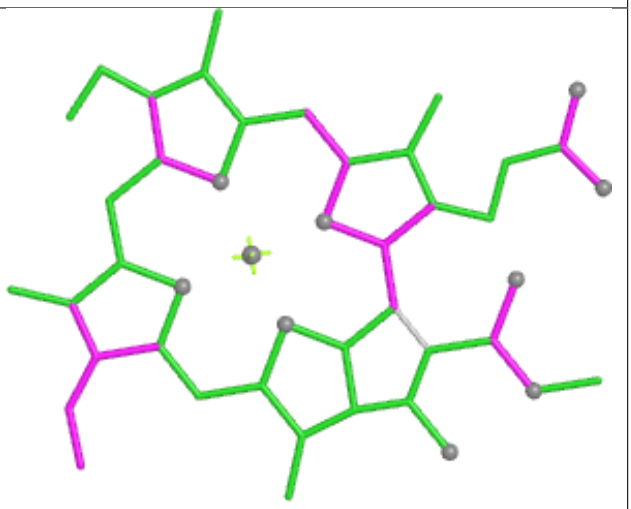


Rings

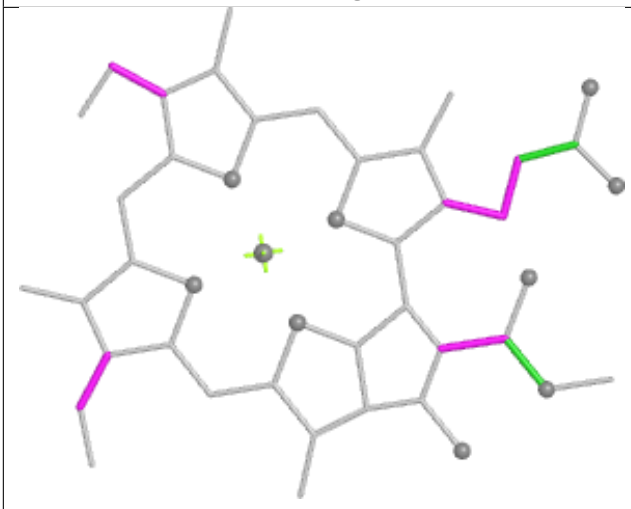
Ligand CLA 3 516



Bond lengths



Bond angles

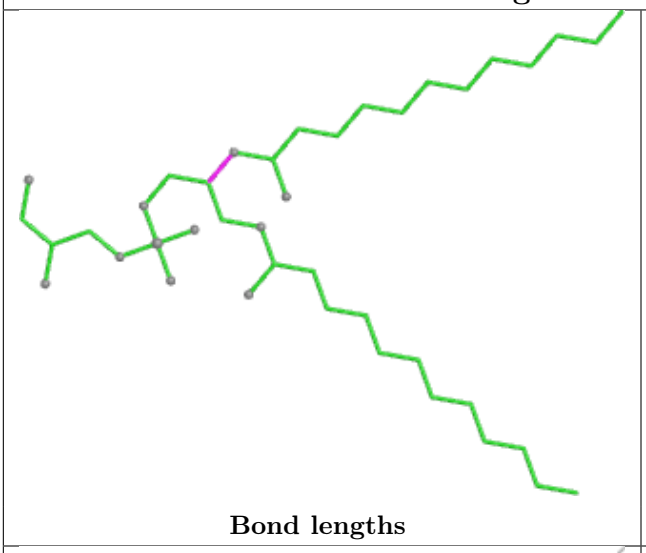


Torsions

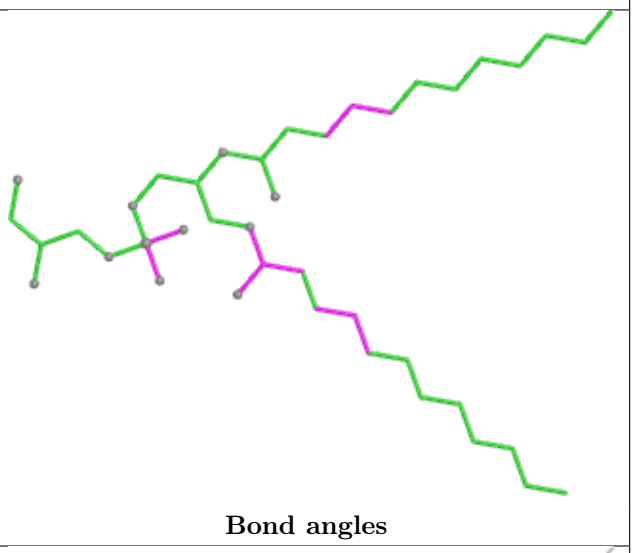


Rings

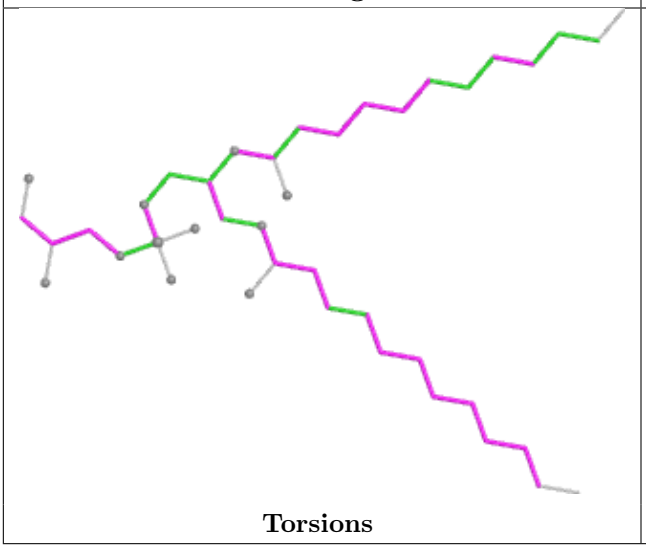
Ligand LHG V 5220



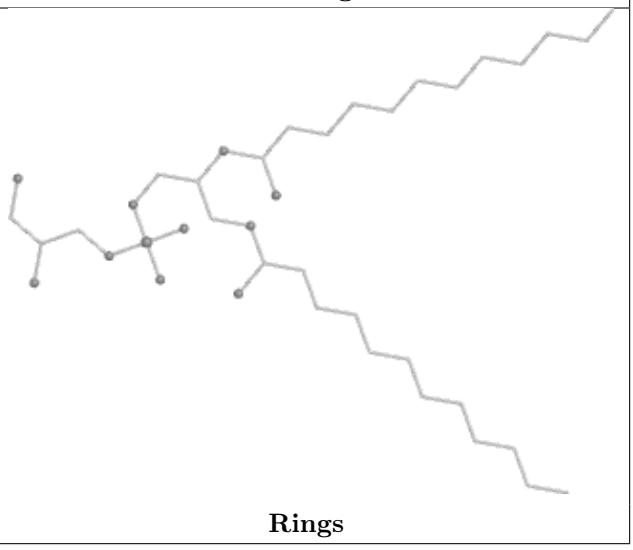
Bond lengths



Bond angles

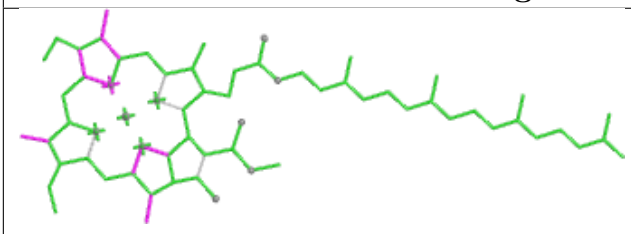


Torsions

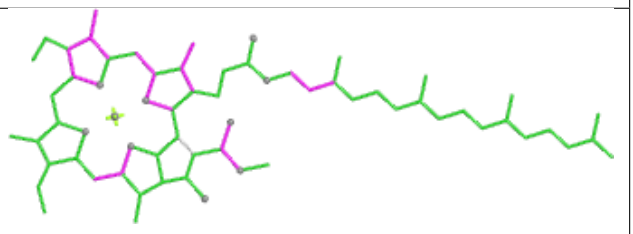


Rings

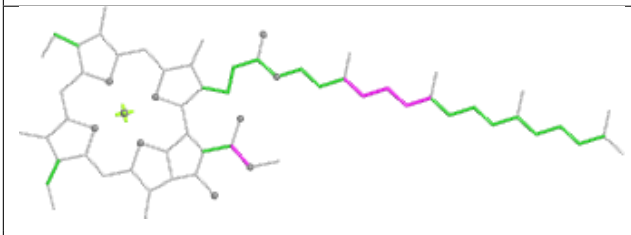
Ligand CLA H 1231



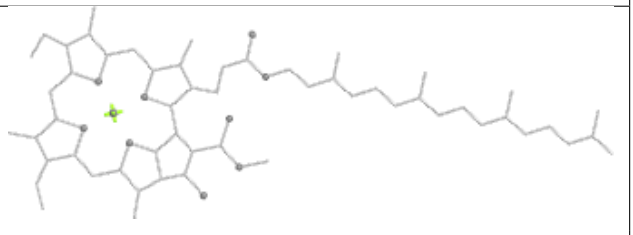
Bond lengths



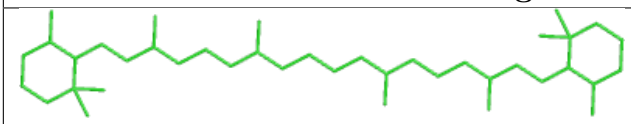
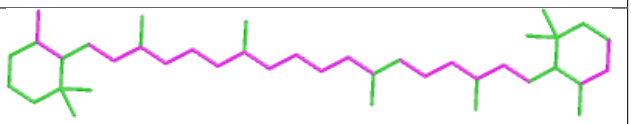
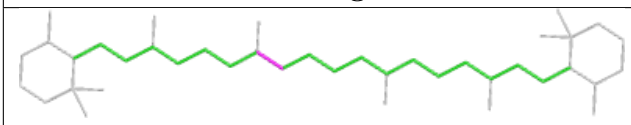
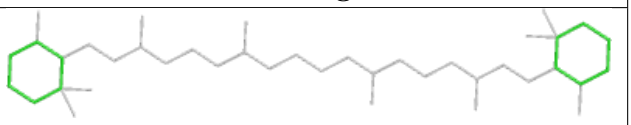
Bond angles

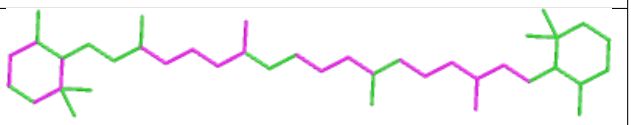
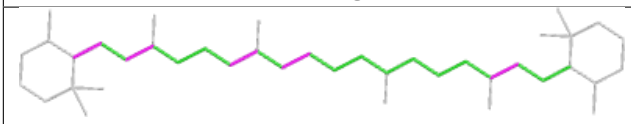
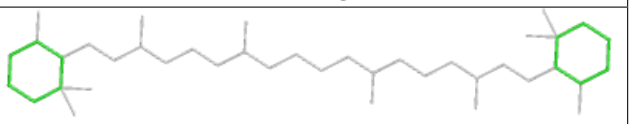


Torsions

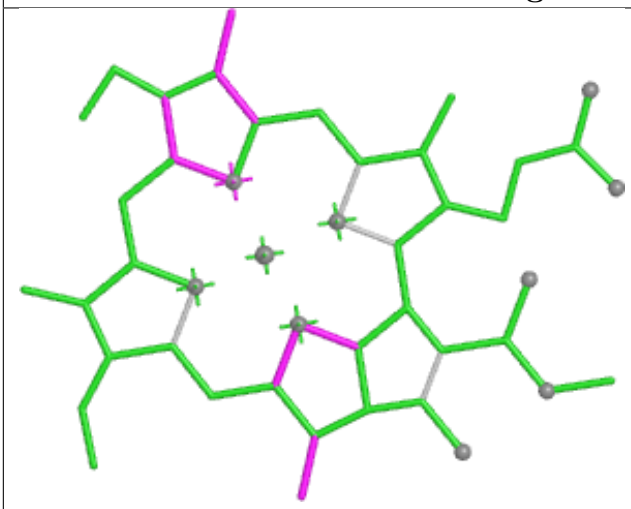


Rings

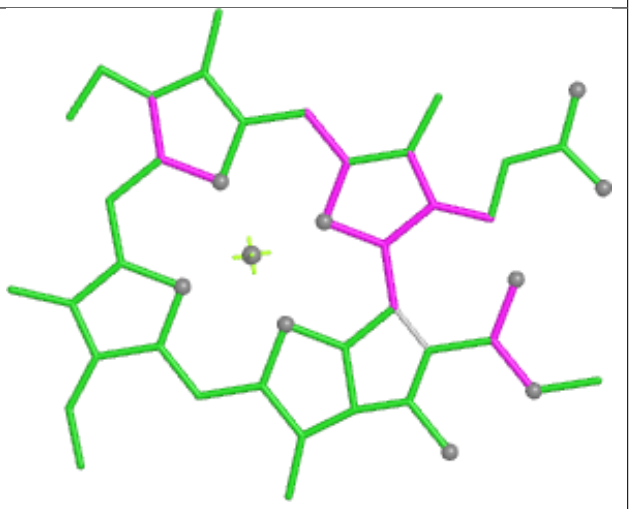
Ligand BCR F 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR G 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

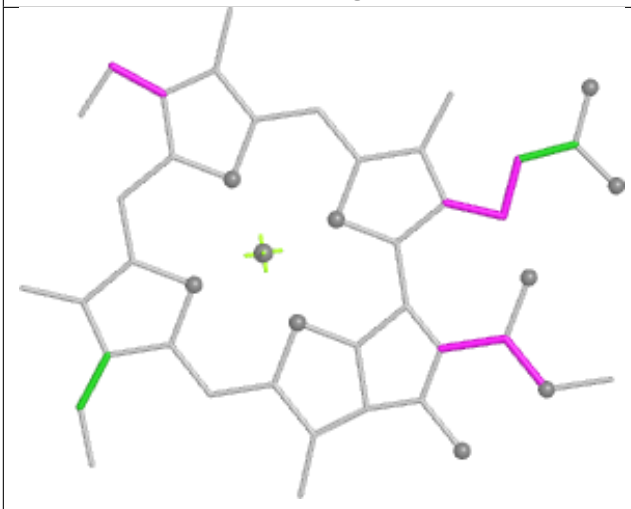
Ligand CLA Z 504



Bond lengths



Bond angles

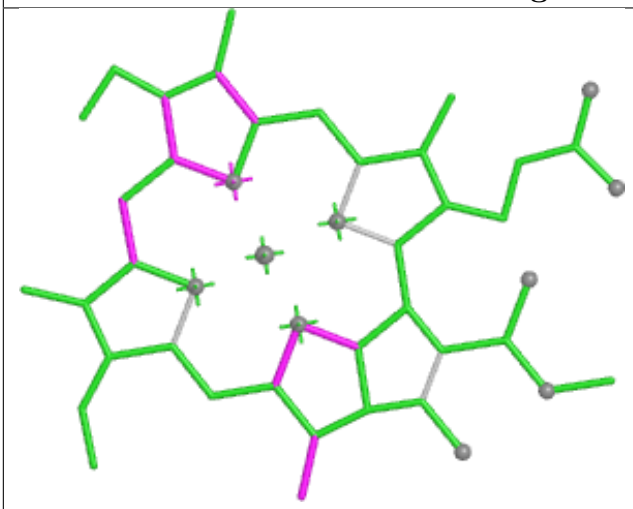


Torsions

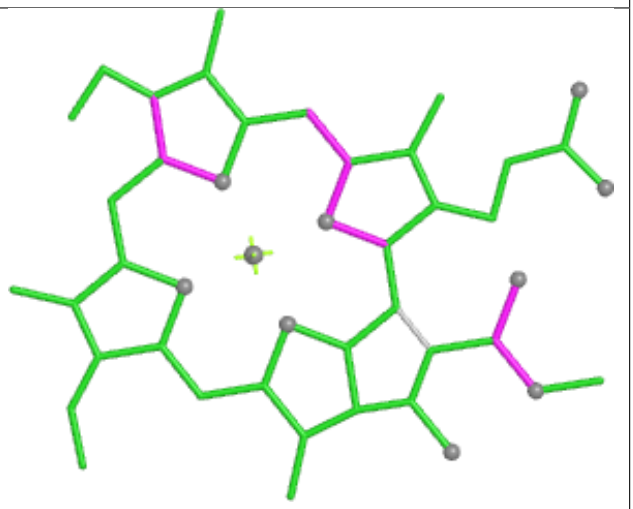


Rings

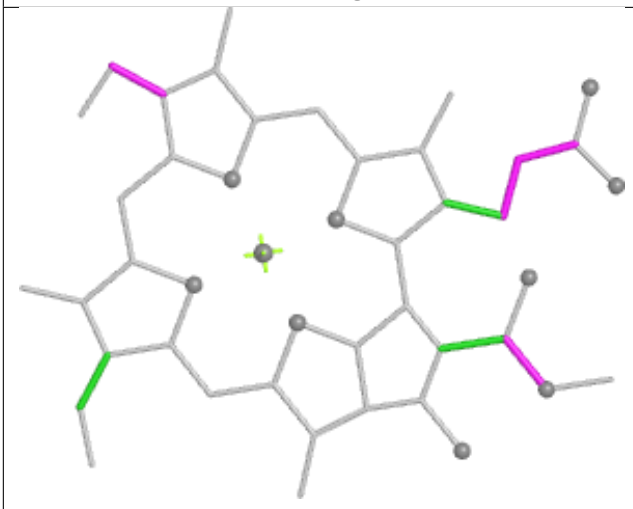
Ligand CLA t 513



Bond lengths



Bond angles

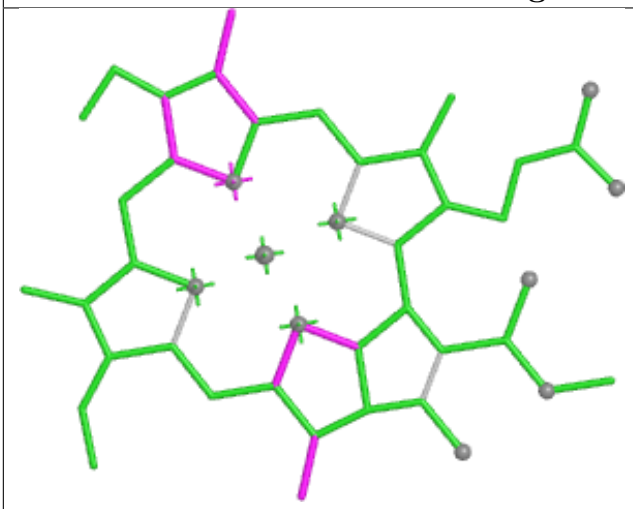


Torsions

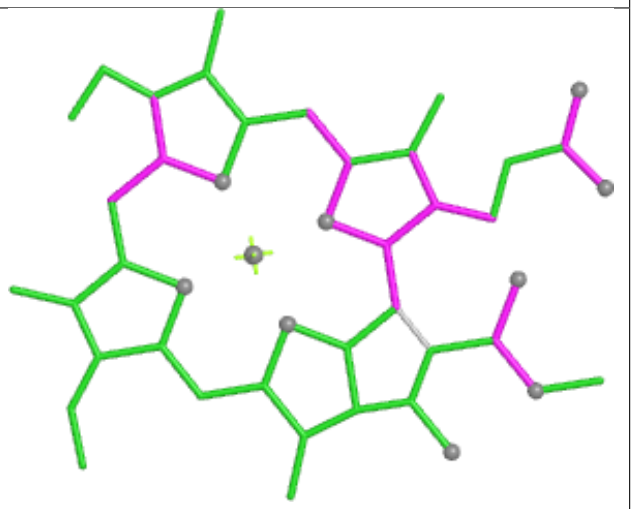


Rings

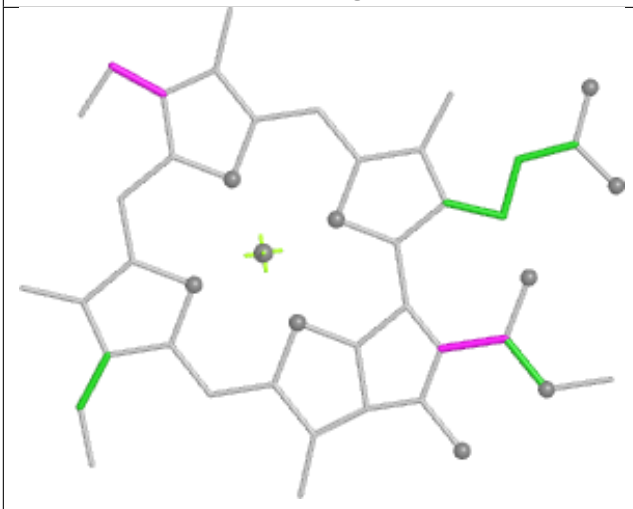
Ligand CLA 3 502



Bond lengths



Bond angles

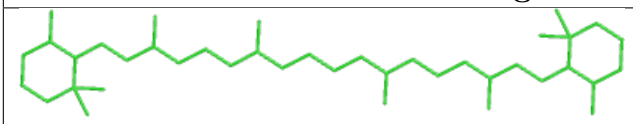


Torsions

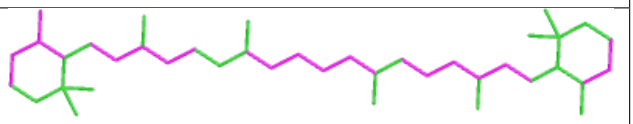


Rings

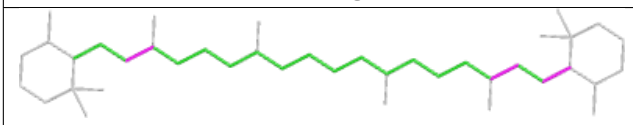
Ligand BCR B 4005



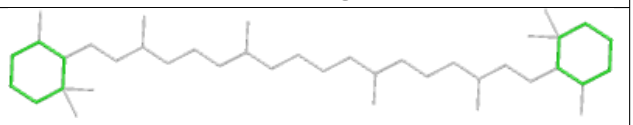
Bond lengths



Bond angles

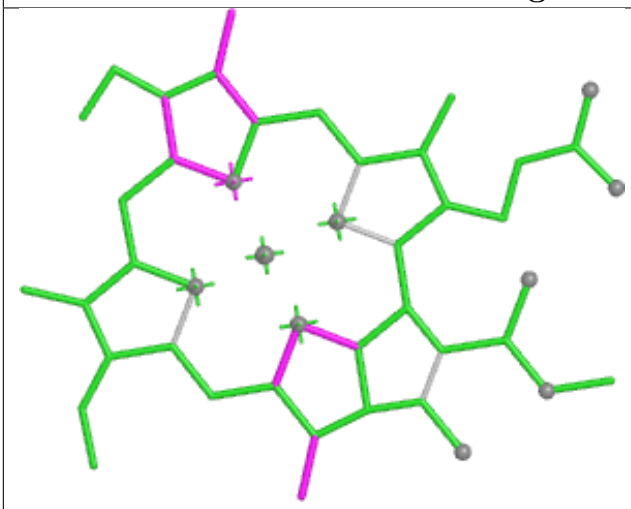


Torsions

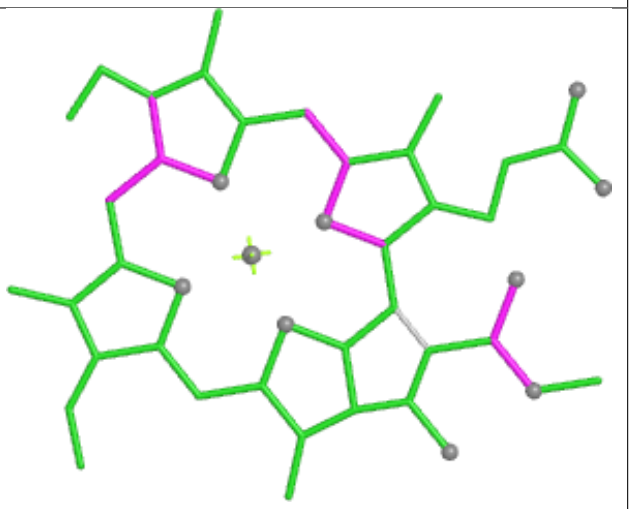


Rings

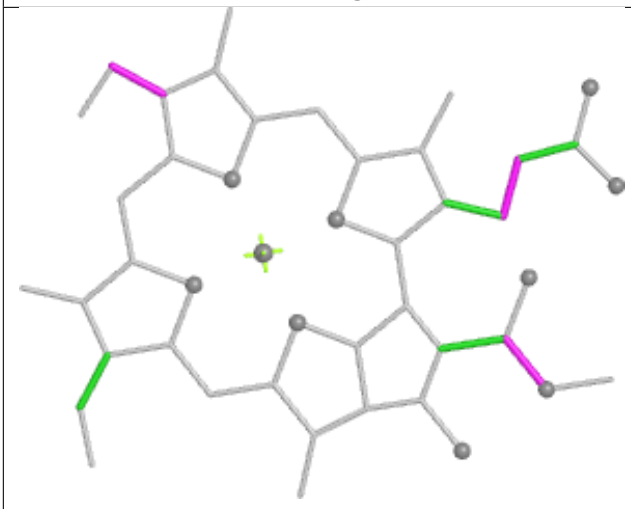
Ligand CLA 3 513



Bond lengths



Bond angles

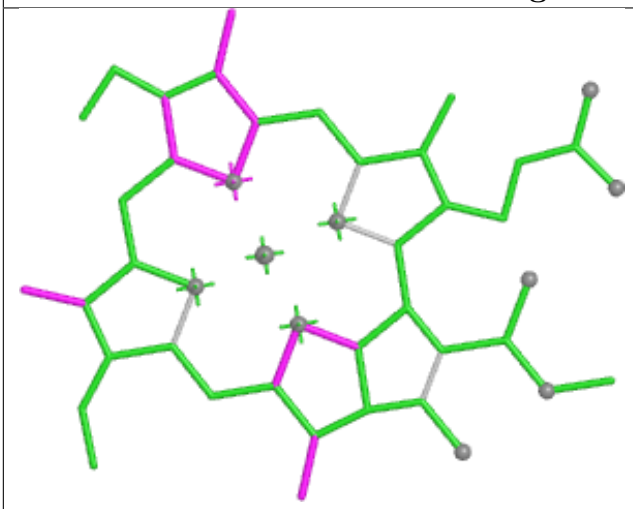


Torsions

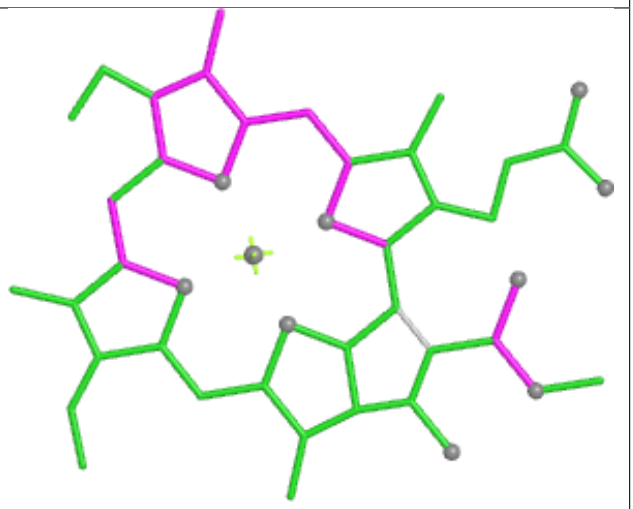


Rings

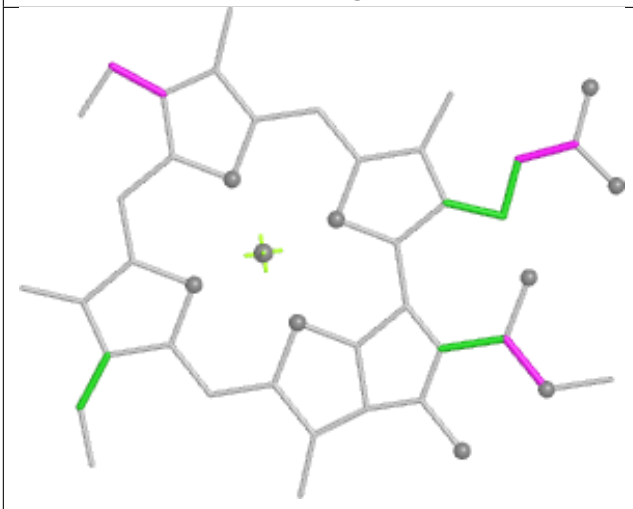
Ligand CLA c 508



Bond lengths



Bond angles

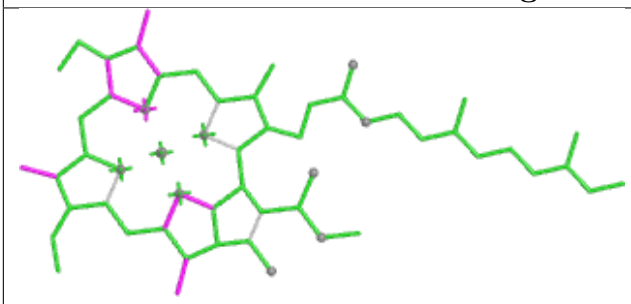


Torsions

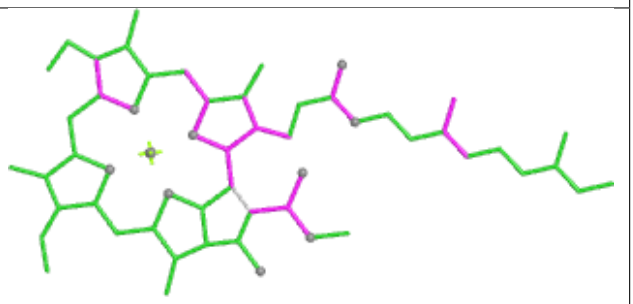


Rings

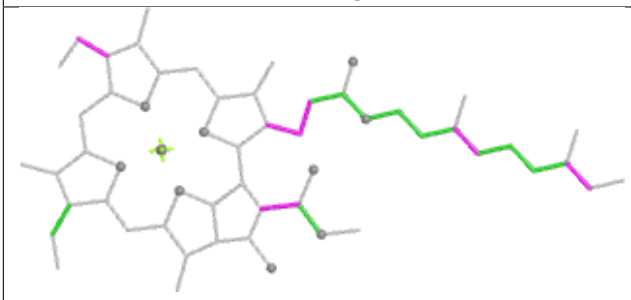
Ligand CLA e 1134



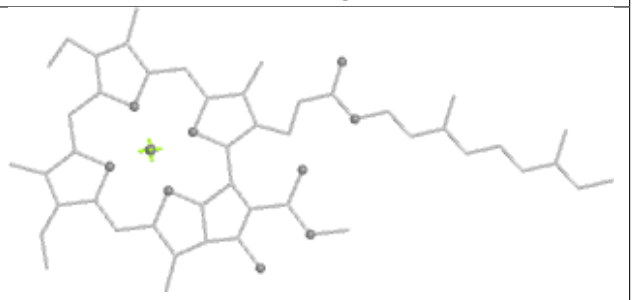
Bond lengths



Bond angles

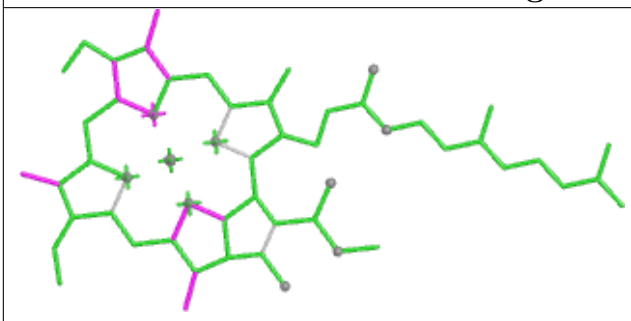


Torsions

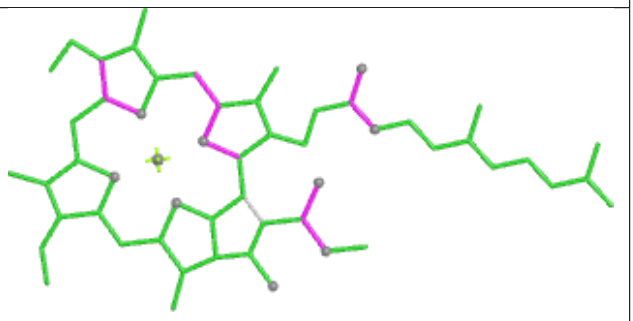


Rings

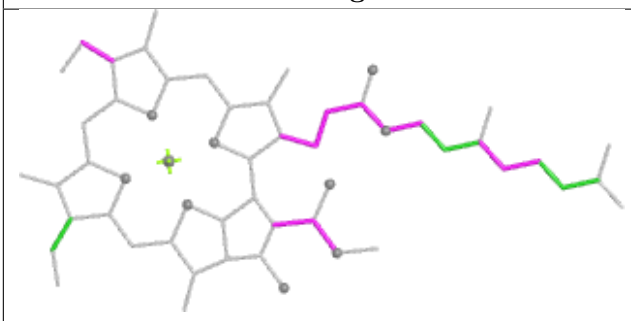
Ligand CLA Z 518



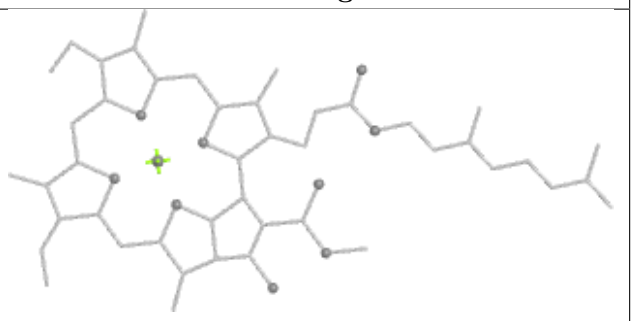
Bond lengths



Bond angles

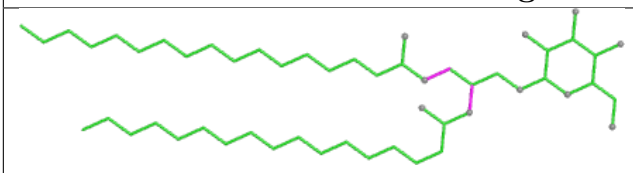


Torsions

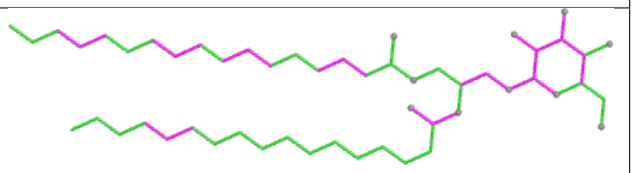


Rings

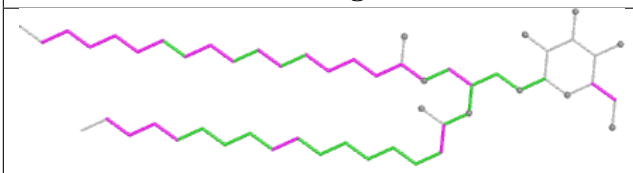
Ligand LMG f 5002



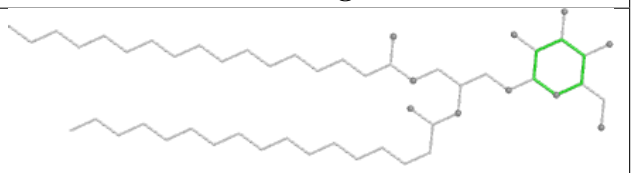
Bond lengths



Bond angles

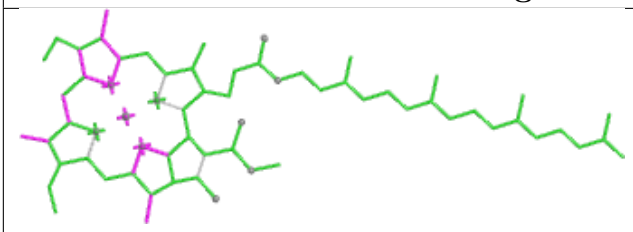


Torsions

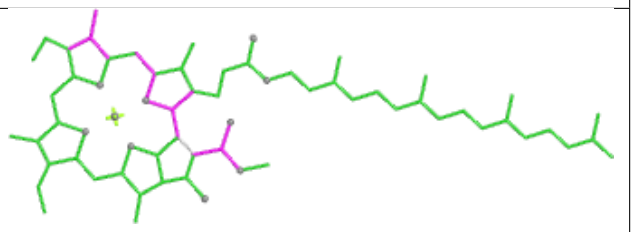


Rings

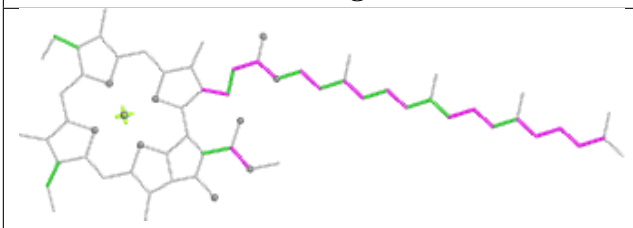
Ligand CLA A 1126



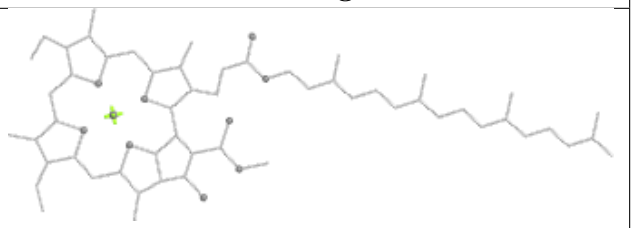
Bond lengths



Bond angles

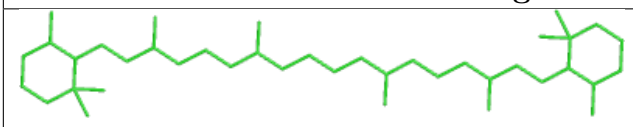


Torsions

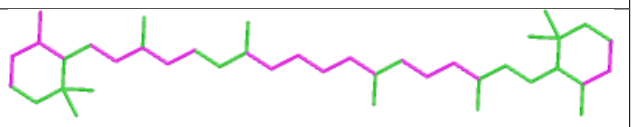


Rings

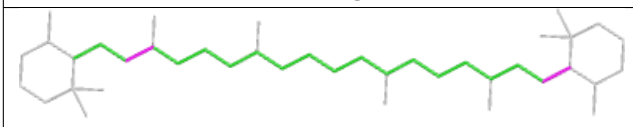
Ligand BCR V 4022



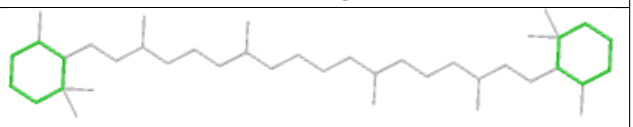
Bond lengths



Bond angles

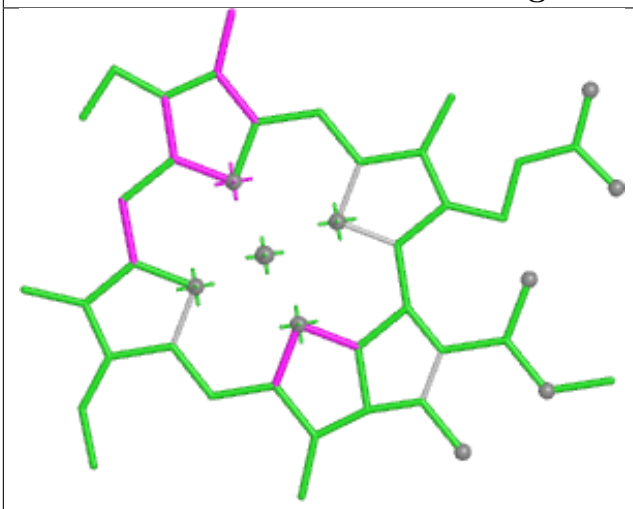


Torsions

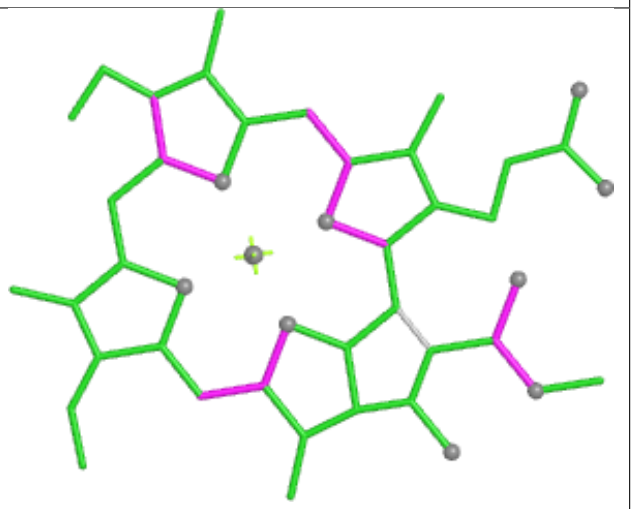


Rings

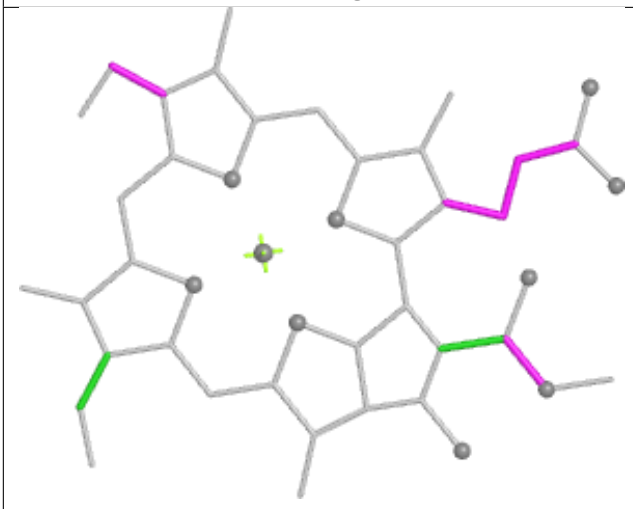
Ligand CLA 4 501



Bond lengths



Bond angles

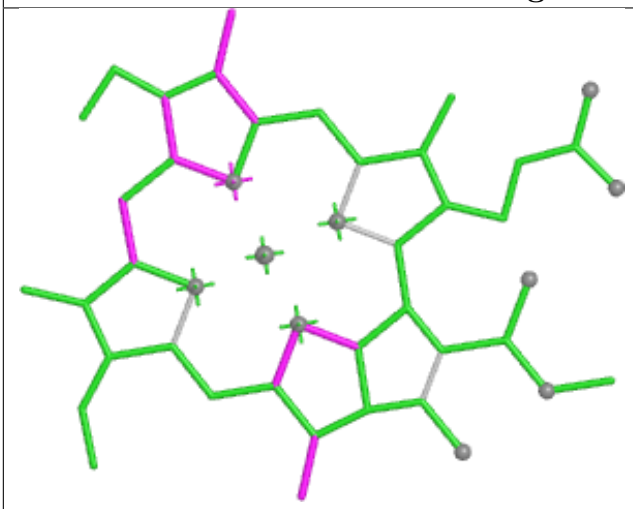


Torsions

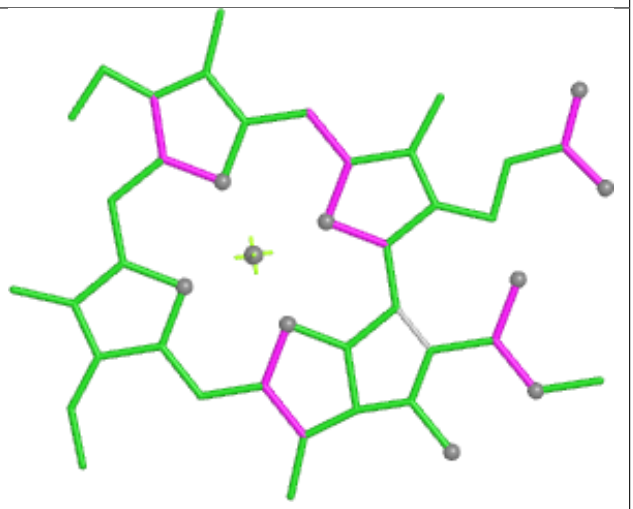


Rings

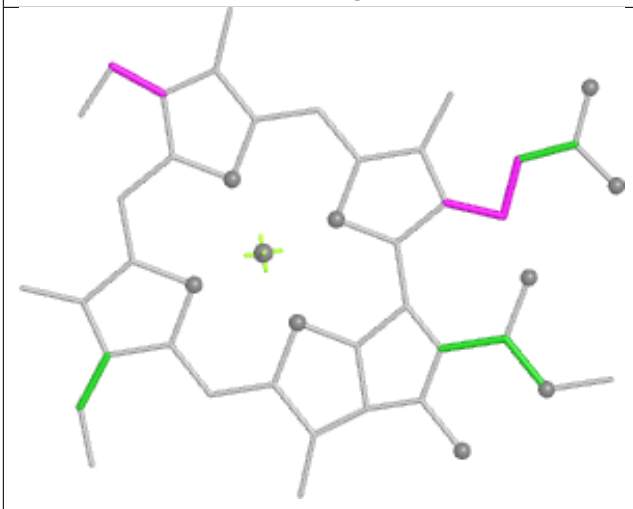
Ligand CLA u 518



Bond lengths



Bond angles

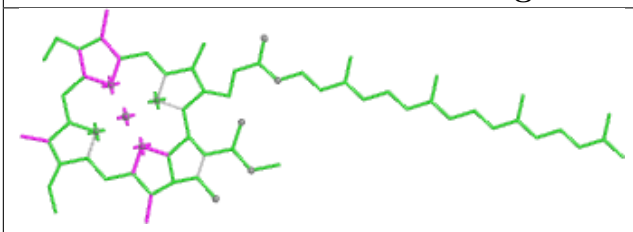


Torsions

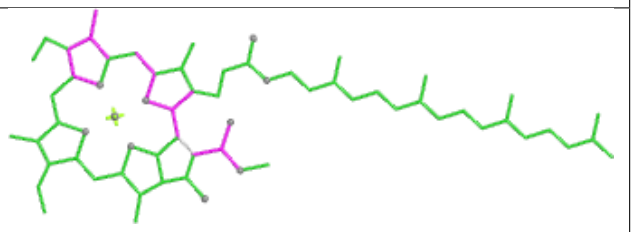


Rings

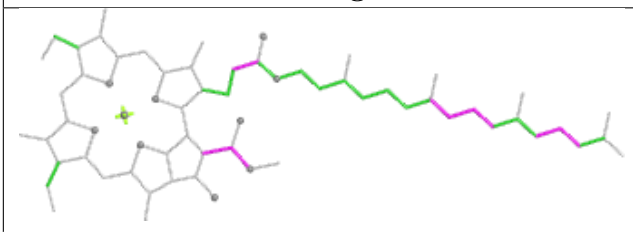
Ligand CLA A 1123



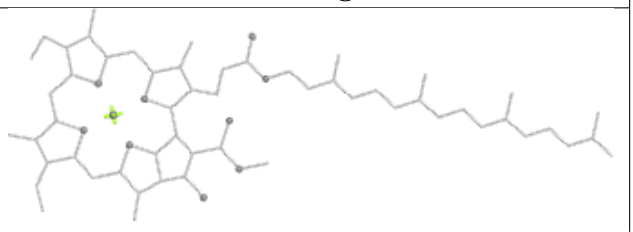
Bond lengths



Bond angles

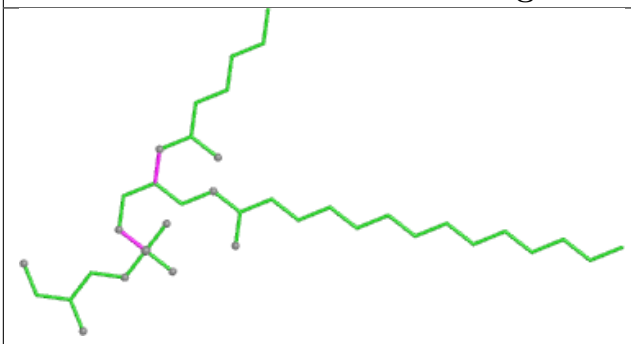


Torsions

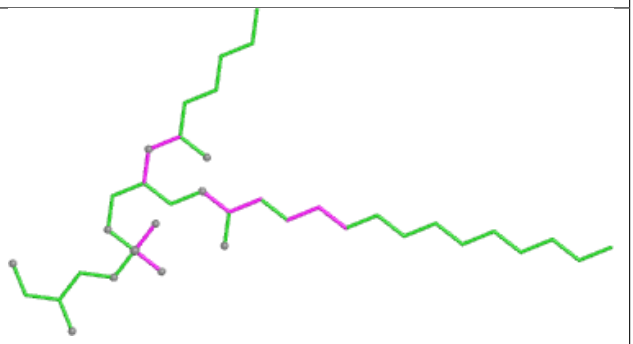


Rings

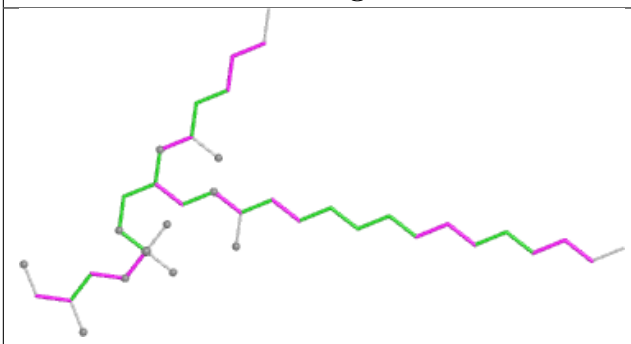
Ligand LHG n 5218



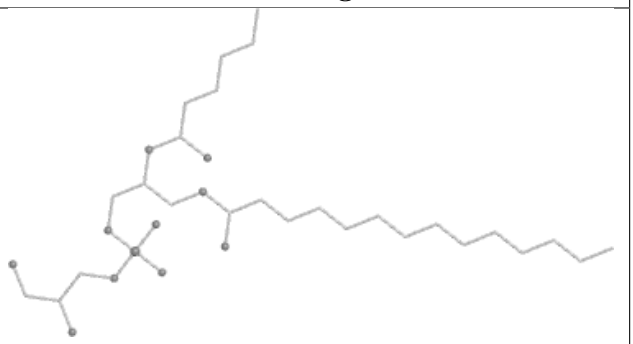
Bond lengths



Bond angles

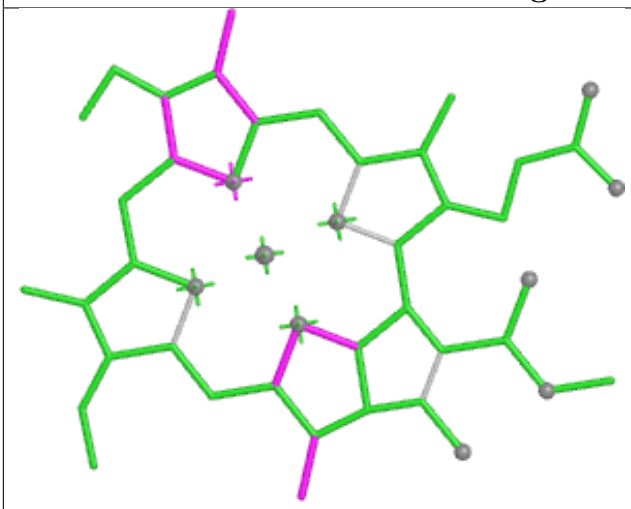


Torsions

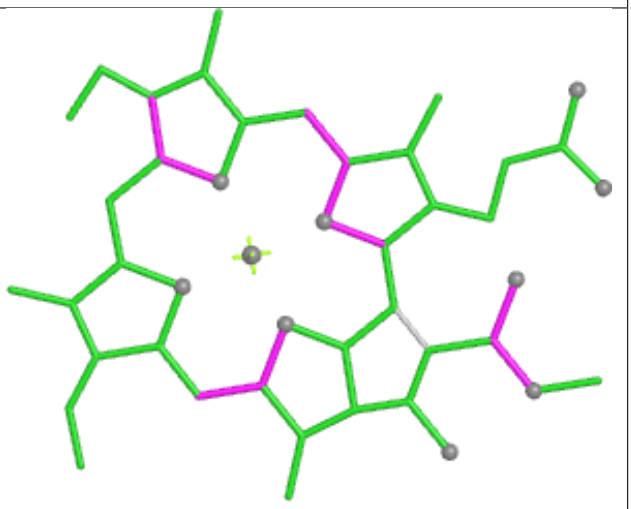


Rings

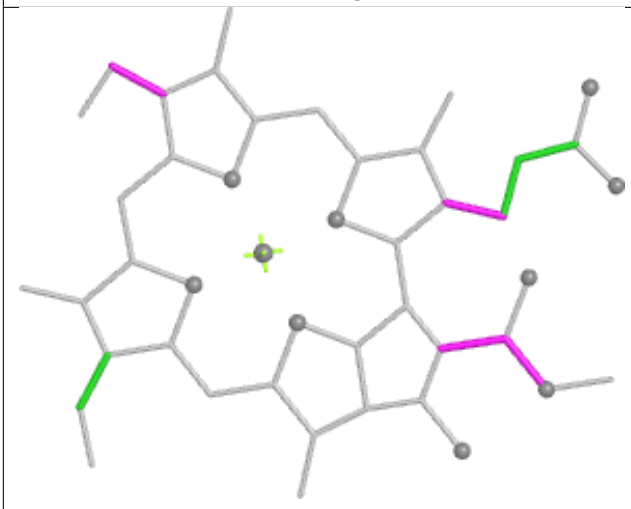
Ligand CLA t 504



Bond lengths



Bond angles

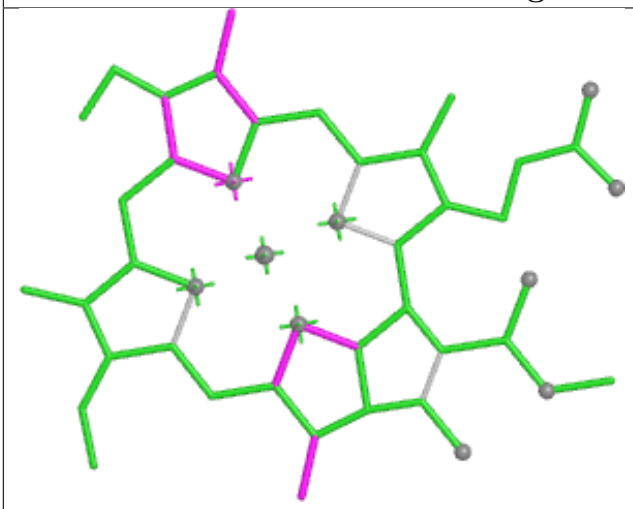


Torsions

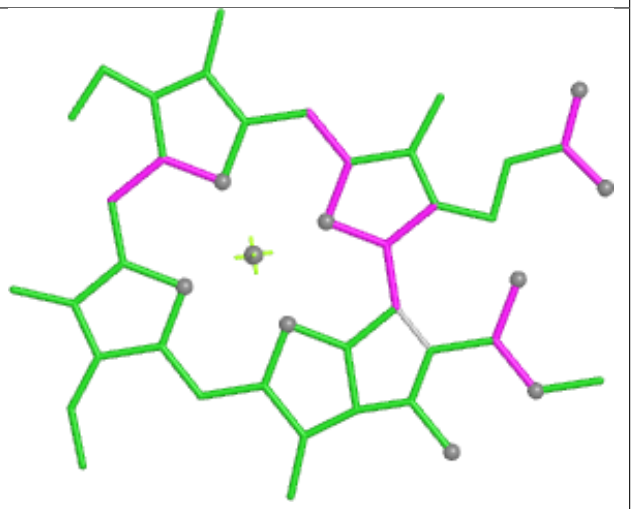


Rings

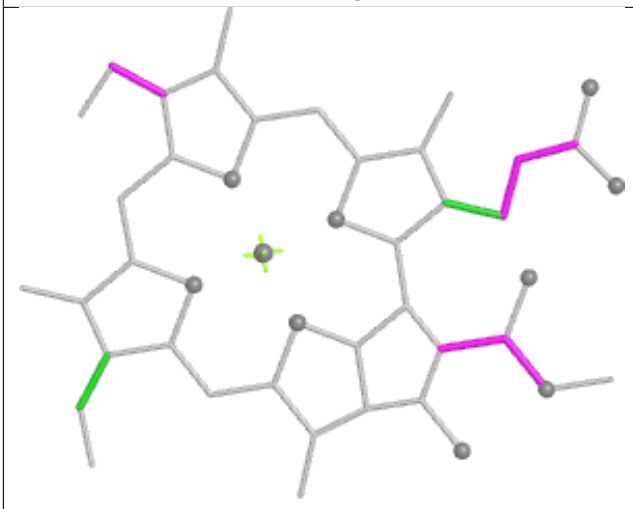
Ligand CLA u 507



Bond lengths



Bond angles

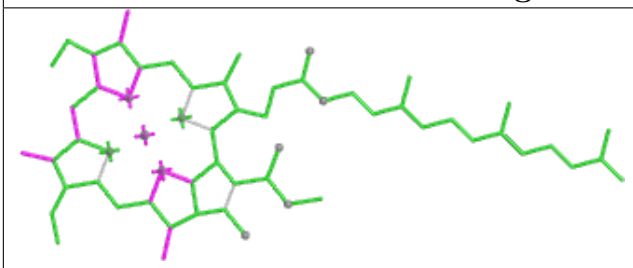


Torsions

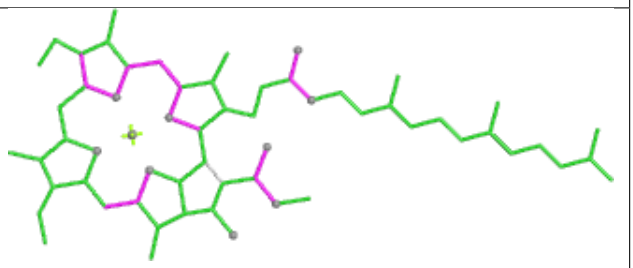


Rings

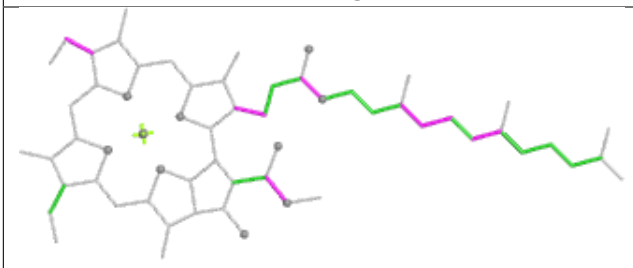
Ligand CLA H 1227



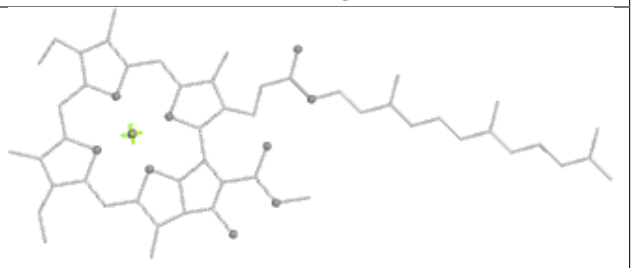
Bond lengths



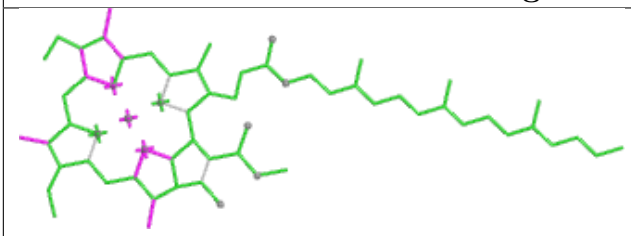
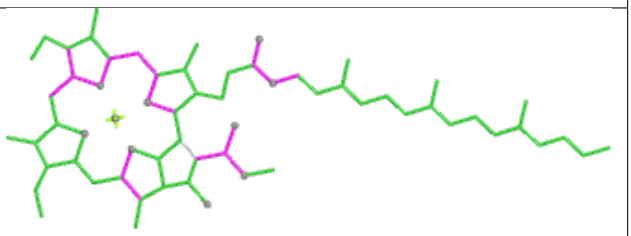
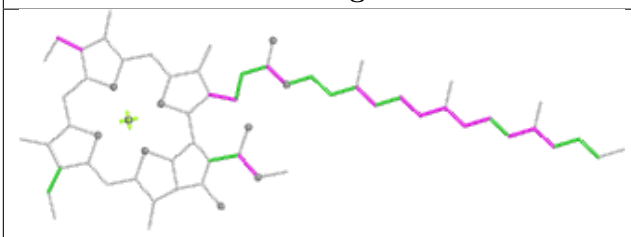
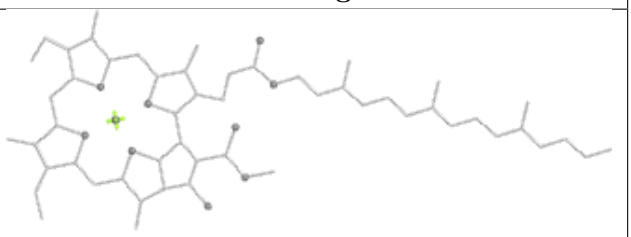
Bond angles

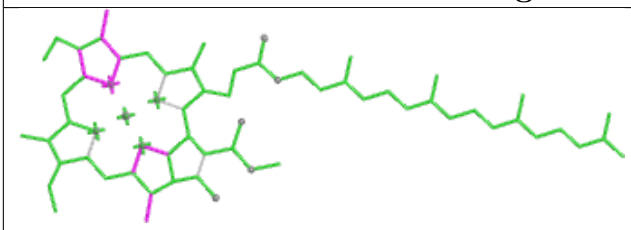
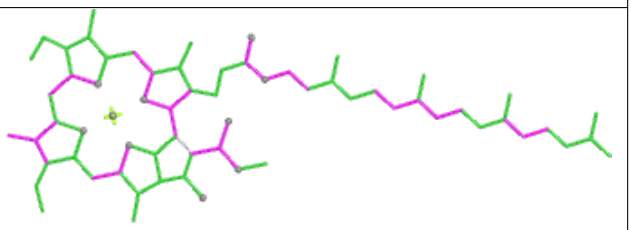
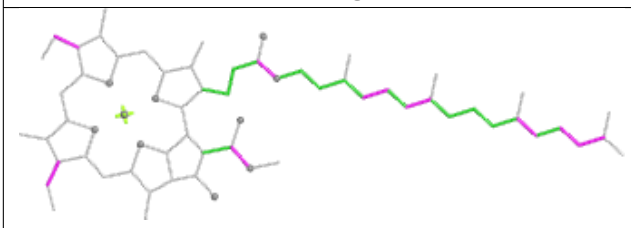
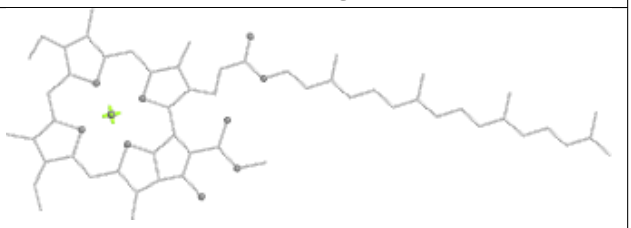


Torsions

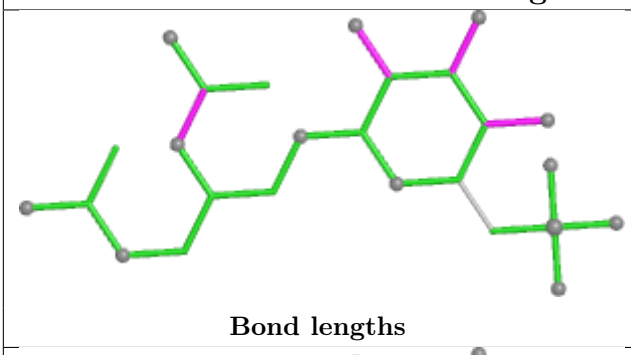


Rings

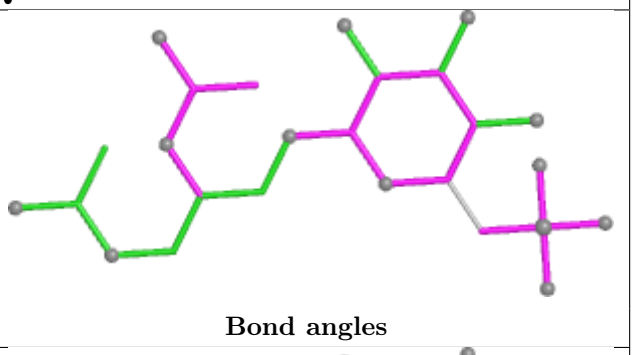
Ligand CLA f 1219	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1239	
	
Bond lengths	Bond angles
	
Torsions	Rings

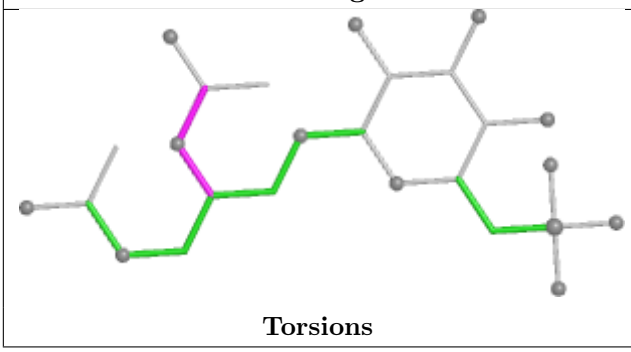
Ligand SQD c 822



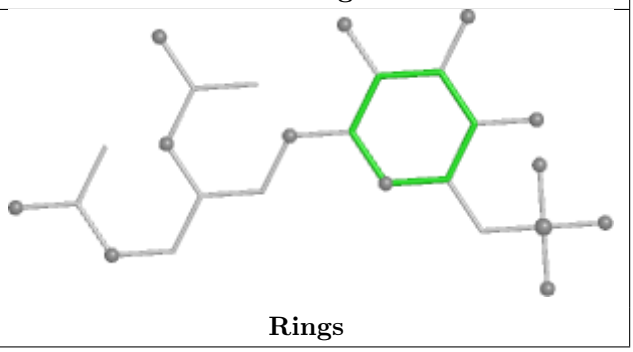
Bond lengths



Bond angles

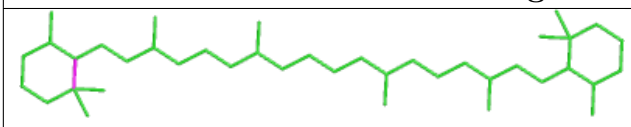


Torsions

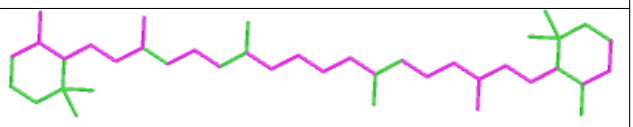


Rings

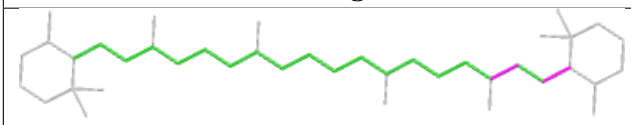
Ligand BCR c 523



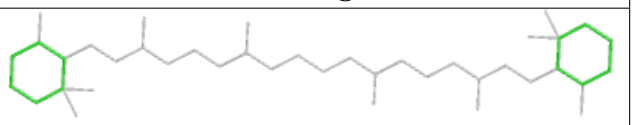
Bond lengths



Bond angles

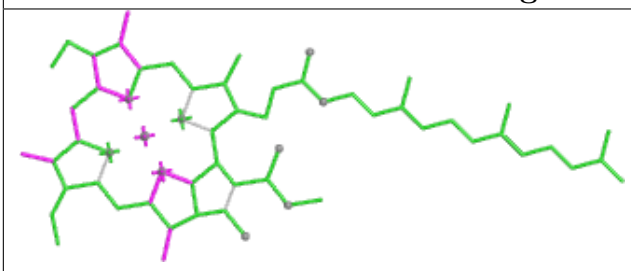


Torsions

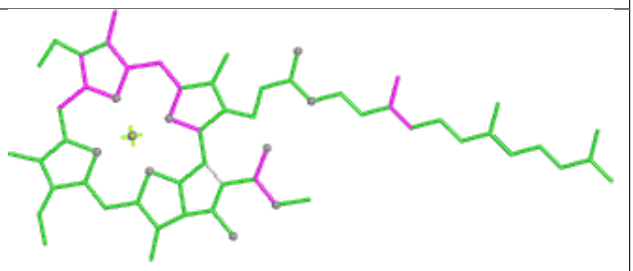


Rings

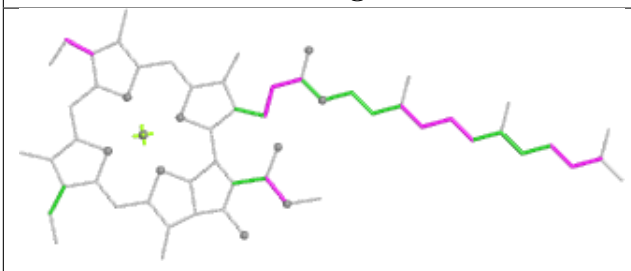
Ligand CLA e 1115



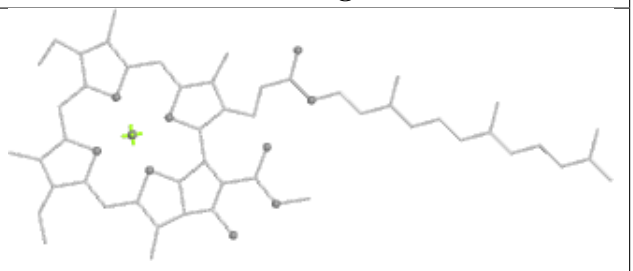
Bond lengths



Bond angles

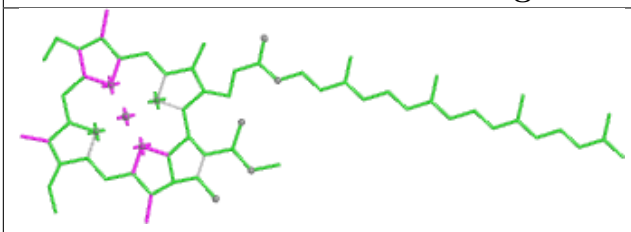


Torsions

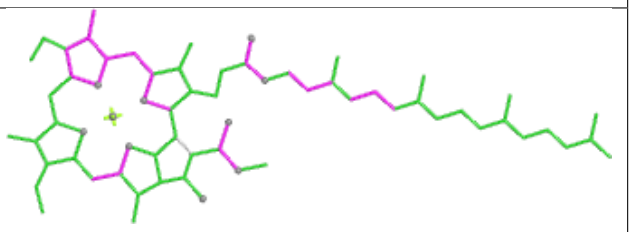


Rings

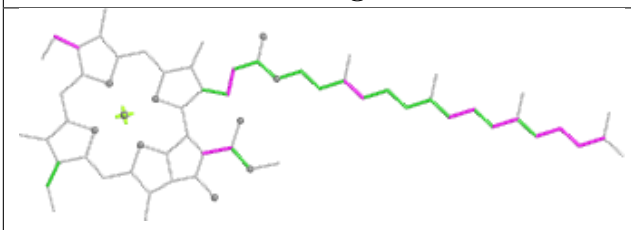
Ligand CLA G 1117



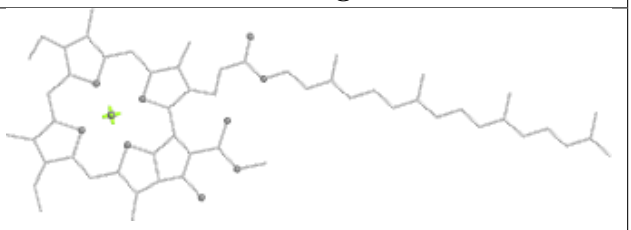
Bond lengths



Bond angles

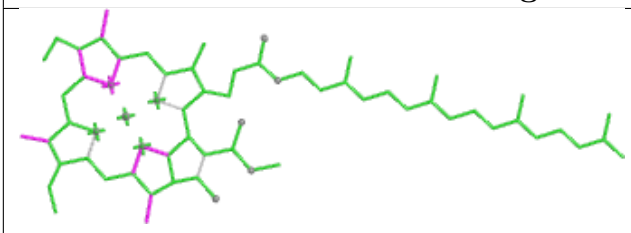


Torsions

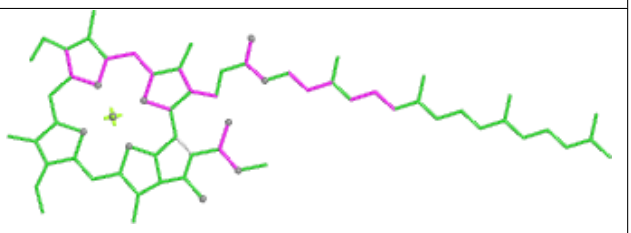


Rings

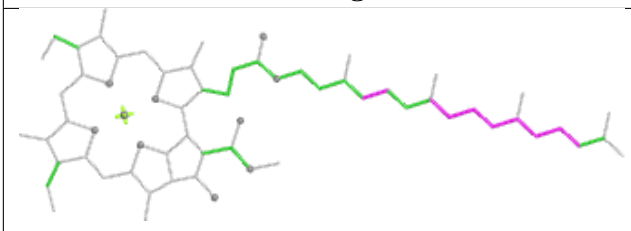
Ligand CLA e 1136



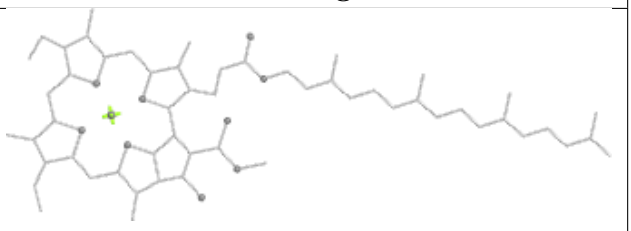
Bond lengths



Bond angles

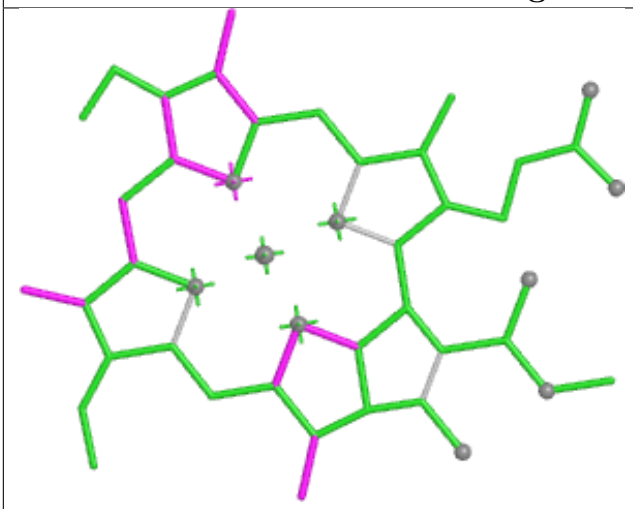


Torsions

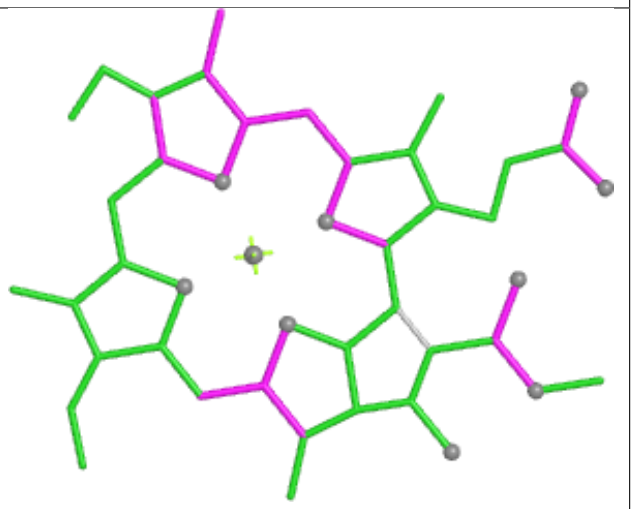


Rings

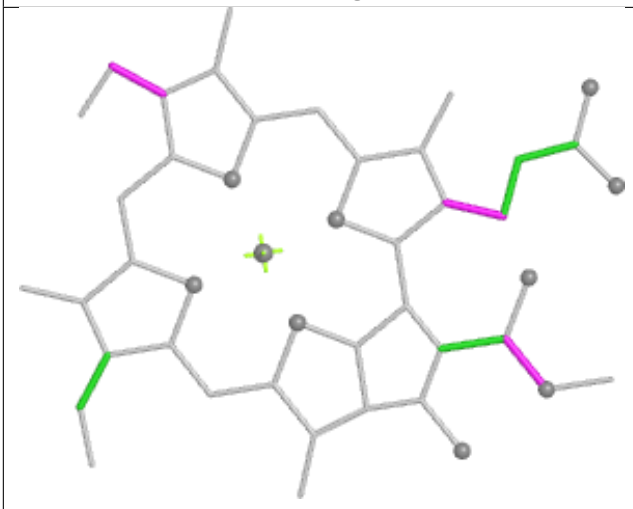
Ligand CLA 4 511



Bond lengths



Bond angles

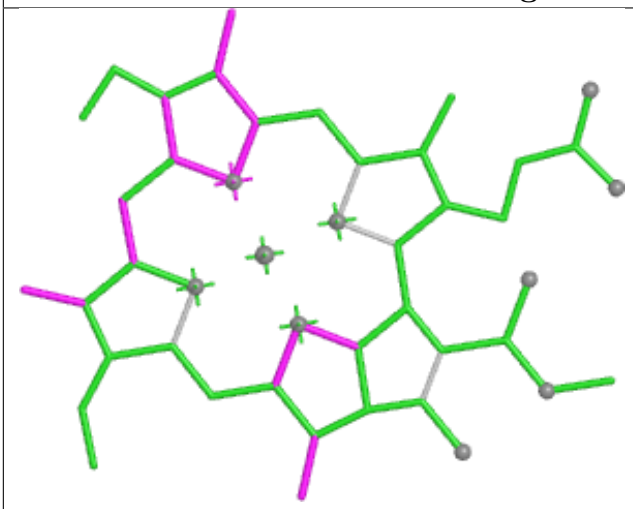


Torsions

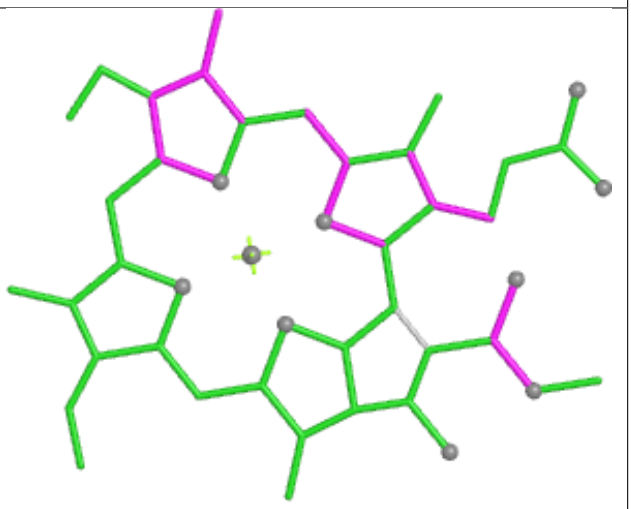


Rings

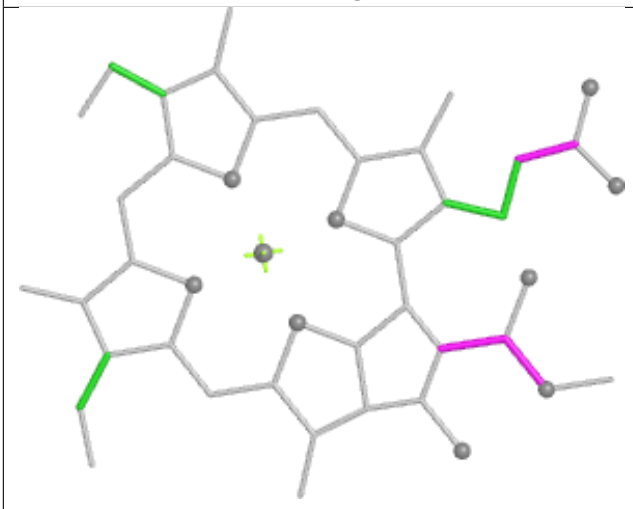
Ligand CLA e 1801



Bond lengths



Bond angles

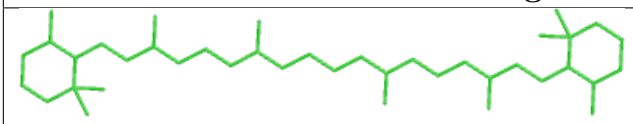


Torsions

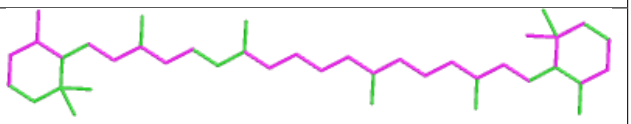


Rings

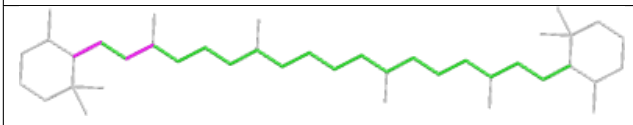
Ligand BCR Z 521



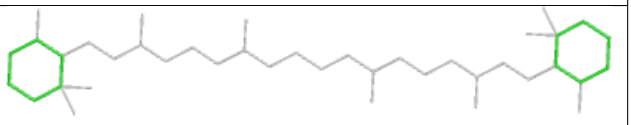
Bond lengths



Bond angles

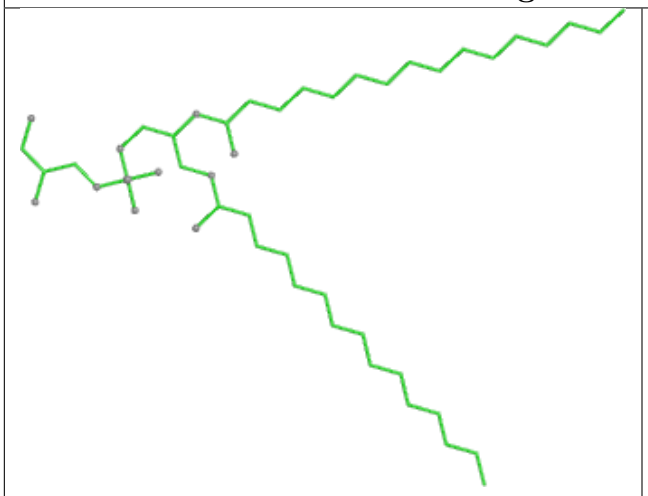


Torsions

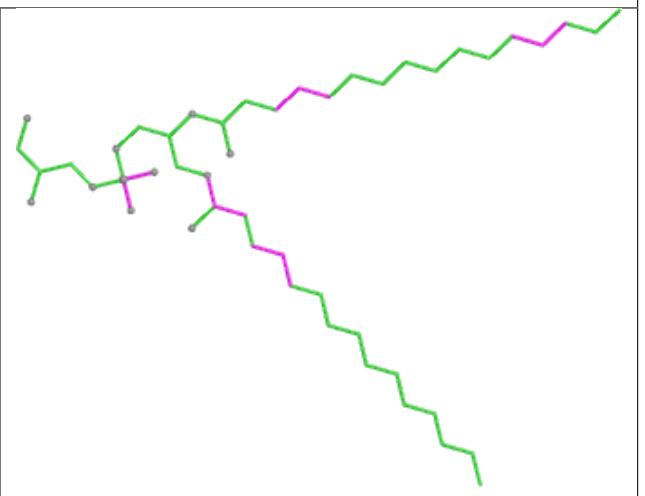


Rings

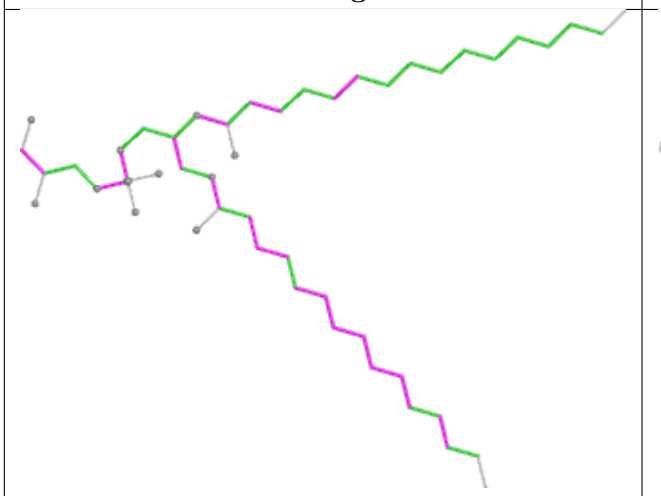
Ligand LHG S 5001



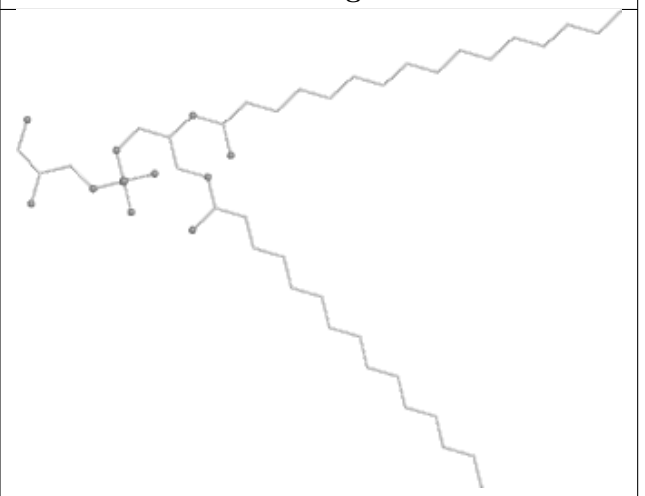
Bond lengths



Bond angles

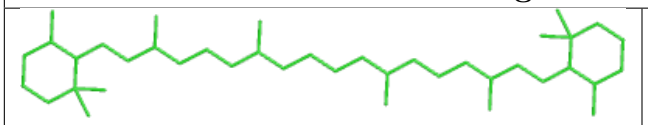


Torsions



Rings

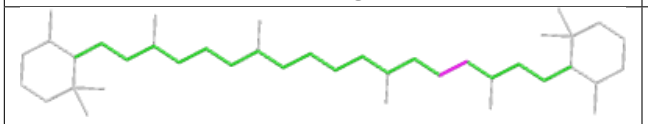
Ligand BCR B 4009



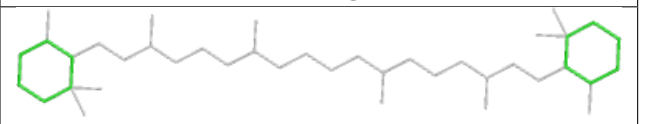
Bond lengths



Bond angles

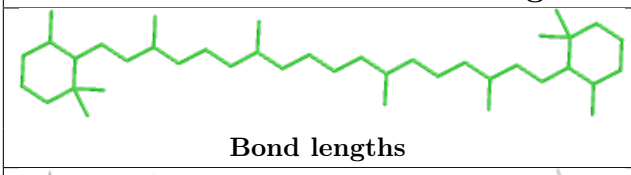


Torsions

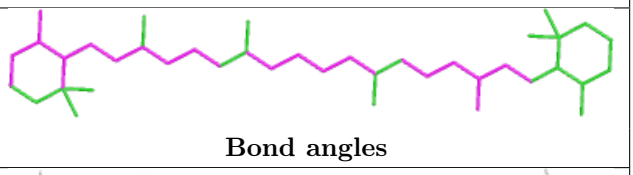


Rings

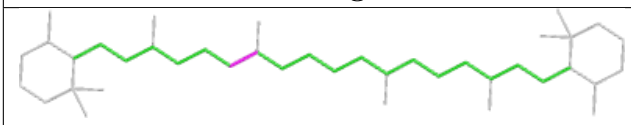
Ligand BCR 1 524



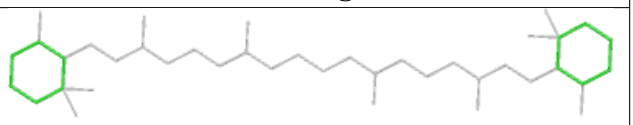
Bond lengths



Bond angles

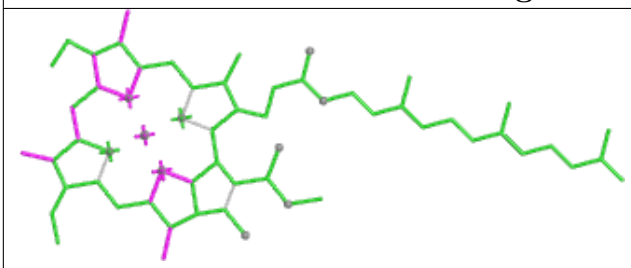


Torsions

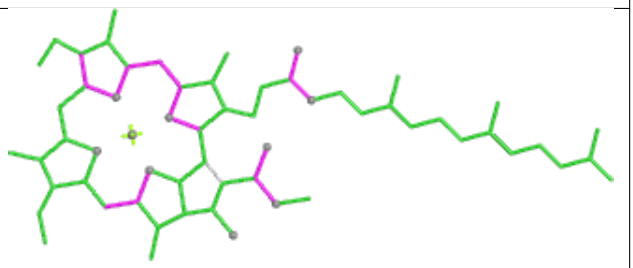


Rings

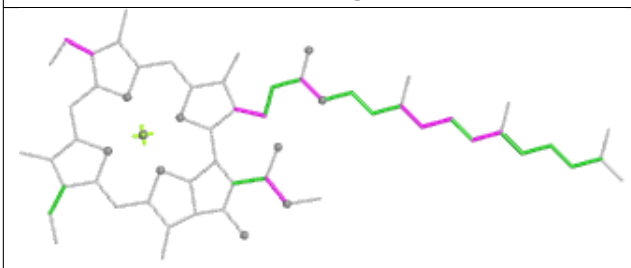
Ligand CLA B 1227



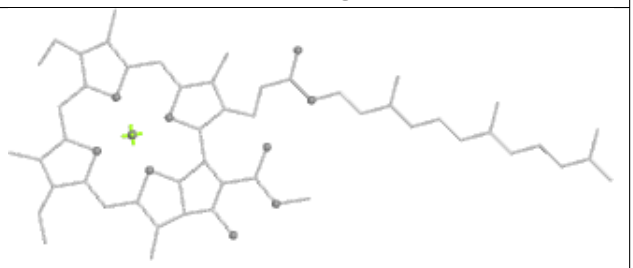
Bond lengths



Bond angles

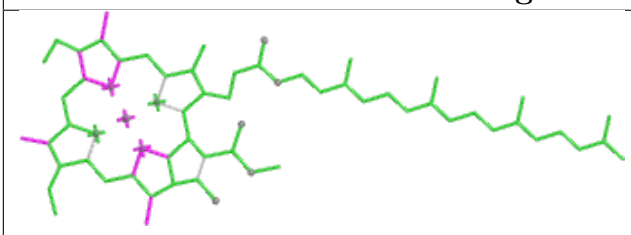


Torsions

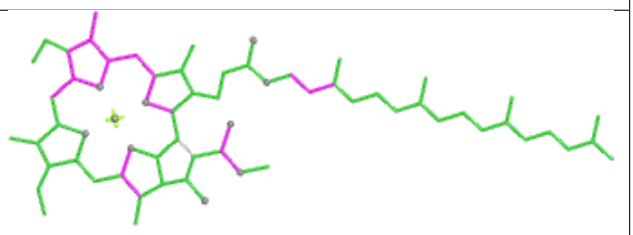


Rings

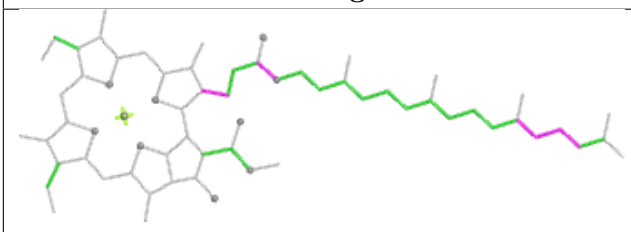
Ligand CLA B 1225



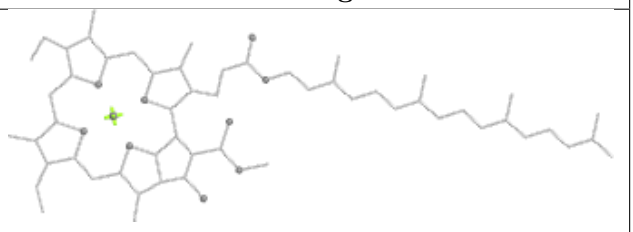
Bond lengths



Bond angles

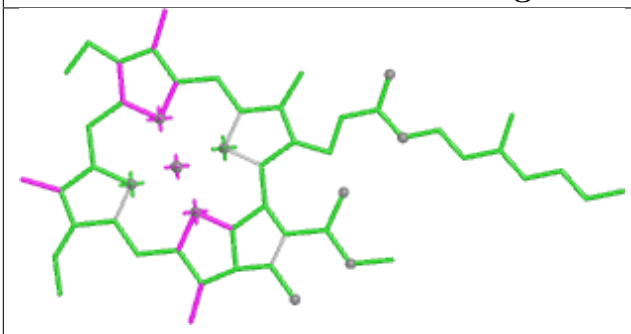


Torsions

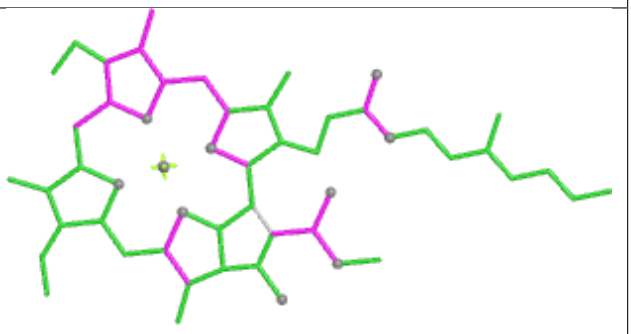


Rings

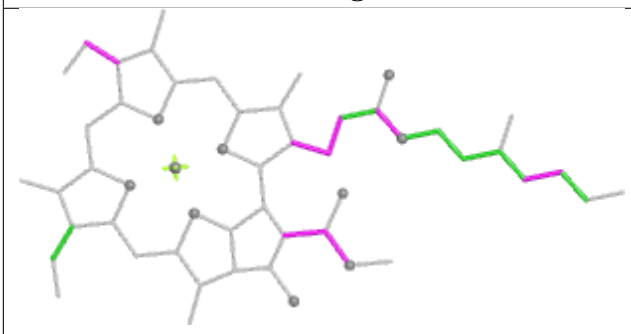
Ligand CLA G 1129



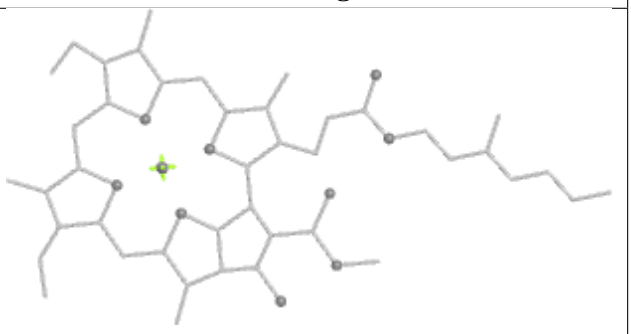
Bond lengths



Bond angles

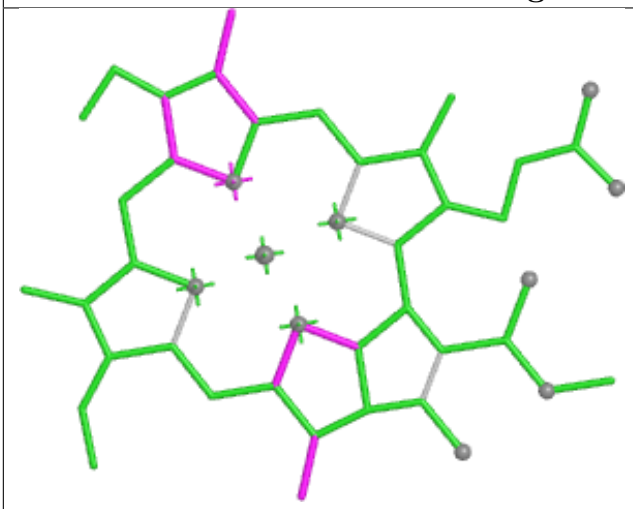


Torsions

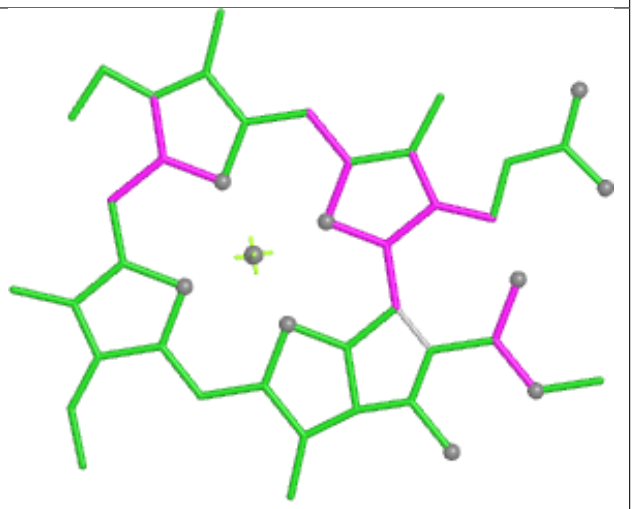


Rings

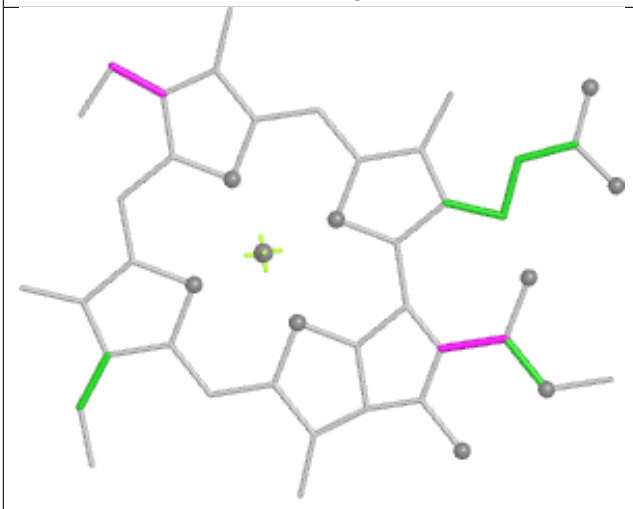
Ligand CLA d 502



Bond lengths



Bond angles

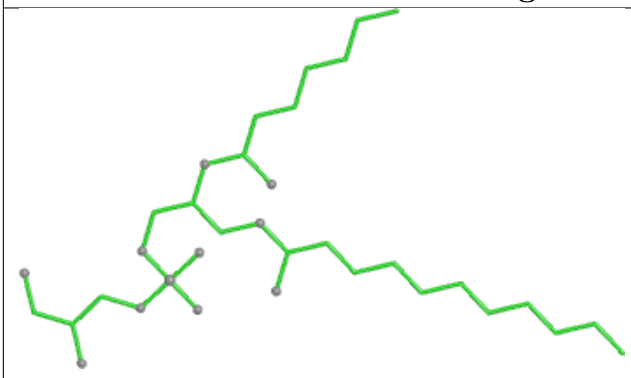


Torsions

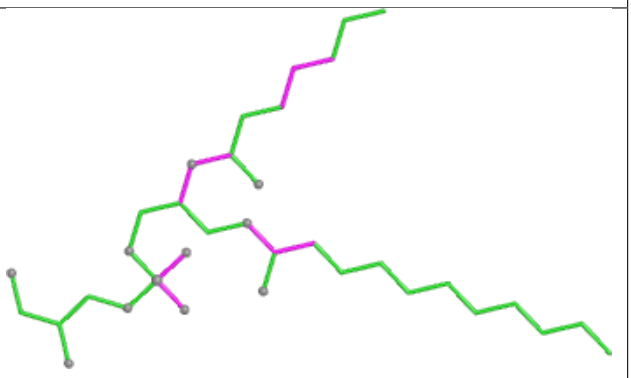


Rings

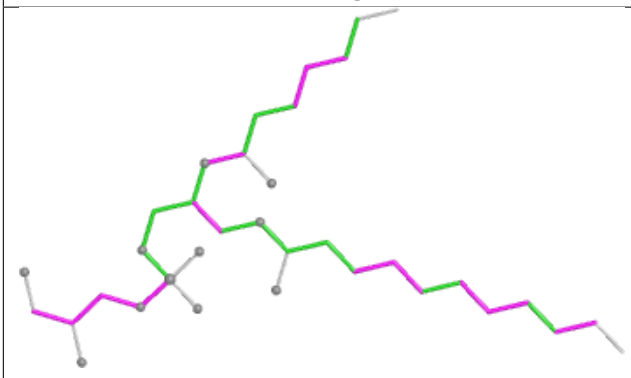
Ligand LHG e 5004



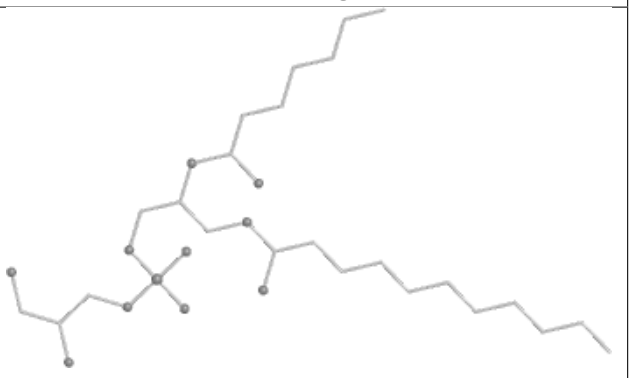
Bond lengths



Bond angles

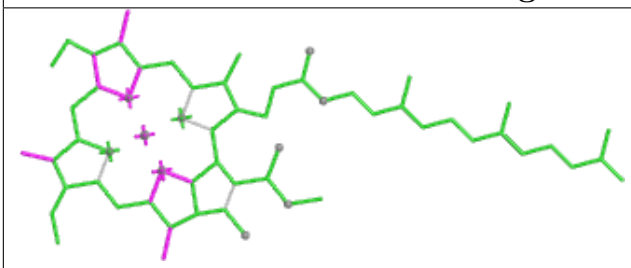


Torsions

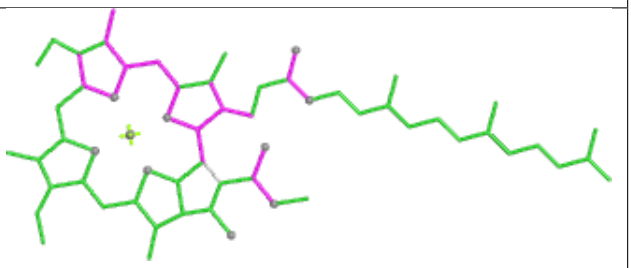


Rings

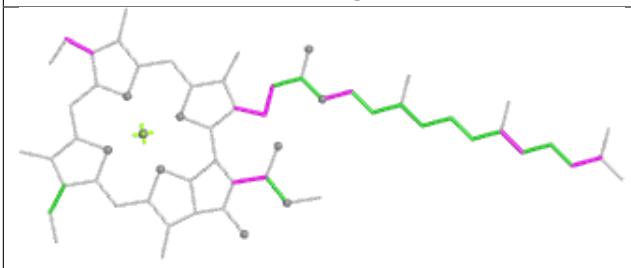
Ligand CLA n 1501



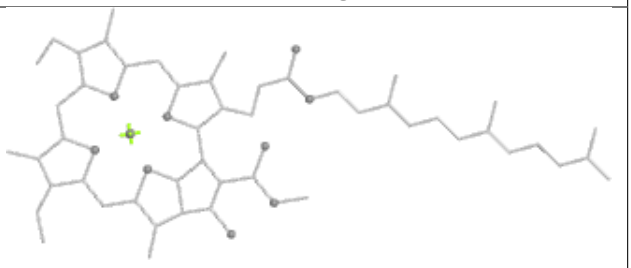
Bond lengths



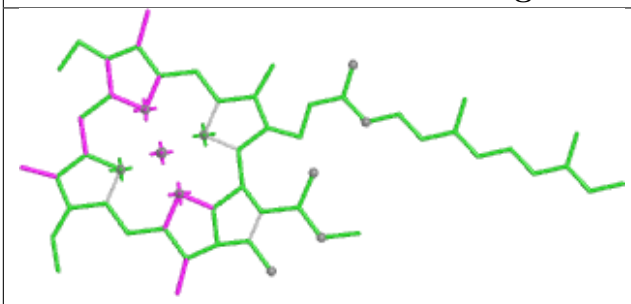
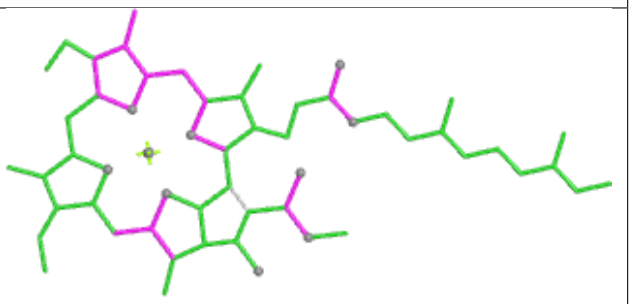
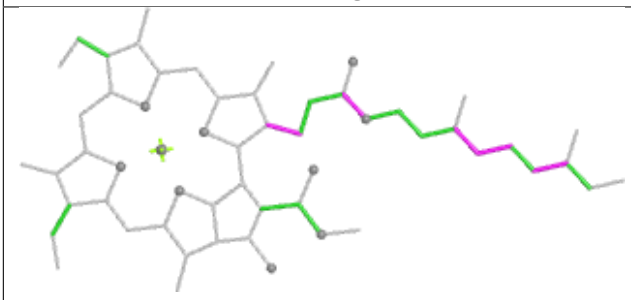
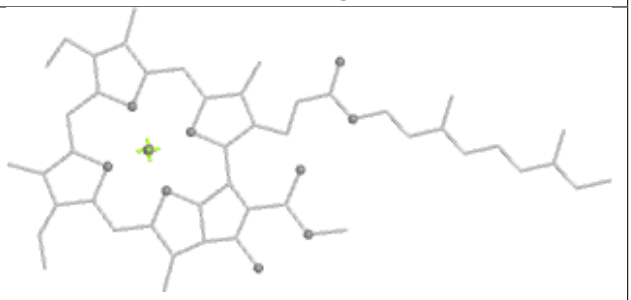
Bond angles

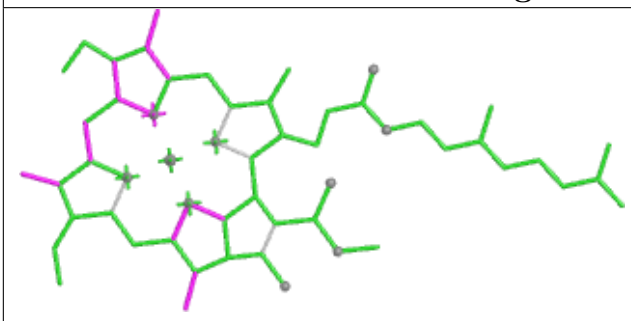
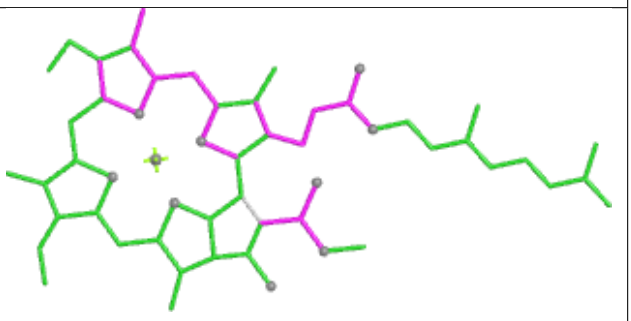
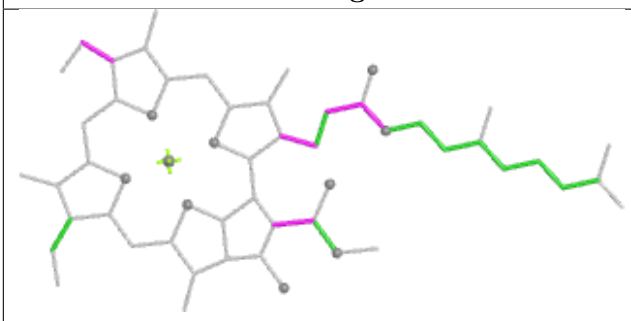
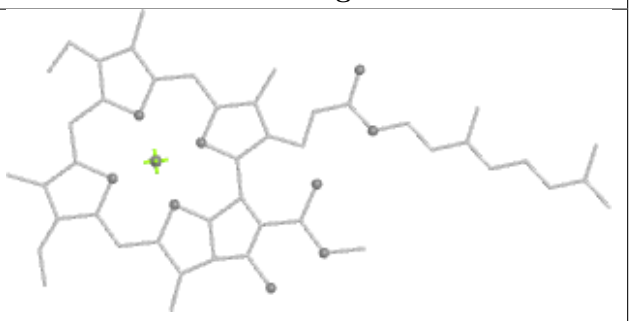


Torsions

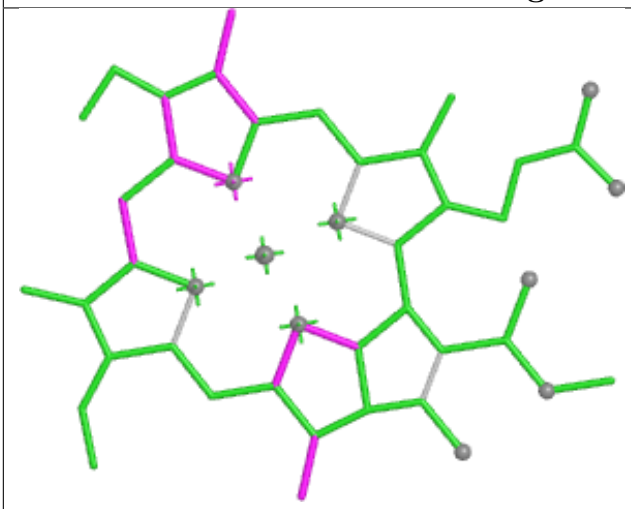


Rings

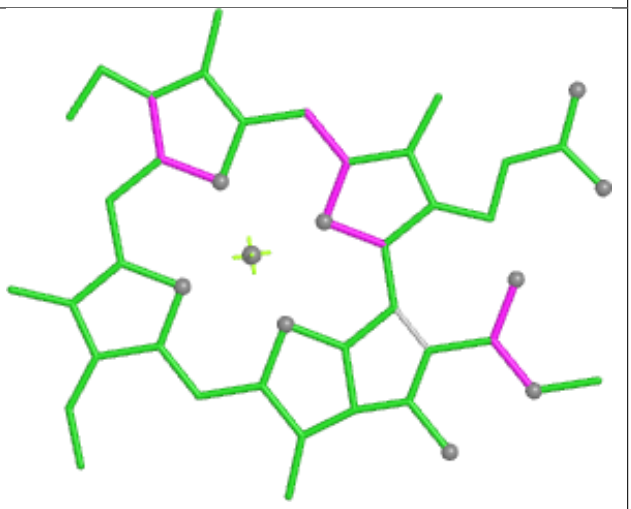
Ligand CLA A 1130	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA U 1401	
	
Bond lengths	Bond angles
	
Torsions	Rings

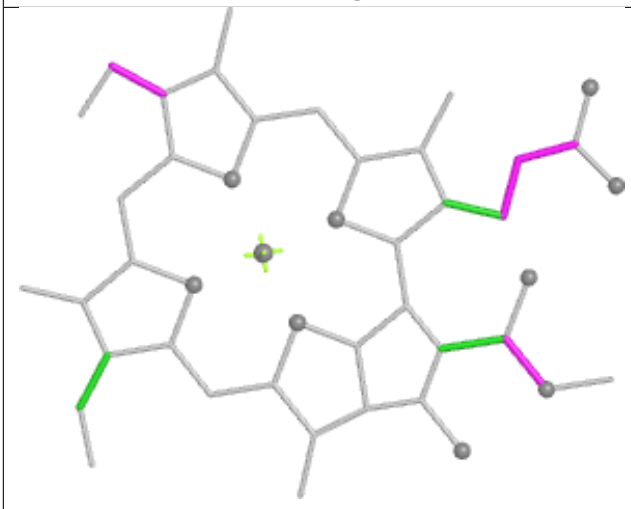
Ligand CLA b 513



Bond lengths



Bond angles

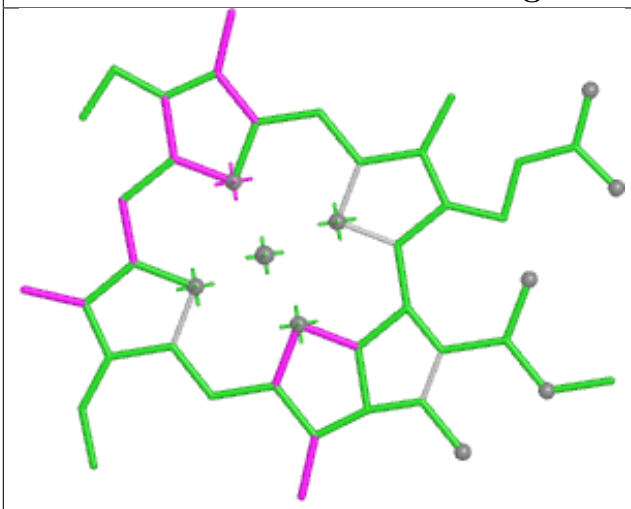


Torsions

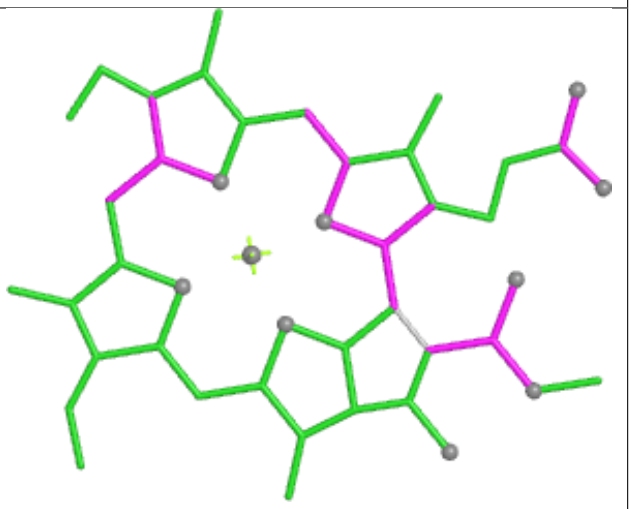


Rings

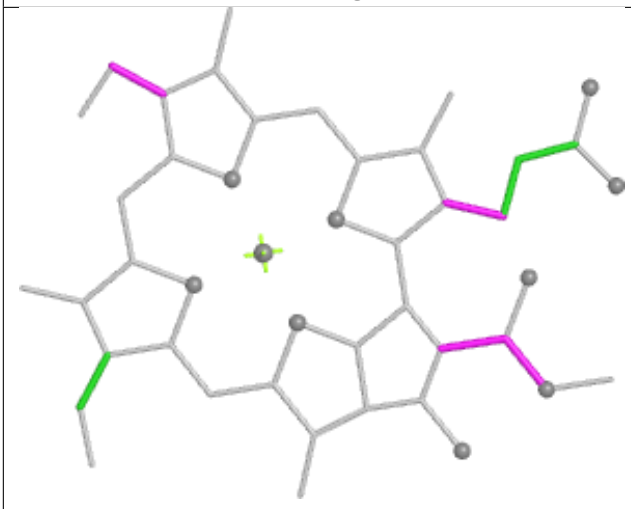
Ligand CLA l 1303



Bond lengths



Bond angles

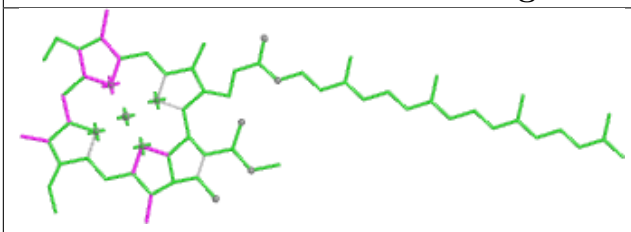


Torsions

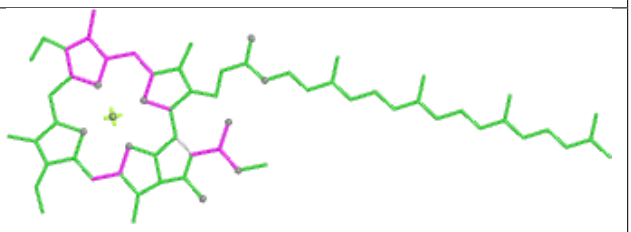


Rings

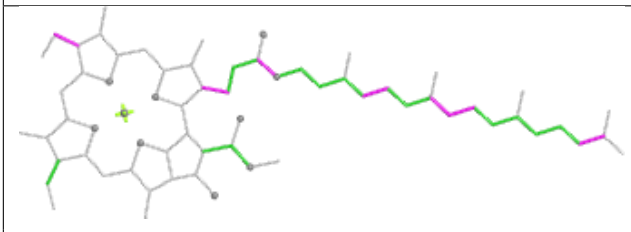
Ligand CLA n 1502



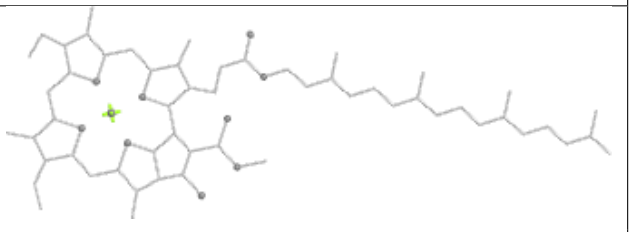
Bond lengths



Bond angles

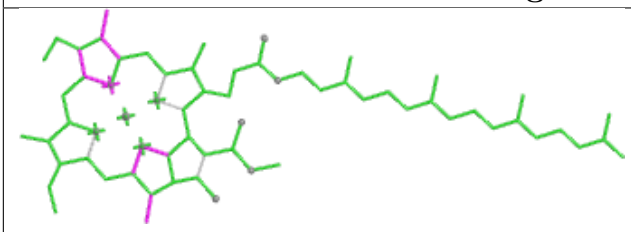


Torsions

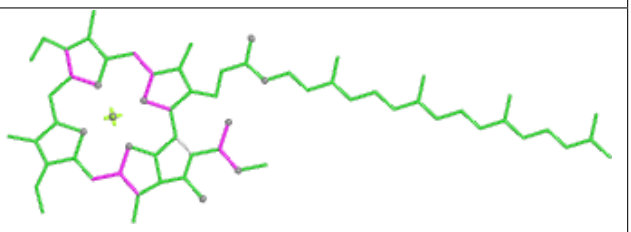


Rings

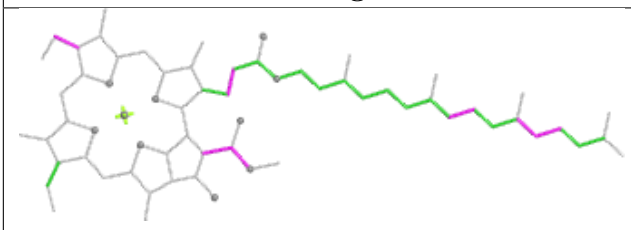
Ligand CLA Z 503



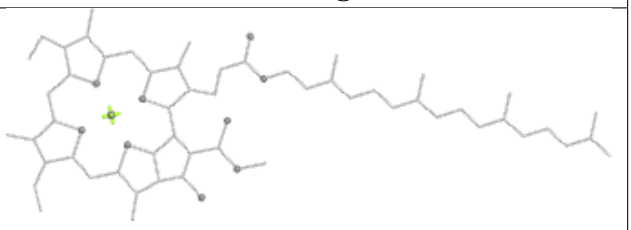
Bond lengths



Bond angles

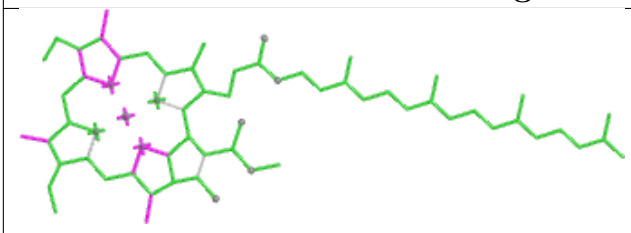


Torsions

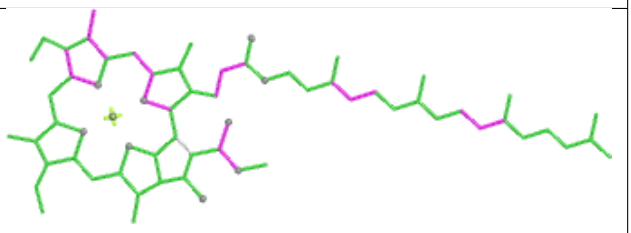


Rings

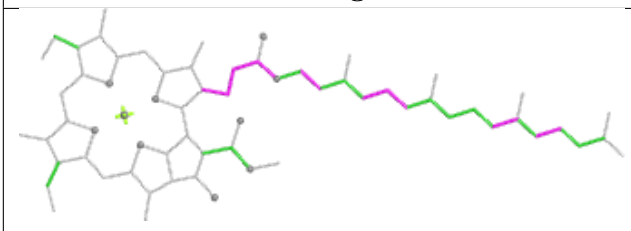
Ligand CLA G 1125



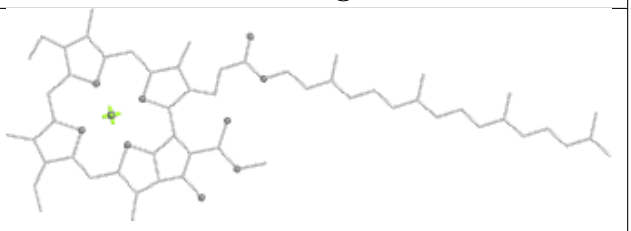
Bond lengths



Bond angles

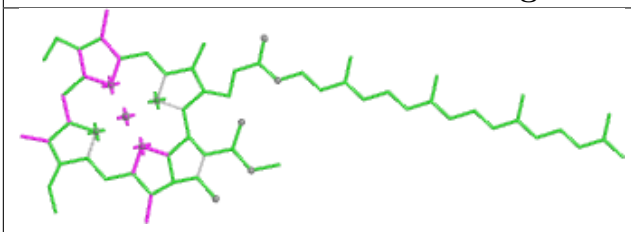


Torsions

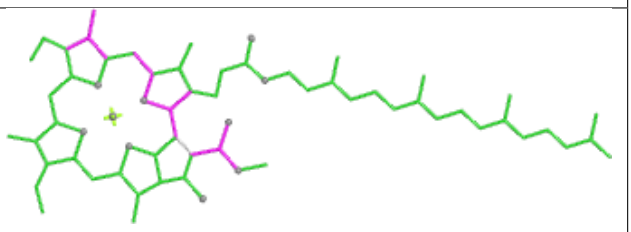


Rings

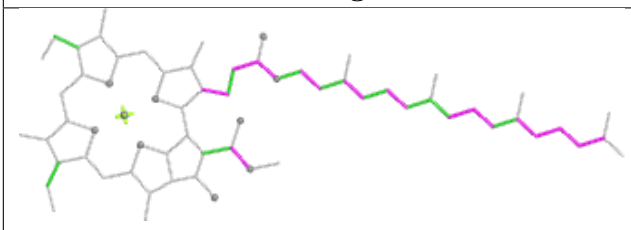
Ligand CLA e 1126



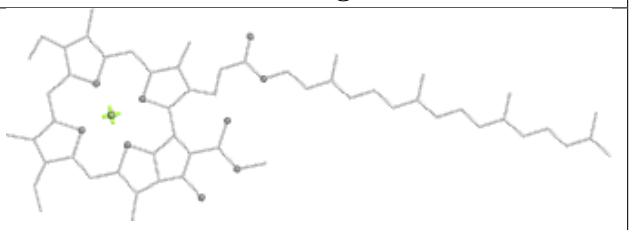
Bond lengths



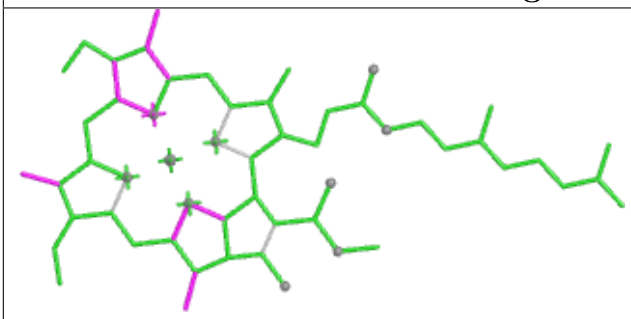
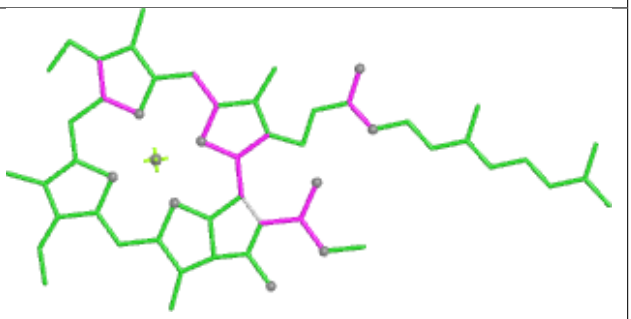
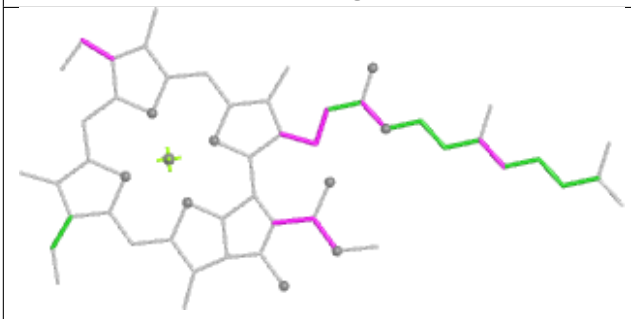
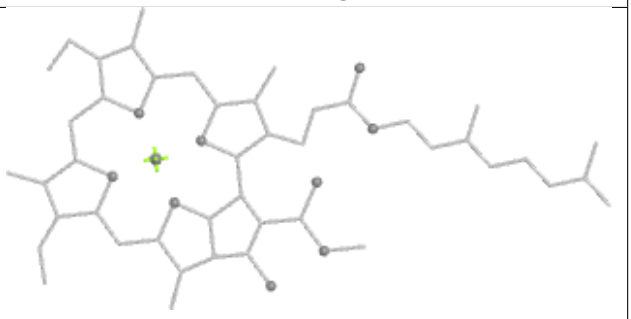
Bond angles

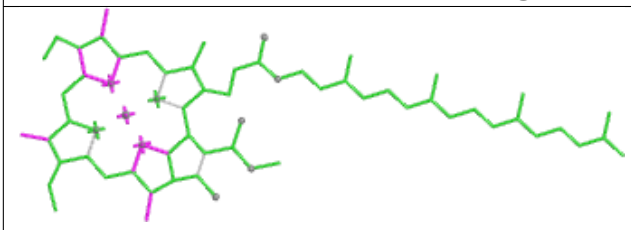
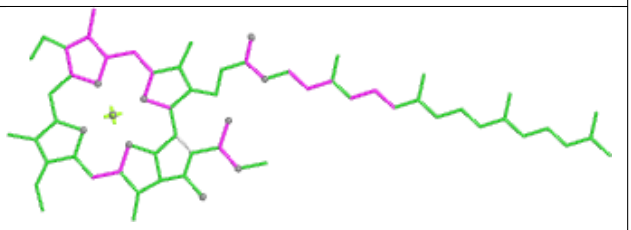
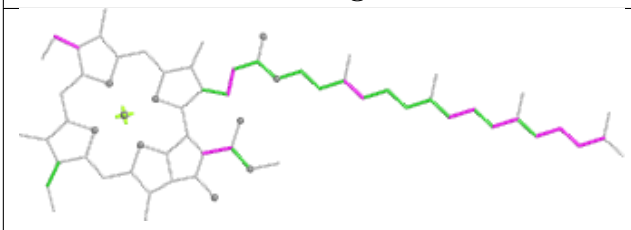
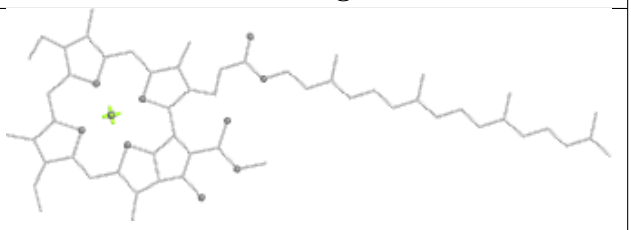


Torsions

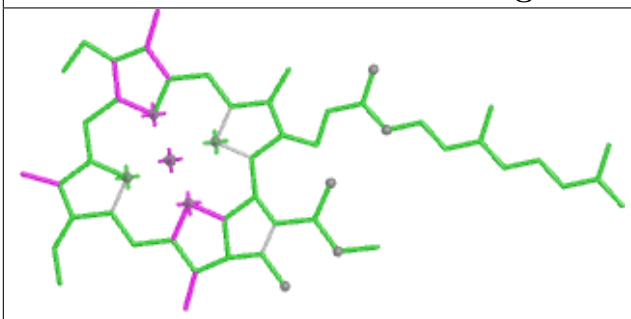


Rings

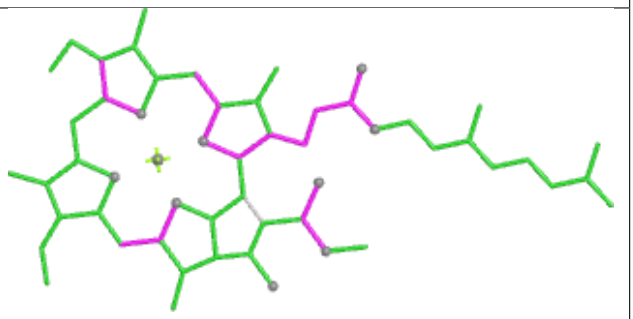
Ligand CLA l 1302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1117	
	
Bond lengths	Bond angles
	
Torsions	Rings

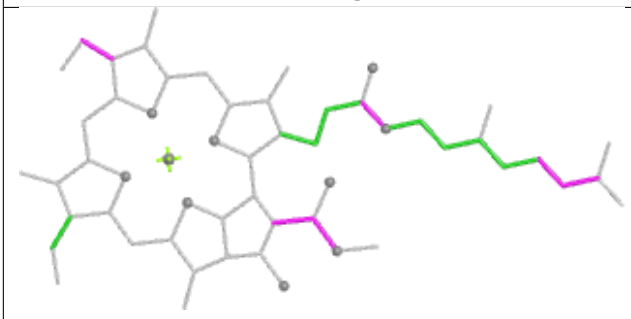
Ligand CLA B 1220



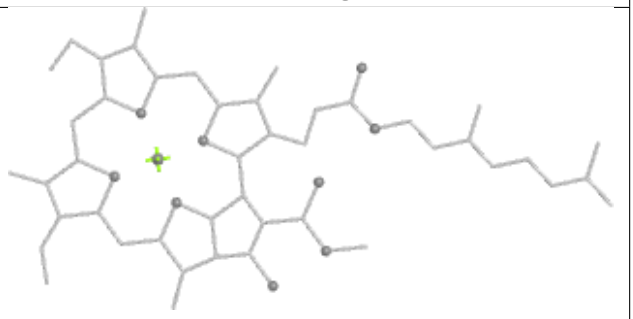
Bond lengths



Bond angles

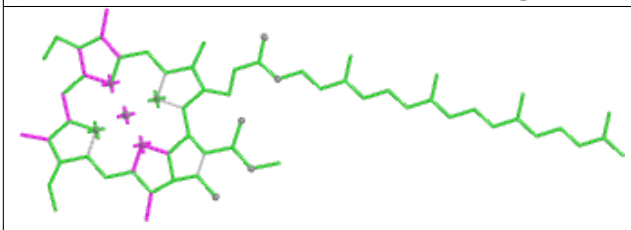


Torsions

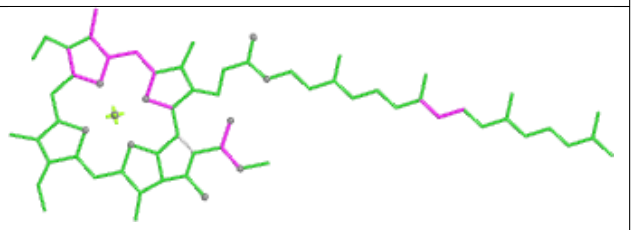


Rings

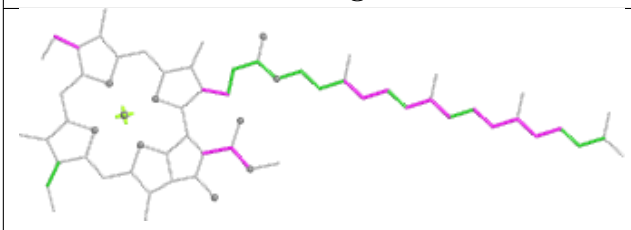
Ligand CLA A 1139



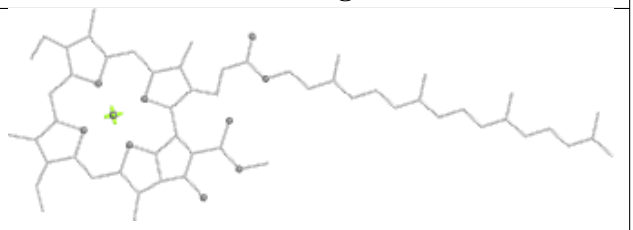
Bond lengths



Bond angles

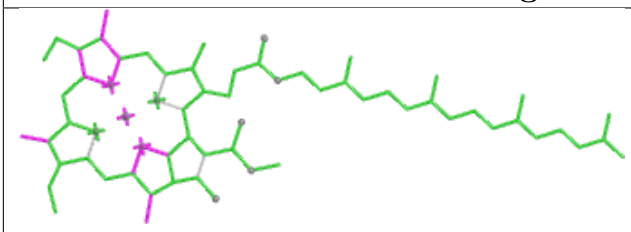


Torsions

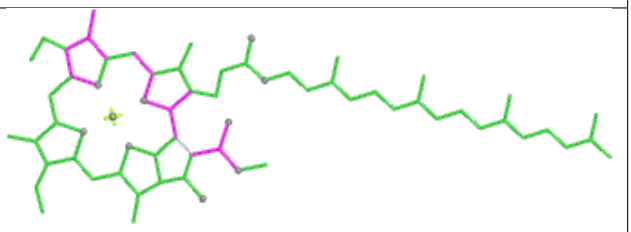


Rings

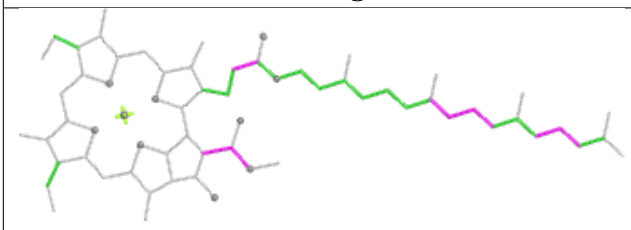
Ligand CLA e 1123



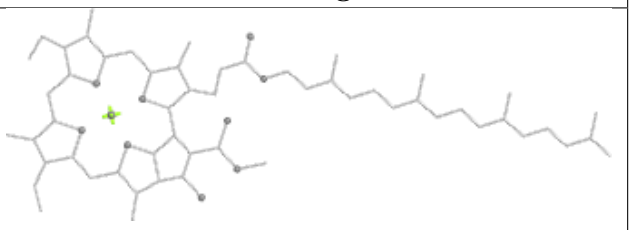
Bond lengths



Bond angles

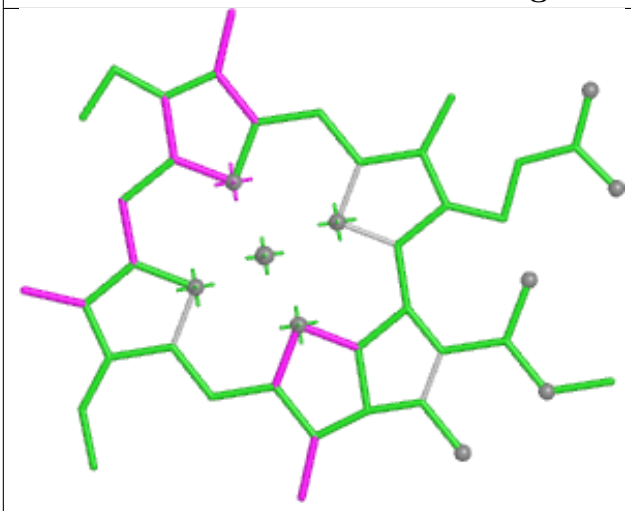


Torsions

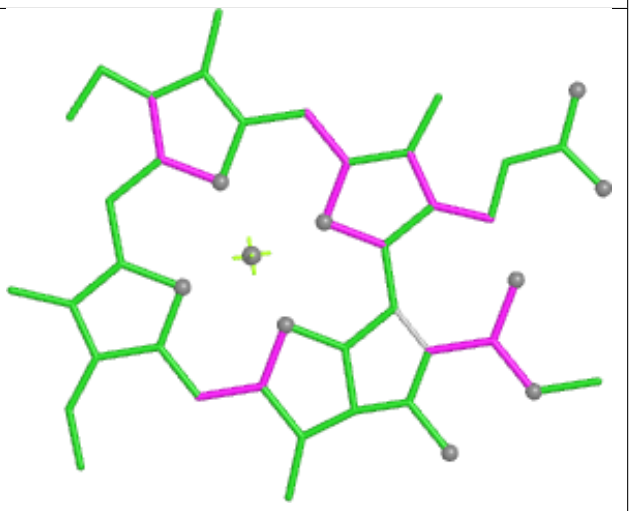


Rings

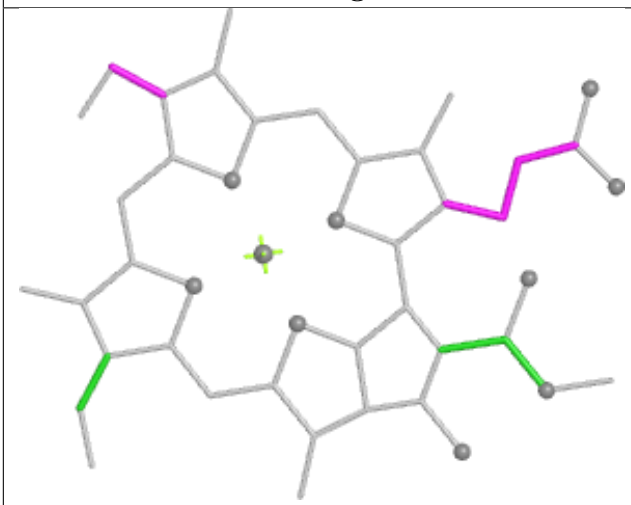
Ligand CLA s 501



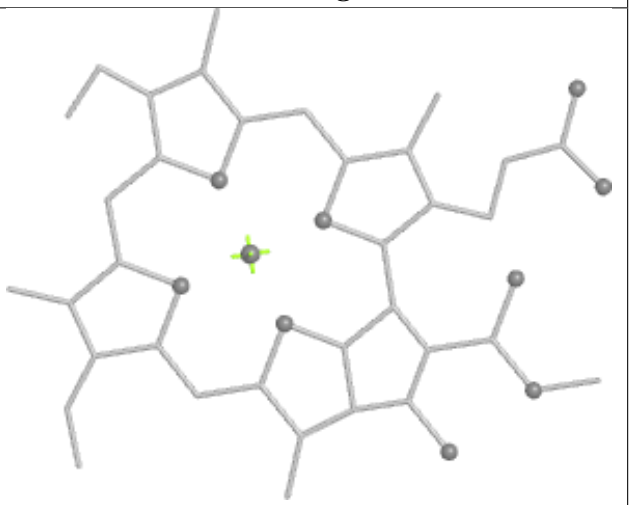
Bond lengths



Bond angles

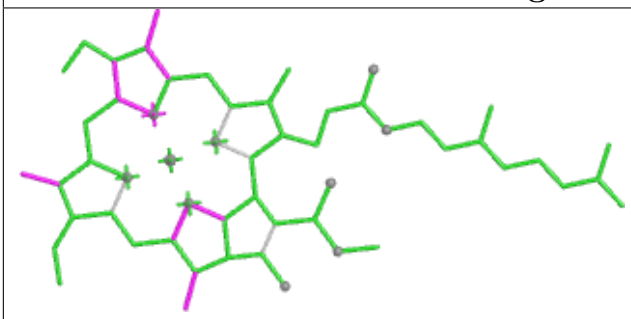


Torsions

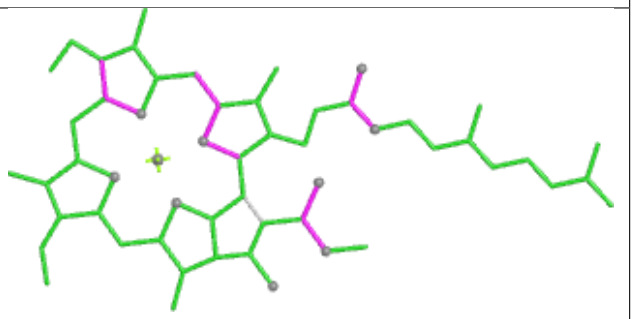


Rings

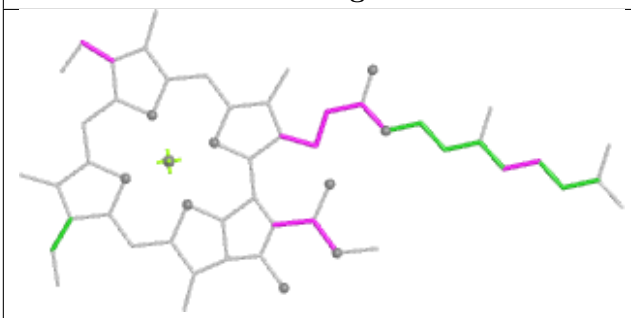
Ligand CLA 3 518



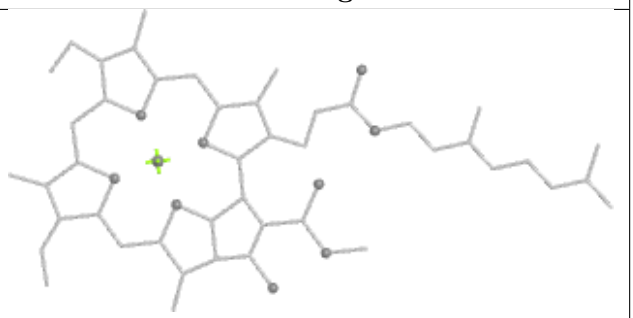
Bond lengths



Bond angles

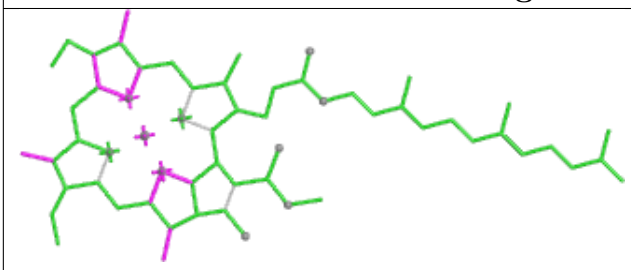


Torsions

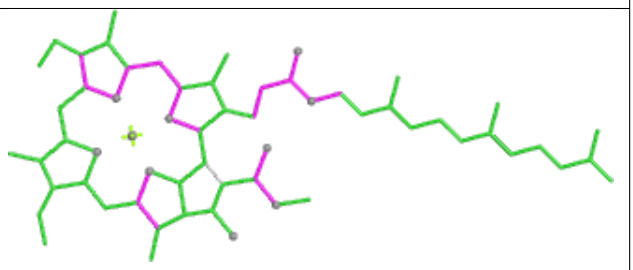


Rings

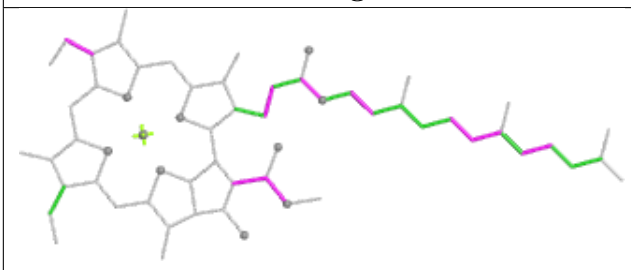
Ligand CLA B 1216



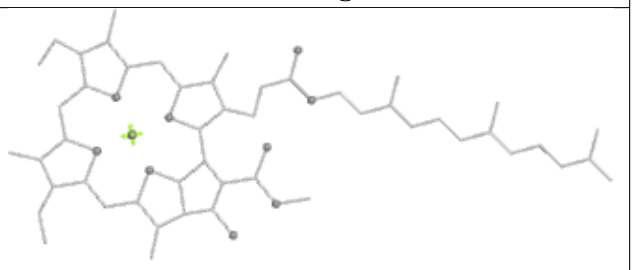
Bond lengths



Bond angles

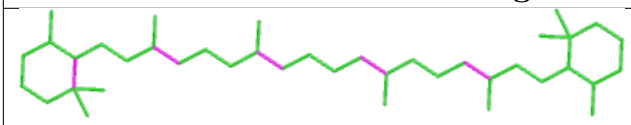


Torsions



Rings

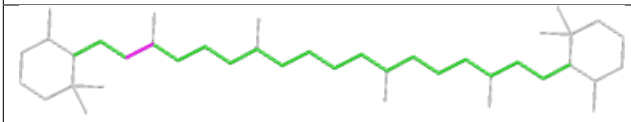
Ligand BCR V 4219



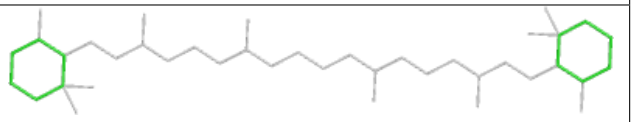
Bond lengths



Bond angles

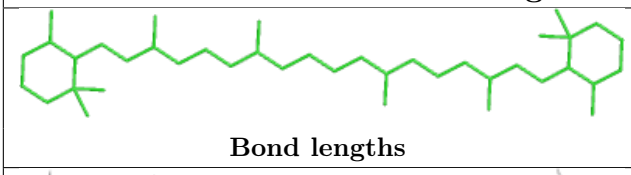


Torsions

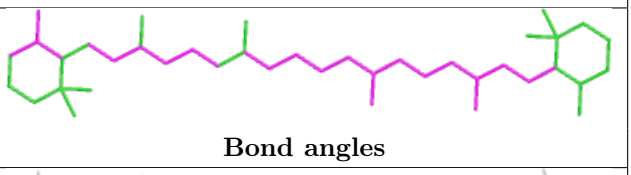


Rings

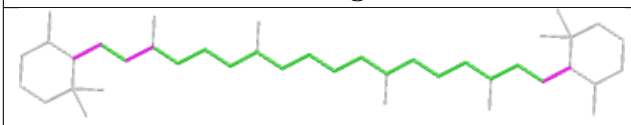
Ligand BCR d 524



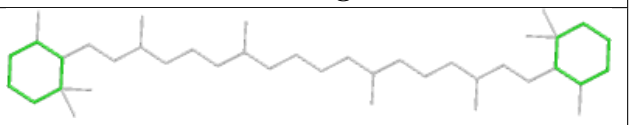
Bond lengths



Bond angles

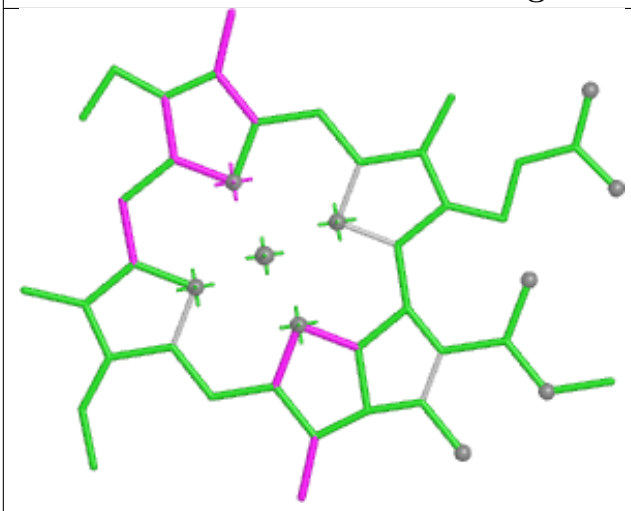


Torsions

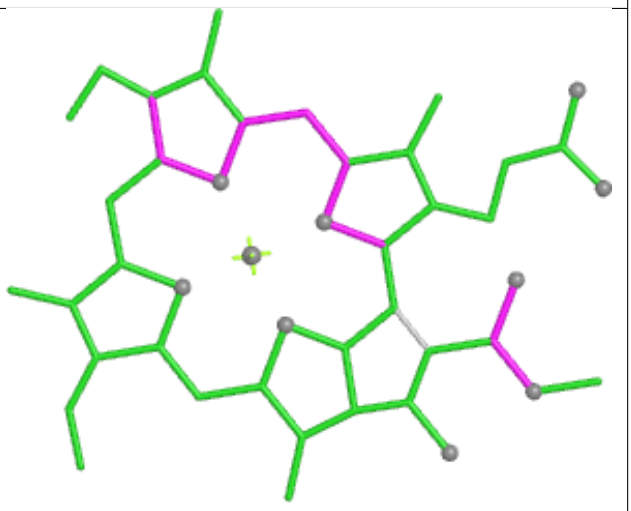


Rings

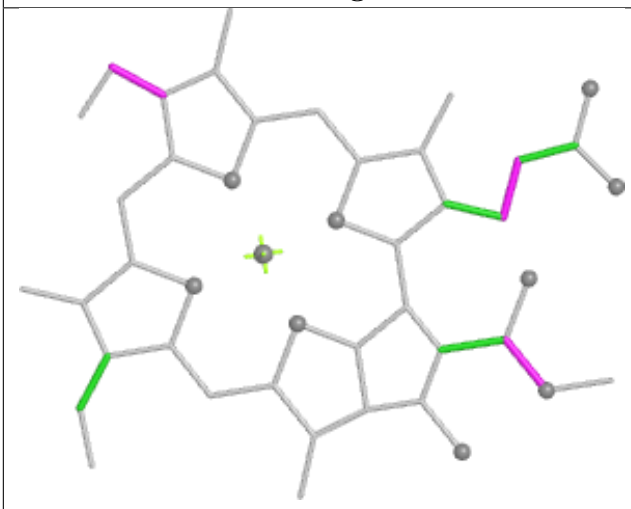
Ligand CLA v 513



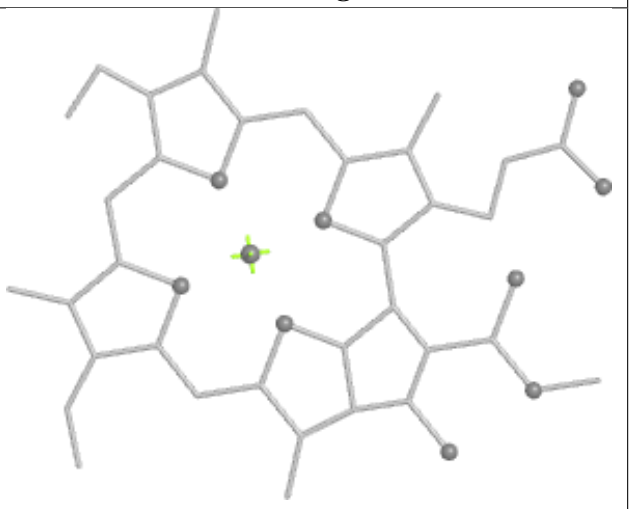
Bond lengths



Bond angles

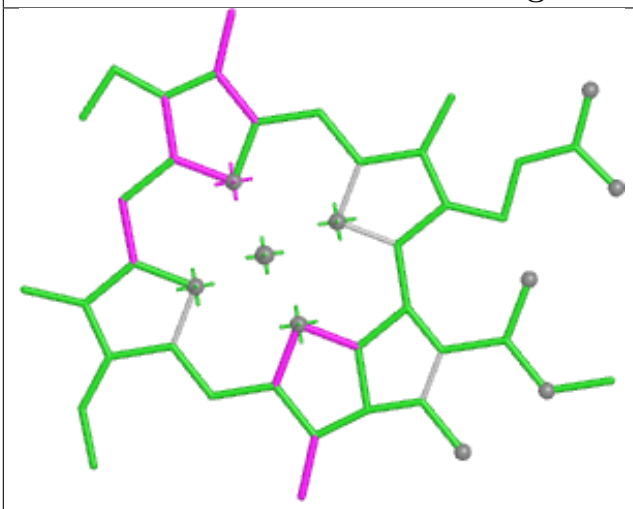


Torsions

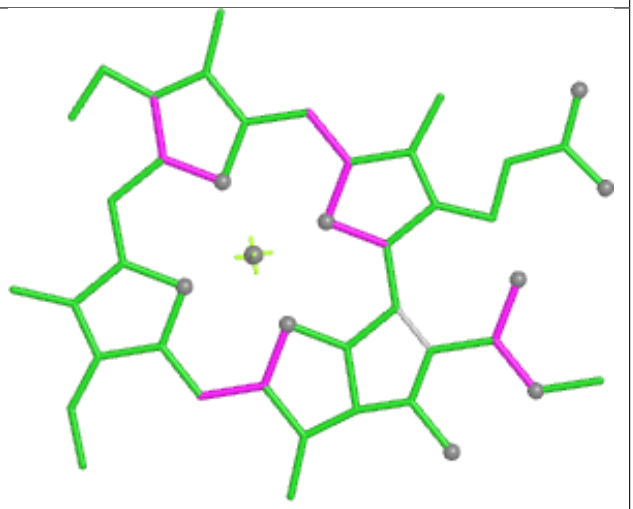


Rings

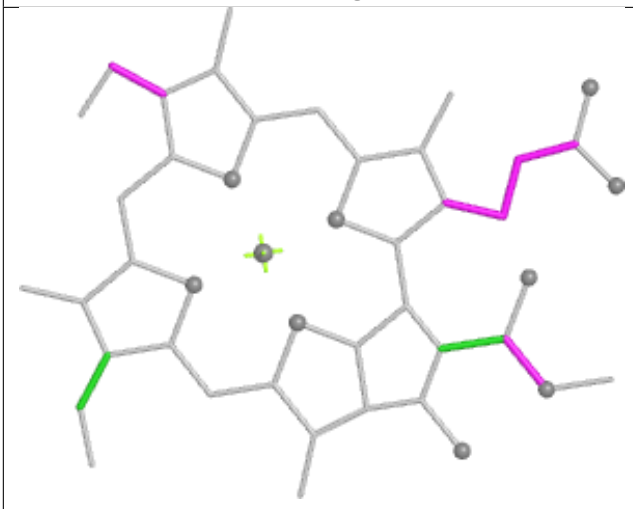
Ligand CLA b 501



Bond lengths



Bond angles

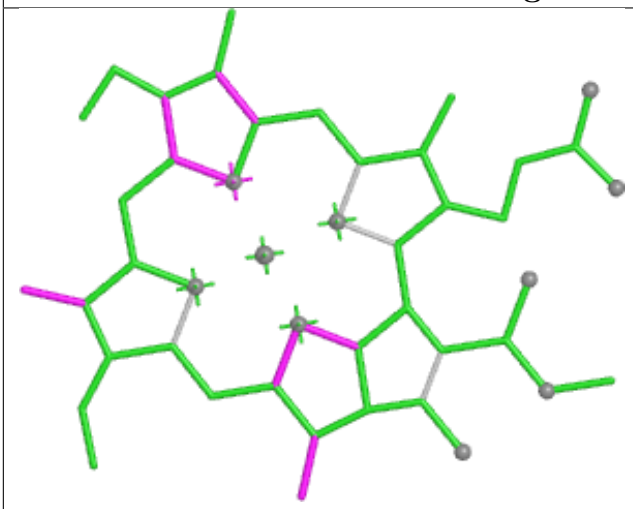


Torsions

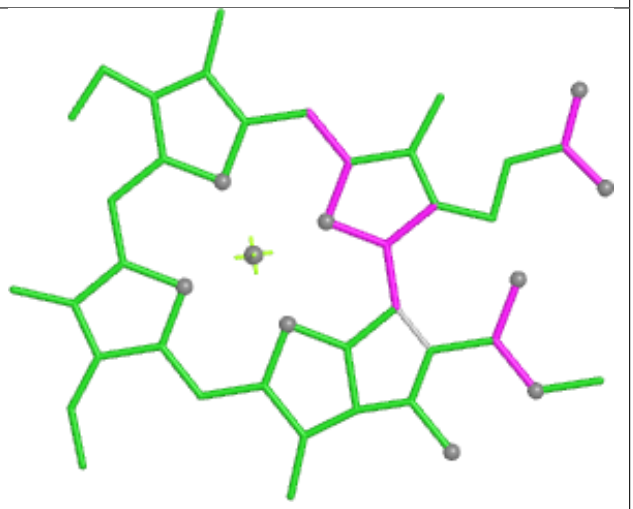


Rings

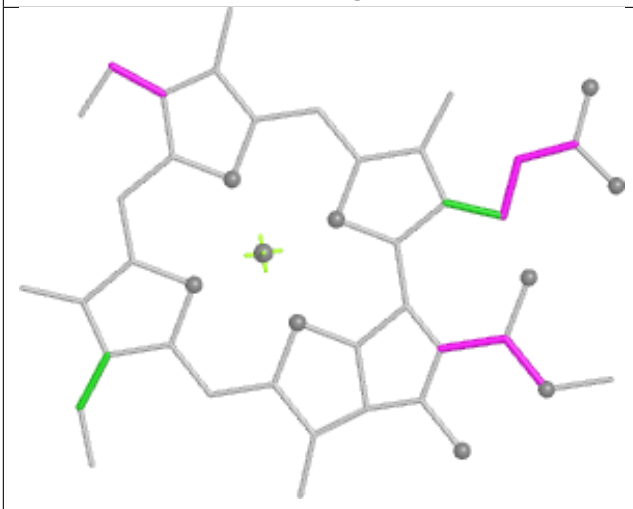
Ligand CLA Y 507



Bond lengths



Bond angles

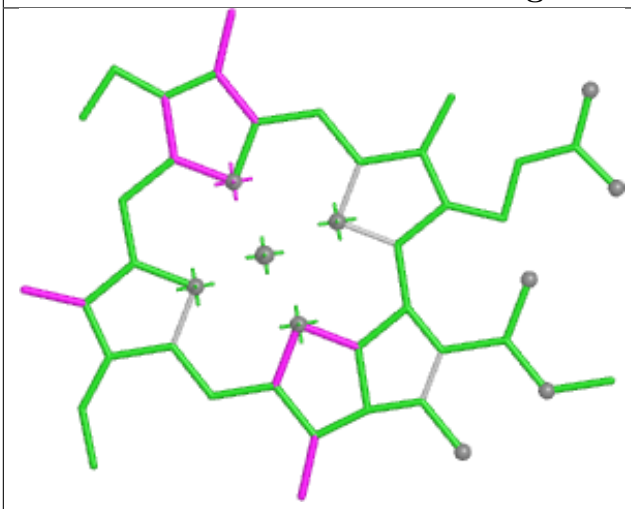


Torsions

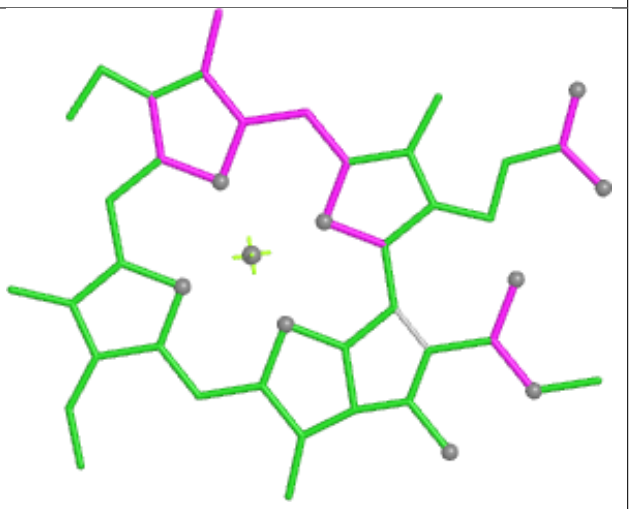


Rings

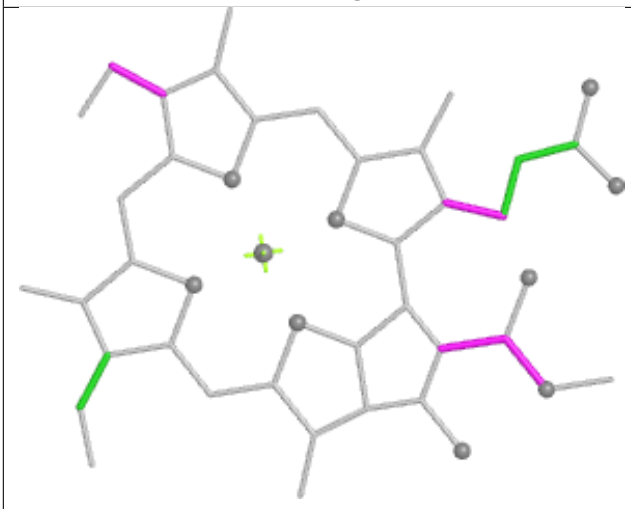
Ligand CLA Z 511



Bond lengths



Bond angles

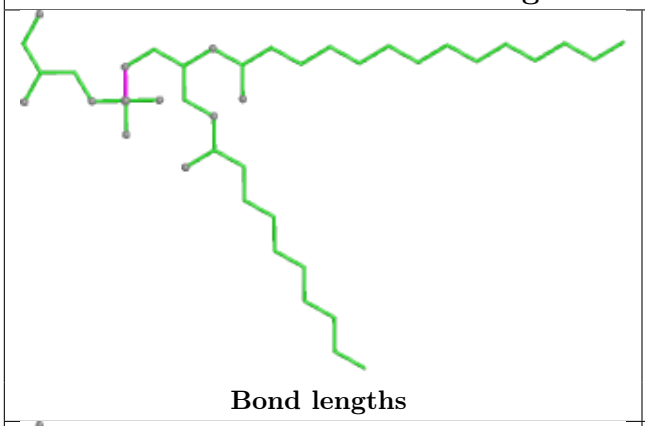


Torsions

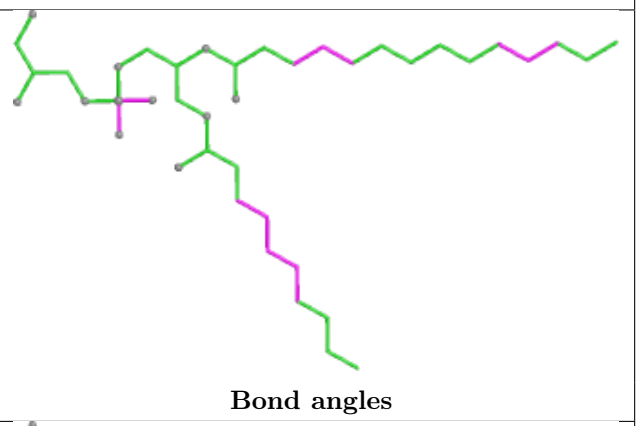


Rings

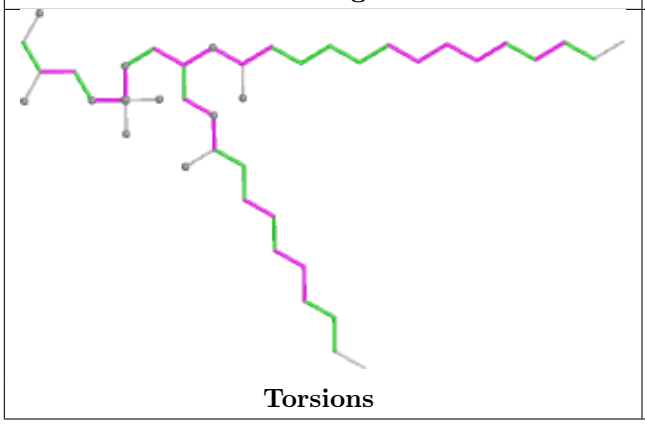
Ligand LHG f 1855



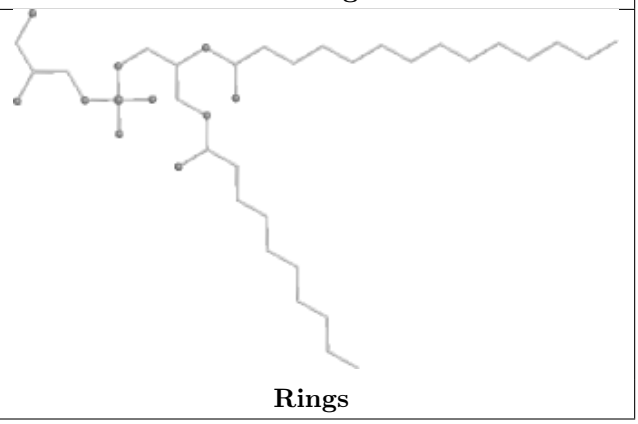
Bond lengths



Bond angles

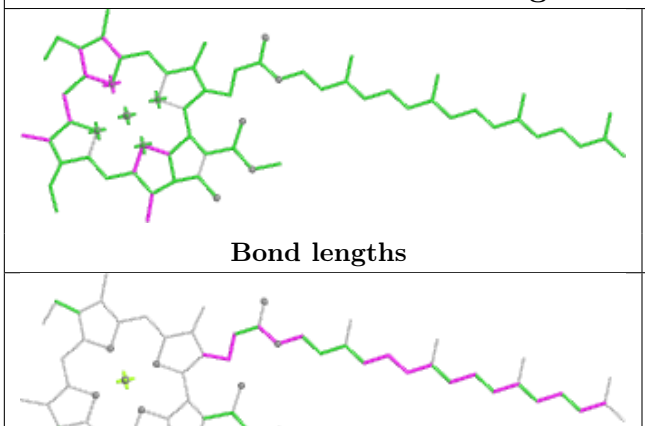


Torsions

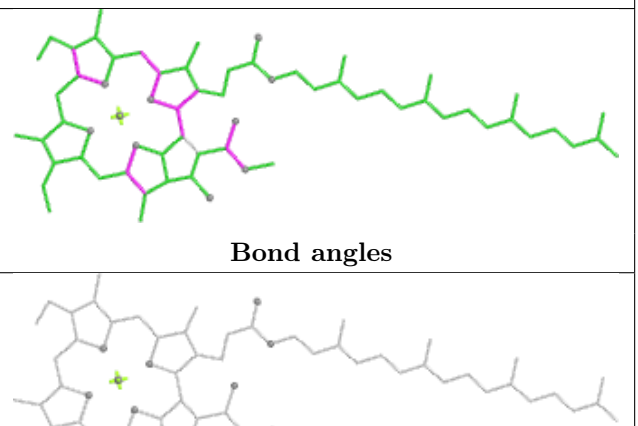


Rings

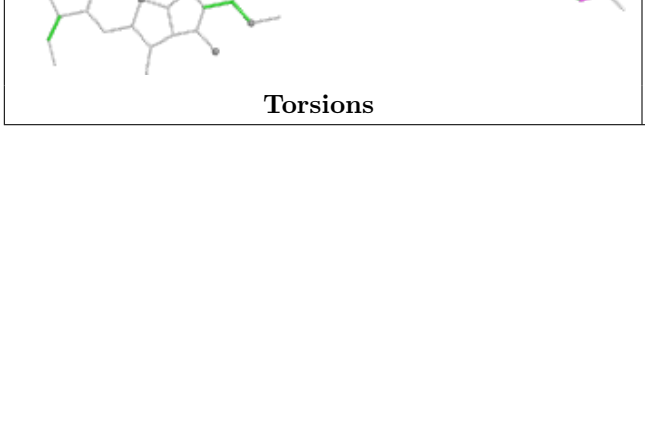
Ligand CLA 6 505



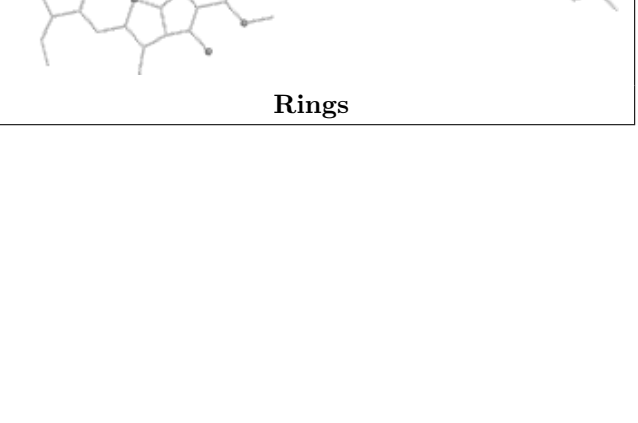
Bond lengths



Bond angles

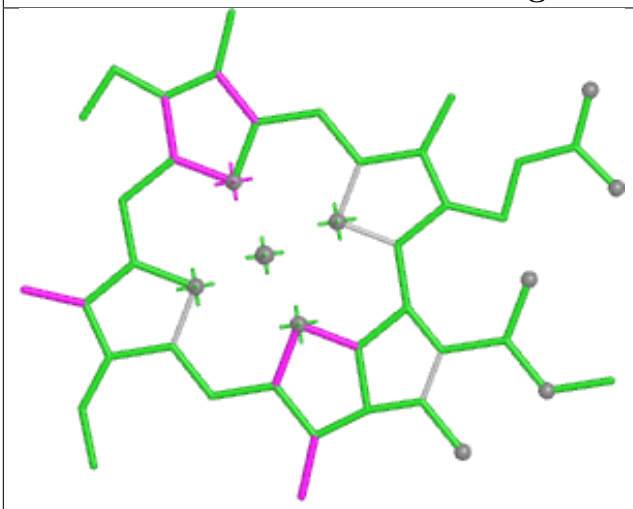


Torsions

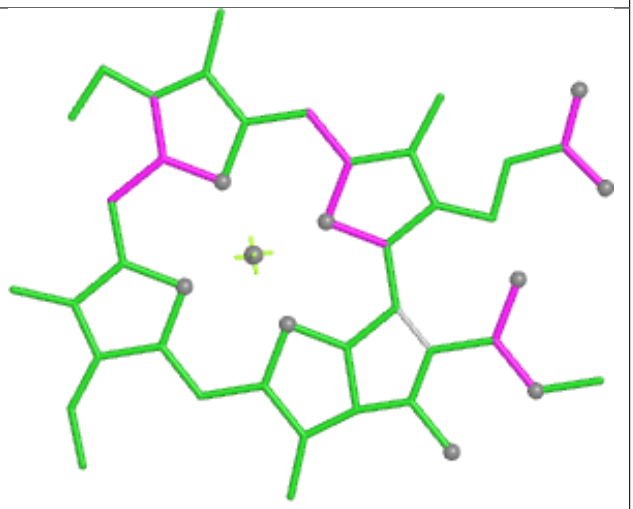


Rings

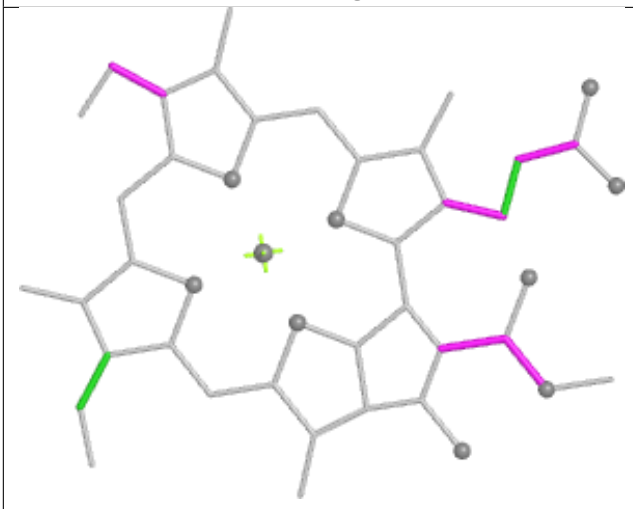
Ligand CLA 6 517



Bond lengths



Bond angles

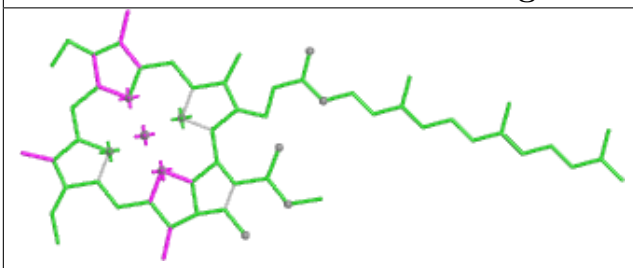


Torsions

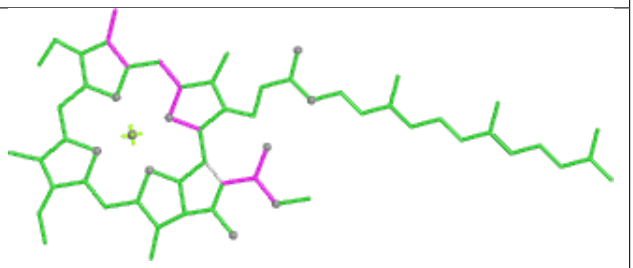


Rings

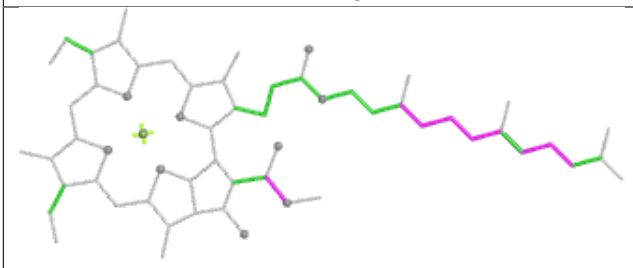
Ligand CLA n 1503



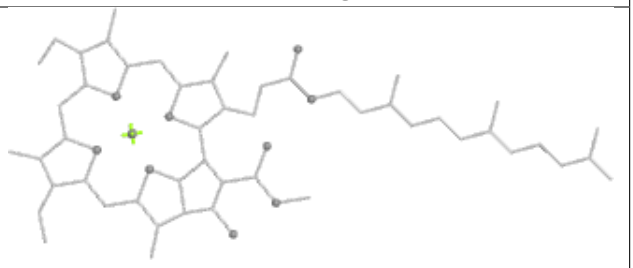
Bond lengths



Bond angles

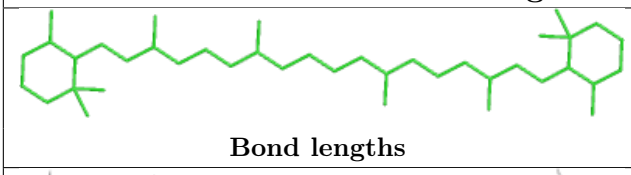


Torsions

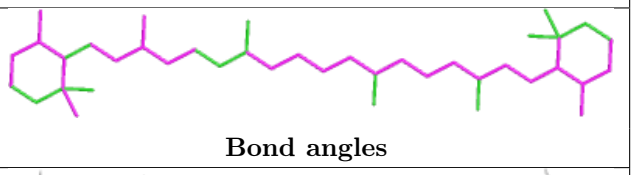


Rings

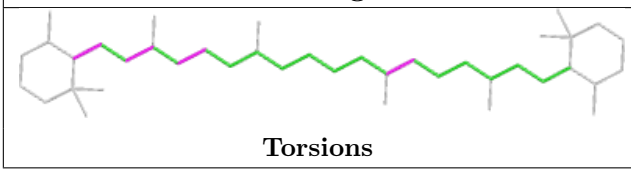
Ligand BCR 5 521



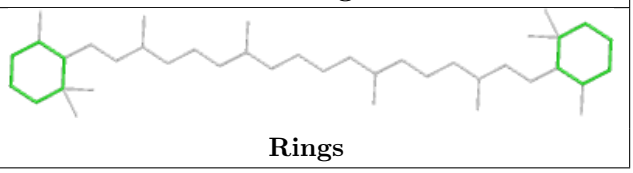
Bond lengths



Bond angles

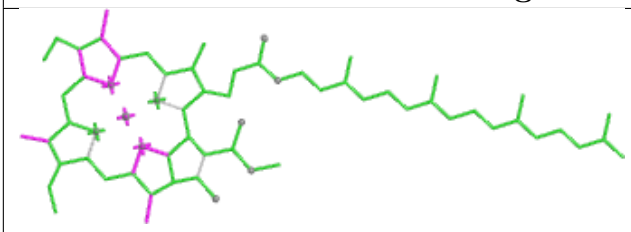


Torsions

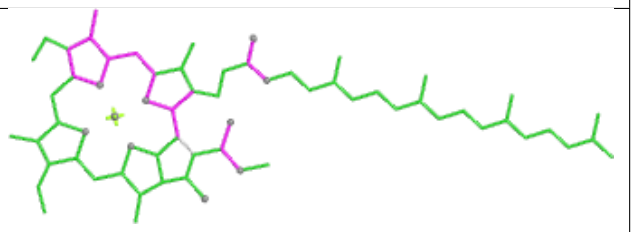


Rings

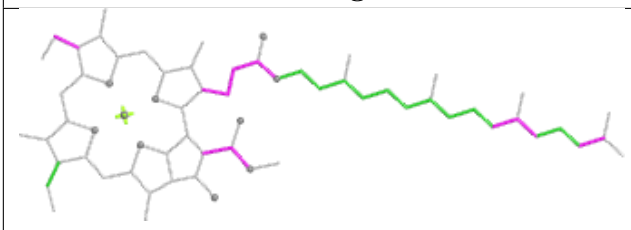
Ligand CLA A 1111



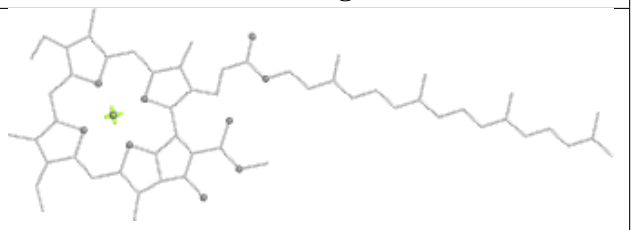
Bond lengths



Bond angles

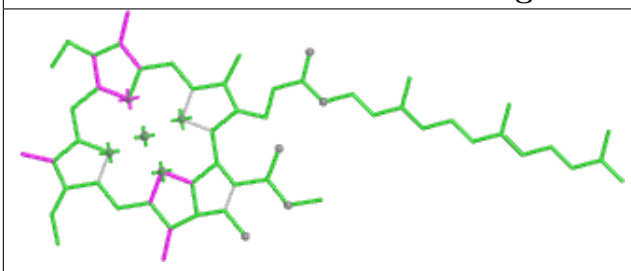


Torsions

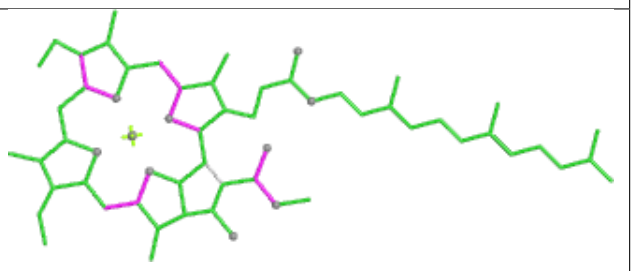


Rings

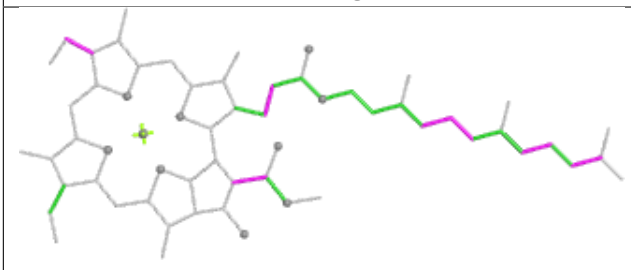
Ligand CLA B 1218



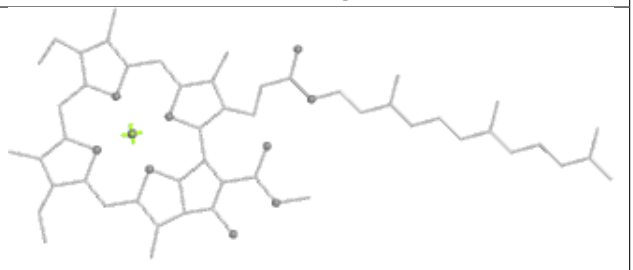
Bond lengths



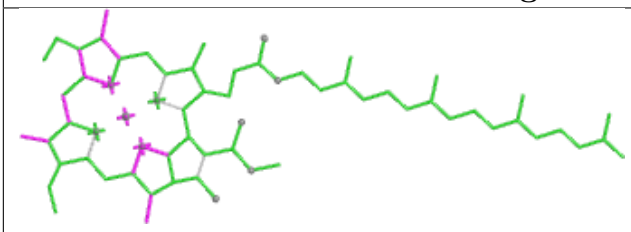
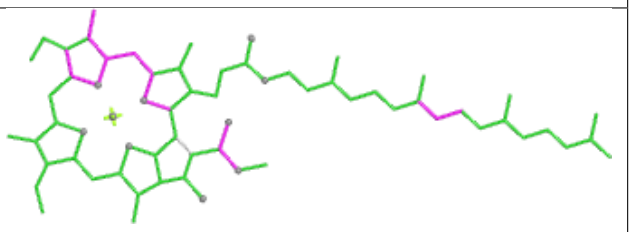
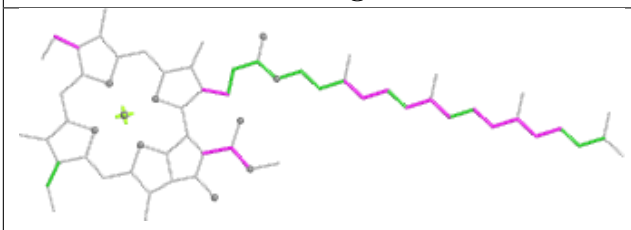
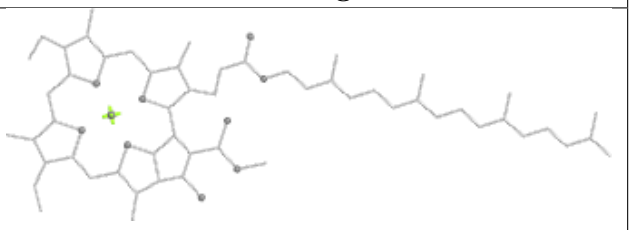
Bond angles

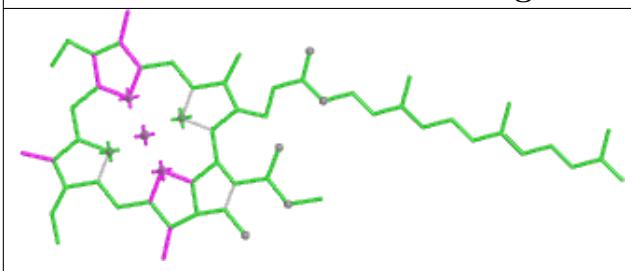
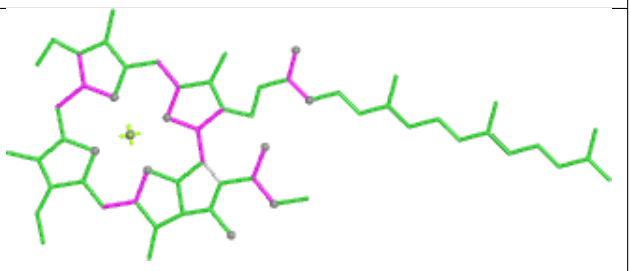
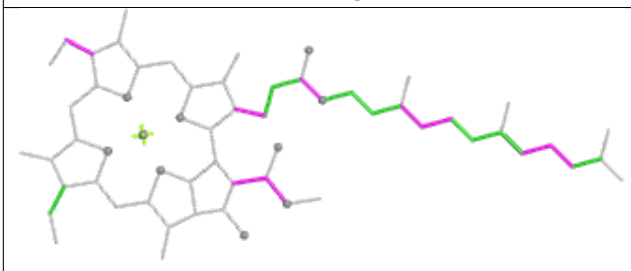
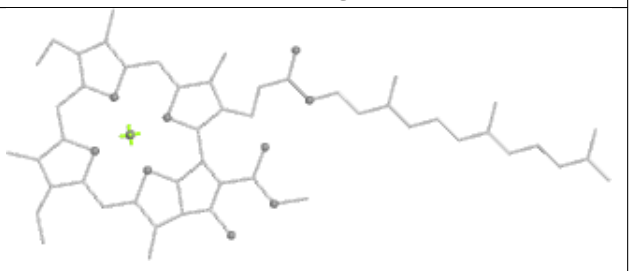


Torsions

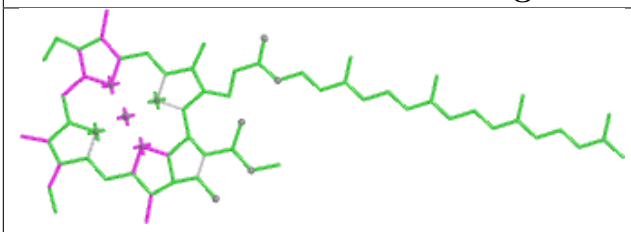


Rings

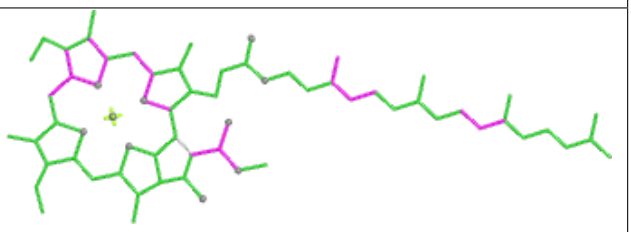
Ligand CLA e 1139	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1122	
 Bond lengths	 Bond angles
 Torsions	 Rings

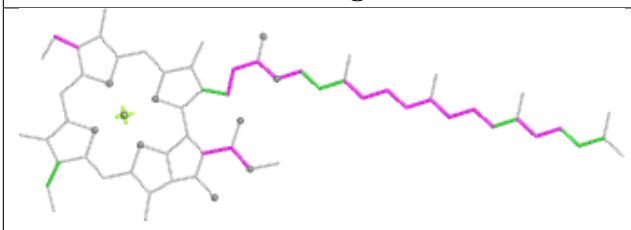
Ligand CLA G 1237



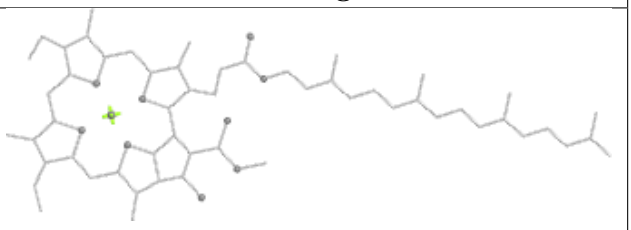
Bond lengths



Bond angles

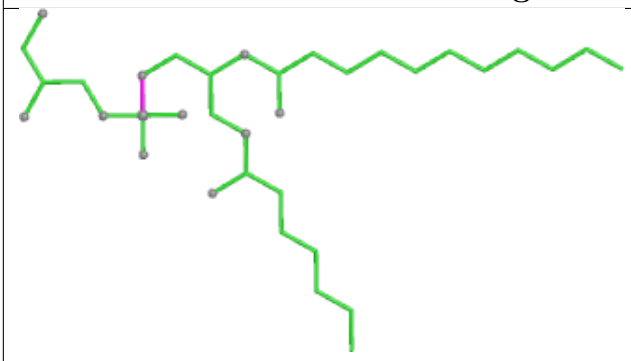


Torsions

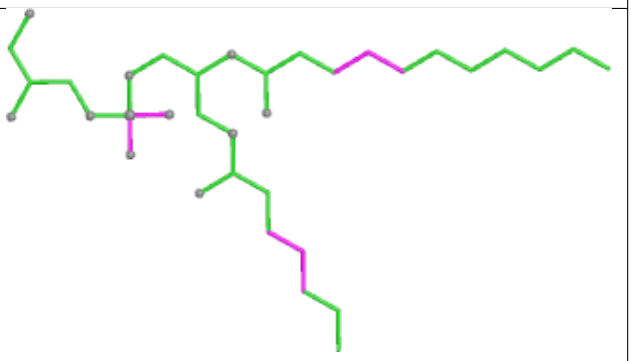


Rings

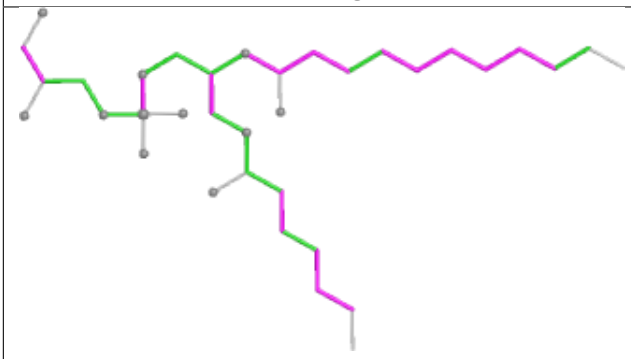
Ligand LHG G 5008



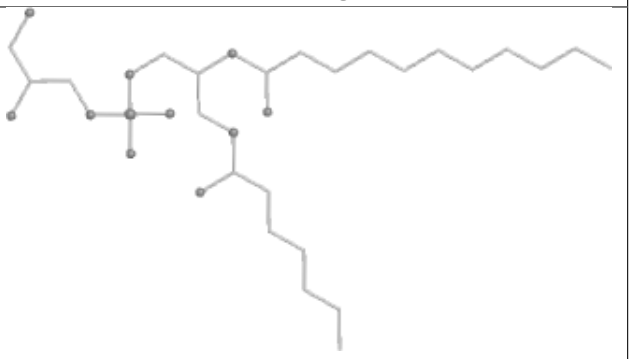
Bond lengths



Bond angles

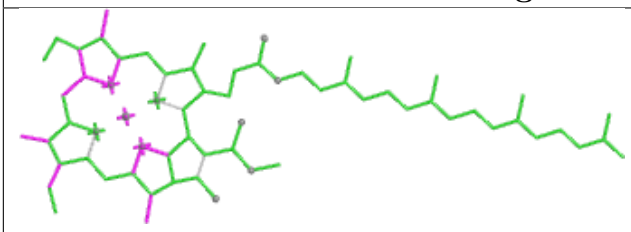


Torsions

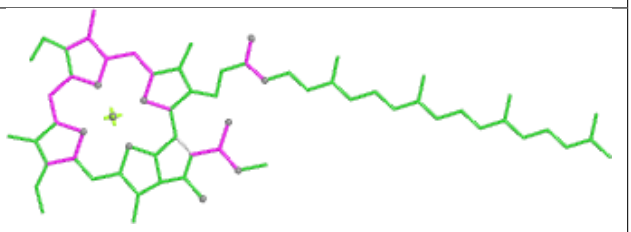


Rings

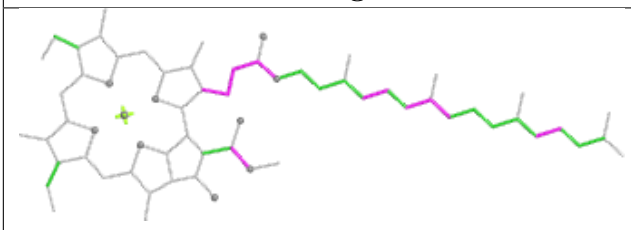
Ligand CLA B 1206



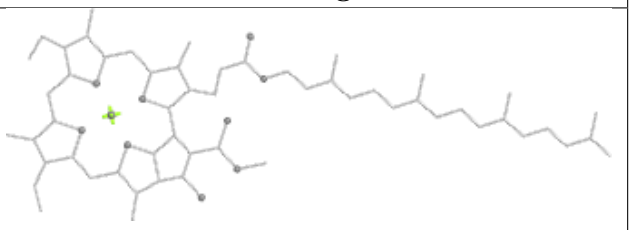
Bond lengths



Bond angles

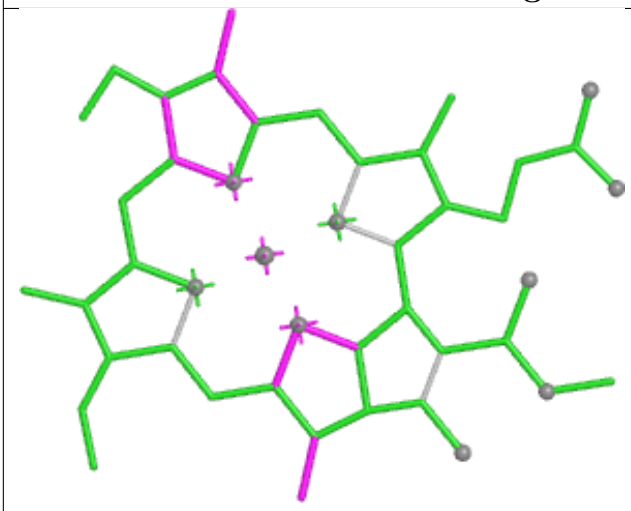


Torsions

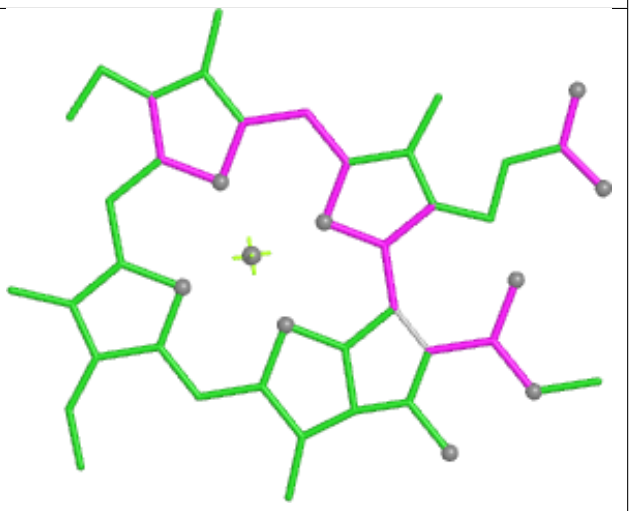


Rings

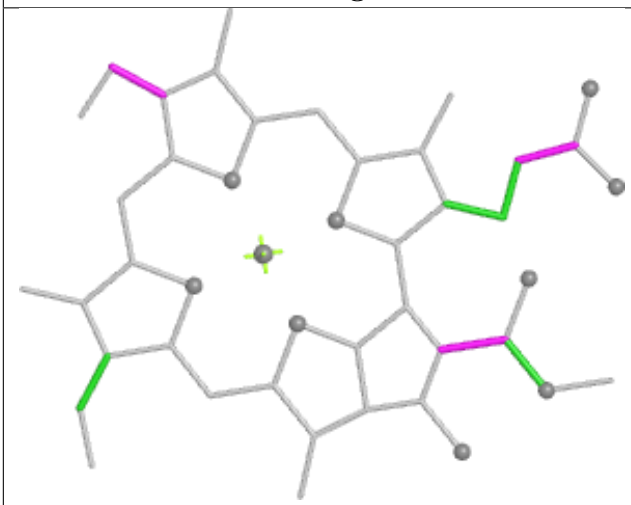
Ligand CLA Y 509



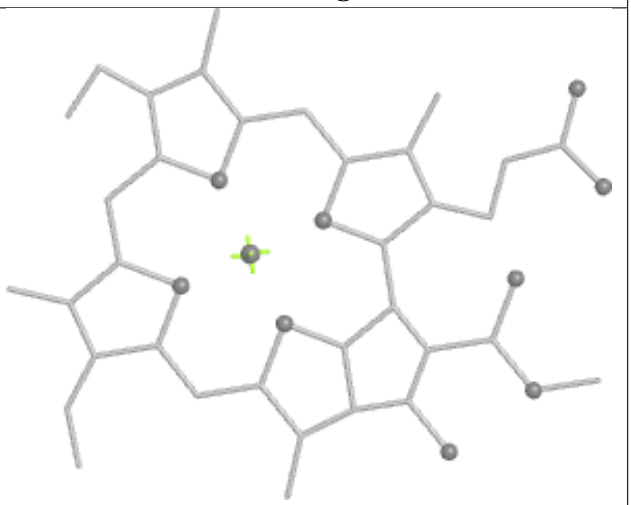
Bond lengths



Bond angles

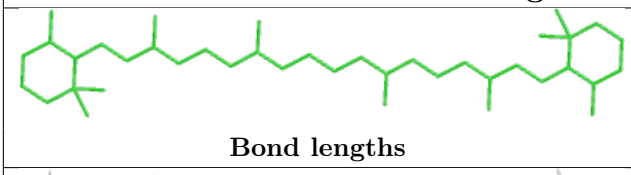


Torsions

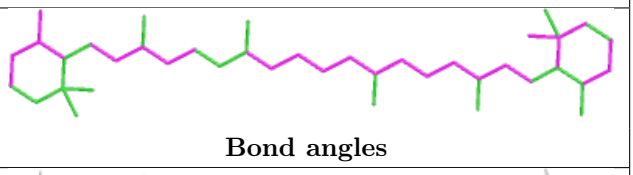


Rings

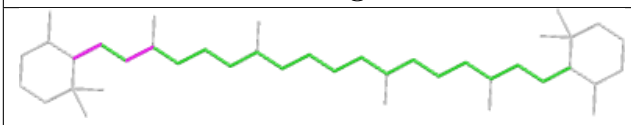
Ligand BCR 2 521



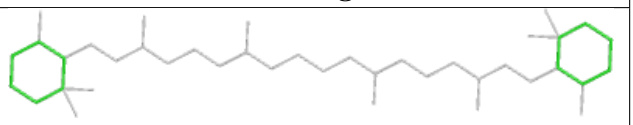
Bond lengths



Bond angles

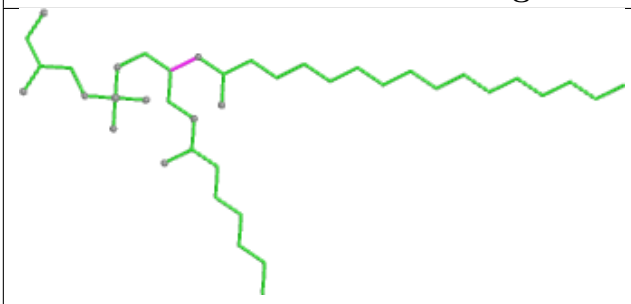


Torsions

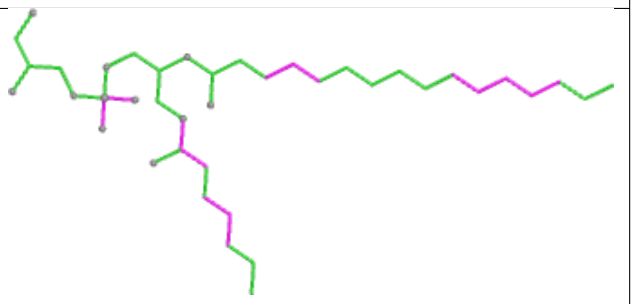


Rings

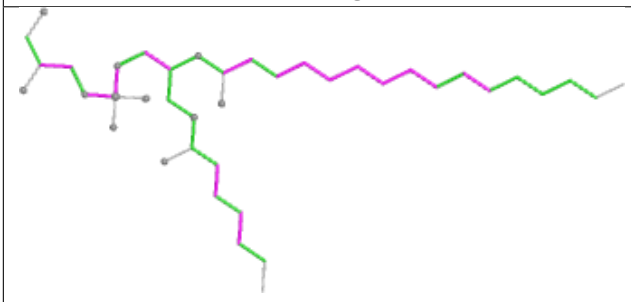
Ligand LHG G 5003



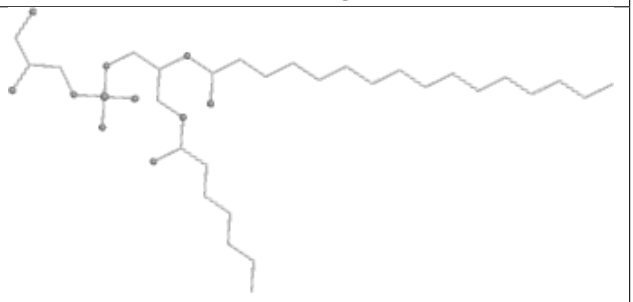
Bond lengths



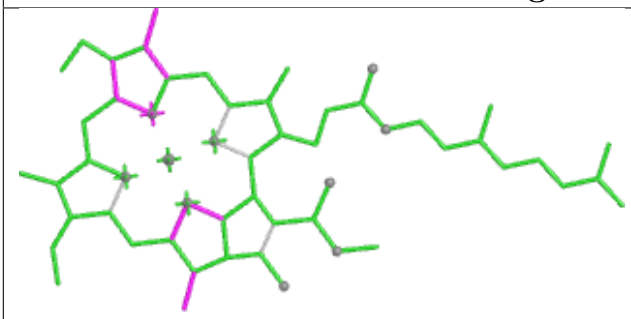
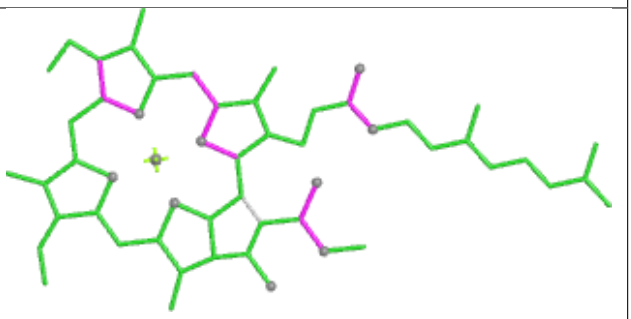
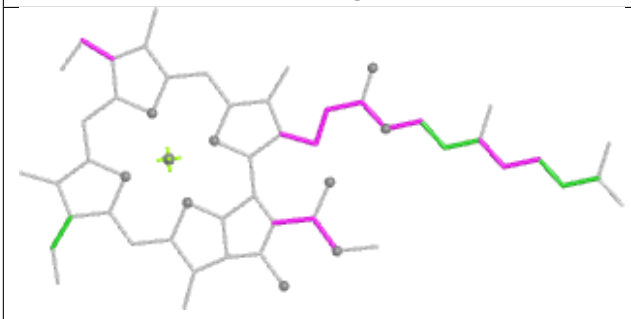
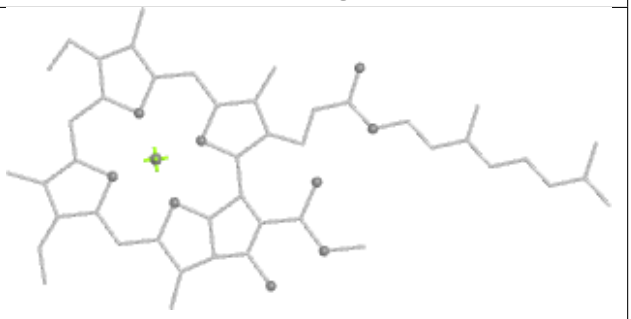
Bond angles

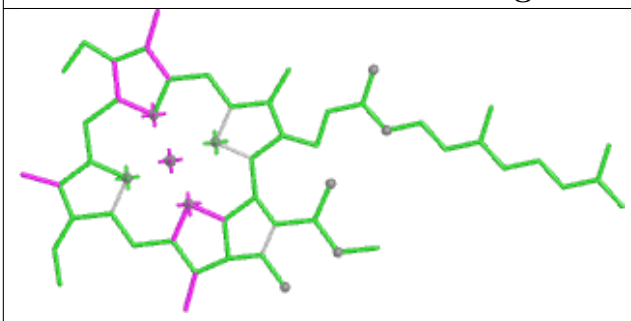
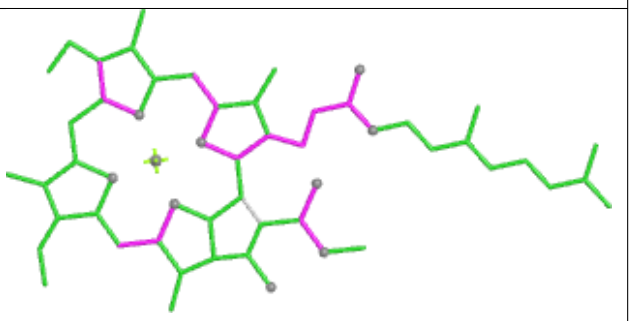
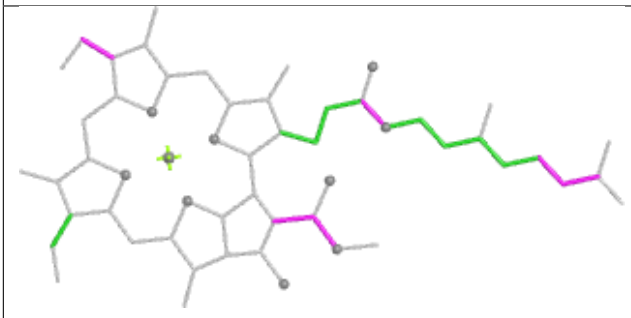
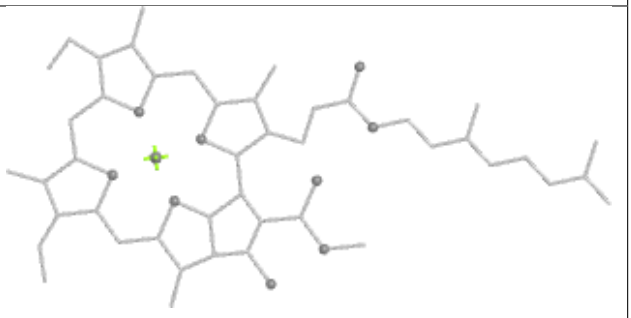


Torsions

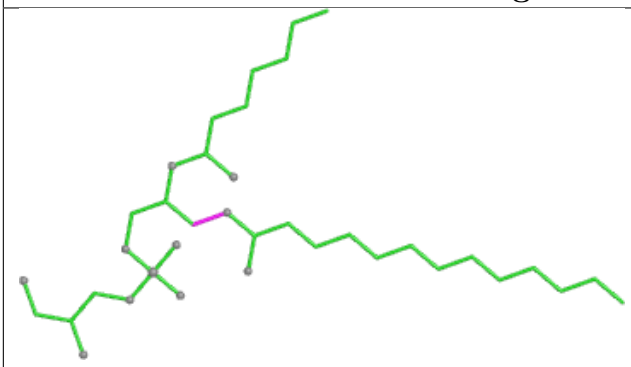


Rings

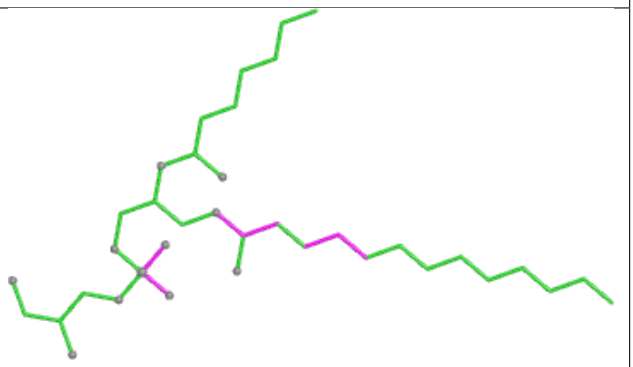
Ligand CLA 2 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1220	
 Bond lengths	 Bond angles
 Torsions	 Rings

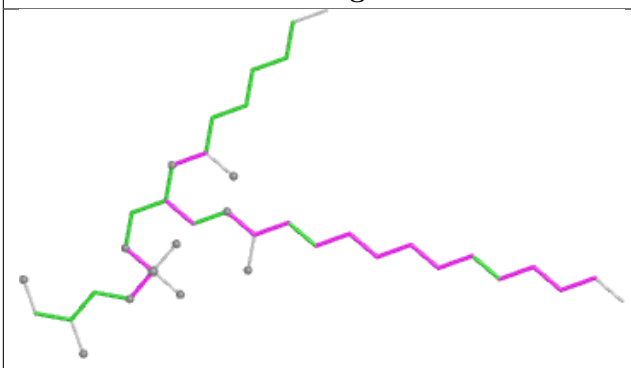
Ligand LHG H 1842



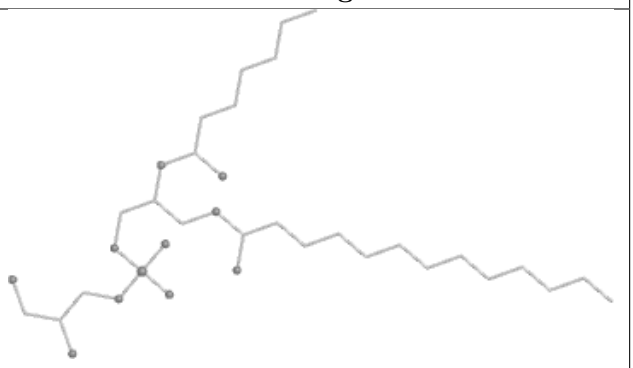
Bond lengths



Bond angles

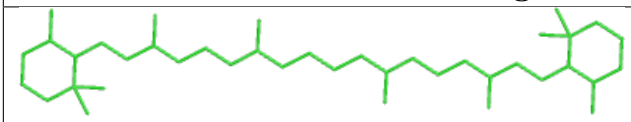


Torsions

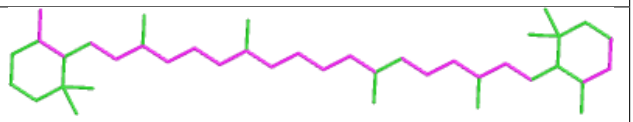


Rings

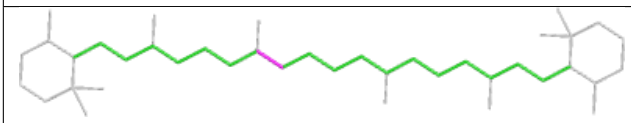
Ligand BCR R 4016



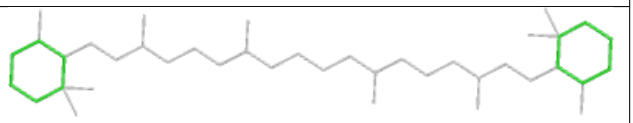
Bond lengths



Bond angles

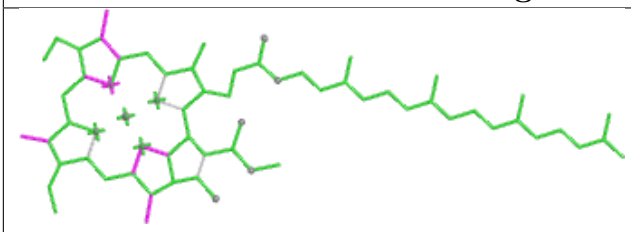


Torsions

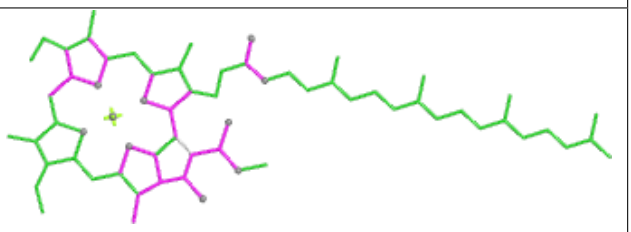


Rings

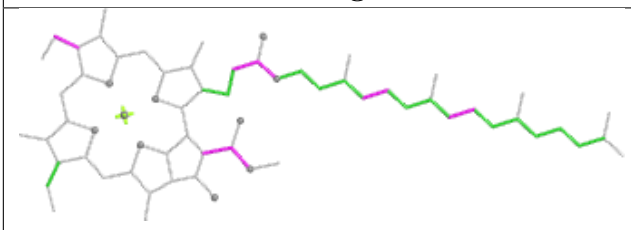
Ligand CLA A 1011



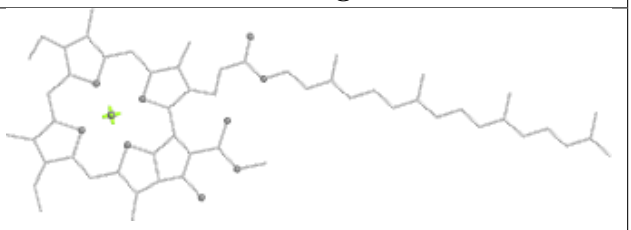
Bond lengths



Bond angles

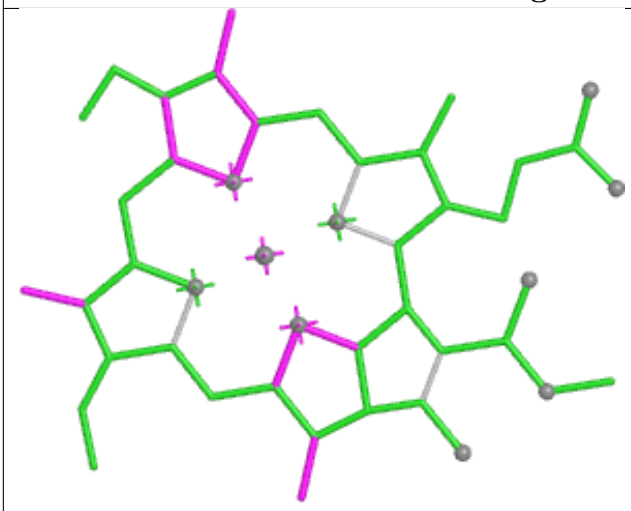


Torsions

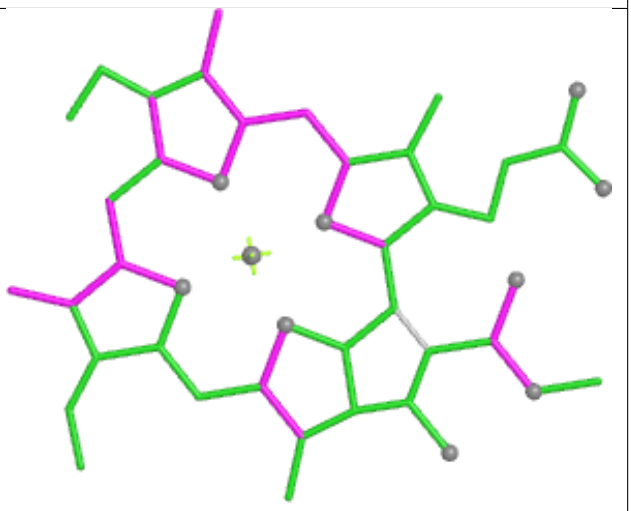


Rings

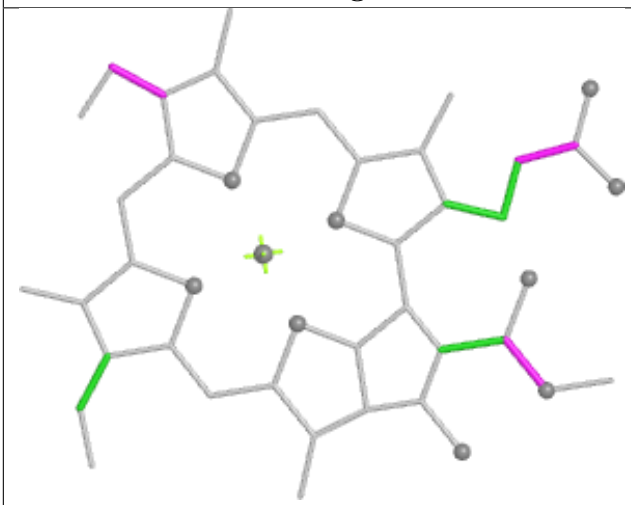
Ligand CLA t 508



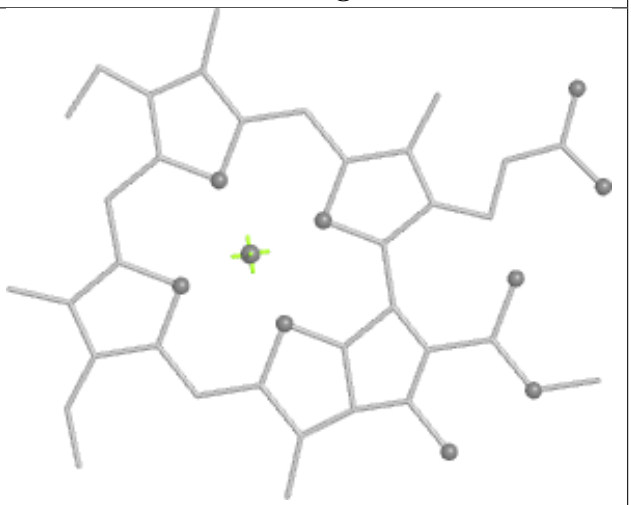
Bond lengths



Bond angles

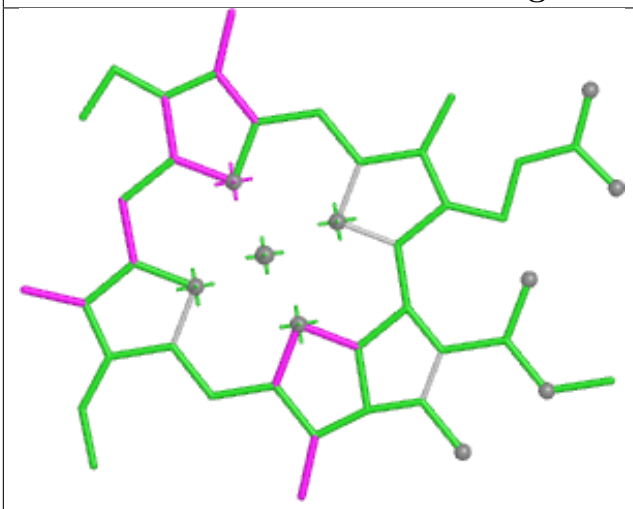


Torsions

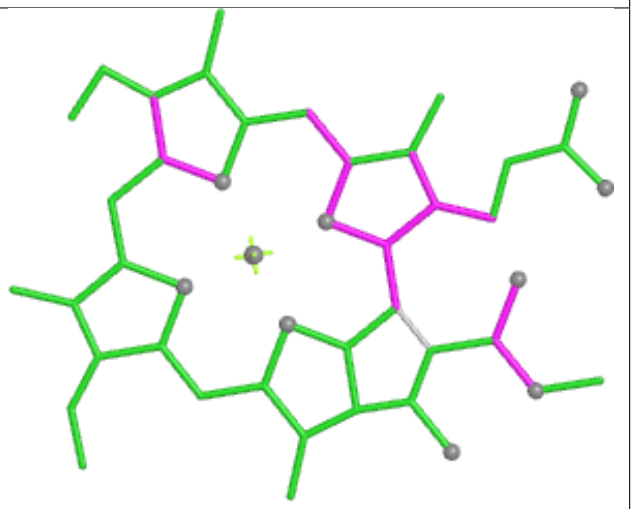


Rings

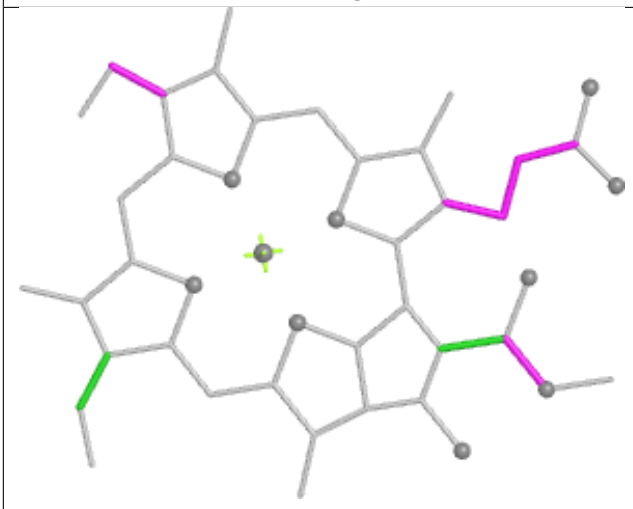
Ligand CLA 5 501



Bond lengths



Bond angles

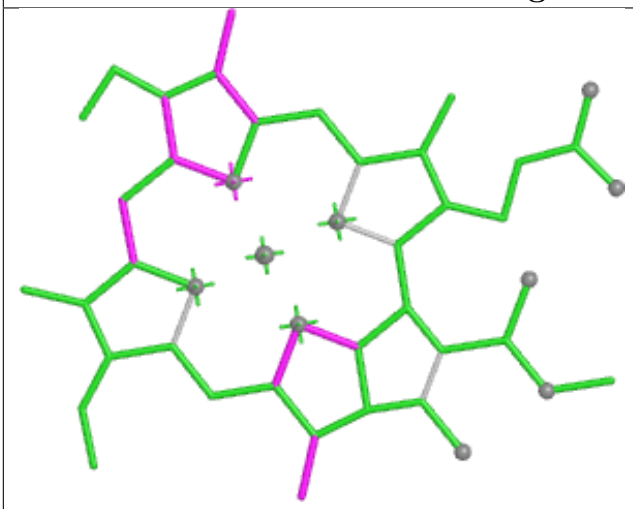


Torsions

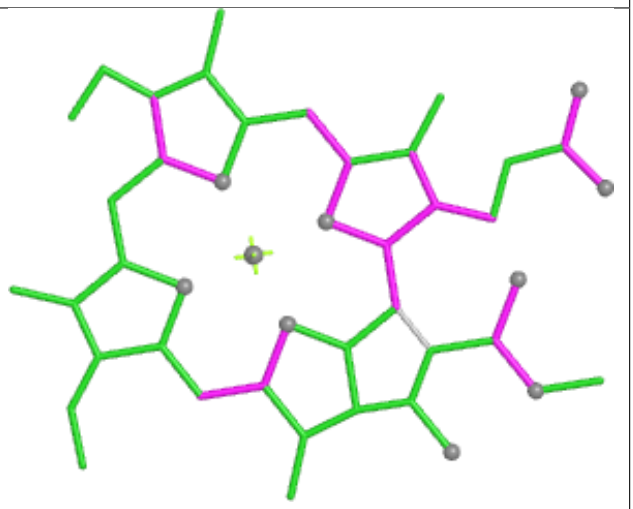


Rings

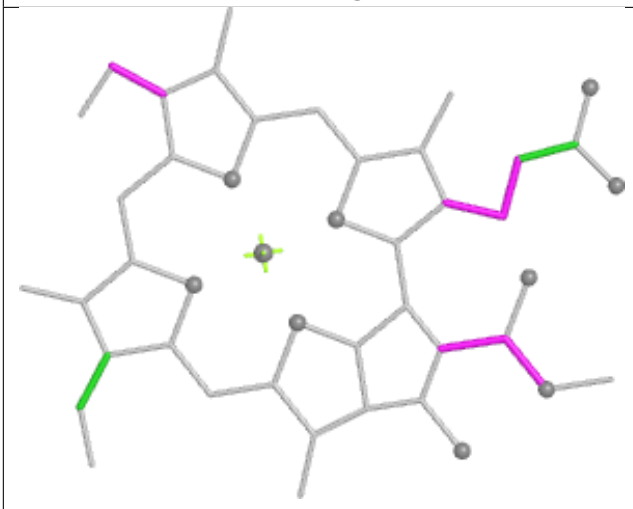
Ligand CLA 5 503



Bond lengths



Bond angles

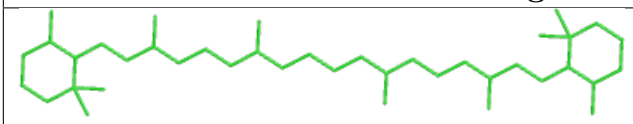


Torsions

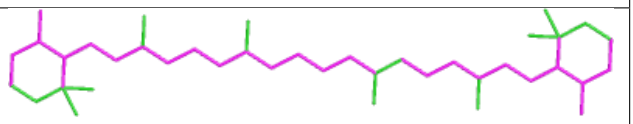


Rings

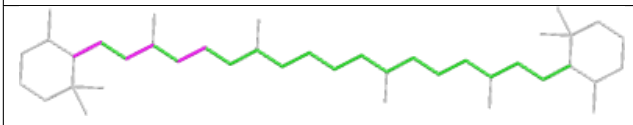
Ligand BCR c 522



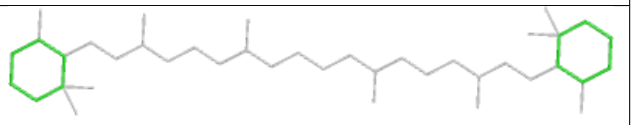
Bond lengths



Bond angles

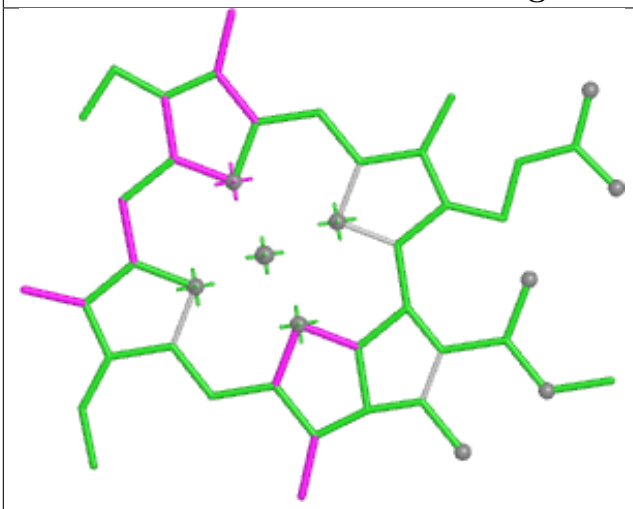


Torsions

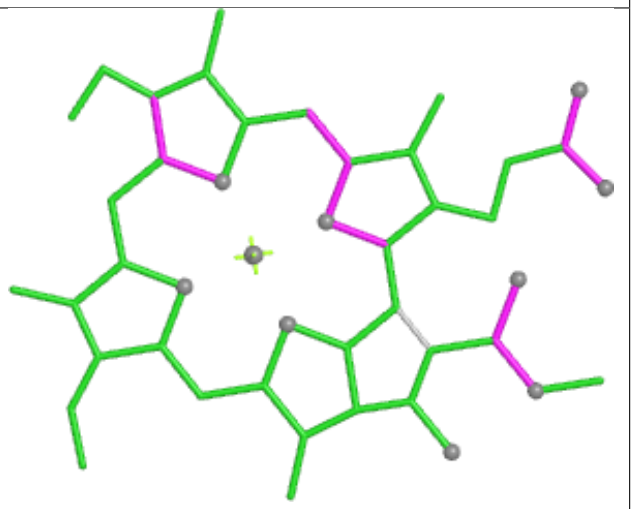


Rings

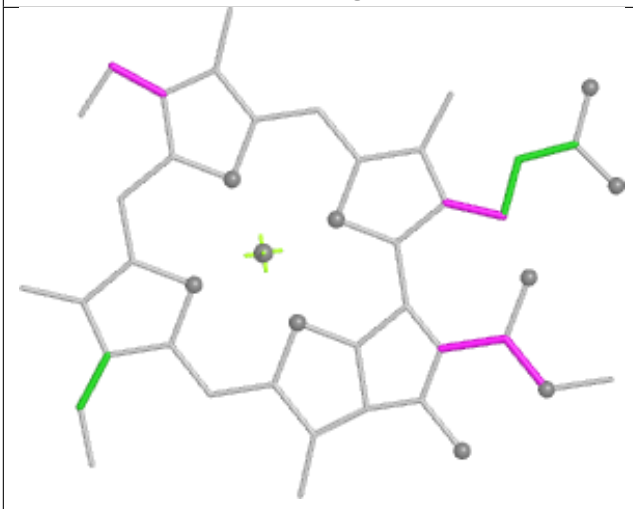
Ligand CLA 5 506



Bond lengths



Bond angles

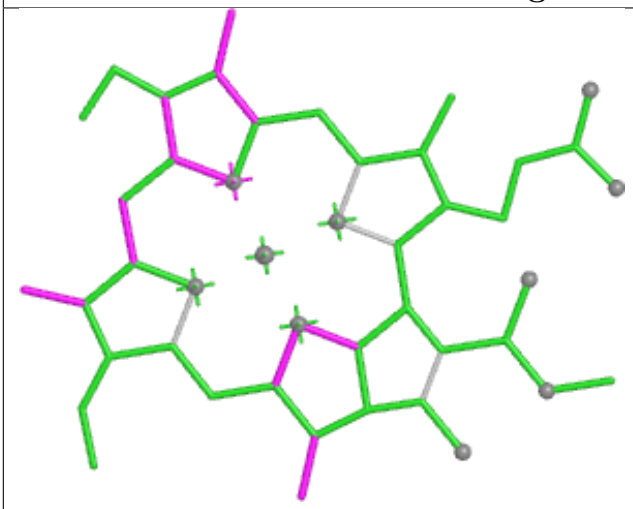


Torsions

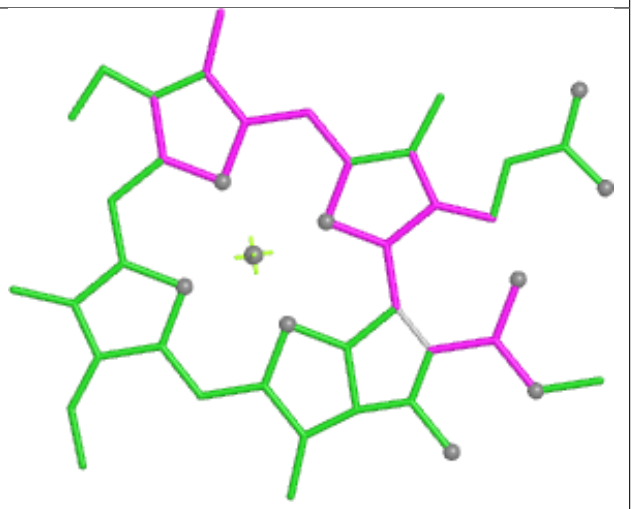


Rings

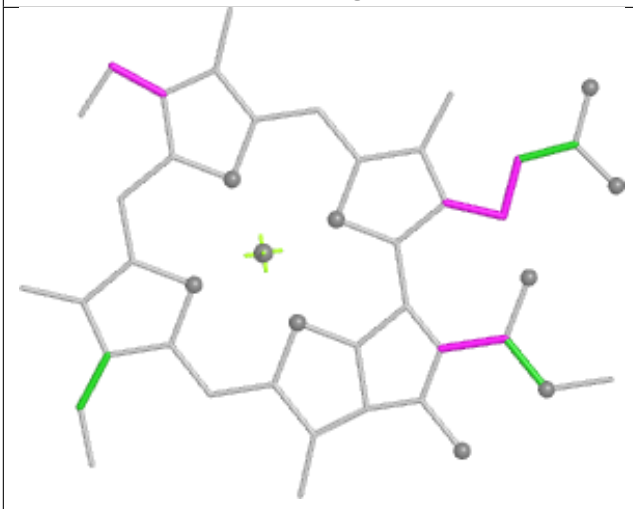
Ligand CLA a 504



Bond lengths



Bond angles

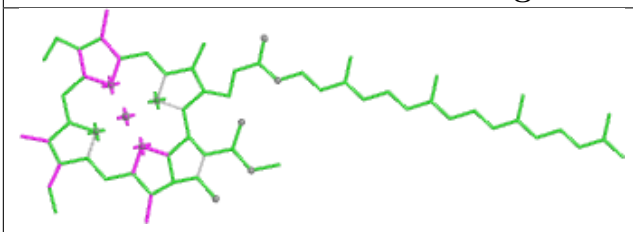


Torsions

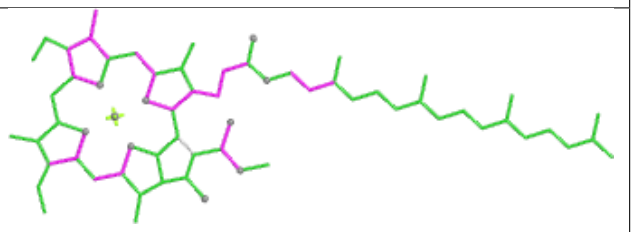


Rings

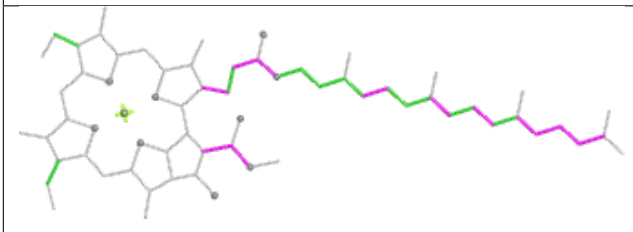
Ligand CLA G 1103



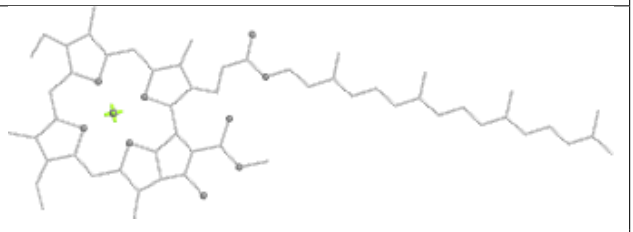
Bond lengths



Bond angles

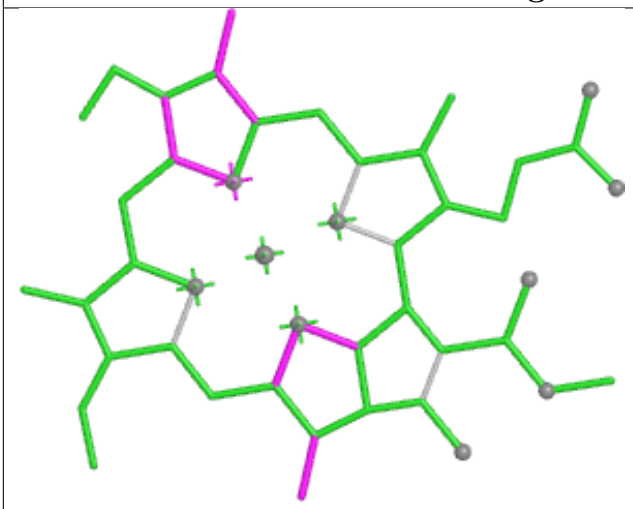


Torsions

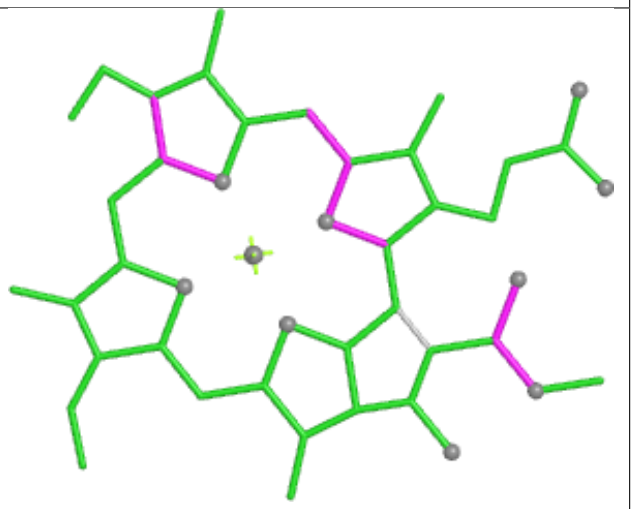


Rings

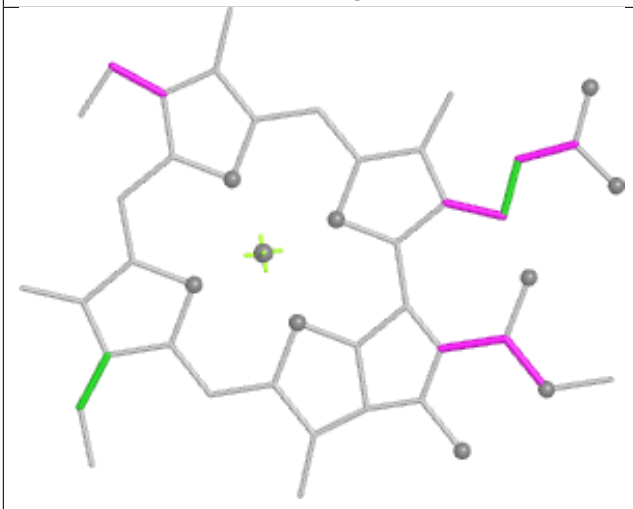
Ligand CLA v 518



Bond lengths



Bond angles

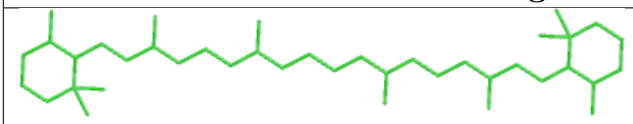


Torsions

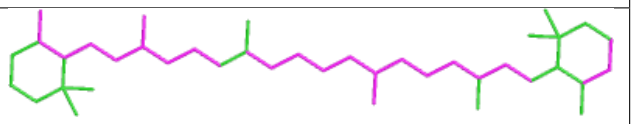


Rings

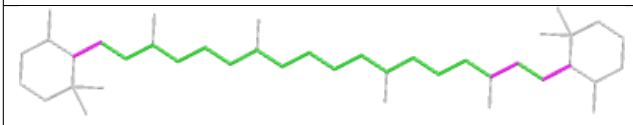
Ligand BCR t 523



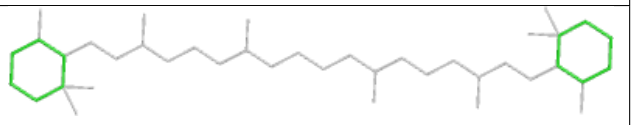
Bond lengths



Bond angles

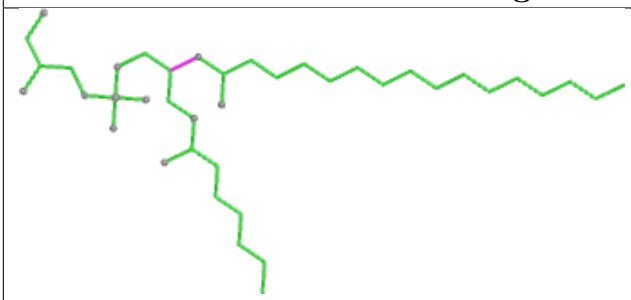


Torsions

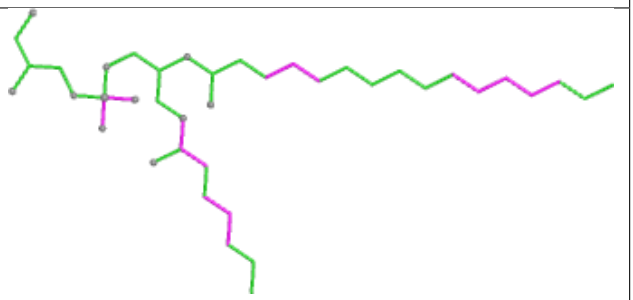


Rings

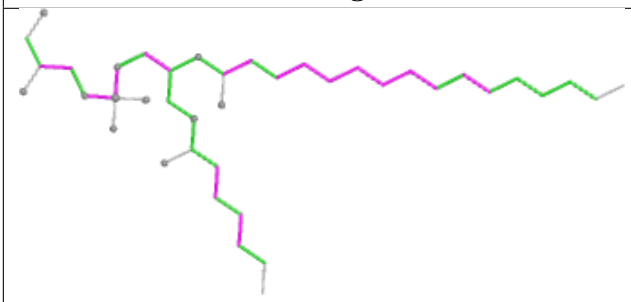
Ligand LHG A 5003



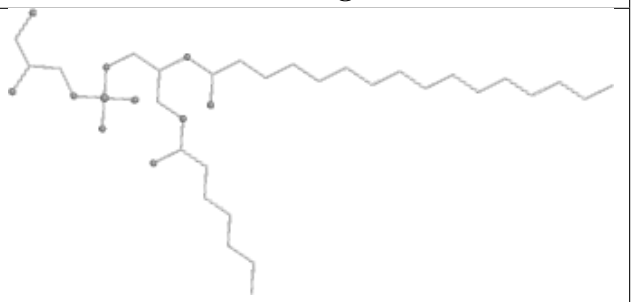
Bond lengths



Bond angles

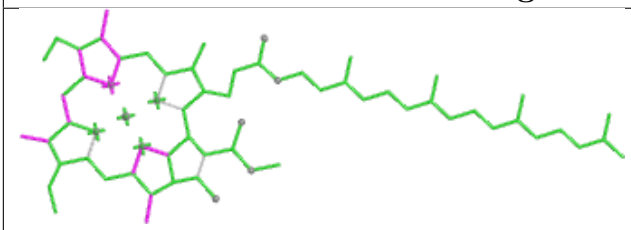


Torsions

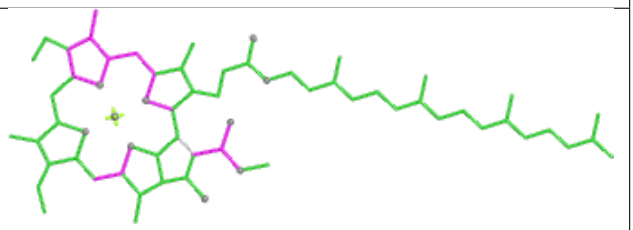


Rings

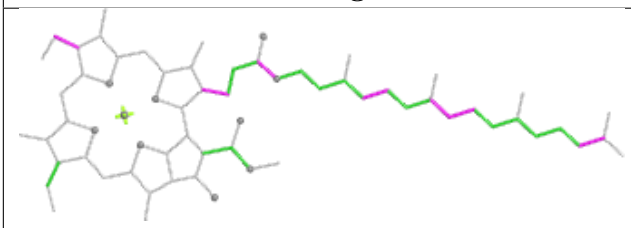
Ligand CLA L 1502



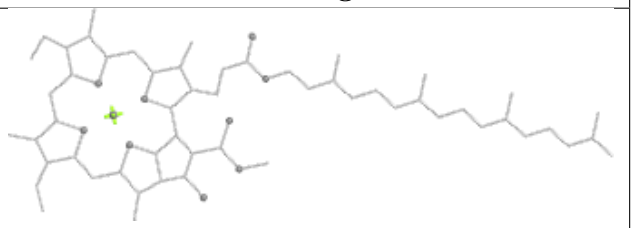
Bond lengths



Bond angles

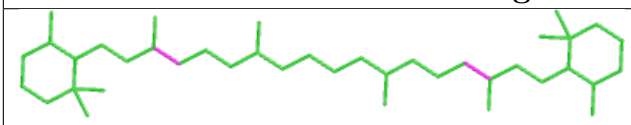


Torsions

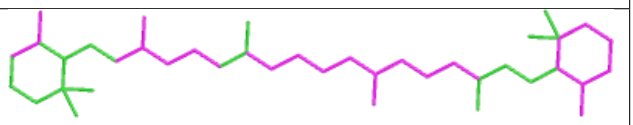


Rings

Ligand BCR V 4020



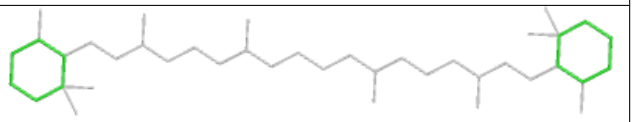
Bond lengths



Bond angles

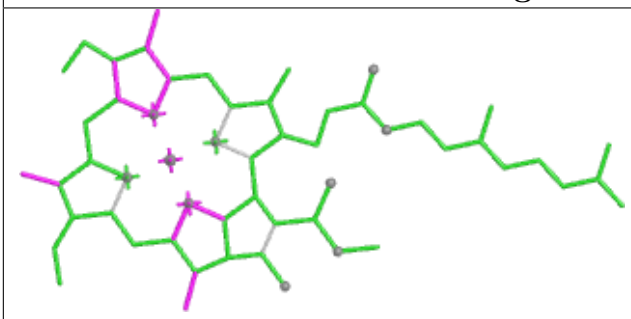


Torsions

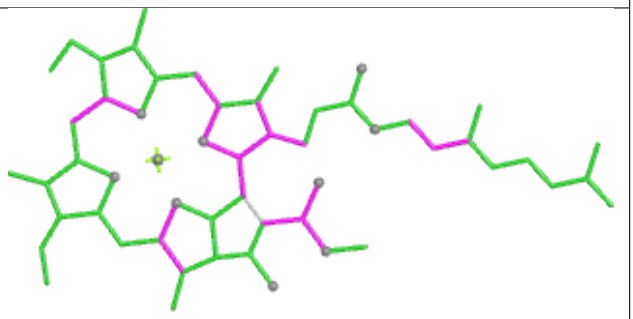


Rings

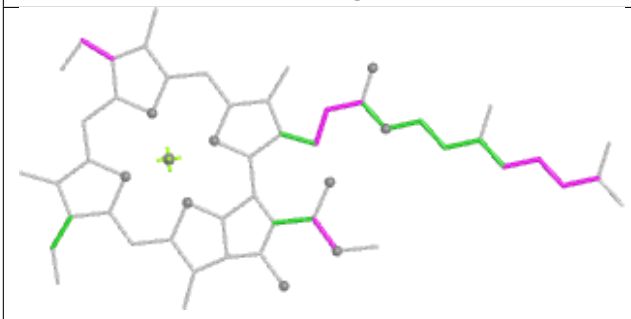
Ligand CLA G 1121



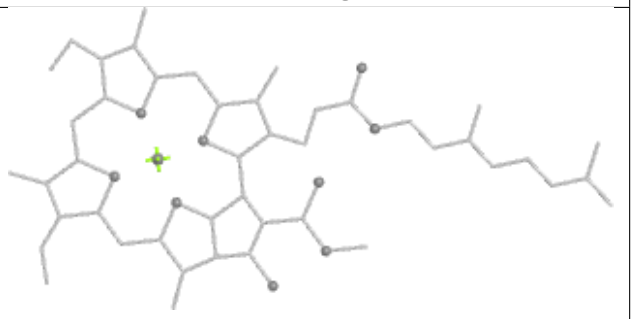
Bond lengths



Bond angles

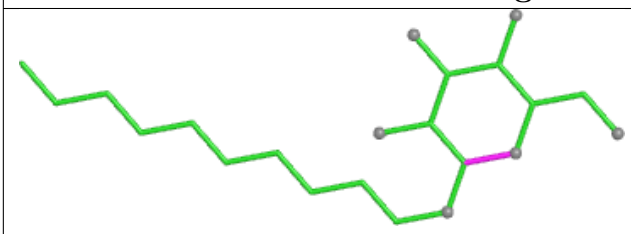


Torsions

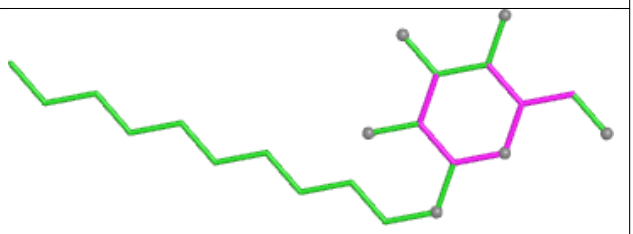


Rings

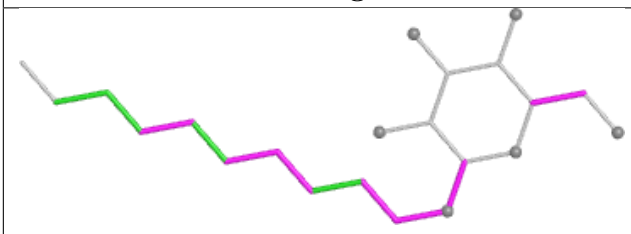
Ligand LMU J 5105



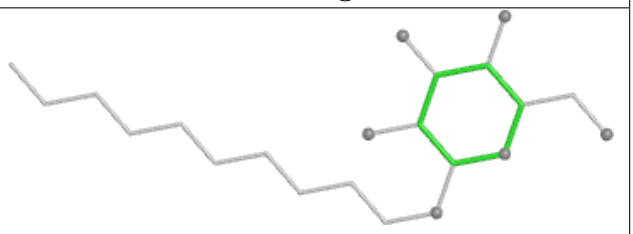
Bond lengths



Bond angles

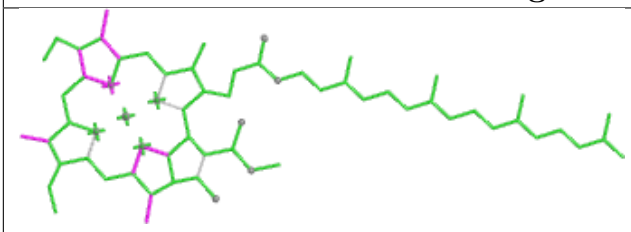


Torsions

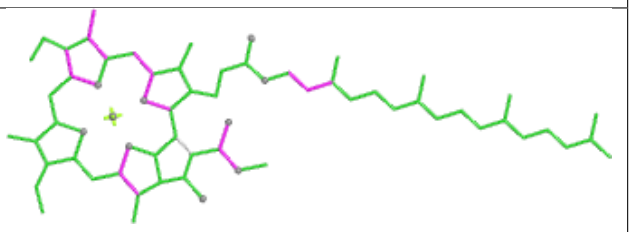


Rings

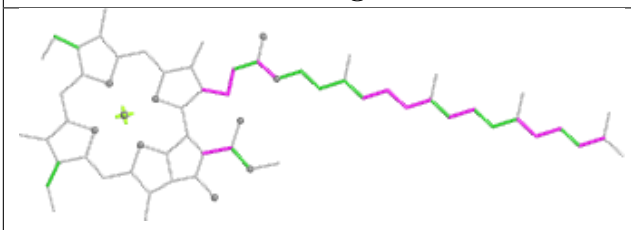
Ligand CLA 2 505



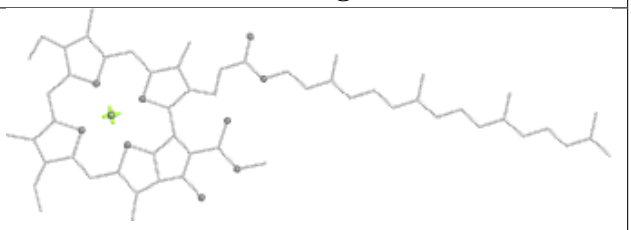
Bond lengths



Bond angles

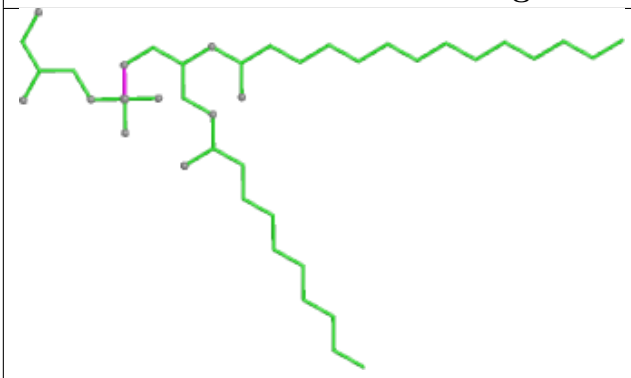


Torsions

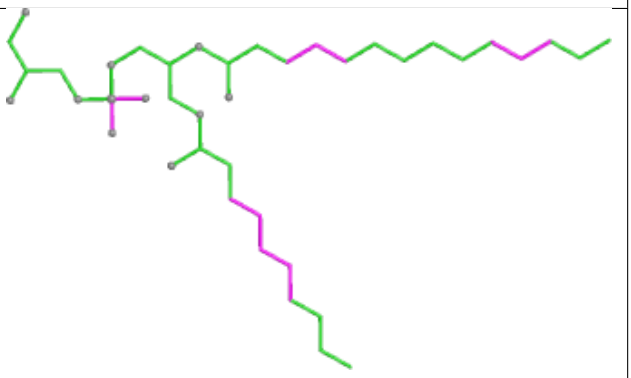


Rings

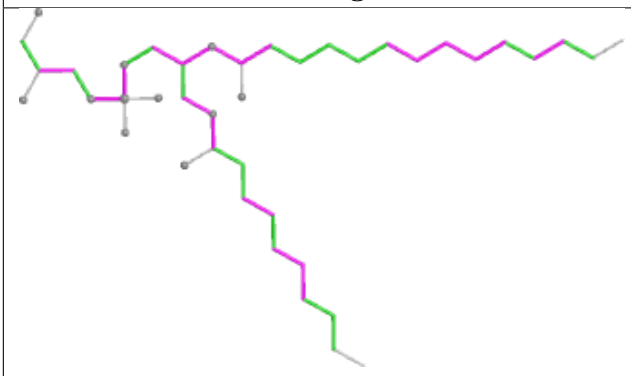
Ligand LHG H 1855



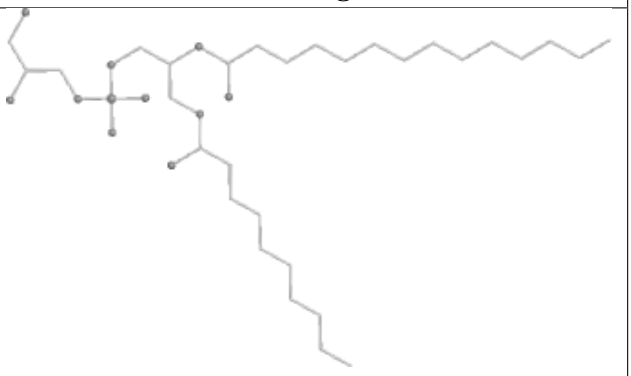
Bond lengths



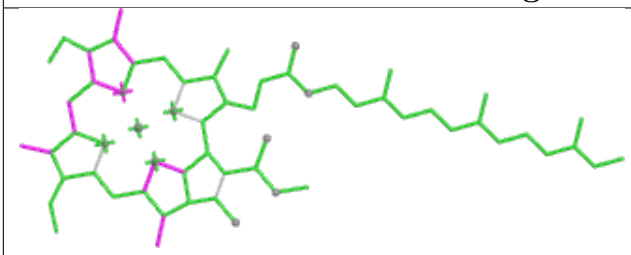
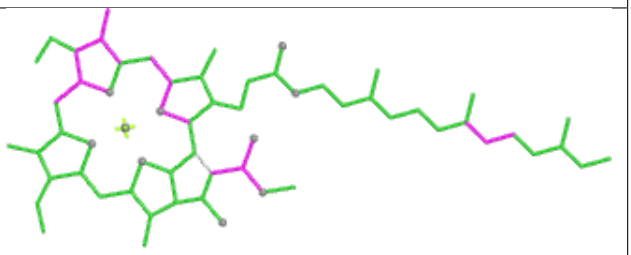
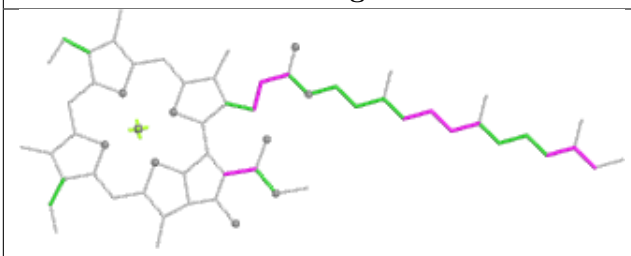
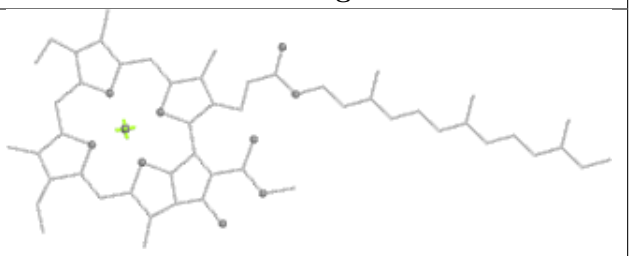
Bond angles

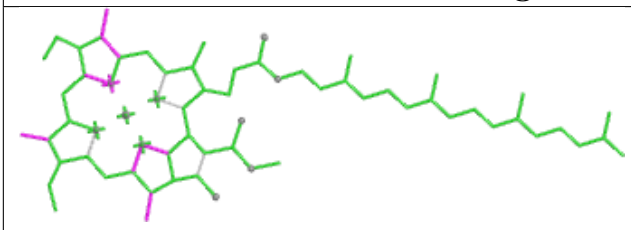
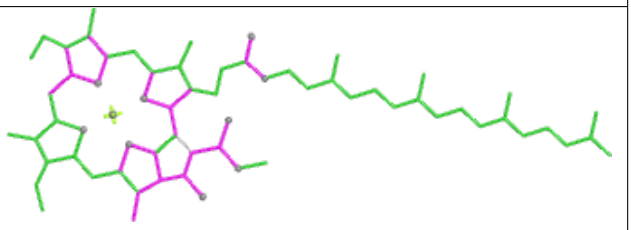
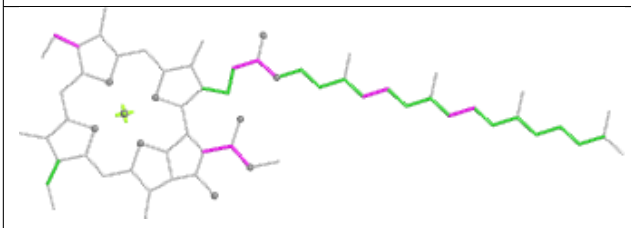
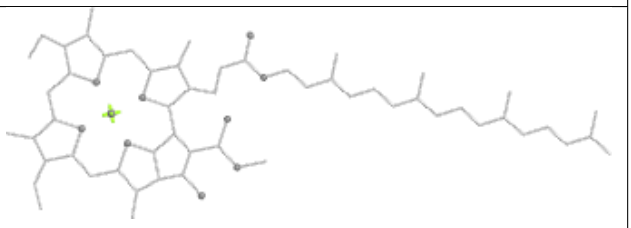


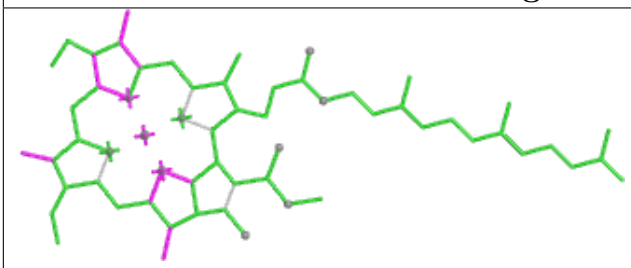
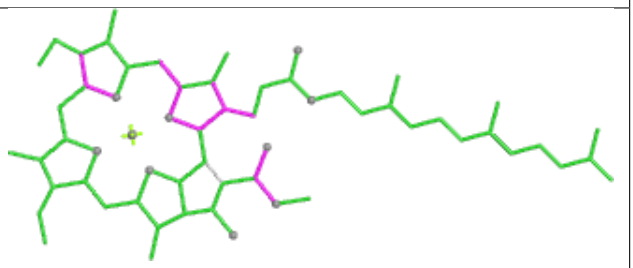
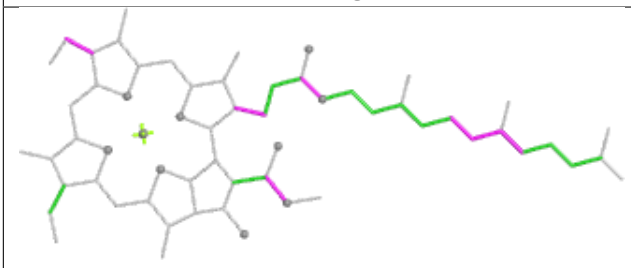
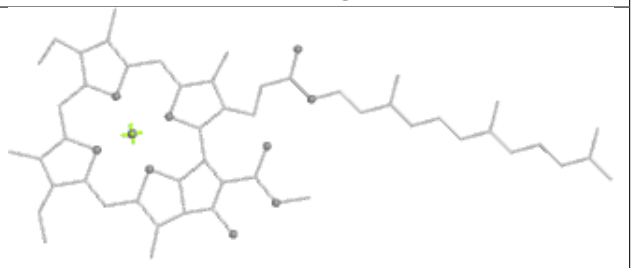
Torsions

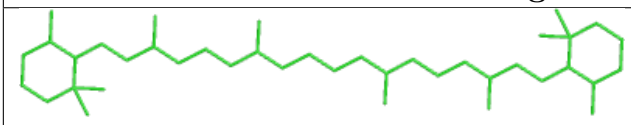
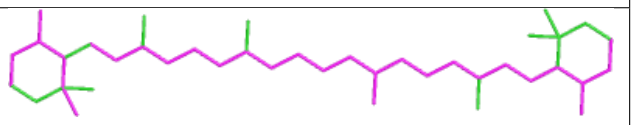
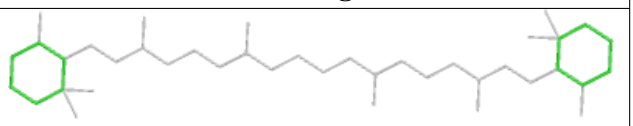


Rings

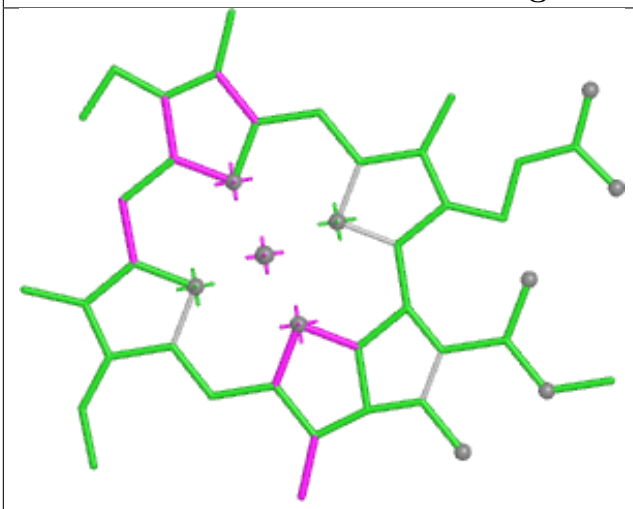
Ligand CLA f 1213	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1011	
 Bond lengths	 Bond angles
 Torsions	 Rings

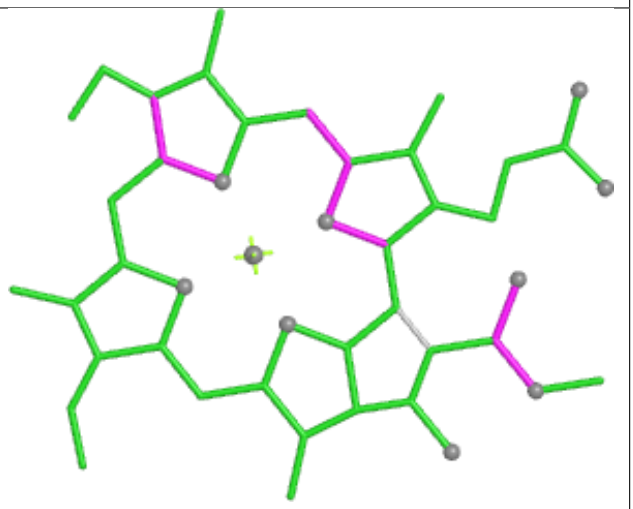
Ligand CLA f 1230	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR s 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

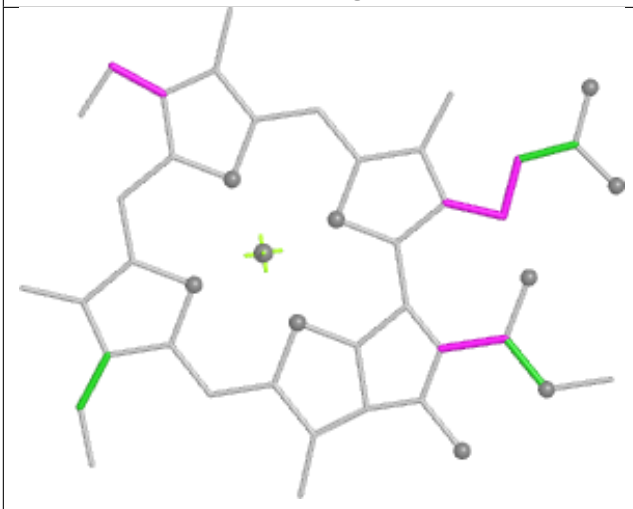
Ligand CLA c 505



Bond lengths



Bond angles

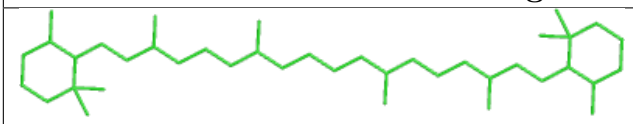


Torsions

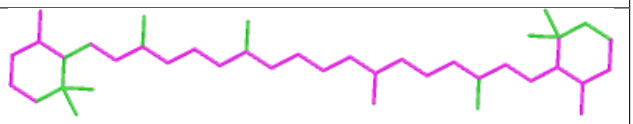


Rings

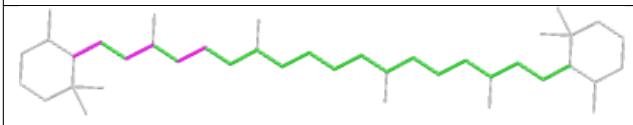
Ligand BCR v 522



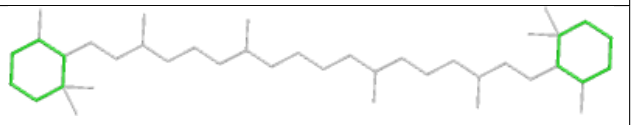
Bond lengths



Bond angles

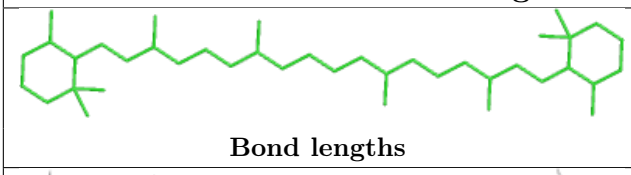


Torsions

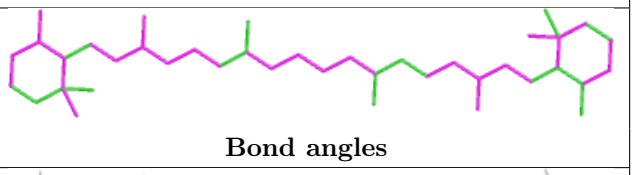


Rings

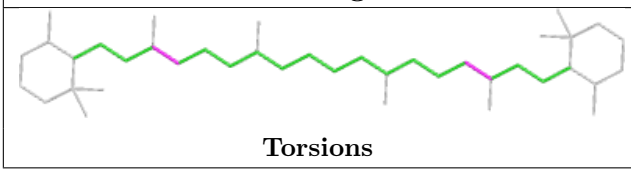
Ligand BCR H 4006



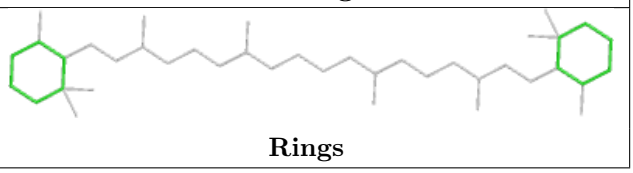
Bond lengths



Bond angles

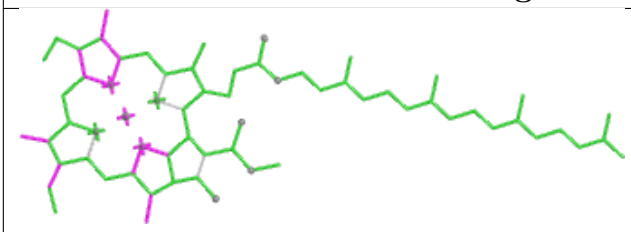


Torsions

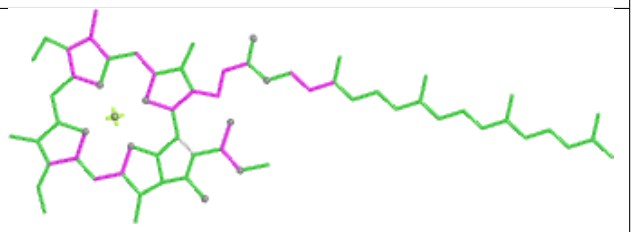


Rings

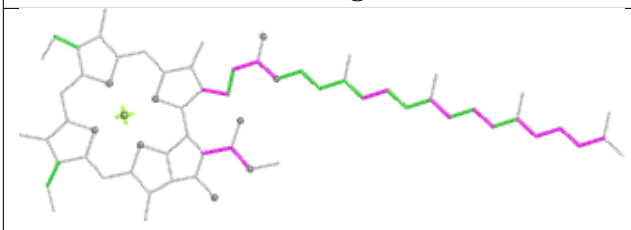
Ligand CLA A 1103



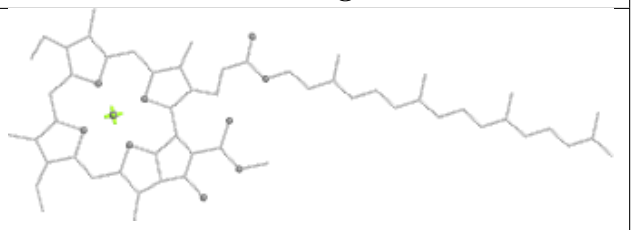
Bond lengths



Bond angles

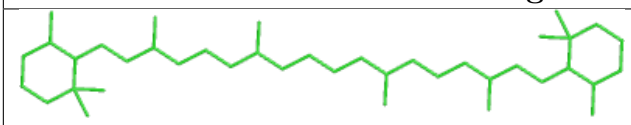


Torsions

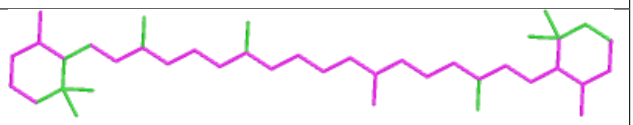


Rings

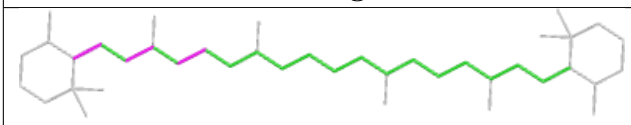
Ligand BCR 6 522



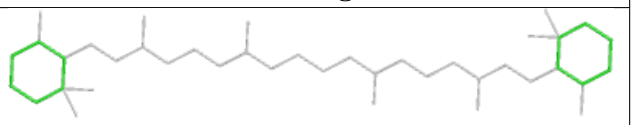
Bond lengths



Bond angles

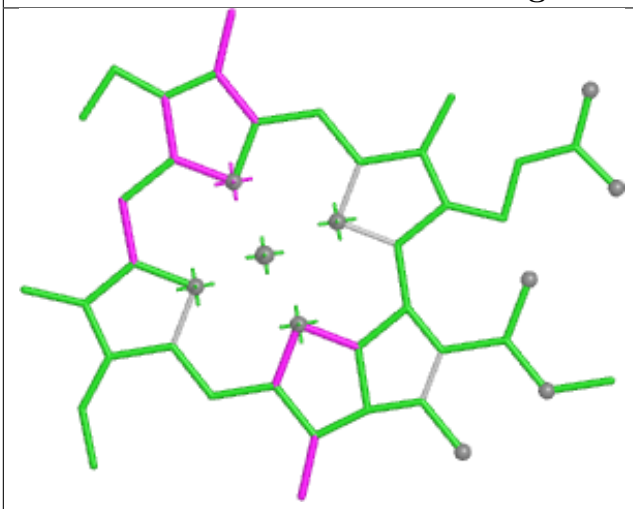


Torsions

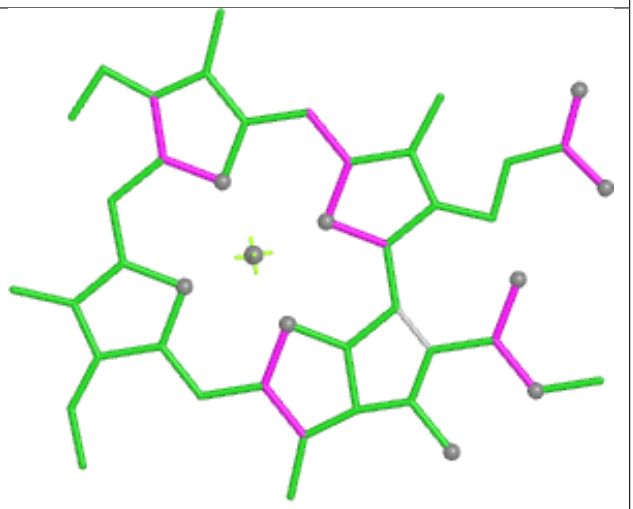


Rings

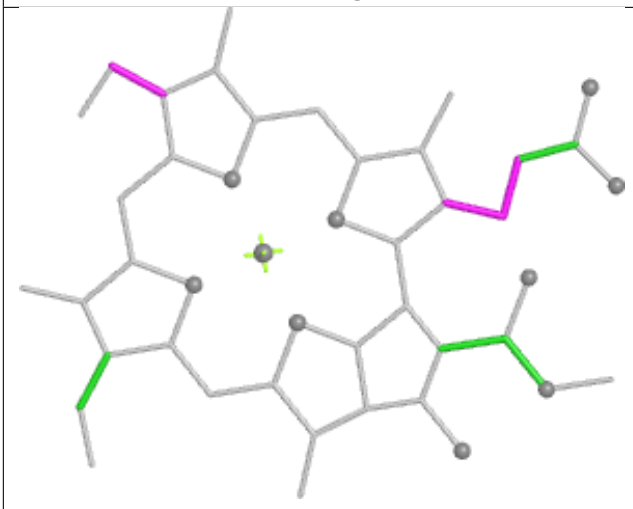
Ligand CLA 5 518



Bond lengths



Bond angles

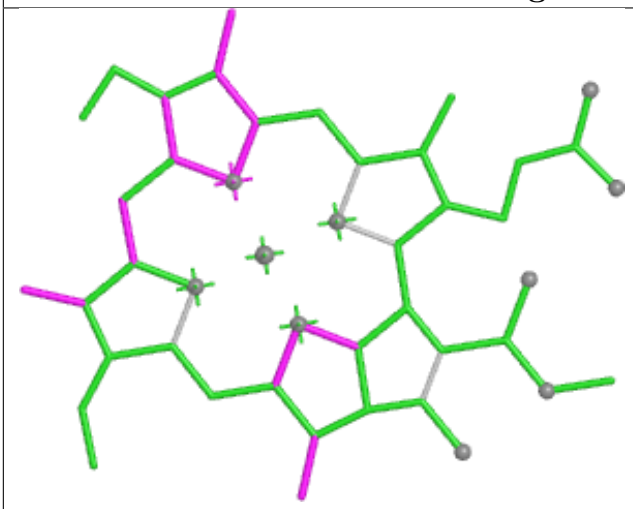


Torsions

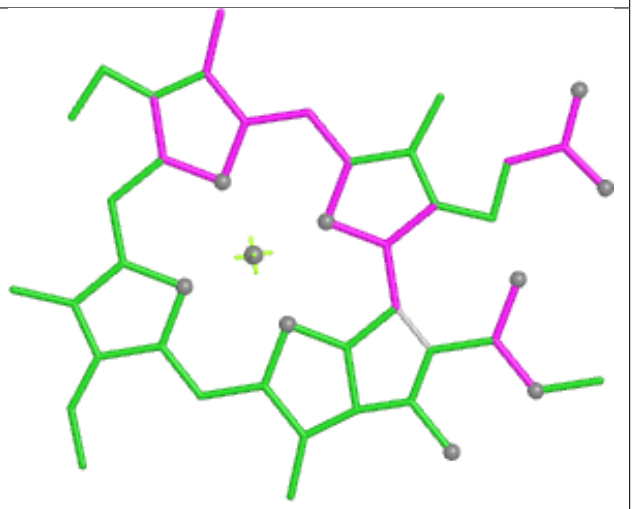


Rings

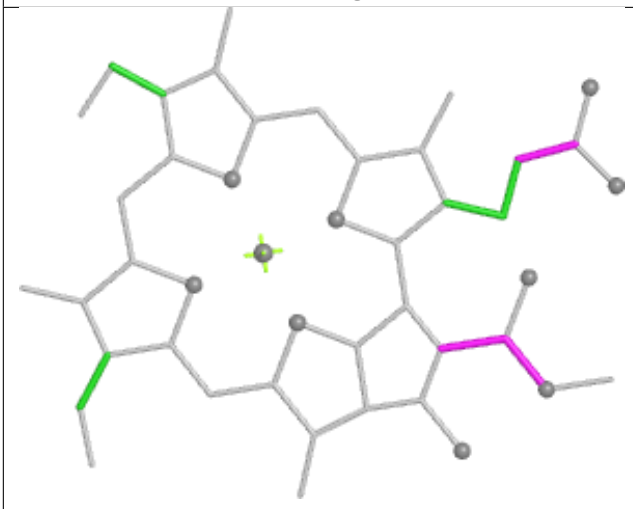
Ligand CLA 4 509



Bond lengths



Bond angles

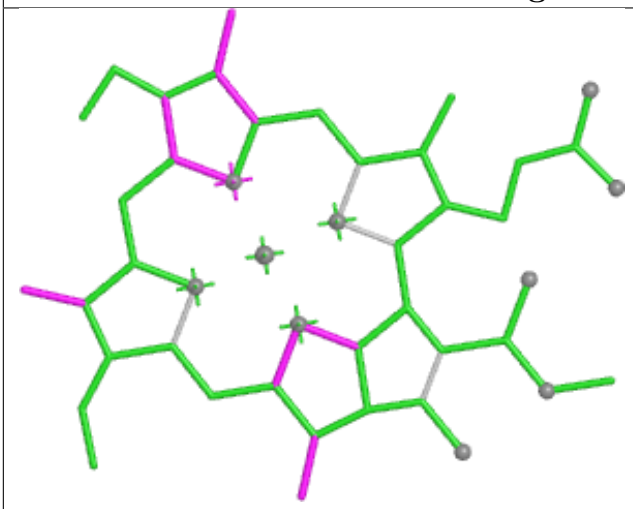


Torsions

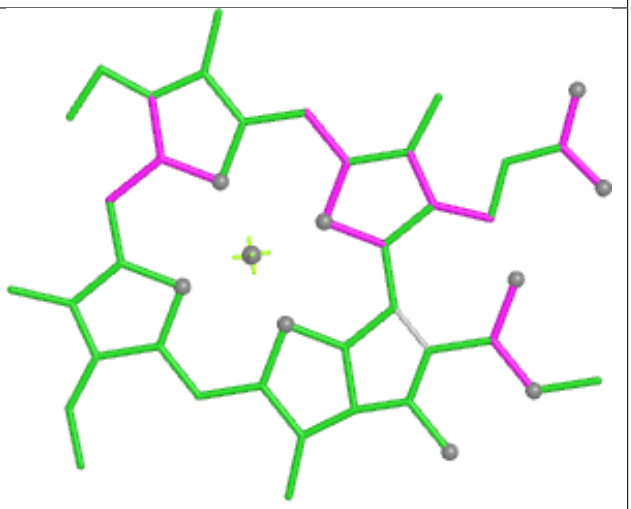


Rings

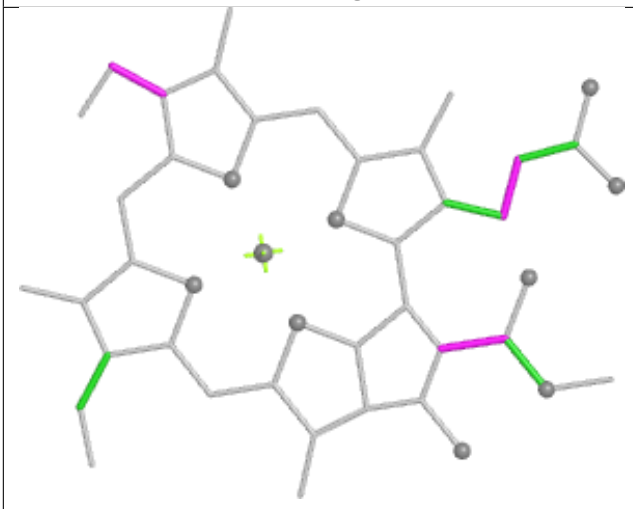
Ligand CLA 1 502



Bond lengths



Bond angles

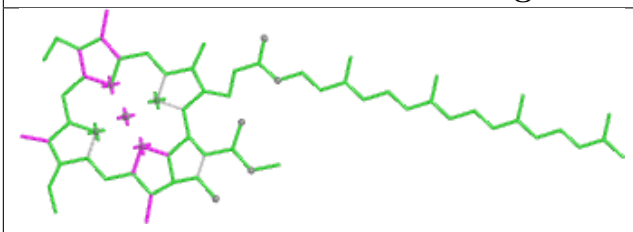


Torsions

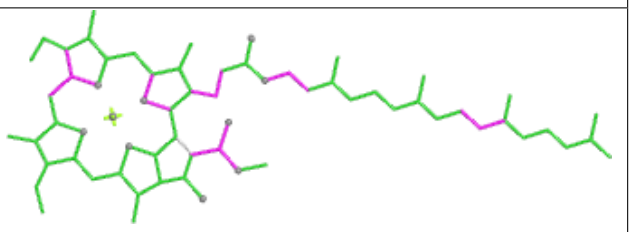


Rings

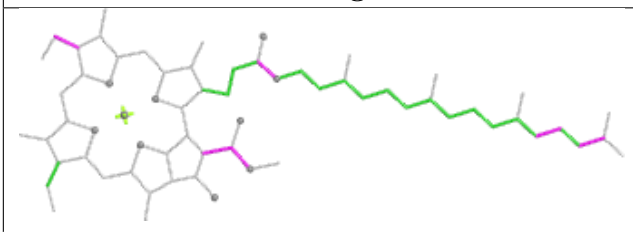
Ligand CLA H 1021



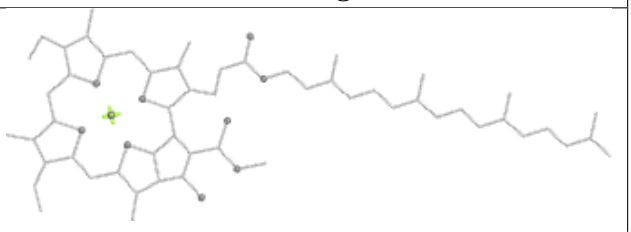
Bond lengths



Bond angles

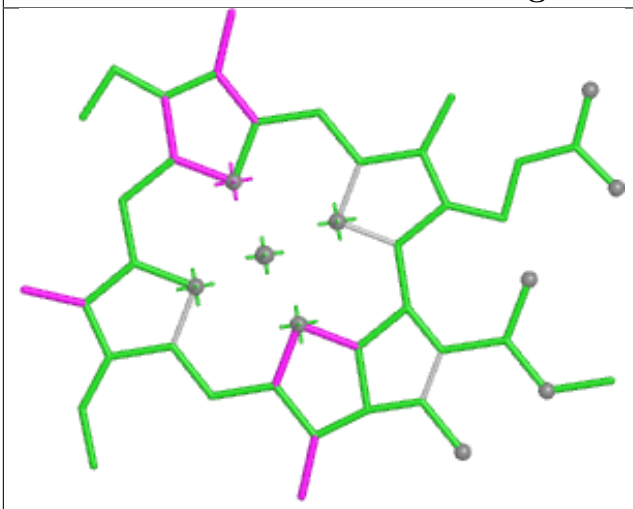


Torsions

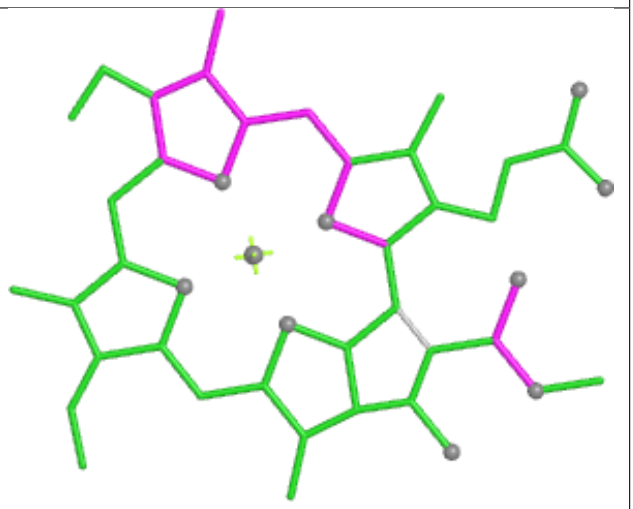


Rings

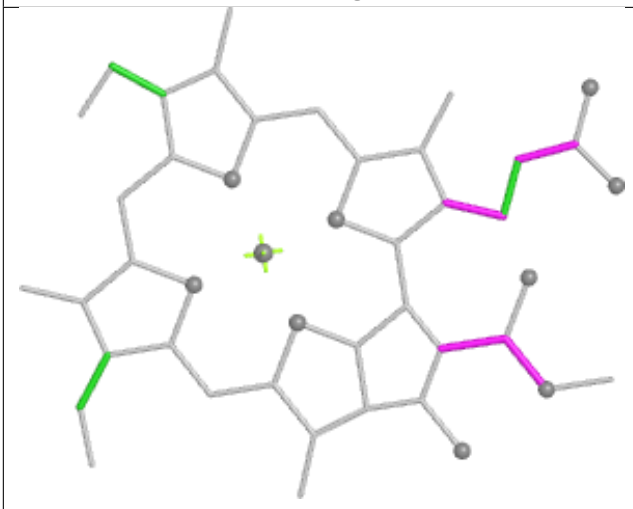
Ligand CLA a 506



Bond lengths



Bond angles

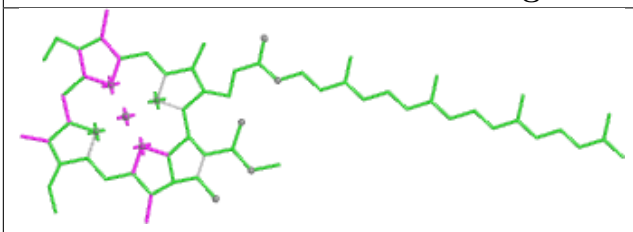


Torsions

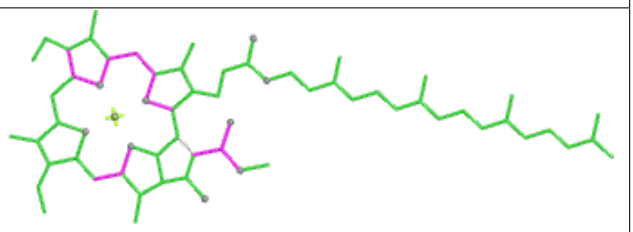


Rings

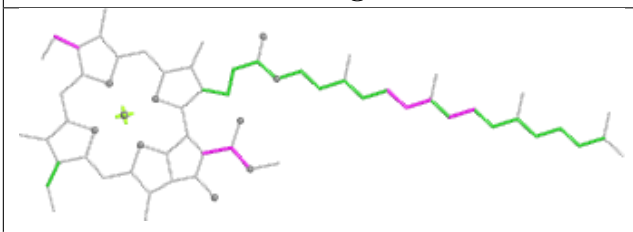
Ligand CLA f 1235



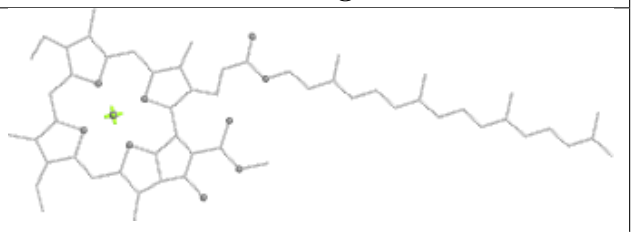
Bond lengths



Bond angles

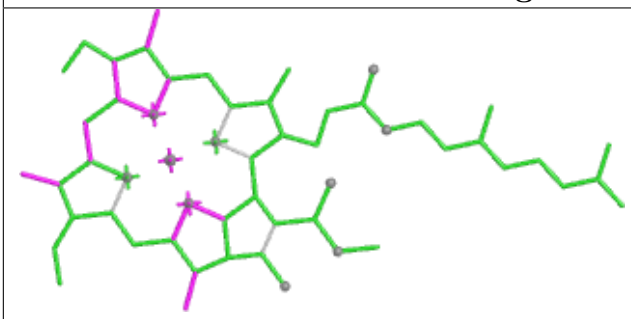


Torsions

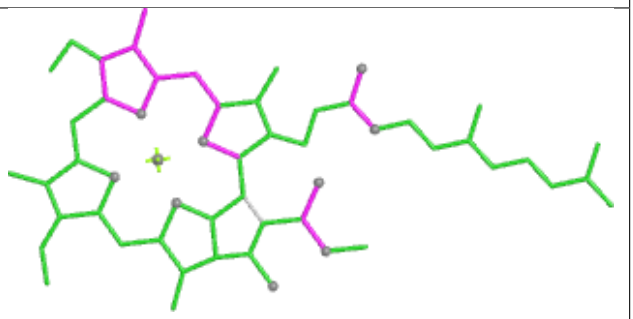


Rings

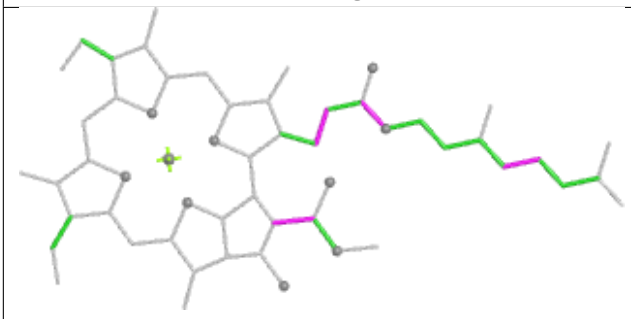
Ligand CLA B 1232



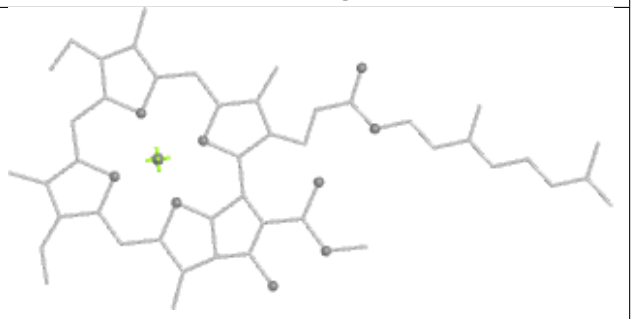
Bond lengths



Bond angles

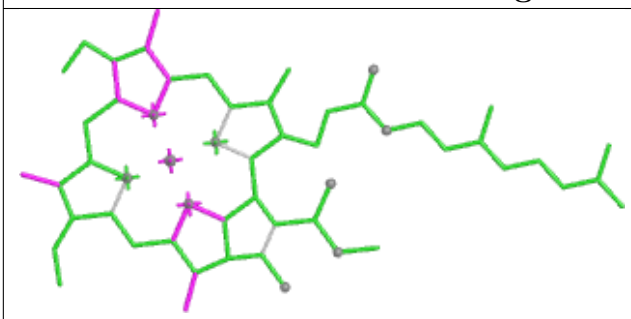


Torsions

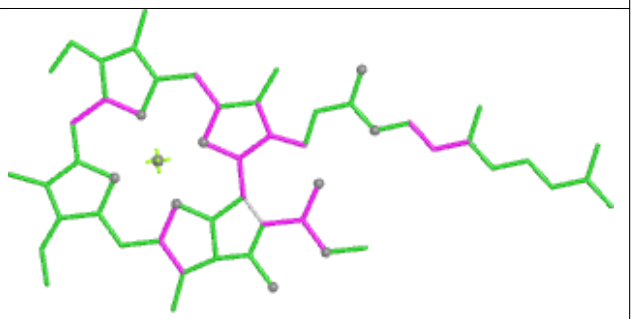


Rings

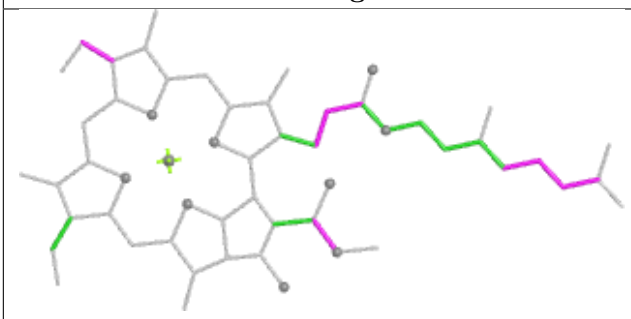
Ligand CLA A 1121



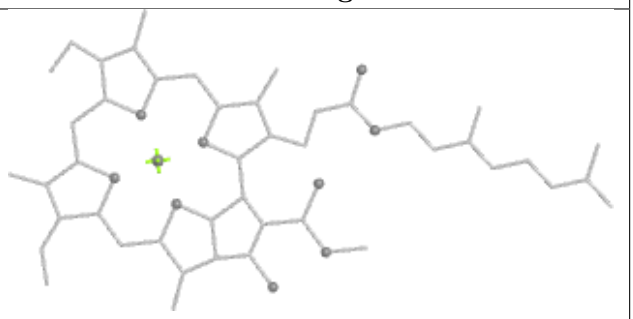
Bond lengths



Bond angles

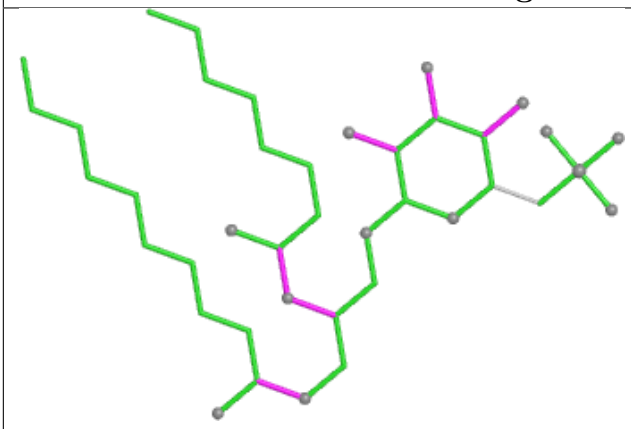


Torsions

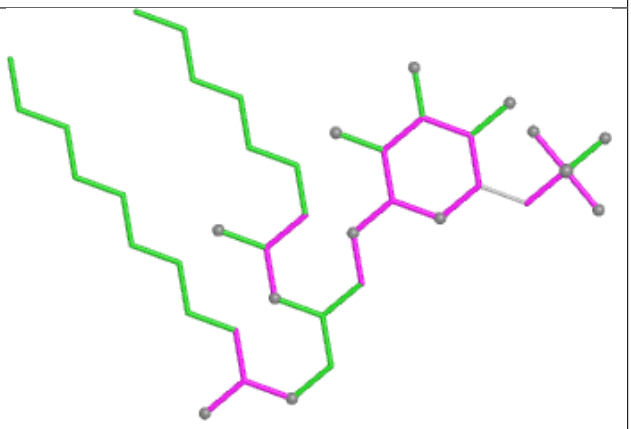


Rings

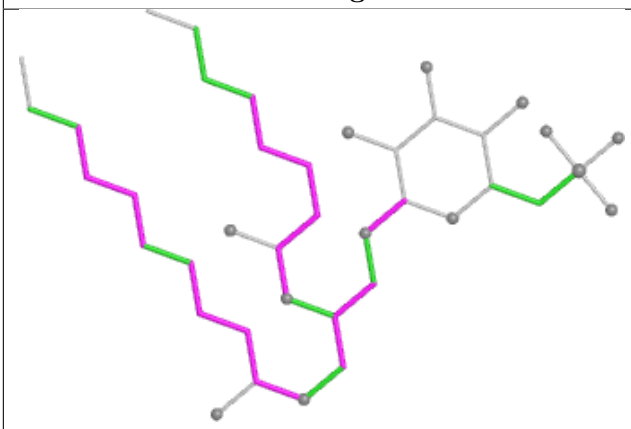
Ligand SQD B 1852



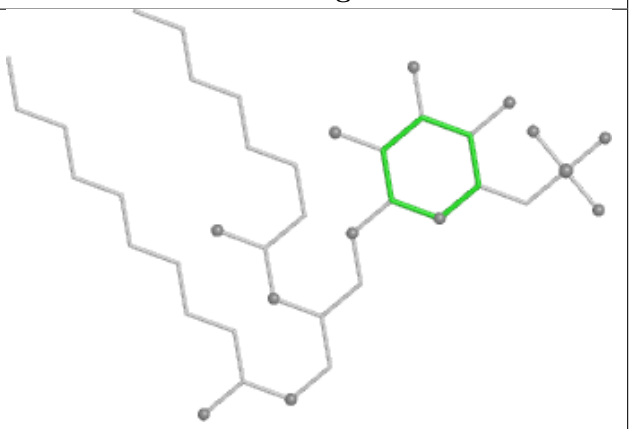
Bond lengths



Bond angles

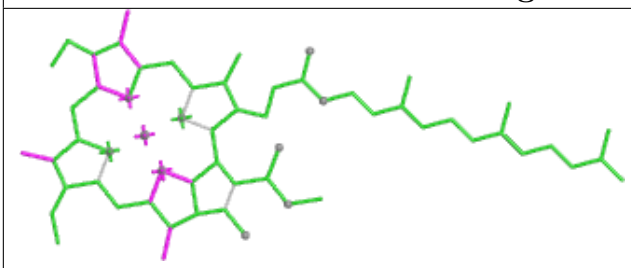


Torsions

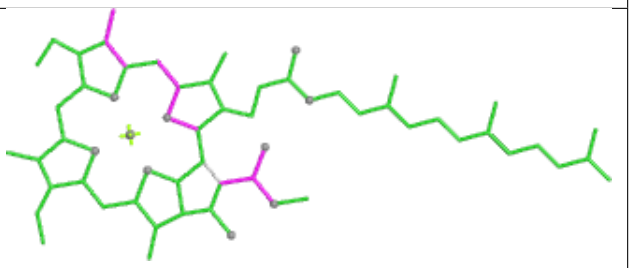


Rings

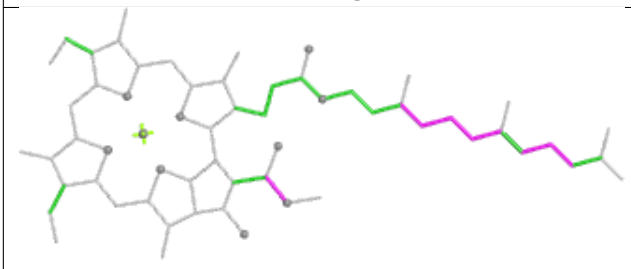
Ligand CLA L 1503



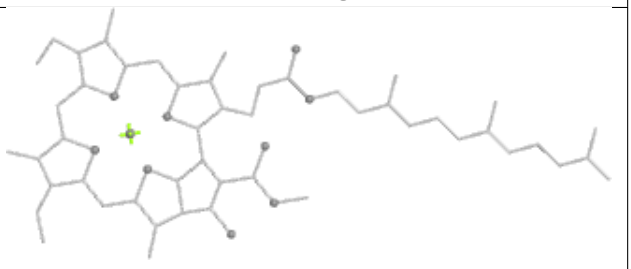
Bond lengths



Bond angles

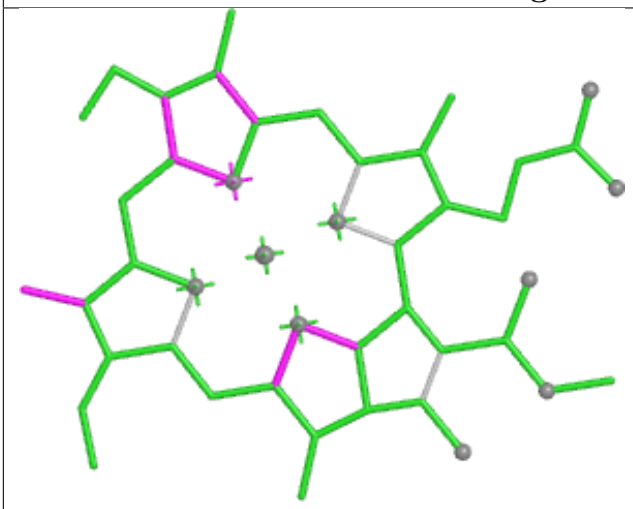


Torsions

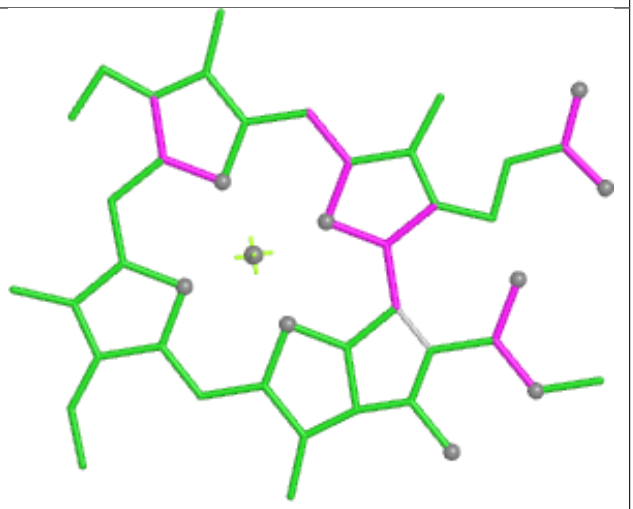


Rings

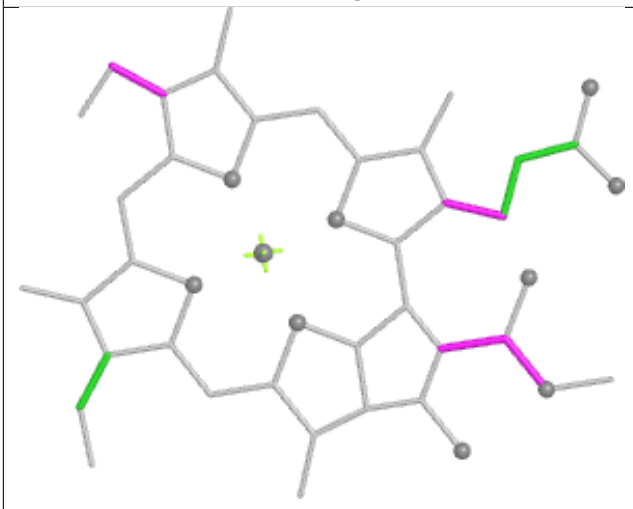
Ligand CLA t 517



Bond lengths



Bond angles

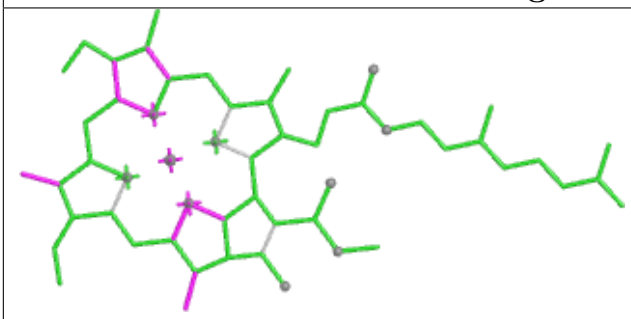


Torsions

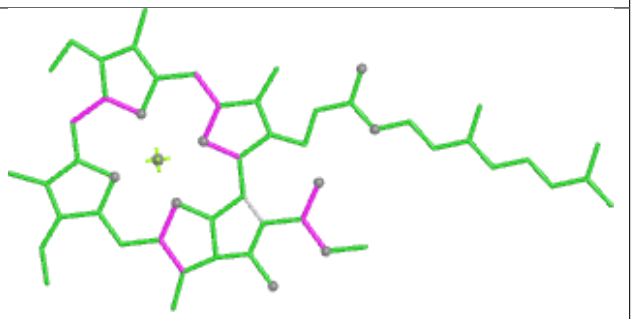


Rings

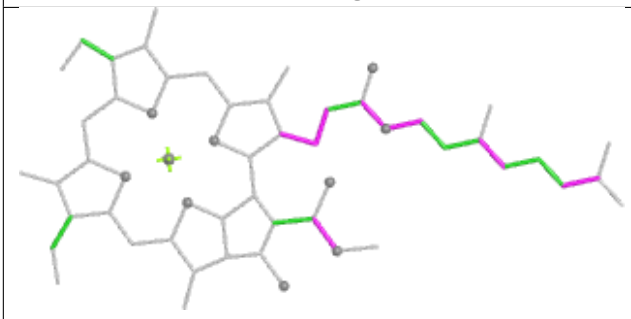
Ligand CLA a 505



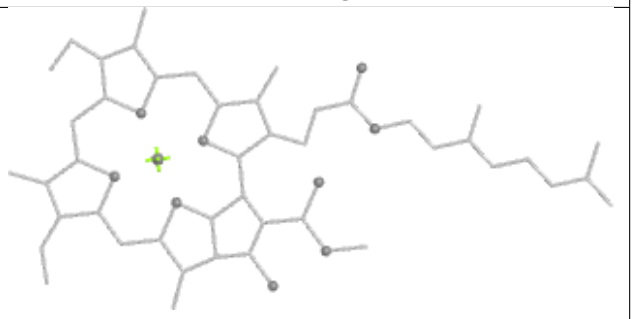
Bond lengths



Bond angles

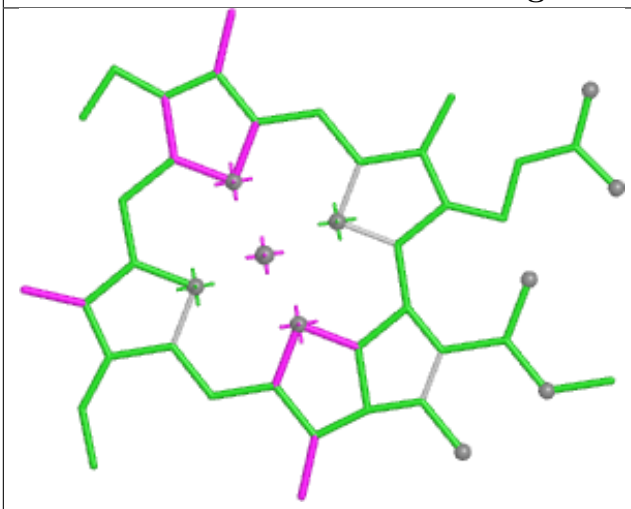


Torsions

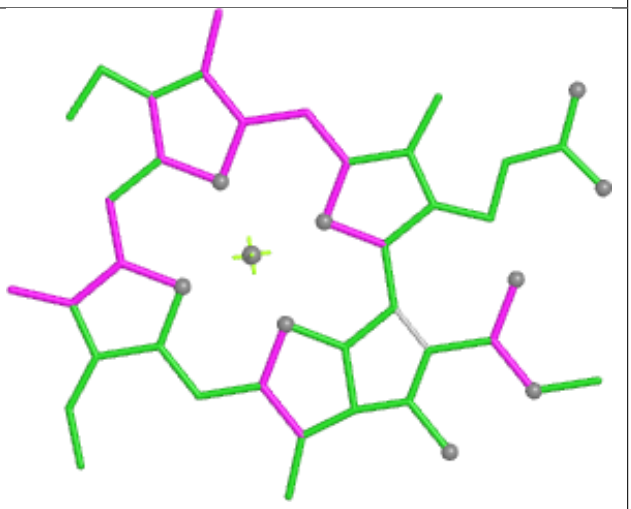


Rings

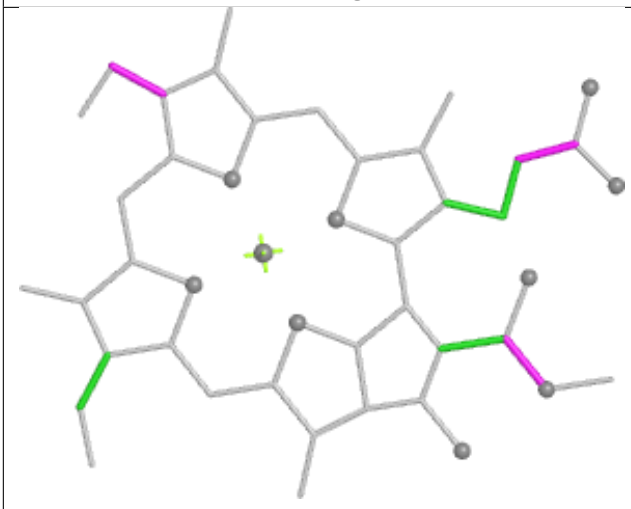
Ligand CLA b 508



Bond lengths



Bond angles

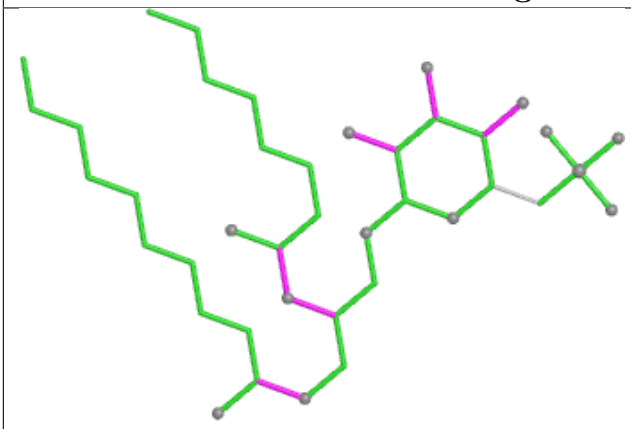


Torsions

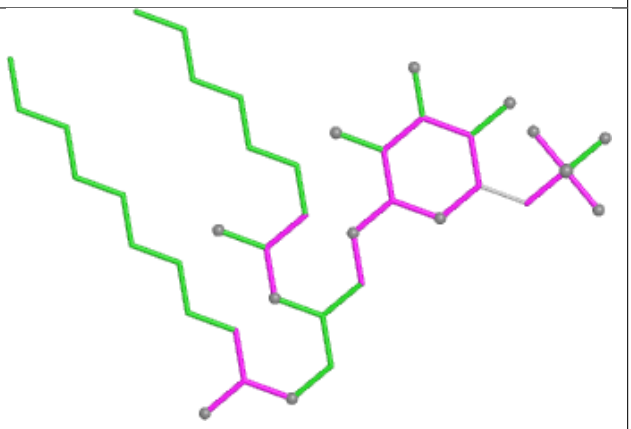


Rings

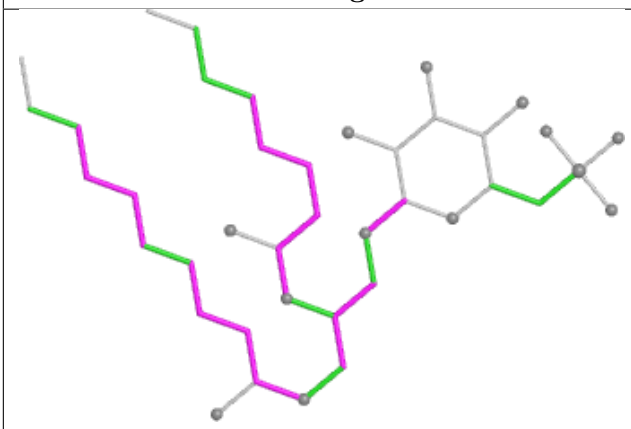
Ligand SQD H 1852



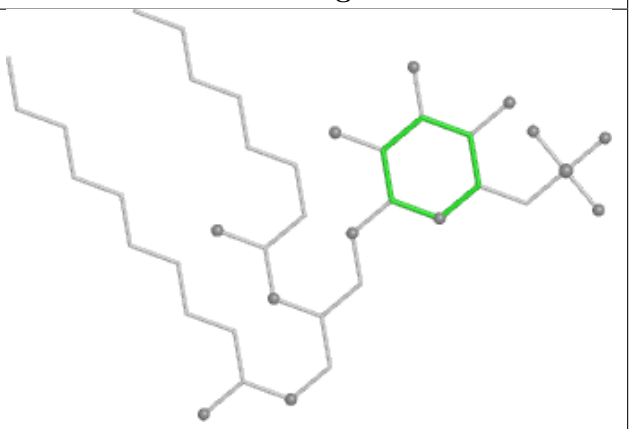
Bond lengths



Bond angles

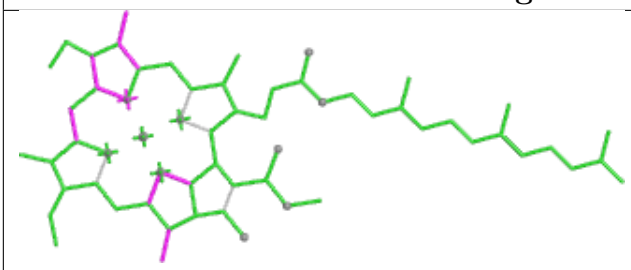


Torsions

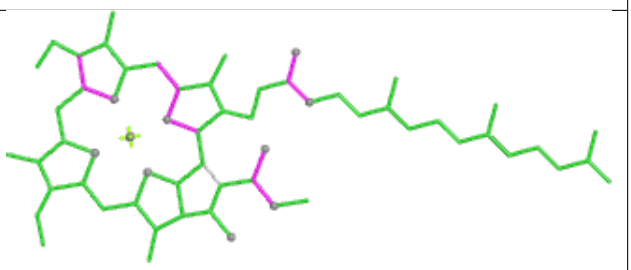


Rings

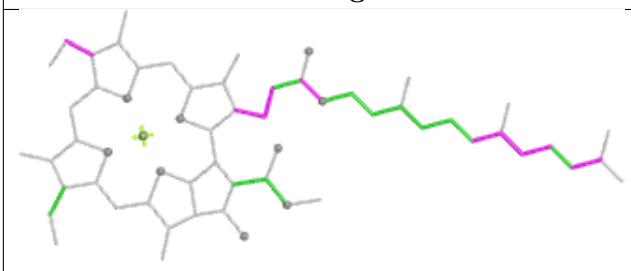
Ligand CLA B 1217



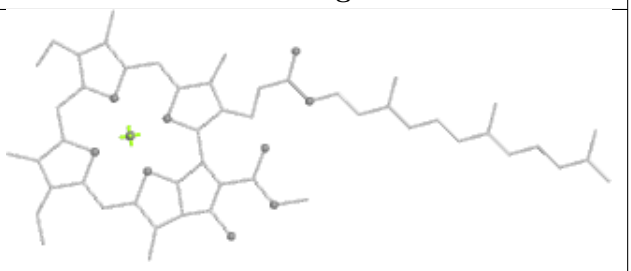
Bond lengths



Bond angles

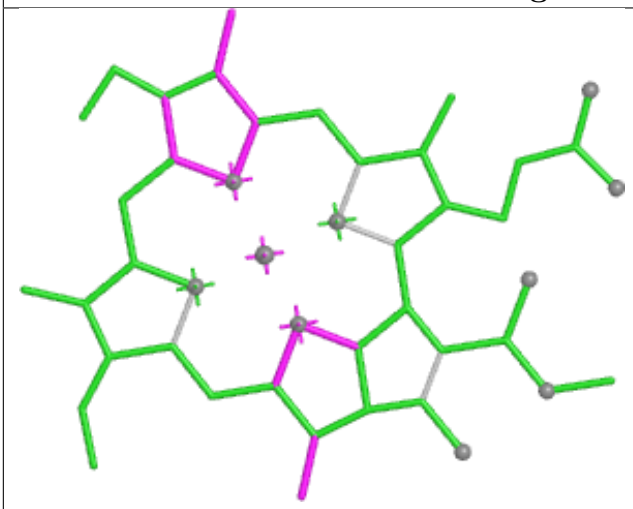


Torsions

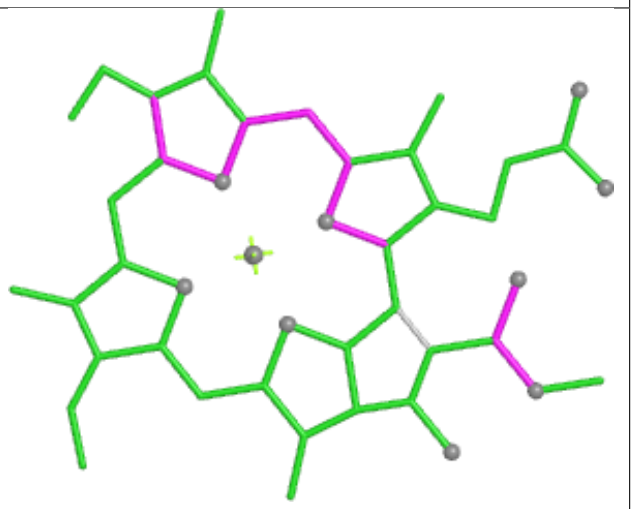


Rings

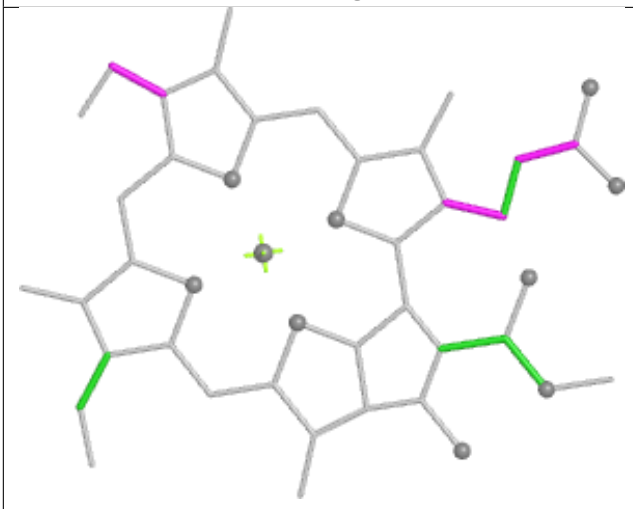
Ligand CLA r 512



Bond lengths



Bond angles

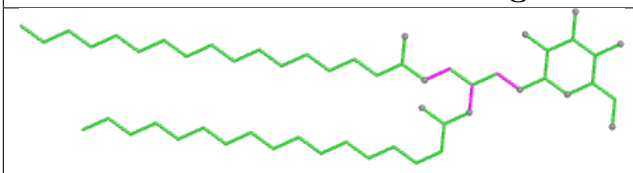


Torsions

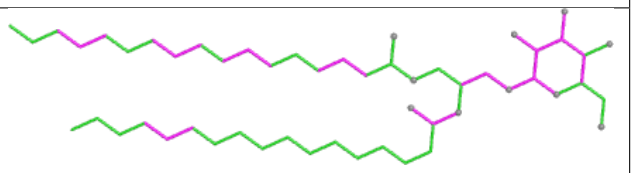


Rings

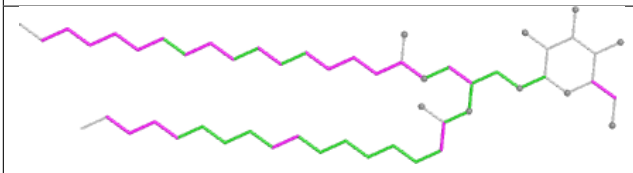
Ligand LMG H 5002



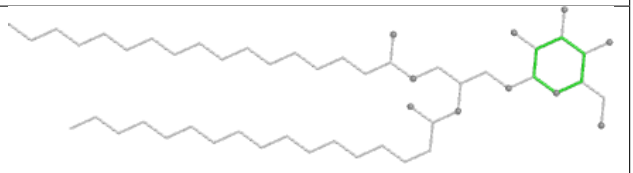
Bond lengths



Bond angles

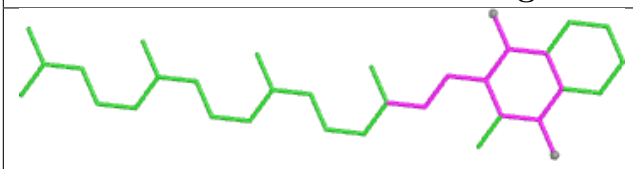


Torsions

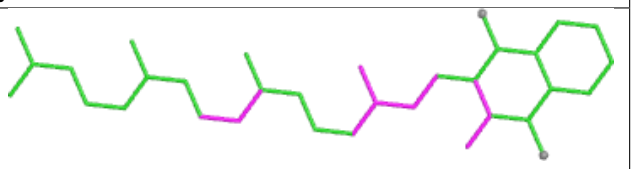


Rings

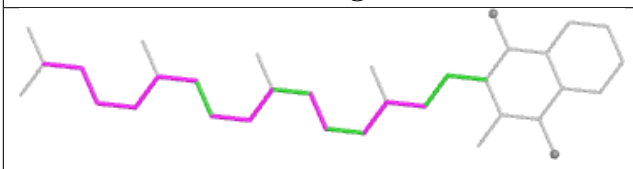
Ligand PQN e 2001



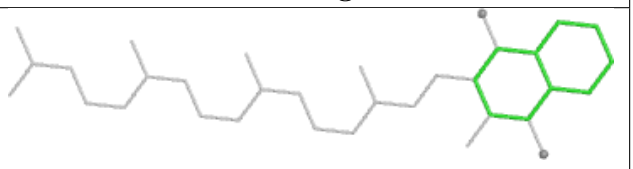
Bond lengths



Bond angles

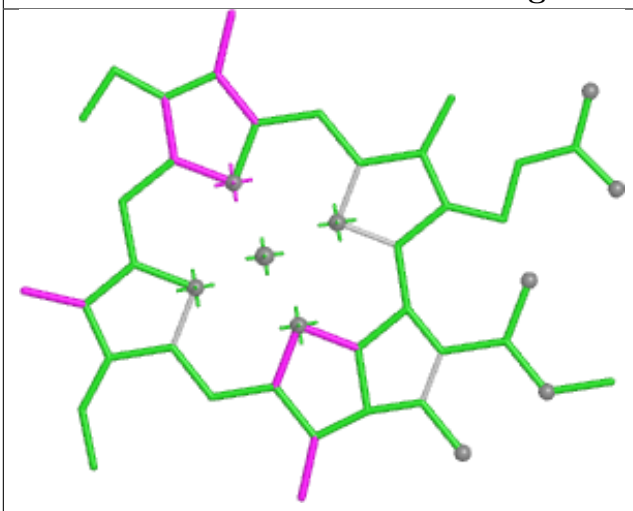


Torsions

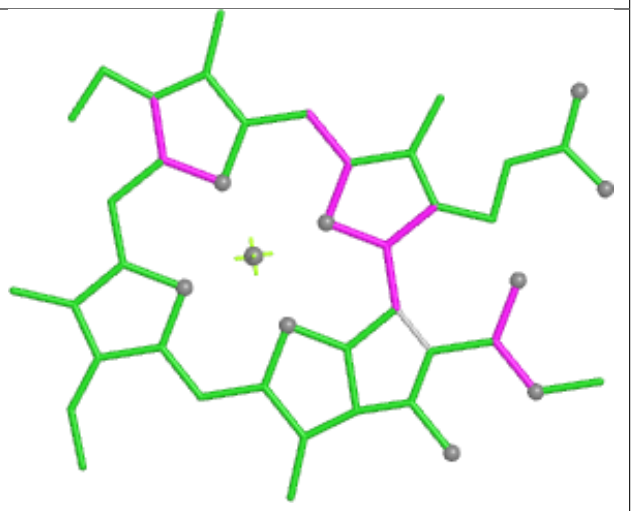


Rings

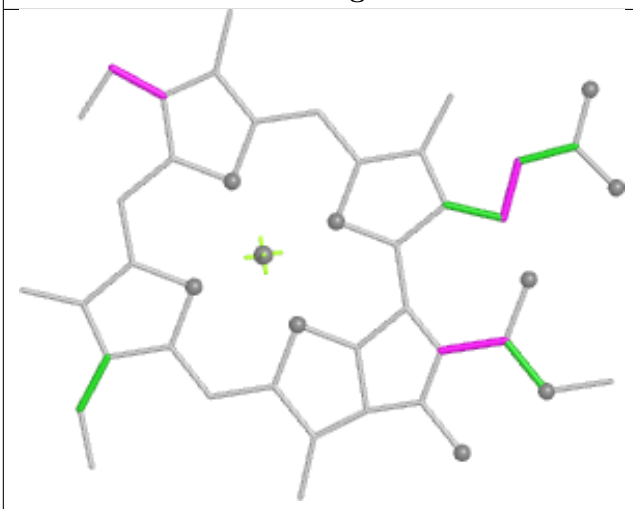
Ligand CLA 4 502



Bond lengths



Bond angles

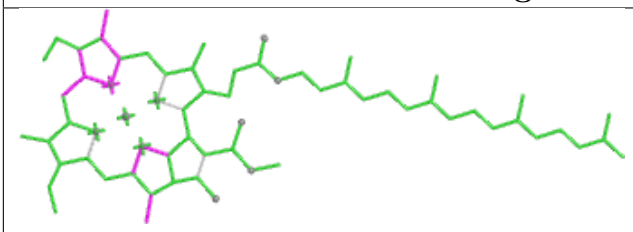


Torsions

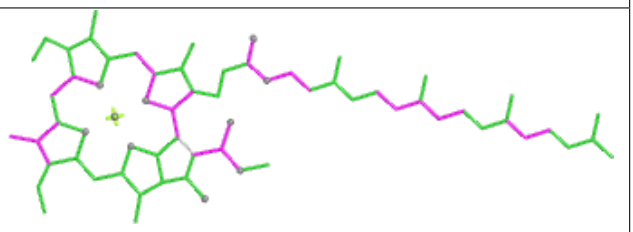


Rings

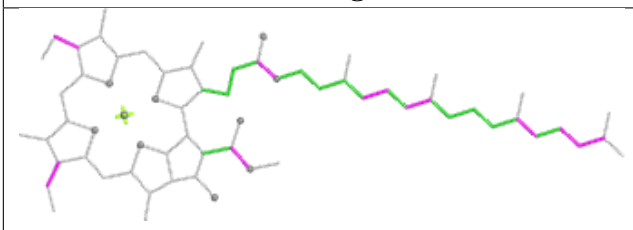
Ligand CLA H 1239



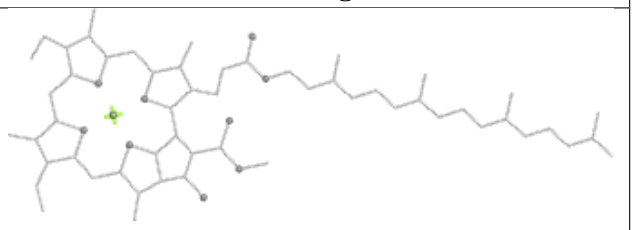
Bond lengths



Bond angles

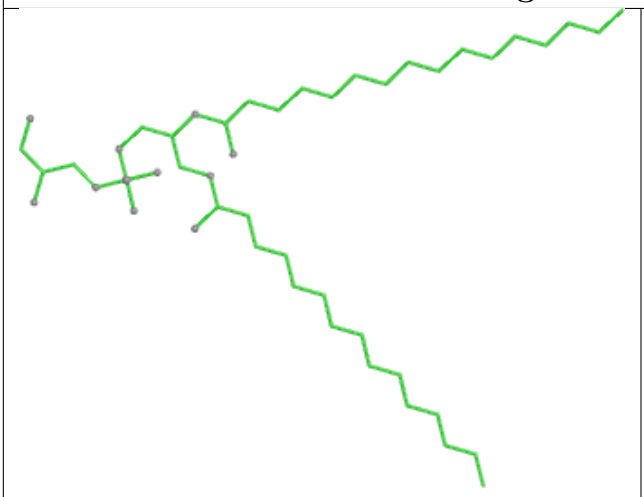


Torsions

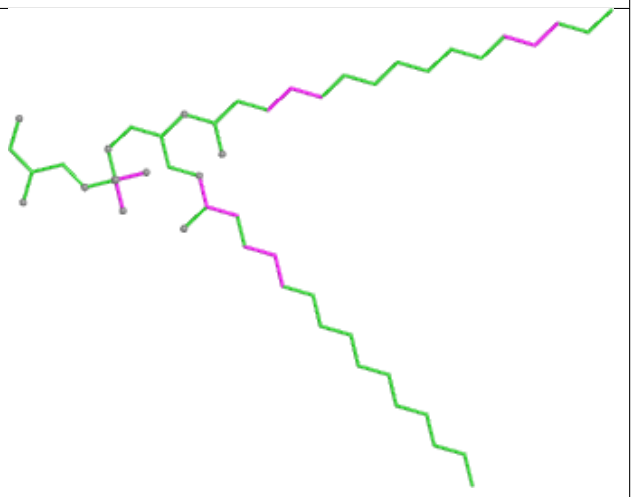


Rings

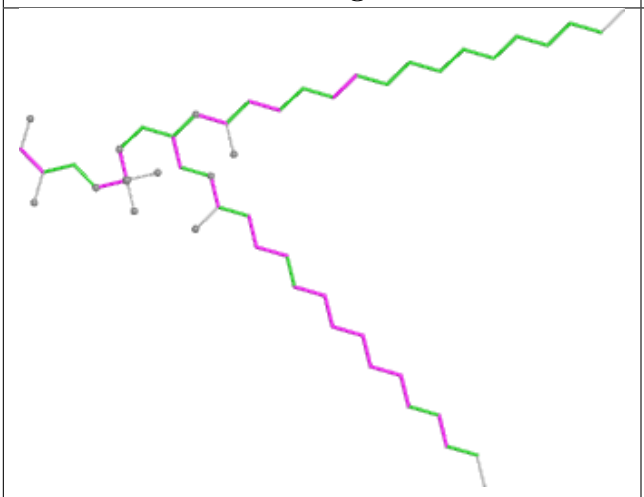
Ligand LHG k 5001



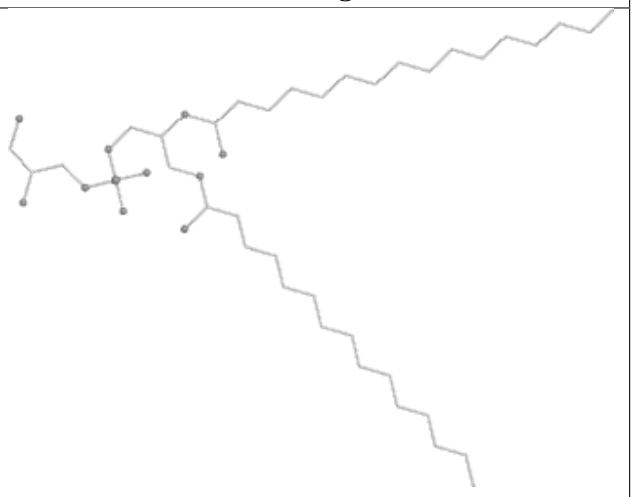
Bond lengths



Bond angles

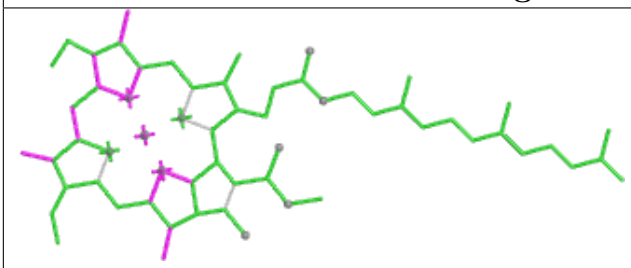


Torsions

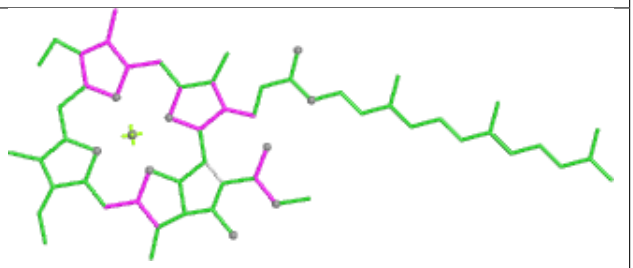


Rings

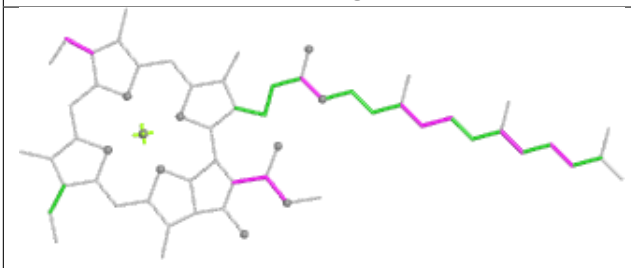
Ligand CLA G 1124



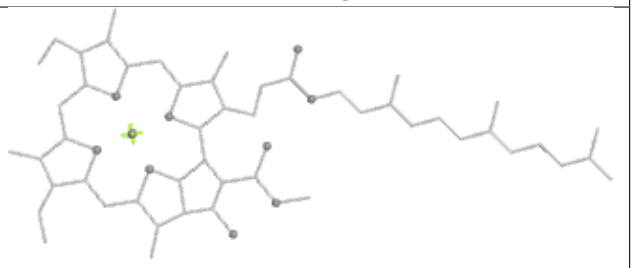
Bond lengths



Bond angles

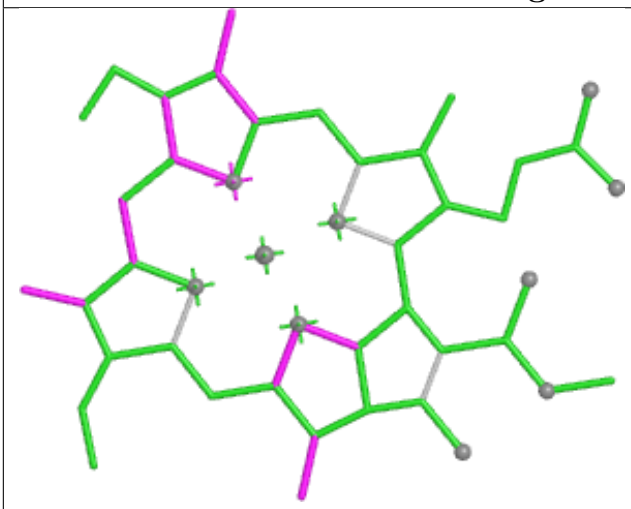


Torsions

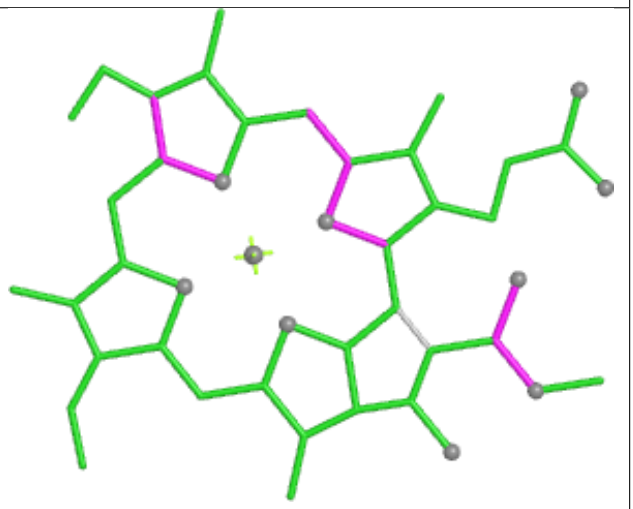


Rings

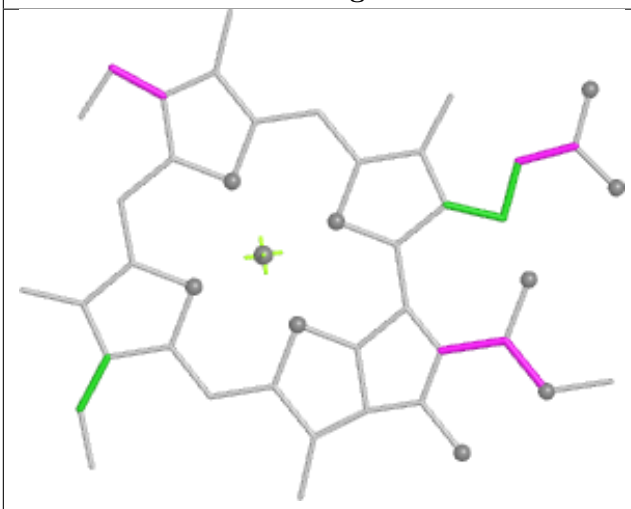
Ligand CLA 6 510



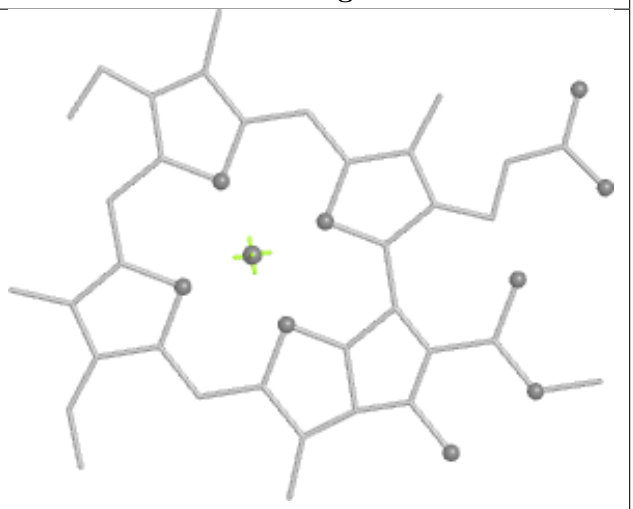
Bond lengths



Bond angles

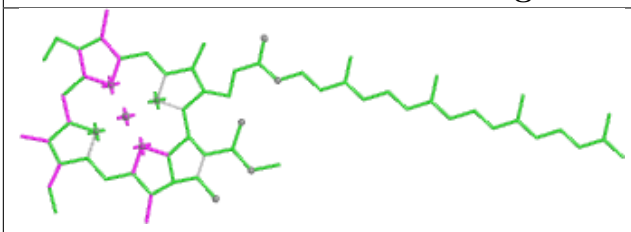


Torsions

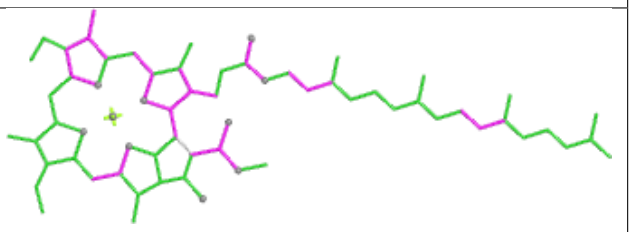


Rings

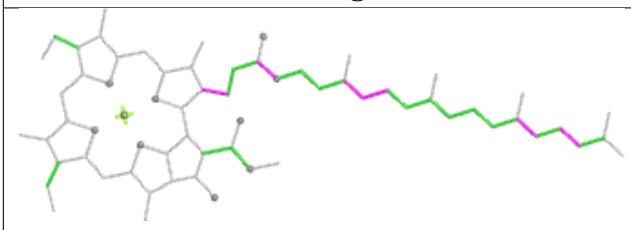
Ligand CLA A 1104



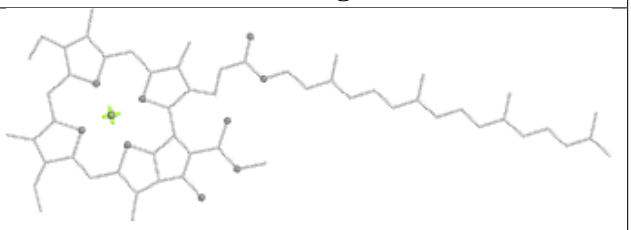
Bond lengths



Bond angles



Torsions

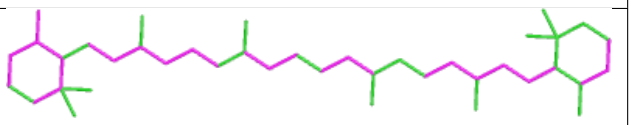


Rings

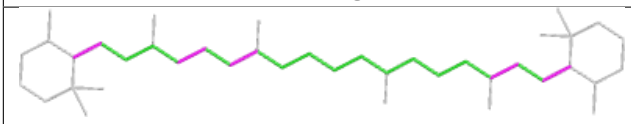
Ligand BCR l 4012



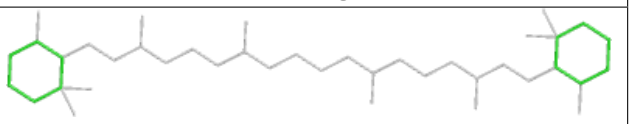
Bond lengths



Bond angles

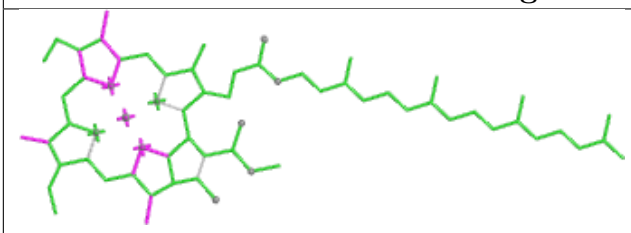


Torsions

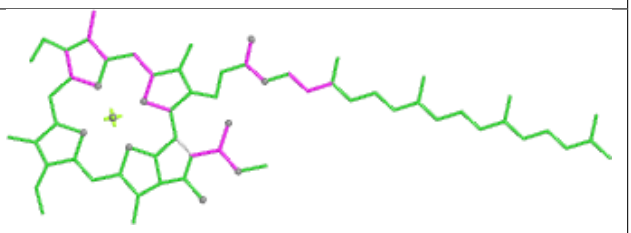


Rings

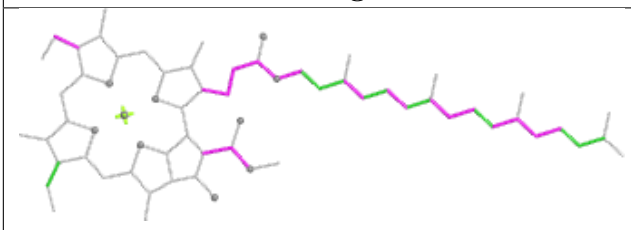
Ligand CLA e 1106



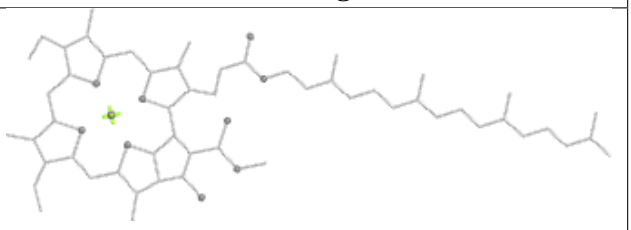
Bond lengths



Bond angles

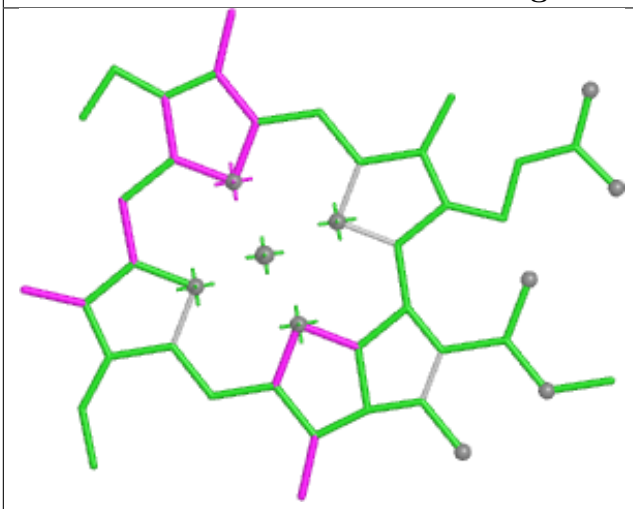


Torsions

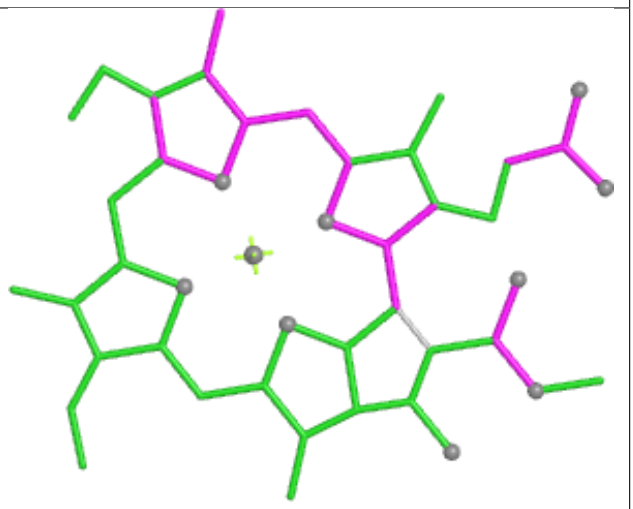


Rings

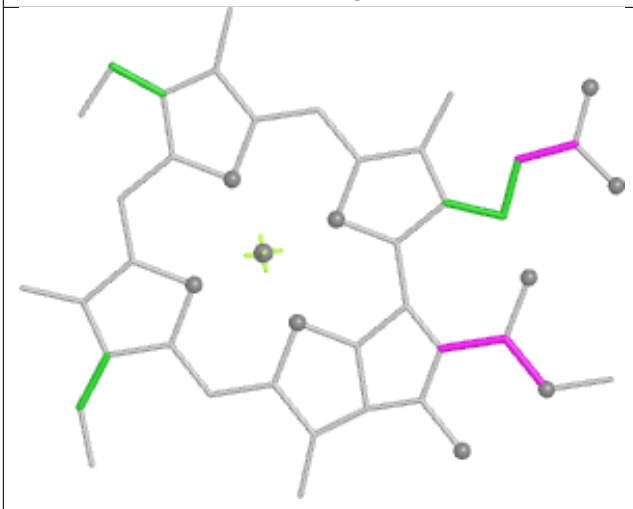
Ligand CLA t 509



Bond lengths



Bond angles

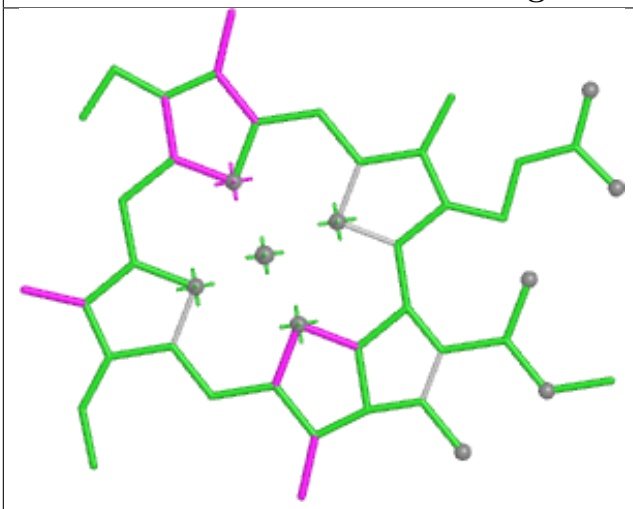


Torsions

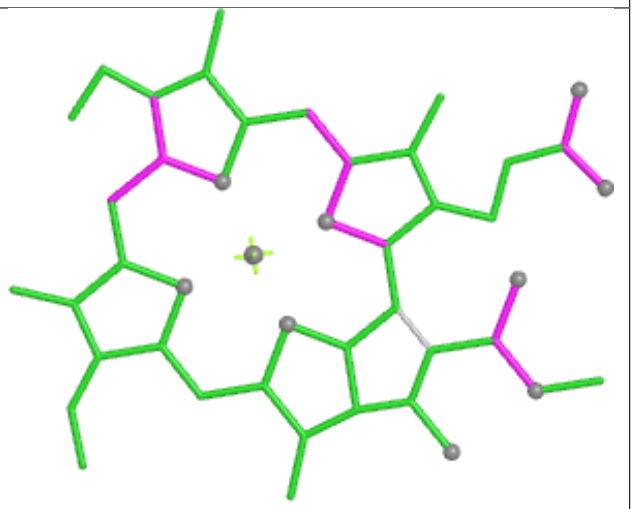


Rings

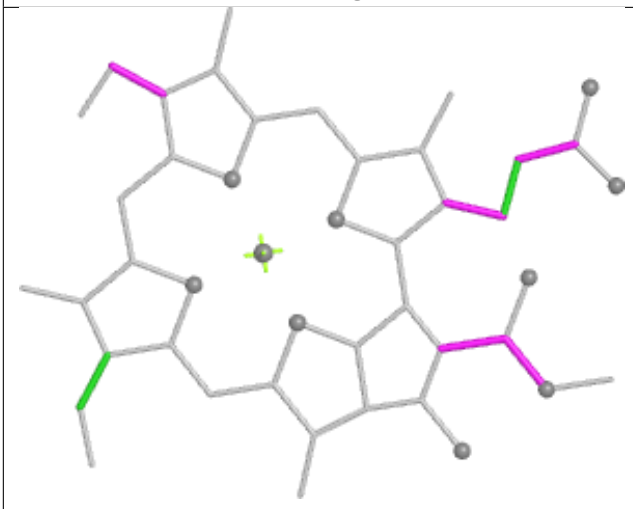
Ligand CLA v 517



Bond lengths



Bond angles

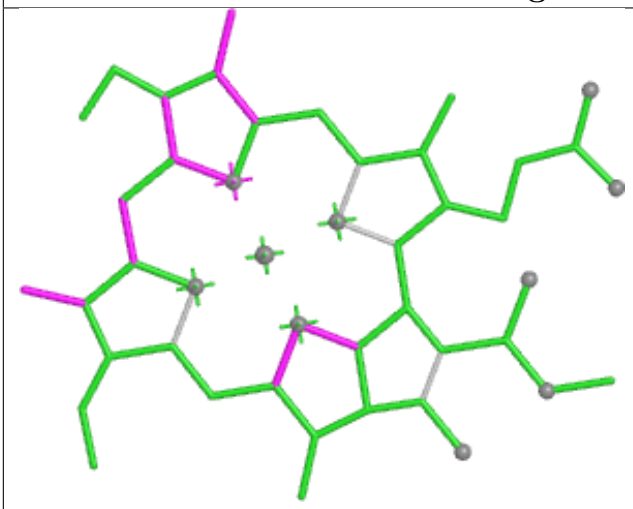


Torsions

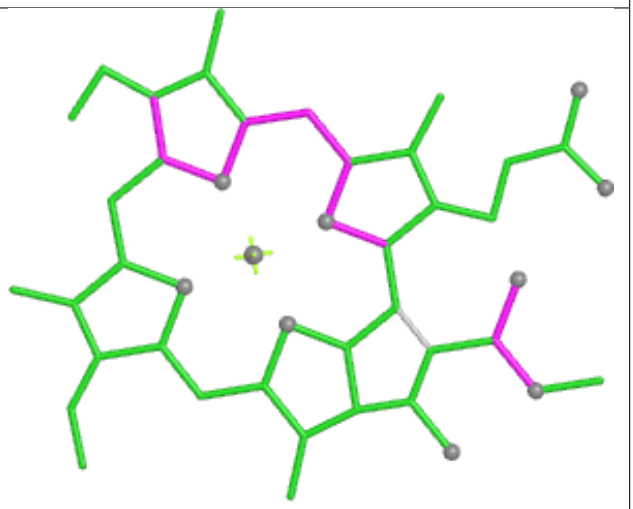


Rings

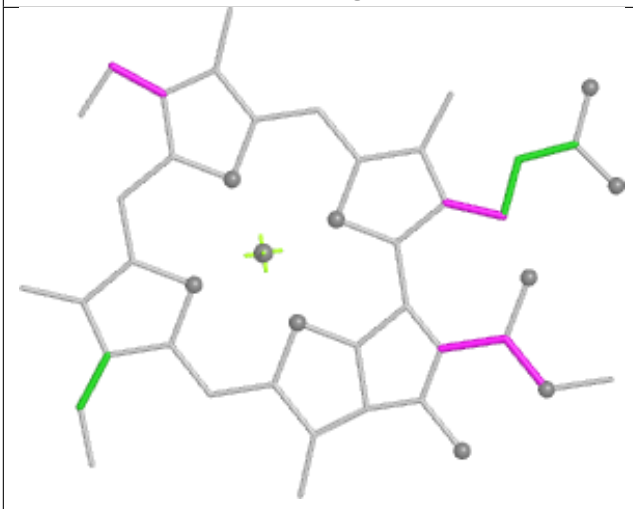
Ligand CLA 4 506



Bond lengths



Bond angles

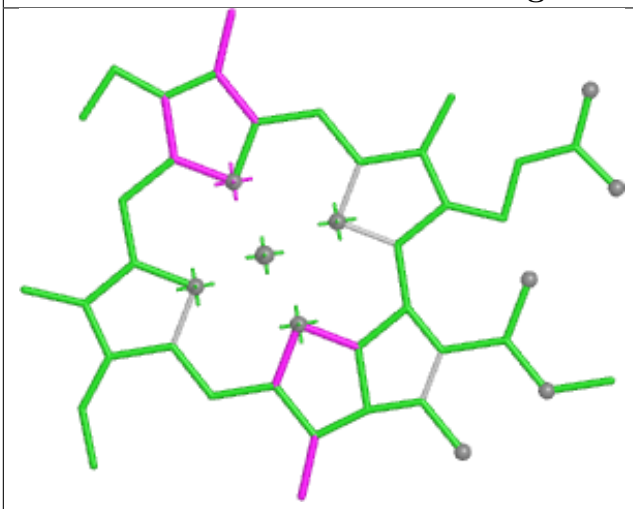


Torsions

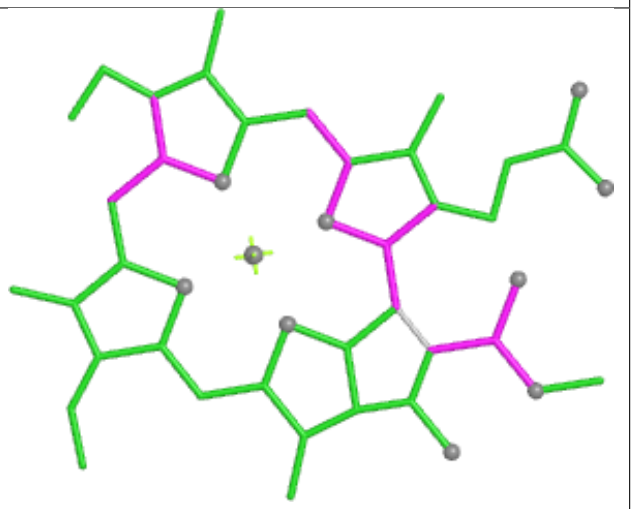


Rings

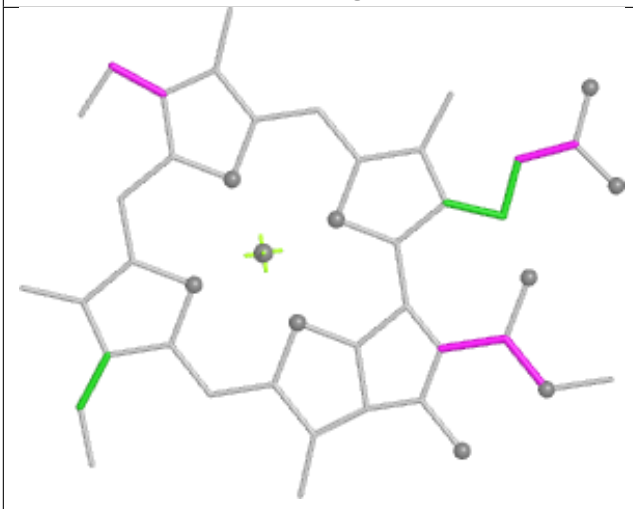
Ligand CLA b 507



Bond lengths



Bond angles

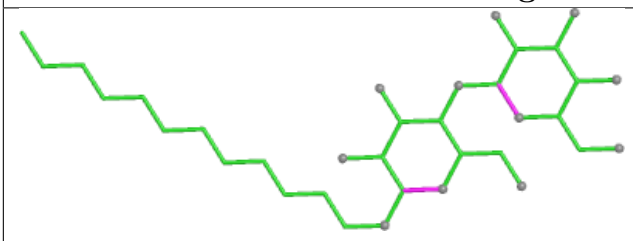


Torsions

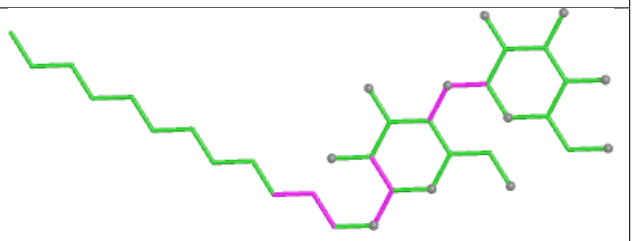


Rings

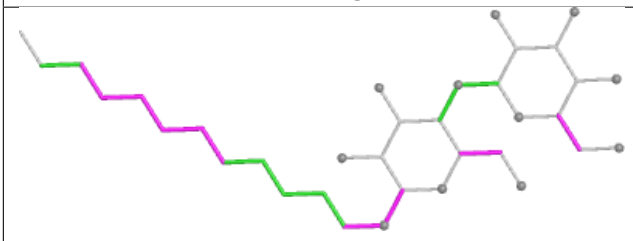
Ligand LMU f 1843



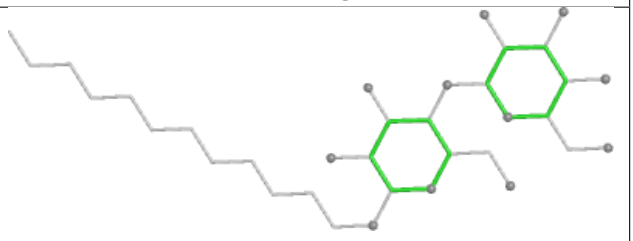
Bond lengths



Bond angles

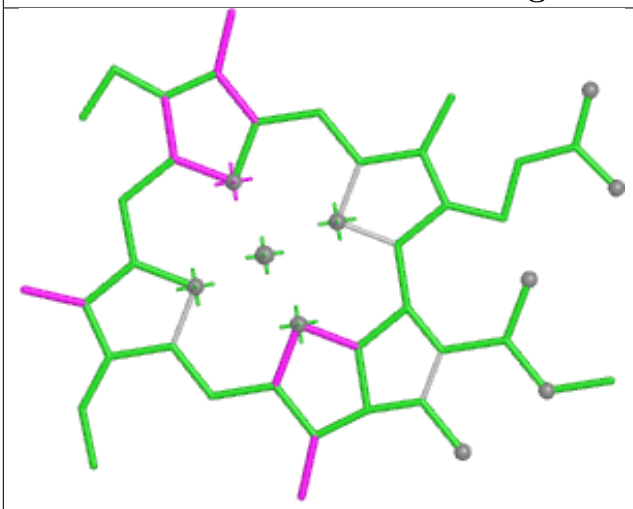


Torsions

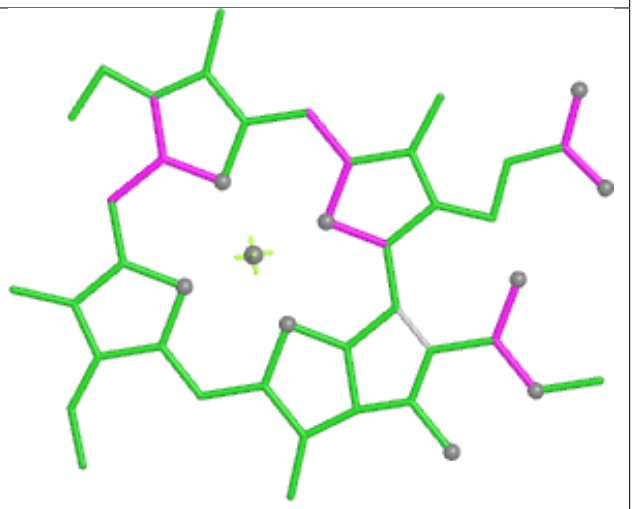


Rings

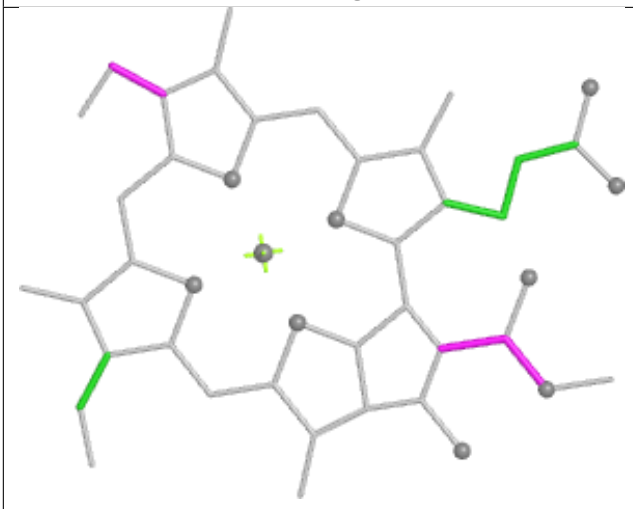
Ligand CLA 2 506



Bond lengths



Bond angles

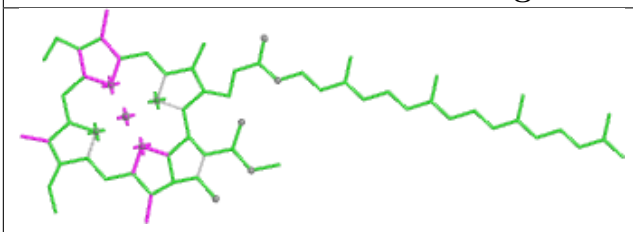


Torsions

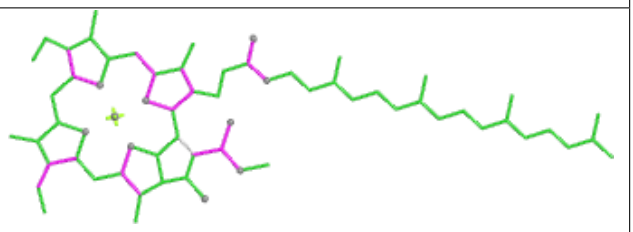


Rings

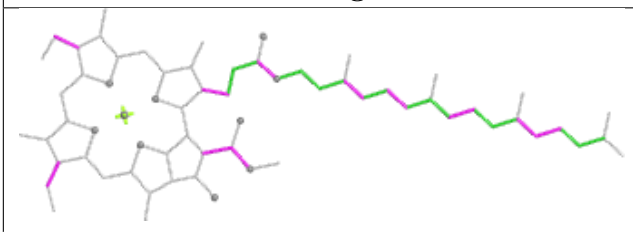
Ligand CLA G 1132



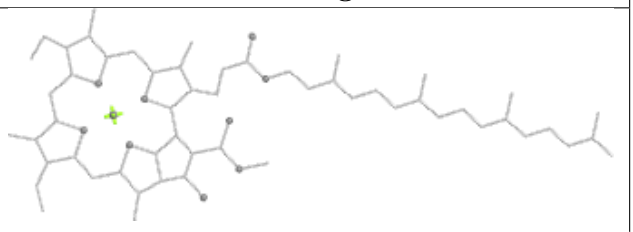
Bond lengths



Bond angles

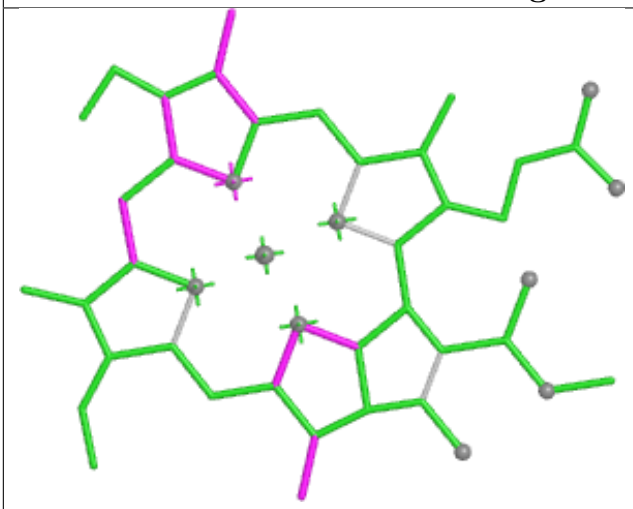


Torsions

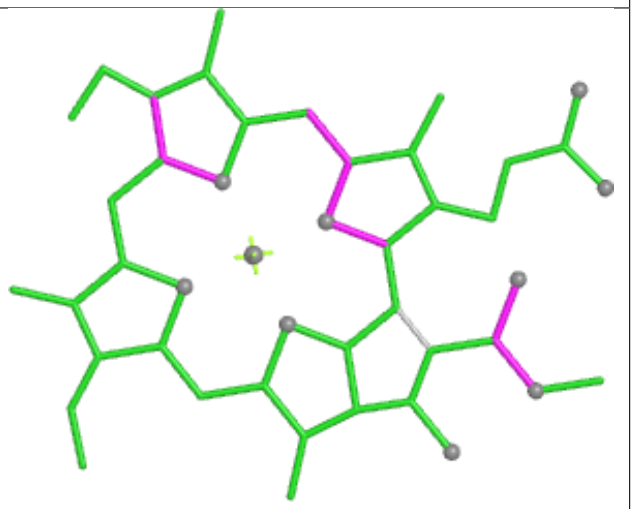


Rings

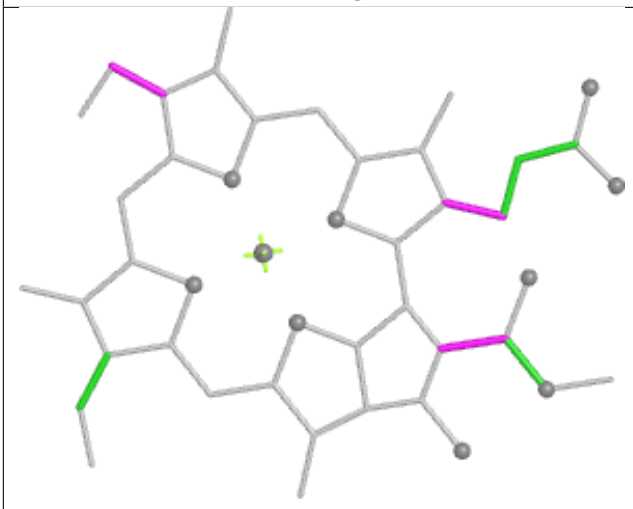
Ligand CLA c 516



Bond lengths



Bond angles

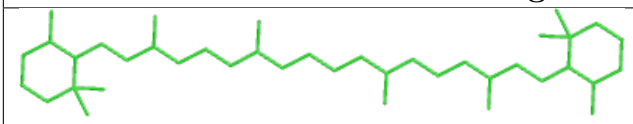


Torsions

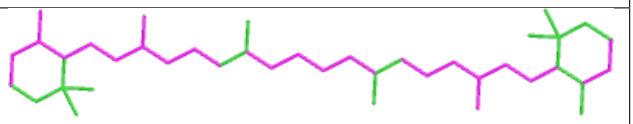


Rings

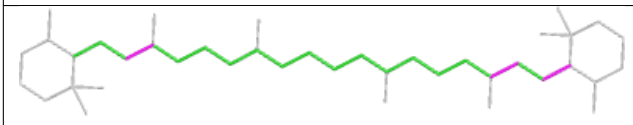
Ligand BCR r 523



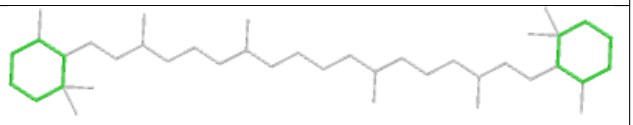
Bond lengths



Bond angles

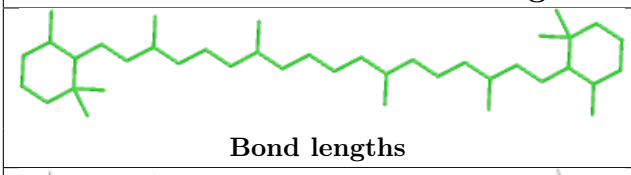


Torsions

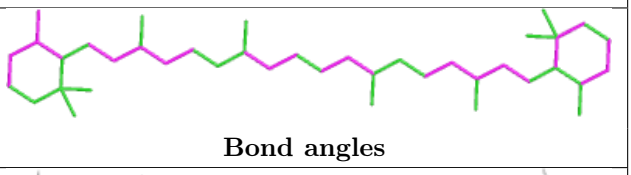


Rings

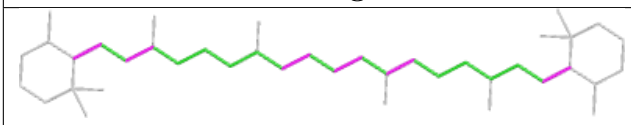
Ligand BCR t 521



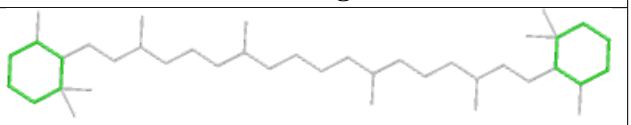
Bond lengths



Bond angles

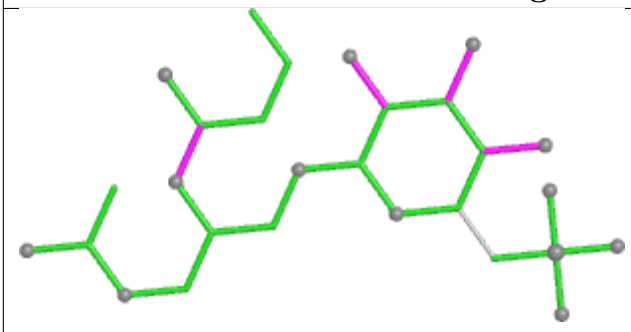


Torsions

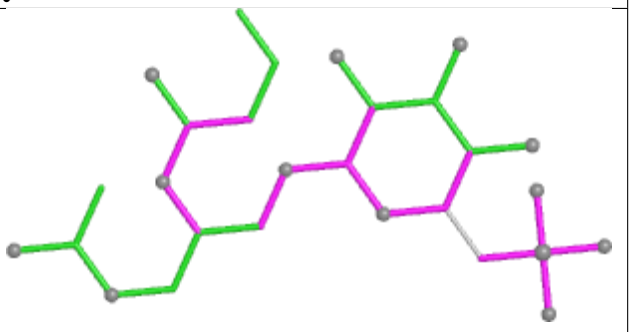


Rings

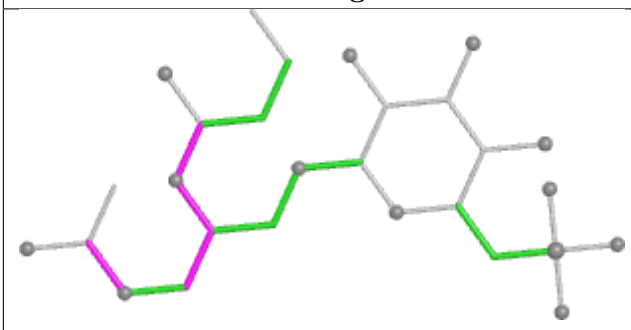
Ligand SQD r 822



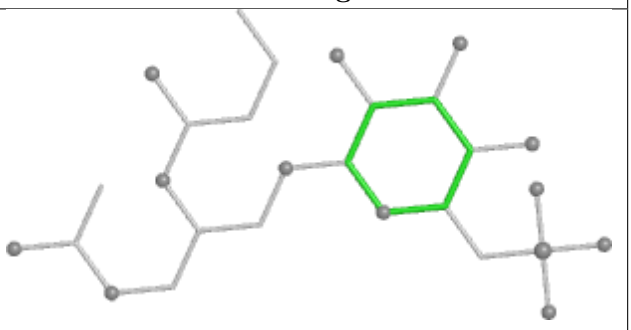
Bond lengths



Bond angles

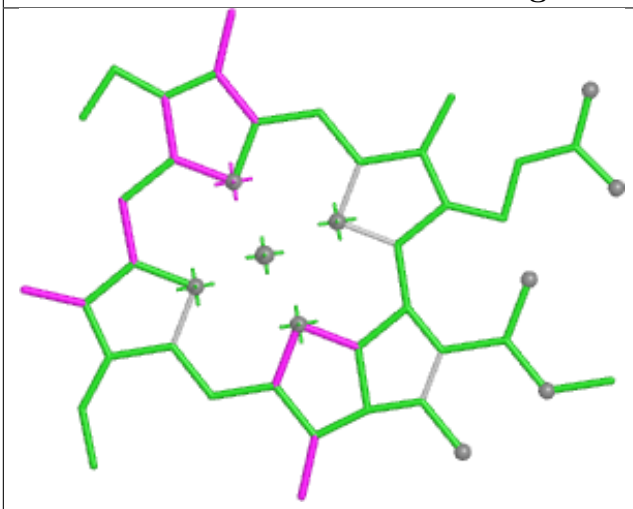


Torsions

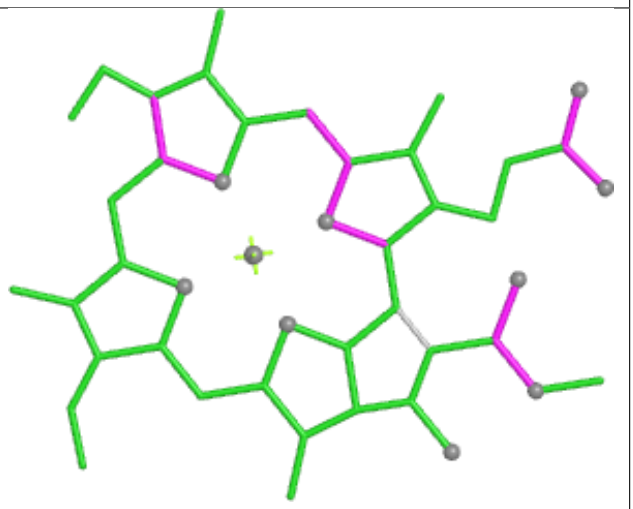


Rings

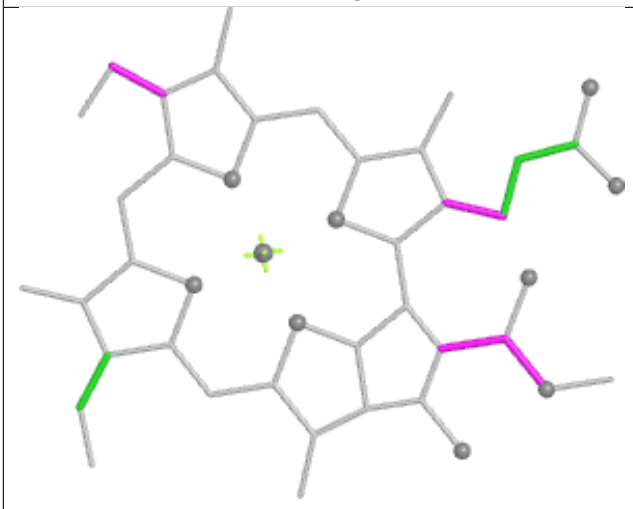
Ligand CLA c 506



Bond lengths



Bond angles

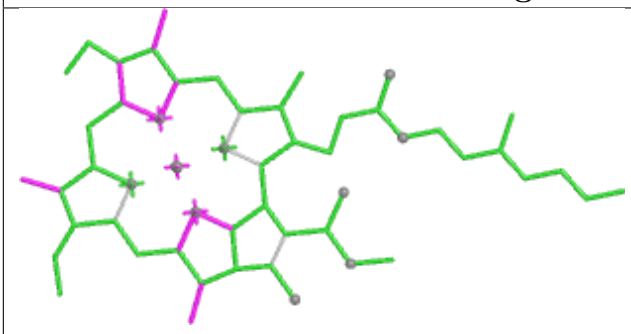


Torsions

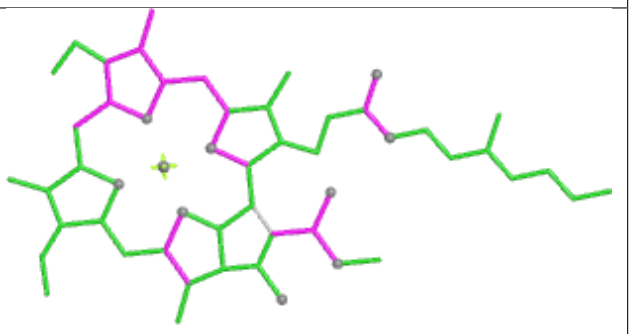


Rings

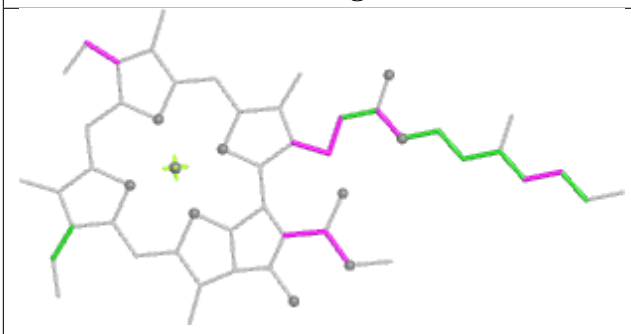
Ligand CLA A 1129



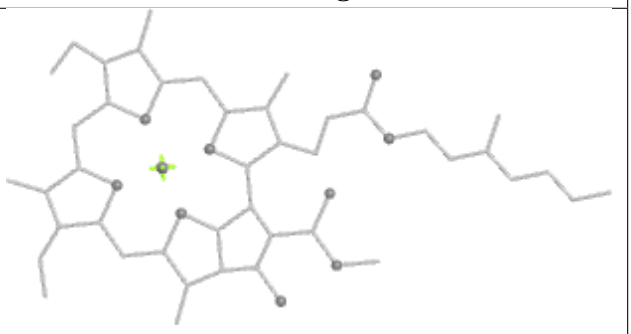
Bond lengths



Bond angles

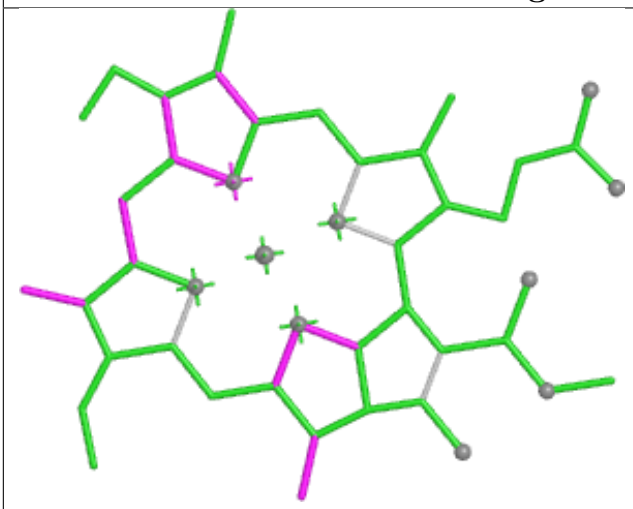


Torsions

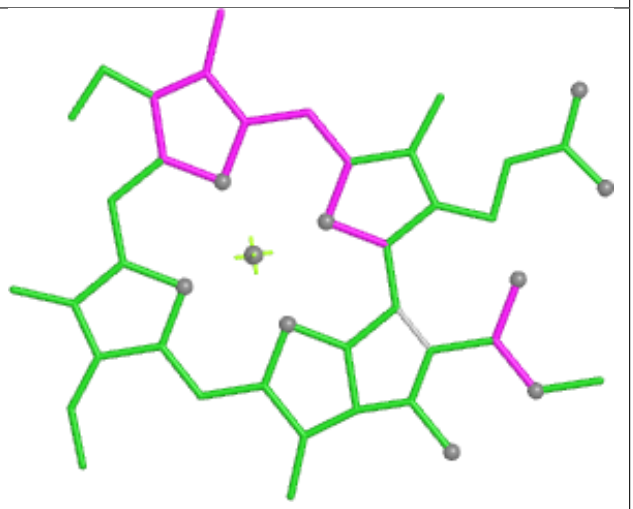


Rings

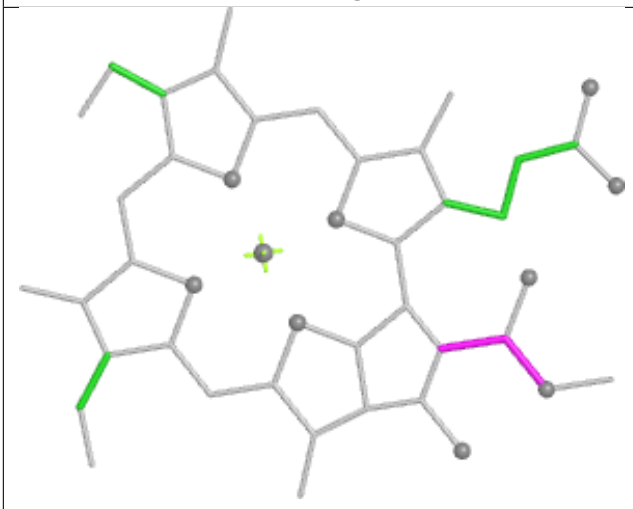
Ligand CLA 1 506



Bond lengths



Bond angles

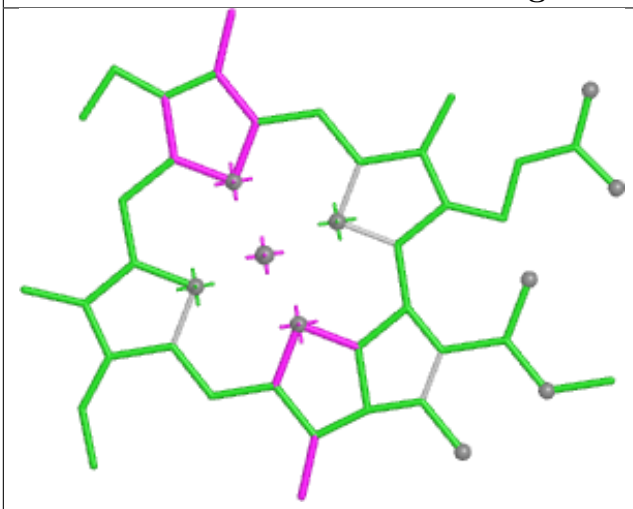


Torsions

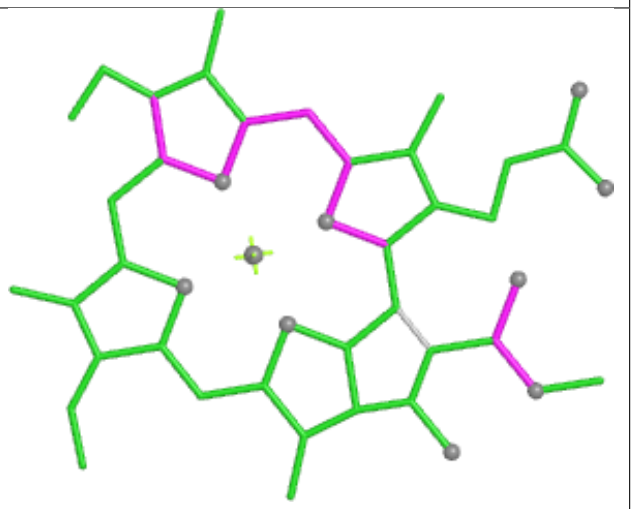


Rings

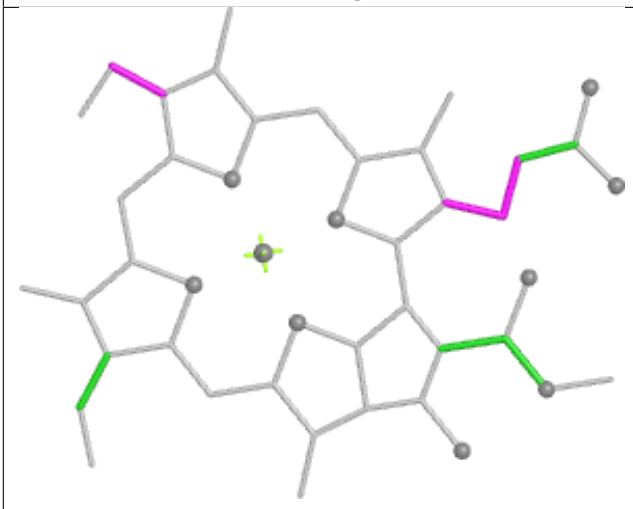
Ligand CLA 3 512



Bond lengths



Bond angles

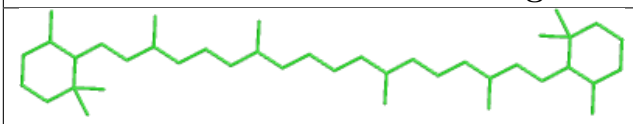


Torsions

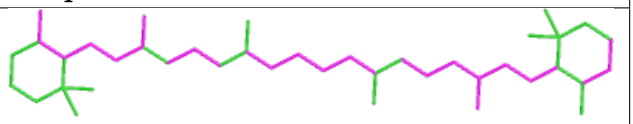


Rings

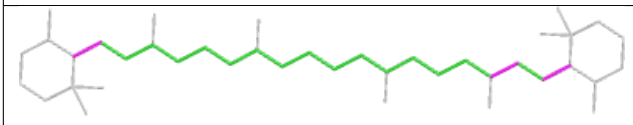
Ligand BCR q 523



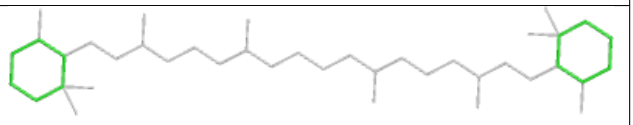
Bond lengths



Bond angles

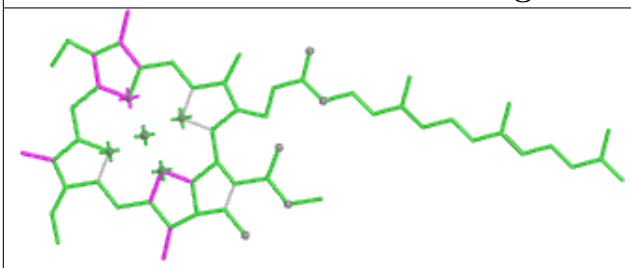


Torsions

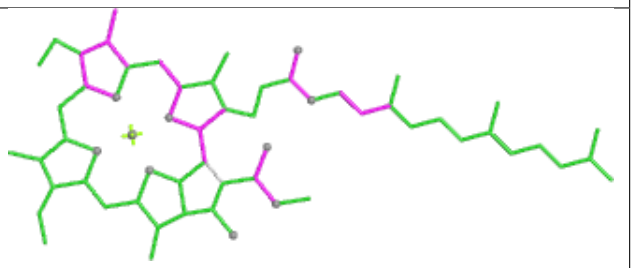


Rings

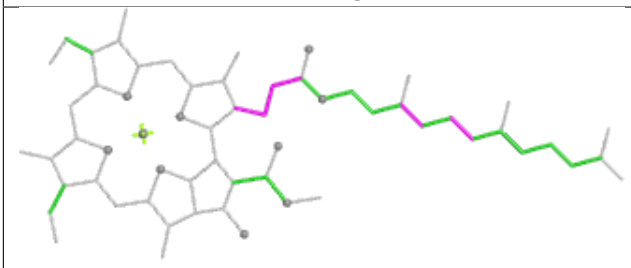
Ligand CLA H 1224



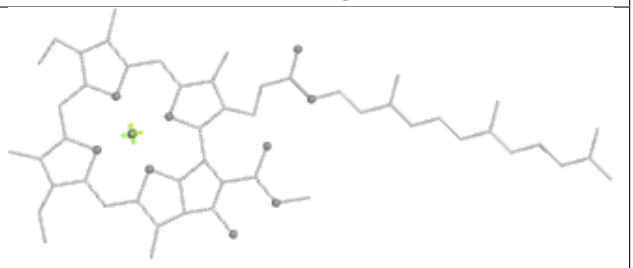
Bond lengths



Bond angles

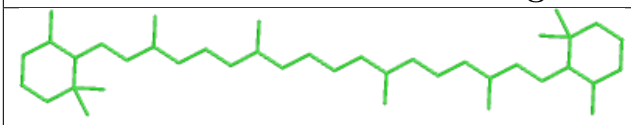


Torsions

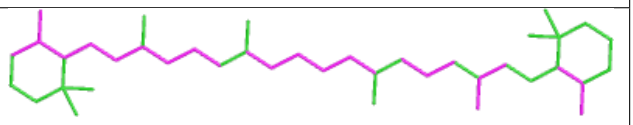


Rings

Ligand BCR c 524



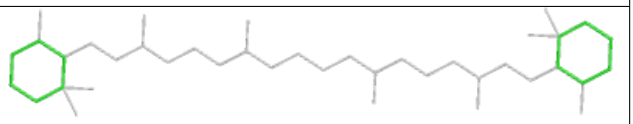
Bond lengths



Bond angles

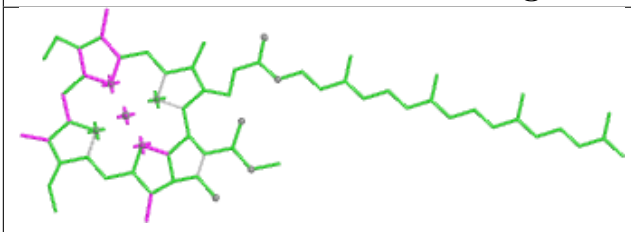


Torsions

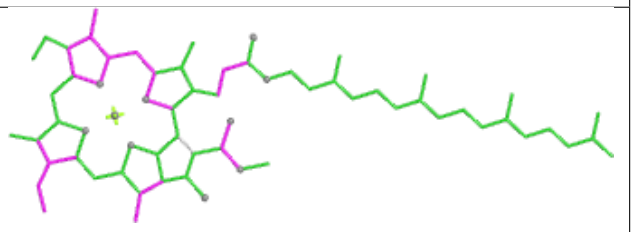


Rings

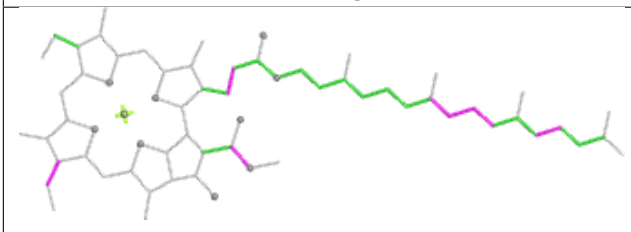
Ligand CLA f 1023



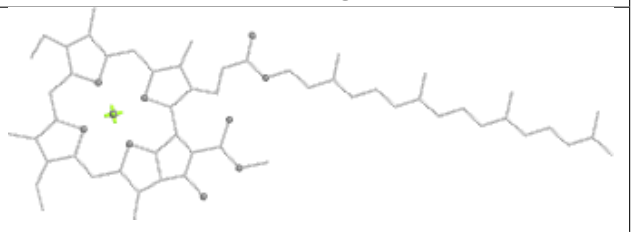
Bond lengths



Bond angles

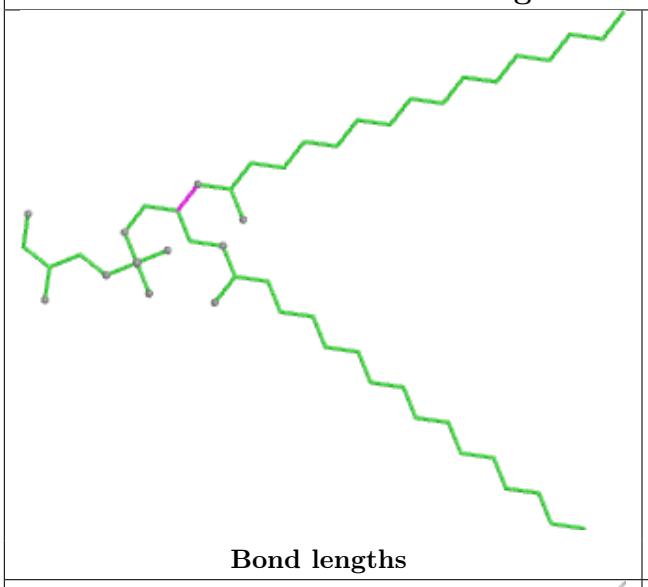


Torsions

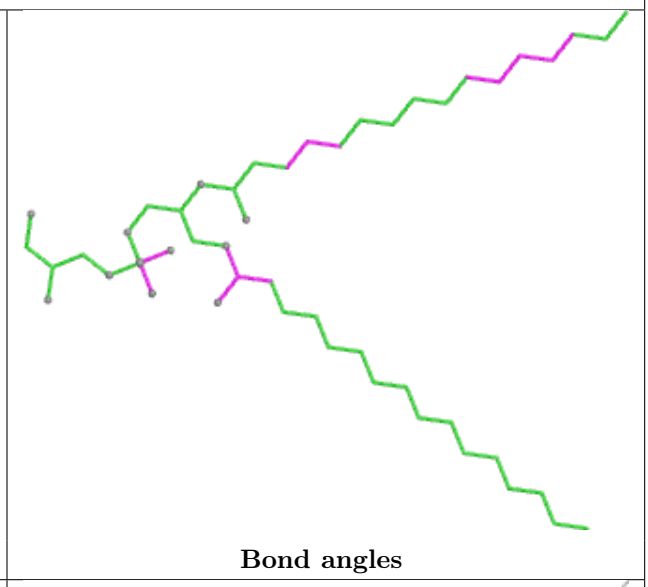


Rings

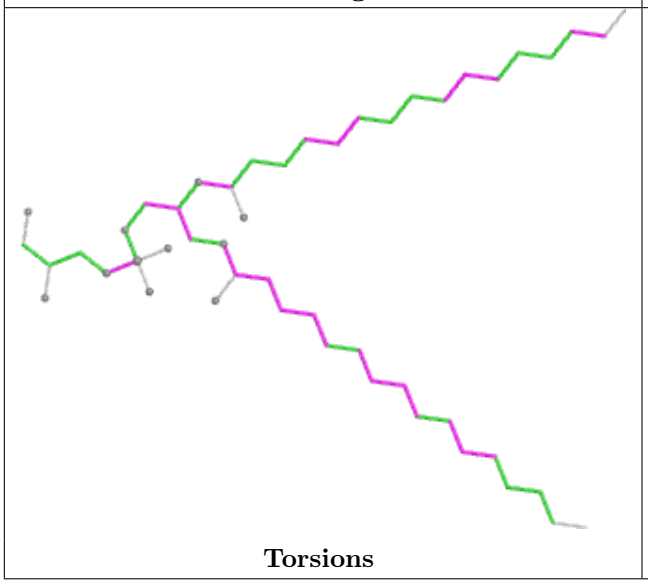
Ligand LHG A 5001



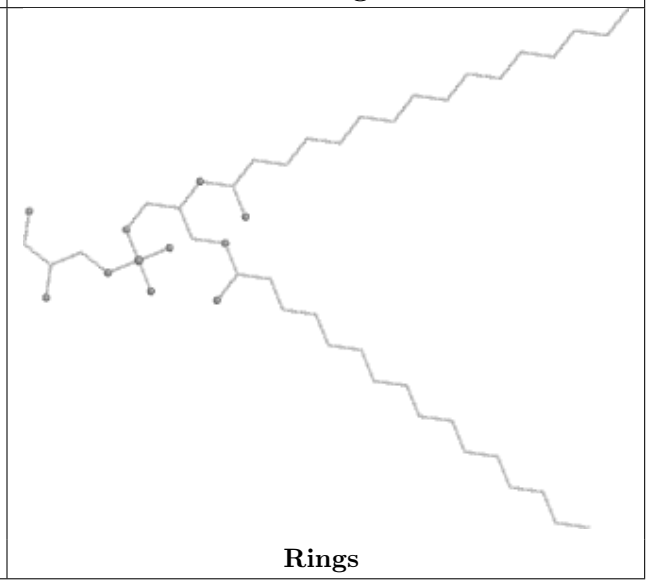
Bond lengths



Bond angles

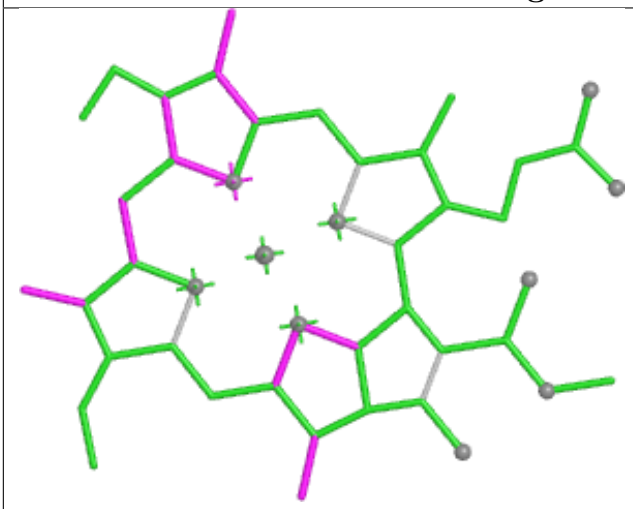


Torsions

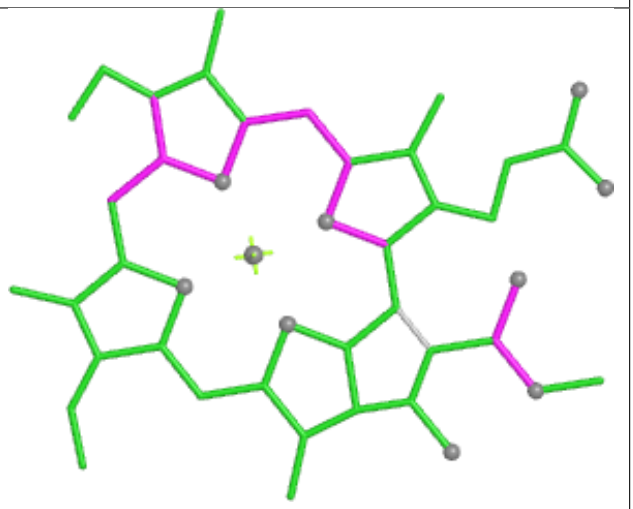


Rings

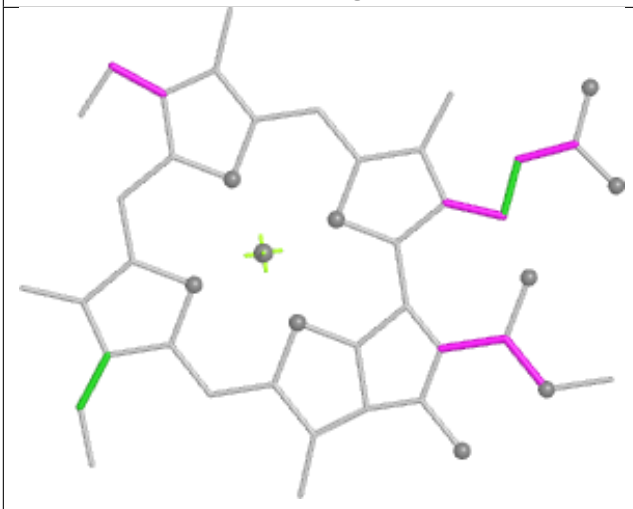
Ligand CLA d 512



Bond lengths



Bond angles

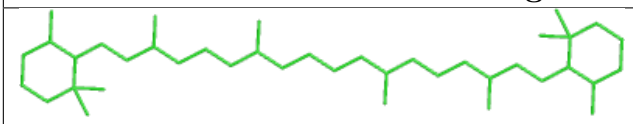


Torsions

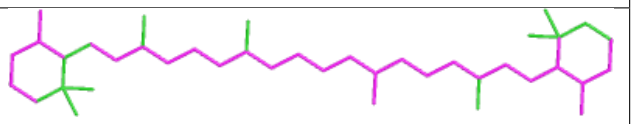


Rings

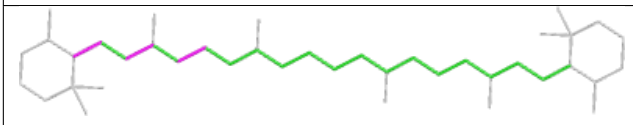
Ligand BCR d 522



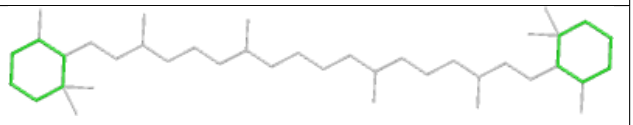
Bond lengths



Bond angles

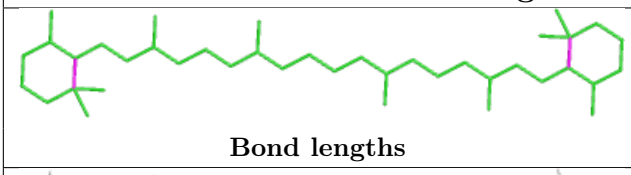


Torsions

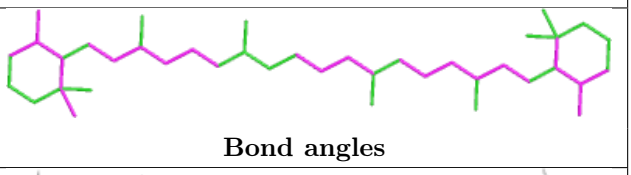


Rings

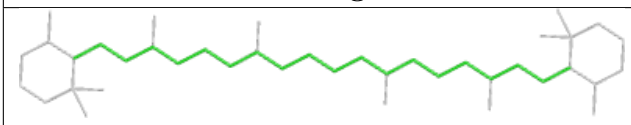
Ligand BCR k 4018



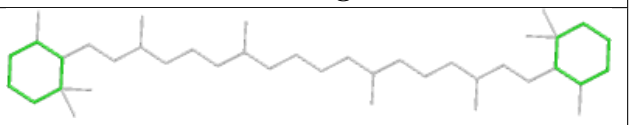
Bond lengths



Bond angles

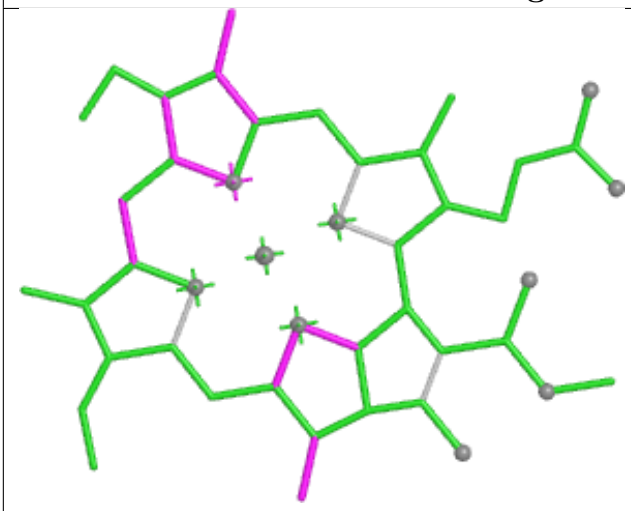


Torsions

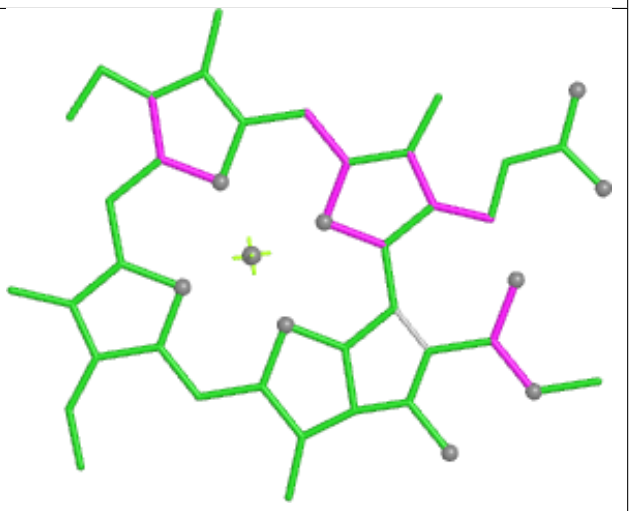


Rings

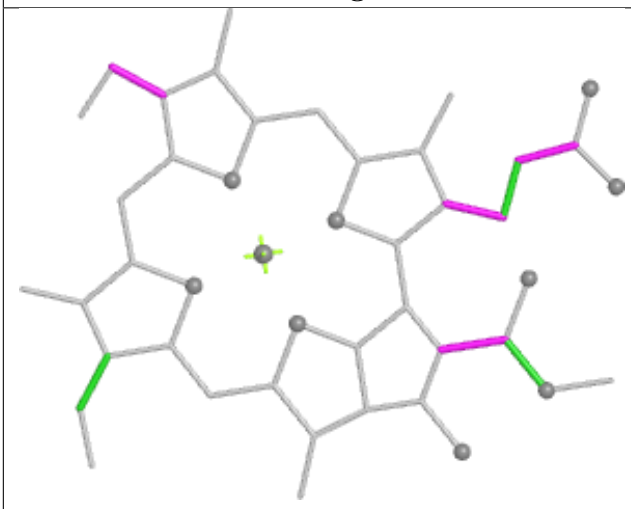
Ligand CLA b 516



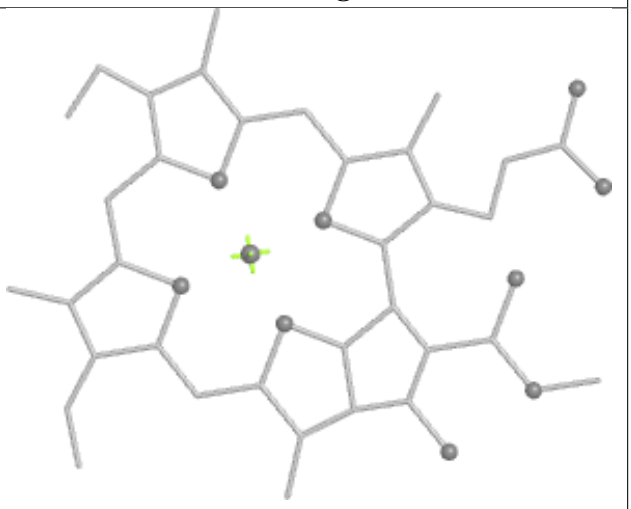
Bond lengths



Bond angles

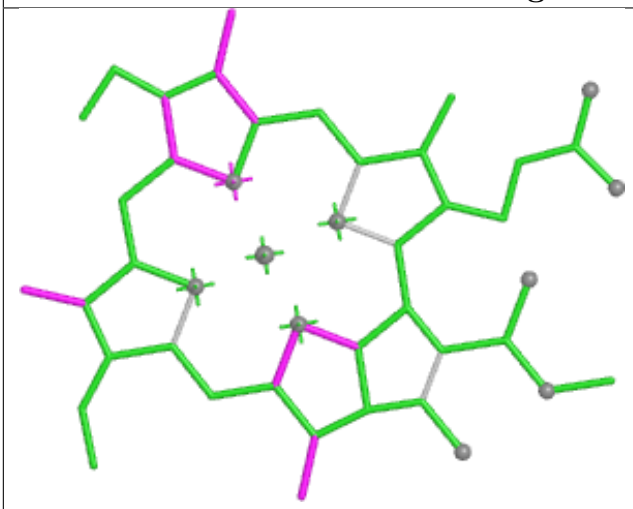


Torsions

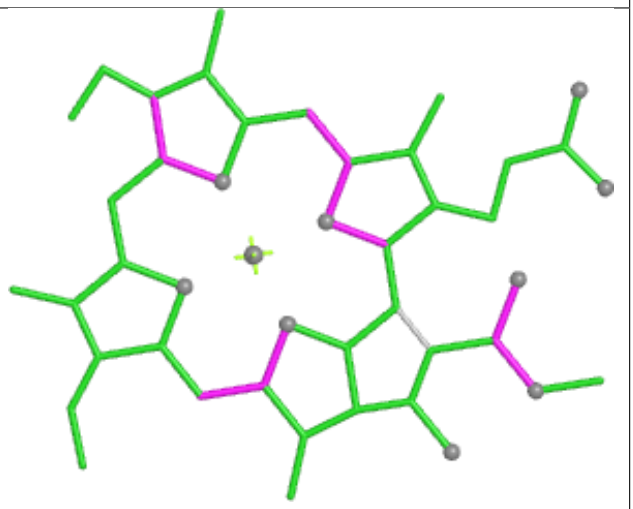


Rings

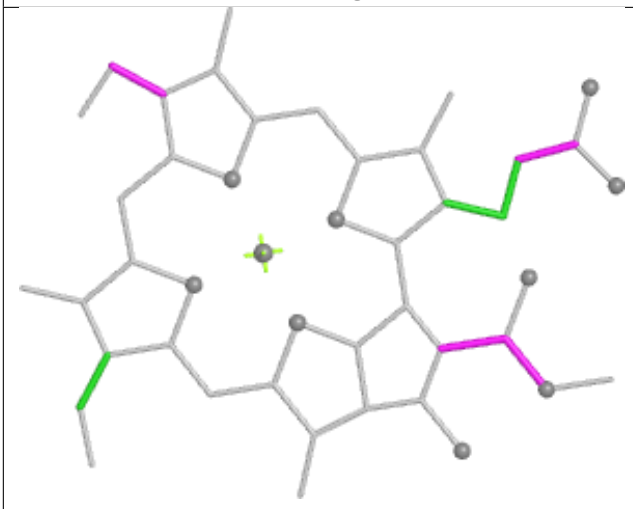
Ligand CLA u 510



Bond lengths



Bond angles

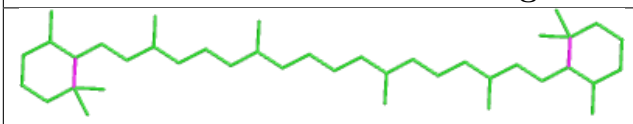


Torsions

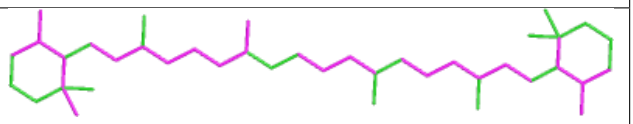


Rings

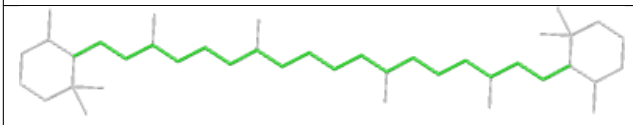
Ligand BCR I 4018



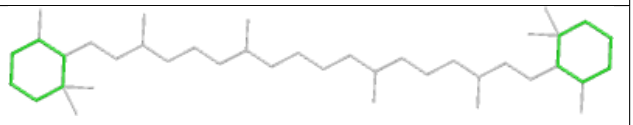
Bond lengths



Bond angles

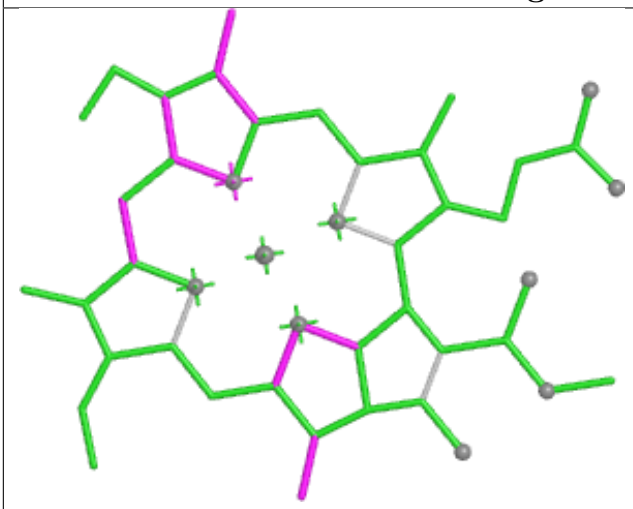


Torsions

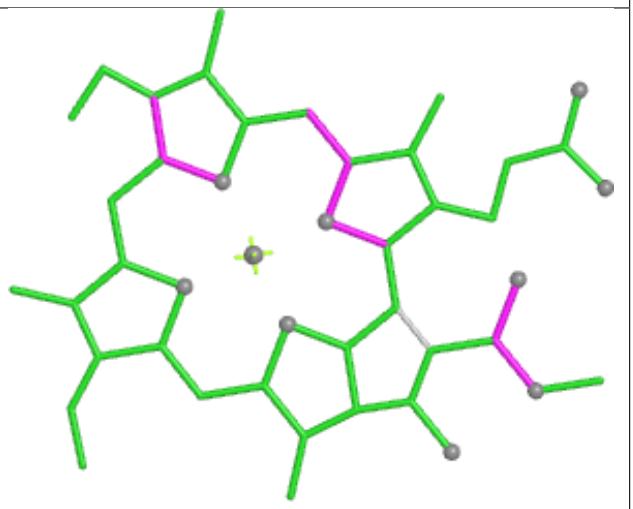


Rings

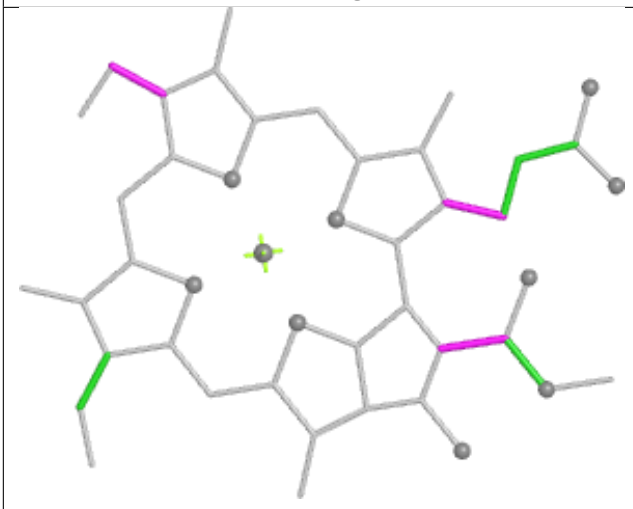
Ligand CLA u 516



Bond lengths



Bond angles

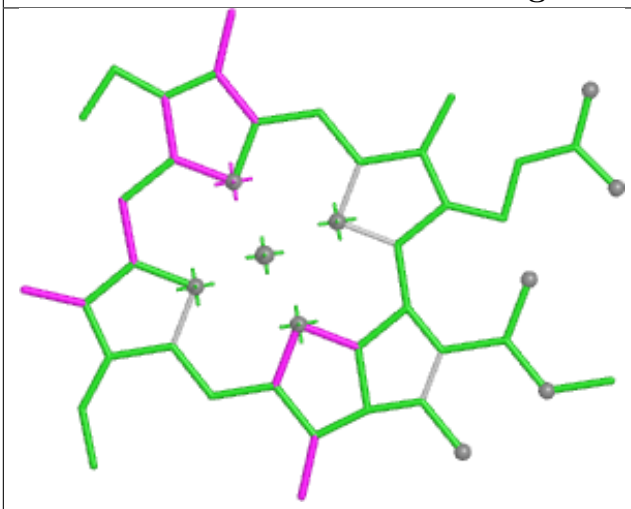


Torsions

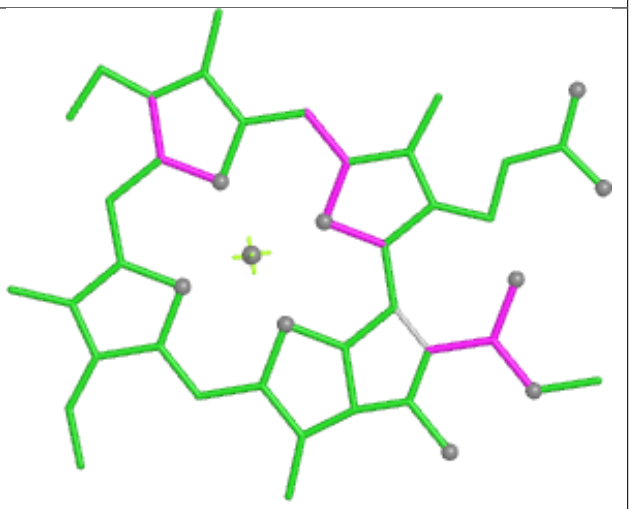


Rings

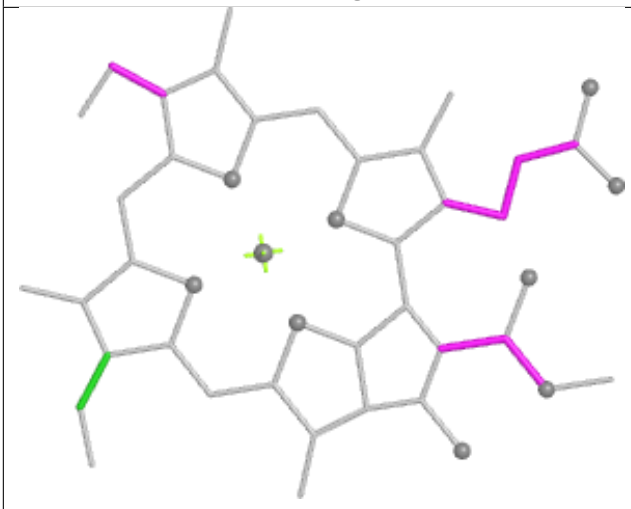
Ligand CLA 6 501



Bond lengths



Bond angles

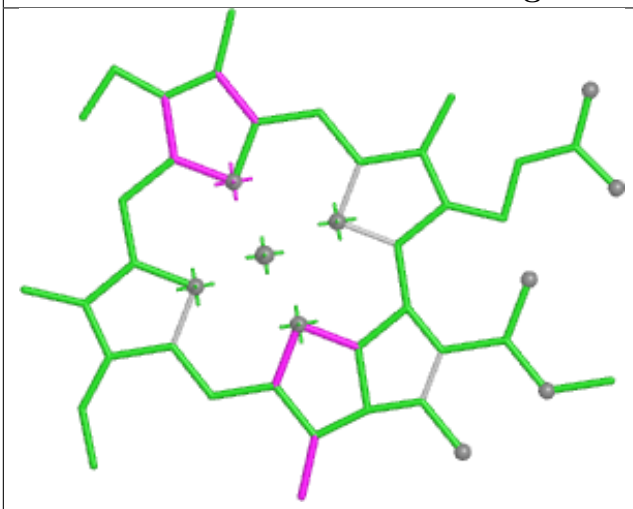


Torsions

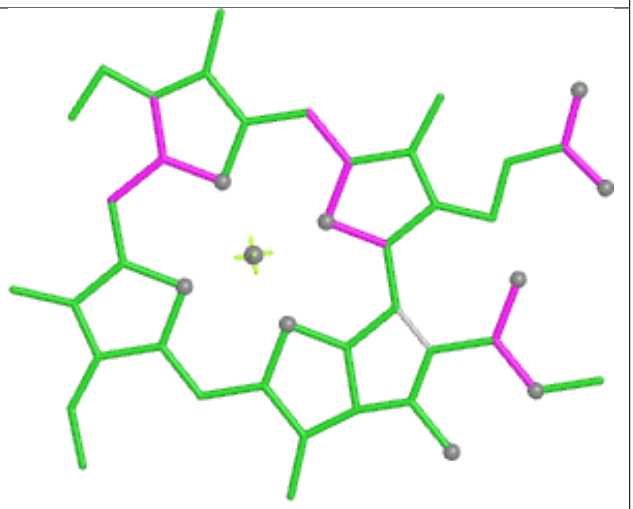


Rings

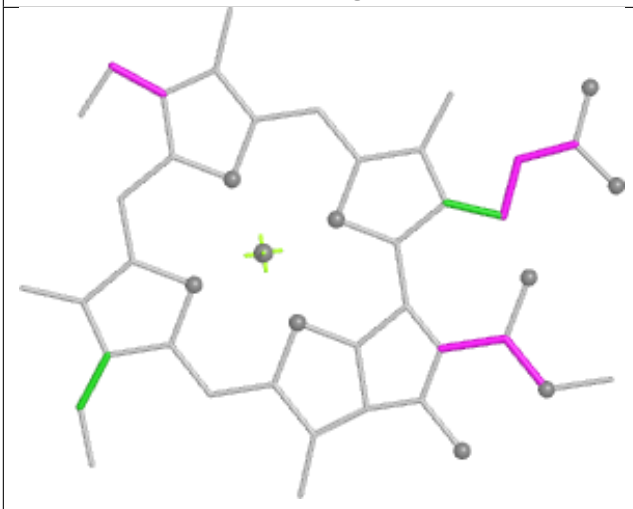
Ligand CLA Y 518



Bond lengths



Bond angles

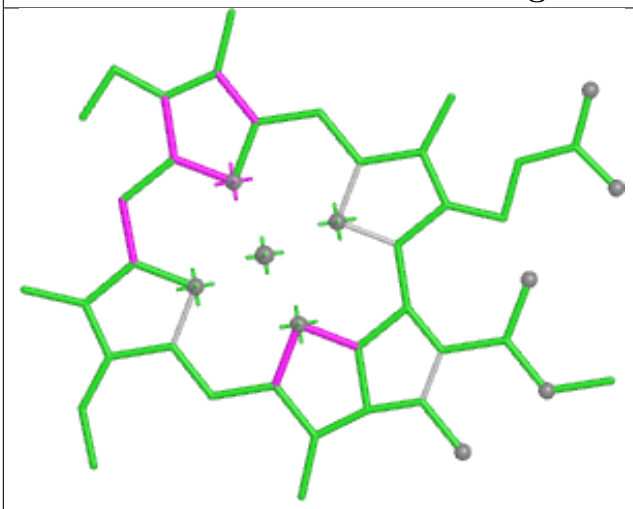


Torsions

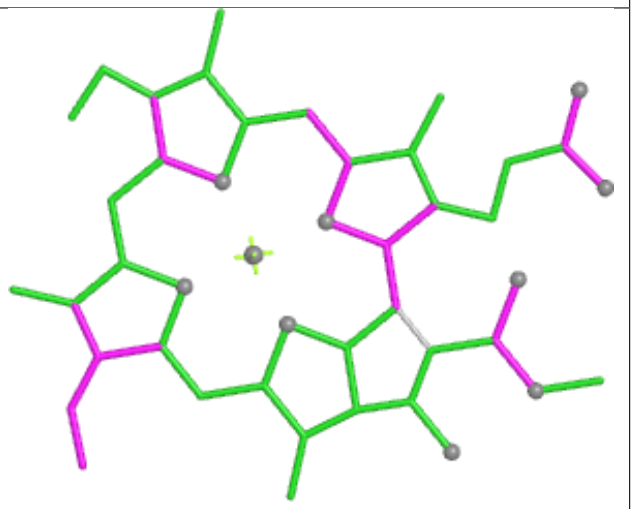


Rings

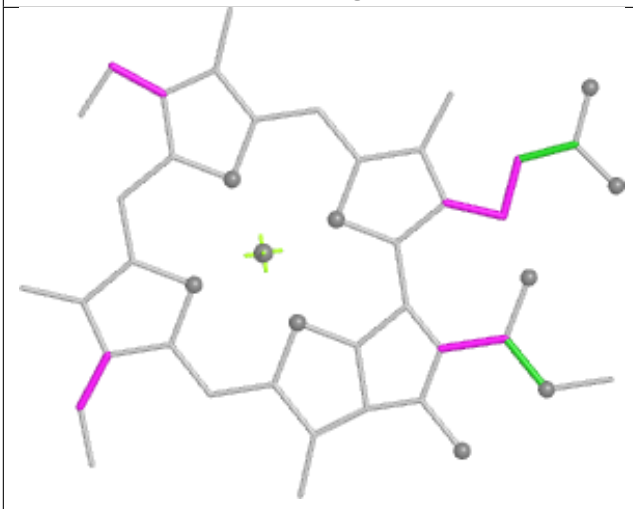
Ligand CLA a 516



Bond lengths



Bond angles

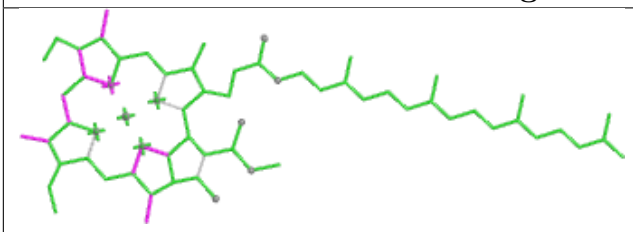


Torsions

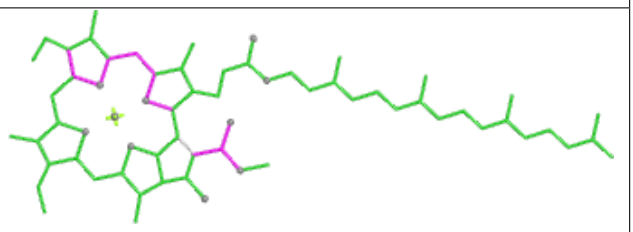


Rings

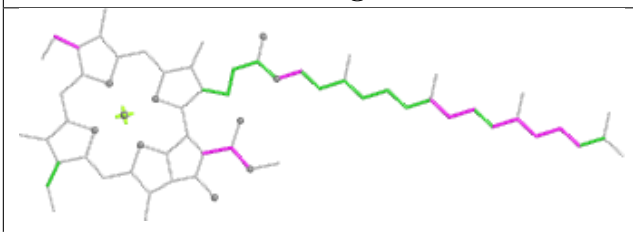
Ligand CLA e 1138



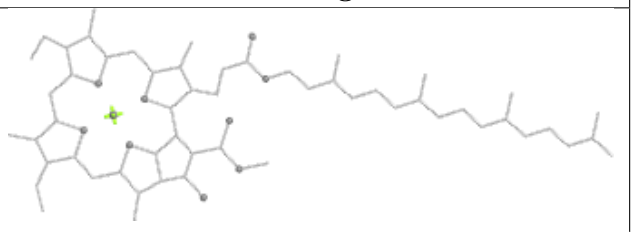
Bond lengths



Bond angles

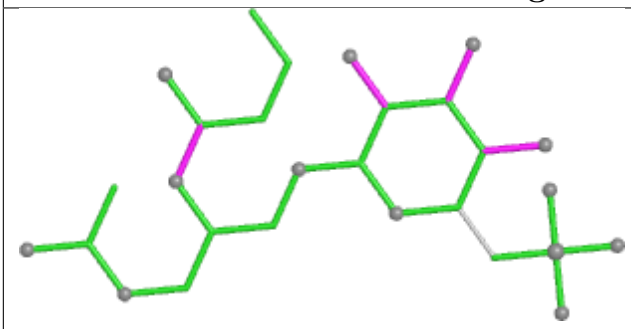


Torsions

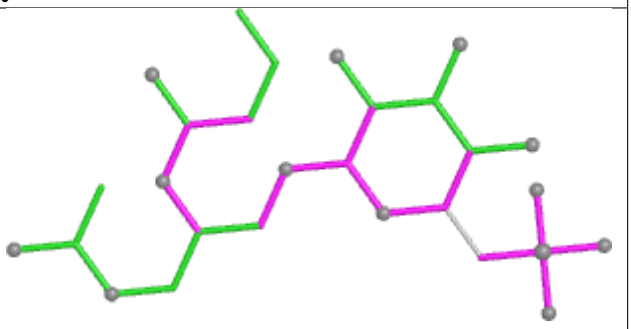


Rings

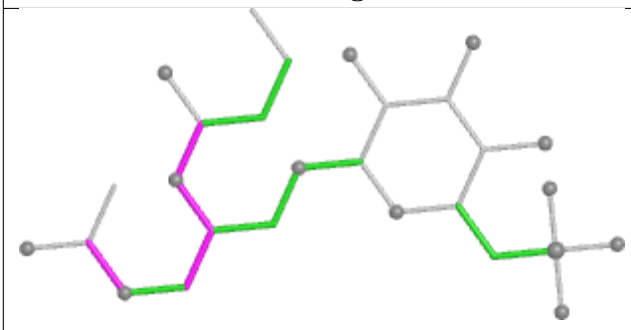
Ligand SQD 2 822



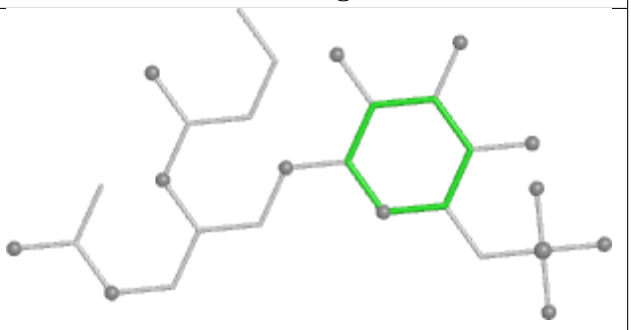
Bond lengths



Bond angles

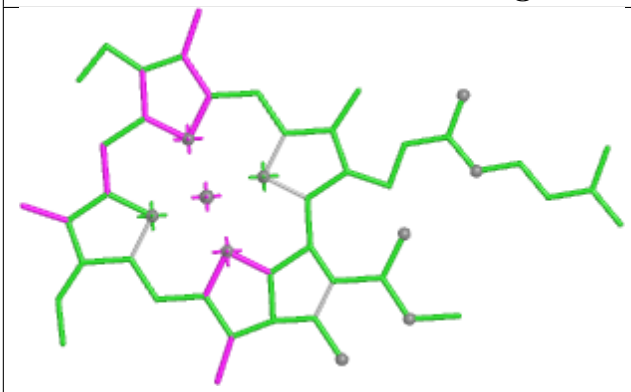


Torsions

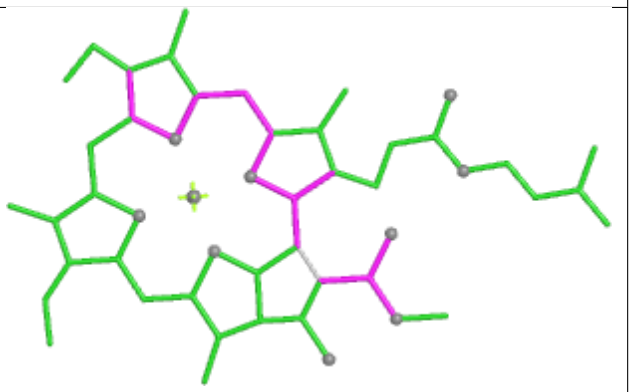


Rings

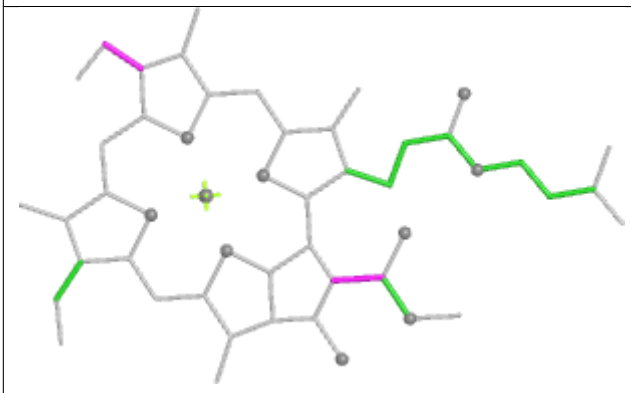
Ligand CLA G 1112



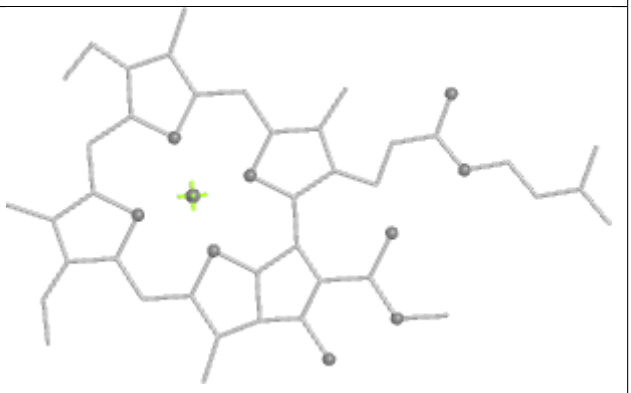
Bond lengths



Bond angles

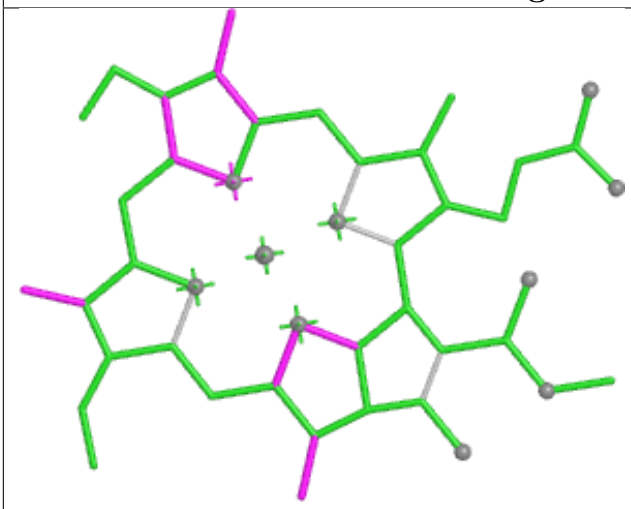


Torsions

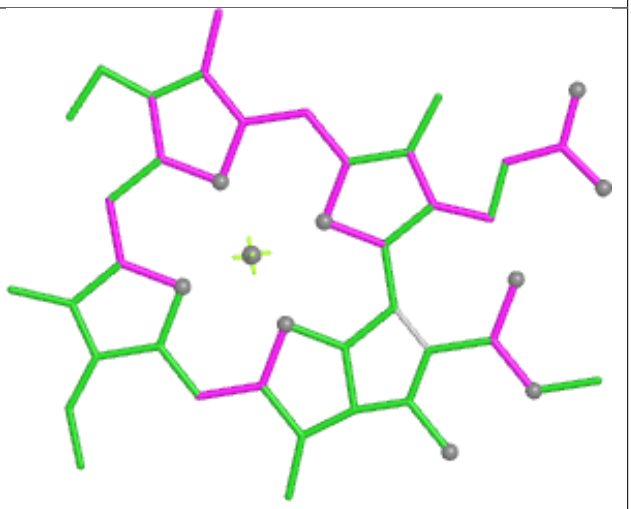


Rings

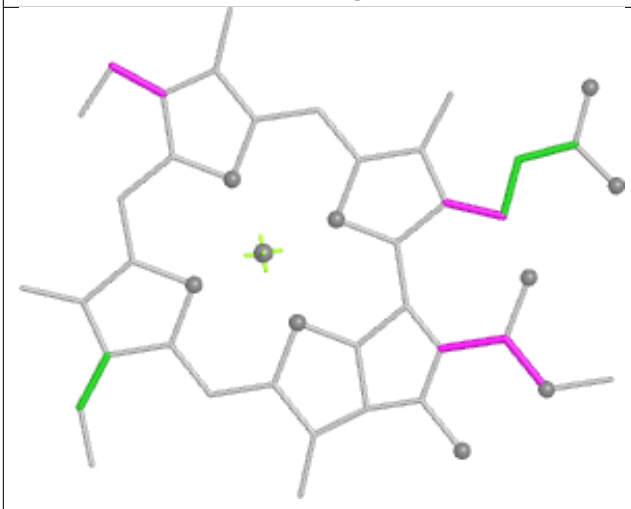
Ligand CLA 6 508



Bond lengths



Bond angles

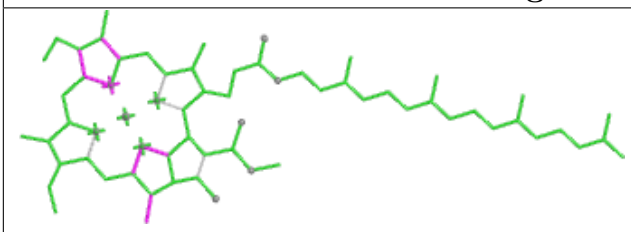


Torsions

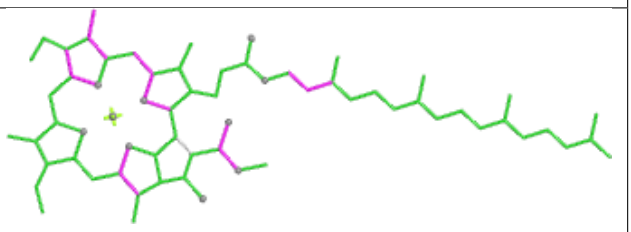


Rings

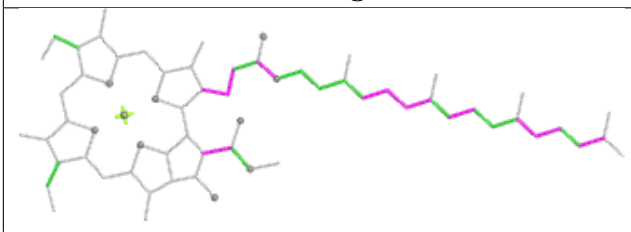
Ligand CLA Z 505



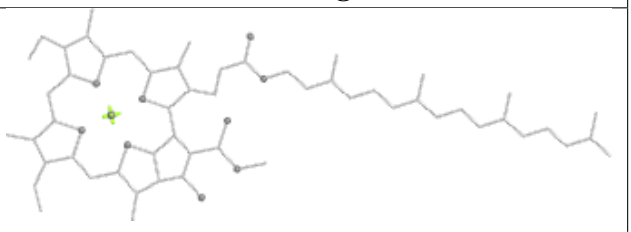
Bond lengths



Bond angles

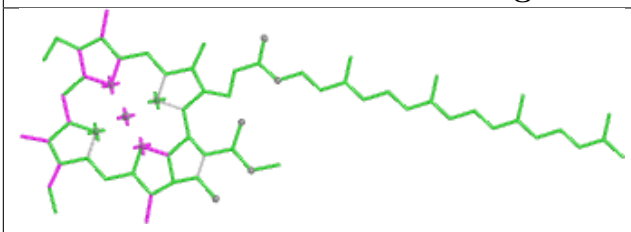


Torsions

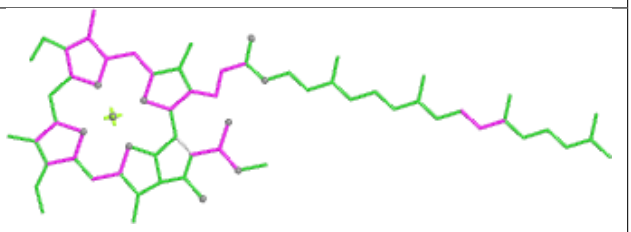


Rings

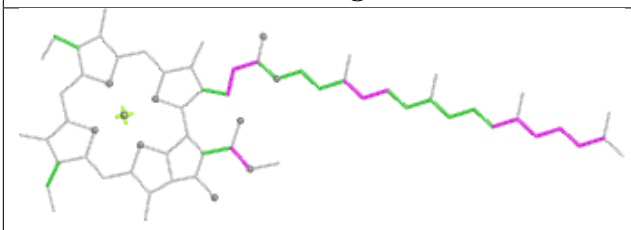
Ligand CLA G 1013



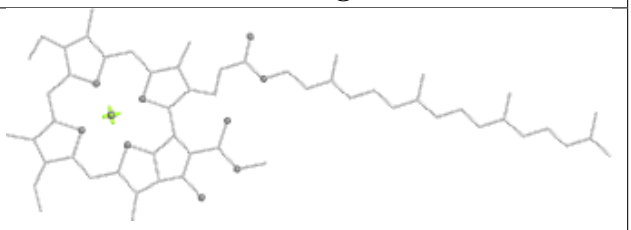
Bond lengths



Bond angles

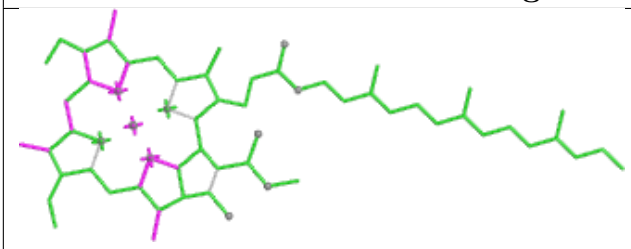


Torsions

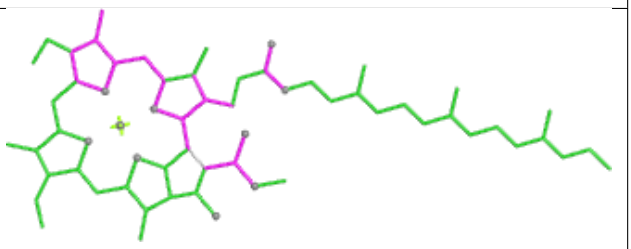


Rings

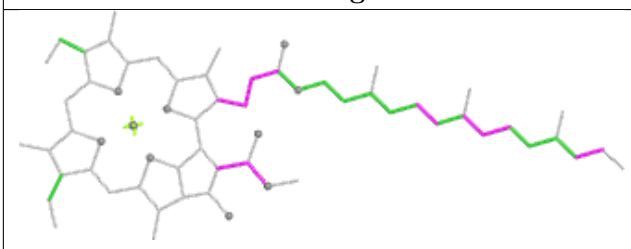
Ligand CLA f 1221



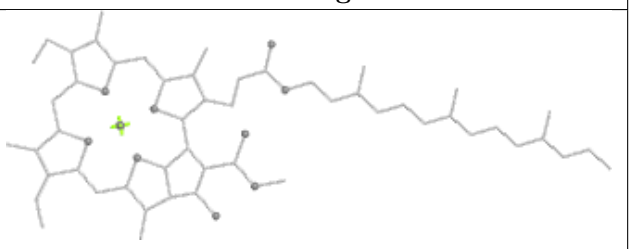
Bond lengths



Bond angles

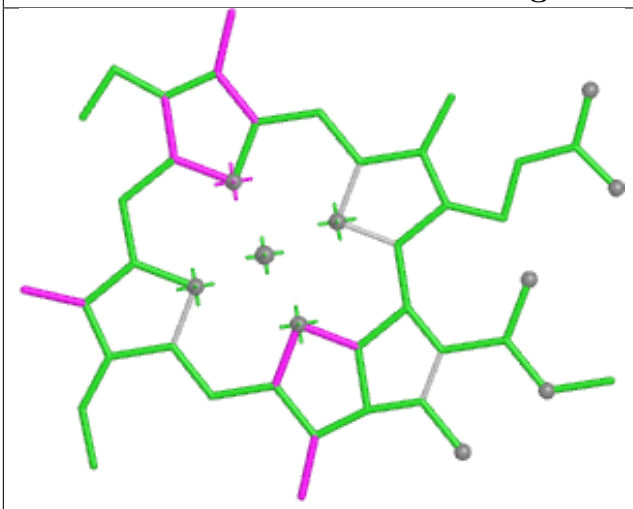


Torsions

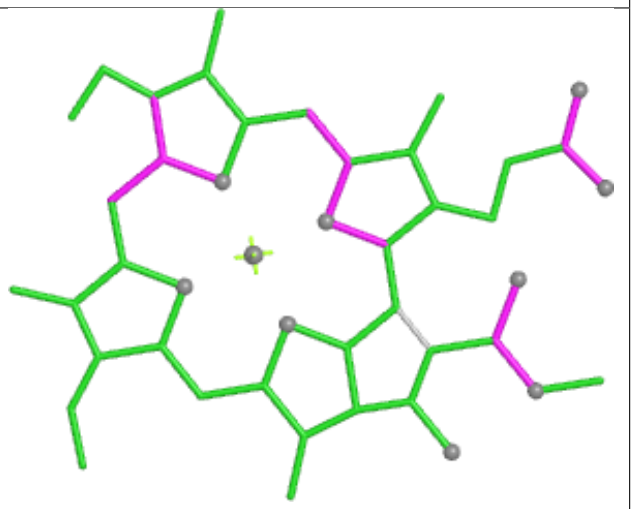


Rings

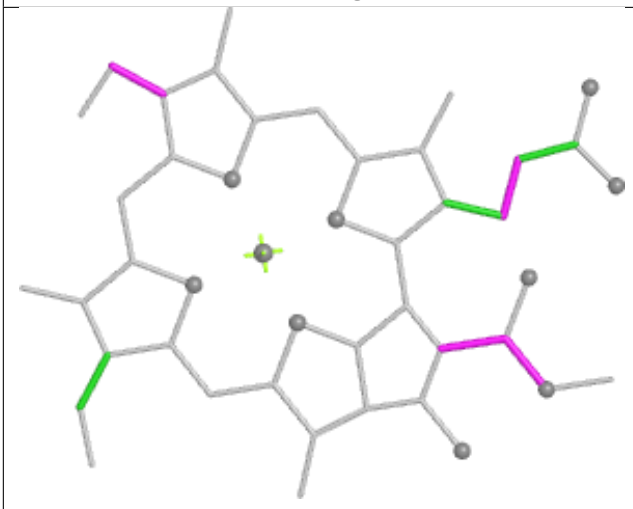
Ligand CLA r 517



Bond lengths



Bond angles

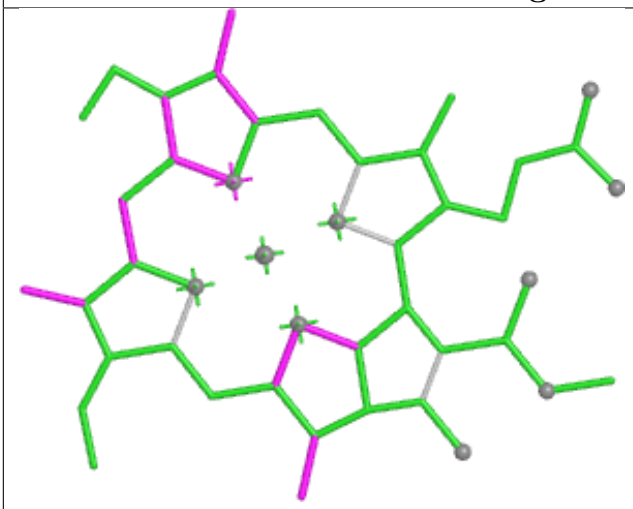


Torsions

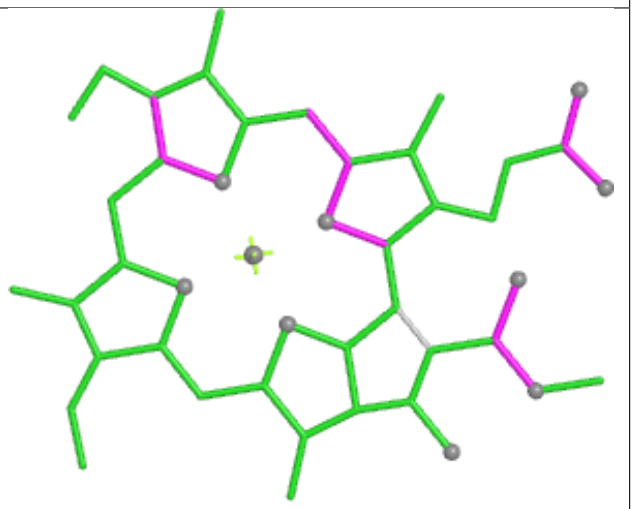


Rings

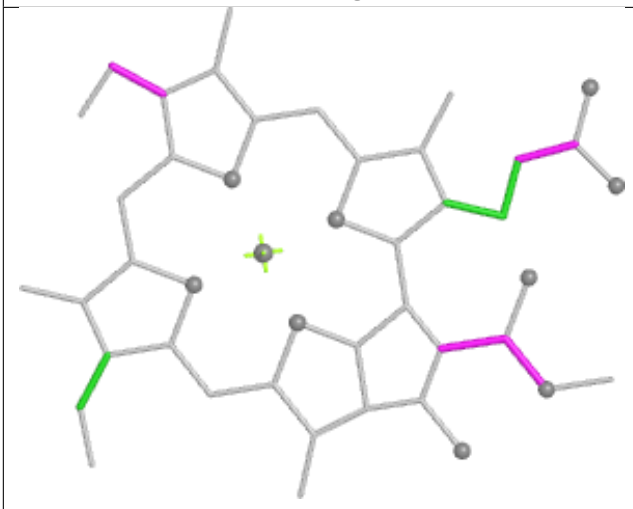
Ligand CLA c 510



Bond lengths



Bond angles

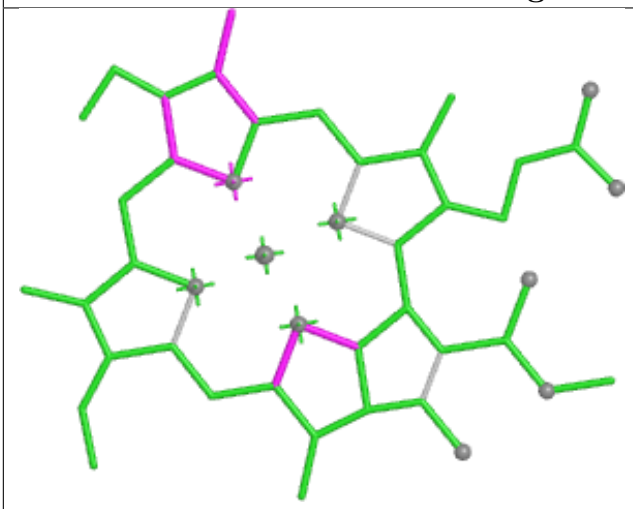


Torsions

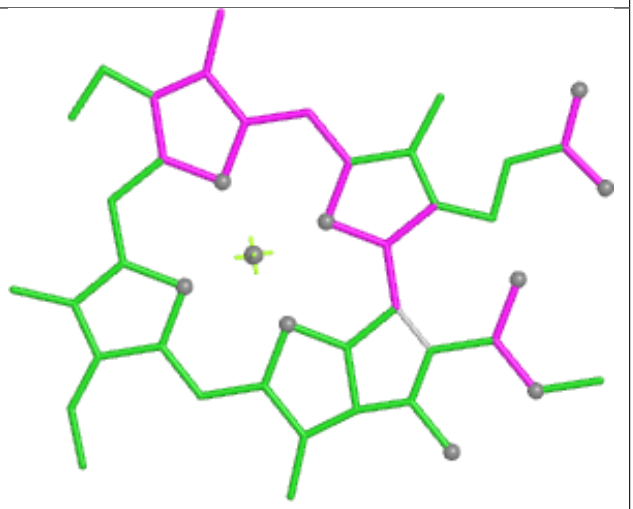


Rings

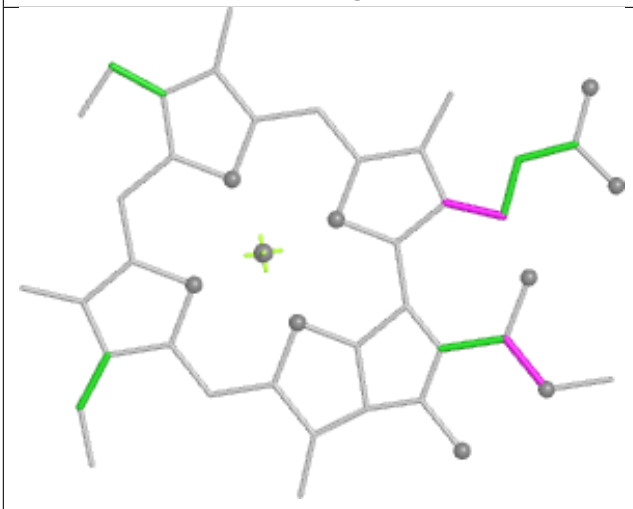
Ligand CLA u 511



Bond lengths



Bond angles

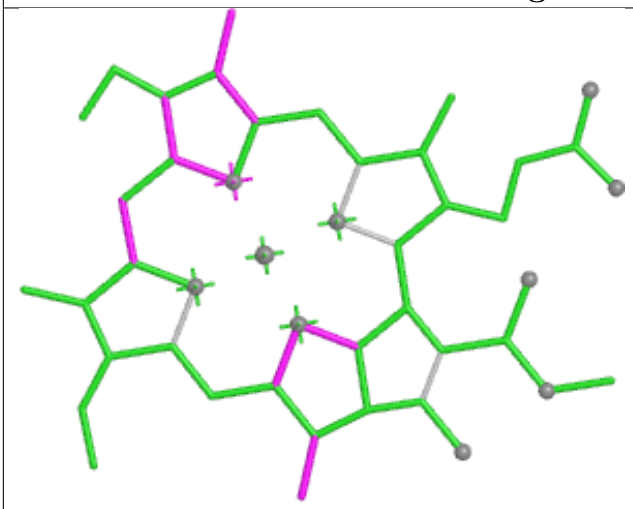


Torsions

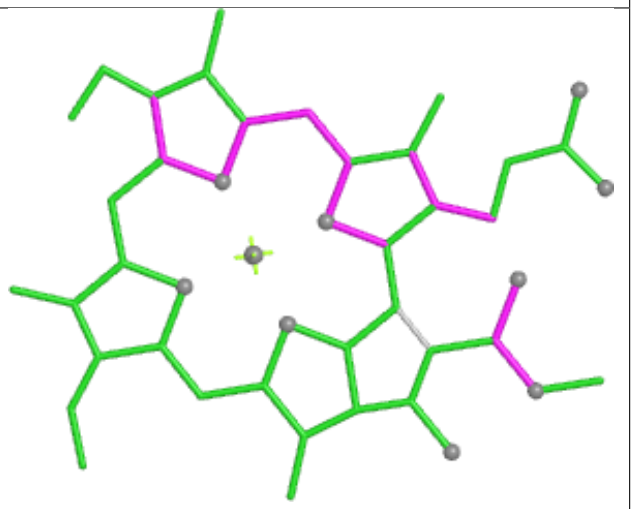


Rings

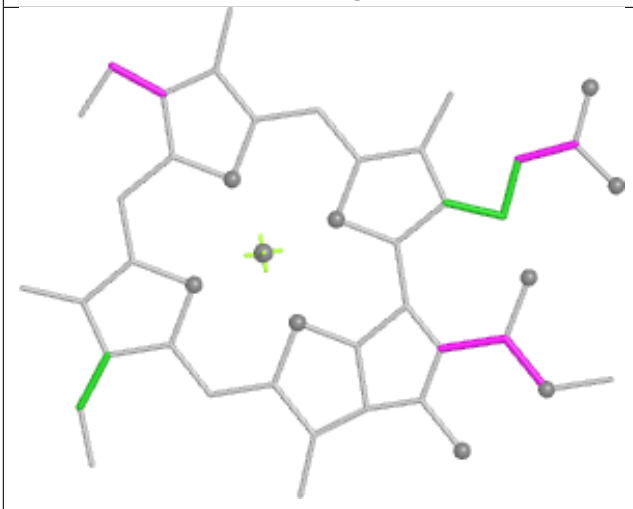
Ligand CLA 5 512



Bond lengths



Bond angles

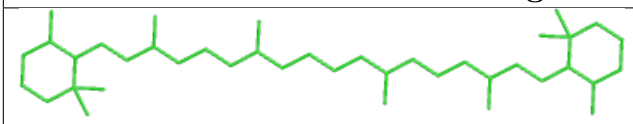


Torsions

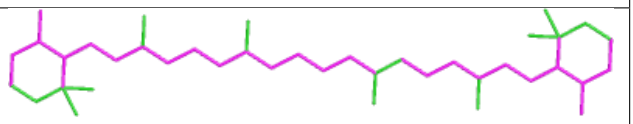


Rings

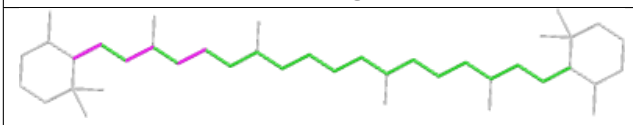
Ligand BCR 5 522



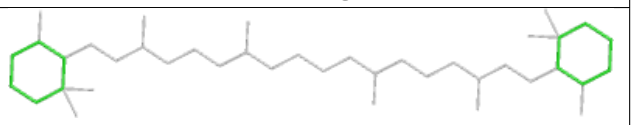
Bond lengths



Bond angles

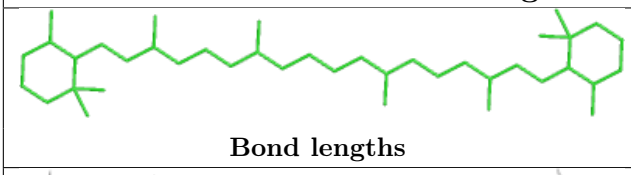


Torsions

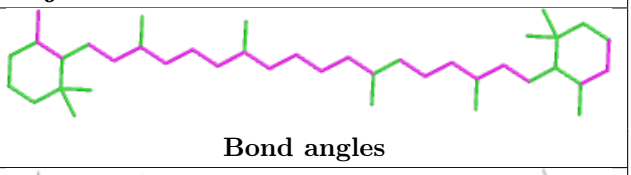


Rings

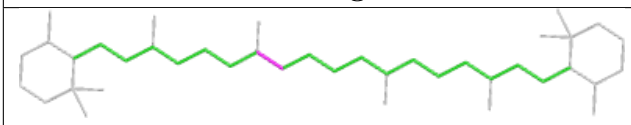
Ligand BCR j 4016



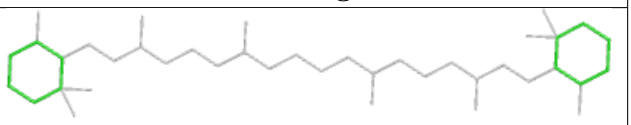
Bond lengths



Bond angles

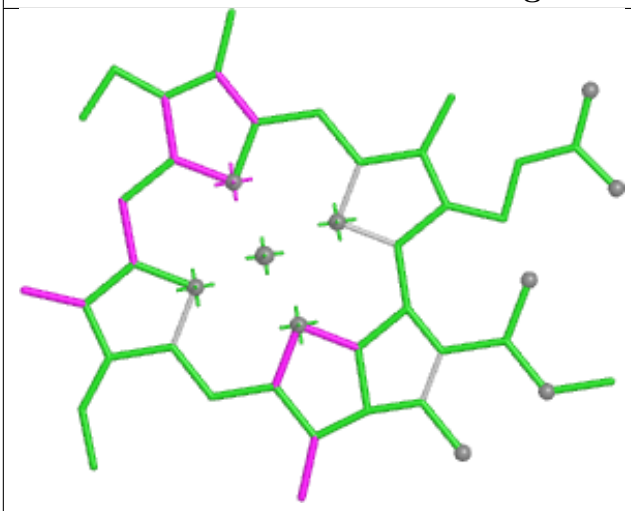


Torsions

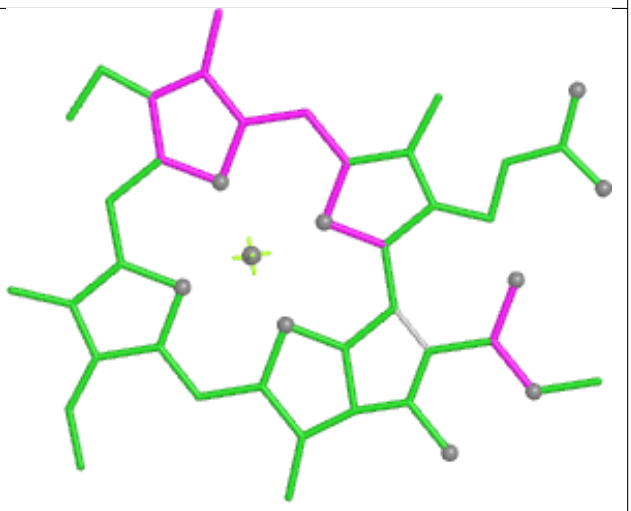


Rings

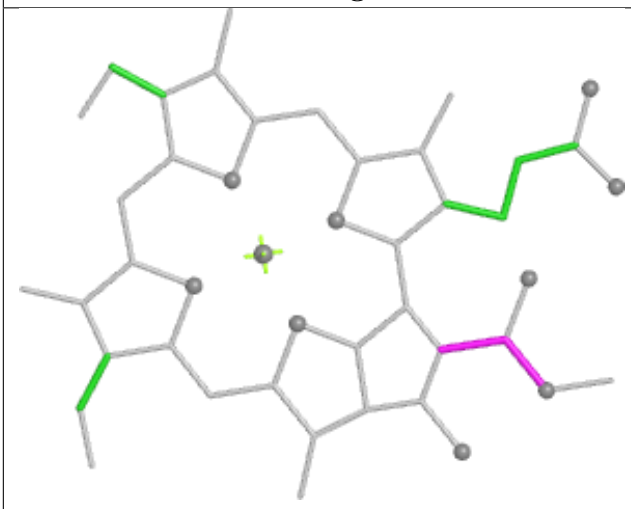
Ligand CLA Y 506



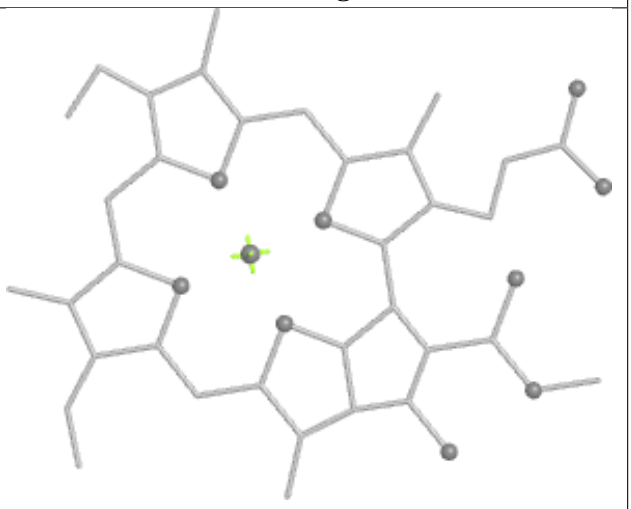
Bond lengths



Bond angles

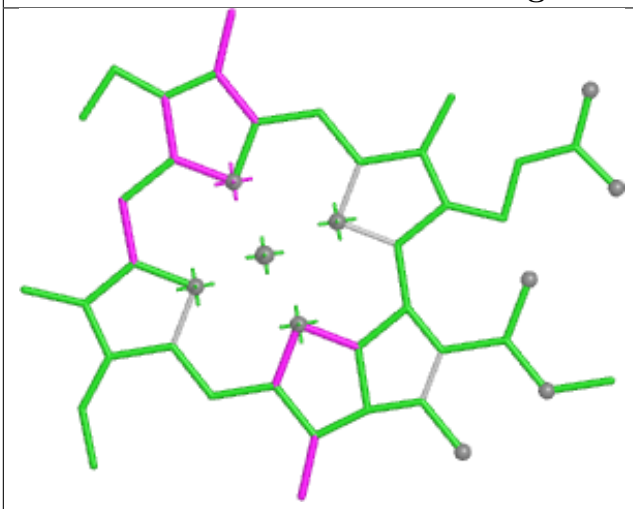


Torsions

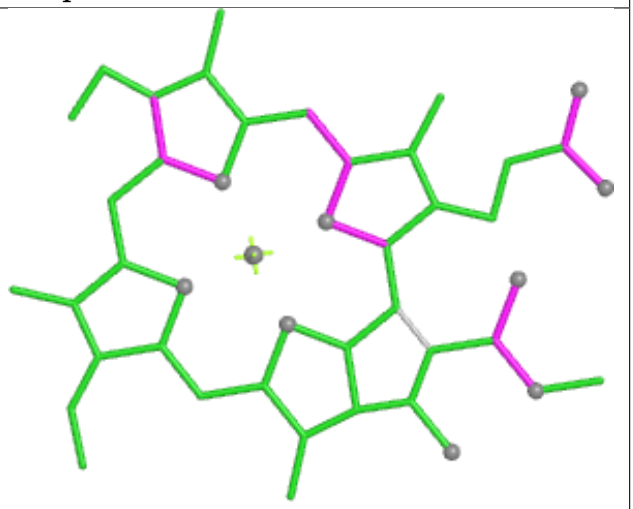


Rings

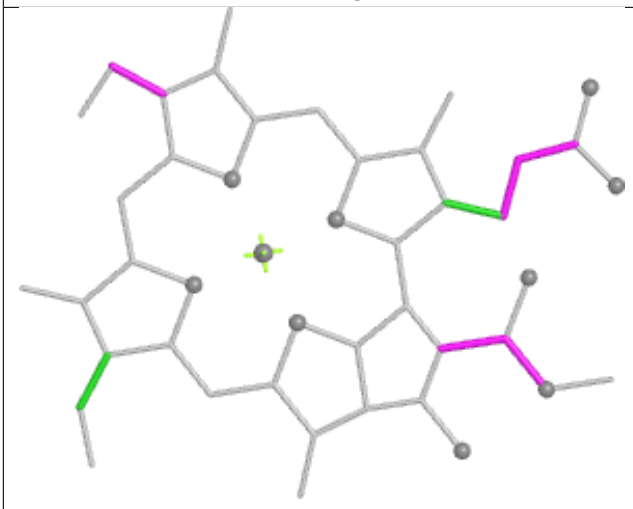
Ligand CLA q 517



Bond lengths



Bond angles

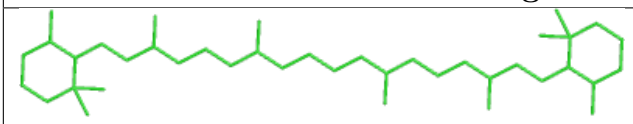


Torsions

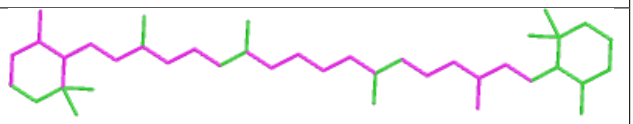


Rings

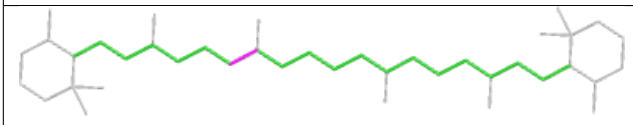
Ligand BCR Y 524



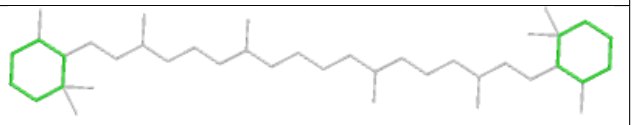
Bond lengths



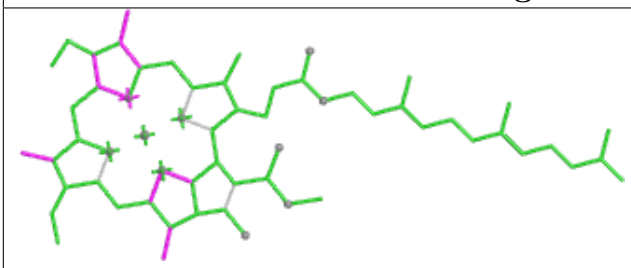
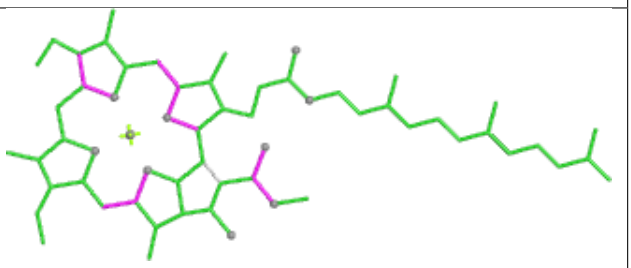
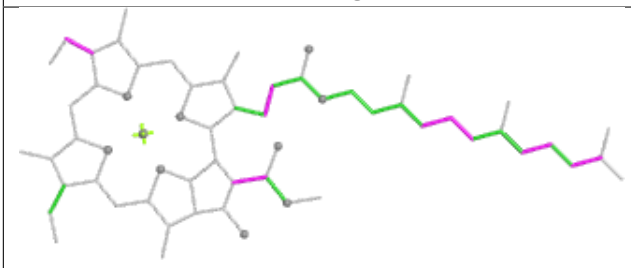
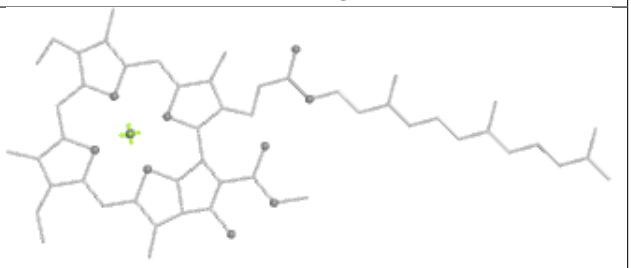
Bond angles

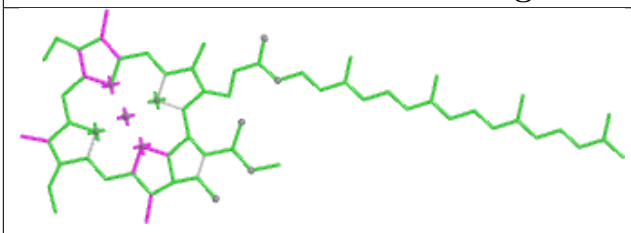
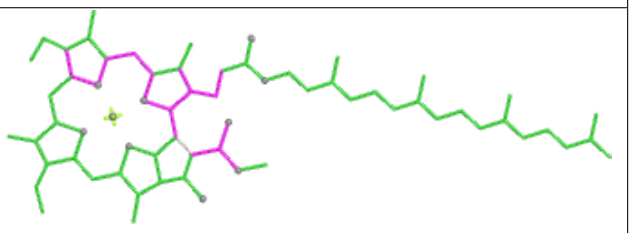
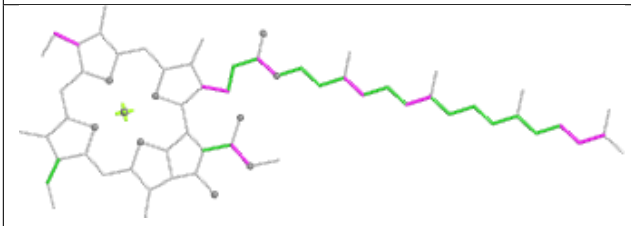
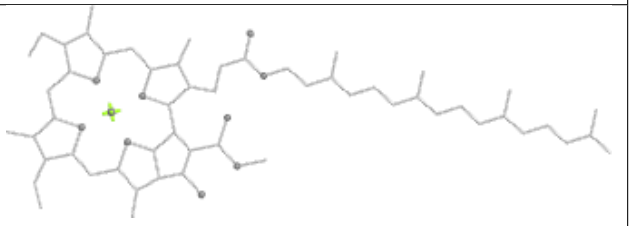


Torsions

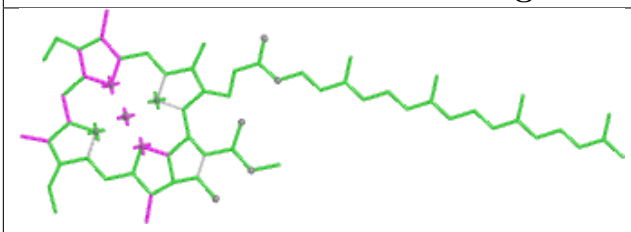


Rings

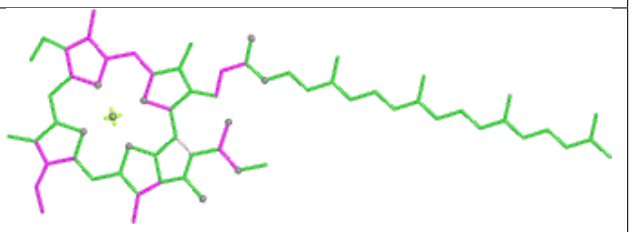
Ligand CLA H 1218	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1140	
 Bond lengths	 Bond angles
 Torsions	 Rings

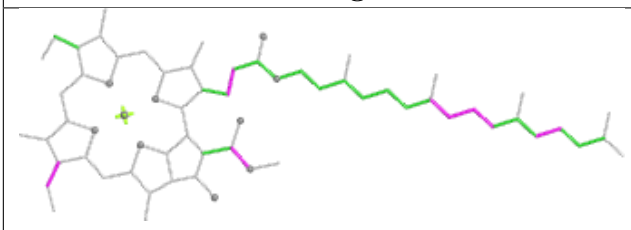
Ligand CLA B 1023



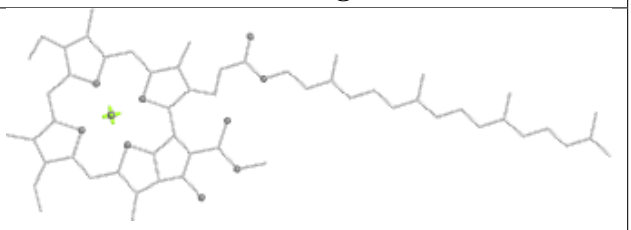
Bond lengths



Bond angles

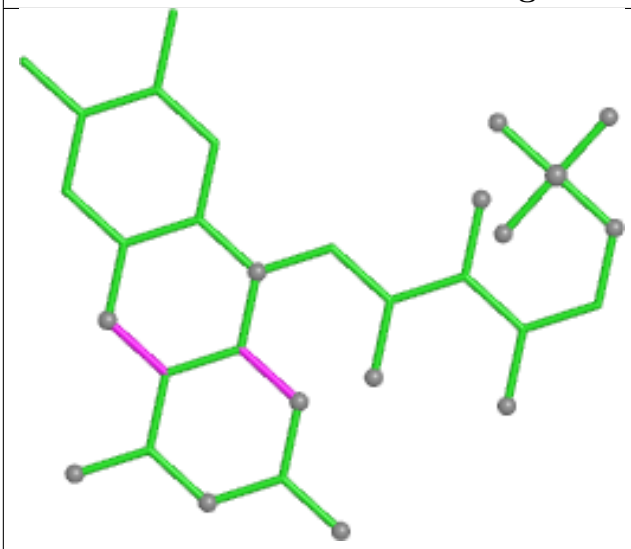


Torsions

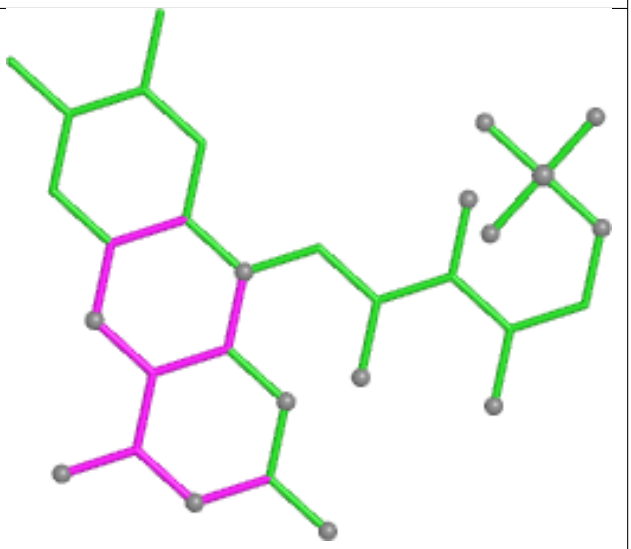


Rings

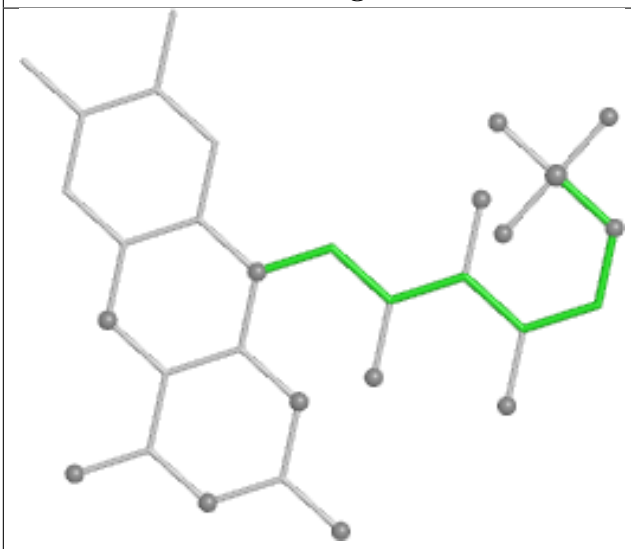
Ligand FMN X 170



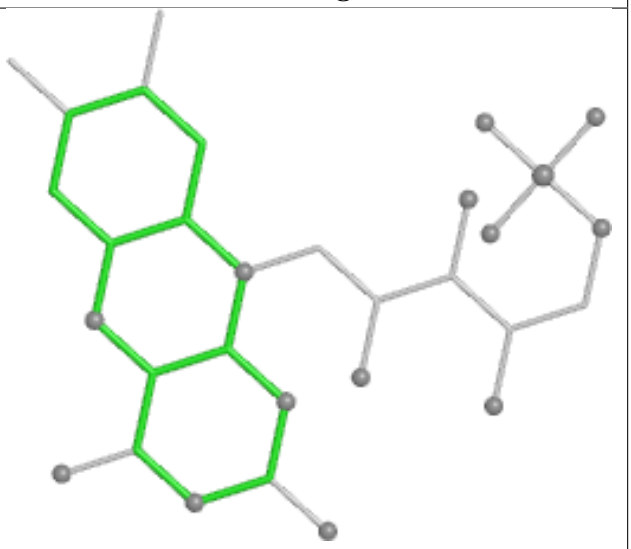
Bond lengths



Bond angles

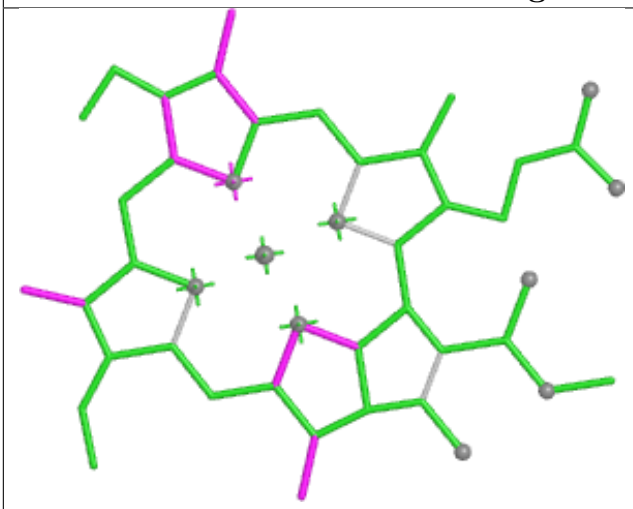


Torsions

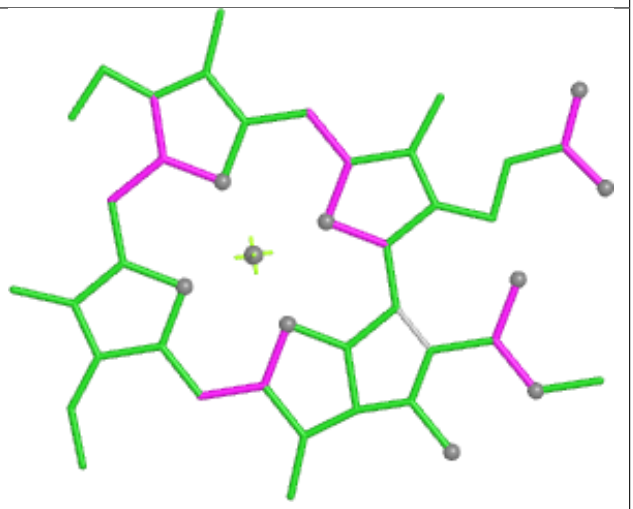


Rings

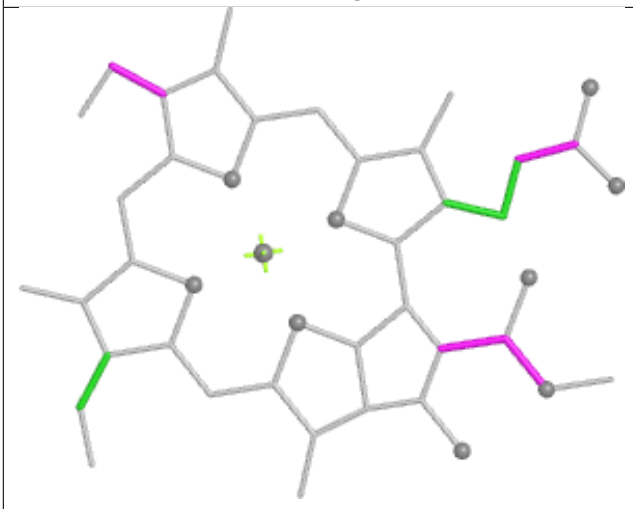
Ligand CLA 2 519



Bond lengths



Bond angles

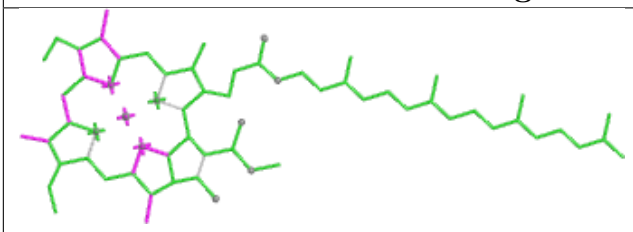


Torsions

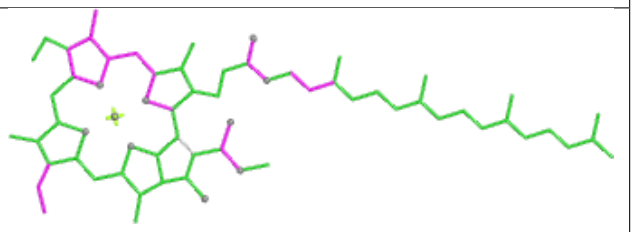


Rings

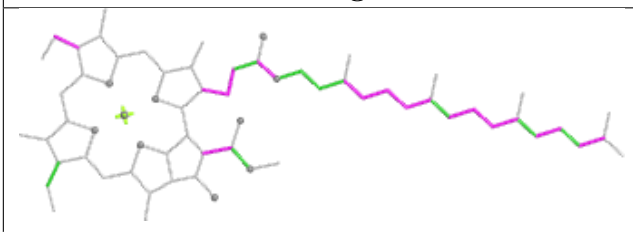
Ligand CLA H 1210



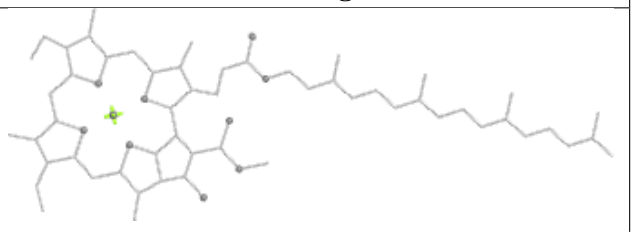
Bond lengths



Bond angles

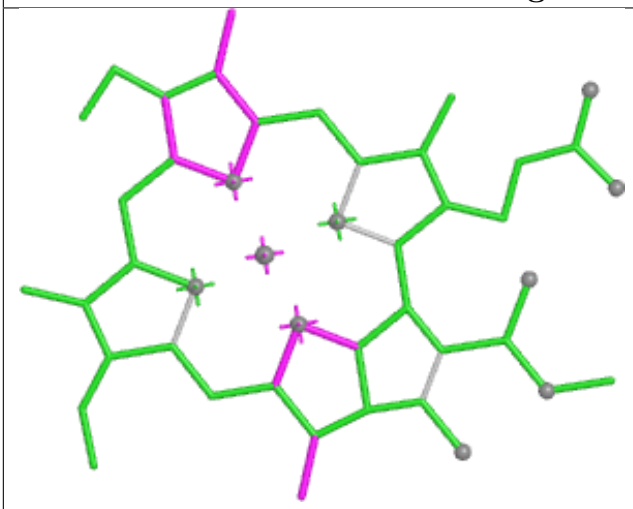


Torsions

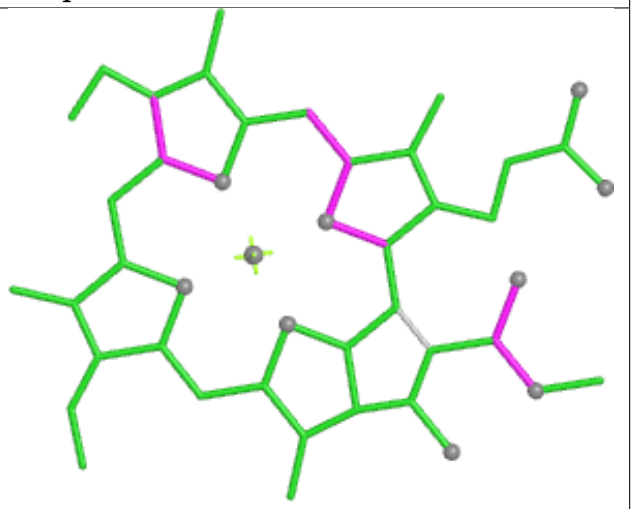


Rings

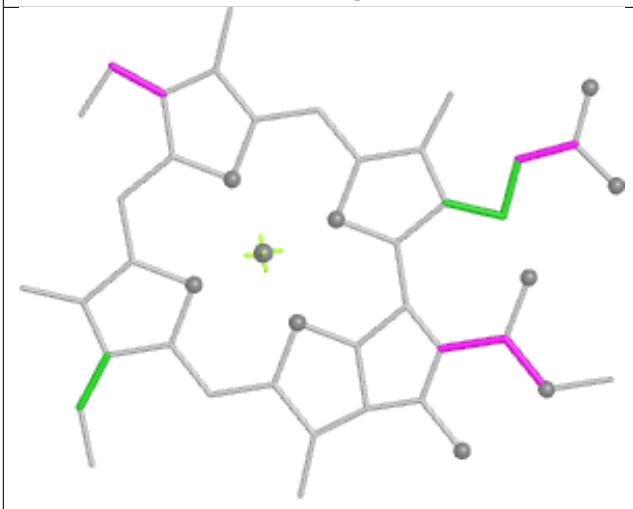
Ligand CLA q 512



Bond lengths



Bond angles

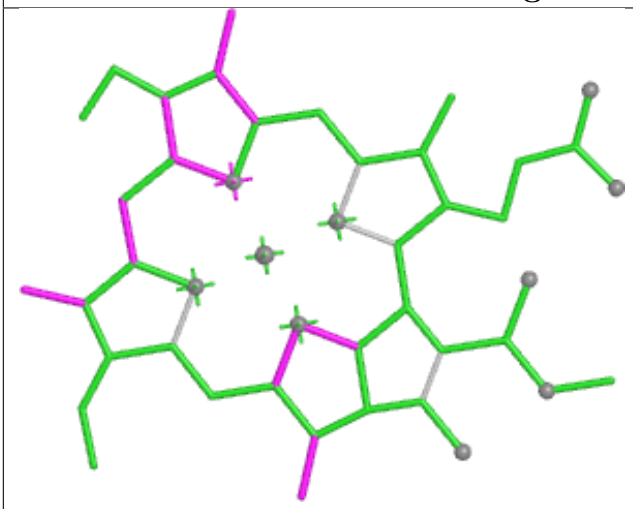


Torsions

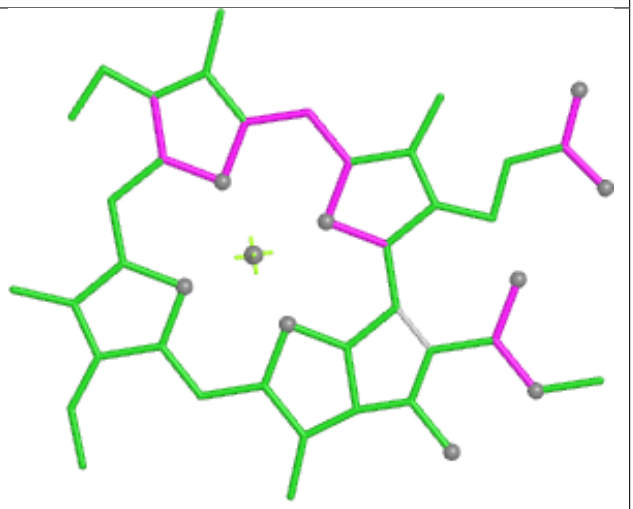


Rings

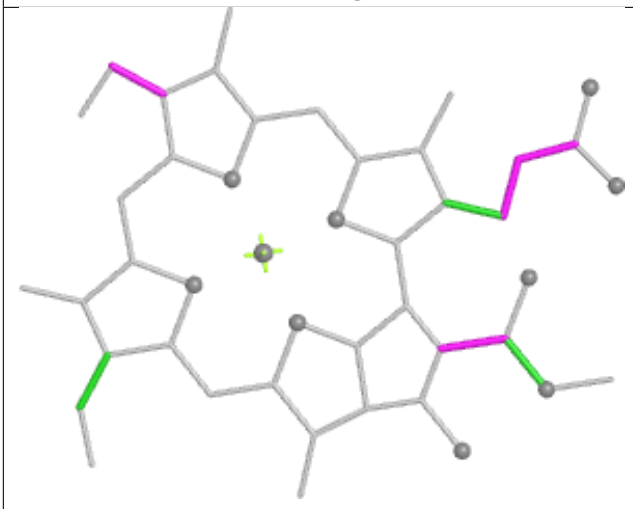
Ligand CLA Y 513



Bond lengths



Bond angles

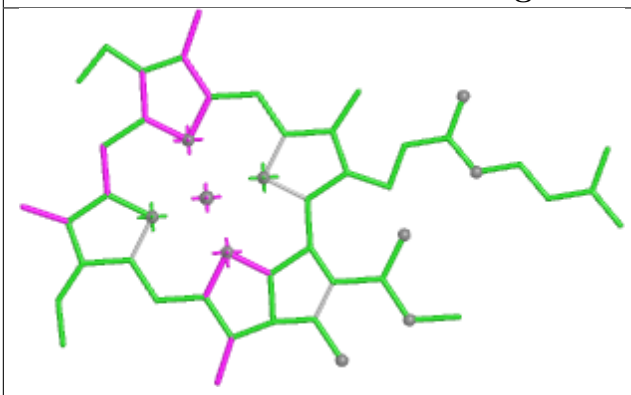


Torsions

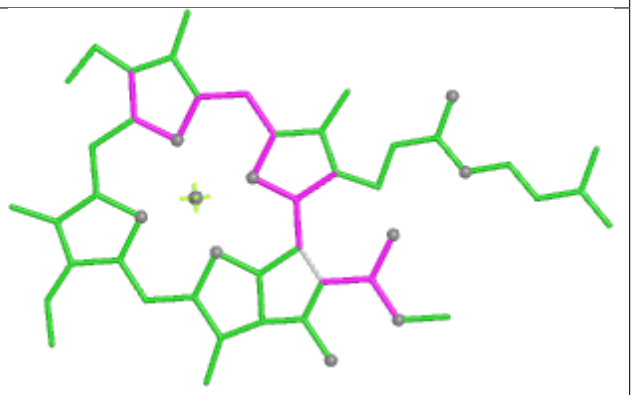


Rings

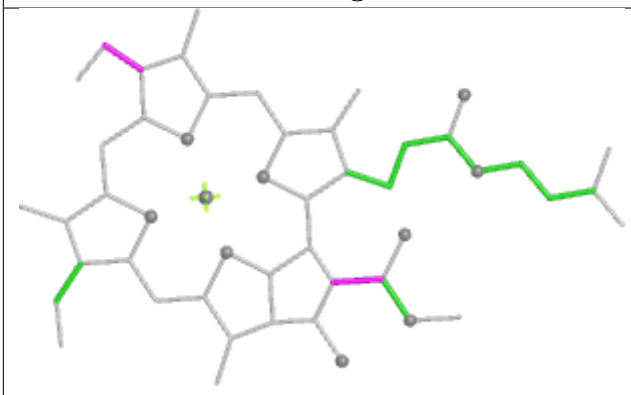
Ligand CLA A 1112



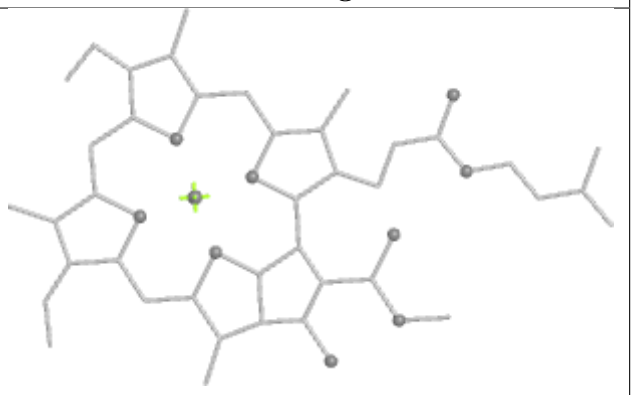
Bond lengths



Bond angles

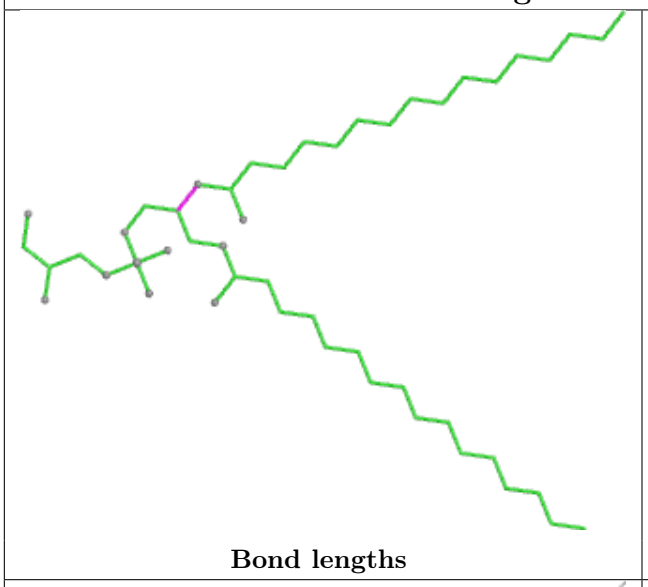


Torsions

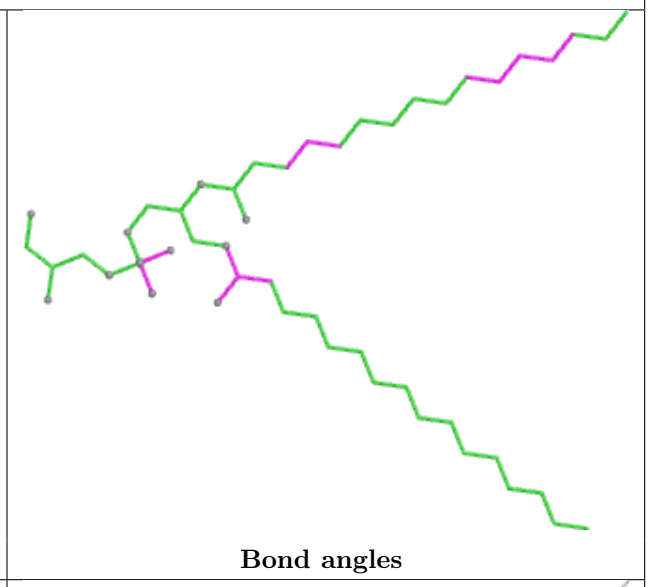


Rings

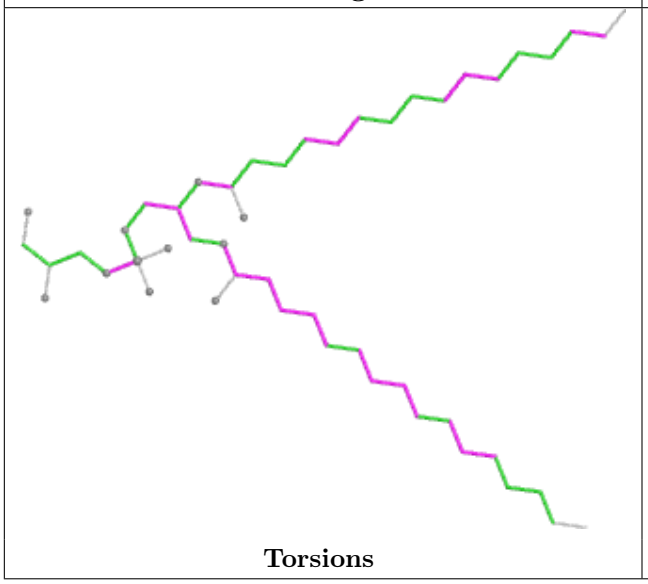
Ligand LHG G 5001



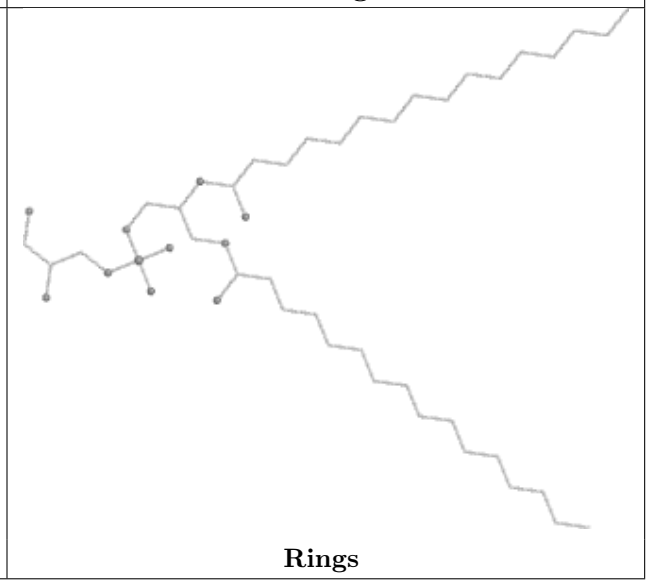
Bond lengths



Bond angles

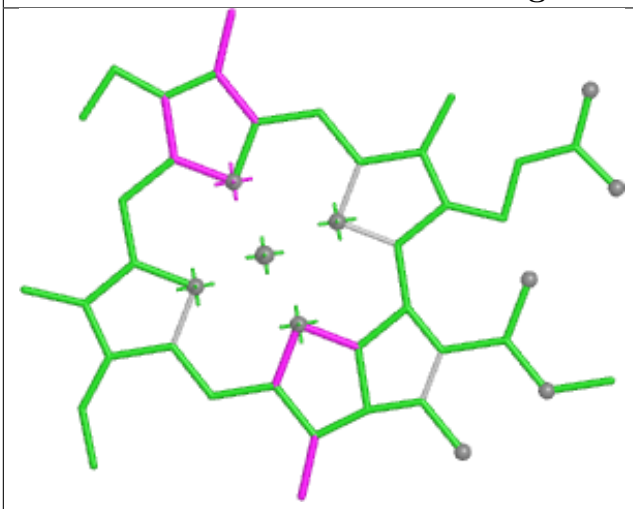


Torsions

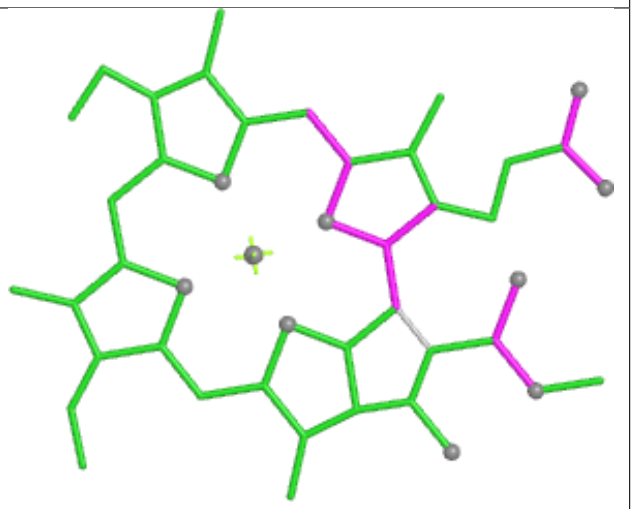


Rings

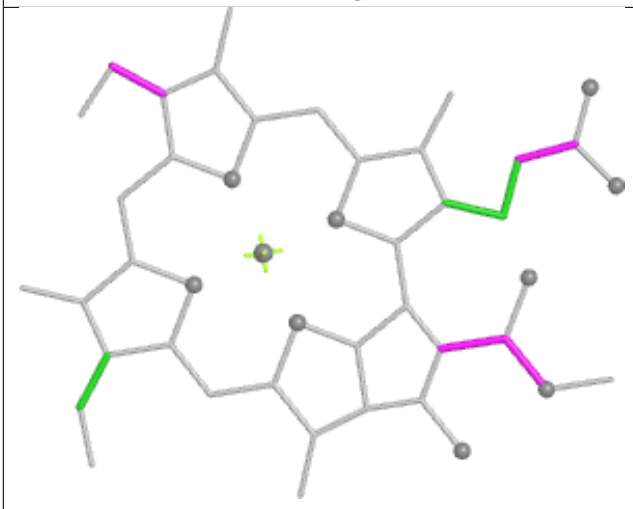
Ligand CLA 6 507



Bond lengths



Bond angles

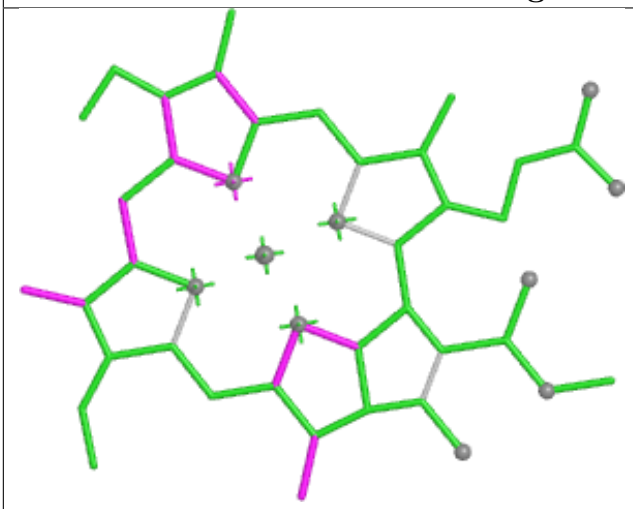


Torsions

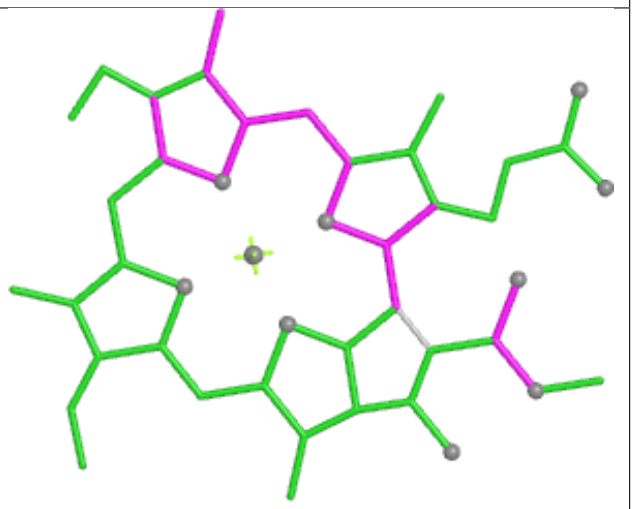


Rings

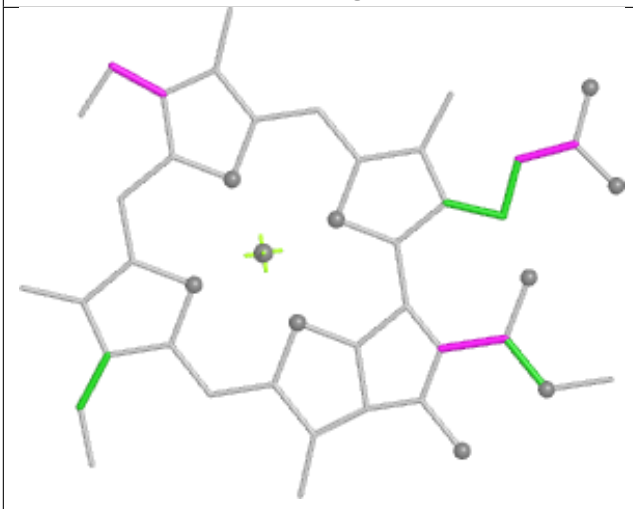
Ligand CLA d 504



Bond lengths



Bond angles

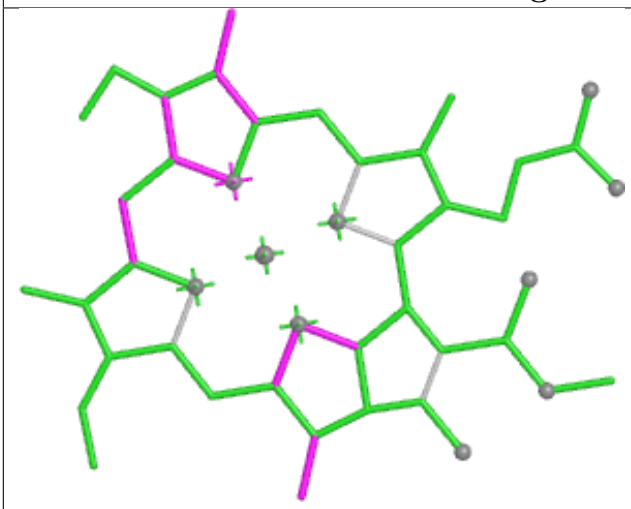


Torsions

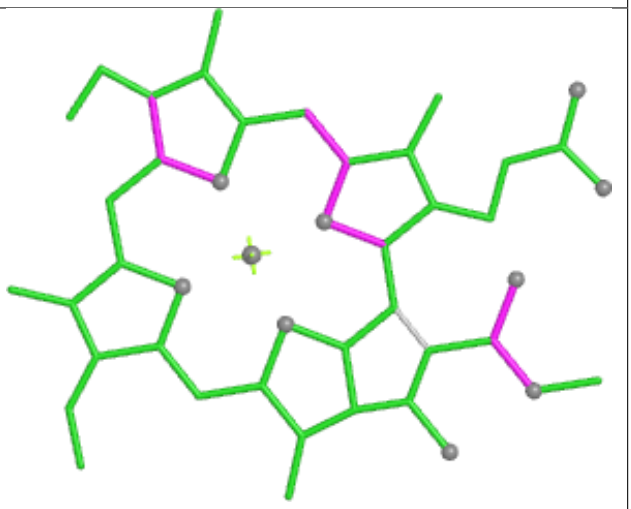


Rings

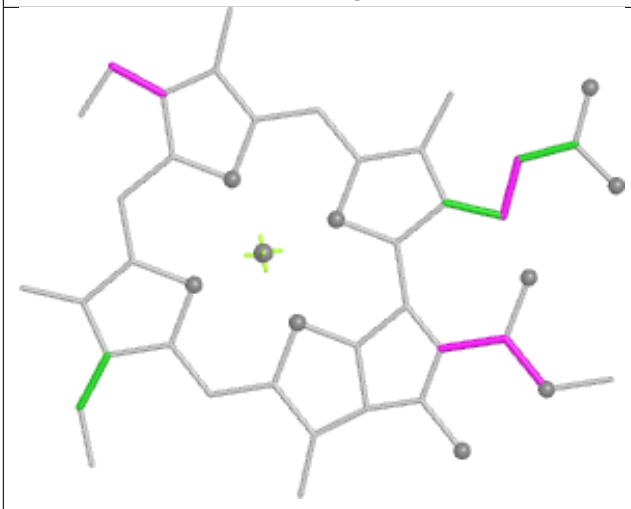
Ligand CLA t 518



Bond lengths



Bond angles

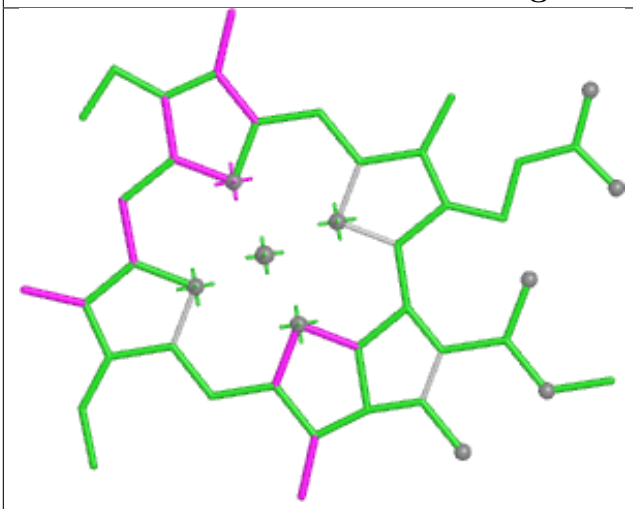


Torsions

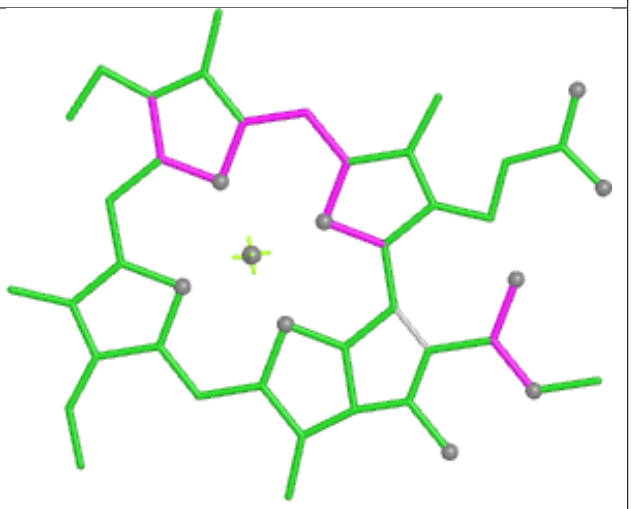


Rings

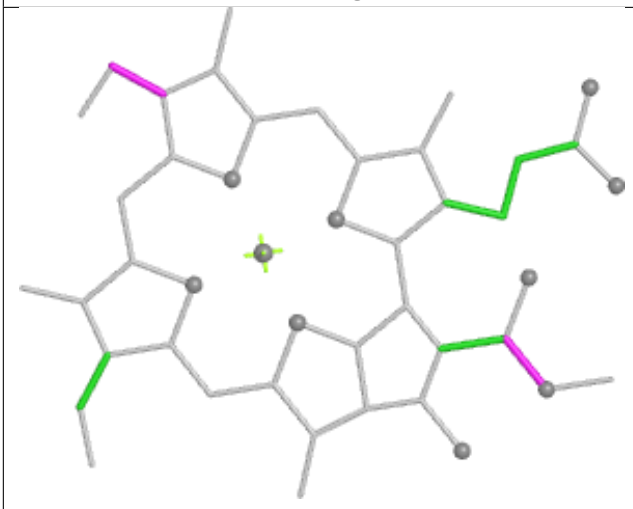
Ligand CLA r 513



Bond lengths



Bond angles

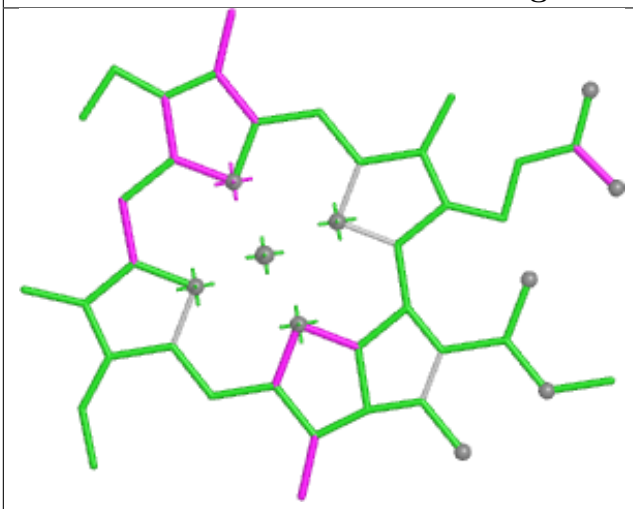


Torsions

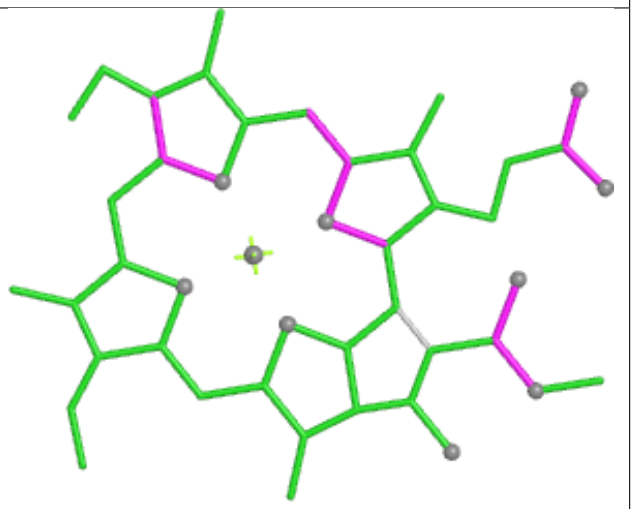


Rings

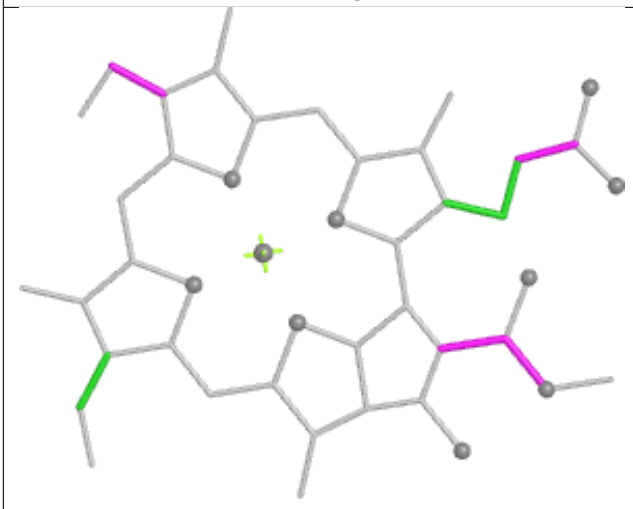
Ligand CLA s 510



Bond lengths



Bond angles

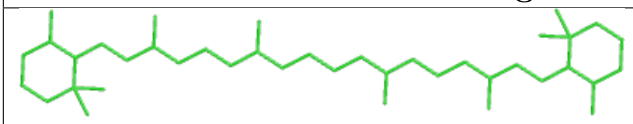


Torsions

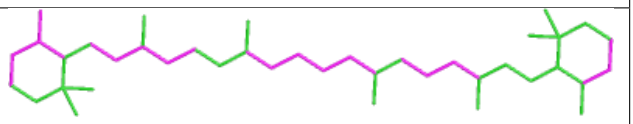


Rings

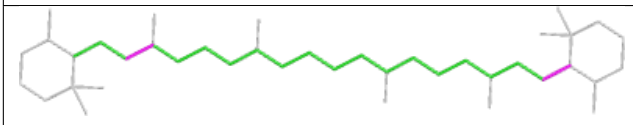
Ligand BCR L 4022



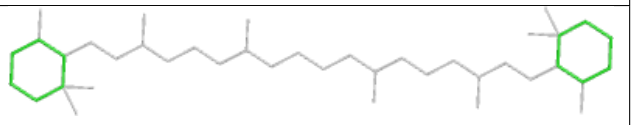
Bond lengths



Bond angles

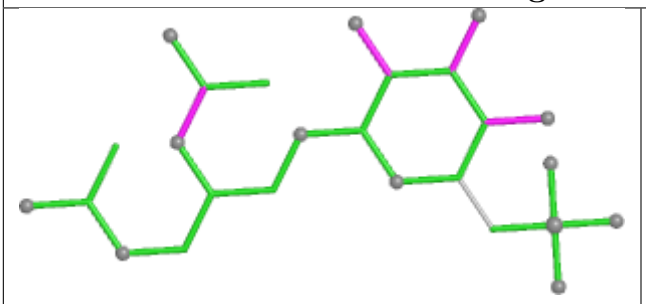


Torsions

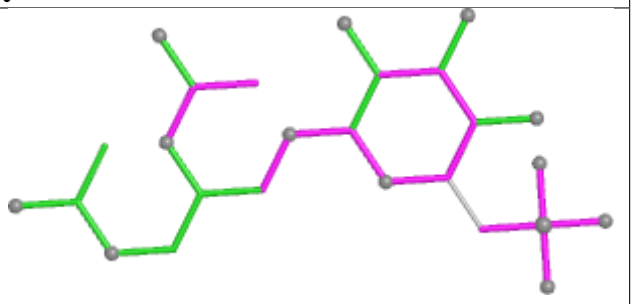


Rings

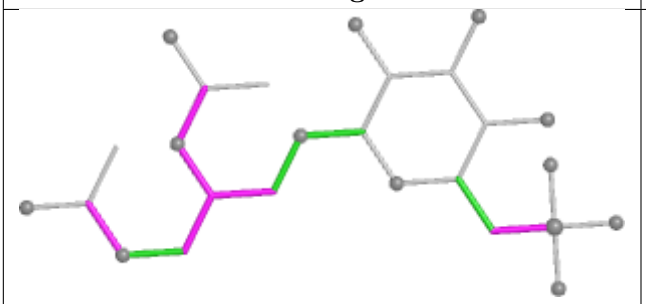
Ligand SQD 4 822



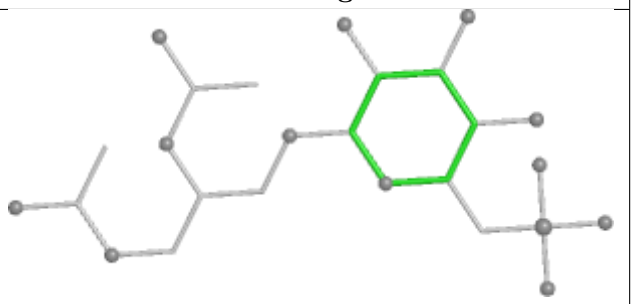
Bond lengths



Bond angles

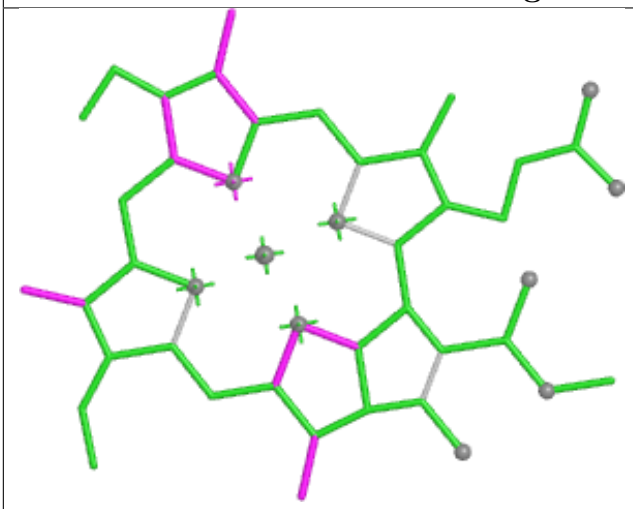


Torsions

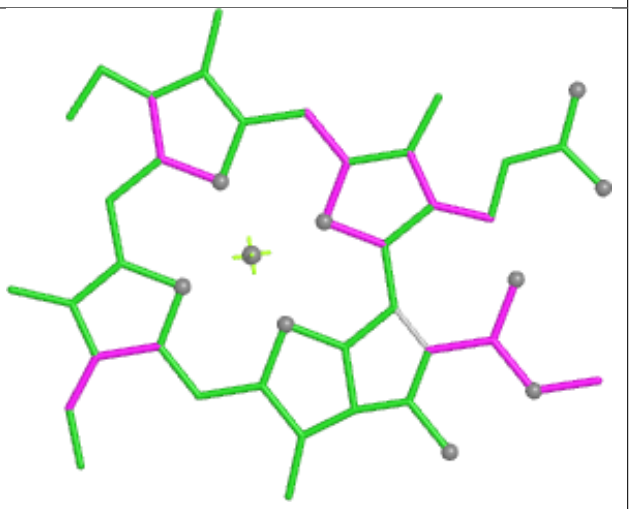


Rings

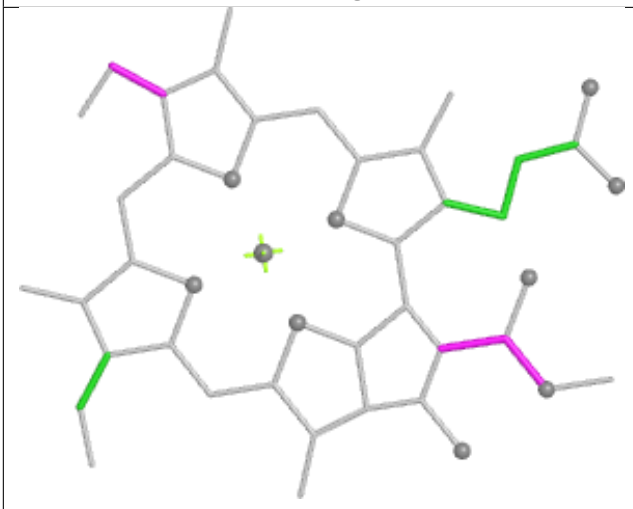
Ligand CLA Y 504



Bond lengths



Bond angles

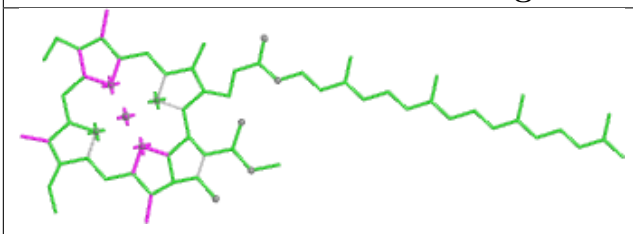


Torsions

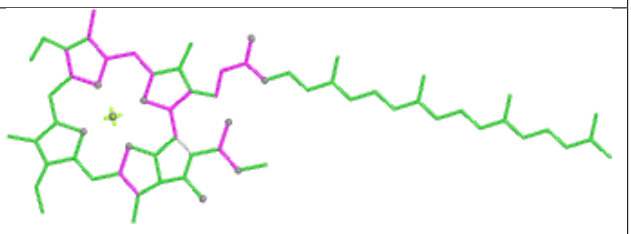


Rings

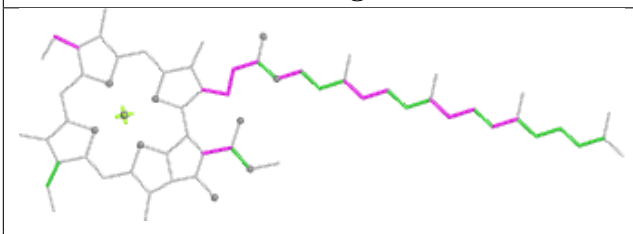
Ligand CLA A 1107



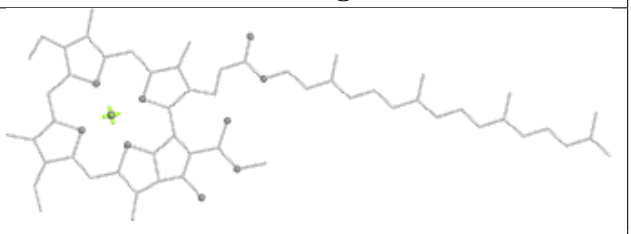
Bond lengths



Bond angles

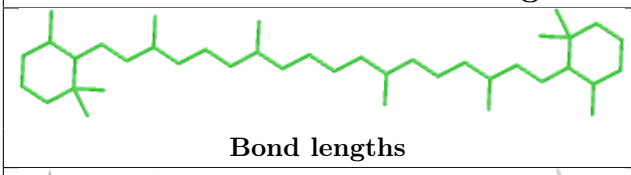


Torsions

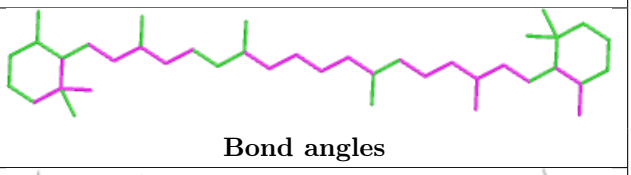


Rings

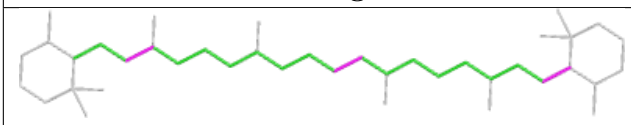
Ligand BCR l 4015



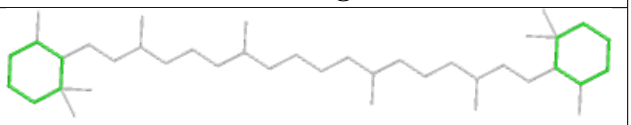
Bond lengths



Bond angles

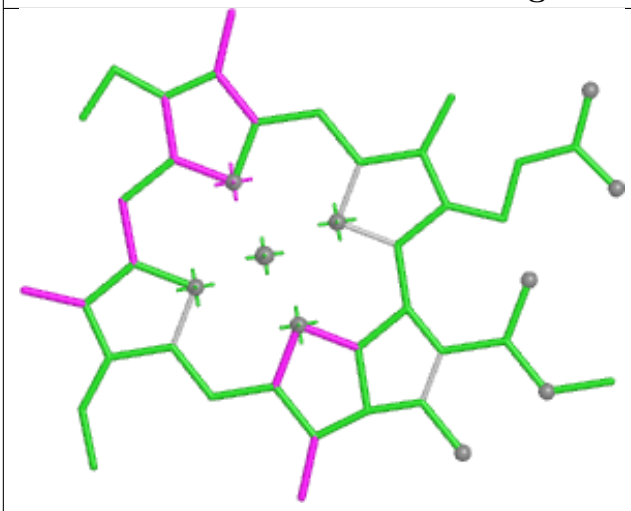


Torsions

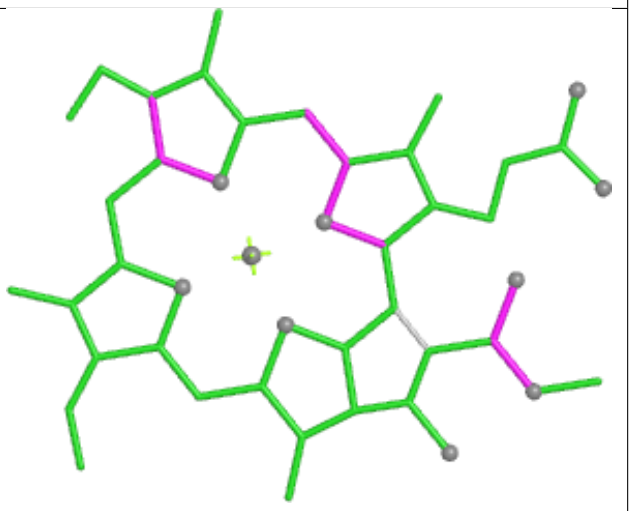


Rings

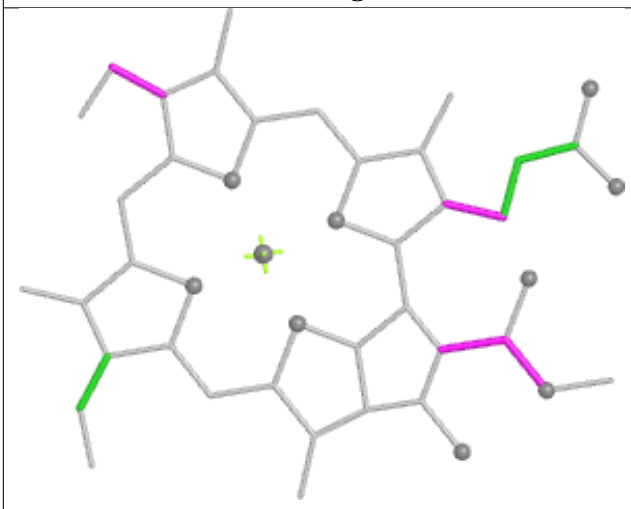
Ligand CLA 3 517



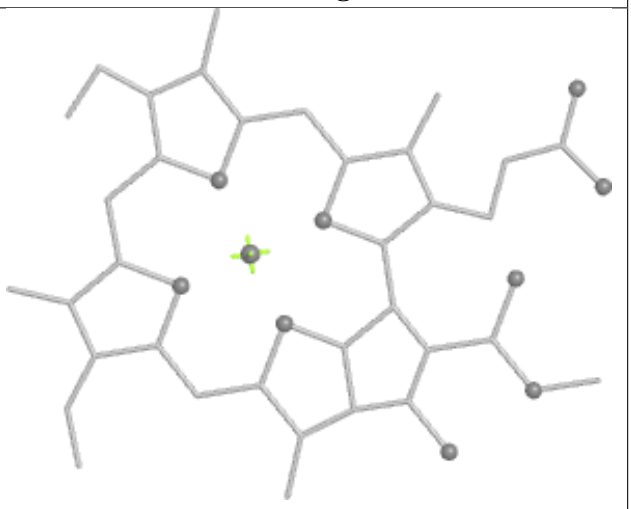
Bond lengths



Bond angles

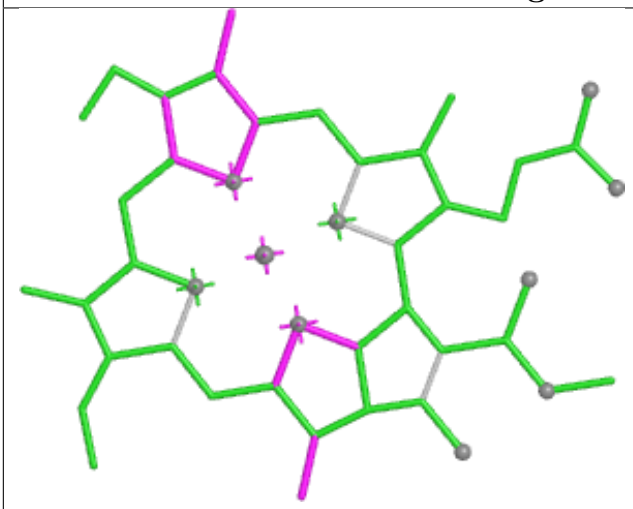


Torsions

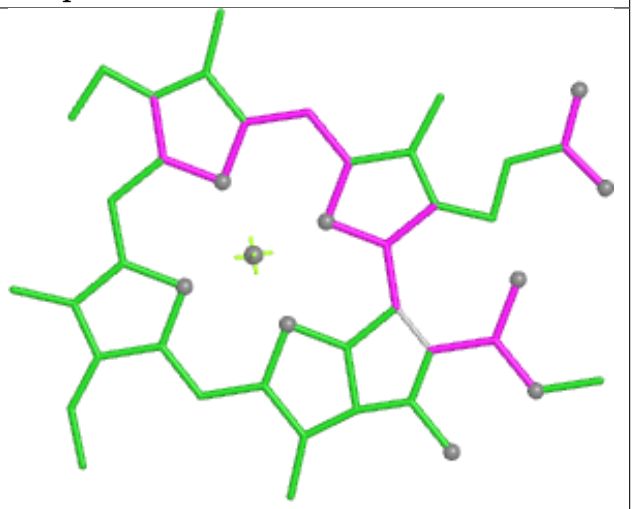


Rings

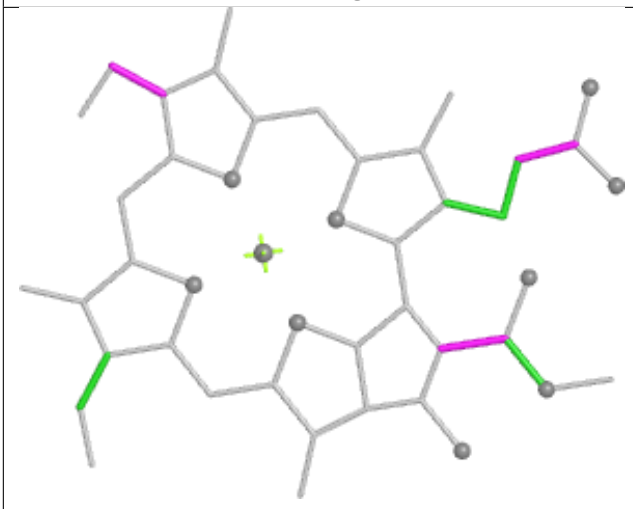
Ligand CLA q 509



Bond lengths



Bond angles

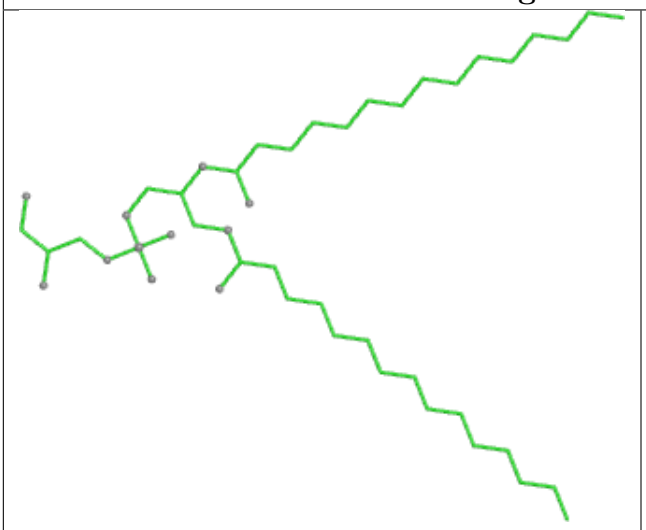


Torsions

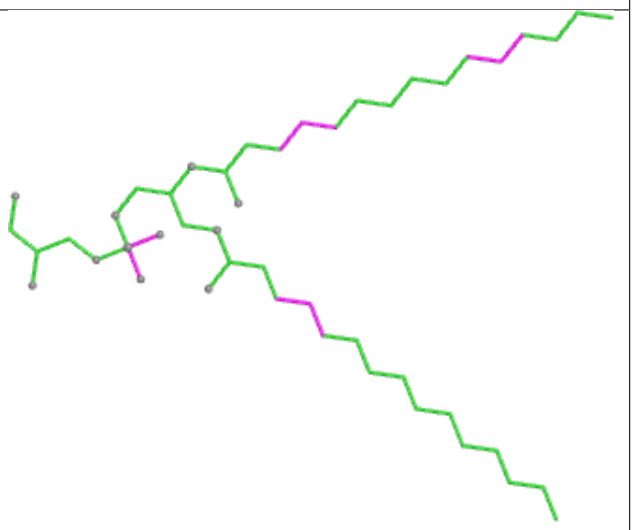


Rings

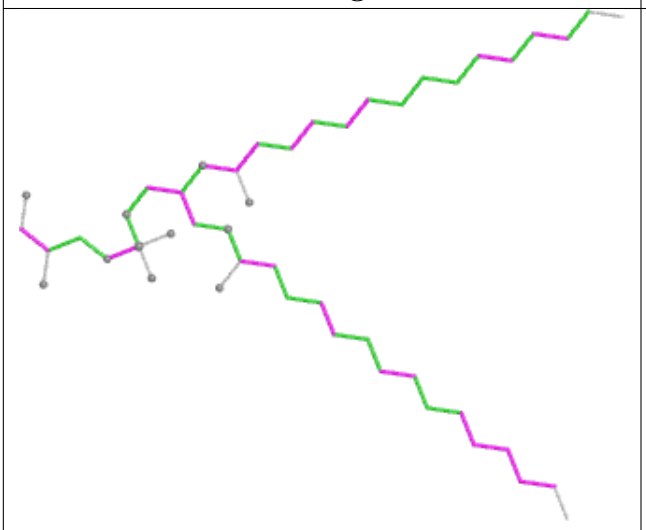
Ligand LHG e 5007



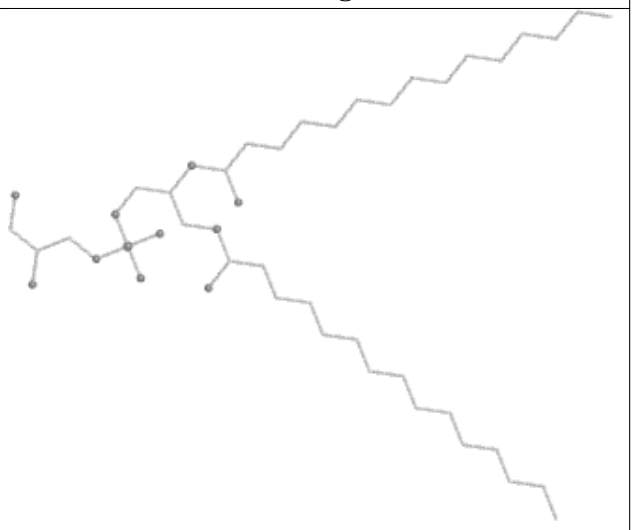
Bond lengths



Bond angles

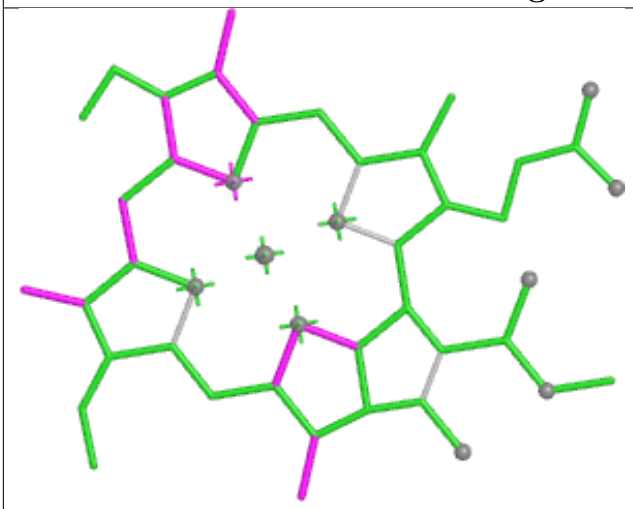


Torsions

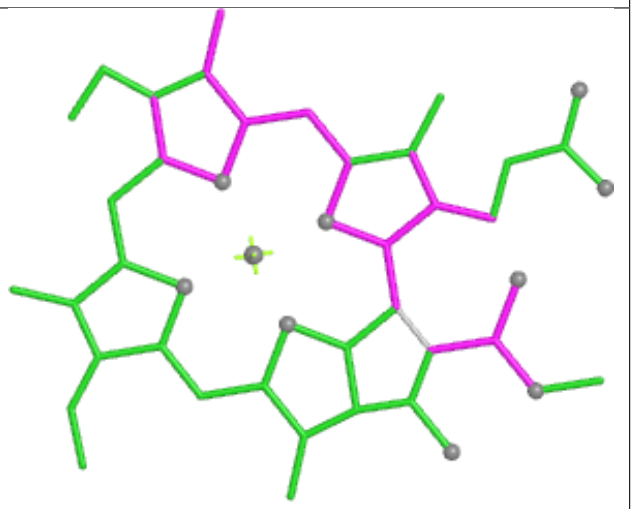


Rings

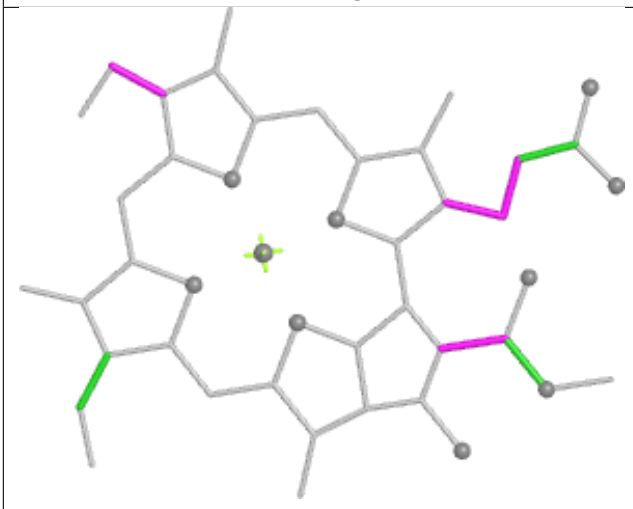
Ligand CLA 3 504



Bond lengths



Bond angles

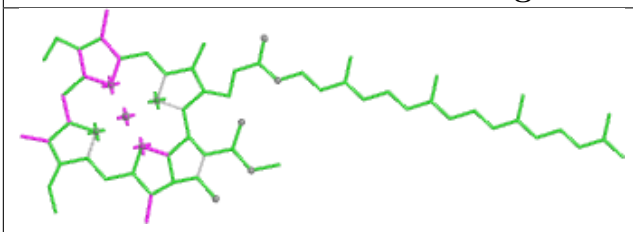


Torsions

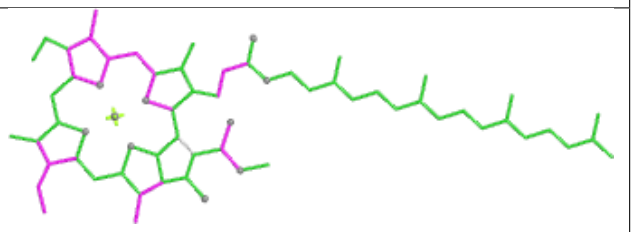


Rings

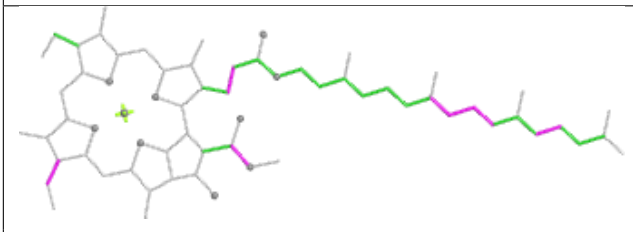
Ligand CLA H 1023



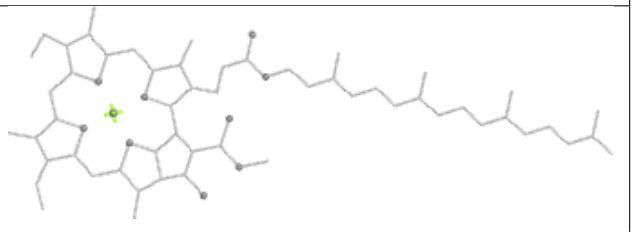
Bond lengths



Bond angles

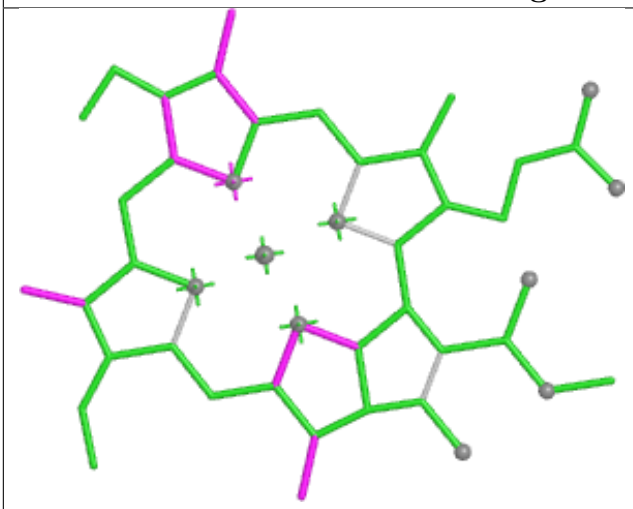


Torsions

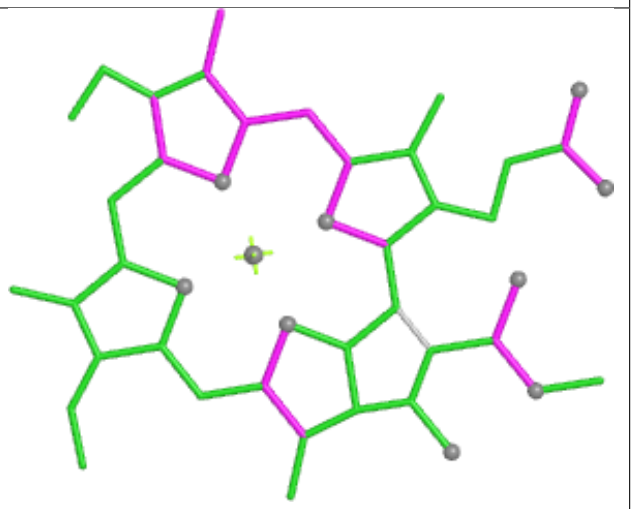


Rings

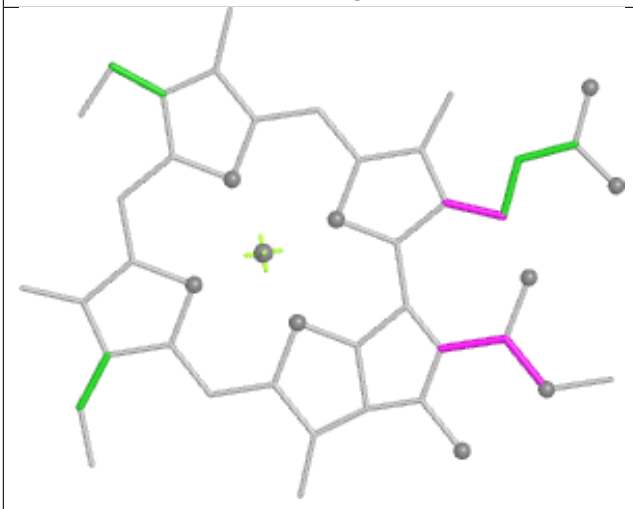
Ligand CLA r 511



Bond lengths



Bond angles

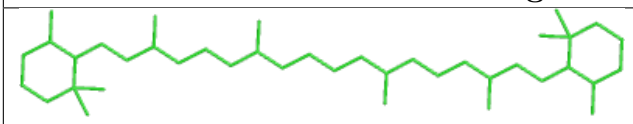


Torsions

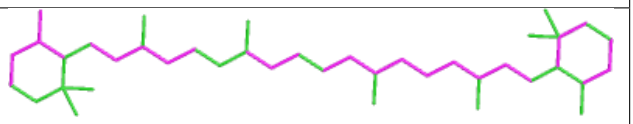


Rings

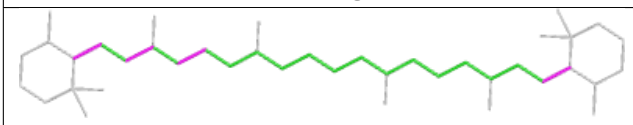
Ligand BCR 3 521



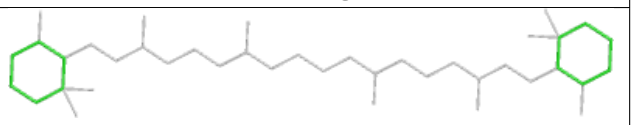
Bond lengths



Bond angles

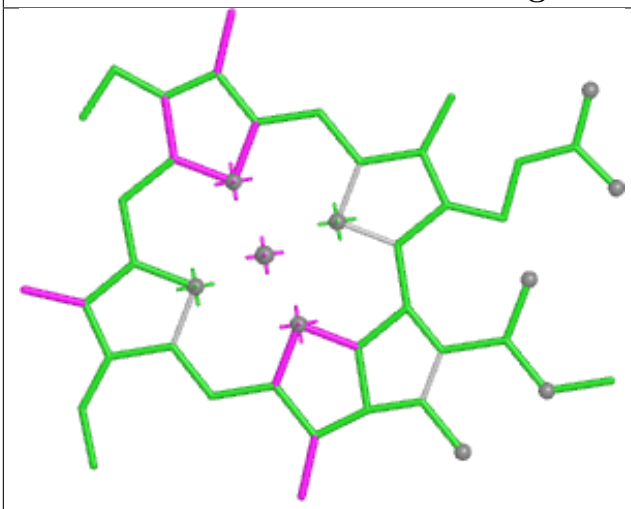


Torsions

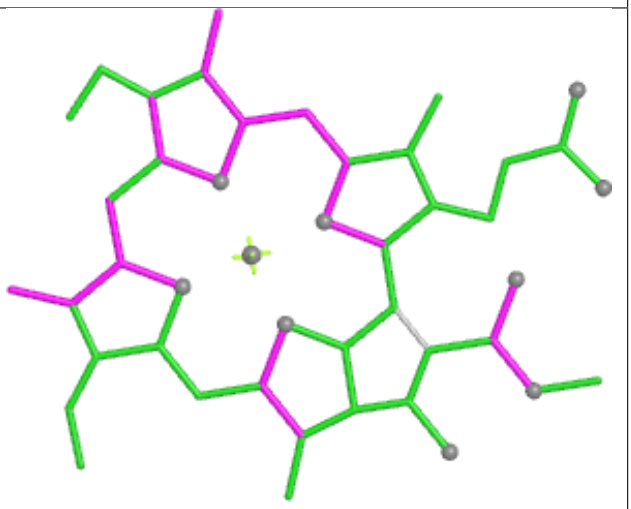


Rings

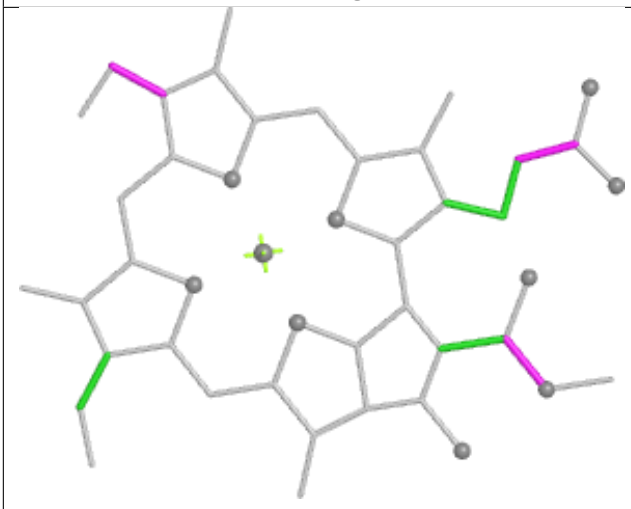
Ligand CLA 4 508



Bond lengths



Bond angles

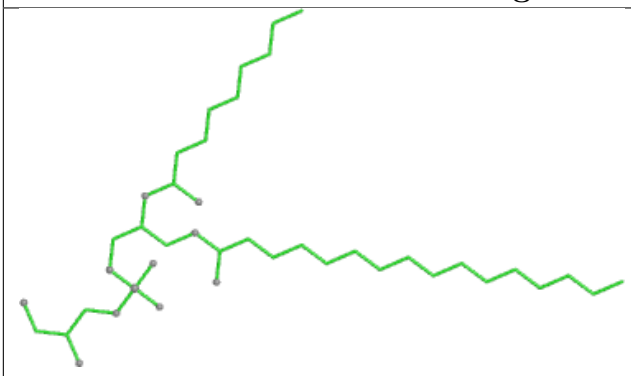


Torsions

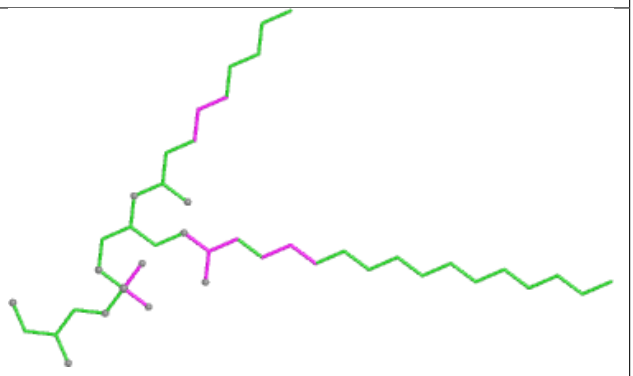


Rings

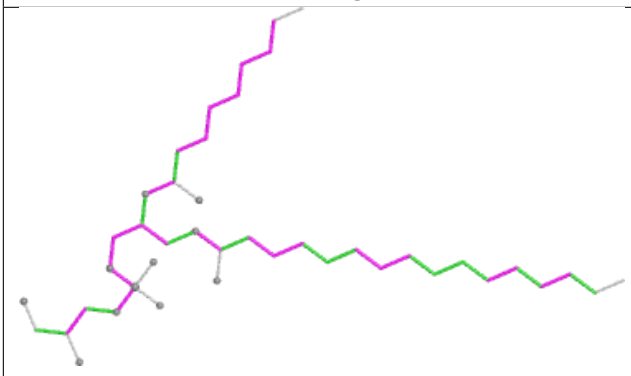
Ligand LHG A 5009



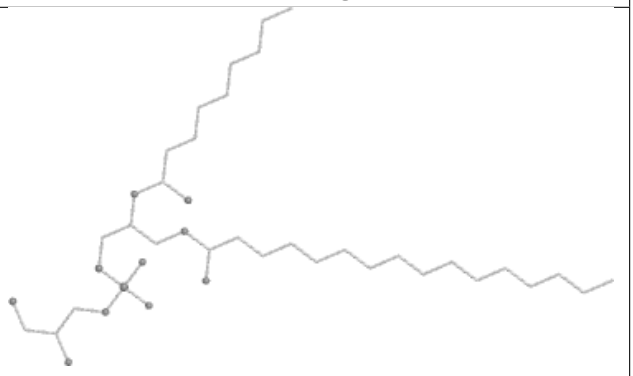
Bond lengths



Bond angles

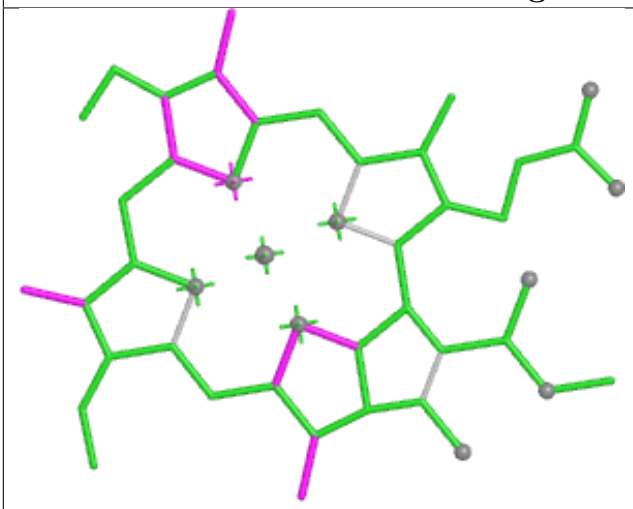


Torsions

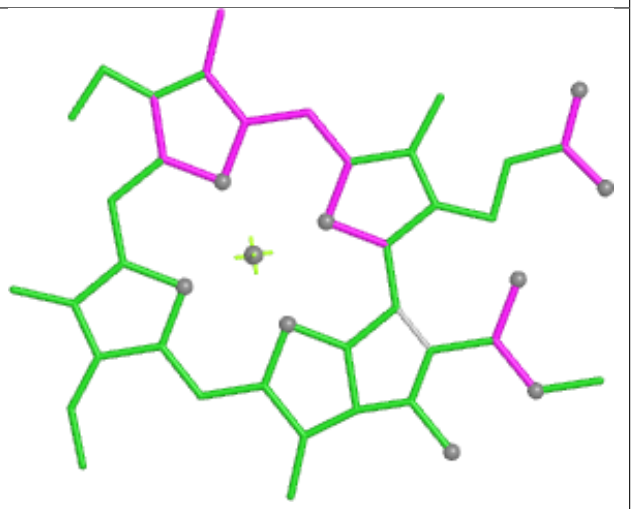


Rings

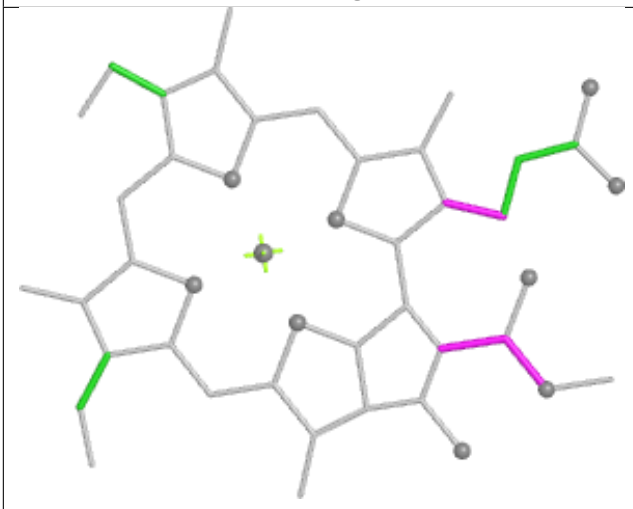
Ligand CLA 2 511



Bond lengths



Bond angles

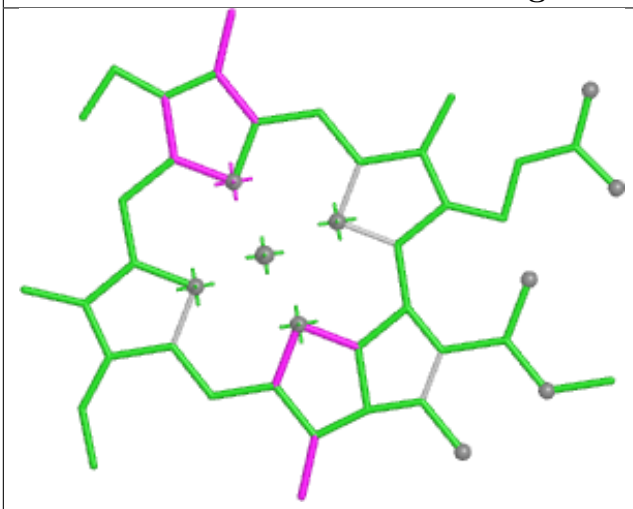


Torsions

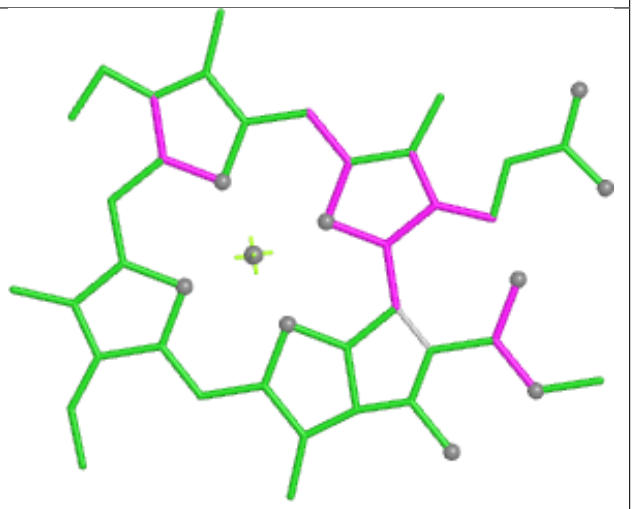


Rings

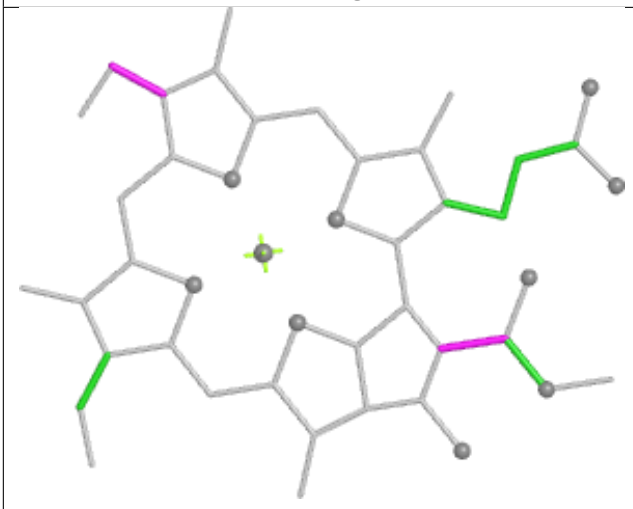
Ligand CLA 6 502



Bond lengths



Bond angles

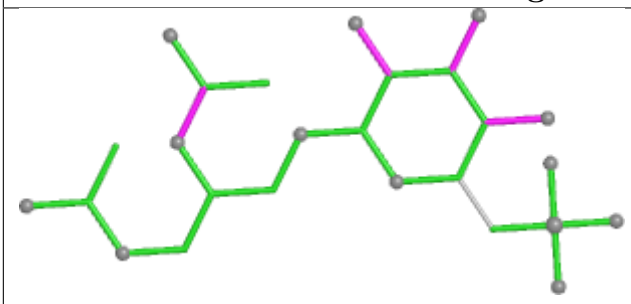


Torsions

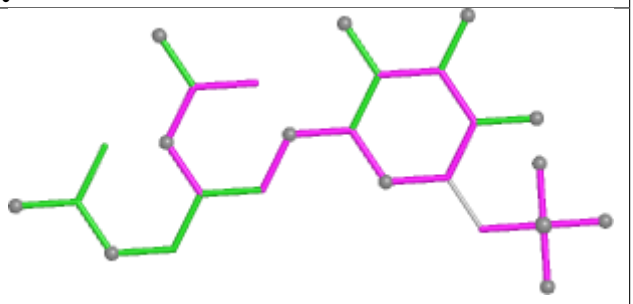


Rings

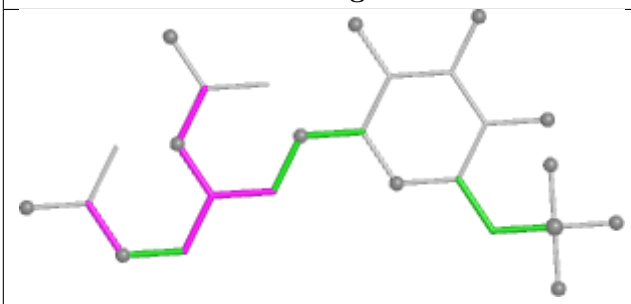
Ligand SQD d 822



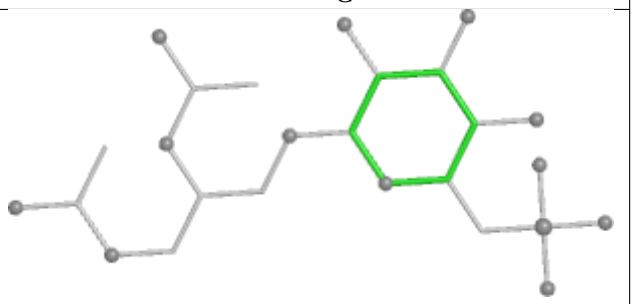
Bond lengths



Bond angles

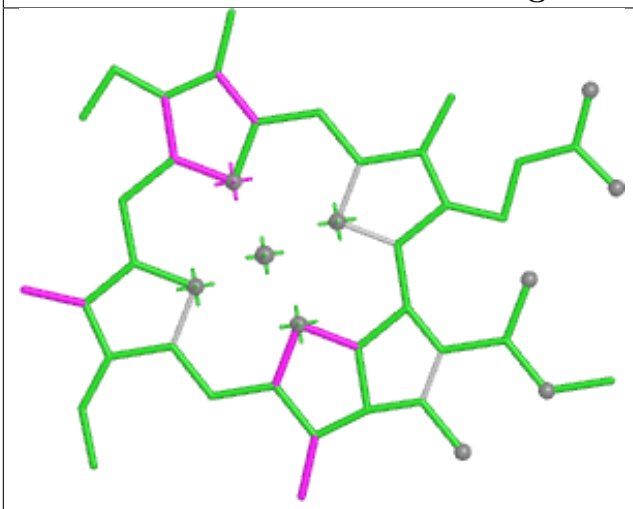


Torsions

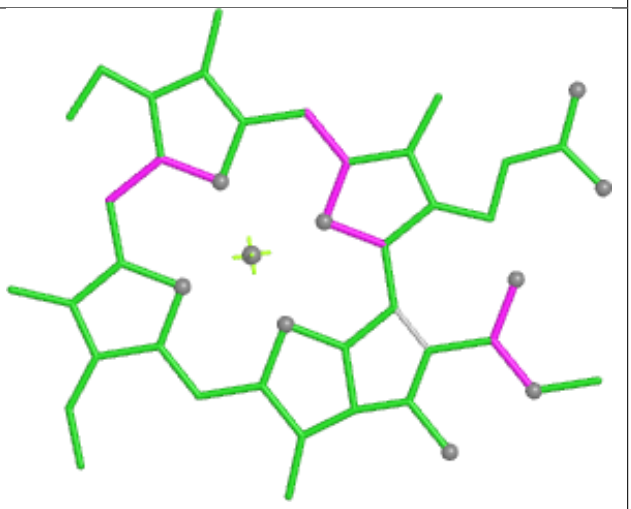


Rings

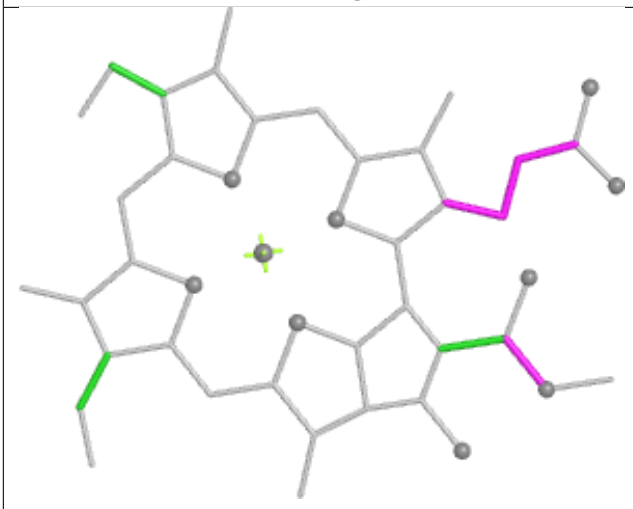
Ligand CLA 1 505



Bond lengths



Bond angles

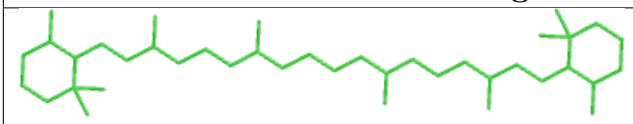


Torsions

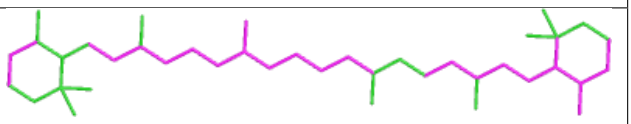


Rings

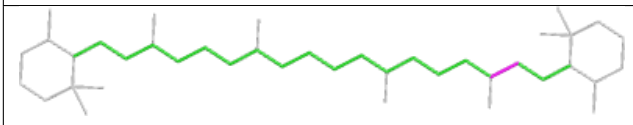
Ligand BCR m 4104



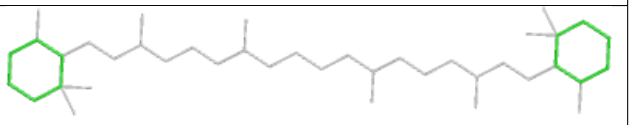
Bond lengths



Bond angles

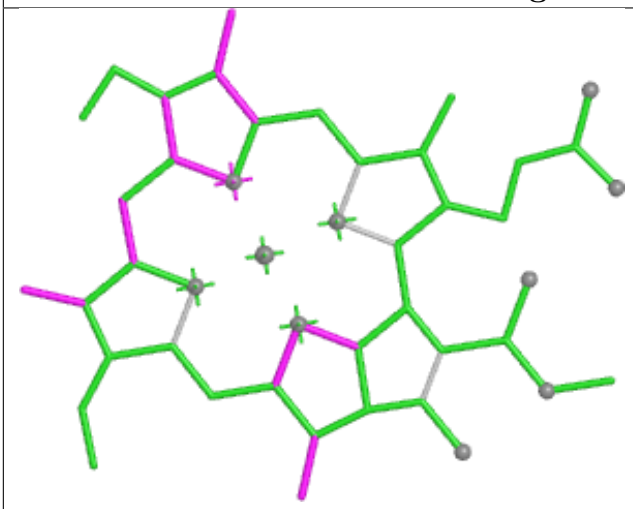


Torsions

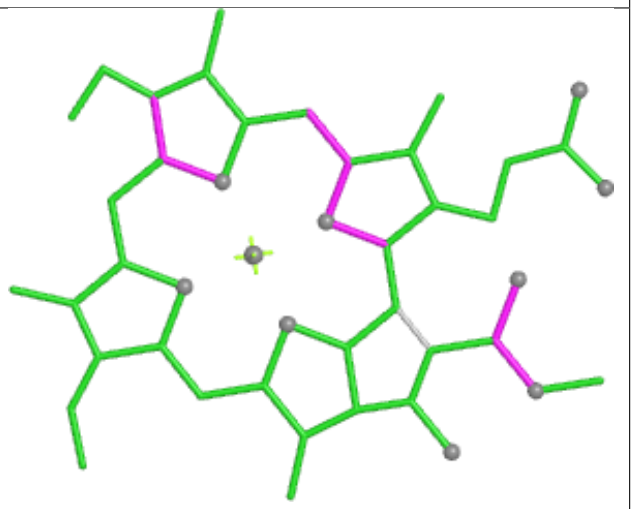


Rings

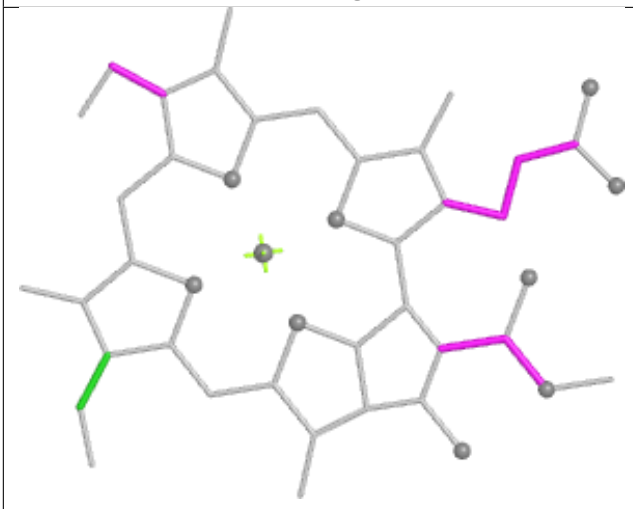
Ligand CLA c 517



Bond lengths



Bond angles

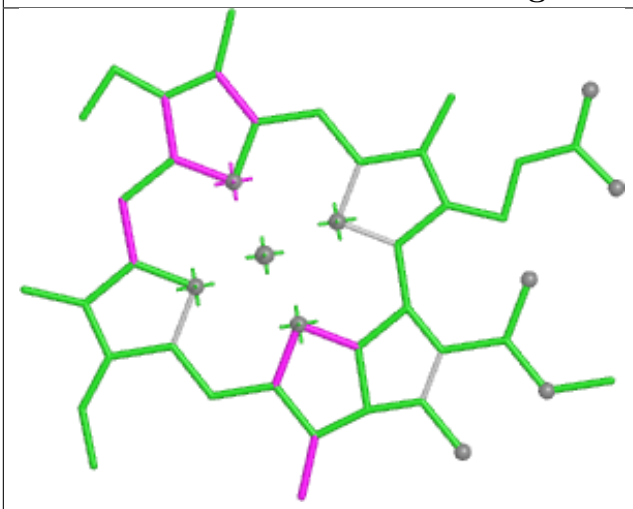


Torsions

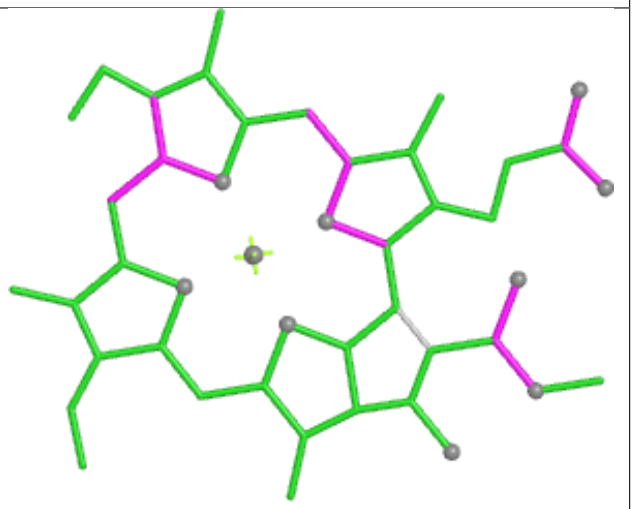


Rings

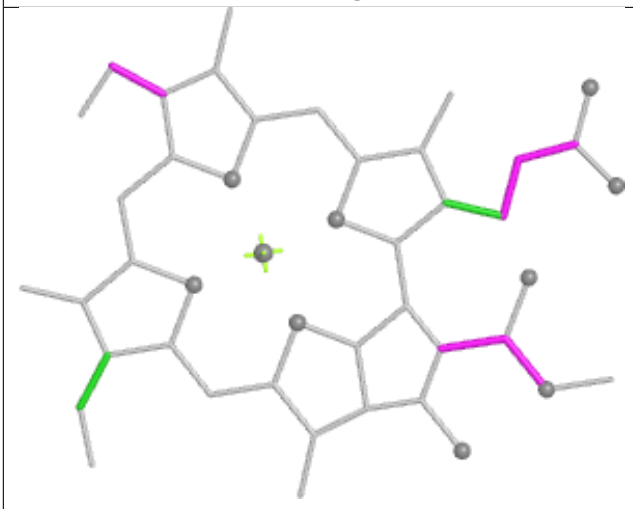
Ligand CLA 1 518



Bond lengths



Bond angles

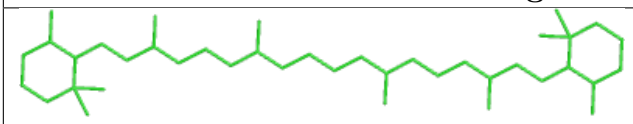


Torsions

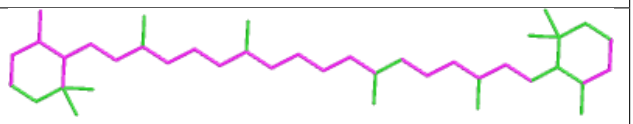


Rings

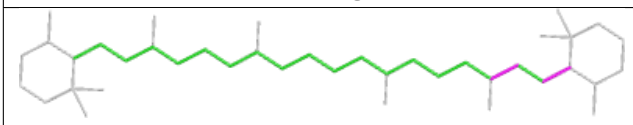
Ligand BCR 3 523



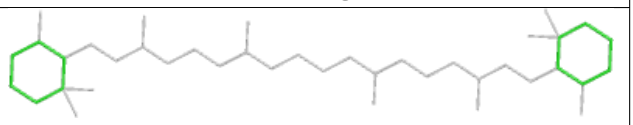
Bond lengths



Bond angles

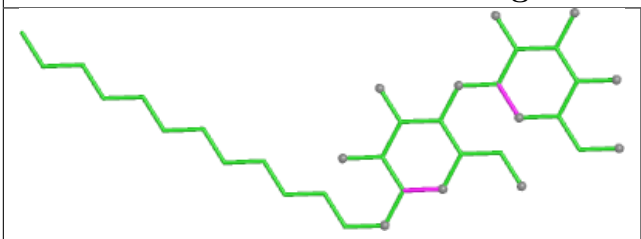


Torsions

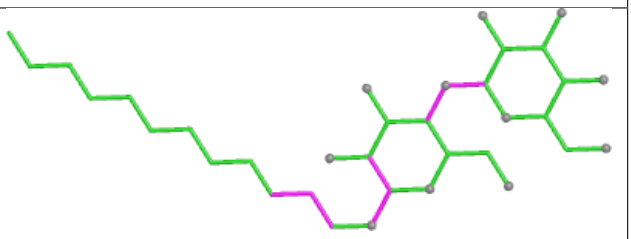


Rings

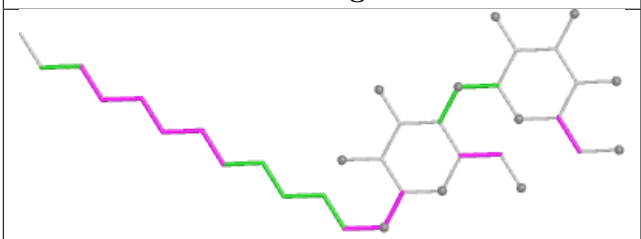
Ligand LMU B 1843



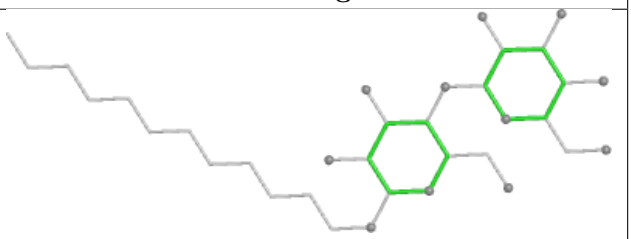
Bond lengths



Bond angles

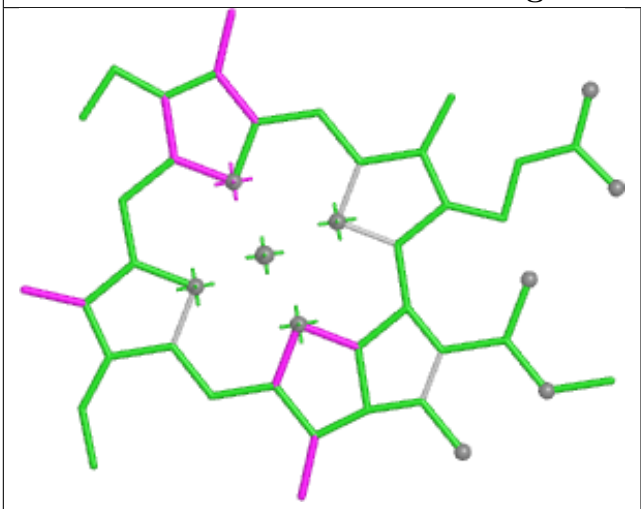


Torsions

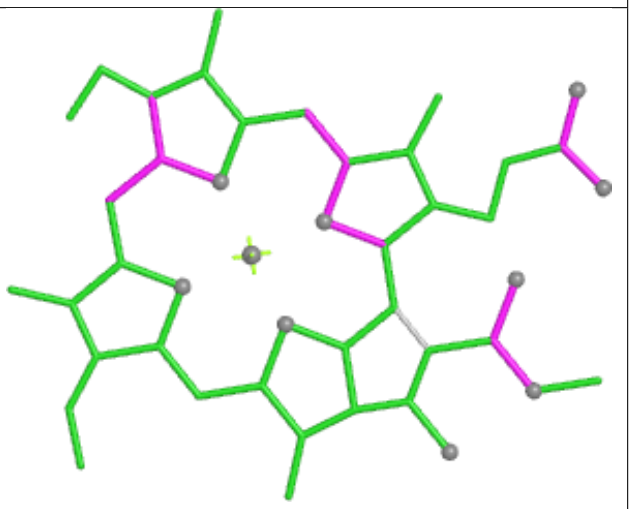


Rings

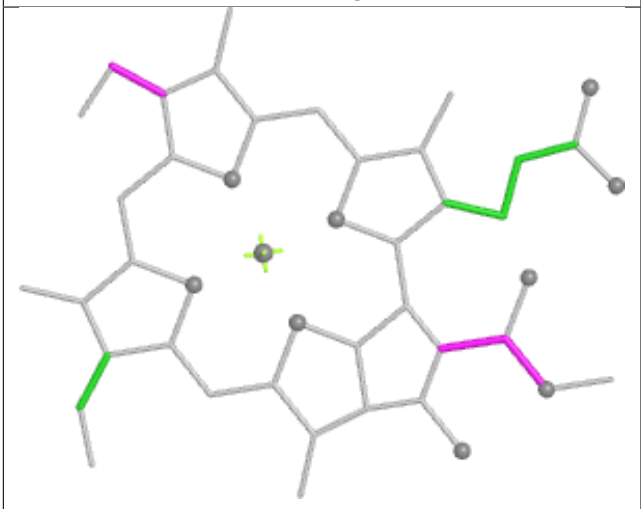
Ligand CLA Z 506



Bond lengths



Bond angles

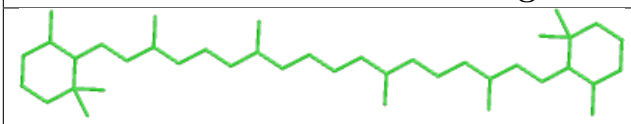


Torsions

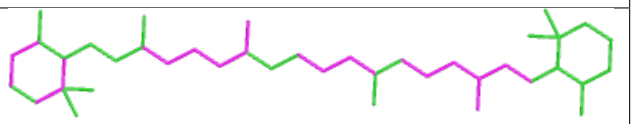


Rings

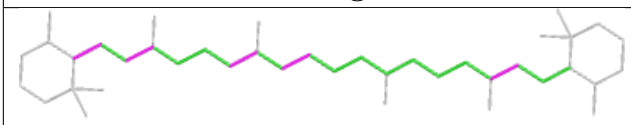
Ligand BCR e 4001



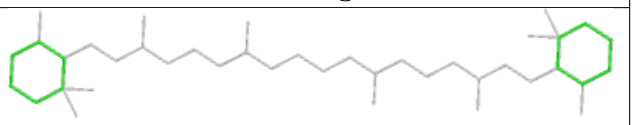
Bond lengths



Bond angles

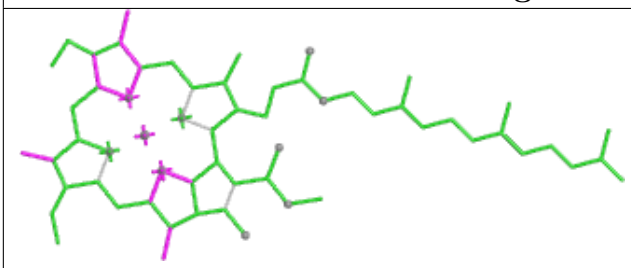


Torsions

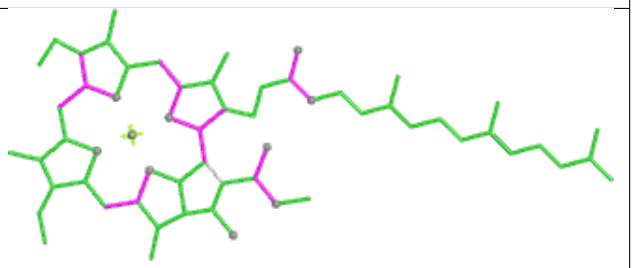


Rings

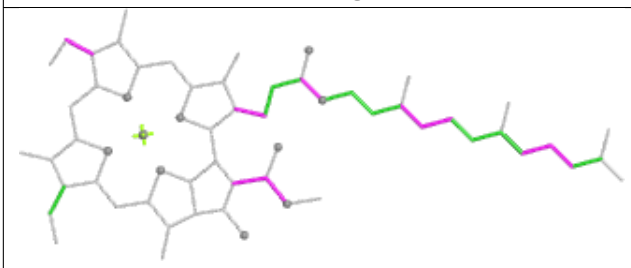
Ligand CLA G 1122



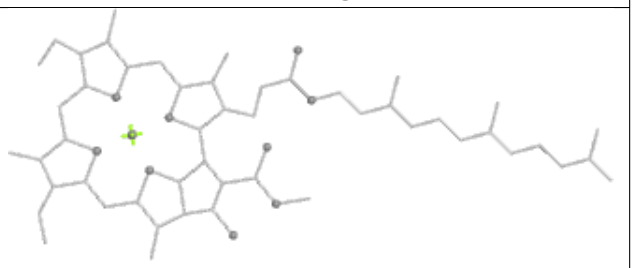
Bond lengths



Bond angles

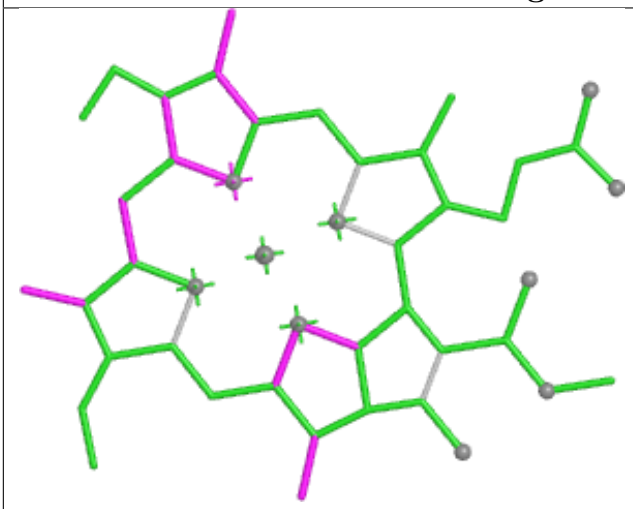


Torsions

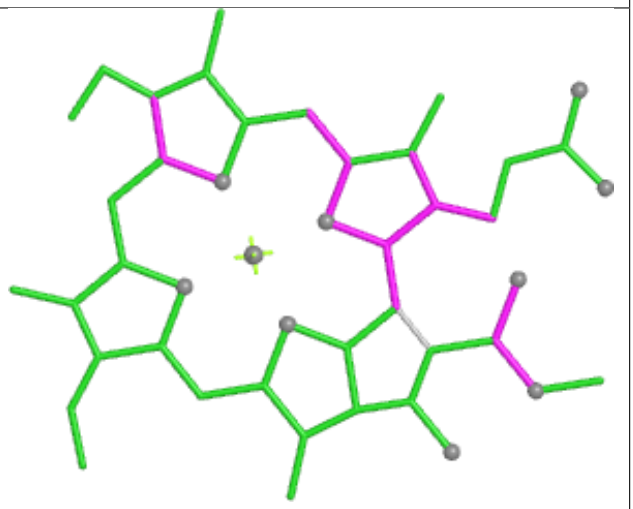


Rings

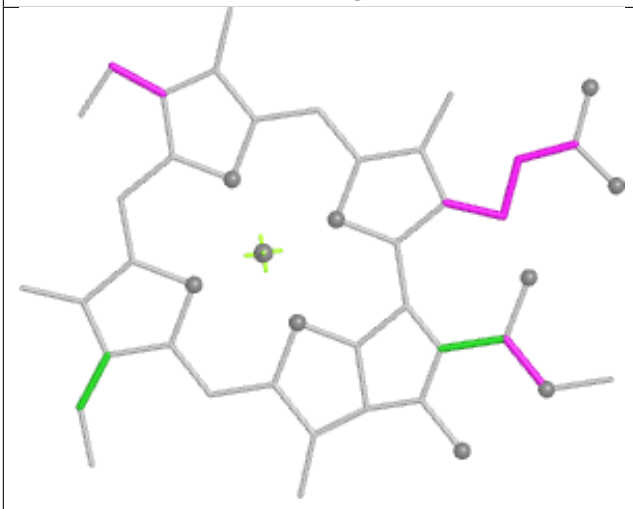
Ligand CLA u 501



Bond lengths



Bond angles

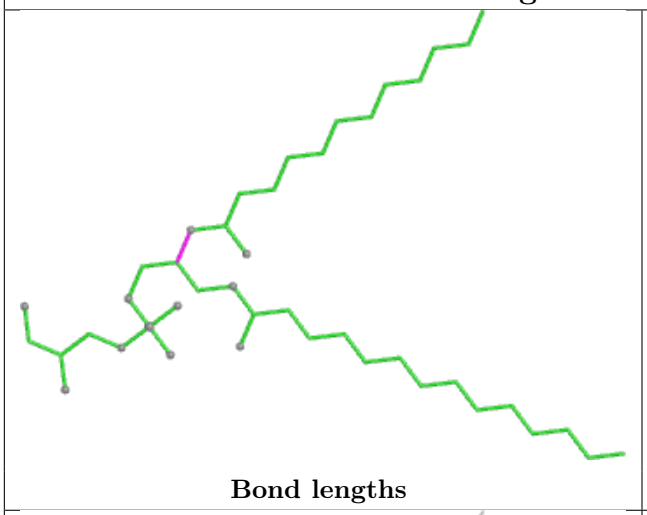


Torsions

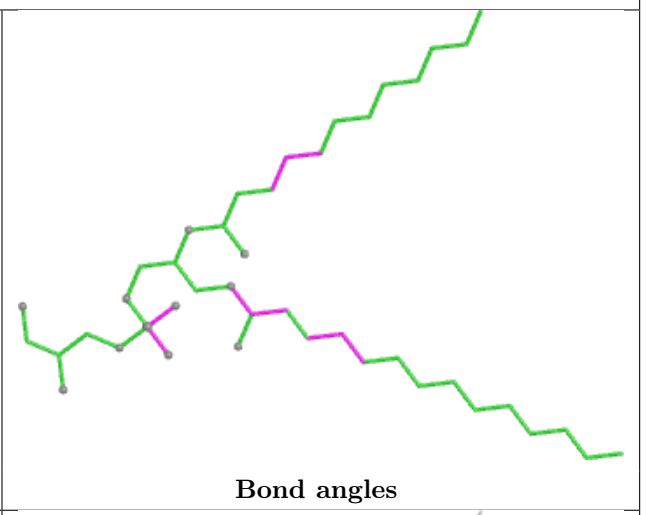


Rings

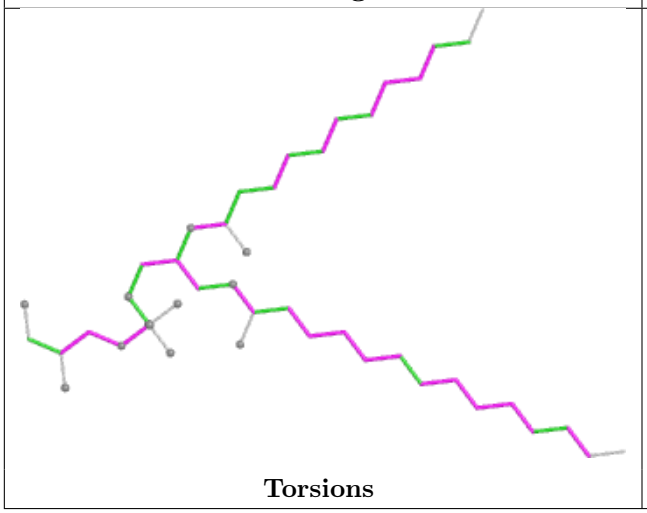
Ligand LHG e 5005



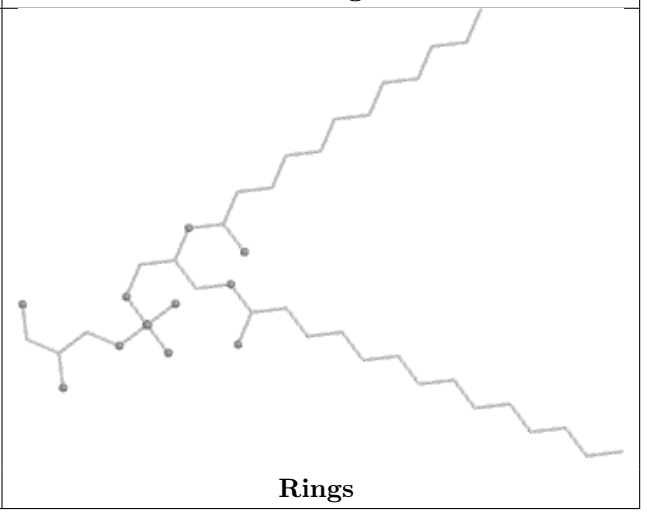
Bond lengths



Bond angles

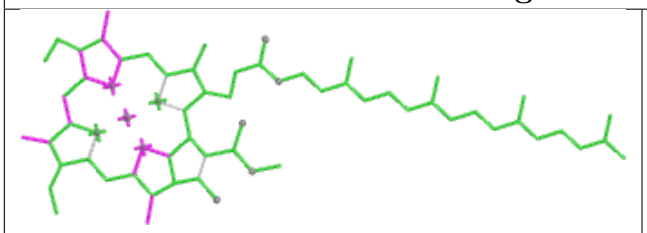


Torsions

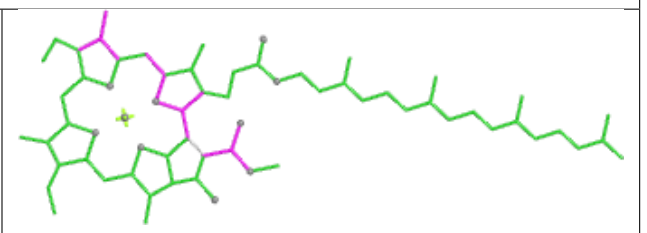


Rings

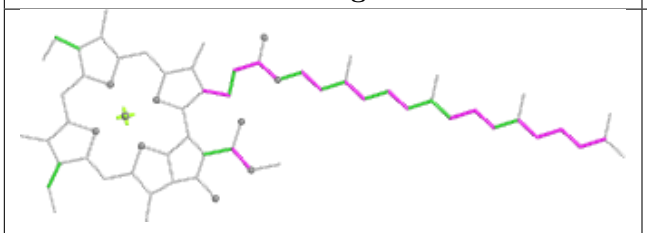
Ligand CLA G 1126



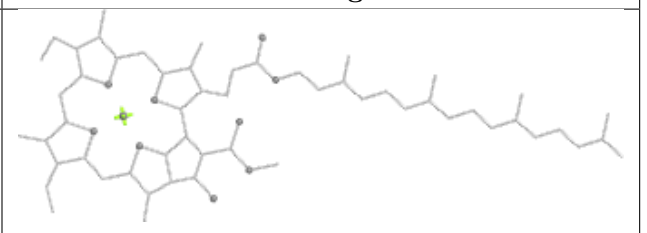
Bond lengths



Bond angles

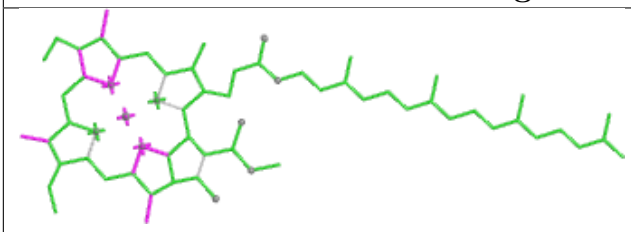


Torsions

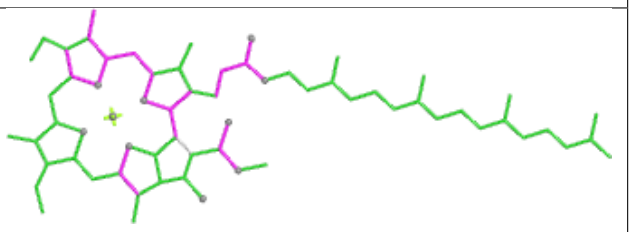


Rings

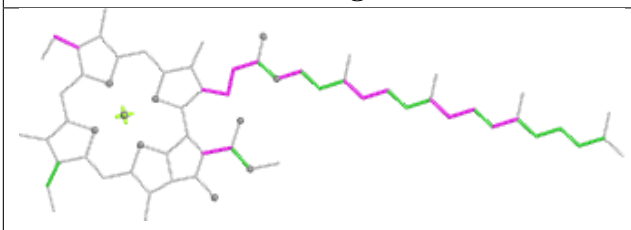
Ligand CLA G 1107



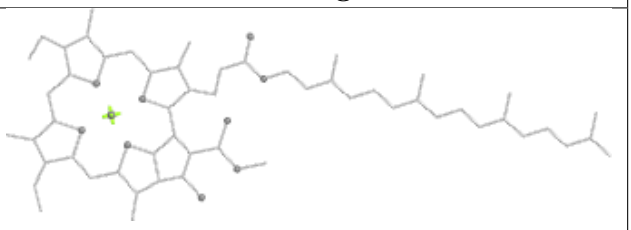
Bond lengths



Bond angles

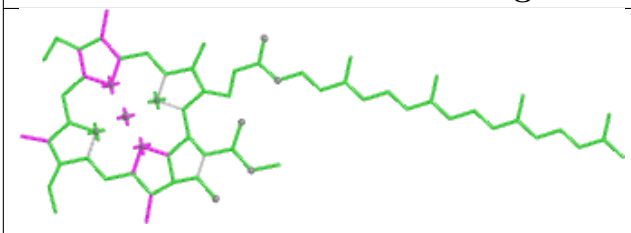


Torsions

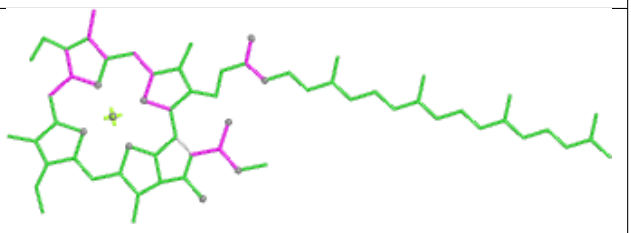


Rings

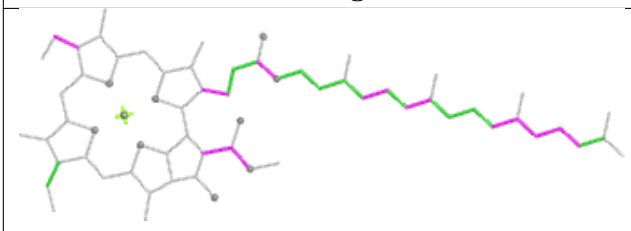
Ligand CLA G 1109



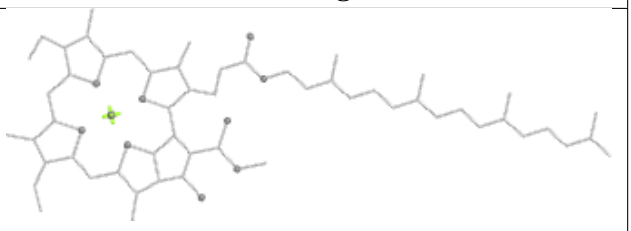
Bond lengths



Bond angles

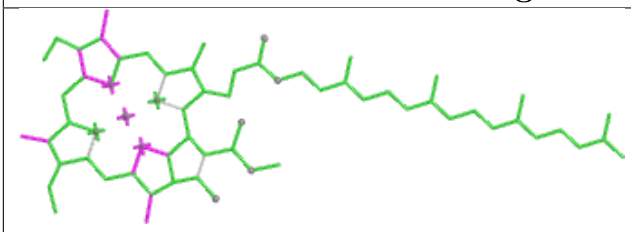


Torsions

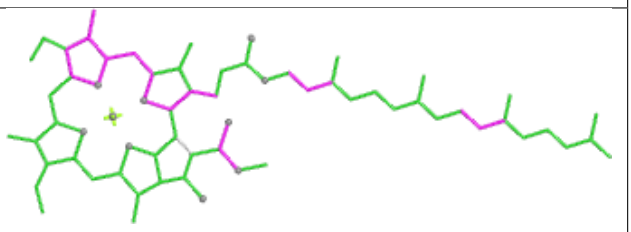


Rings

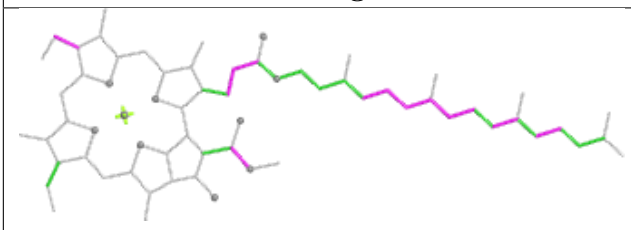
Ligand CLA B 1203



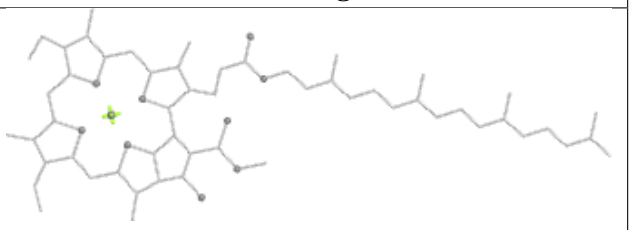
Bond lengths



Bond angles

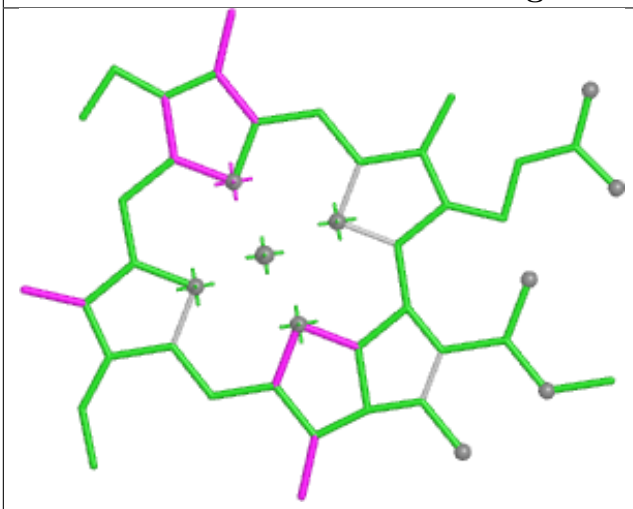


Torsions

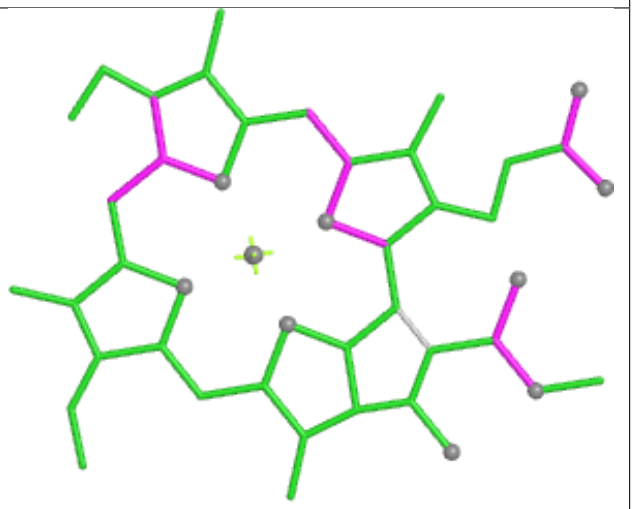


Rings

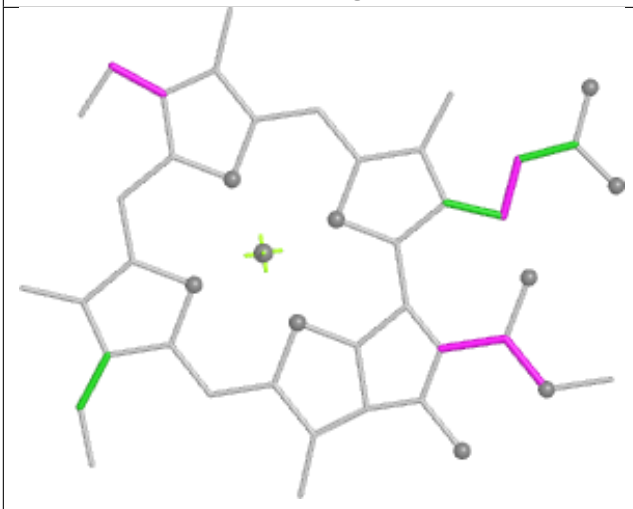
Ligand CLA Z 517



Bond lengths



Bond angles

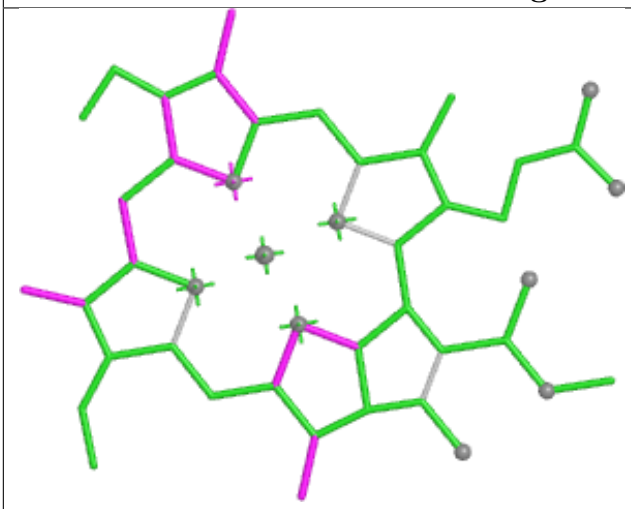


Torsions

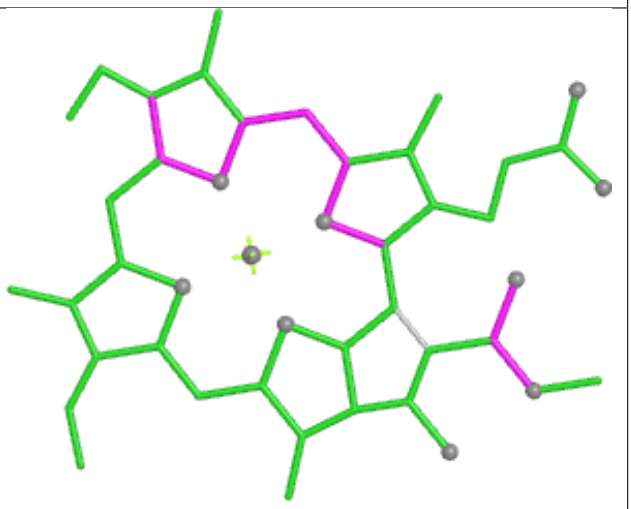


Rings

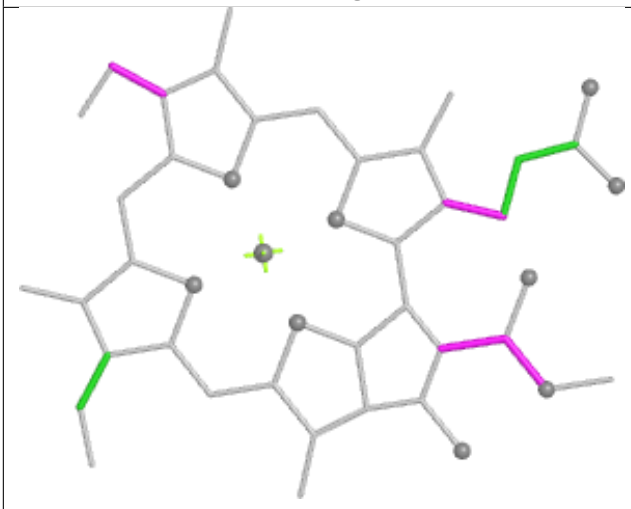
Ligand CLA t 506



Bond lengths



Bond angles

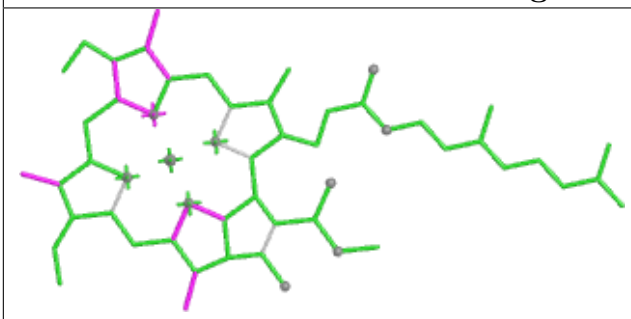


Torsions

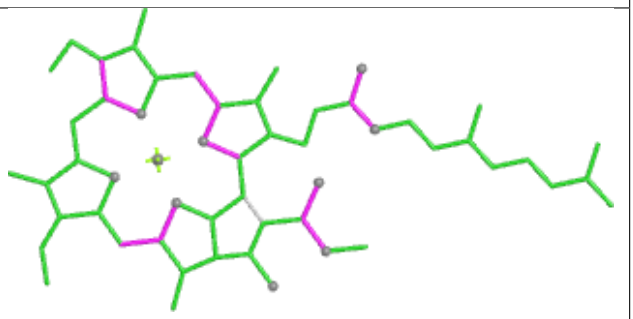


Rings

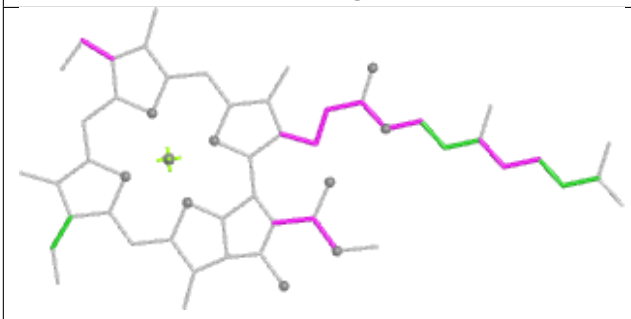
Ligand CLA r 518



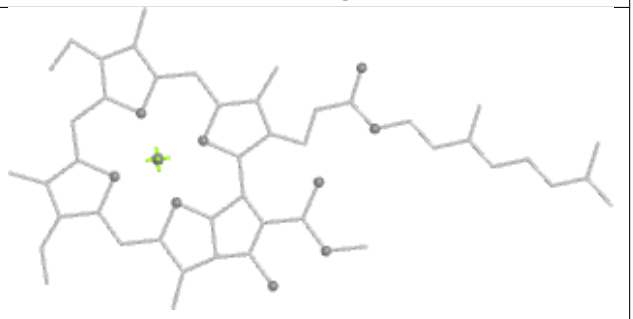
Bond lengths



Bond angles

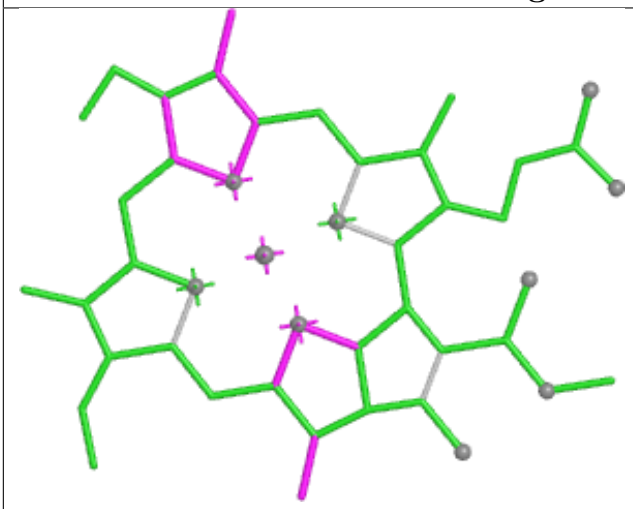


Torsions

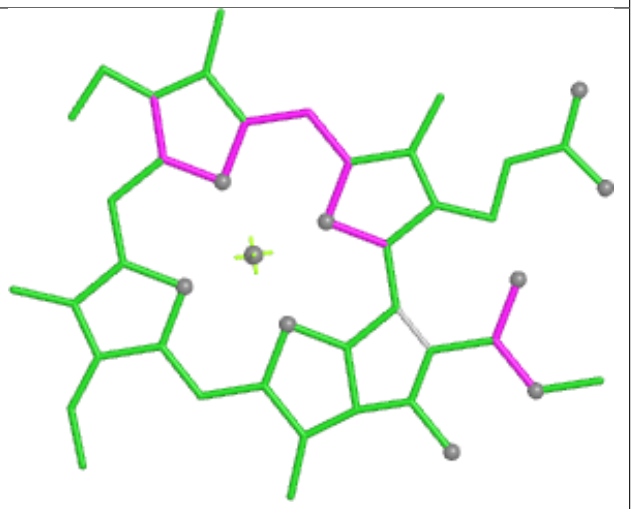


Rings

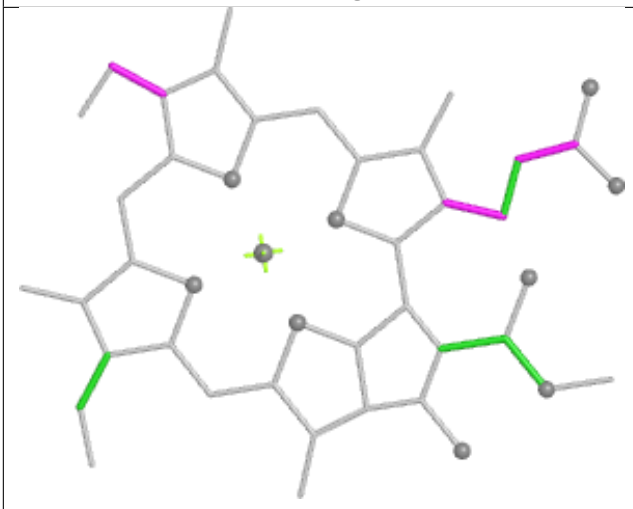
Ligand CLA 2 512



Bond lengths



Bond angles

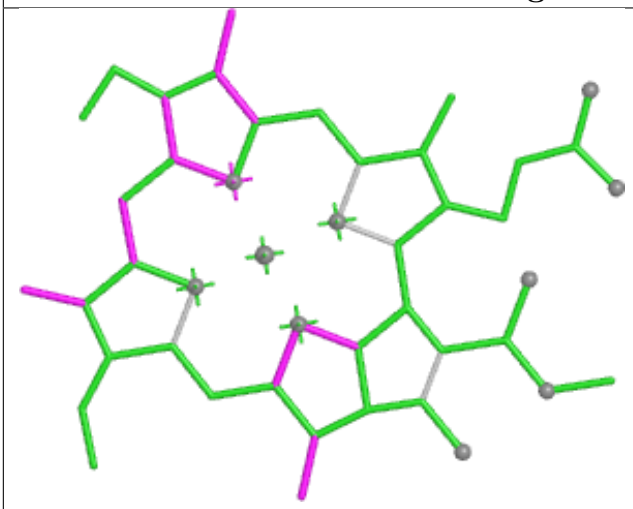


Torsions

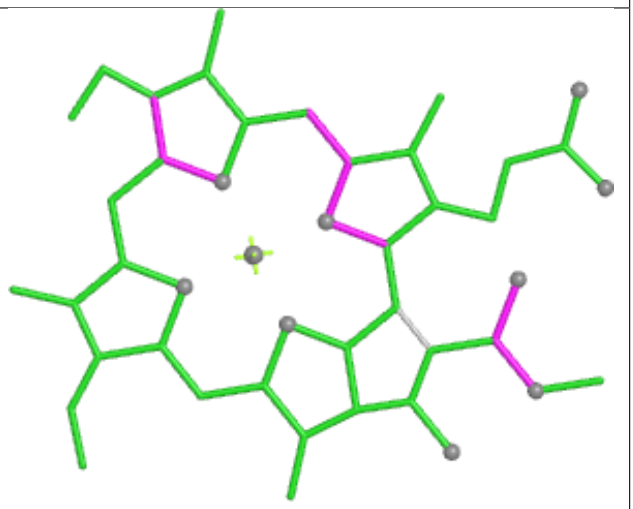


Rings

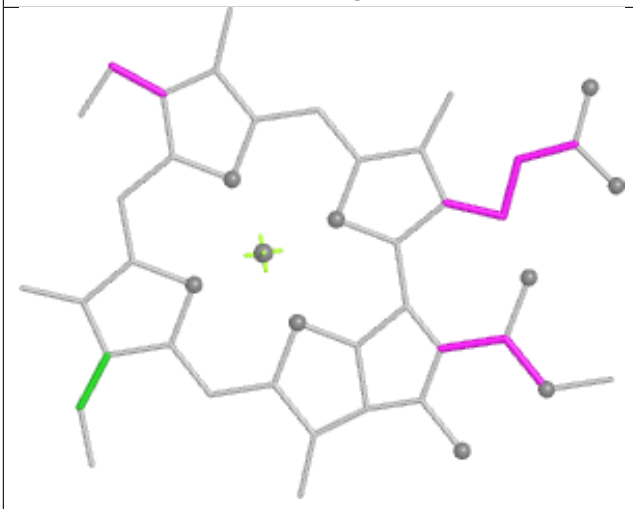
Ligand CLA u 517



Bond lengths



Bond angles

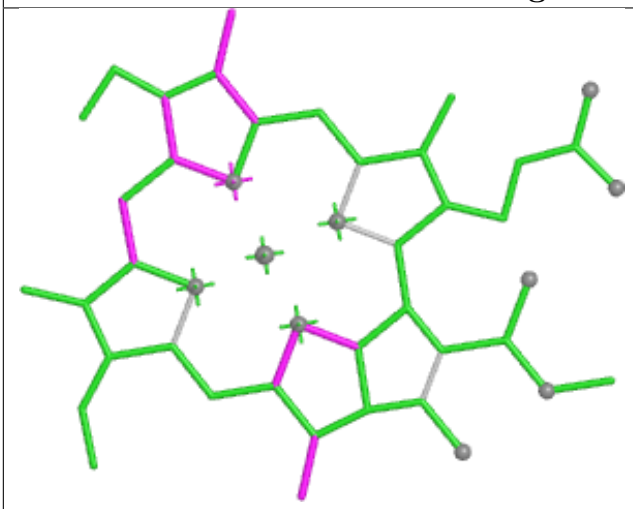


Torsions

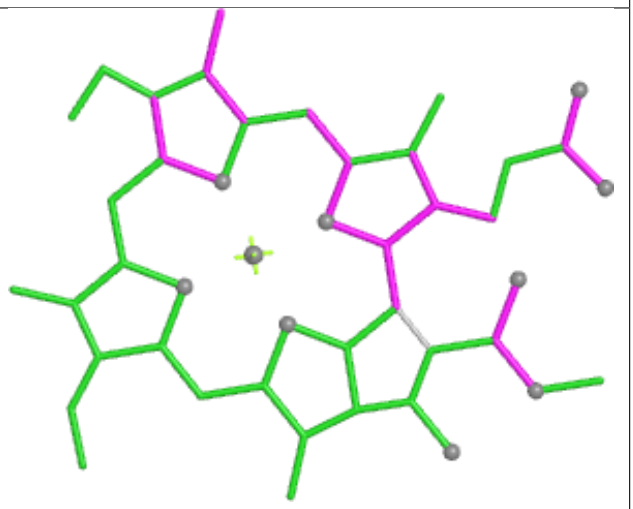


Rings

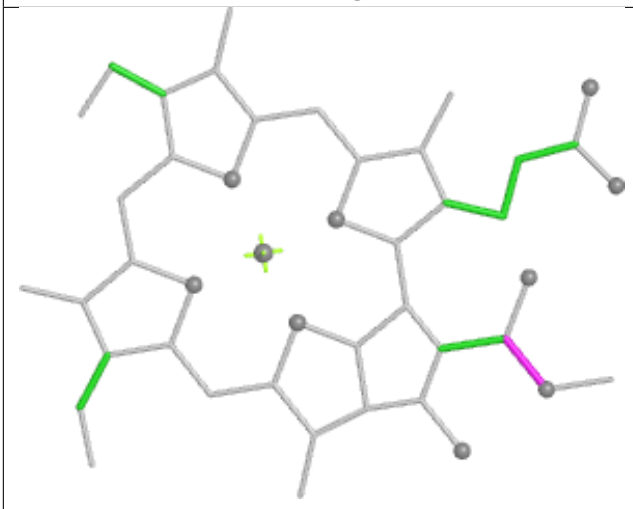
Ligand CLA 3 511



Bond lengths



Bond angles

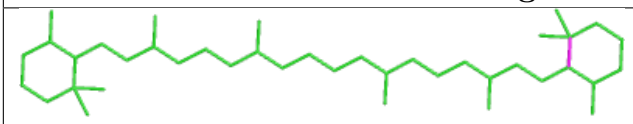


Torsions

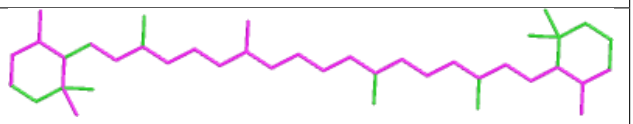


Rings

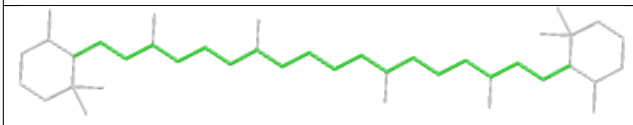
Ligand BCR e 4002



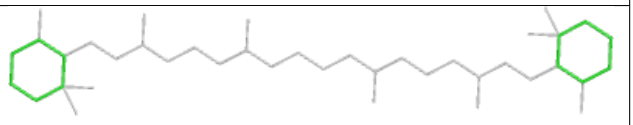
Bond lengths



Bond angles

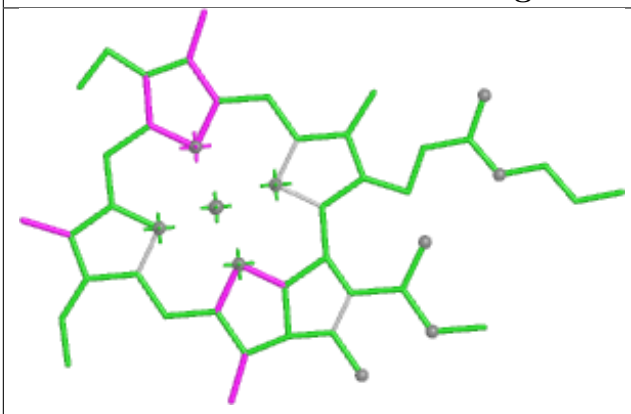


Torsions

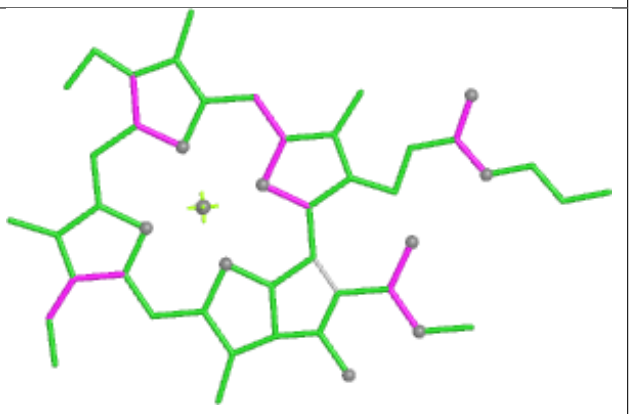


Rings

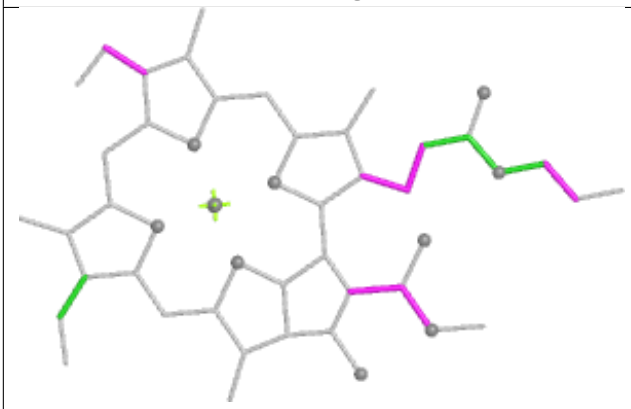
Ligand CLA U 1103



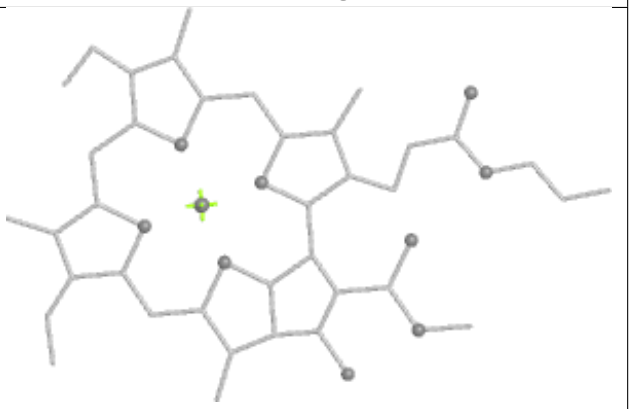
Bond lengths



Bond angles

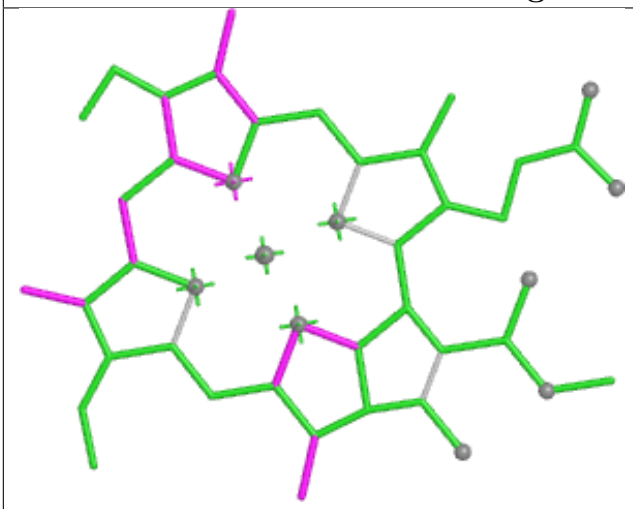


Torsions

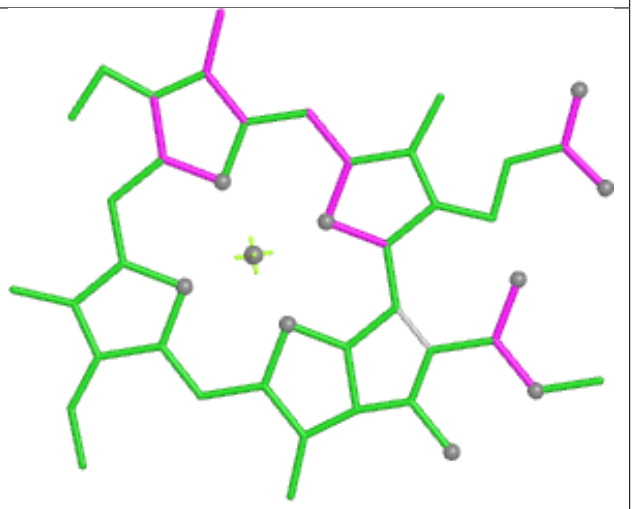


Rings

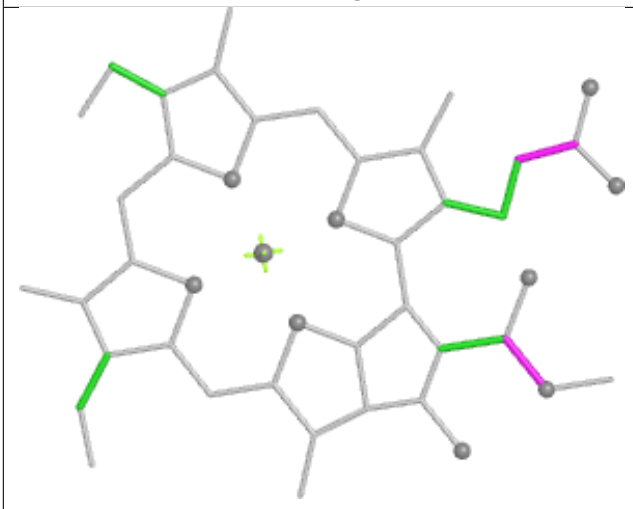
Ligand CLA d 509



Bond lengths



Bond angles

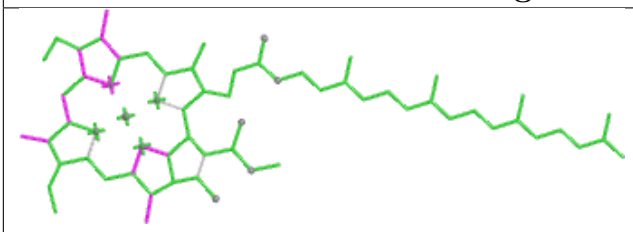


Torsions

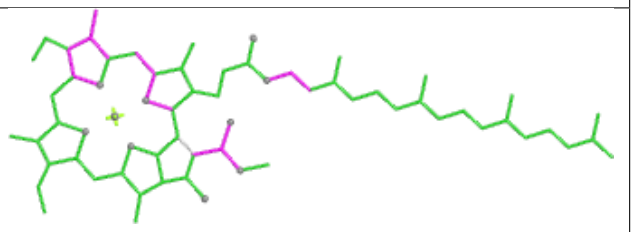


Rings

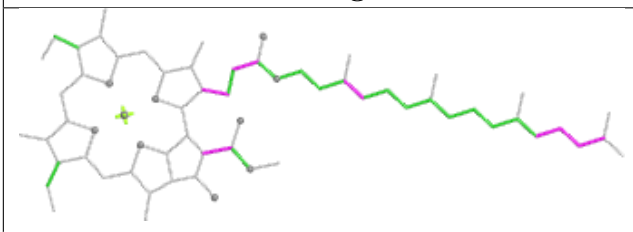
Ligand CLA H 1202



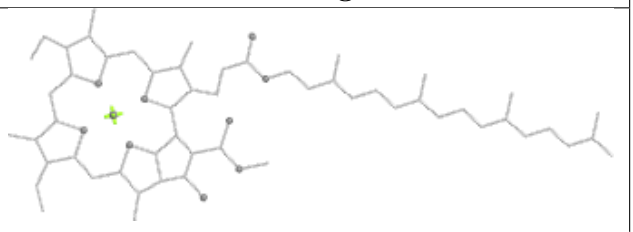
Bond lengths



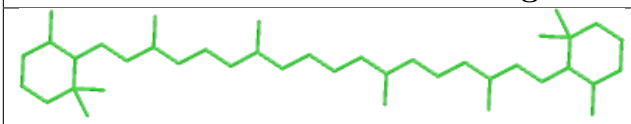
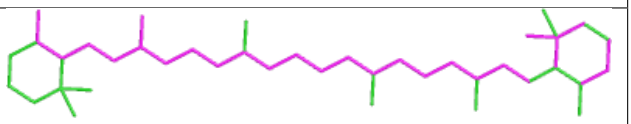
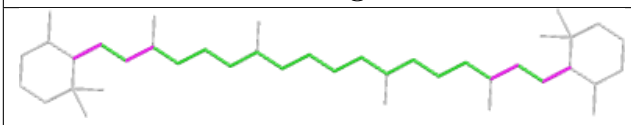
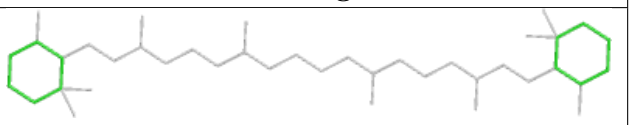
Bond angles



Torsions



Rings

Ligand BCR f 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

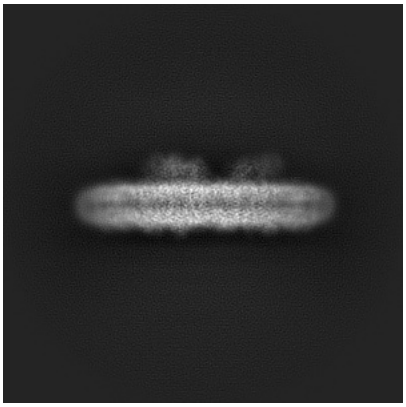
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9994. These allow visual inspection of the internal detail of the map and identification of artifacts.

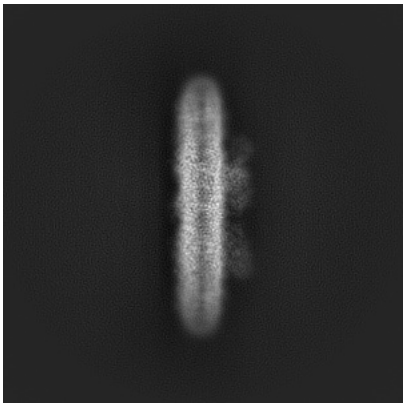
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

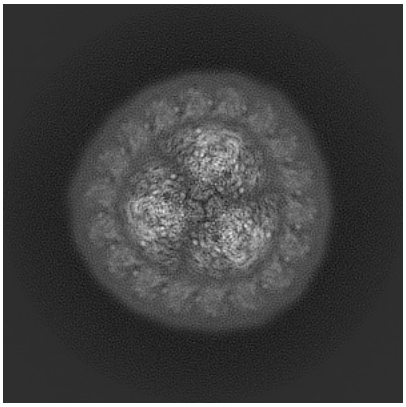
6.1.1 Primary map



X



Y

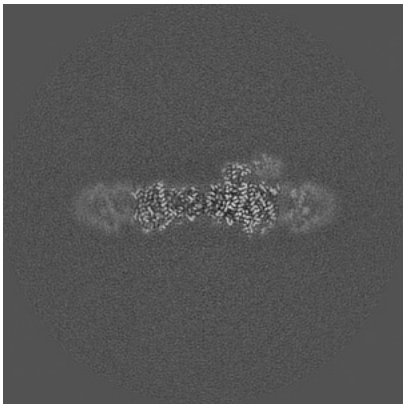


Z

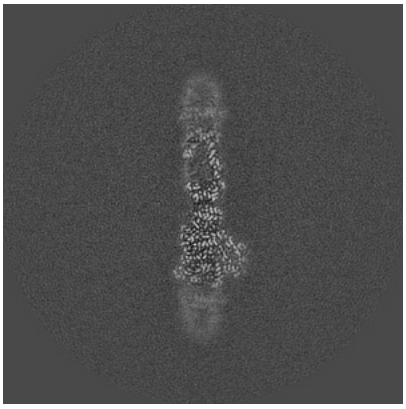
The images above show the map projected in three orthogonal directions.

6.2 Central slices

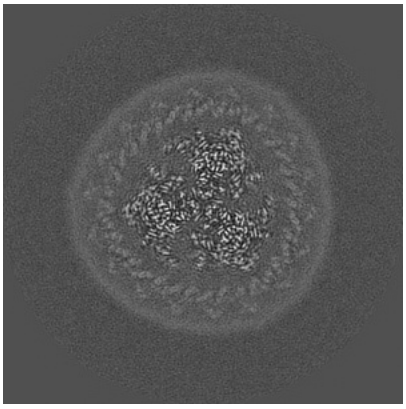
6.2.1 Primary map



X Index: 240



Y Index: 240

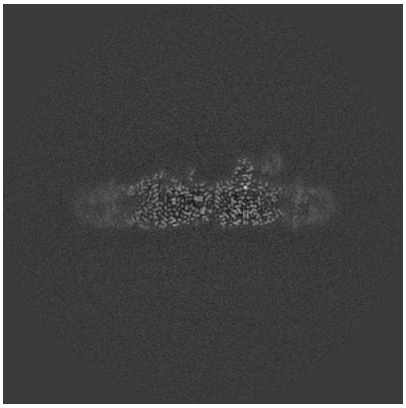


Z Index: 240

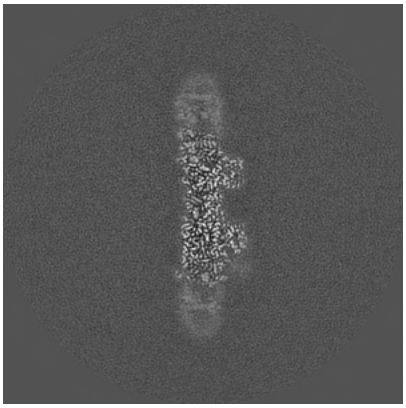
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

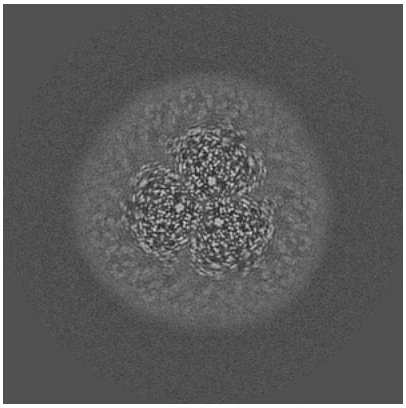
6.3.1 Primary map



X Index: 259



Y Index: 225

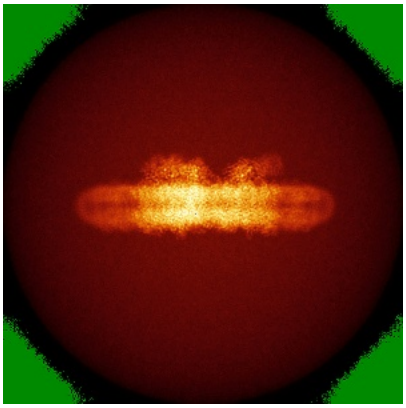


Z Index: 253

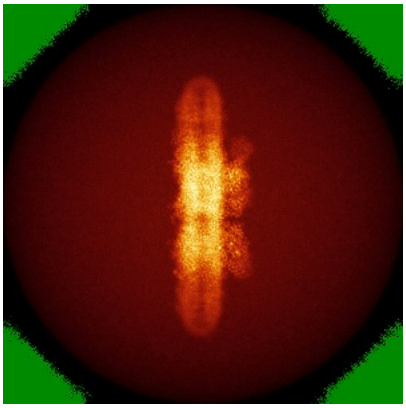
The images above show the largest variance slices of the map in three orthogonal directions.

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

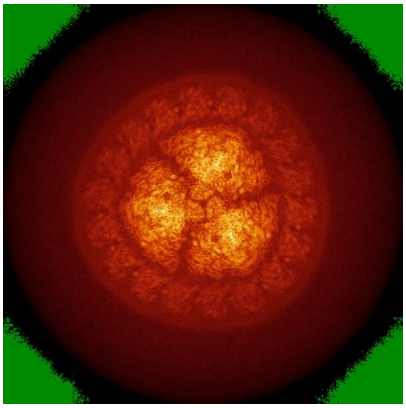
6.4.1 Primary map



X



Y

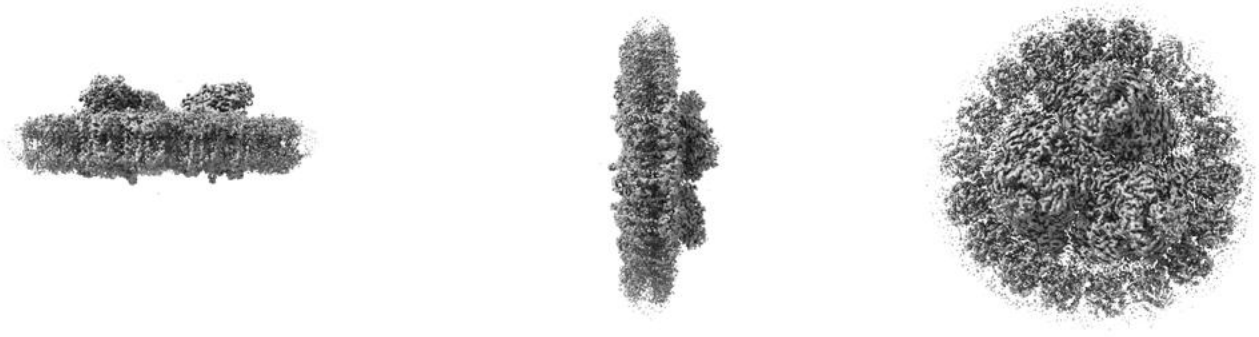


Z

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

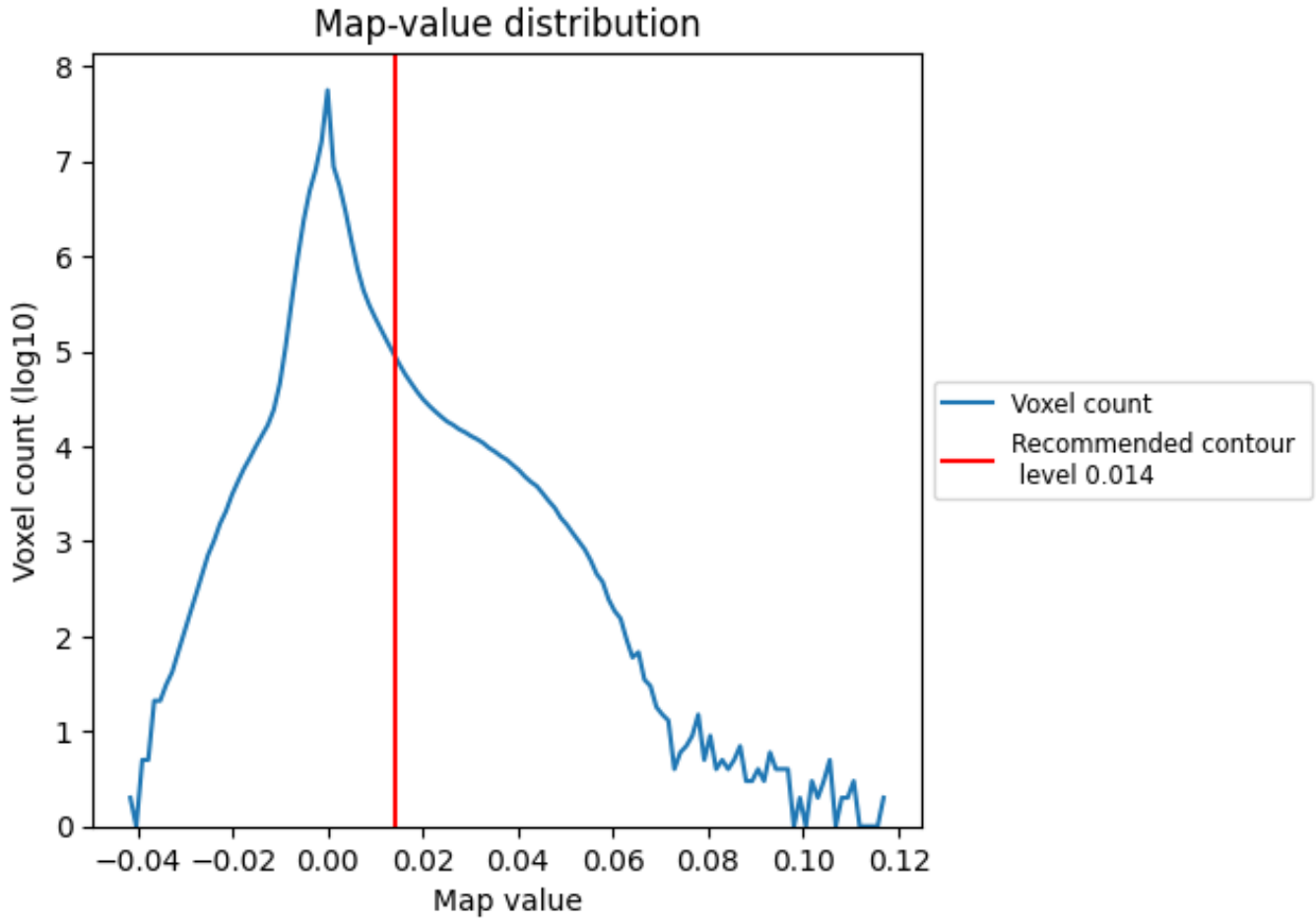
6.6 Mask visualisation (i)

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

7 Map analysis

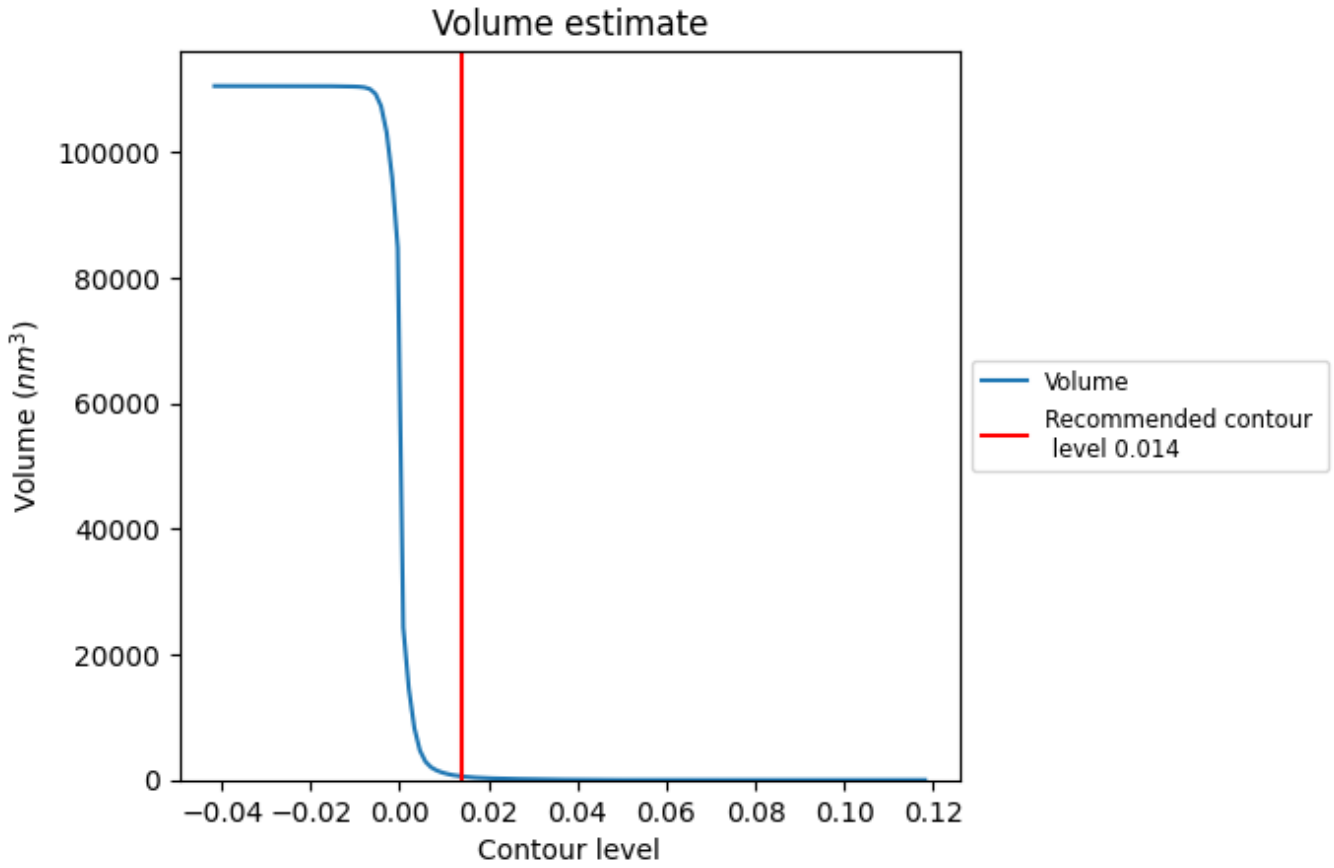
This section contains the results of statistical analysis of the map.

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.

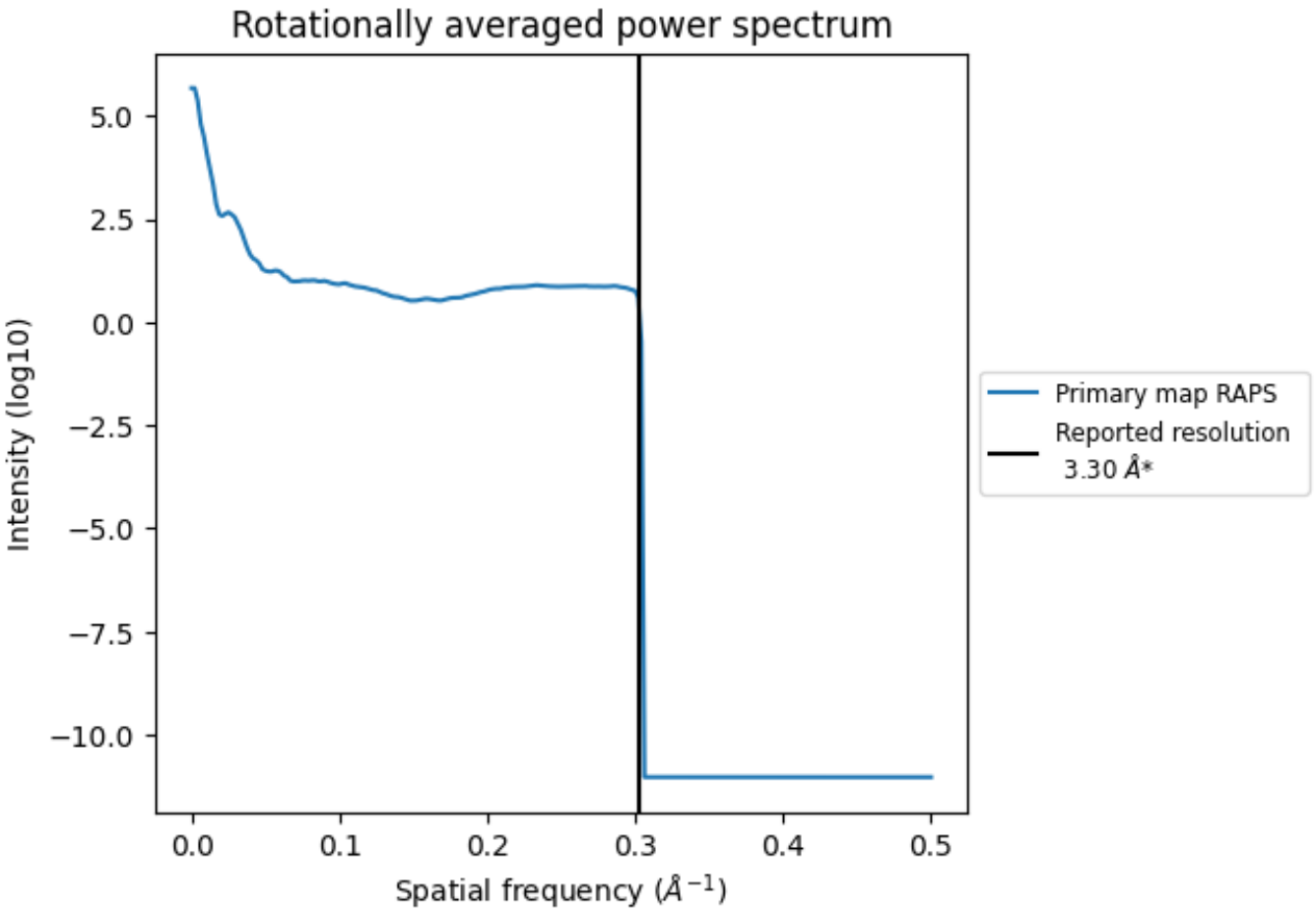
7.2 Volume estimate



The volume at the recommended contour level is 567 nm^3; this corresponds to an approximate mass of 512 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 0.303 $Å^{-1}$

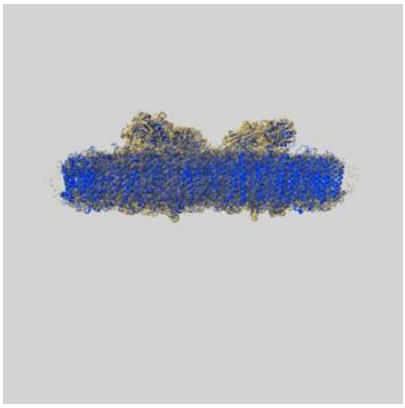
8 Fourier-Shell correlation

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

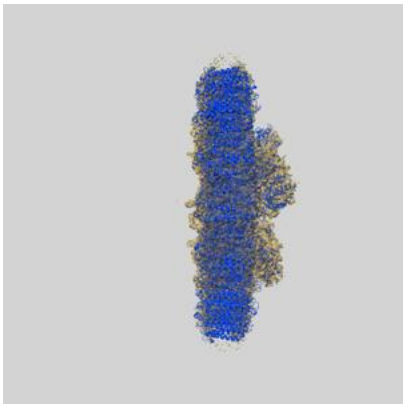
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9994 and PDB model 6KIF. Per-residue inclusion information can be found in section 3 on page 55.

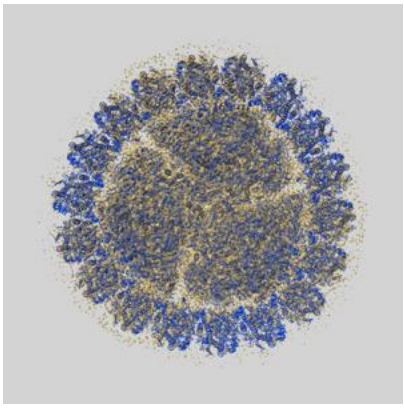
9.1 Map-model overlay



X



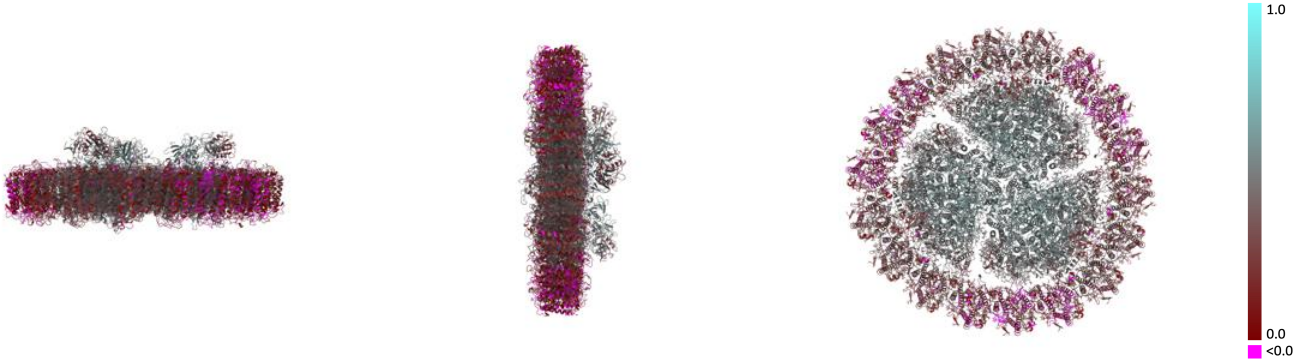
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

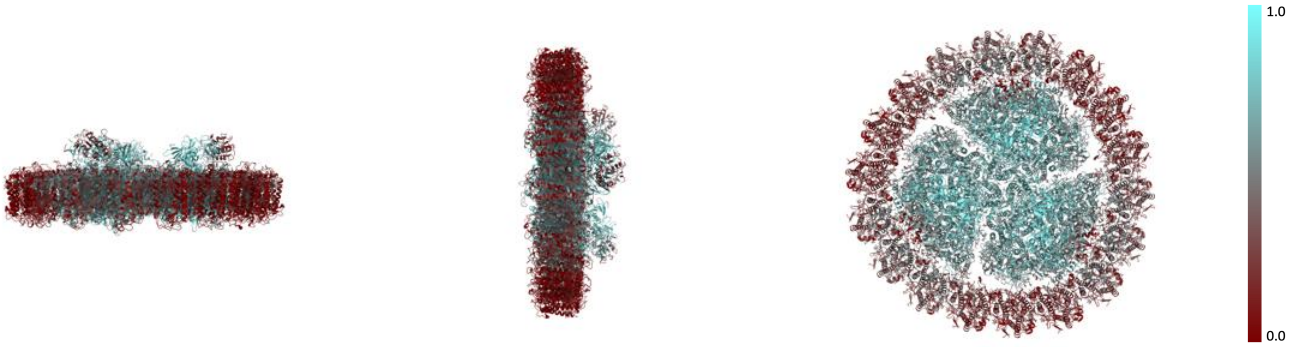
9.2 Q-score mapped to coordinate model



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.

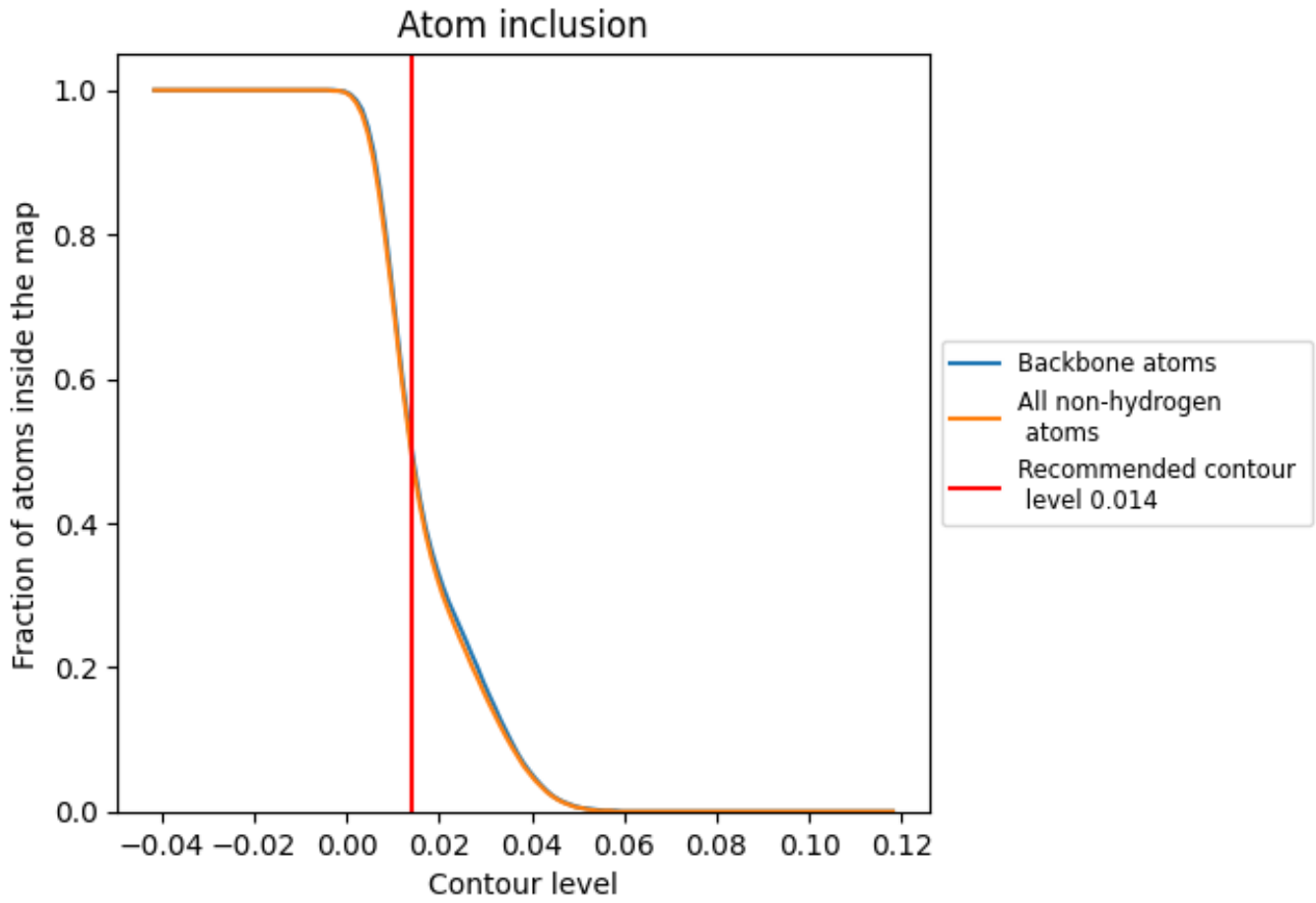
9.3 Atom inclusion mapped to coordinate model



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4950	0.3600
1	0.3260	0.2570
2	0.3300	0.2860
3	0.2650	0.2560
4	0.0820	0.0950
5	0.0790	0.1060
6	0.1420	0.1610
A	0.7560	0.5190
B	0.7500	0.5000
C	0.8750	0.5350
D	0.7920	0.5270
E	0.7270	0.4830
F	0.6900	0.4570
G	0.7550	0.5150
H	0.7500	0.5000
I	0.7510	0.5410
J	0.6790	0.4920
K	0.5300	0.3470
L	0.7810	0.5400
M	0.7060	0.5080
N	0.8720	0.5370
O	0.7930	0.5260
P	0.3710	0.3350
Q	0.7210	0.4810
R	0.6900	0.4570
S	0.7590	0.5440
T	0.6690	0.4930
U	0.5180	0.3330
V	0.7830	0.5400
W	0.6990	0.5040
X	0.3680	0.3320
Y	0.3180	0.2520
Z	0.3280	0.2790
a	0.2610	0.2510
b	0.0830	0.0900



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.0760	0.1030
d	0.1460	0.1570
e	0.7560	0.5190
f	0.7500	0.4990
g	0.8680	0.5350
h	0.7920	0.5260
i	0.7180	0.4760
j	0.6890	0.4540
k	0.7530	0.5370
l	0.6690	0.4910
m	0.5360	0.3490
n	0.7850	0.5390
o	0.7020	0.5050
p	0.3780	0.3340
q	0.3240	0.2590
r	0.3350	0.2880
s	0.2640	0.2580
t	0.0810	0.0950
u	0.0770	0.1070
v	0.1480	0.1590