Full wwPDB EM Validation Report ⓘ

Sep 30, 2026 – 01:21 AM JST

PDB ID	:	9V7T / pdb_00009v7t
EMDB ID	:	EMD-64823
Title	:	PSI-LHCE supercomplex from Euglena gracilis.
Authors	:	Bai, T.Y.; Mao, Z.Y.; Tian, L.R.
Deposited on	:	2025-05-28
Resolution	:	2.23 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:

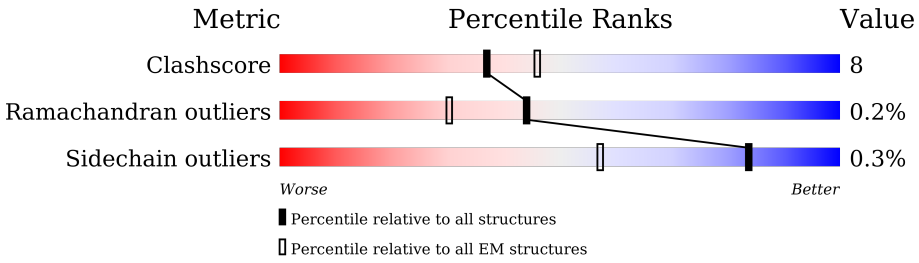
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

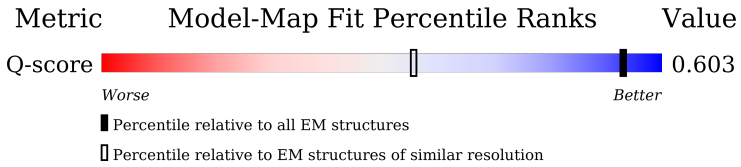
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.23 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	3335 (1.73 - 2.73)

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

Mol	Chain	Length	Quality of chain
1	A	751	83% 16%
2	B	734	84% 16%
3	C	81	6% 89% 10%
4	D	186	34% 86% 13%

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Mol	Chain	Length	Quality of chain
5	E	63	33% 84% 16%
6	F	168	17% 91% 9%
7	J	37	5% 95% 5%
8	M	31	16% 84% 16%
9	a	166	36% 90% 10%
10	b	169	62% 83% 17%
11	c	221	37% 90% 10%
12	d	220	23% 92% 8%
13	e	199	45% 87% 13%
14	h	174	21% 87% 12%
15	i	177	15% 84% 16%
16	j	183	9% 86% 14%
17	k	172	36% 89% 11%
18	l	167	53% 85% 15%
19	m	168	71% 85% 15%
20	f	174	100% 84% 16%
21	g	178	72% 90% 10%
22	n	184	100% 81% 18%
23	o	164	90% 83% 17%
24	p	148	100% 85% 15%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 55406 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
			Total	C	N	O	S		
1	A	741	5878	3860	994	1003	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5861	3855	984	1007	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	596	363	104	118	11	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	186	1393	892	235	262	4	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	481	311	81	89	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	168	1250	801	206	239	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			243	162	37	43	1		

- Molecule 9 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	166	Total	C	N	O	S	0	0
			1274	819	220	228	7		

- Molecule 10 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	169	Total	C	N	O	S	0	0
			1302	842	213	243	4		

- Molecule 11 is a protein called LHCE 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	221	Total	C	N	O	S	0	0
			1676	1087	282	302	5		

- Molecule 12 is a protein called Light harvesting chlorophyll a /b binding protein of PSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

- Molecule 13 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 14 is a protein called LHCE 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	174	Total	C	N	O	S	0	0
			1350	865	233	247	5		

- Molecule 15 is a protein called LHCE 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	177	Total	C	N	O	S	0	0
			1355	865	242	244	4		

- Molecule 16 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	183	Total	C	N	O	S	0	0
			1450	944	246	254	6		

- Molecule 17 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	172	Total	C	N	O	S	0	0
			1338	860	232	241	5		

- Molecule 18 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	167	Total	C	N	O	S	0	0
			1256	811	214	227	4		

- Molecule 19 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		

- Molecule 20 is a protein called Chloroplast light-harvesting complex I protein, Lhca7_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	174	Total	C	N	O	S	0	0
			1332	851	236	241	4		

- Molecule 21 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	178	Total	C	N	O	S	0	0
			1406	914	240	246	6		

- Molecule 22 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	184	Total	C	N	O	S	0	0
			1411	921	232	254	4		

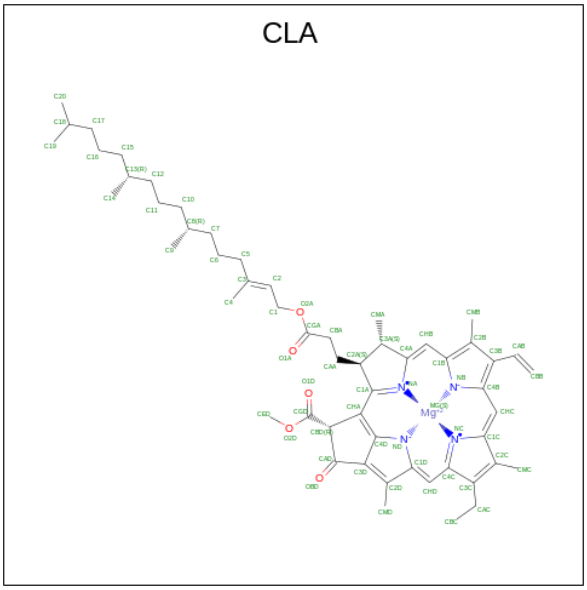
- Molecule 23 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	164	Total	C	N	O	S	0	0
			1230	794	208	224	4		

- Molecule 24 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	148	Total	C	N	O	S	0	0
			1126	727	188	207	4		

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



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

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	h	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	i	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	i	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	j	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	j	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	m	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	m	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	m	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	m	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	m	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	m	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	f	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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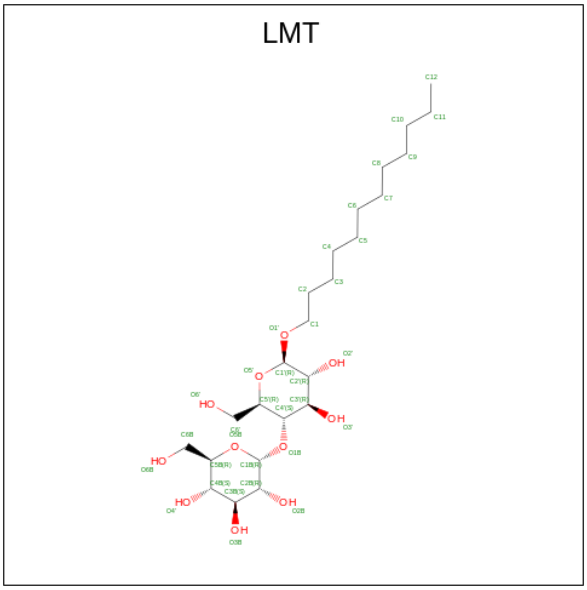
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	n	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	o	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	o	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			42	35	1	4	2	
25	o	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	o	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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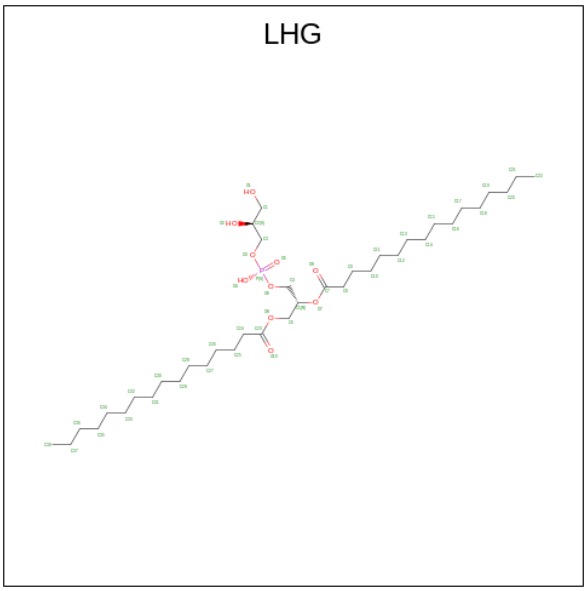
Mol	Chain	Residues	Atoms					AltConf
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



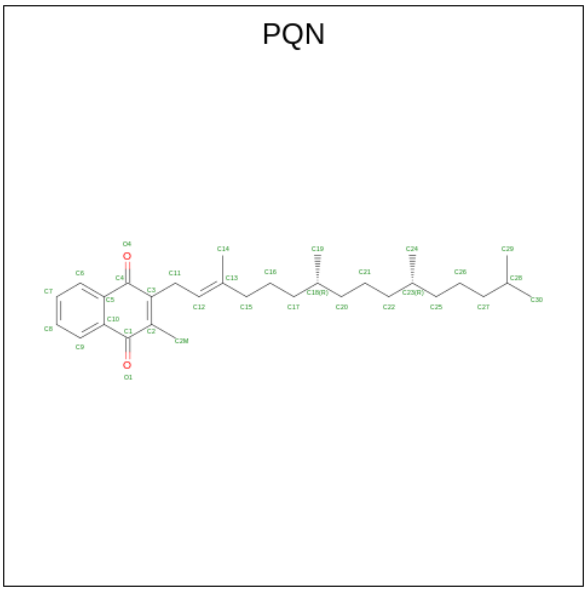
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



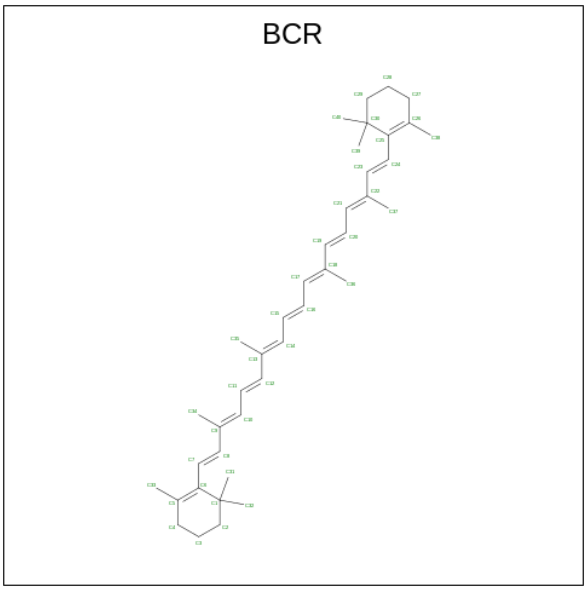
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total 38	C 27	O 10	P 1	0
27	A	1	Total 49	C 38	O 10	P 1	0
27	a	1	Total 26	C 15	O 10	P 1	0
27	b	1	Total 31	C 20	O 10	P 1	0
27	c	1	Total 30	C 19	O 10	P 1	0
27	d	1	Total 29	C 18	O 10	P 1	0
27	h	1	Total 30	C 19	O 10	P 1	0
27	h	1	Total 31	C 20	O 10	P 1	0
27	i	1	Total 36	C 25	O 10	P 1	0
27	j	1	Total 37	C 26	O 10	P 1	0
27	m	1	Total 32	C 21	O 10	P 1	0
27	g	1	Total 35	C 24	O 10	P 1	0

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



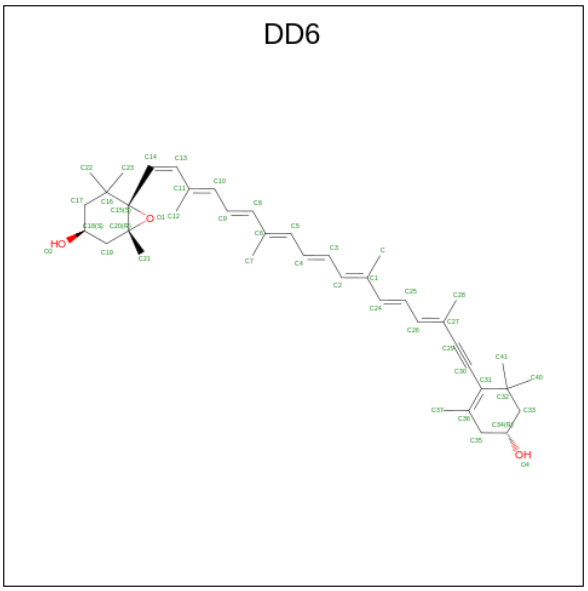
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C O 33 31 2	0
28	B	1	Total C O 33 31 2	0
28	B	1	Total C O 27 25 2	0
28	F	1	Total C O 26 24 2	0

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	M	1	Total C 40 40	0

- Molecule 30 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C O 43 40 3	0
30	A	1	Total C O 43 40 3	0
30	F	1	Total C O 43 40 3	0
30	J	1	Total C O 43 40 3	0
30	J	1	Total C O 43 40 3	0
30	a	1	Total C O 43 40 3	0
30	a	1	Total C O 43 40 3	0
30	b	1	Total C O 43 40 3	0
30	b	1	Total C O 43 40 3	0
30	c	1	Total C O 43 40 3	0
30	c	1	Total C O 43 40 3	0
30	c	1	Total C O 43 40 3	0
30	d	1	Total C O 43 40 3	0
30	d	1	Total C O 43 40 3	0

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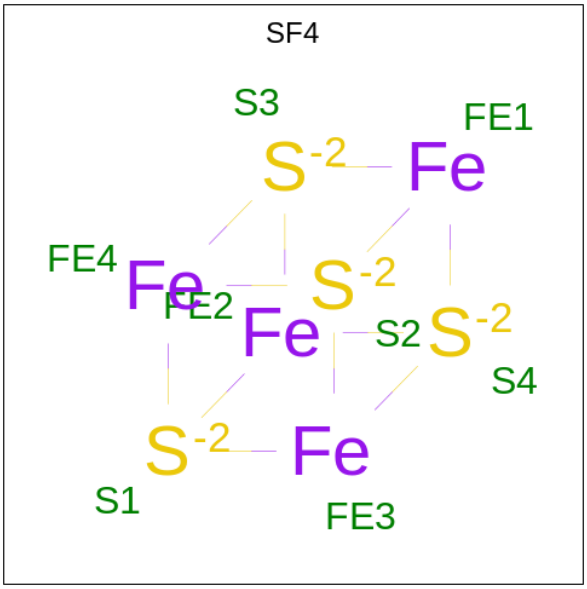
Mol	Chain	Residues	Atoms			AltConf
30	d	1	Total	C	O	0
			43	40	3	
30	e	1	Total	C	O	0
			43	40	3	
30	e	1	Total	C	O	0
			43	40	3	
30	e	1	Total	C	O	0
			43	40	3	
30	h	1	Total	C	O	0
			43	40	3	
30	h	1	Total	C	O	0
			43	40	3	
30	i	1	Total	C	O	0
			43	40	3	
30	i	1	Total	C	O	0
			43	40	3	
30	i	1	Total	C	O	0
			43	40	3	
30	j	1	Total	C	O	0
			43	40	3	
30	j	1	Total	C	O	0
			43	40	3	
30	k	1	Total	C	O	0
			43	40	3	
30	k	1	Total	C	O	0
			43	40	3	
30	l	1	Total	C	O	0
			43	40	3	
30	l	1	Total	C	O	0
			43	40	3	
30	m	1	Total	C	O	0
			43	40	3	
30	m	1	Total	C	O	0
			43	40	3	
30	f	1	Total	C	O	0
			43	40	3	
30	f	1	Total	C	O	0
			43	40	3	
30	g	1	Total	C	O	0
			43	40	3	
30	g	1	Total	C	O	0
			43	40	3	

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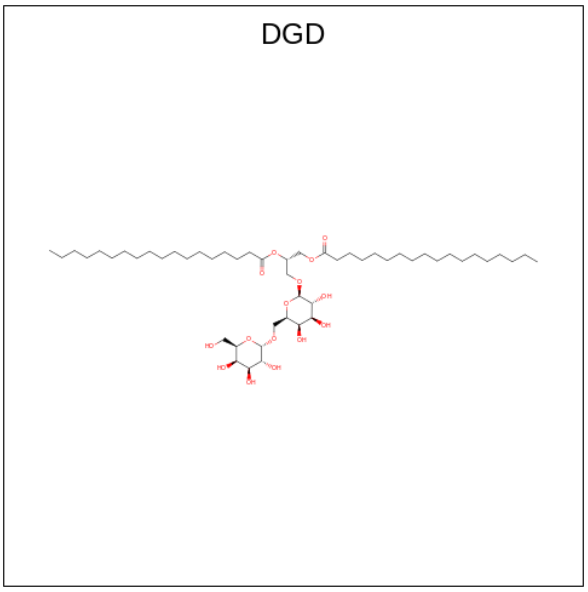
Mol	Chain	Residues	Atoms	AltConf
30	n	1	Total C O 43 40 3	0
30	n	1	Total C O 43 40 3	0
30	n	1	Total C O 43 40 3	0
30	o	1	Total C O 43 40 3	0
30	o	1	Total C O 43 40 3	0
30	p	1	Total C O 43 40 3	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



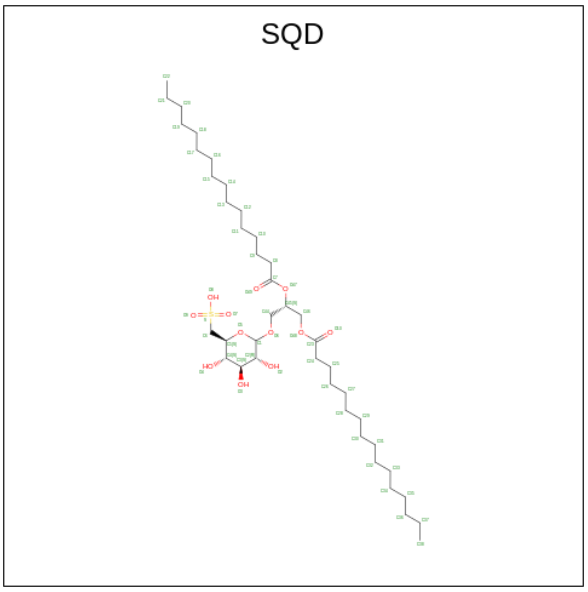
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



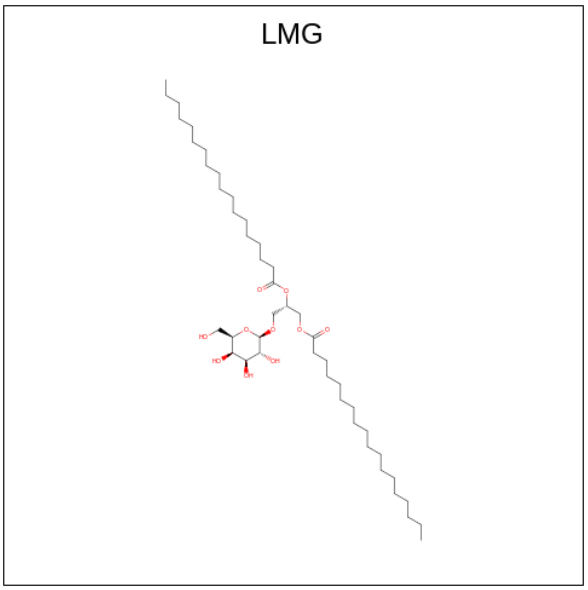
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total 54	C 39	O 15	0
32	b	1	Total 48	C 33	O 15	0
32	e	1	Total 36	C 21	O 15	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



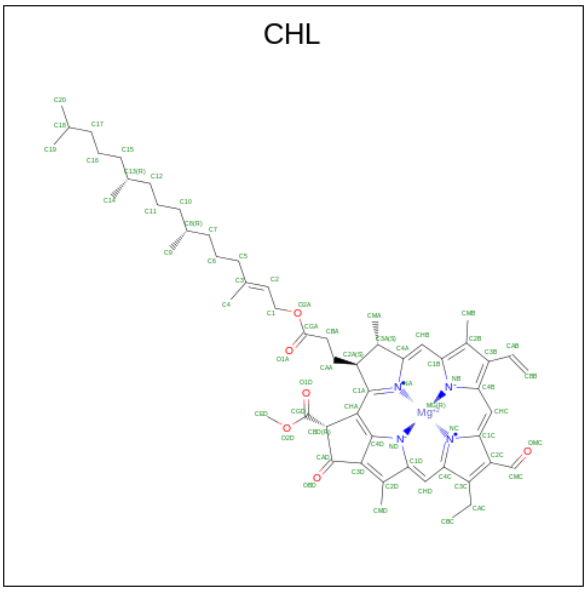
Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	O	S	0
			36	23	12	1	
33	F	1	Total	C	O	S	0
			39	26	12	1	
33	J	1	Total	C	O	S	0
			27	14	12	1	
33	g	1	Total	C	O	S	0
			32	19	12	1	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
34	a	1	Total	C	O	0
			43	33	10	
34	e	1	Total	C	O	0
			52	42	10	
34	j	1	Total	C	O	0
			44	34	10	
34	k	1	Total	C	O	0
			36	26	10	

- Molecule 35 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	e	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

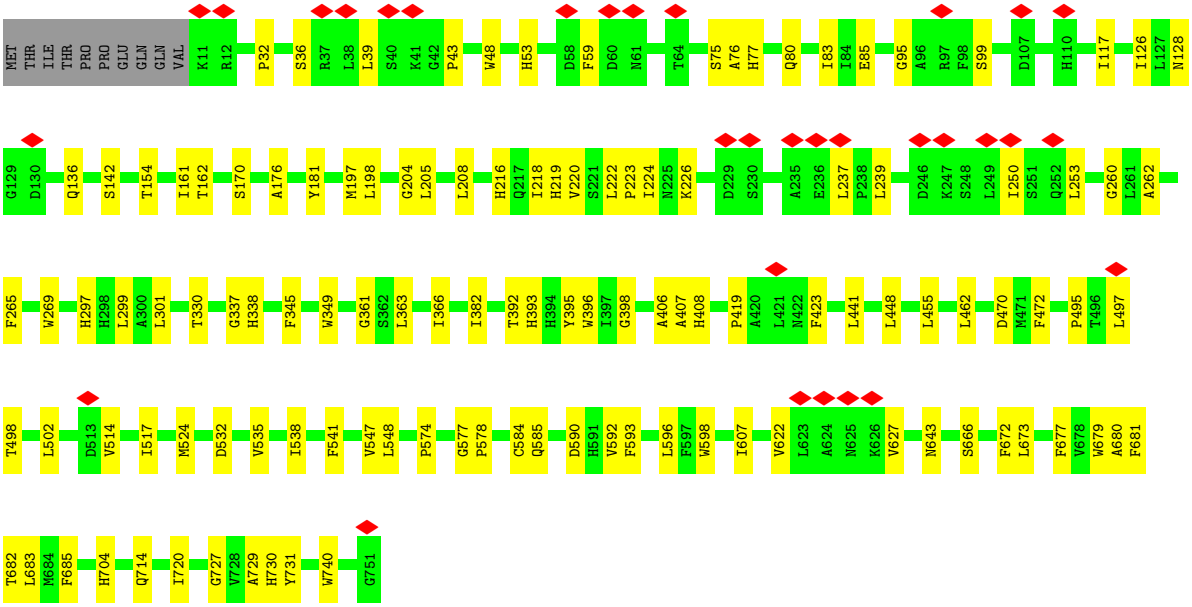
3 Residue-property plots (i)

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:

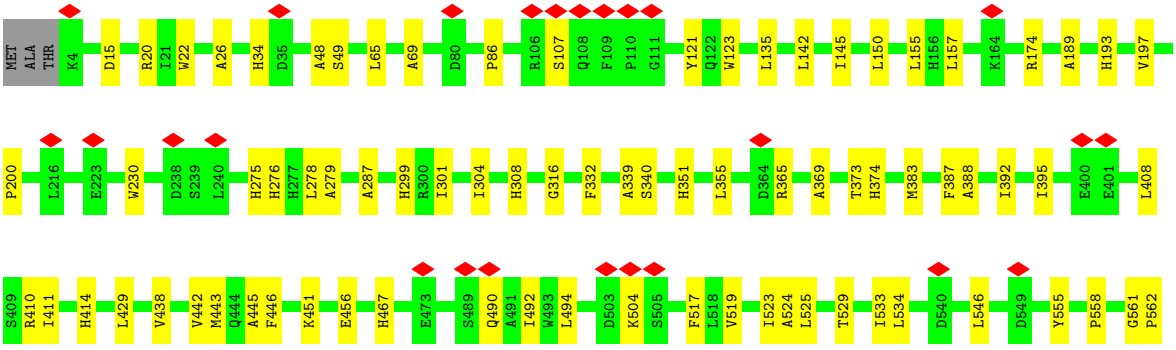


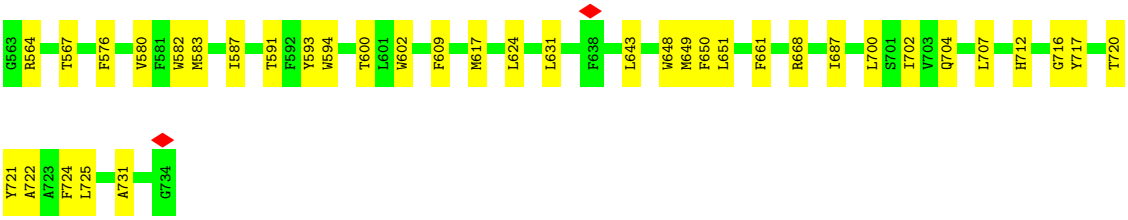


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

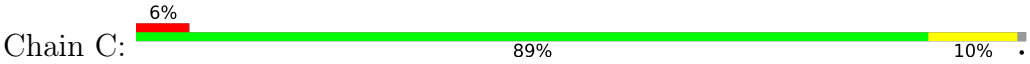
Chain B:

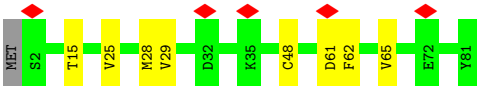




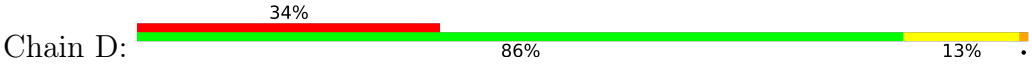


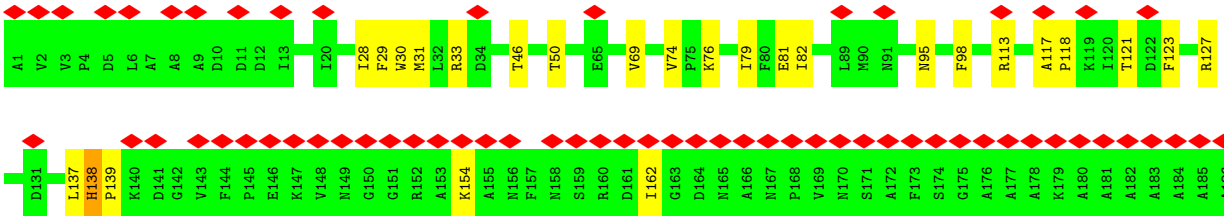
• Molecule 3: Photosystem I iron-sulfur center



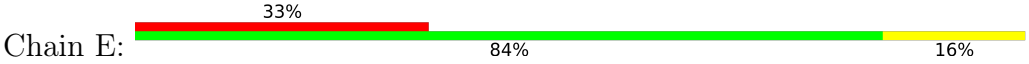


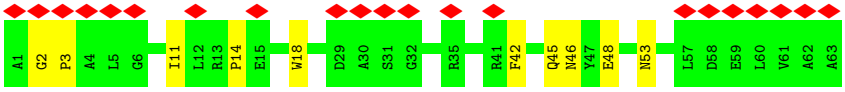
• Molecule 4: PsaD



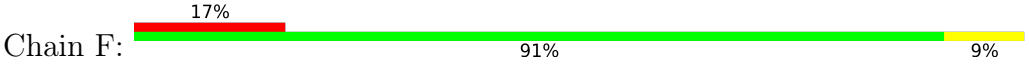


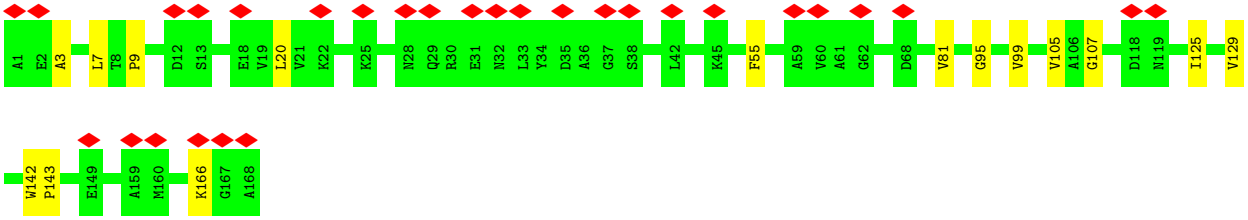
• Molecule 5: PsaE



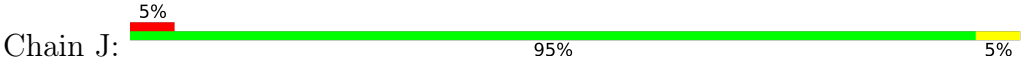


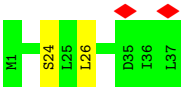
• Molecule 6: PsaF





• Molecule 7: Photosystem I reaction center subunit IX

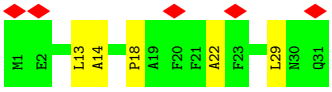




• Molecule 8: Photosystem I reaction center subunit XII

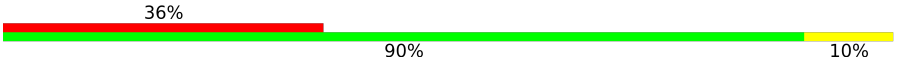
Chain M:

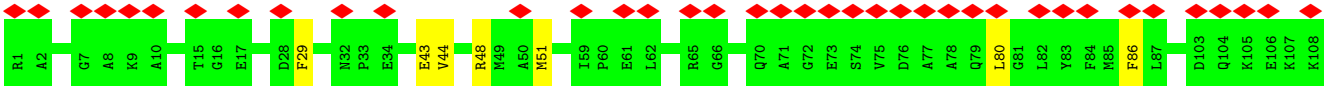




• Molecule 9: Chloroplast light-harvesting complex I protein

Chain a:



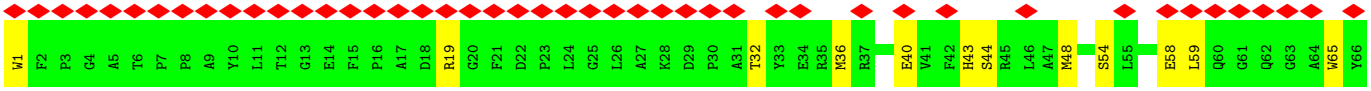


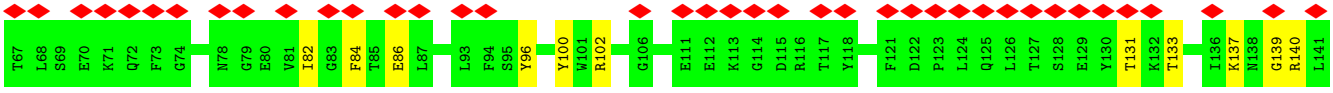


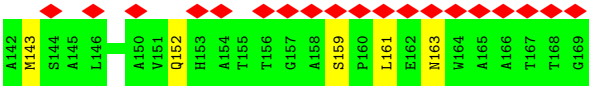
• Molecule 10: Chloroplast light-harvesting complex I protein

Chain b:



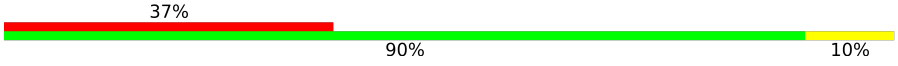


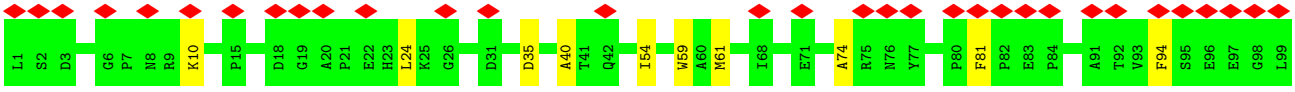


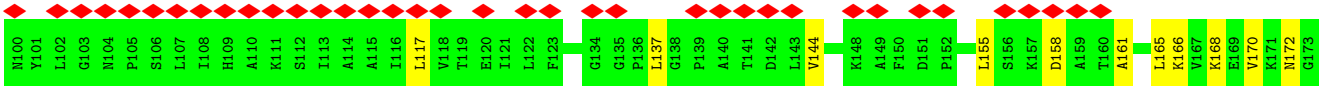


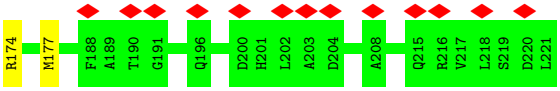
• Molecule 11: LHCE 3

Chain c:



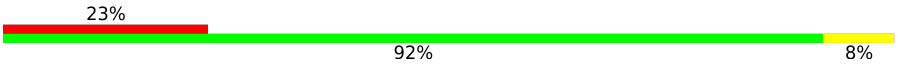


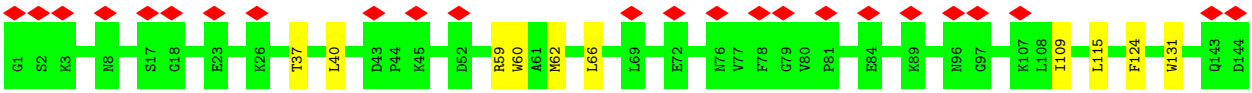


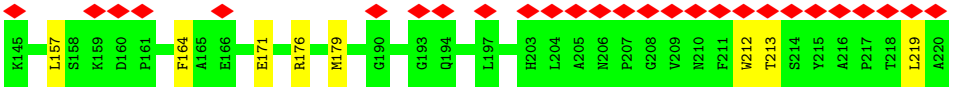


• Molecule 12: Light harvesting chlorophyll a /b binding protein of PSII

Chain d:



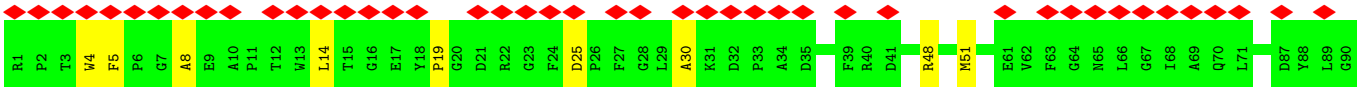


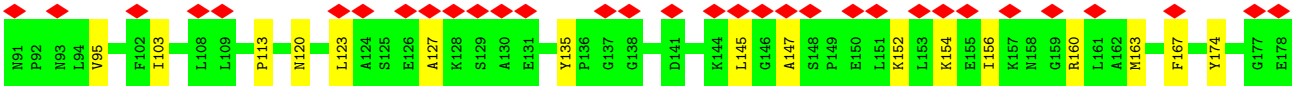


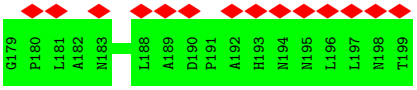
• Molecule 13: Chloroplast light-harvesting complex II protein

Chain e:





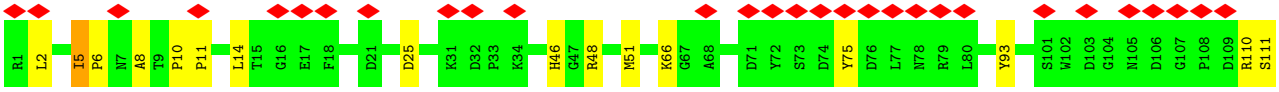




• Molecule 14: LHCE 8

Chain h:



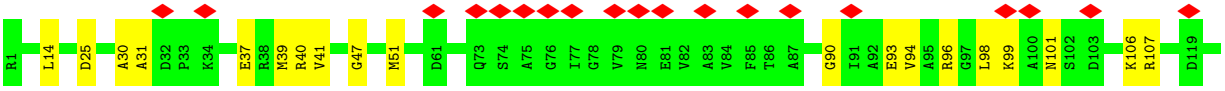


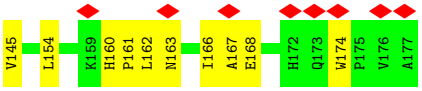


• Molecule 15: LHCE 9

Chain i:



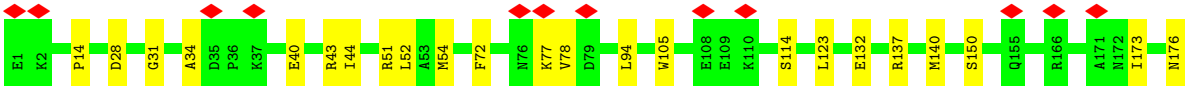


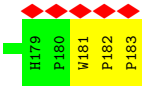


• Molecule 16: Chloroplast light-harvesting complex I protein

Chain j:



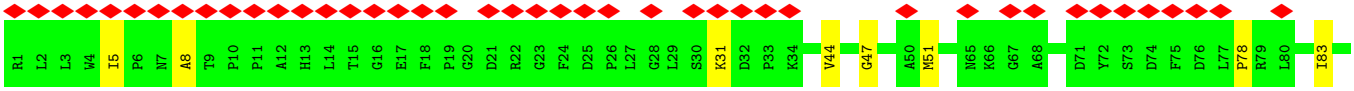


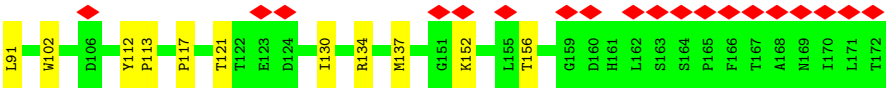


• Molecule 17: Chloroplast light-harvesting complex I protein

Chain k:



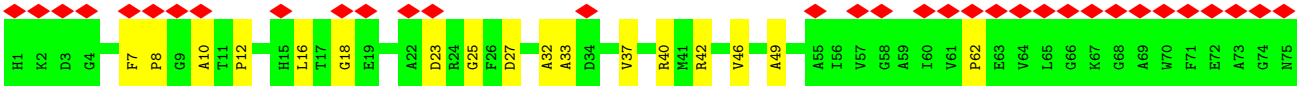


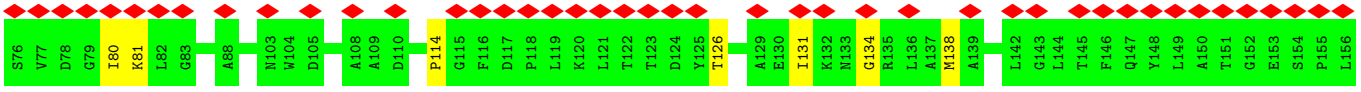


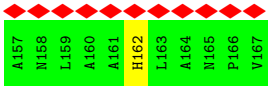
• Molecule 18: Chloroplast light-harvesting complex I protein

Chain l:





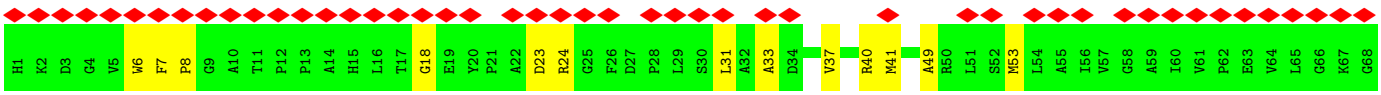


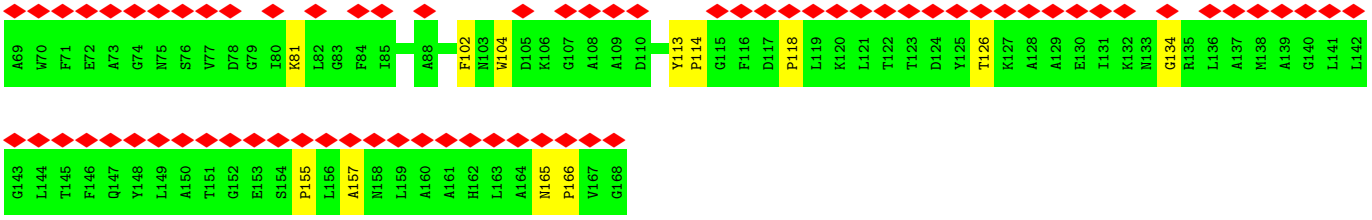


• Molecule 19: Chloroplast light-harvesting complex I protein

Chain m:



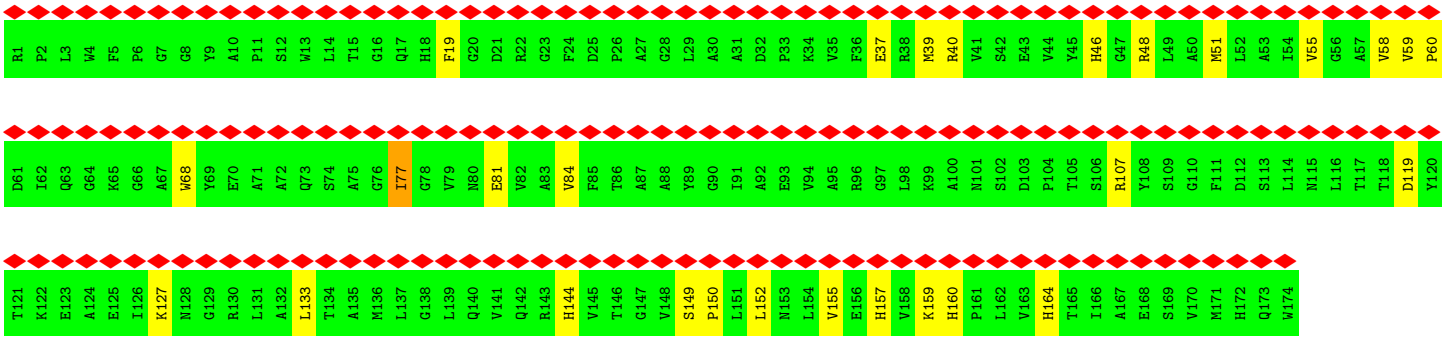




• Molecule 20: Chloroplast light-harvesting complex I protein, Lhca7_2

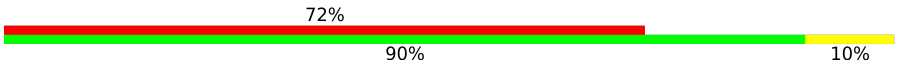
Chain f:

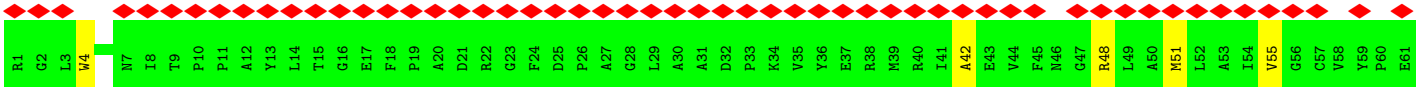


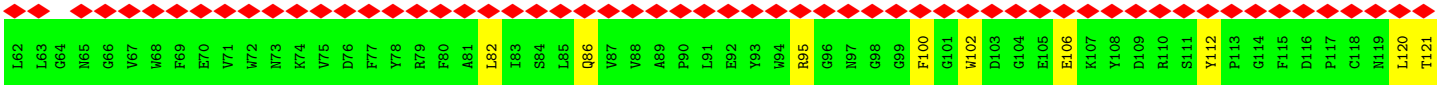


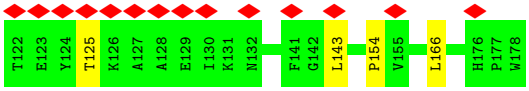
• Molecule 21: Chloroplast light-harvesting complex I protein

Chain g:





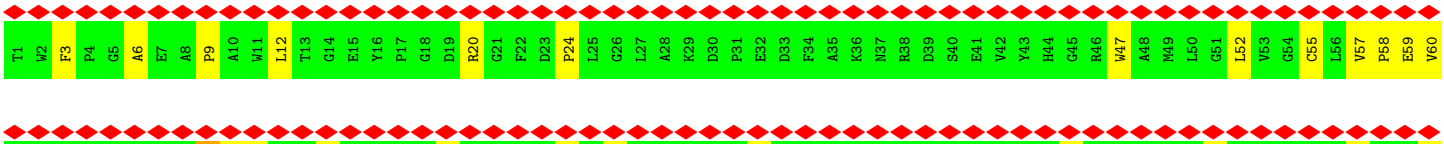


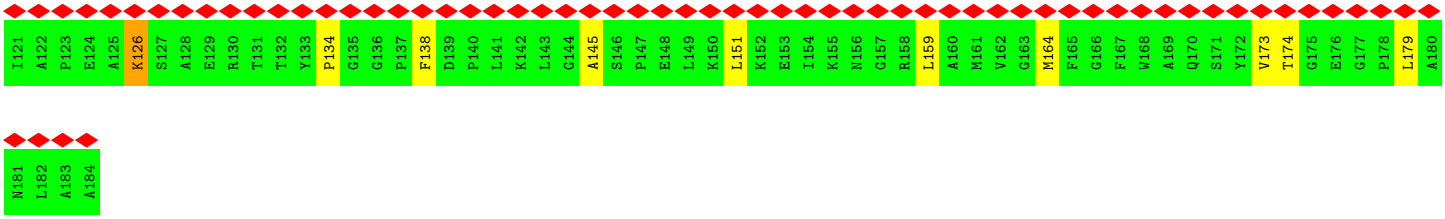


• Molecule 22: Chloroplast light-harvesting complex II protein

Chain n:

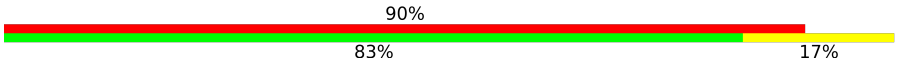


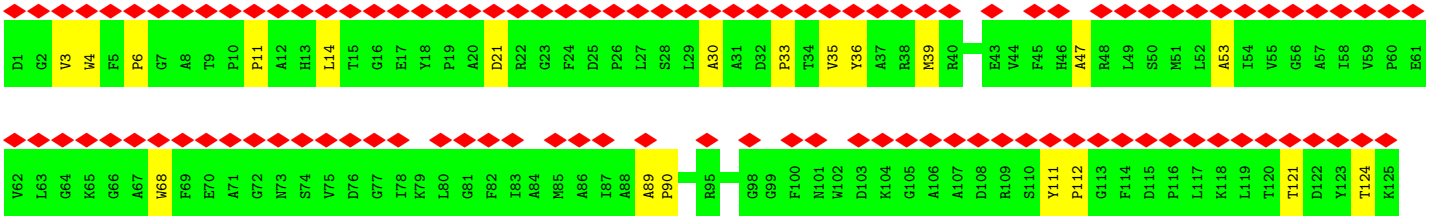




• Molecule 23: Chloroplast light-harvesting complex I protein

Chain o:

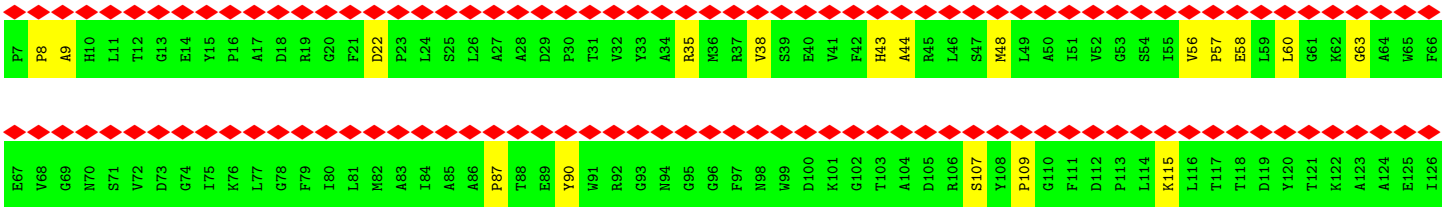




• Molecule 24: Chloroplast light-harvesting complex I protein

Chain p:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	562173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.741	Depositor
Minimum map value	-0.575	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, SQD, LMT, SF4, DGD, BCR, LMG, DD6, CHL, CLA, LHG

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	0.17	0/6079	0.28	0/8287
2	B	0.17	0/6071	0.28	0/8277
3	C	0.16	0/606	0.30	0/819
4	D	0.13	0/1426	0.27	0/1941
5	E	0.13	0/491	0.25	0/669
6	F	0.14	0/1275	0.26	0/1739
7	J	0.14	0/314	0.24	0/429
8	M	0.16	0/247	0.24	0/332
9	a	0.14	0/1311	0.25	0/1772
10	b	0.13	0/1344	0.28	0/1829
11	c	0.14	0/1719	0.25	0/2336
12	d	0.15	0/1719	0.27	0/2343
13	e	0.13	0/1566	0.25	0/2141
14	h	0.14	0/1388	0.28	0/1886
15	i	0.16	0/1391	0.30	0/1894
16	j	0.16	0/1499	0.27	0/2045
17	k	0.14	0/1377	0.26	0/1871
18	l	0.13	0/1293	0.26	0/1763
19	m	0.14	0/1297	0.30	0/1768
20	f	0.10	0/1367	0.26	0/1861
21	g	0.12	0/1452	0.25	0/1980
22	n	0.11	0/1458	0.26	0/1993
23	o	0.12	0/1266	0.28	0/1727
24	p	0.11	0/1156	0.26	0/1572
All	All	0.15	0/39112	0.27	0/53274

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	138	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5878	0	5745	99	0
2	B	5861	0	5659	102	0
3	C	596	0	571	6	0
4	D	1393	0	1371	17	0
5	E	481	0	479	9	0
6	F	1250	0	1259	13	0
7	J	305	0	317	2	0
8	M	243	0	258	4	0
9	a	1274	0	1235	13	0
10	b	1302	0	1244	19	0
11	c	1676	0	1689	16	0
12	d	1669	0	1650	16	0
13	e	1517	0	1468	19	0
14	h	1350	0	1324	18	0
15	i	1355	0	1336	24	0
16	j	1450	0	1401	20	0
17	k	1338	0	1314	13	0
18	l	1256	0	1234	20	0
19	m	1260	0	1236	24	0
20	f	1332	0	1312	16	0
21	g	1406	0	1358	15	0
22	n	1411	0	1372	24	0
23	o	1230	0	1205	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	p	1126	0	1115	13	0
25	A	2599	0	2480	118	0
25	B	2182	0	2078	111	0
25	F	87	0	64	6	0
25	J	50	0	39	2	0
25	a	571	0	488	24	0
25	b	492	0	373	14	0
25	c	638	0	527	22	0
25	d	521	0	418	11	0
25	e	676	0	551	18	0
25	f	553	0	448	10	0
25	g	598	0	467	22	0
25	h	642	0	533	27	0
25	i	603	0	527	15	0
25	j	667	0	568	19	0
25	k	631	0	520	14	0
25	l	562	0	459	17	0
25	m	461	0	369	15	0
25	n	499	0	389	14	0
25	o	429	0	320	12	0
25	p	393	0	297	9	0
26	A	35	0	46	0	0
27	A	87	0	123	7	0
27	a	26	0	22	1	0
27	b	31	0	32	3	0
27	c	30	0	29	3	0
27	d	29	0	28	3	0
27	g	35	0	40	0	0
27	h	61	0	62	3	0
27	i	36	0	42	2	0
27	j	37	0	44	4	0
27	m	32	0	34	2	0
28	A	33	0	46	5	0
28	B	60	0	78	2	0
28	F	26	0	29	0	0
29	A	160	0	224	9	0
29	B	280	0	392	26	0
29	J	40	0	56	3	0
29	M	40	0	56	2	0
30	A	86	0	0	0	0
30	F	43	0	0	0	0
30	J	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	86	0	0	1	0
30	b	86	0	0	0	0
30	c	129	0	0	0	0
30	d	129	0	0	1	0
30	e	129	0	0	0	0
30	f	86	0	0	0	0
30	g	86	0	0	0	0
30	h	86	0	0	0	0
30	i	129	0	0	1	0
30	j	86	0	0	0	0
30	k	86	0	0	0	0
30	l	86	0	0	0	0
30	m	86	0	0	2	0
30	n	129	0	0	1	0
30	o	86	0	0	0	0
30	p	43	0	0	0	0
31	A	8	0	0	0	0
31	C	16	0	0	0	0
32	B	54	0	66	2	0
32	b	48	0	54	3	0
32	e	36	0	30	2	0
33	D	36	0	36	0	0
33	F	39	0	42	0	0
33	J	27	0	18	0	0
33	g	32	0	28	2	0
34	a	43	0	56	0	0
34	e	52	0	77	5	0
34	j	44	0	61	0	0
34	k	36	0	42	3	0
35	c	49	0	34	3	0
35	d	186	0	128	7	0
35	e	46	0	31	0	0
All	All	55406	0	51153	806	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 (806) 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)
19:m:7:PHE:HA	25:m:202:CLA:NB	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:30:ALA:HB2	25:e:205:CLA:HBA1	1.63	0.81
23:o:47:ALA:HB1	23:o:132:GLY:HA3	1.64	0.78
25:A:824:CLA:HBD	25:A:824:CLA:HBA1	1.67	0.76
1:A:740:TRP:HB2	25:A:824:CLA:HBB1	1.69	0.74
1:A:204:GLY:O	1:A:208:LEU:HB2	1.86	0.74
19:m:49:ALA:HB1	19:m:134:GLY:HA3	1.69	0.74
27:a:201:LHG:HC42	25:a:203:CLA:HBD	1.70	0.73
25:a:204:CLA:H51	25:a:204:CLA:HBB1	1.70	0.73
18:l:49:ALA:HB1	18:l:134:GLY:HA3	1.71	0.72
20:f:149:SER:HB2	20:f:152:LEU:HB2	1.72	0.72
23:o:160:HIS:HE1	25:o:610:CLA:NA	1.87	0.72
18:l:46:VAL:HG22	18:l:131:ILE:HD11	1.72	0.70
25:A:833:CLA:HBA2	27:A:835:LHG:H161	1.73	0.69
28:A:834:PQN:H162	29:B:801:BCR:H382	1.74	0.69
25:B:819:CLA:H41	25:B:836:CLA:HBC3	1.73	0.69
14:h:5:ILE:HG22	14:h:8:ALA:HB2	1.74	0.69
23:o:36:TYR:H	23:o:39:MET:HG2	1.59	0.68
3:C:62:PHE:HD2	4:D:162:ILE:HG21	1.59	0.68
1:A:76:ALA:HB1	25:A:809:CLA:HBB1	1.76	0.68
5:E:14:PRO:HB2	6:F:166:LYS:HG3	1.77	0.67
20:f:39:MET:HB3	25:f:602:CLA:H3A	1.75	0.67
25:A:802:CLA:HBB1	25:A:840:CLA:NB	2.10	0.67
2:B:721:TYR:HB2	25:B:802:CLA:HED2	1.77	0.67
25:A:843:CLA:H12	29:J:101:BCR:H12C	1.77	0.66
1:A:223:PRO:HG3	1:A:250:ILE:HD13	1.77	0.66
25:j:203:CLA:HBB1	34:k:201:LMG:H331	1.76	0.66
1:A:83:ILE:HD12	25:A:842:CLA:HAB	1.76	0.66
4:D:74:VAL:HG22	4:D:76:LYS:H	1.59	0.66
6:F:105:VAL:HG21	6:F:142:TRP:HB2	1.77	0.66
23:o:121:THR:H	23:o:124:THR:HG22	1.61	0.66
25:B:817:CLA:H2	25:B:823:CLA:HBB2	1.78	0.65
14:h:120:LEU:HB2	25:h:209:CLA:HBA1	1.77	0.65
1:A:729:ALA:HA	27:A:835:LHG:H342	1.78	0.65
15:i:90:GLY:HA3	25:i:207:CLA:HAB	1.76	0.65
18:l:114:PRO:HB3	25:l:605:CLA:HBC2	1.78	0.65
25:B:842:CLA:H3A	25:B:848:CLA:HED3	1.79	0.65
10:b:44:SER:HB3	10:b:139:GLY:HA3	1.78	0.64
25:i:204:CLA:HBC2	25:i:213:CLA:HBB2	1.79	0.64
2:B:339:ALA:HB2	29:B:832:BCR:H372	1.80	0.64
1:A:265:PHE:HB2	25:a:213:CLA:H41	1.81	0.63
13:e:145:LEU:HB2	25:e:213:CLA:HBA1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:59:LEU:HD12	10:b:161:LEU:HD11	1.81	0.63
25:e:211:CLA:HBA1	25:e:211:CLA:HBD	1.80	0.63
22:n:3:PHE:HD2	22:n:6:ALA:HB2	1.64	0.62
25:B:840:CLA:HAB	34:e:202:LMG:H342	1.80	0.62
25:e:205:CLA:H43	25:e:206:CLA:HBA1	1.81	0.62
27:h:202:LHG:HC82	25:h:210:CLA:HBC3	1.82	0.62
35:c:307:CHL:HBA2	12:d:219:LEU:HB2	1.82	0.61
35:d:309:CHL:HHC	35:d:309:CHL:HBB1	1.82	0.61
14:h:113:PRO:HB3	25:h:207:CLA:HBC2	1.80	0.61
2:B:722:ALA:HB2	25:B:843:CLA:HBB1	1.80	0.61
17:k:113:PRO:HB3	25:k:206:CLA:HBC2	1.82	0.61
20:f:160:HIS:HB2	20:f:164:HIS:HD2	1.66	0.61
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.83	0.61
1:A:269:TRP:CH2	25:A:816:CLA:HBB1	2.36	0.60
1:A:498:THR:HG21	25:A:829:CLA:HMD3	1.83	0.60
2:B:490:GLN:HB2	25:e:201:CLA:HED1	1.82	0.60
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.83	0.60
21:g:143:LEU:HD22	21:g:154:PRO:HB3	1.82	0.60
22:n:120:GLN:HB3	22:n:126:LYS:HE2	1.83	0.60
27:j:202:LHG:HC42	25:j:203:CLA:HBD	1.84	0.60
1:A:226:LYS:HD3	1:A:253:LEU:HB3	1.83	0.60
1:A:538:ILE:HD12	25:A:801:CLA:H171	1.84	0.60
25:i:202:CLA:HED3	25:i:202:CLA:H2A	1.81	0.60
23:o:161:LEU:HD21	25:o:610:CLA:HAC1	1.83	0.59
25:d:315:CLA:HMB2	25:d:316:CLA:HAB	1.84	0.59
4:D:33:ARG:HD2	25:j:210:CLA:HAA2	1.83	0.59
1:A:598:TRP:HH2	25:A:807:CLA:HAB	1.68	0.59
29:B:831:BCR:H332	34:e:202:LMG:H141	1.84	0.59
15:i:160:HIS:HB3	15:i:163:ASN:HD22	1.67	0.59
12:d:60:TRP:CE2	35:d:310:CHL:HED2	2.38	0.58
9:a:124:SER:H	9:a:127:THR:HG22	1.68	0.58
10:b:1:TRP:HB2	10:b:19:ARG:HB3	1.84	0.58
27:A:805:LHG:H292	25:A:849:CLA:HBB1	1.84	0.58
29:B:831:BCR:H373	25:B:845:CLA:H111	1.85	0.58
18:l:7:PHE:HB3	18:l:10:ALA:HB2	1.83	0.58
13:e:123:LEU:HD21	25:e:211:CLA:HBB1	1.84	0.58
10:b:32:THR:O	10:b:36:MET:HG2	2.03	0.58
11:c:40:ALA:HB2	25:c:303:CLA:HBA1	1.86	0.58
23:o:160:HIS:CD2	25:o:610:CLA:NC	2.70	0.58
25:A:822:CLA:H12	25:A:830:CLA:HAA1	1.86	0.58
1:A:682:THR:HG21	1:A:731:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:817:CLA:HED2	25:B:845:CLA:HBD	1.86	0.58
25:l:611:CLA:C1D	25:l:612:CLA:HBB2	2.34	0.58
5:E:11:ILE:HD12	5:E:18:TRP:HB2	1.85	0.57
2:B:395:ILE:HD13	2:B:555:TYR:HA	1.86	0.57
10:b:84:PHE:HE2	32:b:202:DGD:HD1	1.69	0.57
25:A:804:CLA:HAC2	25:A:815:CLA:HAB	1.86	0.57
29:B:828:BCR:HC8	25:B:840:CLA:HMD1	1.85	0.57
25:B:817:CLA:HBB1	29:B:832:BCR:H19C	1.85	0.57
25:A:825:CLA:H61	29:A:836:BCR:H342	1.86	0.57
25:A:807:CLA:C1B	25:B:803:CLA:HBB1	2.35	0.57
2:B:49:SER:HB3	25:B:804:CLA:HBB1	1.86	0.57
25:p:603:CLA:HAA2	25:p:603:CLA:HBD	1.85	0.57
13:e:147:ALA:HB2	25:e:213:CLA:H2A	1.87	0.57
25:A:807:CLA:H143	25:B:808:CLA:HAB	1.85	0.56
25:A:819:CLA:HBB1	25:A:823:CLA:H72	1.86	0.56
27:i:201:LHG:H281	27:i:201:LHG:HC91	1.88	0.56
17:k:83:ILE:HG23	25:k:214:CLA:HMD2	1.87	0.56
21:g:48:ARG:HA	21:g:51:MET:HE3	1.87	0.56
25:A:810:CLA:H3A	25:A:826:CLA:HAB	1.87	0.56
25:B:838:CLA:H42	25:B:845:CLA:HBB2	1.87	0.56
15:i:101:ASN:HA	15:i:106:LYS:HG2	1.87	0.56
25:A:819:CLA:H151	25:A:849:CLA:HBC1	1.87	0.56
12:d:59:ARG:HA	12:d:62:MET:HE3	1.87	0.56
2:B:332:PHE:HE2	2:B:408:LEU:HD11	1.70	0.56
2:B:649:MET:HE1	25:B:807:CLA:H41	1.87	0.56
25:j:203:CLA:HMB2	34:k:201:LMG:H292	1.88	0.56
1:A:673:LEU:HD11	2:B:617:MET:HB2	1.88	0.55
1:A:338:HIS:CD2	25:A:820:CLA:ND	2.73	0.55
1:A:392:THR:HG22	25:A:824:CLA:HAB	1.88	0.55
25:B:805:CLA:H3A	25:B:819:CLA:HAB	1.89	0.55
6:F:81:VAL:HG21	12:d:115:LEU:HD13	1.88	0.55
2:B:442:VAL:HG21	25:B:822:CLA:HAC2	1.88	0.55
12:d:176:ARG:HA	12:d:179:MET:HE3	1.88	0.55
21:g:82:LEU:HG	21:g:86:GLN:HE21	1.71	0.55
25:B:804:CLA:H122	25:B:804:CLA:HBD	1.89	0.55
25:B:821:CLA:HBC2	25:B:847:CLA:HMC2	1.87	0.55
22:n:105:THR:HG22	25:n:205:CLA:C4A	2.29	0.55
25:c:304:CLA:HBC1	35:c:307:CHL:HBB2	1.88	0.55
19:m:8:PRO:HD3	25:m:202:CLA:C1B	2.37	0.55
19:m:165:ASN:HB3	19:m:166:PRO:HD3	1.87	0.55
9:a:136:ARG:HA	9:a:139:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:j:212:CLA:HAB	25:j:212:CLA:H122	1.88	0.55
25:g:207:CLA:HAA1	25:g:207:CLA:HBD	1.88	0.55
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.88	0.55
13:e:5:PHE:HB3	13:e:8:ALA:HB2	1.88	0.55
15:i:30:ALA:HB2	25:i:203:CLA:HBA1	1.89	0.55
16:j:51:ARG:HA	16:j:54:MET:HE3	1.88	0.55
21:g:112:TYR:HB3	25:g:209:CLA:HED2	1.89	0.55
1:A:162:THR:OG1	25:A:844:CLA:HBA1	2.07	0.54
2:B:155:LEU:HD13	25:h:211:CLA:H41	1.89	0.54
13:e:120:ASN:HA	13:e:127:ALA:HA	1.89	0.54
1:A:85:GLU:HB3	1:A:170:SER:HB2	1.89	0.54
1:A:714:GLN:HE22	5:E:45:GLN:H	1.55	0.54
23:o:11:PRO:HD2	23:o:14:LEU:HD12	1.89	0.54
14:h:5:ILE:HG12	14:h:6:PRO:HD2	1.89	0.54
1:A:363:LEU:HD11	25:A:818:CLA:H71	1.89	0.54
25:B:816:CLA:HHC	25:B:842:CLA:HMD3	1.89	0.54
16:j:105:TRP:HB2	19:m:40:ARG:HG3	1.90	0.54
25:f:610:CLA:HAA1	25:f:610:CLA:HBD	1.89	0.54
25:p:607:CLA:HAB	25:p:608:CLA:HAC2	1.90	0.54
1:A:330:THR:HG22	1:A:337:GLY:HA3	1.90	0.54
2:B:301:ILE:HG21	25:B:816:CLA:HAC1	1.90	0.54
11:c:165:LEU:HD23	11:c:168:LYS:HD3	1.89	0.54
29:B:830:BCR:H343	25:B:837:CLA:H3A	1.90	0.54
8:M:13:LEU:HD21	29:M:201:BCR:HC32	1.88	0.54
14:h:134:ARG:HA	14:h:137:MET:HE3	1.89	0.54
4:D:127:ARG:HB2	4:D:137:LEU:HD11	1.89	0.54
13:e:160:ARG:HA	13:e:163:MET:HE3	1.90	0.54
22:n:145:ALA:HB2	25:n:209:CLA:HED3	1.90	0.54
25:A:801:CLA:HAB	25:B:802:CLA:HAA1	1.90	0.53
25:B:816:CLA:H142	25:B:842:CLA:H51	1.89	0.53
25:B:841:CLA:H52	13:e:113:PRO:HG3	1.90	0.53
17:k:5:ILE:HG23	17:k:8:ALA:HB2	1.91	0.53
25:B:818:CLA:H203	29:B:830:BCR:H15C	1.90	0.53
19:m:102:PHE:H	27:m:201:LHG:HC12	1.73	0.53
25:B:819:CLA:H141	25:B:843:CLA:H141	1.90	0.53
19:m:8:PRO:HD3	25:m:202:CLA:C2B	2.39	0.53
25:F:201:CLA:HMB2	7:J:26:LEU:HD21	1.91	0.53
9:a:115:PRO:HB3	25:a:207:CLA:HBC2	1.91	0.53
13:e:19:PRO:HB2	13:e:156:ILE:HD12	1.91	0.53
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.74	0.53
1:A:75:SER:OG	1:A:181:TYR:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:HD11	25:A:814:CLA:H112	1.90	0.53
25:B:824:CLA:H72	25:B:824:CLA:HBB1	1.91	0.53
25:A:809:CLA:H72	25:A:815:CLA:H12	1.90	0.52
2:B:524:ALA:HB2	25:B:824:CLA:HMA1	1.90	0.52
25:n:202:CLA:HAC2	25:n:206:CLA:HBB2	1.90	0.52
1:A:730:HIS:HE1	25:A:833:CLA:ND	2.08	0.52
25:B:839:CLA:H71	25:B:845:CLA:H11	1.91	0.52
25:i:204:CLA:HBB1	30:i:215:DD6:C6	2.38	0.52
21:g:102:TRP:HB2	24:p:35:ARG:HD3	1.91	0.52
10:b:140:ARG:HA	10:b:143:MET:HE3	1.91	0.52
25:i:211:CLA:HBD	25:i:211:CLA:HBA1	1.90	0.52
16:j:77:LYS:HG3	16:j:78:VAL:HG23	1.91	0.52
1:A:361:GLY:HA2	1:A:398:GLY:HA2	1.92	0.52
1:A:495:PRO:HG3	1:A:502:LEU:HD23	1.92	0.52
25:A:833:CLA:HBA1	25:A:833:CLA:HBD	1.91	0.52
2:B:373:THR:HG22	25:B:843:CLA:HAB	1.89	0.52
27:d:302:LHG:HC5	25:d:303:CLA:HMD3	1.92	0.52
25:A:824:CLA:HBC3	29:A:839:BCR:H313	1.91	0.52
14:h:2:LEU:HB3	25:h:203:CLA:HED3	1.91	0.52
2:B:668:ARG:HB2	28:B:827:PQN:H7	1.90	0.52
21:g:120:LEU:HB2	25:g:209:CLA:HBA1	1.92	0.52
16:j:181:TRP:HB2	16:j:182:PRO:HD3	1.92	0.52
17:k:134:ARG:HA	17:k:137:MET:HE3	1.91	0.52
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.92	0.51
18:l:32:ALA:HB2	25:l:602:CLA:HBA1	1.91	0.51
25:l:610:CLA:HBA1	25:l:610:CLA:HBD	1.92	0.51
20:f:157:HIS:CD2	25:f:611:CLA:NC	2.78	0.51
1:A:142:SER:HA	25:A:824:CLA:HMA2	1.92	0.51
1:A:622:VAL:HG22	1:A:627:VAL:HG22	1.91	0.51
13:e:48:ARG:HA	13:e:51:MET:HE3	1.91	0.51
22:n:159:LEU:HD21	25:n:210:CLA:HAA1	1.91	0.51
1:A:349:TRP:HB3	25:A:809:CLA:HAC1	1.91	0.51
10:b:43:HIS:CE1	25:b:209:CLA:HMD3	2.45	0.51
1:A:598:TRP:CH2	25:A:807:CLA:HAB	2.45	0.51
2:B:174:ARG:HB2	25:B:811:CLA:HBC2	1.92	0.51
2:B:564:ARG:HG2	5:E:48:GLU:HG2	1.93	0.51
15:i:31:ALA:HB3	19:m:33:ALA:HB3	1.93	0.51
25:A:823:CLA:HMB1	25:A:829:CLA:HAA2	1.93	0.51
25:B:825:CLA:HBB2	28:B:827:PQN:H141	1.93	0.51
5:E:11:ILE:HD11	5:E:42:PHE:CZ	2.46	0.51
25:k:208:CLA:H43	25:k:210:CLA:HBA1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:203:CLA:HAA1	25:n:203:CLA:HBD	1.91	0.51
19:m:126:THR:HG22	25:m:208:CLA:H3A	1.93	0.51
29:B:830:BCR:H313	25:B:837:CLA:H12	1.92	0.51
17:k:78:PRO:HB2	18:l:80:ILE:HG22	1.93	0.51
23:o:4:TRP:H	23:o:4:TRP:CD1	2.29	0.51
24:p:44:ALA:HB1	24:p:129:GLY:HA3	1.93	0.51
25:A:802:CLA:HMD3	2:B:533:ILE:HG12	1.93	0.51
2:B:411:ILE:HA	2:B:414:HIS:CE1	2.46	0.51
15:i:94:VAL:HG11	22:n:111:PRO:HD3	1.93	0.51
17:k:44:VAL:HG22	17:k:130:ILE:HD11	1.93	0.51
19:m:118:PRO:HD2	30:m:212:DD6:O2	2.11	0.51
2:B:189:ALA:HA	25:B:837:CLA:HAB	1.92	0.50
6:F:20:LEU:HB2	6:F:55:PHE:CD2	2.45	0.50
25:h:209:CLA:HMB1	25:h:209:CLA:H12	1.93	0.50
2:B:519:VAL:HG21	2:B:593:TYR:HB2	1.93	0.50
25:h:212:CLA:HBD	25:h:212:CLA:HBA1	1.92	0.50
16:j:34:ALA:HB3	18:l:33:ALA:HB3	1.93	0.50
19:m:6:TRP:HA	25:m:202:CLA:C4D	2.41	0.50
19:m:18:GLY:HA2	19:m:23:ASP:HB3	1.93	0.50
29:M:201:BCR:H382	29:M:201:BCR:H23C	1.93	0.50
27:c:301:LHG:HC32	25:c:302:CLA:HAC1	1.94	0.50
14:h:46:HIS:CE1	25:h:208:CLA:HMD3	2.46	0.50
10:b:54:SER:HB2	10:b:65:TRP:HB3	1.92	0.50
24:p:38:VAL:HG22	24:p:107:SER:HB2	1.93	0.50
15:i:90:GLY:HA2	15:i:93:GLU:HB2	1.91	0.50
25:A:840:CLA:H51	2:B:438:VAL:HG13	1.94	0.50
22:n:71:ALA:HB3	22:n:74:GLU:HG2	1.92	0.50
15:i:161:PRO:O	15:i:162:LEU:HB2	2.11	0.50
1:A:154:THR:HG21	1:A:237:LEU:HD12	1.94	0.50
25:B:803:CLA:HED3	25:B:803:CLA:HBA2	1.94	0.50
17:k:121:THR:HG21	25:k:208:CLA:HED3	1.94	0.50
21:g:42:ALA:HB2	25:g:208:CLA:HED2	1.92	0.50
25:g:209:CLA:HBB2	25:g:211:CLA:CHB	2.41	0.50
12:d:66:LEU:HD23	25:d:306:CLA:HMC1	1.94	0.50
25:j:208:CLA:H2	27:m:201:LHG:H132	1.94	0.49
2:B:123:TRP:HH2	25:B:818:CLA:H12	1.77	0.49
2:B:340:SER:HA	25:B:845:CLA:H51	1.93	0.49
25:F:202:CLA:HAA1	25:F:202:CLA:HBD	1.93	0.49
15:i:41:VAL:HG22	15:i:107:ARG:HG3	1.94	0.49
22:n:20:ARG:HH21	22:n:151:LEU:HD21	1.76	0.49
25:l:602:CLA:H43	25:l:603:CLA:HBA1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.94	0.49
1:A:683:LEU:HB2	25:A:802:CLA:HMC2	1.95	0.49
2:B:279:ALA:HB2	25:B:838:CLA:HBB1	1.94	0.49
2:B:687:ILE:HD11	16:j:123:LEU:HD21	1.95	0.49
25:a:212:CLA:H11	25:a:213:CLA:H52	1.95	0.49
25:c:309:CLA:HBA1	12:d:37:THR:HG21	1.95	0.49
27:j:202:LHG:H262	25:j:203:CLA:HMD2	1.93	0.49
9:a:29:PHE:CD2	25:a:204:CLA:H12	2.47	0.49
16:j:44:ILE:HG12	16:j:114:SER:HB2	1.94	0.49
18:l:42:ARG:O	18:l:46:VAL:HG23	2.13	0.49
25:A:825:CLA:H12	29:A:836:BCR:H311	1.94	0.49
23:o:89:ALA:HB3	23:o:90:PRO:HD3	1.94	0.49
25:A:807:CLA:NB	25:B:803:CLA:HBB1	2.27	0.49
25:A:832:CLA:HBB2	6:F:107:GLY:HA3	1.94	0.49
27:d:302:LHG:HC61	27:d:302:LHG:H111	1.95	0.49
1:A:677:PHE:CG	29:A:839:BCR:H363	2.47	0.49
25:a:204:CLA:CGA	25:a:204:CLA:H3A	2.43	0.49
25:f:605:CLA:HAA2	25:f:605:CLA:HBD	1.94	0.49
25:n:201:CLA:H43	25:n:202:CLA:HBA1	1.94	0.49
1:A:197:MET:HE2	25:A:815:CLA:HHD	1.94	0.49
12:d:164:PHE:CZ	25:d:312:CLA:HED3	2.48	0.49
15:i:145:VAL:HA	15:i:174:TRP:HB2	1.95	0.49
23:o:142:LEU:HD13	23:o:153:PRO:HB3	1.94	0.49
1:A:59:PHE:CD2	25:A:809:CLA:HMC2	2.48	0.48
19:m:7:PHE:HA	25:m:202:CLA:C1B	2.43	0.48
1:A:198:LEU:HG	25:A:821:CLA:HMD2	1.95	0.48
1:A:345:PHE:HZ	29:A:837:BCR:H24C	1.78	0.48
2:B:355:LEU:HD11	25:B:845:CLA:HBB1	1.95	0.48
22:n:105:THR:HA	25:n:205:CLA:HMA3	1.96	0.48
1:A:218:ILE:HA	1:A:222:LEU:HD12	1.94	0.48
1:A:679:TRP:O	1:A:682:THR:HB	2.14	0.48
25:o:607:CLA:HBB2	25:o:608:CLA:CHB	2.44	0.48
1:A:77:HIS:CE1	25:A:809:CLA:ND	2.81	0.48
25:i:205:CLA:HAB	25:i:206:CLA:H52	1.95	0.48
22:n:47:TRP:CD2	25:n:207:CLA:HED3	2.48	0.48
1:A:682:THR:HG23	1:A:727:GLY:O	2.13	0.48
25:A:840:CLA:HMB3	25:B:802:CLA:H191	1.96	0.48
2:B:643:LEU:HD11	2:B:731:ALA:HB2	1.94	0.48
25:B:807:CLA:O1A	25:B:843:CLA:HBD	2.13	0.48
25:B:822:CLA:HBB1	25:B:844:CLA:C2B	2.44	0.48
9:a:48:ARG:HA	9:a:51:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:48:ARG:HA	14:h:51:MET:HE3	1.94	0.48
27:h:201:LHG:H101	27:h:201:LHG:H131	1.57	0.48
16:j:137:ARG:HA	16:j:140:MET:HE3	1.96	0.48
17:k:47:GLY:O	17:k:51:MET:HG3	2.13	0.48
1:A:419:PRO:HG2	4:D:81:GLU:HB2	1.96	0.48
25:A:826:CLA:H101	27:A:835:LHG:H331	1.94	0.48
17:k:91:LEU:HD13	25:k:206:CLA:HMA1	1.95	0.48
23:o:6:PRO:HD3	25:o:601:CLA:HMA1	1.96	0.48
25:h:214:CLA:HAA2	25:h:214:CLA:HBD	1.95	0.48
15:i:37:GLU:HG3	15:i:40:ARG:HH12	1.78	0.48
25:B:840:CLA:HBB2	34:e:202:LMG:H362	1.96	0.48
25:c:304:CLA:H43	12:d:40:LEU:HD21	1.94	0.48
25:c:310:CLA:H3A	25:c:310:CLA:HBA2	1.45	0.48
25:k:214:CLA:HBB2	25:l:606:CLA:H101	1.96	0.48
1:A:408:HIS:HE1	25:A:826:CLA:NA	2.11	0.47
25:B:804:CLA:HBC2	25:B:819:CLA:HMA1	1.96	0.47
1:A:681:PHE:N	25:A:802:CLA:HAB	2.28	0.47
25:A:804:CLA:H62	25:A:804:CLA:H41	1.56	0.47
25:g:212:CLA:HAA1	25:g:212:CLA:HBD	1.96	0.47
23:o:35:VAL:O	23:o:36:TYR:HB3	2.12	0.47
24:p:58:GLU:HG3	24:p:63:GLY:C	2.40	0.47
2:B:230:TRP:CH2	25:B:813:CLA:HBB1	2.50	0.47
25:B:818:CLA:H192	29:B:829:BCR:H352	1.95	0.47
12:d:157:LEU:HB2	25:d:312:CLA:HBA1	1.94	0.47
25:d:305:CLA:HBC1	35:d:309:CHL:HBB2	1.96	0.47
13:e:174:TYR:CD1	32:e:203:DGD:HG11	2.49	0.47
25:e:205:CLA:H3A	25:e:205:CLA:HBA2	1.55	0.47
20:f:155:VAL:O	20:f:159:LYS:HG2	2.14	0.47
25:A:833:CLA:HAC1	28:A:834:PQN:H192	1.96	0.47
25:c:303:CLA:H3A	25:c:303:CLA:HBA2	1.56	0.47
23:o:112:PRO:HD3	25:o:605:CLA:HMD2	1.97	0.47
25:B:817:CLA:HBB1	29:B:832:BCR:C19	2.44	0.47
14:h:129:GLU:HB2	25:h:209:CLA:CHB	2.45	0.47
25:h:207:CLA:H3A	25:h:207:CLA:HBA2	1.56	0.47
18:l:126:THR:HG22	25:l:607:CLA:HHB	1.96	0.47
21:g:4:TRP:O	25:g:203:CLA:NA	2.48	0.47
2:B:373:THR:HG23	2:B:591:THR:HG21	1.97	0.47
14:h:93:TYR:CE2	25:o:606:CLA:HBA1	2.50	0.47
23:o:30:ALA:HB1	23:o:36:TYR:HB2	1.97	0.47
25:A:812:CLA:H162	25:A:812:CLA:H122	1.71	0.47
2:B:150:LEU:HD22	8:M:22:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.96	0.47
2:B:661:PHE:HB3	25:B:803:CLA:HMC2	1.96	0.47
11:c:74:ALA:HB2	11:c:81:PHE:HD2	1.80	0.47
25:c:308:CLA:HAA1	25:c:308:CLA:HBD	1.97	0.47
13:e:103:ILE:HG12	25:e:208:CLA:HBC2	1.97	0.47
14:h:75:TYR:OH	25:h:206:CLA:H2A	2.14	0.47
15:i:174:TRP:HE1	25:j:215:CLA:CAD	2.27	0.47
25:j:209:CLA:H61	25:j:209:CLA:H41	1.72	0.47
19:m:113:TYR:HB3	25:m:208:CLA:HED2	1.96	0.47
20:f:48:ARG:HA	20:f:51:MET:HE3	1.94	0.47
25:p:602:CLA:H3A	25:p:602:CLA:HBA2	1.66	0.47
1:A:382:ILE:HG21	1:A:517:ILE:HB	1.96	0.47
25:A:844:CLA:H3A	25:A:844:CLA:HBA2	1.49	0.47
25:l:602:CLA:H61	25:l:602:CLA:H41	1.80	0.47
22:n:79:ALA:HB2	22:n:84:LEU:HD11	1.96	0.47
1:A:80:GLN:HG2	25:A:809:CLA:H3A	1.97	0.47
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.33	0.47
25:B:848:CLA:HAC2	34:e:202:LMG:HC71	1.96	0.47
11:c:10:LYS:HE2	27:c:301:LHG:HC2	1.97	0.47
11:c:155:LEU:HB2	25:c:310:CLA:HBA1	1.97	0.47
25:h:207:CLA:HAA1	25:h:207:CLA:HBD	1.97	0.47
16:j:31:GLY:HA3	18:l:37:VAL:HG21	1.96	0.47
25:f:610:CLA:H62	25:f:610:CLA:H92	1.70	0.47
22:n:117:TRP:HZ3	25:n:208:CLA:HED3	1.80	0.47
23:o:133:ARG:HA	23:o:136:MET:HE3	1.97	0.47
25:A:816:CLA:HAA1	25:A:816:CLA:HBD	1.97	0.47
25:A:833:CLA:H61	25:A:833:CLA:H41	1.77	0.47
13:e:14:LEU:HD11	13:e:25:ASP:HB2	1.97	0.47
14:h:125:THR:HG22	25:h:209:CLA:H3A	1.97	0.47
25:o:602:CLA:HBA2	25:o:602:CLA:H3A	1.76	0.47
25:A:824:CLA:H61	25:A:824:CLA:H41	1.69	0.46
3:C:29:VAL:HG21	4:D:154:LYS:HG3	1.97	0.46
25:d:304:CLA:HBB2	25:d:305:CLA:CHB	2.45	0.46
27:j:202:LHG:HC82	27:j:202:LHG:H281	1.97	0.46
18:l:162:HIS:CD2	25:l:611:CLA:NB	2.83	0.46
19:m:31:LEU:HD12	25:m:203:CLA:H12	1.97	0.46
1:A:441:LEU:HG	1:A:548:LEU:HB2	1.97	0.46
25:A:819:CLA:H62	25:A:819:CLA:H92	1.83	0.46
25:B:822:CLA:H8	25:B:822:CLA:H51	1.51	0.46
11:c:24:LEU:HD11	11:c:35:ASP:HB2	1.96	0.46
20:f:68:TRP:HD1	20:f:150:PRO:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:204:CLA:H3A	25:g:204:CLA:HBA2	1.72	0.46
25:A:817:CLA:H3A	25:A:817:CLA:HBA2	1.59	0.46
25:F:202:CLA:HMD3	12:d:115:LEU:HD23	1.97	0.46
25:h:203:CLA:H3A	25:h:203:CLA:HBA2	1.47	0.46
15:i:166:ILE:HD13	25:j:206:CLA:H101	1.97	0.46
27:i:201:LHG:H302	27:i:201:LHG:H112	1.98	0.46
25:i:208:CLA:HMB3	25:i:210:CLA:HAA1	1.98	0.46
21:g:166:LEU:HD12	33:g:202:SQD:H5	1.96	0.46
22:n:86:TYR:HD2	22:n:92:LEU:HD13	1.80	0.46
1:A:704:HIS:HE1	25:A:832:CLA:C4D	2.27	0.46
2:B:26:ALA:HB2	32:B:849:DGD:HB42	1.97	0.46
25:a:204:CLA:H11	30:a:215:DD6:O1	2.15	0.46
25:a:208:CLA:HMB1	10:b:100:TYR:HB2	1.97	0.46
15:i:47:GLY:O	15:i:51:MET:HG3	2.15	0.46
25:i:208:CLA:H41	25:i:208:CLA:H61	1.74	0.46
25:f:607:CLA:H61	25:f:607:CLA:H41	1.56	0.46
25:A:814:CLA:H62	25:A:814:CLA:H41	1.49	0.46
2:B:712:HIS:HE1	25:B:826:CLA:ND	2.12	0.46
9:a:120:LEU:HD12	9:a:122:MET:HE2	1.97	0.46
25:h:204:CLA:H41	25:h:204:CLA:H61	1.58	0.46
16:j:72:PHE:CD2	16:j:150:SER:HB2	2.51	0.46
18:l:126:THR:HG21	25:l:607:CLA:HBA2	1.97	0.46
15:i:167:ALA:O	25:j:206:CLA:H11	2.16	0.46
16:j:173:ILE:HD11	25:k:205:CLA:H161	1.98	0.46
23:o:68:TRP:HE1	23:o:142:LEU:HD11	1.81	0.46
2:B:365:ARG:HB3	2:B:602:TRP:CZ3	2.51	0.46
6:F:142:TRP:CG	6:F:143:PRO:HD3	2.50	0.46
25:e:201:CLA:H62	25:e:201:CLA:H41	1.56	0.46
25:e:213:CLA:HBB2	25:e:215:CLA:CHB	2.45	0.46
17:k:117:PRO:HB3	34:k:201:LMG:H142	1.98	0.46
25:g:212:CLA:H62	25:g:212:CLA:H41	1.70	0.46
22:n:58:PRO:HA	22:n:69:LEU:HB3	1.97	0.46
1:A:36:SER:HB3	1:A:39:LEU:HB2	1.98	0.46
25:A:833:CLA:H142	29:B:801:BCR:H363	1.98	0.46
25:A:841:CLA:H112	6:F:129:VAL:HG13	1.98	0.46
22:n:173:VAL:HG23	22:n:174:THR:HG23	1.97	0.46
24:p:57:PRO:O	24:p:58:GLU:HB2	2.15	0.46
25:A:812:CLA:HAB	29:J:101:BCR:H352	1.98	0.46
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.98	0.46
2:B:707:LEU:HD23	32:B:849:DGD:HB31	1.98	0.46
25:B:841:CLA:HAB	34:e:202:LMG:H132	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:ILE:HD12	4:D:30:TRP:HD1	1.80	0.46
4:D:123:PHE:CE2	4:D:138:HIS:HD2	2.34	0.46
24:p:8:PRO:HG2	24:p:22:ASP:H	1.80	0.46
1:A:216:HIS:HB2	25:A:844:CLA:C1C	2.46	0.46
1:A:301:LEU:HD11	25:A:818:CLA:HBB1	1.97	0.46
2:B:279:ALA:CB	25:B:838:CLA:HBB1	2.46	0.46
2:B:351:HIS:CD2	25:B:845:CLA:NC	2.85	0.46
2:B:648:TRP:CE3	29:B:833:BCR:HC41	2.51	0.46
18:l:134:GLY:O	18:l:138:MET:HG3	2.16	0.46
20:f:144:HIS:HB2	25:f:612:CLA:HED1	1.97	0.46
25:A:821:CLA:HBB2	29:A:837:BCR:H361	1.98	0.45
4:D:113:ARG:HG2	4:D:121:THR:HG22	1.98	0.45
25:l:611:CLA:HAA1	25:l:611:CLA:HBD	1.97	0.45
21:g:125:THR:HG22	25:g:209:CLA:H3A	1.97	0.45
25:g:212:CLA:H3A	25:g:212:CLA:HBA2	1.78	0.45
2:B:278:LEU:HD11	25:B:813:CLA:HAB	1.96	0.45
2:B:301:ILE:HG23	25:B:839:CLA:HED3	1.97	0.45
25:F:202:CLA:H3A	25:F:202:CLA:HBA2	1.65	0.45
25:i:202:CLA:H3A	25:i:202:CLA:HBA2	1.60	0.45
20:f:40:ARG:HB2	20:f:107:ARG:HH21	1.82	0.45
1:A:262:ALA:HA	25:a:213:CLA:H43	1.98	0.45
1:A:643:ASN:HB2	2:B:651:LEU:HD11	1.98	0.45
25:B:824:CLA:HBA2	25:B:846:CLA:CGA	2.47	0.45
29:B:831:BCR:H363	25:B:839:CLA:H2	1.97	0.45
25:h:209:CLA:HMB3	25:h:211:CLA:HAA1	1.96	0.45
15:i:93:GLU:OE1	15:i:96:ARG:HD3	2.16	0.45
20:f:81:GLU:HA	20:f:84:VAL:HG22	1.97	0.45
2:B:523:ILE:CG2	25:B:846:CLA:HBB1	2.45	0.45
11:c:61:MET:HE3	11:c:172:ASN:HB3	1.97	0.45
25:k:206:CLA:HAA1	25:k:206:CLA:HBD	1.99	0.45
18:l:7:PHE:CG	18:l:8:PRO:HD2	2.52	0.45
2:B:276:HIS:HB2	25:B:838:CLA:CHB	2.45	0.45
11:c:137:LEU:HB2	25:c:308:CLA:HMC2	1.98	0.45
11:c:174:ARG:HA	11:c:177:MET:HE3	1.97	0.45
1:A:406:ALA:HB2	29:A:838:BCR:H323	1.98	0.45
25:A:857:CLA:HMD3	29:B:833:BCR:H383	1.99	0.45
2:B:65:LEU:HD11	29:B:830:BCR:H281	1.97	0.45
25:l:607:CLA:HBA2	25:l:607:CLA:H3A	1.49	0.45
1:A:197:MET:HB2	25:A:815:CLA:HBC2	1.98	0.45
25:A:850:CLA:CAD	4:D:29:PHE:HB2	2.47	0.45
2:B:594:TRP:CD1	25:B:846:CLA:HBC2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:h:206:CLA:HBA1	25:h:206:CLA:H3A	1.73	0.45
23:o:160:HIS:HE1	25:o:610:CLA:C4A	2.29	0.45
2:B:523:ILE:HG23	25:B:846:CLA:HBB1	1.99	0.45
25:B:814:CLA:HBA2	25:B:814:CLA:H3A	1.86	0.45
3:C:15:THR:HG22	3:C:28:MET:HG3	1.97	0.45
25:B:807:CLA:H203	25:B:807:CLA:H162	1.70	0.45
25:B:822:CLA:H91	6:F:99:VAL:HG21	1.98	0.45
25:j:209:CLA:HBA2	25:j:209:CLA:H3A	1.50	0.45
25:k:211:CLA:HAA1	25:k:211:CLA:HBD	1.98	0.45
1:A:297:HIS:HB2	25:A:817:CLA:C1B	2.47	0.45
25:A:817:CLA:H102	25:A:817:CLA:HBC3	1.99	0.45
25:B:824:CLA:HBA1	25:B:824:CLA:HBD	1.99	0.45
10:b:152:GLN:HB3	10:b:163:ASN:ND2	2.32	0.45
25:i:208:CLA:H3A	25:i:208:CLA:HBA2	1.45	0.45
21:g:121:THR:HG21	25:g:209:CLA:HED3	1.98	0.45
25:g:214:CLA:HAA2	25:g:214:CLA:HBD	1.99	0.45
22:n:59:GLU:HB2	22:n:179:LEU:HD12	2.00	0.45
1:A:53:HIS:HB3	27:A:835:LHG:H111	1.99	0.44
2:B:576:PHE:O	2:B:580:VAL:HG23	2.16	0.44
3:C:61:ASP:HB2	5:E:53:ASN:ND2	2.31	0.44
25:b:207:CLA:HAA1	25:b:207:CLA:HBD	1.99	0.44
35:d:308:CHL:HBD	35:d:308:CHL:HBA2	1.99	0.44
21:g:95:ARG:HA	25:g:207:CLA:HBC2	2.00	0.44
2:B:308:HIS:HE1	25:B:841:CLA:ND	2.12	0.44
25:B:805:CLA:H112	25:B:805:CLA:H152	1.77	0.44
25:B:805:CLA:H191	25:B:843:CLA:H151	2.00	0.44
22:n:70:PRO:HD2	25:n:203:CLA:HED3	1.99	0.44
23:o:36:TYR:HA	23:o:39:MET:HB2	1.99	0.44
25:A:821:CLA:H193	25:A:821:CLA:H162	1.89	0.44
25:A:832:CLA:HBB1	25:A:841:CLA:HMD3	2.00	0.44
25:A:843:CLA:H62	25:A:843:CLA:H41	1.79	0.44
2:B:123:TRP:CH2	25:B:818:CLA:H12	2.52	0.44
2:B:287:ALA:HB2	25:B:839:CLA:HBC2	1.99	0.44
2:B:443:MET:SD	2:B:451:LYS:HE3	2.57	0.44
25:m:203:CLA:H41	25:m:204:CLA:H3A	2.00	0.44
1:A:532:ASP:HA	1:A:535:VAL:HG12	2.00	0.44
2:B:230:TRP:HB2	25:B:813:CLA:HBA1	2.00	0.44
25:g:209:CLA:H3A	25:g:209:CLA:HBA2	1.68	0.44
1:A:578:PRO:HD3	2:B:561:GLY:HA2	1.99	0.44
25:A:801:CLA:HAA2	25:A:801:CLA:CGD	2.48	0.44
25:B:836:CLA:HAA1	25:B:836:CLA:HBD	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:213:CLA:HED2	25:a:213:CLA:HBD	1.86	0.44
25:b:212:CLA:H62	25:b:212:CLA:H41	1.59	0.44
13:e:123:LEU:HD21	25:e:211:CLA:CBB	2.48	0.44
25:k:203:CLA:H72	25:k:204:CLA:HMB3	1.98	0.44
25:l:607:CLA:H61	25:l:607:CLA:H41	1.66	0.44
2:B:712:HIS:HE1	25:B:826:CLA:C4D	2.31	0.44
29:B:832:BCR:H11C	25:B:847:CLA:H43	2.00	0.44
7:J:24:SER:HB3	25:J:103:CLA:HHC	1.99	0.44
25:b:206:CLA:HBA1	25:b:206:CLA:HBD	1.98	0.44
14:h:10:PRO:HA	14:h:11:PRO:HD3	1.82	0.44
16:j:44:ILE:HD13	19:m:104:TRP:NE1	2.33	0.44
25:l:602:CLA:H3A	25:l:602:CLA:HBA2	1.54	0.44
1:A:176:ALA:HB2	25:A:813:CLA:HBC2	1.99	0.44
25:A:814:CLA:H11	25:A:842:CLA:HBD	1.99	0.44
2:B:583:MET:O	2:B:587:ILE:HG12	2.18	0.44
11:c:59:TRP:CE2	25:c:308:CLA:HED2	2.53	0.44
16:j:94:LEU:HD13	25:j:207:CLA:HMA2	2.00	0.44
25:c:313:CLA:H2	25:c:314:CLA:HMD1	1.99	0.44
13:e:4:TRP:H	13:e:4:TRP:CD1	2.35	0.44
19:m:114:PRO:HB3	25:m:206:CLA:HBC2	1.99	0.44
1:A:117:ILE:O	25:A:843:CLA:HED2	2.18	0.44
25:A:818:CLA:H112	25:A:818:CLA:H72	1.67	0.44
25:A:832:CLA:H92	25:A:832:CLA:H62	1.77	0.44
6:F:99:VAL:HG13	25:F:201:CLA:HAA1	2.00	0.44
25:a:207:CLA:H41	25:a:207:CLA:H62	1.76	0.44
25:c:304:CLA:HMA2	25:c:304:CLA:H11	2.00	0.44
25:c:313:CLA:HAA1	25:c:313:CLA:HBD	1.99	0.44
25:m:203:CLA:H41	25:m:203:CLA:H62	1.92	0.44
2:B:456:GLU:HG3	6:F:7:LEU:HD11	2.00	0.43
11:c:94:PHE:CE1	12:d:213:THR:HG22	2.53	0.43
25:d:313:CLA:HAA1	25:d:313:CLA:HBD	2.00	0.43
16:j:52:LEU:HD22	25:j:208:CLA:HHD	1.99	0.43
24:p:109:PRO:HB3	25:p:605:CLA:HBC2	1.99	0.43
1:A:680:ALA:C	25:A:802:CLA:HAB	2.43	0.43
2:B:48:ALA:HB3	8:M:29:LEU:HD21	2.00	0.43
2:B:387:PHE:HB3	2:B:534:LEU:HB3	2.00	0.43
29:B:832:BCR:H17C	25:B:845:CLA:H112	2.00	0.43
16:j:40:GLU:HG2	16:j:43:ARG:HH22	1.83	0.43
22:n:55:CYS:O	22:n:58:PRO:HD2	2.18	0.43
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.99	0.43
1:A:498:THR:HG21	25:A:829:CLA:CMD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:845:CLA:HBA1	25:A:845:CLA:H3A	1.87	0.43
2:B:383:MET:HE1	29:B:832:BCR:H361	2.01	0.43
25:J:103:CLA:H3A	25:J:103:CLA:HBA2	1.47	0.43
15:i:14:LEU:HD11	15:i:25:ASP:HB2	1.99	0.43
23:o:53:ALA:HB3	23:o:139:LEU:HD11	2.00	0.43
1:A:666:SER:HB2	2:B:445:ALA:HB1	1.99	0.43
2:B:275:HIS:HE1	25:B:813:CLA:C4D	2.31	0.43
25:B:812:CLA:HBB2	25:B:818:CLA:H143	2.00	0.43
1:A:95:GLY:O	1:A:99:SER:HB2	2.19	0.43
1:A:366:ILE:HA	25:A:822:CLA:HED2	2.00	0.43
25:a:205:CLA:H11	25:a:205:CLA:HBA1	1.72	0.43
15:i:99:LYS:HB2	15:i:106:LYS:HD3	1.99	0.43
1:A:393:HIS:HE2	25:A:825:CLA:C1B	2.32	0.43
1:A:455:LEU:HD22	1:A:472:PHE:CE2	2.53	0.43
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.54	0.43
2:B:600:THR:HG21	2:B:609:PHE:HB2	2.00	0.43
25:B:805:CLA:H3A	25:B:819:CLA:CAB	2.48	0.43
25:B:842:CLA:HBA1	25:B:842:CLA:HBD	1.99	0.43
18:l:18:GLY:HA2	18:l:23:ASP:HB3	2.00	0.43
1:A:161:ILE:HG22	25:A:844:CLA:H12	2.00	0.43
25:A:840:CLA:C1D	25:B:802:CLA:H2	2.49	0.43
2:B:142:LEU:HG	29:B:830:BCR:H382	1.99	0.43
25:b:212:CLA:H2	25:c:311:CLA:C1B	2.48	0.43
12:d:124:PHE:HB3	30:d:319:DD6:C3	2.48	0.43
13:e:174:TYR:HD1	32:e:203:DGD:HG11	1.84	0.43
25:f:610:CLA:H3A	25:f:610:CLA:HBA2	1.86	0.43
25:A:801:CLA:C1A	25:B:802:CLA:HAB	2.47	0.43
2:B:145:ILE:HD12	25:B:812:CLA:H152	2.01	0.43
25:B:811:CLA:H152	29:B:829:BCR:H271	2.01	0.43
25:a:210:CLA:H3A	25:a:210:CLA:HBA2	1.69	0.43
10:b:133:THR:HG22	10:b:137:LYS:HD2	2.01	0.43
27:b:201:LHG:HC32	32:b:202:DGD:HA82	2.00	0.43
11:c:166:LYS:O	11:c:170:VAL:HG23	2.19	0.43
25:c:309:CLA:HBA2	25:c:309:CLA:H3A	1.55	0.43
25:h:205:CLA:HBB1	25:h:214:CLA:HMB2	2.01	0.43
25:a:212:CLA:H41	25:a:212:CLA:H62	1.73	0.43
25:m:211:CLA:HED3	25:m:211:CLA:H2A	2.01	0.43
22:n:57:VAL:HA	22:n:60:VAL:HG12	2.01	0.43
24:p:56:VAL:HG13	24:p:60:LEU:HD13	2.01	0.43
2:B:558:PRO:HB3	2:B:702:ILE:HB	2.00	0.43
11:c:54:ILE:HG21	11:c:144:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:e:207:CLA:HAA1	25:e:207:CLA:HBD	2.00	0.43
25:h:208:CLA:HHC	25:h:208:CLA:HBB1	2.01	0.43
25:h:209:CLA:H92	25:h:209:CLA:H61	1.76	0.43
1:A:585:GLN:HA	1:A:590:ASP:OD2	2.19	0.42
25:A:810:CLA:H202	25:A:810:CLA:H162	1.82	0.42
4:D:28:ILE:HG13	4:D:31:MET:H	1.83	0.42
9:a:44:VAL:HG22	9:a:132:ILE:HD11	2.01	0.42
11:c:158:ASP:HB3	11:c:161:ALA:HB3	2.01	0.42
27:h:202:LHG:H112	25:h:203:CLA:HMD2	2.00	0.42
25:h:209:CLA:H12	25:h:209:CLA:CMB	2.47	0.42
21:g:166:LEU:HG	33:g:202:SQD:H81	2.01	0.42
2:B:276:HIS:HB2	25:B:838:CLA:C1B	2.49	0.42
25:B:815:CLA:HBA2	25:B:815:CLA:H3A	1.50	0.42
9:a:86:PHE:HZ	32:b:202:DGD:HG11	1.85	0.42
12:d:131:TRP:CZ3	35:d:310:CHL:HAB	2.53	0.42
17:k:102:TRP:HB2	18:l:40:ARG:HG3	2.01	0.42
18:l:81:LYS:HE2	18:l:81:LYS:HB3	1.83	0.42
22:n:134:PRO:HB3	25:n:207:CLA:HBC2	2.01	0.42
25:A:812:CLA:H192	25:A:812:CLA:H161	1.76	0.42
28:A:834:PQN:H303	28:A:834:PQN:H261	1.79	0.42
2:B:374:HIS:HE2	25:B:818:CLA:C1B	2.33	0.42
23:o:21:ASP:HA	25:o:602:CLA:O1D	2.19	0.42
24:p:43:HIS:HE1	25:p:603:CLA:NA	2.16	0.42
24:p:142:GLN:HE22	25:p:609:CLA:C4C	2.32	0.42
25:A:821:CLA:H62	25:A:821:CLA:H93	1.75	0.42
25:A:832:CLA:H12	25:B:844:CLA:H42	2.00	0.42
2:B:467:HIS:CD2	25:B:823:CLA:ND	2.87	0.42
29:B:828:BCR:HC8	25:B:840:CLA:CMD	2.50	0.42
25:B:843:CLA:HBA2	25:B:843:CLA:H3A	1.78	0.42
5:E:2:GLY:HA2	5:E:3:PRO:HD3	1.90	0.42
17:k:112:TYR:HB3	25:k:208:CLA:HED2	2.00	0.42
25:m:203:CLA:H61	25:m:203:CLA:H92	1.80	0.42
25:g:204:CLA:H62	25:g:205:CLA:HMB1	2.02	0.42
22:n:9:PRO:HG2	22:n:12:LEU:HB3	2.01	0.42
29:B:832:BCR:C17	25:B:845:CLA:H112	2.49	0.42
25:b:212:CLA:H42	25:c:311:CLA:NC	2.35	0.42
15:i:39:MET:HB3	25:i:203:CLA:H3A	2.01	0.42
25:g:203:CLA:HAA1	25:g:203:CLA:HBD	2.01	0.42
23:o:124:THR:HG23	25:o:607:CLA:H3A	2.01	0.42
24:p:48:MET:HE2	24:p:48:MET:HB3	1.93	0.42
25:p:602:CLA:HBB2	25:p:603:CLA:CHD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:HA2	1:A:99:SER:OG	2.18	0.42
1:A:126:ILE:HG21	2:B:446:PHE:HA	2.02	0.42
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.81	0.42
29:J:101:BCR:H20C	29:J:101:BCR:H361	1.92	0.42
10:b:131:THR:HG22	25:b:210:CLA:HHB	2.02	0.42
19:m:37:VAL:O	19:m:41:MET:HG2	2.19	0.42
25:g:208:CLA:H42	24:p:87:PRO:HG3	2.00	0.42
2:B:374:HIS:HB2	25:B:843:CLA:C1B	2.50	0.42
2:B:388:ALA:O	2:B:392:ILE:HG13	2.19	0.42
25:B:839:CLA:HAA1	25:B:842:CLA:OBD	2.20	0.42
14:h:14:LEU:HD11	14:h:25:ASP:HB2	2.02	0.42
25:k:208:CLA:HBA2	25:k:208:CLA:H3A	1.46	0.42
25:k:211:CLA:H62	25:k:211:CLA:H41	1.76	0.42
25:A:831:CLA:HED3	25:A:831:CLA:H2A	2.02	0.42
2:B:624:LEU:HD22	25:B:802:CLA:HMD3	2.02	0.42
2:B:716:GLY:O	2:B:720:THR:HG22	2.20	0.42
2:B:720:THR:HG23	25:B:802:CLA:O1D	2.20	0.42
25:a:209:CLA:HBA2	25:a:209:CLA:H3A	1.85	0.42
25:b:210:CLA:HBB2	25:b:212:CLA:CHB	2.50	0.42
35:d:307:CHL:HHC	35:d:307:CHL:HBB1	2.01	0.42
13:e:154:LYS:HD3	25:e:215:CLA:HAA2	2.01	0.42
25:l:606:CLA:H92	25:l:606:CLA:H61	1.78	0.42
20:f:59:VAL:N	20:f:60:PRO:HD2	2.34	0.42
15:i:154:LEU:HD13	25:i:212:CLA:HBC2	2.01	0.42
19:m:126:THR:CG2	25:m:208:CLA:H3A	2.49	0.42
20:f:37:GLU:HG3	20:f:40:ARG:NH2	2.35	0.42
25:g:208:CLA:HMB1	24:p:90:TYR:HB2	2.02	0.42
1:A:128:ASN:HB3	1:A:136:GLN:HB3	2.02	0.42
1:A:260:GLY:HA3	9:a:151:THR:HG23	2.01	0.42
1:A:301:LEU:CD1	25:A:818:CLA:HBB1	2.50	0.42
4:D:117:ALA:HB3	4:D:118:PRO:HD3	2.01	0.42
25:c:306:CLA:HMC3	35:c:307:CHL:C1C	2.50	0.42
14:h:125:THR:CG2	25:h:209:CLA:H3A	2.50	0.42
20:f:19:PHE:HE1	20:f:119:ASP:HB2	1.84	0.42
1:A:220:VAL:C	1:A:223:PRO:HD2	2.44	0.41
1:A:577:GLY:HA2	2:B:562:PRO:HD3	2.01	0.41
27:A:805:LHG:HC31	25:A:853:CLA:C1C	2.50	0.41
2:B:339:ALA:HB1	29:B:832:BCR:H20C	2.02	0.41
2:B:546:LEU:HD21	2:B:567:THR:HG22	2.01	0.41
25:B:805:CLA:H41	25:B:805:CLA:H61	1.49	0.41
10:b:102:ARG:HH22	25:b:209:CLA:CHA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:301:LHG:H112	27:c:301:LHG:HC82	1.79	0.41
25:c:310:CLA:H43	25:c:312:CLA:HBA1	2.01	0.41
18:l:62:PRO:HG3	25:l:604:CLA:C1D	2.50	0.41
19:m:6:TRP:O	19:m:7:PHE:HB3	2.20	0.41
19:m:155:PRO:C	19:m:157:ALA:H	2.28	0.41
1:A:441:LEU:HD21	1:A:547:VAL:HG12	2.02	0.41
25:A:822:CLA:HBB1	25:A:831:CLA:HHB	2.01	0.41
2:B:197:VAL:C	2:B:200:PRO:HD2	2.45	0.41
15:i:166:ILE:O	15:i:167:ALA:HB3	2.21	0.41
25:i:211:CLA:HBC1	25:i:213:CLA:H43	2.02	0.41
16:j:182:PRO:HA	16:j:183:PRO:HD3	1.91	0.41
25:f:602:CLA:H3A	25:f:602:CLA:HBA2	1.70	0.41
25:p:602:CLA:HBB2	25:p:603:CLA:C1D	2.50	0.41
25:A:802:CLA:CGA	25:A:802:CLA:H3A	2.50	0.41
11:c:168:LYS:HE2	25:c:312:CLA:HBD	2.02	0.41
25:c:311:CLA:HBD	25:c:312:CLA:OBD	2.20	0.41
14:h:110:ARG:O	14:h:111:SER:HB3	2.20	0.41
16:j:14:PRO:HG2	16:j:28:ASP:HB3	2.02	0.41
25:l:606:CLA:HBB1	25:l:606:CLA:HHC	2.02	0.41
25:g:207:CLA:H3A	25:g:207:CLA:HBA2	1.58	0.41
29:B:833:BCR:H23C	29:B:833:BCR:H382	2.02	0.41
11:c:117:LEU:HD11	12:d:212:TRP:CE2	2.55	0.41
16:j:132:GLU:HB2	25:j:209:CLA:CHB	2.50	0.41
19:m:81:LYS:HE2	19:m:81:LYS:HB3	1.84	0.41
1:A:224:ILE:HG23	1:A:237:LEU:HD13	2.03	0.41
25:A:801:CLA:HAA2	25:A:801:CLA:O1D	2.21	0.41
25:A:845:CLA:HHC	25:A:845:CLA:HBB1	2.02	0.41
4:D:69:VAL:HG22	4:D:98:PHE:CD1	2.55	0.41
9:a:43:GLU:HB2	25:a:204:CLA:CHB	2.51	0.41
13:e:135:TYR:CE2	13:e:152:LYS:HE3	2.56	0.41
14:h:66:LYS:HD3	14:h:66:LYS:HA	1.85	0.41
23:o:121:THR:H	23:o:124:THR:CG2	2.29	0.41
25:A:820:CLA:CMB	25:A:853:CLA:HBB1	2.50	0.41
25:A:850:CLA:HBA1	4:D:28:ILE:HB	2.03	0.41
2:B:429:LEU:HB3	2:B:525:LEU:HB2	2.03	0.41
25:B:840:CLA:HBA1	25:B:841:CLA:H2	2.02	0.41
4:D:46:THR:O	4:D:50:THR:HG23	2.20	0.41
12:d:171:GLU:HB2	25:d:312:CLA:CHB	2.51	0.41
25:e:214:CLA:HBD	25:e:215:CLA:OBD	2.20	0.41
25:i:206:CLA:HAA2	25:i:206:CLA:HBD	2.01	0.41
25:p:606:CLA:H3A	25:p:606:CLA:HBA1	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HD11	25:A:816:CLA:HAB	2.03	0.41
27:A:835:LHG:H272	27:A:835:LHG:H242	1.89	0.41
3:C:61:ASP:HB2	5:E:53:ASN:CG	2.45	0.41
25:a:209:CLA:H62	25:a:209:CLA:H41	1.75	0.41
10:b:44:SER:CB	10:b:139:GLY:HA3	2.48	0.41
10:b:44:SER:O	10:b:48:MET:HG3	2.20	0.41
10:b:102:ARG:HG2	25:b:208:CLA:CHD	2.50	0.41
27:b:201:LHG:H281	25:b:206:CLA:CAD	2.51	0.41
25:d:312:CLA:HBA2	25:d:312:CLA:H3A	1.83	0.41
13:e:167:PHE:CE2	25:e:205:CLA:H161	2.56	0.41
25:j:212:CLA:H92	25:j:212:CLA:H61	1.72	0.41
25:g:207:CLA:CAD	25:g:209:CLA:HMD3	2.50	0.41
22:n:52:LEU:HG	22:n:164:MET:HG2	2.03	0.41
1:A:462:LEU:HD13	1:A:470:ASP:HB2	2.02	0.41
1:A:590:ASP:HA	1:A:593:PHE:HB3	2.02	0.41
29:A:836:BCR:H292	25:a:204:CLA:H111	2.02	0.41
2:B:517:PHE:HE2	25:B:824:CLA:C1D	2.34	0.41
2:B:529:THR:HG21	2:B:582:TRP:CE2	2.55	0.41
2:B:687:ILE:HD11	16:j:123:LEU:HD11	2.03	0.41
25:B:811:CLA:H3A	25:B:811:CLA:HBA1	1.64	0.41
4:D:74:VAL:HG12	4:D:95:ASN:HD21	1.86	0.41
9:a:80:LEU:HD13	25:a:206:CLA:HBA1	2.03	0.41
10:b:40:GLU:HB2	25:b:204:CLA:CHB	2.51	0.41
25:d:306:CLA:HBA1	35:d:308:CHL:C1D	2.51	0.41
25:h:209:CLA:H3A	25:h:209:CLA:HBA2	1.72	0.41
15:i:94:VAL:O	15:i:98:LEU:HG	2.20	0.41
25:k:207:CLA:HHC	25:k:207:CLA:HBB1	2.03	0.41
19:m:24:ARG:HA	19:m:24:ARG:HD3	1.91	0.41
25:m:203:CLA:H11	30:m:213:DD6:O1	2.20	0.41
22:n:138:PHE:CE2	25:n:207:CLA:NC	2.89	0.41
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.88	0.41
1:A:219:HIS:HE1	25:A:806:CLA:C4D	2.34	0.41
1:A:396:TRP:CD1	25:A:824:CLA:HAB	2.56	0.41
1:A:407:ALA:HB2	1:A:592:VAL:HG11	2.03	0.41
1:A:423:PHE:HB2	4:D:79:ILE:HD13	2.03	0.41
1:A:596:LEU:HD21	25:A:826:CLA:HBC1	2.03	0.41
1:A:672:PHE:HZ	25:A:801:CLA:CHD	2.34	0.41
25:A:810:CLA:H162	25:A:810:CLA:H122	1.76	0.41
25:A:830:CLA:HBA1	25:A:830:CLA:HBD	2.03	0.41
25:A:846:CLA:HBA2	25:A:846:CLA:H3A	1.60	0.41
2:B:650:PHE:HZ	25:B:802:CLA:C1D	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:VAL:HG21	3:C:48:CYS:HA	2.03	0.41
6:F:3:ALA:HB2	6:F:9:PRO:HD3	2.03	0.41
25:F:201:CLA:HBD	25:F:201:CLA:HAA2	2.02	0.41
8:M:14:ALA:O	8:M:18:PRO:HD2	2.21	0.41
9:a:122:MET:HE3	25:a:209:CLA:O2A	2.20	0.41
25:a:213:CLA:H12	25:a:213:CLA:HBA1	1.73	0.41
27:j:202:LHG:H252	25:j:210:CLA:HBC3	2.03	0.41
20:f:77:ILE:HG13	25:f:604:CLA:HMA2	2.03	0.41
21:g:100:PHE:H	21:g:106:GLU:CD	2.28	0.41
25:g:204:CLA:H61	25:g:204:CLA:H41	1.62	0.41
22:n:24:PRO:O	30:n:213:DD6:O2	2.38	0.41
25:n:201:CLA:HBA2	25:n:201:CLA:H3A	1.84	0.41
25:n:202:CLA:H62	25:n:202:CLA:H41	1.81	0.41
1:A:216:HIS:HB2	25:A:844:CLA:CHC	2.51	0.41
1:A:685:PHE:HA	28:A:834:PQN:H9	2.03	0.41
27:b:201:LHG:HC41	25:b:206:CLA:HBB1	2.03	0.41
25:c:304:CLA:H11	25:c:304:CLA:H2A	2.03	0.41
21:g:51:MET:O	21:g:55:VAL:HG22	2.20	0.41
1:A:43:PRO:HG3	6:F:125:ILE:HG21	2.03	0.40
25:A:802:CLA:HBB1	25:A:840:CLA:C1B	2.49	0.40
2:B:34:HIS:HE1	25:B:836:CLA:HED1	1.85	0.40
25:a:204:CLA:CHB	25:a:204:CLA:H2	2.51	0.40
18:l:12:PRO:HB3	18:l:25:GLY:HA3	2.03	0.40
18:l:16:LEU:HD11	18:l:27:ASP:HB2	2.02	0.40
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.91	0.40
1:A:297:HIS:HE2	25:A:818:CLA:C1B	2.33	0.40
25:A:801:CLA:H161	25:A:807:CLA:HMA1	2.03	0.40
25:A:815:CLA:H41	25:A:815:CLA:H62	1.53	0.40
28:A:834:PQN:H141	25:A:841:CLA:HBB2	2.02	0.40
2:B:717:TYR:CZ	25:B:802:CLA:HED1	2.56	0.40
5:E:46:ASN:C	5:E:48:GLU:H	2.29	0.40
10:b:58:GLU:OE2	10:b:159:SER:HB3	2.21	0.40
19:m:53:MET:HE2	19:m:134:GLY:N	2.37	0.40
20:f:46:HIS:HB3	20:f:133:LEU:HD21	2.03	0.40
20:f:55:VAL:HA	20:f:58:VAL:HG22	2.02	0.40
1:A:514:VAL:HG13	1:A:524:MET:HB3	2.03	0.40
25:A:819:CLA:HBB1	25:A:823:CLA:C7	2.51	0.40
2:B:193:HIS:HB2	25:B:812:CLA:C1C	2.51	0.40
2:B:576:PHE:CE1	25:B:819:CLA:HAC2	2.56	0.40
25:B:821:CLA:HMC1	25:B:847:CLA:HAC1	2.04	0.40
9:a:117:PHE:HB2	25:a:207:CLA:H43	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:203:CLA:HED3	25:b:203:CLA:H2A	2.02	0.40
25:e:216:CLA:HBD	25:e:216:CLA:HAA1	2.03	0.40
14:h:170:LEU:HD13	25:h:212:CLA:HMD3	2.04	0.40
15:i:145:VAL:HG22	15:i:174:TRP:CE3	2.56	0.40
25:j:212:CLA:C1C	25:j:212:CLA:H51	2.51	0.40
17:k:152:LYS:HD2	17:k:156:THR:HG21	2.03	0.40
25:A:833:CLA:H93	25:A:833:CLA:H62	1.86	0.40
2:B:316:GLY:HA3	2:B:410:ARG:HD2	2.03	0.40
2:B:492:ILE:H	2:B:492:ILE:HG12	1.66	0.40
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.37	0.40
25:B:816:CLA:HBD	25:B:816:CLA:HAA2	2.04	0.40
25:B:826:CLA:HHC	25:B:826:CLA:HBB1	2.04	0.40
10:b:82:ILE:HB	10:b:86:GLU:HB2	2.02	0.40
27:d:302:LHG:H131	27:d:302:LHG:H102	1.68	0.40
25:e:213:CLA:HBA2	25:e:213:CLA:H3A	1.77	0.40
25:h:212:CLA:H41	25:h:212:CLA:H62	1.55	0.40
15:i:166:ILE:C	15:i:168:GLU:H	2.29	0.40
29:A:837:BCR:H24C	29:A:837:BCR:H371	1.87	0.40
25:A:840:CLA:HAB	2:B:582:TRP:HH2	1.86	0.40
2:B:48:ALA:HB2	2:B:157:LEU:HG	2.02	0.40
2:B:504:LYS:HB2	2:B:504:LYS:HE2	1.82	0.40
25:B:810:CLA:H3A	25:B:810:CLA:HBA2	1.87	0.40
29:B:831:BCR:H24C	29:B:831:BCR:H371	1.84	0.40
6:F:95:GLY:O	6:F:99:VAL:HG23	2.21	0.40
16:j:176:ASN:HD21	25:j:212:CLA:HED2	1.87	0.40
23:o:111:TYR:HB3	25:o:607:CLA:HED2	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	739/751 (98%)	713 (96%)	24 (3%)	2 (0%)	36 38
2	B	729/734 (99%)	705 (97%)	23 (3%)	1 (0%)	48 54
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100 100
4	D	184/186 (99%)	173 (94%)	10 (5%)	1 (0%)	24 23
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
6	F	166/168 (99%)	163 (98%)	3 (2%)	0	100 100
7	J	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
8	M	29/31 (94%)	29 (100%)	0	0	100 100
9	a	164/166 (99%)	158 (96%)	6 (4%)	0	100 100
10	b	167/169 (99%)	158 (95%)	9 (5%)	0	100 100
11	c	219/221 (99%)	208 (95%)	11 (5%)	0	100 100
12	d	218/220 (99%)	207 (95%)	10 (5%)	1 (0%)	24 23
13	e	197/199 (99%)	190 (96%)	6 (3%)	1 (0%)	24 23
14	h	172/174 (99%)	166 (96%)	6 (4%)	0	100 100
15	i	175/177 (99%)	166 (95%)	9 (5%)	0	100 100
16	j	181/183 (99%)	179 (99%)	2 (1%)	0	100 100
17	k	170/172 (99%)	162 (95%)	8 (5%)	0	100 100
18	l	165/167 (99%)	162 (98%)	3 (2%)	0	100 100
19	m	166/168 (99%)	155 (93%)	11 (7%)	0	100 100
20	f	172/174 (99%)	151 (88%)	20 (12%)	1 (1%)	21 20
21	g	176/178 (99%)	173 (98%)	3 (2%)	0	100 100
22	n	182/184 (99%)	155 (85%)	25 (14%)	2 (1%)	11 7
23	o	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	21 20
24	p	146/148 (99%)	131 (90%)	14 (10%)	1 (1%)	18 16
All	All	4853/4915 (99%)	4619 (95%)	223 (5%)	11 (0%)	44 48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	f	77	ILE
1	A	205	LEU
1	A	497	LEU
2	B	107	SER
13	e	95	VAL
22	n	126	LYS

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Mol	Chain	Res	Type
24	p	9	ALA
22	n	69	LEU
4	D	139	PRO
23	o	33	PRO
12	d	109	ILE

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	621/632 (98%)	619 (100%)	2 (0%)	86 90
2	B	607/609 (100%)	607 (100%)	0	100 100
3	C	69/70 (99%)	68 (99%)	1 (1%)	59 69
4	D	140/140 (100%)	139 (99%)	1 (1%)	76 81
5	E	49/49 (100%)	49 (100%)	0	100 100
6	F	127/127 (100%)	127 (100%)	0	100 100
7	J	34/34 (100%)	34 (100%)	0	100 100
8	M	26/26 (100%)	26 (100%)	0	100 100
9	a	125/125 (100%)	125 (100%)	0	100 100
10	b	130/130 (100%)	129 (99%)	1 (1%)	73 80
11	c	172/172 (100%)	172 (100%)	0	100 100
12	d	167/167 (100%)	167 (100%)	0	100 100
13	e	152/152 (100%)	152 (100%)	0	100 100
14	h	142/142 (100%)	140 (99%)	2 (1%)	59 69
15	i	137/137 (100%)	137 (100%)	0	100 100
16	j	145/145 (100%)	145 (100%)	0	100 100
17	k	141/141 (100%)	140 (99%)	1 (1%)	76 81
18	l	122/122 (100%)	122 (100%)	0	100 100
19	m	122/122 (100%)	122 (100%)	0	100 100
20	f	135/135 (100%)	134 (99%)	1 (1%)	76 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	g	140/140 (100%)	140 (100%)	0	100 100
22	n	140/140 (100%)	140 (100%)	0	100 100
23	o	119/119 (100%)	118 (99%)	1 (1%)	73 80
24	p	114/114 (100%)	111 (97%)	3 (3%)	40 48
All	All	3876/3890 (100%)	3863 (100%)	13 (0%)	84 90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	TYR
1	A	584	CYS
3	C	65	VAL
4	D	82	ILE
10	b	96	TYR
14	h	5	ILE
14	h	120	LEU
17	k	31	LYS
20	f	127	LYS
23	o	3	VAL
24	p	115	LYS
24	p	127	LYS
24	p	134	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	225	ASN
1	A	252	GLN
1	A	714	GLN
2	B	294	ASN
2	B	444	GLN
2	B	452	GLN
2	B	475	ASN
2	B	627	ASN
2	B	630	GLN
4	D	138	HIS
4	D	170	ASN
5	E	21	GLN
9	a	70	GLN

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Mol	Chain	Res	Type
9	a	158	GLN
9	a	159	ASN
10	b	60	GLN
10	b	78	ASN
11	c	51	GLN
12	d	143	GLN
13	e	198	ASN
14	h	37	GLN
14	h	97	ASN
14	h	164	HIS
15	i	63	GLN
15	i	163	ASN
15	i	164	HIS
16	j	49	ASN
16	j	89	GLN
16	j	179	HIS
19	m	165	ASN
20	f	140	GLN
20	f	164	HIS
21	g	152	GLN
22	n	37	ASN
22	n	63	ASN
24	p	70	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

367 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	$\#\|Z\| > 2$
25	CLA	j	211	16	59,63,73	1.33	8 (13%)	71,101,113	1.74	11 (15%)
25	CLA	j	206	-	61,65,73	1.32	8 (13%)	73,103,113	1.77	10 (13%)
25	CLA	e	215	13	47,51,73	1.41	8 (17%)	56,86,113	1.89	8 (14%)
25	CLA	m	203	19	64,68,73	1.28	7 (10%)	77,107,113	1.54	11 (14%)
25	CLA	d	312	12	63,67,73	1.29	7 (11%)	75,105,113	1.77	9 (12%)
25	CLA	k	210	17	47,51,73	1.40	8 (17%)	56,86,113	1.83	8 (14%)
25	CLA	A	801	1	69,73,73	1.21	8 (11%)	83,113,113	1.75	15 (18%)
25	CLA	h	206	-	64,68,73	1.28	8 (12%)	77,107,113	1.73	9 (11%)
25	CLA	B	840	2	54,58,73	1.39	7 (12%)	65,95,113	1.65	10 (15%)
25	CLA	o	608	23	47,50,73	1.55	10 (21%)	51,84,113	2.04	9 (17%)
25	CLA	l	603	18	47,51,73	1.41	8 (17%)	56,86,113	1.89	8 (14%)
25	CLA	h	204	14	59,63,73	1.35	8 (13%)	71,101,113	1.75	11 (15%)
25	CLA	A	820	1	61,65,73	1.30	8 (13%)	73,103,113	1.79	11 (15%)
25	CLA	l	604	-	47,51,73	1.41	8 (17%)	56,86,113	1.74	7 (12%)
25	CLA	n	203	-	52,56,73	1.40	7 (13%)	62,92,113	1.81	9 (14%)
25	CLA	j	213	16	46,50,73	1.41	8 (17%)	55,85,113	1.85	9 (16%)
25	CLA	B	819	2	69,73,73	1.23	8 (11%)	83,113,113	1.54	9 (10%)
30	DD6	e	220	-	39,45,45	1.58	8 (20%)	52,67,67	1.69	9 (17%)
25	CLA	i	210	15	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	a	203	9	54,58,73	1.39	7 (12%)	65,95,113	1.70	9 (13%)
27	LHG	a	201	25	25,25,48	1.86	2 (8%)	28,31,54	1.42	5 (17%)
25	CLA	g	205	21	46,50,73	1.44	7 (15%)	55,85,113	1.76	5 (9%)
25	CLA	f	605	20	46,50,73	1.42	7 (15%)	55,85,113	1.93	7 (12%)
25	CLA	m	208	19	46,50,73	1.40	7 (15%)	55,85,113	1.76	7 (12%)
30	DD6	a	215	-	39,45,45	1.42	5 (12%)	52,67,67	2.10	16 (30%)
25	CLA	b	208	-	45,49,73	1.45	8 (17%)	54,84,113	1.88	9 (16%)
25	CLA	d	304	12	61,65,73	1.30	7 (11%)	73,103,113	1.75	11 (15%)
25	CLA	B	841	2	63,67,73	1.30	8 (12%)	75,105,113	1.76	10 (13%)
25	CLA	g	215	21	49,53,73	1.42	7 (14%)	59,89,113	1.79	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	814	1	63,67,73	1.29	8 (12%)	75,105,113	1.77	12 (16%)
25	CLA	B	802	2	69,73,73	1.20	8 (11%)	83,113,113	1.58	12 (14%)
25	CLA	c	305	-	52,56,73	1.38	8 (15%)	62,92,113	1.81	10 (16%)
25	CLA	b	210	10	46,50,73	1.41	7 (15%)	55,85,113	1.84	8 (14%)
25	CLA	n	208	22	49,53,73	1.43	8 (16%)	59,89,113	1.87	6 (10%)
25	CLA	k	206	-	54,58,73	1.38	8 (14%)	65,95,113	1.84	10 (15%)
30	DD6	o	611	-	39,45,45	1.30	4 (10%)	52,67,67	2.13	15 (28%)
25	CLA	e	207	-	54,58,73	1.38	8 (14%)	65,95,113	1.78	11 (16%)
25	CLA	B	816	-	64,68,73	1.26	7 (10%)	77,107,113	1.75	14 (18%)
25	CLA	c	309	11	64,68,73	1.28	8 (12%)	77,107,113	1.75	10 (12%)
25	CLA	B	823	2	64,68,73	1.27	6 (9%)	77,107,113	1.60	12 (15%)
25	CLA	a	208	9	54,58,73	1.39	8 (14%)	65,95,113	1.82	9 (13%)
30	DD6	m	213	-	39,45,45	1.36	5 (12%)	52,67,67	2.12	17 (32%)
27	LHG	c	301	25	29,29,48	1.76	2 (6%)	32,35,54	1.37	5 (15%)
25	CLA	B	803	-	59,63,73	1.32	6 (10%)	71,101,113	1.93	10 (14%)
27	LHG	b	201	-	30,30,48	1.77	2 (6%)	33,36,54	1.35	5 (15%)
25	CLA	a	205	9	57,61,73	1.35	8 (14%)	68,98,113	1.77	11 (16%)
30	DD6	a	214	-	39,45,45	1.38	4 (10%)	52,67,67	2.22	15 (28%)
30	DD6	e	219	-	39,45,45	1.41	5 (12%)	52,67,67	2.14	14 (26%)
25	CLA	A	804	1	64,68,73	1.29	8 (12%)	77,107,113	1.75	10 (12%)
30	DD6	i	214	-	39,45,45	1.42	5 (12%)	52,67,67	2.13	14 (26%)
25	CLA	l	610	18	52,56,73	1.38	7 (13%)	62,92,113	1.76	9 (14%)
25	CLA	g	203	21	46,50,73	1.41	8 (17%)	55,85,113	1.82	8 (14%)
25	CLA	p	605	-	46,50,73	1.42	8 (17%)	55,85,113	1.84	8 (14%)
25	CLA	A	808	1	64,68,73	1.26	8 (12%)	77,107,113	1.77	12 (15%)
30	DD6	n	213	-	39,45,45	1.52	8 (20%)	52,67,67	1.48	9 (17%)
25	CLA	l	602	18	63,67,73	1.30	8 (12%)	75,105,113	1.69	12 (16%)
34	LMG	j	201	-	44,44,55	0.86	1 (2%)	52,52,63	1.08	2 (3%)
30	DD6	n	212	-	39,45,45	1.29	4 (10%)	52,67,67	2.54	16 (30%)
25	CLA	a	204	9	64,68,73	1.27	6 (9%)	77,107,113	1.61	15 (19%)
35	CHL	d	309	-	47,51,74	1.41	5 (10%)	52,86,114	2.09	11 (21%)
30	DD6	c	317	-	39,45,45	1.42	5 (12%)	52,67,67	2.12	16 (30%)
25	CLA	o	603	23	47,51,73	1.46	8 (17%)	56,86,113	1.81	7 (12%)
25	CLA	B	834	2	59,63,73	1.33	7 (11%)	71,101,113	1.75	10 (14%)
25	CLA	B	839	-	64,68,73	1.29	8 (12%)	77,107,113	1.77	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	CHL	e	209	-	50,54,74	1.51	7 (14%)	56,90,114	2.13	10 (17%)
25	CLA	n	204	22	46,50,73	1.42	7 (15%)	55,85,113	1.83	9 (16%)
35	CHL	d	308	-	50,54,74	1.51	7 (14%)	56,90,114	2.11	11 (19%)
30	DD6	d	317	-	39,45,45	1.38	4 (10%)	52,67,67	2.14	15 (28%)
25	CLA	m	210	19	47,51,73	1.40	8 (17%)	56,86,113	1.84	8 (14%)
25	CLA	g	209	21	59,63,73	1.32	7 (11%)	71,101,113	1.71	9 (12%)
25	CLA	B	845	2	69,73,73	1.23	7 (10%)	83,113,113	1.71	11 (13%)
25	CLA	e	217	13	46,50,73	1.39	7 (15%)	55,85,113	1.84	6 (10%)
25	CLA	m	207	19	54,58,73	1.39	8 (14%)	65,95,113	1.82	9 (13%)
25	CLA	d	314	12	46,50,73	1.41	8 (17%)	55,85,113	1.90	5 (9%)
27	LHG	g	201	25	34,34,48	1.60	2 (5%)	37,40,54	1.31	5 (13%)
25	CLA	B	809	2	46,50,73	1.40	7 (15%)	55,85,113	1.87	7 (12%)
25	CLA	g	212	21	59,63,73	1.33	8 (13%)	71,101,113	1.78	11 (15%)
25	CLA	c	306	-	47,51,73	1.41	8 (17%)	56,86,113	1.82	8 (14%)
33	SQD	F	204	-	38,39,54	1.73	8 (21%)	47,50,65	1.54	7 (14%)
29	BCR	A	839	-	41,41,41	0.74	0	56,56,56	1.03	4 (7%)
25	CLA	l	606	18	64,68,73	1.27	8 (12%)	77,107,113	1.75	10 (12%)
25	CLA	l	609	18	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	n	210	22	46,50,73	1.42	8 (17%)	55,85,113	1.92	7 (12%)
25	CLA	A	810	1	69,73,73	1.21	7 (10%)	83,113,113	1.72	12 (14%)
25	CLA	m	211	19	46,50,73	1.42	7 (15%)	55,85,113	1.82	7 (12%)
25	CLA	l	608	-	47,51,73	1.40	7 (14%)	56,86,113	1.86	8 (14%)
25	CLA	p	609	24	47,51,73	1.43	7 (14%)	56,86,113	1.90	9 (16%)
25	CLA	A	806	1	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
25	CLA	B	826	2	47,51,73	1.39	7 (14%)	56,86,113	1.83	7 (12%)
26	LMT	A	803	-	36,36,36	0.55	0	47,47,47	0.66	0
25	CLA	h	209	14	58,62,73	1.32	7 (12%)	69,99,113	1.77	10 (14%)
25	CLA	k	203	17	57,61,73	1.35	8 (14%)	68,98,113	1.75	11 (16%)
25	CLA	e	208	13	46,50,73	1.42	8 (17%)	55,85,113	1.91	7 (12%)
25	CLA	A	846	1	69,73,73	1.22	8 (11%)	83,113,113	1.71	13 (15%)
25	CLA	A	841	-	61,65,73	1.29	8 (13%)	73,103,113	1.71	10 (13%)
25	CLA	m	205	-	47,51,73	1.41	8 (17%)	56,86,113	1.93	6 (10%)
25	CLA	g	213	21	46,50,73	1.41	7 (15%)	55,85,113	1.89	8 (14%)
25	CLA	J	103	7	54,58,73	1.39	8 (14%)	65,95,113	1.80	11 (16%)
25	CLA	n	205	-	46,50,73	1.41	7 (15%)	55,85,113	1.84	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LHG	m	201	-	31,31,48	1.73	2 (6%)	34,37,54	1.34	5 (14%)
35	CHL	d	307	12	55,59,74	1.47	7 (12%)	62,96,114	2.07	16 (25%)
27	LHG	i	201	25	35,35,48	1.55	2 (5%)	38,41,54	1.29	5 (13%)
25	CLA	B	821	2	64,68,73	1.28	8 (12%)	77,107,113	1.72	12 (15%)
25	CLA	i	209	27	47,51,73	1.40	8 (17%)	56,86,113	1.88	7 (12%)
28	PQN	B	827	-	34,34,34	1.13	4 (11%)	42,45,45	1.87	10 (23%)
25	CLA	i	212	15	46,50,73	1.41	7 (15%)	55,85,113	1.77	9 (16%)
25	CLA	i	204	15	47,51,73	1.40	8 (17%)	56,86,113	1.75	8 (14%)
25	CLA	n	211	22	46,50,73	1.43	8 (17%)	55,85,113	1.74	6 (10%)
34	LMG	a	202	-	43,43,55	0.89	1 (2%)	51,51,63	1.18	2 (3%)
25	CLA	k	207	17	54,58,73	1.38	8 (14%)	65,95,113	1.77	8 (12%)
25	CLA	l	611	18	46,50,73	1.44	7 (15%)	55,85,113	1.91	8 (14%)
30	DD6	k	216	-	39,45,45	1.36	4 (10%)	52,67,67	2.10	16 (30%)
25	CLA	A	851	1	49,53,73	1.40	8 (16%)	59,89,113	1.84	9 (15%)
30	DD6	F	203	-	39,45,45	1.53	7 (17%)	52,67,67	1.51	11 (21%)
25	CLA	e	214	-	46,50,73	1.42	7 (15%)	55,85,113	1.74	8 (14%)
31	SF4	A	856	1,2	0,12,12	-	-	-		
25	CLA	k	212	17	46,50,73	1.41	7 (15%)	55,85,113	1.82	6 (10%)
25	CLA	p	601	-	46,50,73	1.41	7 (15%)	55,85,113	1.71	9 (16%)
30	DD6	d	319	-	39,45,45	1.32	4 (10%)	52,67,67	2.40	19 (36%)
25	CLA	j	208	16	54,58,73	1.39	8 (14%)	65,95,113	1.83	9 (13%)
25	CLA	a	207	-	57,61,73	1.34	8 (14%)	68,98,113	1.74	11 (16%)
25	CLA	b	209	10	49,53,73	1.41	8 (16%)	59,89,113	1.82	10 (16%)
25	CLA	f	606	20	46,50,73	1.43	7 (15%)	55,85,113	1.82	8 (14%)
25	CLA	f	608	-	46,50,73	1.43	7 (15%)	55,85,113	1.93	7 (12%)
31	SF4	C	101	3	0,12,12	-	-	-		
25	CLA	A	823	1	68,72,73	1.22	7 (10%)	81,111,113	1.81	8 (9%)
25	CLA	i	207	15	47,51,73	1.39	8 (17%)	56,86,113	1.87	4 (7%)
30	DD6	j	217	-	39,45,45	1.42	5 (12%)	52,67,67	2.15	15 (28%)
25	CLA	j	212	16	66,70,73	1.24	6 (9%)	79,109,113	1.70	11 (13%)
25	CLA	p	604	-	47,51,73	1.43	8 (17%)	56,86,113	1.88	8 (14%)
30	DD6	J	105	-	39,45,45	1.54	8 (20%)	52,67,67	1.53	9 (17%)
25	CLA	f	603	20	47,51,73	1.43	8 (17%)	56,86,113	1.84	7 (12%)
30	DD6	h	217	-	39,45,45	1.38	4 (10%)	52,67,67	2.10	14 (26%)
25	CLA	b	207	-	49,53,73	1.42	8 (16%)	59,89,113	1.85	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	829	1	62,66,73	1.30	7 (11%)	74,104,113	1.70	10 (13%)
25	CLA	B	837	2	54,58,73	1.39	8 (14%)	65,95,113	1.81	7 (10%)
34	LMG	e	202	-	52,52,55	0.81	2 (3%)	60,60,63	1.07	3 (5%)
30	DD6	i	215	-	39,45,45	1.46	5 (12%)	52,67,67	2.12	15 (28%)
30	DD6	c	318	-	39,45,45	1.32	4 (10%)	52,67,67	2.38	19 (36%)
25	CLA	n	201	22	63,67,73	1.28	6 (9%)	75,105,113	1.83	13 (17%)
25	CLA	o	610	23	47,51,73	1.43	7 (14%)	56,86,113	1.83	8 (14%)
25	CLA	h	203	14	54,58,73	1.39	8 (14%)	65,95,113	1.81	11 (16%)
25	CLA	F	201	-	46,50,73	1.42	8 (17%)	55,85,113	1.90	5 (9%)
25	CLA	c	311	27	47,51,73	1.41	7 (14%)	56,86,113	1.79	8 (14%)
25	CLA	B	848	-	69,73,73	1.21	8 (11%)	83,113,113	1.70	11 (13%)
25	CLA	d	313	27	49,53,73	1.42	8 (16%)	59,89,113	1.82	9 (15%)
25	CLA	m	204	19	58,62,73	1.34	8 (13%)	69,99,113	1.73	12 (17%)
27	LHG	A	805	25	37,37,48	1.49	2 (5%)	40,43,54	1.24	5 (12%)
25	CLA	g	204	21	57,61,73	1.34	7 (12%)	68,98,113	1.71	9 (13%)
25	CLA	A	821	-	68,72,73	1.24	8 (11%)	81,111,113	1.64	12 (14%)
25	CLA	d	316	12	46,50,73	1.39	7 (15%)	55,85,113	1.79	7 (12%)
25	CLA	A	826	1	69,73,73	1.24	8 (11%)	83,113,113	1.74	9 (10%)
25	CLA	j	205	16	46,50,73	1.42	8 (17%)	55,85,113	1.86	8 (14%)
25	CLA	A	817	1	60,64,73	1.31	9 (15%)	72,102,113	1.71	9 (12%)
29	BCR	B	828	-	41,41,41	0.78	1 (2%)	56,56,56	1.18	6 (10%)
25	CLA	h	213	14	47,51,73	1.39	8 (17%)	56,86,113	1.74	7 (12%)
30	DD6	d	318	-	39,45,45	1.47	5 (12%)	52,67,67	2.19	16 (30%)
25	CLA	e	206	13	49,53,73	1.42	8 (16%)	59,89,113	1.84	9 (15%)
25	CLA	g	207	-	49,53,73	1.45	7 (14%)	59,89,113	1.86	7 (11%)
30	DD6	c	316	-	39,45,45	1.46	5 (12%)	52,67,67	2.14	18 (34%)
25	CLA	i	203	15	68,72,73	1.26	8 (11%)	81,111,113	1.67	12 (14%)
25	CLA	B	807	2	69,73,73	1.22	7 (10%)	83,113,113	1.67	10 (12%)
29	BCR	M	201	-	41,41,41	0.78	0	56,56,56	1.16	5 (8%)
30	DD6	n	214	-	39,45,45	1.63	7 (17%)	52,67,67	1.72	10 (19%)
31	SF4	C	102	3	0,12,12	-	-	-		
25	CLA	A	832	1	69,73,73	1.22	8 (11%)	83,113,113	1.59	11 (13%)
30	DD6	o	612	-	39,45,45	1.34	4 (10%)	52,67,67	2.13	16 (30%)
25	CLA	p	602	24	47,51,73	1.44	9 (19%)	56,86,113	1.96	9 (16%)
25	CLA	i	206	-	69,73,73	1.23	8 (11%)	83,113,113	1.68	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	842	2	57,61,73	1.35	8 (14%)	68,98,113	1.67	11 (16%)
25	CLA	d	306	-	56,60,73	1.37	8 (14%)	67,97,113	1.76	8 (11%)
25	CLA	n	209	22	45,49,73	1.47	7 (15%)	54,84,113	1.79	10 (18%)
25	CLA	b	203	-	46,50,73	1.42	7 (15%)	55,85,113	1.87	7 (12%)
30	DD6	l	613	-	39,45,45	1.35	4 (10%)	52,67,67	2.14	16 (30%)
25	CLA	A	816	1	47,51,73	1.40	8 (17%)	56,86,113	1.80	6 (10%)
35	CHL	c	307	-	53,57,74	1.44	6 (11%)	59,93,114	2.10	14 (23%)
25	CLA	j	210	27	54,58,73	1.38	8 (14%)	65,95,113	1.80	8 (12%)
25	CLA	c	314	11	46,50,73	1.42	8 (17%)	55,85,113	1.79	8 (14%)
25	CLA	B	814	2	63,67,73	1.30	8 (12%)	75,105,113	1.75	11 (14%)
25	CLA	o	601	23	45,49,73	1.48	9 (20%)	54,84,113	1.76	11 (20%)
25	CLA	A	827	1	47,51,73	1.40	8 (17%)	56,86,113	1.85	9 (16%)
25	CLA	B	811	2	67,71,73	1.23	8 (11%)	80,110,113	1.74	10 (12%)
25	CLA	m	202	19	46,50,73	1.43	7 (15%)	55,85,113	1.68	8 (14%)
25	CLA	A	815	1	62,66,73	1.28	7 (11%)	74,104,113	1.86	11 (14%)
25	CLA	a	213	-	67,71,73	1.25	8 (11%)	80,110,113	1.72	11 (13%)
29	BCR	B	829	-	41,41,41	0.75	0	56,56,56	1.08	4 (7%)
25	CLA	i	208	15	59,63,73	1.31	6 (10%)	71,101,113	1.73	10 (14%)
25	CLA	B	822	2	64,68,73	1.27	8 (12%)	77,107,113	1.73	11 (14%)
25	CLA	i	202	15	57,61,73	1.35	8 (14%)	68,98,113	1.76	10 (14%)
25	CLA	B	846	2	54,58,73	1.37	7 (12%)	65,95,113	1.91	11 (16%)
25	CLA	B	808	2	47,51,73	1.40	8 (17%)	56,86,113	1.83	6 (10%)
25	CLA	B	815	2	53,57,73	1.37	8 (15%)	62,93,113	1.74	10 (16%)
25	CLA	k	205	17	69,73,73	1.23	8 (11%)	83,113,113	1.64	10 (12%)
25	CLA	o	607	23	45,49,73	1.46	7 (15%)	54,84,113	1.79	10 (18%)
25	CLA	h	214	14	46,50,73	1.41	8 (17%)	55,85,113	1.91	7 (12%)
25	CLA	A	843	1	56,60,73	1.37	7 (12%)	67,97,113	1.86	10 (14%)
25	CLA	g	206	-	47,51,73	1.40	8 (17%)	56,86,113	1.72	6 (10%)
25	CLA	A	849	1	54,58,73	1.38	7 (12%)	65,95,113	1.76	10 (15%)
33	SQD	g	202	-	31,32,54	1.85	7 (22%)	40,43,65	1.58	6 (15%)
25	CLA	j	215	16	54,58,73	1.39	8 (14%)	65,95,113	1.84	9 (13%)
25	CLA	e	201	-	57,61,73	1.36	8 (14%)	68,98,113	1.84	9 (13%)
25	CLA	A	813	1	62,66,73	1.29	7 (11%)	74,104,113	1.71	11 (14%)
25	CLA	A	807	-	69,73,73	1.21	8 (11%)	83,113,113	1.67	10 (12%)
32	DGD	e	203	-	37,37,67	1.23	1 (2%)	51,51,81	1.10	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	811	1	54,58,73	1.41	8 (14%)	65,95,113	1.84	12 (18%)
25	CLA	k	202	17	47,51,73	1.40	7 (14%)	56,86,113	1.79	8 (14%)
28	PQN	A	834	-	34,34,34	1.02	3 (8%)	42,45,45	1.80	10 (23%)
25	CLA	h	211	14	62,66,73	1.30	8 (12%)	74,104,113	1.73	9 (12%)
25	CLA	A	842	1	53,57,73	1.37	7 (13%)	62,93,113	1.83	8 (12%)
25	CLA	B	844	2	69,73,73	1.25	8 (11%)	83,113,113	1.73	15 (18%)
25	CLA	k	211	17	56,60,73	1.35	8 (14%)	67,97,113	1.82	11 (16%)
25	CLA	h	210	27	47,51,73	1.39	8 (17%)	56,86,113	1.81	8 (14%)
25	CLA	B	836	2	57,61,73	1.35	8 (14%)	68,98,113	1.75	10 (14%)
30	DD6	J	104	-	39,45,45	1.42	4 (10%)	52,67,67	2.22	15 (28%)
25	CLA	e	211	-	52,56,73	1.37	8 (15%)	62,92,113	1.75	8 (12%)
33	SQD	J	102	-	26,27,54	1.81	7 (26%)	35,38,65	1.69	8 (22%)
35	CHL	d	310	-	50,54,74	1.51	7 (14%)	56,90,114	2.03	13 (23%)
25	CLA	A	822	-	57,61,73	1.35	8 (14%)	68,98,113	1.76	10 (14%)
25	CLA	b	213	10	46,50,73	1.42	8 (17%)	55,85,113	1.85	8 (14%)
25	CLA	k	214	17	54,58,73	1.38	7 (12%)	65,95,113	1.80	9 (13%)
25	CLA	B	847	2	54,58,73	1.38	8 (14%)	65,95,113	1.81	9 (13%)
25	CLA	e	216	13	59,63,73	1.34	8 (13%)	71,101,113	1.72	9 (12%)
25	CLA	c	310	11	59,63,73	1.32	8 (13%)	71,101,113	1.75	10 (14%)
30	DD6	j	216	-	39,45,45	1.44	5 (12%)	52,67,67	2.13	15 (28%)
25	CLA	d	311	12	53,57,73	1.37	8 (15%)	62,93,113	1.88	8 (12%)
25	CLA	l	605	-	47,51,73	1.40	8 (17%)	56,86,113	1.82	6 (10%)
25	CLA	k	208	17	61,65,73	1.29	8 (13%)	73,103,113	1.71	11 (15%)
25	CLA	B	825	-	47,51,73	1.39	8 (17%)	56,86,113	1.66	7 (12%)
25	CLA	A	845	-	52,56,73	1.38	8 (15%)	62,92,113	1.77	10 (16%)
25	CLA	B	818	2	69,73,73	1.23	8 (11%)	83,113,113	1.63	11 (13%)
25	CLA	j	214	16	47,51,73	1.39	8 (17%)	56,86,113	1.86	6 (10%)
29	BCR	B	832	-	41,41,41	1.67	8 (19%)	56,56,56	1.40	9 (16%)
25	CLA	e	204	13	45,49,73	1.43	7 (15%)	54,84,113	1.86	9 (16%)
25	CLA	d	301	12	45,49,73	1.45	8 (17%)	54,84,113	2.03	8 (14%)
25	CLA	a	211	9	47,51,73	1.41	8 (17%)	56,86,113	1.87	6 (10%)
25	CLA	A	812	1	69,73,73	1.22	7 (10%)	83,113,113	1.63	9 (10%)
30	DD6	b	215	-	39,45,45	1.38	4 (10%)	52,67,67	2.13	16 (30%)
25	CLA	B	806	2	46,50,73	1.41	8 (17%)	55,85,113	1.84	7 (12%)
25	CLA	A	828	1	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	g	211	21	46,50,73	1.43	8 (17%)	55,85,113	1.89	6 (10%)
25	CLA	p	607	24	49,53,73	1.45	8 (16%)	59,89,113	1.73	8 (13%)
25	CLA	l	601	18	46,50,73	1.42	7 (15%)	55,85,113	1.76	6 (10%)
32	DGD	b	202	-	49,49,67	1.23	6 (12%)	63,63,81	1.08	4 (6%)
25	CLA	e	213	13	59,63,73	1.30	7 (11%)	71,101,113	1.73	11 (15%)
25	CLA	f	610	20	63,67,73	1.29	8 (12%)	75,105,113	1.70	11 (14%)
25	CLA	B	824	2	69,73,73	1.23	8 (11%)	83,113,113	1.62	11 (13%)
25	CLA	f	602	20	63,67,73	1.29	7 (11%)	75,105,113	1.69	12 (16%)
25	CLA	i	213	15	54,58,73	1.38	8 (14%)	65,95,113	1.81	9 (13%)
25	CLA	A	844	1	64,68,73	1.29	8 (12%)	77,107,113	1.77	13 (16%)
25	CLA	k	204	17	46,50,73	1.41	8 (17%)	55,85,113	2.02	6 (10%)
32	DGD	B	849	-	55,55,67	1.10	0	69,69,81	1.04	2 (2%)
25	CLA	A	840	-	67,71,73	1.24	8 (11%)	80,110,113	1.64	11 (13%)
29	BCR	J	101	-	41,41,41	1.71	8 (19%)	56,56,56	1.58	11 (19%)
25	CLA	j	209	16	68,72,73	1.22	6 (8%)	81,111,113	1.59	11 (13%)
25	CLA	b	204	10	57,61,73	1.36	8 (14%)	68,98,113	1.76	9 (13%)
25	CLA	A	825	1	69,73,73	1.24	8 (11%)	83,113,113	1.61	11 (13%)
30	DD6	A	855	-	39,45,45	1.35	4 (10%)	52,67,67	2.35	20 (38%)
25	CLA	B	843	2	67,71,73	1.23	7 (10%)	80,110,113	1.61	11 (13%)
25	CLA	j	203	16	54,58,73	1.39	8 (14%)	65,95,113	1.73	11 (16%)
30	DD6	f	614	-	39,45,45	1.28	4 (10%)	52,67,67	2.47	19 (36%)
30	DD6	g	217	-	39,45,45	1.37	5 (12%)	52,67,67	2.21	14 (26%)
25	CLA	A	850	1	59,63,73	1.31	7 (11%)	71,101,113	1.66	10 (14%)
25	CLA	o	606	23	49,53,73	1.41	7 (14%)	59,89,113	1.86	9 (15%)
25	CLA	d	305	12	46,50,73	1.39	8 (17%)	55,85,113	1.92	7 (12%)
25	CLA	A	830	1	56,60,73	1.36	7 (12%)	67,97,113	1.73	13 (19%)
25	CLA	j	207	-	51,55,73	1.40	8 (15%)	61,91,113	1.89	8 (13%)
29	BCR	A	837	-	41,41,41	1.65	10 (24%)	56,56,56	1.50	12 (21%)
30	DD6	l	614	-	39,45,45	1.41	5 (12%)	52,67,67	2.10	18 (34%)
25	CLA	f	601	20	46,50,73	1.43	7 (15%)	55,85,113	1.77	7 (12%)
25	CLA	A	824	1	62,66,73	1.29	7 (11%)	74,104,113	1.72	10 (13%)
25	CLA	c	303	11	63,67,73	1.28	8 (12%)	75,105,113	1.69	13 (17%)
27	LHG	A	835	-	48,48,48	1.35	2 (4%)	51,54,54	1.18	5 (9%)
25	CLA	A	802	-	67,71,73	1.25	6 (8%)	80,110,113	1.65	11 (13%)
25	CLA	A	857	-	57,61,73	1.35	8 (14%)	68,98,113	1.72	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	h	205	14	47,51,73	1.39	8 (17%)	56,86,113	1.94	9 (16%)
25	CLA	c	302	11	46,50,73	1.40	8 (17%)	55,85,113	1.76	8 (14%)
30	DD6	m	212	-	39,45,45	1.32	4 (10%)	52,67,67	2.14	14 (26%)
30	DD6	b	214	-	39,45,45	1.34	4 (10%)	52,67,67	2.25	16 (30%)
25	CLA	e	210	-	47,51,73	1.39	8 (17%)	56,86,113	1.89	7 (12%)
25	CLA	B	817	-	54,58,73	1.39	7 (12%)	65,95,113	1.74	9 (13%)
27	LHG	h	202	25	30,30,48	1.69	2 (6%)	33,36,54	1.38	5 (15%)
25	CLA	f	607	20	59,63,73	1.35	7 (11%)	71,101,113	1.75	11 (15%)
25	CLA	A	847	1	47,51,73	1.39	6 (12%)	56,86,113	1.72	6 (10%)
25	CLA	e	212	13	56,60,73	1.36	8 (14%)	67,97,113	1.79	9 (13%)
25	CLA	g	208	21	54,58,73	1.39	8 (14%)	65,95,113	1.78	8 (12%)
25	CLA	i	205	-	47,51,73	1.40	8 (17%)	56,86,113	1.78	5 (8%)
25	CLA	a	210	27	49,53,73	1.42	8 (16%)	59,89,113	1.84	9 (15%)
30	DD6	e	218	-	39,45,45	1.52	8 (20%)	52,67,67	1.49	9 (17%)
25	CLA	A	853	27	57,61,73	1.34	8 (14%)	68,98,113	1.88	13 (19%)
27	LHG	d	302	25	28,28,48	1.76	2 (7%)	31,34,54	1.33	5 (16%)
25	CLA	o	604	-	46,50,73	1.43	7 (15%)	55,85,113	1.84	8 (14%)
25	CLA	B	810	2	47,51,73	1.40	8 (17%)	56,86,113	1.81	7 (12%)
28	PQN	F	205	-	27,27,34	1.04	2 (7%)	33,36,45	1.99	9 (27%)
25	CLA	c	313	11	57,61,73	1.34	8 (14%)	68,98,113	1.74	10 (14%)
29	BCR	A	838	-	41,41,41	0.78	1 (2%)	56,56,56	1.06	4 (7%)
25	CLA	c	315	11	51,55,73	1.37	8 (15%)	61,91,113	1.76	10 (16%)
27	LHG	h	201	-	29,29,48	1.74	2 (6%)	32,35,54	1.10	2 (6%)
25	CLA	g	214	21	46,50,73	1.42	8 (17%)	55,85,113	1.88	7 (12%)
25	CLA	n	206	-	46,50,73	1.43	7 (15%)	55,85,113	1.82	6 (10%)
25	CLA	A	809	1	69,73,73	1.22	7 (10%)	83,113,113	1.68	10 (12%)
29	BCR	B	831	-	41,41,41	1.66	8 (19%)	56,56,56	1.42	10 (17%)
33	SQD	D	200	-	35,36,54	1.75	7 (20%)	44,47,65	1.75	10 (22%)
25	CLA	A	848	1	55,59,73	1.35	7 (12%)	66,96,113	1.85	11 (16%)
25	CLA	B	812	2	68,72,73	1.26	8 (11%)	81,111,113	1.70	10 (12%)
25	CLA	d	315	12	46,50,73	1.41	8 (17%)	55,85,113	1.85	6 (10%)
25	CLA	m	209	-	47,51,73	1.40	7 (14%)	56,86,113	1.77	7 (12%)
25	CLA	f	609	20	46,50,73	1.46	7 (15%)	55,85,113	1.63	7 (12%)
25	CLA	a	206	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	9 (15%)
25	CLA	f	612	20	47,51,73	1.42	7 (14%)	56,86,113	1.84	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	819	-	69,73,73	1.22	8 (11%)	83,113,113	1.59	13 (15%)
25	CLA	A	818	1	69,73,73	1.23	8 (11%)	83,113,113	1.60	13 (15%)
25	CLA	A	831	1	52,56,73	1.39	8 (15%)	62,92,113	1.81	9 (14%)
25	CLA	f	611	20	46,50,73	1.41	7 (15%)	55,85,113	1.78	9 (16%)
25	CLA	B	805	2	69,73,73	1.21	7 (10%)	83,113,113	1.71	13 (15%)
25	CLA	h	207	-	52,56,73	1.39	8 (15%)	62,92,113	1.84	7 (11%)
25	CLA	A	833	1	69,73,73	1.21	7 (10%)	83,113,113	1.54	13 (15%)
25	CLA	l	607	18	58,62,73	1.33	6 (10%)	69,99,113	1.73	9 (13%)
30	DD6	h	216	-	39,45,45	1.39	4 (10%)	52,67,67	2.11	16 (30%)
25	CLA	c	312	11	47,51,73	1.40	8 (17%)	56,86,113	1.84	9 (16%)
25	CLA	g	210	27	46,50,73	1.41	7 (15%)	55,85,113	1.88	8 (14%)
25	CLA	B	813	2	53,57,73	1.43	8 (15%)	63,93,113	1.74	11 (17%)
25	CLA	o	602	23	51,55,73	1.39	7 (13%)	61,91,113	1.83	9 (14%)
29	BCR	B	833	-	41,41,41	0.80	1 (2%)	56,56,56	1.12	4 (7%)
25	CLA	m	206	-	46,50,73	1.42	8 (17%)	55,85,113	1.85	4 (7%)
25	CLA	o	609	23	46,50,73	1.41	7 (15%)	55,85,113	1.86	6 (10%)
25	CLA	B	820	2	47,51,73	1.40	8 (17%)	56,86,113	1.82	6 (10%)
30	DD6	p	610	-	39,45,45	1.29	4 (10%)	52,67,67	2.28	17 (32%)
25	CLA	n	202	22	59,63,73	1.35	8 (13%)	71,101,113	1.76	9 (12%)
25	CLA	l	612	-	46,50,73	1.43	7 (15%)	55,85,113	2.00	6 (10%)
25	CLA	p	608	24	47,51,73	1.40	7 (14%)	56,86,113	1.70	8 (14%)
25	CLA	j	204	16	59,63,73	1.29	6 (10%)	71,101,113	1.78	11 (15%)
25	CLA	B	838	2	65,69,73	1.28	8 (12%)	78,108,113	1.75	12 (15%)
25	CLA	b	212	10	56,60,73	1.36	8 (14%)	67,97,113	1.82	9 (13%)
25	CLA	c	308	-	54,58,73	1.38	8 (14%)	65,95,113	1.73	9 (13%)
25	CLA	A	852	1	52,56,73	1.38	7 (13%)	62,92,113	1.93	10 (16%)
25	CLA	h	212	14	57,61,73	1.34	7 (12%)	68,98,113	1.79	12 (17%)
29	BCR	B	830	-	41,41,41	0.77	2 (4%)	56,56,56	1.01	3 (5%)
25	CLA	p	603	24	46,50,73	1.47	7 (15%)	55,85,113	1.63	6 (10%)
30	DD6	g	216	-	39,45,45	1.31	4 (10%)	52,67,67	2.28	16 (30%)
25	CLA	h	215	14	47,51,73	1.40	8 (17%)	56,86,113	1.79	7 (12%)
25	CLA	b	211	-	46,50,73	1.41	7 (15%)	55,85,113	1.86	6 (10%)
25	CLA	b	206	-	49,53,73	1.42	8 (16%)	59,89,113	1.83	6 (10%)
25	CLA	o	605	-	47,51,73	1.40	8 (17%)	56,86,113	1.81	8 (14%)
27	LHG	j	202	25	36,36,48	1.55	2 (5%)	39,42,54	1.28	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	DD6	A	854	-	39,45,45	1.36	4 (10%)	52,67,67	2.35	17 (32%)
25	CLA	a	209	9	58,62,73	1.33	7 (12%)	69,99,113	1.83	10 (14%)
25	CLA	a	212	9	59,63,73	1.33	6 (10%)	71,101,113	1.77	9 (12%)
25	CLA	f	604	-	46,50,73	1.43	7 (15%)	55,85,113	1.83	6 (10%)
29	BCR	A	836	-	41,41,41	0.83	1 (2%)	56,56,56	1.10	4 (7%)
29	BCR	B	801	-	41,41,41	0.71	0	56,56,56	1.24	7 (12%)
25	CLA	p	606	24	54,58,73	1.42	7 (12%)	65,95,113	1.79	8 (12%)
25	CLA	c	304	11	57,61,73	1.34	8 (14%)	68,98,113	1.77	11 (16%)
25	CLA	i	211	15	63,67,73	1.29	8 (12%)	75,105,113	1.75	11 (14%)
25	CLA	k	213	17	46,50,73	1.42	8 (17%)	55,85,113	1.91	7 (12%)
25	CLA	d	303	12	54,58,73	1.38	8 (14%)	65,95,113	1.90	11 (16%)
25	CLA	F	202	6	49,53,73	1.41	7 (14%)	59,89,113	1.78	8 (13%)
25	CLA	n	207	-	45,49,73	1.46	9 (20%)	54,84,113	1.89	11 (20%)
25	CLA	b	205	10	47,51,73	1.40	8 (17%)	56,86,113	1.86	8 (14%)
25	CLA	B	804	2	69,73,73	1.22	7 (10%)	83,113,113	1.70	8 (9%)
25	CLA	k	209	-	46,50,73	1.41	7 (15%)	55,85,113	1.83	7 (12%)
30	DD6	k	215	-	39,45,45	1.37	4 (10%)	52,67,67	2.12	14 (26%)
25	CLA	e	205	13	69,73,73	1.23	8 (11%)	83,113,113	1.60	11 (13%)
30	DD6	i	216	-	39,45,45	1.32	4 (10%)	52,67,67	2.17	16 (30%)
28	PQN	B	835	-	28,28,34	1.04	2 (7%)	34,37,45	2.00	10 (29%)
25	CLA	h	208	14	54,58,73	1.38	8 (14%)	65,95,113	1.78	9 (13%)
30	DD6	f	613	-	39,45,45	1.27	4 (10%)	52,67,67	2.31	15 (28%)
34	LMG	k	201	-	36,36,55	0.96	1 (2%)	44,44,63	1.12	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	j	211	16	-	11/27/103/115	-
25	CLA	j	206	-	-	11/30/106/115	-
25	CLA	e	215	13	-	2/13/89/115	-
25	CLA	m	203	19	-	16/33/109/115	-
25	CLA	d	312	12	-	14/32/108/115	-
25	CLA	k	210	17	-	2/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	801	1	-	18/39/115/115	-
25	CLA	h	206	-	-	8/33/109/115	-
25	CLA	B	840	2	-	8/21/97/115	-
25	CLA	o	608	23	-	4/13/85/115	-
25	CLA	l	603	18	-	2/13/89/115	-
25	CLA	h	204	14	-	15/27/103/115	-
25	CLA	A	820	1	-	10/30/106/115	-
25	CLA	l	604	-	-	4/13/89/115	-
25	CLA	n	203	-	-	8/19/95/115	-
25	CLA	j	213	16	-	3/12/88/115	-
25	CLA	B	819	2	-	15/39/115/115	-
30	DD6	e	220	-	-	15/26/80/80	0/3/3/3
25	CLA	i	210	15	-	5/13/89/115	-
25	CLA	a	203	9	-	6/21/97/115	-
27	LHG	a	201	25	-	9/30/30/53	-
25	CLA	g	205	21	-	4/12/88/115	-
25	CLA	f	605	20	-	2/12/88/115	-
25	CLA	m	208	19	-	6/12/88/115	-
30	DD6	a	215	-	-	0/26/80/80	0/3/3/3
25	CLA	b	208	-	-	2/10/86/115	-
25	CLA	d	304	12	-	5/30/106/115	-
25	CLA	B	841	2	-	10/32/108/115	-
25	CLA	g	215	21	-	4/15/91/115	-
25	CLA	A	814	1	-	10/32/108/115	-
25	CLA	B	802	2	-	10/39/115/115	-
25	CLA	c	305	-	-	6/19/95/115	-
25	CLA	b	210	10	-	4/12/88/115	-
25	CLA	n	208	22	-	7/15/91/115	-
25	CLA	k	206	-	-	2/21/97/115	-
30	DD6	o	611	-	-	5/26/80/80	0/3/3/3
25	CLA	e	207	-	-	4/21/97/115	-
25	CLA	B	816	-	-	10/33/109/115	-
25	CLA	c	309	11	-	16/33/109/115	-
25	CLA	B	823	2	-	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	208	9	-	5/21/97/115	-
30	DD6	m	213	-	-	6/26/80/80	0/3/3/3
27	LHG	c	301	25	-	11/34/34/53	-
25	CLA	B	803	-	-	9/27/103/115	-
27	LHG	b	201	-	-	24/35/35/53	-
25	CLA	a	205	9	-	8/25/101/115	-
30	DD6	a	214	-	-	5/26/80/80	0/3/3/3
30	DD6	e	219	-	-	5/26/80/80	0/3/3/3
25	CLA	A	804	1	-	8/33/109/115	-
30	DD6	i	214	-	-	2/26/80/80	0/3/3/3
25	CLA	l	610	18	-	7/19/95/115	-
25	CLA	g	203	21	-	6/12/88/115	-
25	CLA	p	605	-	-	6/12/88/115	-
25	CLA	A	808	1	-	11/33/109/115	-
30	DD6	n	213	-	-	13/26/80/80	0/3/3/3
25	CLA	l	602	18	-	12/32/108/115	-
34	LMG	j	201	-	-	11/39/59/70	0/1/1/1
30	DD6	n	212	-	-	5/26/80/80	0/3/3/3
25	CLA	a	204	9	-	17/33/109/115	-
35	CHL	d	309	-	-	4/14/90/117	-
30	DD6	c	317	-	-	0/26/80/80	0/3/3/3
25	CLA	o	603	23	-	6/13/89/115	-
25	CLA	B	834	2	-	6/27/103/115	-
25	CLA	B	839	-	-	15/33/109/115	-
35	CHL	e	209	-	-	10/17/93/117	-
25	CLA	n	204	22	-	6/12/88/115	-
35	CHL	d	308	-	-	8/17/93/117	-
30	DD6	d	317	-	-	2/26/80/80	0/3/3/3
25	CLA	m	210	19	-	3/13/89/115	-
25	CLA	g	209	21	-	10/27/103/115	-
25	CLA	B	845	2	-	11/39/115/115	-
25	CLA	e	217	13	-	4/12/88/115	-
25	CLA	m	207	19	-	4/21/97/115	-
25	CLA	d	314	12	-	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	g	201	25	-	25/39/39/53	-
25	CLA	B	809	2	-	4/12/88/115	-
25	CLA	g	212	21	-	12/27/103/115	-
25	CLA	c	306	-	-	4/13/89/115	-
33	SQD	F	204	-	-	21/34/54/69	0/1/1/1
29	BCR	A	839	-	-	12/29/63/63	0/2/2/2
25	CLA	l	606	18	-	13/33/109/115	-
25	CLA	l	609	18	-	6/13/89/115	-
25	CLA	n	210	22	-	4/12/88/115	-
25	CLA	A	810	1	-	14/39/115/115	-
25	CLA	m	211	19	-	5/12/88/115	-
25	CLA	l	608	-	-	3/13/89/115	-
25	CLA	p	609	24	-	5/13/89/115	-
25	CLA	A	806	1	-	7/15/91/115	-
25	CLA	B	826	2	-	4/13/89/115	-
26	LMT	A	803	-	-	7/21/61/61	0/2/2/2
25	CLA	h	209	14	-	10/26/102/115	-
25	CLA	k	203	17	-	10/25/101/115	-
25	CLA	e	208	13	-	3/12/88/115	-
25	CLA	A	846	1	-	18/39/115/115	-
25	CLA	A	841	-	-	8/30/106/115	-
25	CLA	m	205	-	-	5/13/89/115	-
25	CLA	g	213	21	-	3/12/88/115	-
25	CLA	J	103	7	-	14/21/97/115	-
25	CLA	n	205	-	-	6/12/88/115	-
27	LHG	m	201	-	-	20/36/36/53	-
35	CHL	d	307	12	-	8/23/99/117	-
27	LHG	i	201	25	-	19/40/40/53	-
25	CLA	B	821	2	-	17/33/109/115	-
25	CLA	i	209	27	-	4/13/89/115	-
28	PQN	B	827	-	-	7/23/43/43	0/2/2/2
25	CLA	i	212	15	-	3/12/88/115	-
25	CLA	i	204	15	-	8/13/89/115	-
25	CLA	n	211	22	-	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	a	202	-	-	18/38/58/70	0/1/1/1
25	CLA	k	207	17	-	2/21/97/115	-
25	CLA	l	611	18	-	5/12/88/115	-
30	DD6	k	216	-	-	3/26/80/80	0/3/3/3
25	CLA	A	851	1	-	2/15/91/115	-
30	DD6	F	203	-	-	18/26/80/80	0/3/3/3
25	CLA	e	214	-	-	3/12/88/115	-
31	SF4	A	856	1,2	-	-	0/6/5/5
25	CLA	k	212	17	-	4/12/88/115	-
25	CLA	p	601	-	-	3/12/88/115	-
30	DD6	d	319	-	-	4/26/80/80	0/3/3/3
25	CLA	j	208	16	-	5/21/97/115	-
25	CLA	a	207	-	-	13/25/101/115	-
25	CLA	b	209	10	-	3/15/91/115	-
25	CLA	f	606	20	-	4/12/88/115	-
25	CLA	f	608	-	-	2/12/88/115	-
31	SF4	C	101	3	-	-	0/6/5/5
25	CLA	A	823	1	-	16/38/114/115	-
25	CLA	i	207	15	-	4/13/89/115	-
30	DD6	j	217	-	-	3/26/80/80	0/3/3/3
25	CLA	j	212	16	-	10/36/112/115	-
25	CLA	p	604	-	-	5/13/89/115	-
30	DD6	J	105	-	-	15/26/80/80	0/3/3/3
25	CLA	f	603	20	-	1/13/89/115	-
30	DD6	h	217	-	-	0/26/80/80	0/3/3/3
25	CLA	b	207	-	-	6/15/91/115	-
25	CLA	A	829	1	-	14/31/107/115	-
25	CLA	B	837	2	-	12/21/97/115	-
34	LMG	e	202	-	-	19/47/67/70	0/1/1/1
30	DD6	i	215	-	-	3/26/80/80	0/3/3/3
30	DD6	c	318	-	-	8/26/80/80	0/3/3/3
25	CLA	n	201	22	-	14/32/108/115	-
25	CLA	o	610	23	-	5/13/89/115	-
25	CLA	h	203	14	-	9/21/97/115	-
25	CLA	F	201	-	-	0/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	311	27	-	1/13/89/115	-
25	CLA	B	848	-	-	18/39/115/115	-
25	CLA	d	313	27	-	5/15/91/115	-
25	CLA	m	204	19	-	10/26/102/115	-
27	LHG	A	805	25	-	19/42/42/53	-
25	CLA	g	204	21	-	16/25/101/115	-
25	CLA	A	821	-	-	13/37/113/115	-
25	CLA	d	316	12	-	4/12/88/115	-
25	CLA	A	826	1	-	13/39/115/115	-
25	CLA	j	205	16	-	2/12/88/115	-
25	CLA	A	817	1	-	10/29/105/115	-
29	BCR	B	828	-	-	7/29/63/63	0/2/2/2
25	CLA	h	213	14	-	4/13/89/115	-
30	DD6	d	318	-	-	3/26/80/80	0/3/3/3
25	CLA	e	206	13	-	5/15/91/115	-
25	CLA	g	207	-	-	7/15/91/115	-
30	DD6	c	316	-	-	4/26/80/80	0/3/3/3
25	CLA	i	203	15	-	11/38/114/115	-
25	CLA	B	807	2	-	15/39/115/115	-
29	BCR	M	201	-	-	6/29/63/63	0/2/2/2
30	DD6	n	214	-	-	8/26/80/80	0/3/3/3
31	SF4	C	102	3	-	-	0/6/5/5
25	CLA	A	832	1	-	12/39/115/115	-
30	DD6	o	612	-	-	3/26/80/80	0/3/3/3
25	CLA	p	602	24	-	9/13/89/115	-
25	CLA	i	206	-	-	13/39/115/115	-
25	CLA	B	842	2	-	13/25/101/115	-
25	CLA	d	306	-	-	7/24/100/115	-
25	CLA	n	209	22	-	3/10/86/115	-
25	CLA	b	203	-	-	4/12/88/115	-
30	DD6	l	613	-	-	2/26/80/80	0/3/3/3
25	CLA	A	816	1	-	6/13/89/115	-
35	CHL	c	307	-	-	6/21/97/117	-
25	CLA	j	210	27	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	314	11	-	6/12/88/115	-
25	CLA	B	814	2	-	12/32/108/115	-
25	CLA	o	601	23	-	2/10/86/115	-
25	CLA	A	827	1	-	3/13/89/115	-
25	CLA	B	811	2	-	19/37/113/115	-
25	CLA	m	202	19	-	5/12/88/115	-
25	CLA	A	815	1	-	18/31/107/115	-
25	CLA	a	213	-	-	12/37/113/115	-
29	BCR	B	829	-	-	2/29/63/63	0/2/2/2
25	CLA	i	208	15	-	12/27/103/115	-
25	CLA	B	822	2	-	18/33/109/115	-
25	CLA	i	202	15	-	14/25/101/115	-
25	CLA	B	846	2	-	6/21/97/115	-
25	CLA	B	808	2	-	3/13/89/115	-
25	CLA	B	815	2	-	8/20/96/115	-
25	CLA	k	205	17	-	20/39/115/115	-
25	CLA	o	607	23	-	2/10/86/115	-
25	CLA	h	214	14	-	6/12/88/115	-
25	CLA	A	843	1	-	12/24/100/115	-
25	CLA	g	206	-	-	5/13/89/115	-
25	CLA	A	849	1	-	10/21/97/115	-
33	SQD	g	202	-	-	13/27/47/69	0/1/1/1
25	CLA	j	215	16	-	6/21/97/115	-
25	CLA	e	201	-	-	7/25/101/115	-
25	CLA	A	813	1	-	11/31/107/115	-
25	CLA	A	807	-	-	10/39/115/115	-
32	DGD	e	203	-	-	6/24/64/95	0/2/2/2
25	CLA	A	811	1	-	2/21/97/115	-
25	CLA	k	202	17	-	3/13/89/115	-
28	PQN	A	834	-	-	8/23/43/43	0/2/2/2
25	CLA	h	211	14	-	8/31/107/115	-
25	CLA	A	842	1	-	9/20/96/115	-
25	CLA	B	844	2	-	15/39/115/115	-
25	CLA	k	211	17	-	10/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	h	210	27	-	5/13/89/115	-
25	CLA	B	836	2	-	9/25/101/115	-
30	DD6	J	104	-	-	2/26/80/80	0/3/3/3
25	CLA	e	211	-	-	6/19/95/115	-
33	SQD	J	102	-	-	10/21/41/69	0/1/1/1
35	CHL	d	310	-	-	8/17/93/117	-
25	CLA	A	822	-	-	8/25/101/115	-
25	CLA	b	213	10	-	5/12/88/115	-
25	CLA	k	214	17	-	3/21/97/115	-
25	CLA	B	847	2	-	3/21/97/115	-
25	CLA	e	216	13	-	4/27/103/115	-
25	CLA	c	310	11	-	13/27/103/115	-
30	DD6	j	216	-	-	4/26/80/80	0/3/3/3
25	CLA	d	311	12	-	5/20/96/115	-
25	CLA	l	605	-	-	6/13/89/115	-
25	CLA	k	208	17	-	14/30/106/115	-
25	CLA	B	825	-	-	5/13/89/115	-
25	CLA	A	845	-	-	5/19/95/115	-
25	CLA	B	818	2	-	13/39/115/115	-
25	CLA	j	214	16	-	5/13/89/115	-
29	BCR	B	832	-	-	14/29/63/63	0/2/2/2
25	CLA	e	204	13	-	5/10/86/115	-
25	CLA	d	301	12	-	5/10/86/115	-
25	CLA	a	211	9	-	5/13/89/115	-
25	CLA	A	812	1	-	16/39/115/115	-
30	DD6	b	215	-	-	1/26/80/80	0/3/3/3
25	CLA	B	806	2	-	2/12/88/115	-
25	CLA	A	828	1	-	7/13/89/115	-
25	CLA	g	211	21	-	4/12/88/115	-
25	CLA	p	607	24	-	11/15/91/115	-
25	CLA	l	601	18	-	4/12/88/115	-
32	DGD	b	202	-	-	18/37/77/95	0/2/2/2
25	CLA	e	213	13	-	8/27/103/115	-
25	CLA	f	610	20	-	14/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	824	2	-	22/39/115/115	-
25	CLA	f	602	20	-	14/32/108/115	-
25	CLA	i	213	15	-	4/21/97/115	-
25	CLA	A	844	1	-	17/33/109/115	-
25	CLA	k	204	17	-	5/12/88/115	-
32	DGD	B	849	-	-	19/43/83/95	0/2/2/2
25	CLA	A	840	-	-	12/37/113/115	-
29	BCR	J	101	-	-	17/29/63/63	0/2/2/2
25	CLA	j	209	16	-	20/38/114/115	-
25	CLA	b	204	10	-	11/25/101/115	-
25	CLA	A	825	1	-	8/39/115/115	-
30	DD6	A	855	-	-	9/26/80/80	0/3/3/3
25	CLA	B	843	2	-	14/37/113/115	-
25	CLA	j	203	16	-	8/21/97/115	-
30	DD6	f	614	-	-	7/26/80/80	0/3/3/3
30	DD6	g	217	-	-	4/26/80/80	0/3/3/3
25	CLA	A	850	1	-	8/27/103/115	-
25	CLA	o	606	23	-	5/15/91/115	-
25	CLA	d	305	12	-	5/12/88/115	-
25	CLA	A	830	1	-	8/24/100/115	-
25	CLA	j	207	-	-	5/18/94/115	-
29	BCR	A	837	-	-	11/29/63/63	0/2/2/2
30	DD6	l	614	-	-	3/26/80/80	0/3/3/3
25	CLA	f	601	20	-	7/12/88/115	-
25	CLA	A	824	1	-	16/31/107/115	-
25	CLA	c	303	11	-	14/32/108/115	-
27	LHG	A	835	-	-	22/53/53/53	-
25	CLA	A	802	-	-	10/37/113/115	-
25	CLA	A	857	-	-	8/25/101/115	-
25	CLA	h	205	14	-	5/13/89/115	-
25	CLA	c	302	11	-	6/12/88/115	-
30	DD6	m	212	-	-	5/26/80/80	0/3/3/3
30	DD6	b	214	-	-	5/26/80/80	0/3/3/3
25	CLA	e	210	-	-	7/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	817	-	-	8/21/97/115	-
27	LHG	h	202	25	-	11/35/35/53	-
25	CLA	f	607	20	-	15/27/103/115	-
25	CLA	A	847	1	-	6/13/89/115	-
25	CLA	e	212	13	-	8/24/100/115	-
25	CLA	g	208	21	-	5/21/97/115	-
25	CLA	i	205	-	-	3/13/89/115	-
25	CLA	a	210	27	-	6/15/91/115	-
30	DD6	e	218	-	-	9/26/80/80	0/3/3/3
25	CLA	A	853	27	-	12/25/101/115	-
27	LHG	d	302	25	-	14/33/33/53	-
25	CLA	o	604	-	-	3/12/88/115	-
25	CLA	B	810	2	-	3/13/89/115	-
28	PQN	F	205	-	-	5/15/35/43	0/2/2/2
25	CLA	c	313	11	-	8/25/101/115	-
29	BCR	A	838	-	-	5/29/63/63	0/2/2/2
25	CLA	c	315	11	-	5/18/94/115	-
27	LHG	h	201	-	-	14/33/33/53	-
25	CLA	g	214	21	-	0/12/88/115	-
25	CLA	n	206	-	-	3/12/88/115	-
25	CLA	A	809	1	-	23/39/115/115	-
29	BCR	B	831	-	-	11/29/63/63	0/2/2/2
33	SQD	D	200	-	-	12/31/51/69	0/1/1/1
25	CLA	A	848	1	-	8/23/99/115	-
25	CLA	B	812	2	-	13/38/114/115	-
25	CLA	d	315	12	-	4/12/88/115	-
25	CLA	m	209	-	-	3/13/89/115	-
25	CLA	f	609	20	-	4/12/88/115	-
25	CLA	a	206	-	-	7/15/91/115	-
25	CLA	f	612	20	-	9/13/89/115	-
25	CLA	A	819	-	-	12/39/115/115	-
25	CLA	A	818	1	-	15/39/115/115	-
25	CLA	A	831	1	-	4/19/95/115	-
25	CLA	f	611	20	-	6/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	805	2	-	13/39/115/115	-
25	CLA	h	207	-	-	7/19/95/115	-
25	CLA	A	833	1	-	15/39/115/115	-
25	CLA	l	607	18	-	14/26/102/115	-
30	DD6	h	216	-	-	3/26/80/80	0/3/3/3
25	CLA	c	312	11	-	4/13/89/115	-
25	CLA	g	210	27	-	3/12/88/115	-
25	CLA	B	813	2	-	5/19/95/115	-
25	CLA	o	602	23	-	10/18/94/115	-
29	BCR	B	833	-	-	5/29/63/63	0/2/2/2
25	CLA	m	206	-	-	2/12/88/115	-
25	CLA	o	609	23	-	8/12/88/115	-
25	CLA	B	820	2	-	7/13/89/115	-
30	DD6	p	610	-	-	3/26/80/80	0/3/3/3
25	CLA	n	202	22	-	14/27/103/115	-
25	CLA	l	612	-	-	6/12/88/115	-
25	CLA	p	608	24	-	5/13/89/115	-
25	CLA	j	204	16	-	4/27/103/115	-
25	CLA	B	838	2	-	6/35/111/115	-
25	CLA	b	212	10	-	11/24/100/115	-
25	CLA	c	308	-	-	11/21/97/115	-
25	CLA	A	852	1	-	5/19/95/115	-
25	CLA	h	212	14	-	10/25/101/115	-
29	BCR	B	830	-	-	7/29/63/63	0/2/2/2
25	CLA	p	603	24	-	4/12/88/115	-
30	DD6	g	216	-	-	4/26/80/80	0/3/3/3
25	CLA	h	215	14	-	2/13/89/115	-
25	CLA	b	211	-	-	4/12/88/115	-
25	CLA	b	206	-	-	5/15/91/115	-
25	CLA	o	605	-	-	5/13/89/115	-
27	LHG	j	202	25	-	24/41/41/53	-
30	DD6	A	854	-	-	3/26/80/80	0/3/3/3
25	CLA	a	209	9	-	10/26/102/115	-
25	CLA	a	212	9	-	14/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	604	-	-	5/12/88/115	-
29	BCR	A	836	-	-	5/29/63/63	0/2/2/2
29	BCR	B	801	-	-	9/29/63/63	0/2/2/2
25	CLA	p	606	24	-	10/21/97/115	-
25	CLA	c	304	11	-	6/25/101/115	-
25	CLA	i	211	15	-	10/32/108/115	-
25	CLA	k	213	17	-	5/12/88/115	-
25	CLA	d	303	12	-	6/21/97/115	-
25	CLA	F	202	6	-	9/15/91/115	-
25	CLA	n	207	-	-	2/10/86/115	-
25	CLA	b	205	10	-	6/13/89/115	-
25	CLA	B	804	2	-	18/39/115/115	-
25	CLA	k	209	-	-	5/12/88/115	-
30	DD6	k	215	-	-	2/26/80/80	0/3/3/3
25	CLA	e	205	13	-	20/39/115/115	-
30	DD6	i	216	-	-	1/26/80/80	0/3/3/3
28	PQN	B	835	-	-	5/16/36/43	0/2/2/2
25	CLA	h	208	14	-	8/21/97/115	-
30	DD6	f	613	-	-	5/26/80/80	0/3/3/3
34	LMG	k	201	-	-	16/31/51/70	0/1/1/1

All (2451) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	201	LHG	P-O3	6.37	1.85	1.59
27	m	201	LHG	P-O3	6.32	1.84	1.59
27	c	301	LHG	P-O3	6.28	1.84	1.59
27	d	302	LHG	P-O3	6.22	1.84	1.59
27	h	201	LHG	P-O3	6.19	1.84	1.59
27	a	201	LHG	P-O3	6.15	1.84	1.59
27	h	202	LHG	P-O3	6.10	1.84	1.59
27	g	201	LHG	P-O3	6.02	1.83	1.59
27	A	835	LHG	P-O3	6.02	1.83	1.59
27	i	201	LHG	P-O3	5.94	1.83	1.59
27	j	202	LHG	P-O3	5.90	1.83	1.59
27	A	805	LHG	P-O3	5.69	1.82	1.59
25	p	603	CLA	MG-NA	5.49	2.19	2.06
35	e	209	CHL	CMC-C2C	5.37	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	609	CLA	MG-NA	5.34	2.19	2.06
25	g	205	CLA	MG-NA	5.34	2.19	2.06
35	d	310	CHL	CMC-C2C	5.34	1.56	1.45
35	d	308	CHL	CMC-C2C	5.34	1.56	1.45
27	b	201	LHG	P-O6	5.30	1.80	1.59
27	m	201	LHG	P-O6	5.29	1.80	1.59
25	o	603	CLA	MG-NA	5.23	2.18	2.06
35	d	307	CHL	CMC-C2C	5.22	1.56	1.45
25	f	603	CLA	MG-NA	5.21	2.18	2.06
35	c	307	CHL	CMC-C2C	5.20	1.56	1.45
27	h	201	LHG	P-O6	5.19	1.80	1.59
25	p	609	CLA	MG-NA	5.19	2.18	2.06
35	d	309	CHL	CMC-C2C	5.16	1.56	1.45
25	m	204	CLA	MG-NA	5.15	2.18	2.06
25	j	205	CLA	MG-NA	5.14	2.18	2.06
27	a	201	LHG	P-O6	5.14	1.80	1.59
25	l	603	CLA	MG-NA	5.14	2.18	2.06
25	i	204	CLA	MG-NA	5.14	2.18	2.06
25	l	611	CLA	MG-NA	5.14	2.18	2.06
25	m	202	CLA	MG-NA	5.13	2.18	2.06
27	j	202	LHG	P-O6	5.12	1.80	1.59
25	p	607	CLA	MG-NA	5.11	2.18	2.06
27	c	301	LHG	P-O6	5.10	1.79	1.59
25	d	305	CLA	MG-NA	5.09	2.18	2.06
27	A	835	LHG	P-O6	5.08	1.79	1.59
25	n	203	CLA	MG-NA	5.08	2.18	2.06
25	a	211	CLA	MG-NA	5.08	2.18	2.06
25	g	211	CLA	MG-NA	5.07	2.18	2.06
25	b	212	CLA	MG-NA	5.07	2.18	2.06
25	g	207	CLA	MG-NA	5.06	2.18	2.06
25	j	211	CLA	MG-NA	5.06	2.18	2.06
25	f	612	CLA	MG-NA	5.06	2.18	2.06
25	o	610	CLA	MG-NA	5.06	2.18	2.06
27	g	201	LHG	P-O6	5.05	1.79	1.59
25	F	201	CLA	MG-NA	5.05	2.18	2.06
25	n	210	CLA	MG-NA	5.03	2.18	2.06
27	A	805	LHG	P-O6	5.03	1.79	1.59
25	n	202	CLA	MG-NA	5.03	2.18	2.06
25	c	312	CLA	MG-NA	5.03	2.18	2.06
25	m	210	CLA	MG-NA	5.03	2.18	2.06
25	k	210	CLA	MG-NA	5.02	2.18	2.06
25	a	205	CLA	MG-NA	5.02	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	302	LHG	P-O6	5.02	1.79	1.59
25	p	606	CLA	MG-NA	5.02	2.18	2.06
25	j	207	CLA	MG-NA	5.02	2.18	2.06
25	e	215	CLA	MG-NA	5.02	2.18	2.06
25	i	210	CLA	MG-NA	5.02	2.18	2.06
25	d	314	CLA	MG-NA	5.02	2.18	2.06
25	l	609	CLA	MG-NA	5.01	2.18	2.06
25	o	601	CLA	MG-NA	5.01	2.18	2.06
25	h	211	CLA	MG-NA	5.01	2.18	2.06
25	n	208	CLA	MG-NA	5.01	2.18	2.06
25	b	205	CLA	MG-NA	5.01	2.18	2.06
25	e	206	CLA	MG-NA	5.00	2.18	2.06
25	b	203	CLA	MG-NA	5.00	2.18	2.06
25	A	831	CLA	MG-NA	4.99	2.18	2.06
25	n	206	CLA	MG-NA	4.99	2.18	2.06
25	A	821	CLA	MG-NA	4.99	2.18	2.06
25	n	207	CLA	MG-NA	4.99	2.18	2.06
25	d	306	CLA	MG-NA	4.99	2.18	2.06
25	d	316	CLA	MG-NA	4.99	2.18	2.06
25	f	601	CLA	MG-NA	4.98	2.18	2.06
25	n	211	CLA	MG-NA	4.98	2.18	2.06
25	l	612	CLA	MG-NA	4.98	2.18	2.06
25	n	205	CLA	MG-NA	4.98	2.18	2.06
25	o	608	CLA	MG-NA	4.97	2.18	2.06
25	B	813	CLA	MG-NA	4.97	2.18	2.06
25	B	844	CLA	MG-NA	4.97	2.18	2.06
25	n	204	CLA	MG-NA	4.97	2.18	2.06
25	e	207	CLA	MG-NA	4.97	2.18	2.06
25	A	814	CLA	MG-NA	4.97	2.18	2.06
25	o	602	CLA	MG-NA	4.97	2.18	2.06
27	i	201	LHG	P-O6	4.97	1.79	1.59
25	c	304	CLA	MG-NA	4.97	2.18	2.06
25	A	811	CLA	MG-NA	4.96	2.18	2.06
25	p	605	CLA	MG-NA	4.96	2.18	2.06
25	c	305	CLA	MG-NA	4.96	2.18	2.06
25	g	203	CLA	MG-NA	4.96	2.18	2.06
25	a	210	CLA	MG-NA	4.96	2.18	2.06
25	f	605	CLA	MG-NA	4.96	2.18	2.06
25	A	825	CLA	MG-NA	4.96	2.18	2.06
25	o	609	CLA	MG-NA	4.96	2.18	2.06
25	o	604	CLA	MG-NA	4.96	2.18	2.06
25	A	826	CLA	MG-NA	4.96	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	841	CLA	MG-NA	4.96	2.18	2.06
25	B	808	CLA	MG-NA	4.95	2.18	2.06
25	f	606	CLA	MG-NA	4.95	2.18	2.06
25	A	827	CLA	MG-NA	4.95	2.18	2.06
25	p	604	CLA	MG-NA	4.95	2.18	2.06
25	j	213	CLA	MG-NA	4.95	2.18	2.06
25	e	217	CLA	MG-NA	4.95	2.18	2.06
25	k	204	CLA	MG-NA	4.95	2.18	2.06
25	d	313	CLA	MG-NA	4.95	2.18	2.06
25	a	213	CLA	MG-NA	4.94	2.18	2.06
25	f	604	CLA	MG-NA	4.94	2.18	2.06
25	b	207	CLA	MG-NA	4.94	2.18	2.06
25	a	203	CLA	MG-NA	4.94	2.18	2.06
25	g	212	CLA	MG-NA	4.94	2.18	2.06
25	c	311	CLA	MG-NA	4.94	2.18	2.06
25	k	213	CLA	MG-NA	4.94	2.18	2.06
25	d	301	CLA	MG-NA	4.94	2.18	2.06
25	p	602	CLA	MG-NA	4.94	2.18	2.06
25	l	601	CLA	MG-NA	4.94	2.18	2.06
25	f	608	CLA	MG-NA	4.93	2.18	2.06
25	B	807	CLA	MG-NA	4.93	2.18	2.06
25	g	215	CLA	MG-NA	4.93	2.18	2.06
25	e	212	CLA	MG-NA	4.93	2.18	2.06
25	B	834	CLA	MG-NA	4.93	2.18	2.06
25	m	205	CLA	MG-NA	4.93	2.18	2.06
25	J	103	CLA	MG-NA	4.93	2.18	2.06
25	g	213	CLA	MG-NA	4.93	2.18	2.06
27	h	202	LHG	P-O6	4.93	1.79	1.59
25	c	306	CLA	MG-NA	4.93	2.18	2.06
25	B	809	CLA	MG-NA	4.93	2.18	2.06
25	g	214	CLA	MG-NA	4.93	2.18	2.06
25	e	204	CLA	MG-NA	4.93	2.18	2.06
25	p	601	CLA	MG-NA	4.93	2.18	2.06
25	h	215	CLA	MG-NA	4.93	2.18	2.06
25	h	203	CLA	MG-NA	4.92	2.18	2.06
25	l	604	CLA	MG-NA	4.92	2.18	2.06
25	e	208	CLA	MG-NA	4.92	2.18	2.06
25	h	204	CLA	MG-NA	4.92	2.18	2.06
25	f	607	CLA	MG-NA	4.92	2.18	2.06
25	k	212	CLA	MG-NA	4.92	2.18	2.06
25	l	608	CLA	MG-NA	4.92	2.18	2.06
25	A	852	CLA	MG-NA	4.92	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	206	CLA	MG-NA	4.92	2.18	2.06
25	B	812	CLA	MG-NA	4.92	2.18	2.06
25	e	214	CLA	MG-NA	4.92	2.18	2.06
25	h	207	CLA	MG-NA	4.92	2.17	2.06
25	b	211	CLA	MG-NA	4.92	2.17	2.06
25	m	206	CLA	MG-NA	4.92	2.17	2.06
25	A	816	CLA	MG-NA	4.92	2.17	2.06
25	e	201	CLA	MG-NA	4.92	2.17	2.06
25	B	836	CLA	MG-NA	4.91	2.17	2.06
25	B	846	CLA	MG-NA	4.91	2.17	2.06
25	A	828	CLA	MG-NA	4.91	2.17	2.06
25	m	209	CLA	MG-NA	4.91	2.17	2.06
25	A	813	CLA	MG-NA	4.91	2.17	2.06
25	F	202	CLA	MG-NA	4.91	2.17	2.06
25	m	211	CLA	MG-NA	4.91	2.17	2.06
25	h	206	CLA	MG-NA	4.91	2.17	2.06
25	f	611	CLA	MG-NA	4.91	2.17	2.06
25	j	206	CLA	MG-NA	4.91	2.17	2.06
25	A	804	CLA	MG-NA	4.90	2.17	2.06
25	A	823	CLA	MG-NA	4.90	2.17	2.06
25	c	314	CLA	MG-NA	4.90	2.17	2.06
25	B	837	CLA	MG-NA	4.90	2.17	2.06
25	c	315	CLA	MG-NA	4.90	2.17	2.06
25	l	605	CLA	MG-NA	4.90	2.17	2.06
25	e	216	CLA	MG-NA	4.90	2.17	2.06
25	c	309	CLA	MG-NA	4.90	2.17	2.06
25	j	215	CLA	MG-NA	4.90	2.17	2.06
25	A	818	CLA	MG-NA	4.89	2.17	2.06
25	k	202	CLA	MG-NA	4.89	2.17	2.06
25	B	820	CLA	MG-NA	4.89	2.17	2.06
25	i	209	CLA	MG-NA	4.89	2.17	2.06
25	A	857	CLA	MG-NA	4.89	2.17	2.06
25	i	212	CLA	MG-NA	4.89	2.17	2.06
25	A	853	CLA	MG-NA	4.89	2.17	2.06
25	d	303	CLA	MG-NA	4.89	2.17	2.06
25	B	826	CLA	MG-NA	4.89	2.17	2.06
25	h	205	CLA	MG-NA	4.89	2.17	2.06
25	g	210	CLA	MG-NA	4.89	2.17	2.06
25	B	839	CLA	MG-NA	4.89	2.17	2.06
25	d	311	CLA	MG-NA	4.89	2.17	2.06
25	o	605	CLA	MG-NA	4.88	2.17	2.06
25	k	206	CLA	MG-NA	4.88	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	206	CLA	MG-NA	4.88	2.17	2.06
25	o	606	CLA	MG-NA	4.88	2.17	2.06
25	d	312	CLA	MG-NA	4.88	2.17	2.06
25	i	202	CLA	MG-NA	4.88	2.17	2.06
25	A	829	CLA	MG-NA	4.88	2.17	2.06
25	c	313	CLA	MG-NA	4.88	2.17	2.06
25	b	213	CLA	MG-NA	4.88	2.17	2.06
25	B	804	CLA	MG-NA	4.88	2.17	2.06
25	f	610	CLA	MG-NA	4.88	2.17	2.06
25	n	209	CLA	MG-NA	4.87	2.17	2.06
25	B	845	CLA	MG-NA	4.87	2.17	2.06
25	h	214	CLA	MG-NA	4.87	2.17	2.06
25	B	821	CLA	MG-NA	4.87	2.17	2.06
25	i	213	CLA	MG-NA	4.87	2.17	2.06
25	B	814	CLA	MG-NA	4.87	2.17	2.06
25	h	208	CLA	MG-NA	4.87	2.17	2.06
25	A	810	CLA	MG-NA	4.87	2.17	2.06
25	b	208	CLA	MG-NA	4.87	2.17	2.06
25	a	208	CLA	MG-NA	4.86	2.17	2.06
25	e	210	CLA	MG-NA	4.86	2.17	2.06
25	l	606	CLA	MG-NA	4.86	2.17	2.06
25	h	213	CLA	MG-NA	4.86	2.17	2.06
25	k	205	CLA	MG-NA	4.86	2.17	2.06
25	A	845	CLA	MG-NA	4.86	2.17	2.06
25	f	602	CLA	MG-NA	4.86	2.17	2.06
25	A	849	CLA	MG-NA	4.86	2.17	2.06
25	h	210	CLA	MG-NA	4.85	2.17	2.06
25	A	843	CLA	MG-NA	4.85	2.17	2.06
25	B	815	CLA	MG-NA	4.85	2.17	2.06
25	b	204	CLA	MG-NA	4.85	2.17	2.06
25	j	214	CLA	MG-NA	4.85	2.17	2.06
25	p	608	CLA	MG-NA	4.85	2.17	2.06
25	k	209	CLA	MG-NA	4.85	2.17	2.06
25	g	206	CLA	MG-NA	4.85	2.17	2.06
25	b	206	CLA	MG-NA	4.85	2.17	2.06
25	B	847	CLA	MG-NA	4.84	2.17	2.06
25	j	208	CLA	MG-NA	4.84	2.17	2.06
25	B	818	CLA	MG-NA	4.84	2.17	2.06
25	B	810	CLA	MG-NA	4.84	2.17	2.06
25	B	806	CLA	MG-NA	4.84	2.17	2.06
25	j	203	CLA	MG-NA	4.84	2.17	2.06
25	B	842	CLA	MG-NA	4.84	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	848	CLA	MG-NA	4.84	2.17	2.06
25	j	210	CLA	MG-NA	4.84	2.17	2.06
25	c	302	CLA	MG-NA	4.83	2.17	2.06
25	l	610	CLA	MG-NA	4.83	2.17	2.06
25	b	209	CLA	MG-NA	4.83	2.17	2.06
25	B	848	CLA	MG-NA	4.83	2.17	2.06
25	A	847	CLA	MG-NA	4.83	2.17	2.06
25	k	214	CLA	MG-NA	4.83	2.17	2.06
25	A	846	CLA	MG-NA	4.83	2.17	2.06
25	l	602	CLA	MG-NA	4.83	2.17	2.06
25	B	825	CLA	MG-NA	4.82	2.17	2.06
25	b	210	CLA	MG-NA	4.82	2.17	2.06
25	m	207	CLA	MG-NA	4.82	2.17	2.06
25	A	822	CLA	MG-NA	4.82	2.17	2.06
25	i	207	CLA	MG-NA	4.82	2.17	2.06
25	A	841	CLA	MG-NA	4.82	2.17	2.06
25	d	315	CLA	MG-NA	4.82	2.17	2.06
25	A	820	CLA	MG-NA	4.81	2.17	2.06
25	B	811	CLA	MG-NA	4.81	2.17	2.06
25	A	815	CLA	MG-NA	4.81	2.17	2.06
25	A	809	CLA	MG-NA	4.81	2.17	2.06
25	A	806	CLA	MG-NA	4.81	2.17	2.06
25	A	851	CLA	MG-NA	4.81	2.17	2.06
25	A	817	CLA	MG-NA	4.81	2.17	2.06
25	i	205	CLA	MG-NA	4.81	2.17	2.06
25	m	208	CLA	MG-NA	4.81	2.17	2.06
25	B	843	CLA	MG-NA	4.81	2.17	2.06
25	A	844	CLA	MG-NA	4.81	2.17	2.06
25	B	824	CLA	MG-NA	4.81	2.17	2.06
25	c	308	CLA	MG-NA	4.80	2.17	2.06
25	k	203	CLA	MG-NA	4.80	2.17	2.06
25	e	205	CLA	MG-NA	4.80	2.17	2.06
25	B	805	CLA	MG-NA	4.80	2.17	2.06
25	a	212	CLA	MG-NA	4.80	2.17	2.06
25	a	207	CLA	MG-NA	4.80	2.17	2.06
25	B	819	CLA	MG-NA	4.80	2.17	2.06
25	e	213	CLA	MG-NA	4.80	2.17	2.06
25	B	840	CLA	MG-NA	4.80	2.17	2.06
25	c	303	CLA	MG-NA	4.79	2.17	2.06
25	g	208	CLA	MG-NA	4.79	2.17	2.06
25	B	838	CLA	MG-NA	4.79	2.17	2.06
25	A	808	CLA	MG-NA	4.78	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	k	207	CLA	MG-NA	4.78	2.17	2.06
25	A	830	CLA	MG-NA	4.77	2.17	2.06
25	k	211	CLA	MG-NA	4.77	2.17	2.06
25	A	819	CLA	MG-NA	4.77	2.17	2.06
25	A	842	CLA	MG-NA	4.77	2.17	2.06
25	d	304	CLA	MG-NA	4.77	2.17	2.06
25	e	211	CLA	MG-NA	4.77	2.17	2.06
25	A	801	CLA	MG-NA	4.77	2.17	2.06
25	A	824	CLA	MG-NA	4.76	2.17	2.06
25	c	310	CLA	MG-NA	4.76	2.17	2.06
25	B	823	CLA	MG-NA	4.75	2.17	2.06
25	i	203	CLA	MG-NA	4.75	2.17	2.06
25	B	817	CLA	MG-NA	4.74	2.17	2.06
25	A	812	CLA	MG-NA	4.74	2.17	2.06
25	a	204	CLA	MG-NA	4.74	2.17	2.06
25	A	833	CLA	MG-NA	4.74	2.17	2.06
25	g	204	CLA	MG-NA	4.73	2.17	2.06
25	B	822	CLA	MG-NA	4.73	2.17	2.06
25	k	208	CLA	MG-NA	4.73	2.17	2.06
25	m	203	CLA	MG-NA	4.73	2.17	2.06
25	o	607	CLA	MG-NA	4.73	2.17	2.06
25	i	211	CLA	MG-NA	4.73	2.17	2.06
25	a	209	CLA	MG-NA	4.71	2.17	2.06
25	B	802	CLA	MG-NA	4.71	2.17	2.06
25	B	816	CLA	MG-NA	4.71	2.17	2.06
25	i	208	CLA	MG-NA	4.71	2.17	2.06
25	n	201	CLA	MG-NA	4.71	2.17	2.06
33	g	202	SQD	O48-C23	4.70	1.47	1.33
25	j	212	CLA	MG-NA	4.70	2.17	2.06
25	l	607	CLA	MG-NA	4.69	2.17	2.06
25	h	212	CLA	MG-NA	4.68	2.17	2.06
33	D	200	SQD	O48-C23	4.67	1.47	1.33
25	A	840	CLA	MG-NA	4.67	2.17	2.06
25	A	802	CLA	MG-NA	4.66	2.17	2.06
25	j	209	CLA	MG-NA	4.66	2.17	2.06
25	A	832	CLA	MG-NA	4.65	2.17	2.06
25	g	209	CLA	MG-NA	4.65	2.17	2.06
25	j	204	CLA	MG-NA	4.64	2.17	2.06
33	F	204	SQD	O48-C23	4.63	1.46	1.33
25	h	209	CLA	MG-NA	4.60	2.17	2.06
25	B	803	CLA	MG-NA	4.60	2.17	2.06
25	A	807	CLA	MG-NA	4.57	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	850	CLA	MG-NA	4.57	2.17	2.06
30	n	212	DD6	C29-C27	-4.39	1.34	1.42
30	p	610	DD6	C29-C27	-4.38	1.34	1.42
30	c	316	DD6	C29-C27	-4.36	1.34	1.42
30	c	318	DD6	C29-C27	-4.35	1.34	1.42
30	i	215	DD6	C29-C27	-4.35	1.34	1.42
30	g	217	DD6	C29-C27	-4.33	1.34	1.42
30	j	216	DD6	C29-C27	-4.33	1.34	1.42
30	d	319	DD6	C29-C27	-4.33	1.34	1.42
30	m	212	DD6	C29-C27	-4.31	1.34	1.42
30	k	216	DD6	C29-C27	-4.31	1.34	1.42
30	J	104	DD6	C29-C27	-4.31	1.34	1.42
30	o	612	DD6	C29-C27	-4.31	1.34	1.42
30	b	215	DD6	C29-C27	-4.31	1.34	1.42
30	o	611	DD6	C29-C27	-4.30	1.34	1.42
30	d	317	DD6	C29-C27	-4.29	1.34	1.42
30	i	216	DD6	C29-C27	-4.29	1.34	1.42
30	e	219	DD6	C29-C27	-4.28	1.34	1.42
30	A	854	DD6	C29-C27	-4.28	1.34	1.42
30	h	217	DD6	C29-C27	-4.28	1.34	1.42
30	c	317	DD6	C29-C27	-4.28	1.34	1.42
30	b	214	DD6	C29-C27	-4.27	1.34	1.42
30	a	214	DD6	C29-C27	-4.27	1.34	1.42
30	i	214	DD6	C29-C27	-4.26	1.34	1.42
30	d	318	DD6	C29-C27	-4.26	1.34	1.42
30	A	855	DD6	C29-C27	-4.25	1.34	1.42
30	j	217	DD6	C29-C27	-4.24	1.34	1.42
30	h	216	DD6	C29-C27	-4.24	1.34	1.42
30	m	213	DD6	C29-C27	-4.24	1.34	1.42
30	g	216	DD6	C29-C27	-4.23	1.34	1.42
30	a	215	DD6	C29-C27	-4.23	1.34	1.42
30	f	613	DD6	C29-C27	-4.23	1.34	1.42
30	l	613	DD6	C29-C27	-4.21	1.34	1.42
30	f	614	DD6	C29-C27	-4.21	1.34	1.42
30	k	215	DD6	C29-C27	-4.21	1.34	1.42
30	l	614	DD6	C29-C27	-4.20	1.34	1.42
30	n	214	DD6	C5-C6	4.09	1.41	1.35
30	n	214	DD6	C2-C1	4.02	1.41	1.35
30	e	220	DD6	C10-C11	3.93	1.41	1.35
29	J	101	BCR	C21-C22	3.93	1.41	1.35
30	n	214	DD6	C10-C11	3.93	1.41	1.35
30	p	610	DD6	C30-C31	-3.91	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	316	DD6	C30-C31	-3.87	1.34	1.42
30	g	217	DD6	C30-C31	-3.86	1.34	1.42
30	c	318	DD6	C30-C31	-3.86	1.34	1.42
30	A	854	DD6	C30-C31	-3.86	1.34	1.42
30	i	216	DD6	C30-C31	-3.85	1.34	1.42
30	i	215	DD6	C30-C31	-3.85	1.34	1.42
30	m	212	DD6	C30-C31	-3.84	1.34	1.42
30	d	318	DD6	C30-C31	-3.84	1.34	1.42
30	o	612	DD6	C30-C31	-3.84	1.34	1.42
30	o	611	DD6	C30-C31	-3.83	1.34	1.42
30	e	219	DD6	C30-C31	-3.83	1.34	1.42
30	n	212	DD6	C30-C31	-3.83	1.34	1.42
30	d	319	DD6	C30-C31	-3.82	1.34	1.42
30	f	614	DD6	C30-C31	-3.82	1.34	1.42
30	b	215	DD6	C30-C31	-3.80	1.34	1.42
30	d	317	DD6	C30-C31	-3.79	1.34	1.42
30	e	220	DD6	C5-C6	3.79	1.40	1.35
30	j	216	DD6	C30-C31	-3.79	1.34	1.42
30	J	104	DD6	C30-C31	-3.79	1.34	1.42
30	b	214	DD6	C30-C31	-3.79	1.34	1.42
30	h	217	DD6	C30-C31	-3.78	1.34	1.42
30	k	216	DD6	C30-C31	-3.78	1.34	1.42
30	c	317	DD6	C30-C31	-3.78	1.34	1.42
29	B	832	BCR	C23-C22	-3.78	1.37	1.45
30	f	613	DD6	C30-C31	-3.77	1.34	1.42
30	a	214	DD6	C30-C31	-3.77	1.34	1.42
30	h	216	DD6	C30-C31	-3.76	1.34	1.42
30	j	217	DD6	C30-C31	-3.76	1.34	1.42
30	i	214	DD6	C30-C31	-3.76	1.34	1.42
30	a	215	DD6	C30-C31	-3.75	1.34	1.42
30	l	614	DD6	C30-C31	-3.75	1.34	1.42
30	A	855	DD6	C30-C31	-3.74	1.34	1.42
30	l	613	DD6	C30-C31	-3.74	1.34	1.42
30	m	213	DD6	C30-C31	-3.74	1.34	1.42
30	k	215	DD6	C30-C31	-3.72	1.34	1.42
30	g	216	DD6	C30-C31	-3.69	1.34	1.42
29	J	101	BCR	C17-C18	3.68	1.40	1.35
25	o	608	CLA	CAD-C3D	-3.68	1.44	1.50
30	d	318	DD6	O1-C20	-3.61	1.41	1.46
29	J	101	BCR	C14-C13	3.60	1.40	1.35
29	A	837	BCR	C23-C22	-3.60	1.38	1.45
33	D	200	SQD	O47-C45	-3.55	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	e	220	DD6	C2-C1	3.50	1.40	1.35
33	g	202	SQD	O47-C45	-3.47	1.37	1.46
30	c	316	DD6	O1-C20	-3.47	1.41	1.46
30	J	105	DD6	C10-C11	3.47	1.40	1.35
33	J	102	SQD	O47-C45	-3.46	1.37	1.46
29	J	101	BCR	C10-C9	3.45	1.40	1.35
33	F	204	SQD	O47-C45	-3.44	1.38	1.46
29	B	832	BCR	C8-C9	-3.43	1.38	1.45
35	e	209	CHL	O2D-CGD	3.42	1.41	1.33
30	e	219	DD6	O1-C20	-3.41	1.41	1.46
30	J	104	DD6	O1-C20	-3.41	1.41	1.46
33	g	202	SQD	O5-C1	3.40	1.50	1.41
35	c	307	CHL	O2D-CGD	3.39	1.41	1.33
35	d	307	CHL	O2D-CGD	3.38	1.41	1.33
33	J	102	SQD	O5-C1	3.38	1.50	1.41
35	d	309	CHL	O2D-CGD	3.36	1.41	1.33
30	j	216	DD6	O1-C20	-3.35	1.41	1.46
35	d	308	CHL	O2D-CGD	3.35	1.41	1.33
29	B	831	BCR	C23-C22	-3.35	1.38	1.45
30	a	215	DD6	O1-C20	-3.35	1.41	1.46
30	F	203	DD6	C2-C1	3.35	1.40	1.35
33	F	204	SQD	O47-C7	3.33	1.43	1.34
35	d	310	CHL	O2A-CGA	3.33	1.41	1.30
30	i	214	DD6	O1-C20	-3.32	1.41	1.46
35	e	209	CHL	O2A-CGA	3.32	1.41	1.30
35	d	310	CHL	O2D-CGD	3.31	1.41	1.33
29	A	837	BCR	C8-C9	-3.31	1.38	1.45
30	m	213	DD6	O1-C20	-3.31	1.41	1.46
29	A	837	BCR	C10-C9	3.31	1.40	1.35
33	J	102	SQD	O47-C7	3.30	1.43	1.34
30	k	215	DD6	O1-C20	-3.30	1.41	1.46
30	j	217	DD6	O1-C20	-3.29	1.41	1.46
35	d	308	CHL	O2A-CGA	3.29	1.41	1.30
29	B	831	BCR	C8-C9	-3.29	1.38	1.45
29	B	831	BCR	C10-C9	3.26	1.40	1.35
30	c	317	DD6	O1-C20	-3.26	1.41	1.46
30	J	105	DD6	C5-C6	3.26	1.40	1.35
33	g	202	SQD	O47-C7	3.23	1.43	1.34
30	l	614	DD6	O1-C20	-3.23	1.41	1.46
33	F	204	SQD	O5-C1	3.22	1.50	1.41
30	h	216	DD6	O1-C20	-3.21	1.41	1.46
30	g	216	DD6	O1-C20	-3.20	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	215	DD6	O1-C20	-3.20	1.41	1.46
29	J	101	BCR	C8-C9	-3.19	1.39	1.45
30	d	317	DD6	O1-C20	-3.18	1.41	1.46
29	B	831	BCR	C14-C13	3.17	1.40	1.35
30	n	213	DD6	C5-C6	3.17	1.40	1.35
30	F	203	DD6	C10-C11	3.16	1.40	1.35
33	D	200	SQD	O47-C7	3.16	1.43	1.34
30	l	613	DD6	O1-C20	-3.16	1.41	1.46
29	B	831	BCR	C21-C22	3.15	1.40	1.35
30	J	105	DD6	C2-C1	3.14	1.39	1.35
30	h	217	DD6	O1-C20	-3.13	1.41	1.46
25	A	802	CLA	C1D-ND	-3.12	1.33	1.37
28	B	827	PQN	C2M-C2	-3.10	1.44	1.50
30	n	213	DD6	C10-C11	3.08	1.39	1.35
30	F	203	DD6	C24-C1	-3.08	1.39	1.45
29	B	832	BCR	C10-C9	3.07	1.39	1.35
25	A	829	CLA	C1D-ND	-3.07	1.34	1.37
25	B	803	CLA	C1D-ND	-3.07	1.34	1.37
30	n	213	DD6	C2-C1	3.07	1.39	1.35
29	J	101	BCR	C23-C22	-3.07	1.39	1.45
29	A	837	BCR	C14-C13	3.05	1.39	1.35
25	A	843	CLA	C1D-ND	-3.05	1.34	1.37
30	b	215	DD6	O1-C20	-3.05	1.41	1.46
30	a	214	DD6	O1-C20	-3.04	1.41	1.46
30	F	203	DD6	C25-C26	-3.04	1.34	1.43
33	D	200	SQD	C24-C23	3.02	1.59	1.50
35	d	310	CHL	MG-NA	3.02	2.13	2.06
33	F	204	SQD	C24-C23	3.02	1.59	1.50
30	e	218	DD6	C24-C1	-3.02	1.39	1.45
30	g	217	DD6	O1-C20	-3.02	1.41	1.46
25	A	840	CLA	C1D-ND	-3.02	1.34	1.37
29	B	831	BCR	C17-C18	3.01	1.39	1.35
35	d	308	CHL	MG-NA	3.01	2.13	2.06
30	k	216	DD6	O1-C20	-3.00	1.41	1.46
33	g	202	SQD	C24-C23	2.99	1.59	1.50
30	o	612	DD6	O1-C20	-2.99	1.41	1.46
28	B	827	PQN	C10-C5	-2.98	1.35	1.40
30	e	218	DD6	C13-C11	-2.98	1.39	1.45
25	j	209	CLA	C1D-ND	-2.97	1.34	1.37
35	c	307	CHL	O2A-CGA	2.96	1.42	1.33
25	A	832	CLA	C1D-ND	-2.95	1.34	1.37
29	B	831	BCR	C19-C18	-2.95	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	807	CLA	C1D-ND	-2.95	1.34	1.37
29	A	837	BCR	C19-C18	-2.95	1.39	1.45
29	B	832	BCR	C17-C18	2.94	1.39	1.35
35	d	307	CHL	MG-NA	2.94	2.13	2.06
25	h	209	CLA	C1D-ND	-2.94	1.34	1.37
29	B	832	BCR	C19-C18	-2.94	1.39	1.45
30	e	218	DD6	C10-C11	2.94	1.39	1.35
25	B	822	CLA	C1D-ND	-2.94	1.34	1.37
33	J	102	SQD	C24-C23	2.94	1.59	1.49
35	d	309	CHL	MG-NA	2.93	2.13	2.06
28	A	834	PQN	C10-C5	-2.92	1.35	1.40
25	A	822	CLA	C1D-ND	-2.92	1.34	1.37
25	A	849	CLA	C1D-ND	-2.92	1.34	1.37
25	k	207	CLA	C1D-ND	-2.92	1.34	1.37
25	B	838	CLA	C1D-ND	-2.92	1.34	1.37
30	e	218	DD6	C8-C6	-2.91	1.39	1.45
25	i	203	CLA	C1D-ND	-2.91	1.34	1.37
25	a	208	CLA	C1D-ND	-2.91	1.34	1.37
25	A	846	CLA	C1D-ND	-2.91	1.34	1.37
35	e	209	CHL	MG-NA	2.91	2.13	2.06
25	e	216	CLA	C1D-ND	-2.90	1.34	1.37
25	h	204	CLA	C1D-ND	-2.90	1.34	1.37
25	A	842	CLA	C1D-ND	-2.89	1.34	1.37
35	d	307	CHL	O2A-CGA	2.89	1.41	1.33
30	A	855	DD6	O1-C20	-2.88	1.42	1.46
33	D	200	SQD	O5-C1	2.88	1.49	1.41
25	A	850	CLA	C1D-ND	-2.88	1.34	1.37
29	B	832	BCR	C21-C22	2.88	1.39	1.35
30	e	220	DD6	C26-C27	2.88	1.43	1.37
30	d	318	DD6	C19-C20	-2.87	1.48	1.52
30	J	105	DD6	C24-C1	-2.87	1.39	1.45
25	B	840	CLA	C1D-ND	-2.87	1.34	1.37
25	j	210	CLA	C1D-ND	-2.87	1.34	1.37
30	n	213	DD6	C24-C1	-2.87	1.39	1.45
29	B	832	BCR	C12-C13	-2.86	1.39	1.45
25	a	209	CLA	C1D-ND	-2.86	1.34	1.37
25	j	206	CLA	C1D-ND	-2.86	1.34	1.37
30	F	203	DD6	C13-C11	-2.86	1.39	1.45
25	g	209	CLA	C1D-ND	-2.86	1.34	1.37
25	B	818	CLA	C1D-ND	-2.85	1.34	1.37
25	k	203	CLA	C1D-ND	-2.85	1.34	1.37
25	m	203	CLA	C1D-ND	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	j	216	DD6	C35-C36	-2.85	1.46	1.51
25	B	814	CLA	C1D-ND	-2.85	1.34	1.37
25	i	208	CLA	C1D-ND	-2.85	1.34	1.37
30	F	203	DD6	C5-C6	2.84	1.39	1.35
29	A	837	BCR	C12-C13	-2.84	1.39	1.45
25	B	843	CLA	C1D-ND	-2.84	1.34	1.37
30	e	218	DD6	C5-C6	2.84	1.39	1.35
25	A	845	CLA	C1D-ND	-2.84	1.34	1.37
25	B	806	CLA	C1D-ND	-2.84	1.34	1.37
25	i	207	CLA	C1D-ND	-2.84	1.34	1.37
25	B	825	CLA	C1D-ND	-2.83	1.34	1.37
30	n	213	DD6	C8-C6	-2.83	1.39	1.45
25	A	809	CLA	C1D-ND	-2.83	1.34	1.37
25	B	812	CLA	C1D-ND	-2.83	1.34	1.37
25	B	802	CLA	C1D-ND	-2.83	1.34	1.37
25	b	204	CLA	C1D-ND	-2.83	1.34	1.37
25	B	836	CLA	C1D-ND	-2.83	1.34	1.37
25	j	208	CLA	C1D-ND	-2.83	1.34	1.37
25	B	837	CLA	C1D-ND	-2.82	1.34	1.37
25	A	825	CLA	C1D-ND	-2.82	1.34	1.37
25	A	844	CLA	C1D-ND	-2.82	1.34	1.37
25	B	819	CLA	C1D-ND	-2.82	1.34	1.37
25	A	830	CLA	C1D-ND	-2.82	1.34	1.37
35	c	307	CHL	MG-NA	2.81	2.13	2.06
25	B	810	CLA	C1D-ND	-2.81	1.34	1.37
25	B	839	CLA	C1D-ND	-2.81	1.34	1.37
25	A	857	CLA	C1D-ND	-2.81	1.34	1.37
25	B	824	CLA	C1D-ND	-2.81	1.34	1.37
25	c	310	CLA	C1D-ND	-2.81	1.34	1.37
25	d	315	CLA	C1D-ND	-2.81	1.34	1.37
25	A	826	CLA	C1D-ND	-2.81	1.34	1.37
25	A	811	CLA	C1D-ND	-2.81	1.34	1.37
25	B	842	CLA	C1D-ND	-2.81	1.34	1.37
25	a	212	CLA	C1D-ND	-2.81	1.34	1.37
25	B	826	CLA	C1D-ND	-2.80	1.34	1.37
25	d	312	CLA	C1D-ND	-2.80	1.34	1.37
25	A	817	CLA	C1D-ND	-2.80	1.34	1.37
25	B	820	CLA	C1D-ND	-2.80	1.34	1.37
25	o	605	CLA	C1D-ND	-2.80	1.34	1.37
25	k	208	CLA	C1D-ND	-2.80	1.34	1.37
25	j	203	CLA	C1D-ND	-2.80	1.34	1.37
25	k	214	CLA	C1D-ND	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	e	205	CLA	C1D-ND	-2.80	1.34	1.37
25	g	203	CLA	C1D-ND	-2.80	1.34	1.37
25	n	208	CLA	C1D-ND	-2.80	1.34	1.37
30	n	213	DD6	C13-C11	-2.80	1.39	1.45
25	i	202	CLA	C1D-ND	-2.79	1.34	1.37
25	d	304	CLA	C1D-ND	-2.79	1.34	1.37
25	A	806	CLA	C1D-ND	-2.79	1.34	1.37
25	B	821	CLA	C1D-ND	-2.79	1.34	1.37
25	B	813	CLA	C1D-ND	-2.79	1.34	1.37
25	A	812	CLA	C1D-ND	-2.79	1.34	1.37
30	F	203	DD6	C8-C6	-2.79	1.40	1.45
25	B	844	CLA	C1D-ND	-2.79	1.34	1.37
25	b	208	CLA	C1D-ND	-2.79	1.34	1.37
25	j	204	CLA	C1D-ND	-2.79	1.34	1.37
25	b	206	CLA	C1D-ND	-2.78	1.34	1.37
25	A	847	CLA	C1D-ND	-2.78	1.34	1.37
25	B	804	CLA	C1D-ND	-2.78	1.34	1.37
25	A	819	CLA	C1D-ND	-2.78	1.34	1.37
25	A	841	CLA	C1D-ND	-2.78	1.34	1.37
33	J	102	SQD	O48-C23	2.78	1.47	1.33
25	i	209	CLA	C1D-ND	-2.77	1.34	1.37
25	A	810	CLA	C1D-ND	-2.77	1.34	1.37
30	m	212	DD6	O1-C20	-2.77	1.42	1.46
25	B	841	CLA	C1D-ND	-2.77	1.34	1.37
25	e	213	CLA	C1D-ND	-2.77	1.34	1.37
25	j	215	CLA	C1D-ND	-2.77	1.34	1.37
25	B	834	CLA	C1D-ND	-2.77	1.34	1.37
25	l	602	CLA	C1D-ND	-2.77	1.34	1.37
25	o	607	CLA	C1D-ND	-2.77	1.34	1.37
25	d	306	CLA	C1D-ND	-2.77	1.34	1.37
25	B	817	CLA	C1D-ND	-2.77	1.34	1.37
25	h	212	CLA	C1D-ND	-2.77	1.34	1.37
25	i	206	CLA	C1D-ND	-2.76	1.34	1.37
25	p	603	CLA	MG-NB	2.76	2.11	2.05
25	A	824	CLA	C1D-ND	-2.76	1.34	1.37
25	m	206	CLA	C1D-ND	-2.76	1.34	1.37
25	a	204	CLA	C1D-ND	-2.76	1.34	1.37
25	o	602	CLA	C1D-ND	-2.76	1.34	1.37
30	e	218	DD6	C2-C1	2.76	1.39	1.35
25	h	208	CLA	C1D-ND	-2.76	1.34	1.37
25	b	210	CLA	C1D-ND	-2.76	1.34	1.37
25	B	807	CLA	C1D-ND	-2.75	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	808	CLA	C1D-ND	-2.75	1.34	1.37
25	e	201	CLA	C1D-ND	-2.75	1.34	1.37
25	A	814	CLA	C1D-ND	-2.75	1.34	1.37
25	d	311	CLA	C1D-ND	-2.75	1.34	1.37
25	k	205	CLA	C1D-ND	-2.75	1.34	1.37
25	l	605	CLA	C1D-ND	-2.75	1.34	1.37
25	k	212	CLA	C1D-ND	-2.75	1.34	1.37
25	A	833	CLA	C1D-ND	-2.75	1.34	1.37
25	h	206	CLA	C1D-ND	-2.75	1.34	1.37
25	l	606	CLA	C1D-ND	-2.75	1.34	1.37
25	j	213	CLA	C1D-ND	-2.75	1.34	1.37
25	A	804	CLA	C1D-ND	-2.74	1.34	1.37
25	b	209	CLA	C1D-ND	-2.74	1.34	1.37
25	m	207	CLA	C1D-ND	-2.74	1.34	1.37
25	l	607	CLA	C1D-ND	-2.74	1.34	1.37
25	A	827	CLA	C1D-ND	-2.74	1.34	1.37
25	g	206	CLA	C1D-ND	-2.74	1.34	1.37
25	A	816	CLA	C1D-ND	-2.74	1.34	1.37
25	k	209	CLA	C1D-ND	-2.74	1.34	1.37
25	a	206	CLA	C1D-ND	-2.74	1.34	1.37
25	i	211	CLA	C1D-ND	-2.74	1.34	1.37
29	B	831	BCR	C12-C13	-2.74	1.40	1.45
25	o	610	CLA	C1D-ND	-2.74	1.34	1.37
25	B	845	CLA	C1D-ND	-2.74	1.34	1.37
25	A	828	CLA	C1D-ND	-2.74	1.34	1.37
25	g	204	CLA	C1D-ND	-2.74	1.34	1.37
29	B	832	BCR	C14-C13	2.74	1.39	1.35
25	f	608	CLA	C1D-ND	-2.73	1.34	1.37
25	c	311	CLA	C1D-ND	-2.73	1.34	1.37
25	c	303	CLA	C1D-ND	-2.73	1.34	1.37
25	c	308	CLA	C1D-ND	-2.73	1.34	1.37
29	A	837	BCR	C17-C18	2.73	1.39	1.35
25	A	813	CLA	C1D-ND	-2.73	1.34	1.37
25	h	203	CLA	C1D-ND	-2.73	1.34	1.37
25	d	313	CLA	C1D-ND	-2.72	1.34	1.37
25	h	215	CLA	C1D-ND	-2.72	1.34	1.37
25	g	212	CLA	C1D-ND	-2.72	1.34	1.37
25	k	211	CLA	C1D-ND	-2.72	1.34	1.37
25	B	815	CLA	C1D-ND	-2.72	1.34	1.37
25	h	210	CLA	C1D-ND	-2.72	1.34	1.37
25	l	612	CLA	C1D-ND	-2.72	1.34	1.37
25	c	313	CLA	C1D-ND	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	801	CLA	C1D-ND	-2.71	1.34	1.37
25	c	305	CLA	C1D-ND	-2.71	1.34	1.37
25	F	201	CLA	C1D-ND	-2.71	1.34	1.37
25	c	302	CLA	C1D-ND	-2.71	1.34	1.37
25	j	207	CLA	C1D-ND	-2.71	1.34	1.37
25	f	602	CLA	C1D-ND	-2.71	1.34	1.37
25	A	851	CLA	C1D-ND	-2.71	1.34	1.37
25	e	212	CLA	C1D-ND	-2.71	1.34	1.37
25	i	205	CLA	C1D-ND	-2.71	1.34	1.37
28	B	835	PQN	C10-C5	-2.71	1.36	1.40
25	a	210	CLA	C1D-ND	-2.71	1.34	1.37
25	e	211	CLA	C1D-ND	-2.70	1.34	1.37
25	k	206	CLA	C1D-ND	-2.70	1.34	1.37
25	o	606	CLA	C1D-ND	-2.70	1.34	1.37
25	j	212	CLA	C1D-ND	-2.69	1.34	1.37
25	m	208	CLA	C1D-ND	-2.69	1.34	1.37
25	A	853	CLA	C1D-ND	-2.68	1.34	1.37
25	B	823	CLA	C1D-ND	-2.68	1.34	1.37
25	i	212	CLA	C1D-ND	-2.68	1.34	1.37
25	d	301	CLA	C1D-ND	-2.68	1.34	1.37
30	i	216	DD6	O1-C20	-2.68	1.42	1.46
25	l	610	CLA	C1D-ND	-2.68	1.34	1.37
25	J	103	CLA	C1D-ND	-2.68	1.34	1.37
25	h	213	CLA	C1D-ND	-2.68	1.34	1.37
25	i	213	CLA	C1D-ND	-2.68	1.34	1.37
25	g	213	CLA	C1D-ND	-2.68	1.34	1.37
25	A	831	CLA	C1D-ND	-2.68	1.34	1.37
25	l	604	CLA	C1D-ND	-2.68	1.34	1.37
30	A	854	DD6	C35-C36	-2.67	1.46	1.51
30	o	611	DD6	O1-C20	-2.67	1.42	1.46
25	m	211	CLA	C1D-ND	-2.67	1.34	1.37
25	n	209	CLA	C3B-C4B	2.67	1.49	1.42
25	m	205	CLA	C1D-ND	-2.67	1.34	1.37
25	n	206	CLA	C1D-ND	-2.67	1.34	1.37
25	e	208	CLA	C1D-ND	-2.67	1.34	1.37
25	g	214	CLA	C1D-ND	-2.67	1.34	1.37
30	J	104	DD6	C35-C36	-2.67	1.46	1.51
25	m	202	CLA	MG-NB	2.67	2.11	2.05
25	e	206	CLA	C1D-ND	-2.67	1.34	1.37
25	f	607	CLA	C3B-C4B	2.66	1.49	1.42
25	B	847	CLA	C1D-ND	-2.66	1.34	1.37
25	j	214	CLA	C1D-ND	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	214	DD6	O1-C20	-2.66	1.42	1.46
25	a	207	CLA	C1D-ND	-2.66	1.34	1.37
30	A	854	DD6	O1-C20	-2.66	1.42	1.46
25	o	604	CLA	C1D-ND	-2.66	1.34	1.37
30	c	318	DD6	C35-C36	-2.65	1.46	1.51
25	g	210	CLA	C1D-ND	-2.65	1.34	1.37
25	B	816	CLA	C1D-ND	-2.65	1.34	1.37
25	f	604	CLA	C1D-ND	-2.65	1.34	1.37
25	c	314	CLA	C1D-ND	-2.65	1.34	1.37
30	J	105	DD6	C8-C6	-2.65	1.40	1.45
25	A	852	CLA	C1D-ND	-2.65	1.34	1.37
25	k	213	CLA	C1D-ND	-2.65	1.34	1.37
25	A	818	CLA	C1D-ND	-2.65	1.34	1.37
25	o	608	CLA	C4D-C3D	-2.64	1.40	1.45
29	J	101	BCR	C12-C13	-2.64	1.40	1.45
25	A	848	CLA	C1D-ND	-2.64	1.34	1.37
25	A	820	CLA	C1D-ND	-2.64	1.34	1.37
25	g	208	CLA	C1D-ND	-2.64	1.34	1.37
30	n	214	DD6	C25-C26	-2.64	1.35	1.43
30	i	215	DD6	C35-C36	-2.64	1.47	1.51
25	c	306	CLA	C1D-ND	-2.63	1.34	1.37
25	o	603	CLA	C1D-ND	-2.63	1.34	1.37
25	B	811	CLA	C1D-ND	-2.63	1.34	1.37
25	h	207	CLA	C1D-ND	-2.63	1.34	1.37
25	k	202	CLA	C1D-ND	-2.63	1.34	1.37
28	F	205	PQN	C10-C5	-2.62	1.36	1.40
30	a	214	DD6	C35-C36	-2.62	1.47	1.51
25	A	815	CLA	C1D-ND	-2.62	1.34	1.37
25	b	207	CLA	C1D-ND	-2.62	1.34	1.37
25	e	207	CLA	C1D-ND	-2.62	1.34	1.37
25	m	203	CLA	C3B-C4B	2.62	1.48	1.42
25	e	214	CLA	C1D-ND	-2.62	1.34	1.37
25	c	309	CLA	C1D-ND	-2.62	1.34	1.37
25	g	215	CLA	C1D-ND	-2.62	1.34	1.37
30	i	214	DD6	C35-C36	-2.62	1.47	1.51
25	p	607	CLA	C1D-ND	-2.62	1.34	1.37
25	e	210	CLA	C1D-ND	-2.61	1.34	1.37
30	c	316	DD6	C35-C36	-2.61	1.47	1.51
25	a	203	CLA	C1D-ND	-2.60	1.34	1.37
25	h	214	CLA	C1D-ND	-2.60	1.34	1.37
25	c	312	CLA	C1D-ND	-2.60	1.34	1.37
25	f	607	CLA	C1D-ND	-2.60	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	606	CLA	C1D-ND	-2.60	1.34	1.37
25	p	604	CLA	C3B-C4B	2.60	1.48	1.42
25	p	604	CLA	C1D-ND	-2.60	1.34	1.37
25	m	209	CLA	C1D-ND	-2.60	1.34	1.37
25	A	823	CLA	C1D-ND	-2.60	1.34	1.37
25	f	601	CLA	C1D-ND	-2.59	1.34	1.37
25	o	603	CLA	MG-NB	2.59	2.10	2.05
25	b	211	CLA	C1D-ND	-2.59	1.34	1.37
25	i	210	CLA	C1D-ND	-2.59	1.34	1.37
25	n	201	CLA	C1D-ND	-2.59	1.34	1.37
30	p	610	DD6	O1-C20	-2.59	1.42	1.46
25	b	213	CLA	C1D-ND	-2.59	1.34	1.37
25	p	609	CLA	C3B-C4B	2.59	1.48	1.42
25	A	808	CLA	C1D-ND	-2.58	1.34	1.37
25	n	203	CLA	C1D-ND	-2.58	1.34	1.37
25	f	609	CLA	MG-NB	2.58	2.10	2.05
25	F	202	CLA	C1D-ND	-2.58	1.34	1.37
25	f	604	CLA	C3B-C4B	2.58	1.48	1.42
25	n	201	CLA	CHC-C1C	2.58	1.43	1.38
25	B	805	CLA	C1D-ND	-2.58	1.34	1.37
25	l	608	CLA	C1D-ND	-2.58	1.34	1.37
25	g	207	CLA	C3B-C4B	2.57	1.48	1.42
25	n	207	CLA	C3B-C4B	2.57	1.48	1.42
25	d	303	CLA	C1D-ND	-2.57	1.34	1.37
25	l	601	CLA	C1D-ND	-2.57	1.34	1.37
25	n	209	CLA	C1D-ND	-2.57	1.34	1.37
29	A	838	BCR	C1-C6	-2.57	1.50	1.53
25	d	314	CLA	C1D-ND	-2.57	1.34	1.37
25	B	817	CLA	C3B-C4B	2.57	1.48	1.42
30	n	213	DD6	C26-C27	2.57	1.42	1.37
25	m	202	CLA	MG-NC	2.57	2.12	2.06
25	n	207	CLA	CHC-C1C	2.57	1.43	1.38
25	n	202	CLA	C3B-C4B	2.57	1.48	1.42
25	l	611	CLA	C1D-ND	-2.57	1.34	1.37
25	a	213	CLA	C1D-ND	-2.56	1.34	1.37
25	o	610	CLA	CHC-C1C	2.56	1.43	1.38
30	e	220	DD6	C24-C1	-2.56	1.40	1.45
28	A	834	PQN	C2M-C2	-2.56	1.45	1.50
29	A	837	BCR	C21-C22	2.56	1.39	1.35
25	o	603	CLA	C3B-C4B	2.56	1.48	1.42
25	o	607	CLA	C3B-C4B	2.56	1.48	1.42
25	f	605	CLA	C3B-C4B	2.56	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	609	CLA	C1D-ND	-2.56	1.34	1.37
25	p	608	CLA	CHC-C1C	2.56	1.43	1.38
25	f	611	CLA	C1D-ND	-2.56	1.34	1.37
25	i	203	CLA	C3B-C4B	2.55	1.48	1.42
25	B	845	CLA	CHC-C1C	2.55	1.43	1.38
25	B	846	CLA	C1D-ND	-2.55	1.34	1.37
25	n	211	CLA	C3B-C4B	2.55	1.48	1.42
30	b	215	DD6	C35-C36	-2.55	1.47	1.51
25	o	604	CLA	C3B-C4B	2.55	1.48	1.42
25	B	809	CLA	C1D-ND	-2.55	1.34	1.37
25	g	207	CLA	C1D-ND	-2.55	1.34	1.37
25	a	205	CLA	C1D-ND	-2.55	1.34	1.37
30	h	216	DD6	C35-C36	-2.54	1.47	1.51
25	A	821	CLA	C1D-ND	-2.54	1.34	1.37
25	o	609	CLA	C1D-ND	-2.54	1.34	1.37
30	b	214	DD6	C35-C36	-2.54	1.47	1.51
25	h	211	CLA	C1D-ND	-2.54	1.34	1.37
25	g	204	CLA	C3B-C4B	2.54	1.48	1.42
25	c	310	CLA	C3B-C4B	2.54	1.48	1.42
25	p	604	CLA	CHC-C1C	2.53	1.43	1.38
25	e	206	CLA	C3B-C4B	2.53	1.48	1.42
25	n	204	CLA	C1D-ND	-2.53	1.34	1.37
25	p	602	CLA	CHB-C1B	-2.53	1.33	1.39
30	d	317	DD6	C35-C36	-2.53	1.47	1.51
30	J	105	DD6	C13-C11	-2.53	1.40	1.45
30	d	319	DD6	C35-C36	-2.53	1.47	1.51
25	f	610	CLA	C1D-ND	-2.53	1.34	1.37
25	p	606	CLA	C3B-C4B	2.53	1.48	1.42
25	p	603	CLA	C3B-C4B	2.53	1.48	1.42
25	p	605	CLA	C1D-ND	-2.53	1.34	1.37
25	n	201	CLA	C3B-C4B	2.52	1.48	1.42
25	b	212	CLA	C3B-C4B	2.52	1.48	1.42
25	g	215	CLA	C3B-C4B	2.52	1.48	1.42
25	b	203	CLA	C1D-ND	-2.52	1.34	1.37
25	k	210	CLA	C1D-ND	-2.52	1.34	1.37
25	B	848	CLA	C1D-ND	-2.52	1.34	1.37
25	o	601	CLA	C1D-ND	-2.52	1.34	1.37
25	A	818	CLA	CHB-C1B	-2.52	1.33	1.39
25	l	602	CLA	C3B-C4B	2.52	1.48	1.42
25	g	205	CLA	MG-NC	2.52	2.12	2.06
25	p	601	CLA	C3B-C4B	2.52	1.48	1.42
25	e	211	CLA	C3B-C4B	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	j	211	CLA	C1D-ND	-2.51	1.34	1.37
25	f	606	CLA	C3B-C4B	2.51	1.48	1.42
25	l	609	CLA	C1D-ND	-2.51	1.34	1.37
25	n	210	CLA	C3B-C4B	2.51	1.48	1.42
25	A	804	CLA	C3B-C4B	2.51	1.48	1.42
25	p	608	CLA	C3B-C4B	2.51	1.48	1.42
30	g	217	DD6	C35-C36	-2.51	1.47	1.51
28	B	827	PQN	C11-C12	-2.51	1.47	1.50
25	o	610	CLA	C3B-C4B	2.51	1.48	1.42
25	p	603	CLA	MG-NC	2.51	2.12	2.06
25	g	208	CLA	C3B-C4B	2.51	1.48	1.42
25	a	211	CLA	C1D-ND	-2.50	1.34	1.37
25	m	209	CLA	C3B-C4B	2.50	1.48	1.42
25	n	203	CLA	C3B-C4B	2.50	1.48	1.42
25	k	202	CLA	C3B-C4B	2.50	1.48	1.42
30	e	219	DD6	C35-C36	-2.50	1.47	1.51
25	p	607	CLA	MG-NB	2.50	2.10	2.05
30	J	105	DD6	C26-C27	2.50	1.42	1.37
25	p	608	CLA	C1D-ND	-2.50	1.34	1.37
25	l	612	CLA	C3B-C4B	2.50	1.48	1.42
25	o	601	CLA	C3B-C4B	2.49	1.48	1.42
25	B	838	CLA	C3B-C4B	2.49	1.48	1.42
25	A	844	CLA	C3B-C4B	2.49	1.48	1.42
25	f	612	CLA	C3B-C4B	2.49	1.48	1.42
30	d	318	DD6	C35-C36	-2.49	1.47	1.51
25	B	844	CLA	C3B-C4B	2.49	1.48	1.42
25	d	301	CLA	C3B-C4B	2.49	1.48	1.42
25	b	203	CLA	C3B-C4B	2.49	1.48	1.42
25	A	802	CLA	C1B-NB	-2.49	1.34	1.37
25	n	206	CLA	C3B-C4B	2.49	1.48	1.42
25	i	203	CLA	CHC-C1C	2.48	1.43	1.38
25	f	608	CLA	C3B-C4B	2.48	1.48	1.42
25	g	205	CLA	MG-NB	2.48	2.10	2.05
25	f	610	CLA	C3B-C4B	2.48	1.48	1.42
25	A	830	CLA	C3B-C4B	2.48	1.48	1.42
30	l	614	DD6	C19-C20	-2.48	1.48	1.52
25	h	207	CLA	C3B-C4B	2.48	1.48	1.42
25	e	204	CLA	C1D-ND	-2.48	1.34	1.37
25	a	213	CLA	C3B-C4B	2.48	1.48	1.42
25	A	811	CLA	C3B-C4B	2.48	1.48	1.42
25	o	608	CLA	C3B-C4B	2.48	1.48	1.42
25	A	802	CLA	C3B-C4B	2.47	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	205	CLA	C1D-ND	-2.47	1.34	1.37
30	n	214	DD6	C13-C11	-2.47	1.40	1.45
25	f	603	CLA	C3B-C4B	2.47	1.48	1.42
25	f	609	CLA	MG-NC	2.47	2.12	2.06
25	e	214	CLA	C3B-C4B	2.47	1.48	1.42
25	k	209	CLA	C3B-C4B	2.47	1.48	1.42
30	a	215	DD6	C19-C20	-2.47	1.48	1.52
25	A	843	CLA	C3B-C4B	2.47	1.48	1.42
30	h	217	DD6	C35-C36	-2.47	1.47	1.51
25	g	211	CLA	C1D-ND	-2.47	1.34	1.37
25	b	211	CLA	C3B-C4B	2.47	1.48	1.42
25	B	845	CLA	C3B-C4B	2.47	1.48	1.42
25	j	207	CLA	C3B-C4B	2.47	1.48	1.42
25	f	603	CLA	MG-NB	2.47	2.10	2.05
25	B	809	CLA	CHC-C1C	2.47	1.43	1.38
25	n	202	CLA	C1D-ND	-2.47	1.34	1.37
25	n	211	CLA	C1D-ND	-2.47	1.34	1.37
25	m	210	CLA	C3B-C4B	2.47	1.48	1.42
25	f	609	CLA	C3B-C4B	2.47	1.48	1.42
25	g	211	CLA	C3B-C4B	2.47	1.48	1.42
25	a	206	CLA	C3B-C4B	2.47	1.48	1.42
25	b	212	CLA	C1D-ND	-2.47	1.34	1.37
25	g	205	CLA	CHB-C1B	-2.46	1.33	1.39
25	A	843	CLA	C1B-NB	-2.46	1.34	1.37
25	h	209	CLA	C3B-C4B	2.46	1.48	1.42
25	h	205	CLA	C3B-C4B	2.46	1.48	1.42
25	l	603	CLA	C3B-C4B	2.46	1.48	1.42
25	n	209	CLA	CHC-C1C	2.46	1.43	1.38
25	B	841	CLA	C3B-C4B	2.46	1.48	1.42
25	n	205	CLA	C1D-ND	-2.46	1.34	1.37
25	g	204	CLA	CHC-C1C	2.46	1.43	1.38
25	B	823	CLA	CHC-C1C	2.46	1.43	1.38
25	h	211	CLA	C3B-C4B	2.46	1.48	1.42
30	j	217	DD6	C35-C36	-2.46	1.47	1.51
25	e	201	CLA	C3B-C4B	2.46	1.48	1.42
25	l	607	CLA	C3B-C4B	2.46	1.48	1.42
25	f	602	CLA	C3B-C4B	2.46	1.48	1.42
25	A	818	CLA	C3B-C4B	2.46	1.48	1.42
25	g	210	CLA	C3B-C4B	2.46	1.48	1.42
25	j	211	CLA	CHB-C1B	-2.46	1.33	1.39
30	a	215	DD6	C35-C36	-2.46	1.47	1.51
25	c	306	CLA	C3B-C4B	2.46	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	601	CLA	MG-NB	2.45	2.10	2.05
25	b	213	CLA	C3B-C4B	2.45	1.48	1.42
25	c	315	CLA	C1D-ND	-2.45	1.34	1.37
25	l	601	CLA	C3B-C4B	2.45	1.48	1.42
25	l	608	CLA	C3B-C4B	2.45	1.48	1.42
25	e	215	CLA	C1D-ND	-2.45	1.34	1.37
30	c	317	DD6	C19-C20	-2.45	1.48	1.52
25	b	205	CLA	C3B-C4B	2.45	1.48	1.42
25	j	205	CLA	C3B-C4B	2.45	1.48	1.42
25	c	304	CLA	C1D-ND	-2.45	1.34	1.37
25	l	604	CLA	C3B-C4B	2.45	1.48	1.42
25	m	208	CLA	C3B-C4B	2.45	1.48	1.42
25	f	605	CLA	C1D-ND	-2.45	1.34	1.37
25	o	603	CLA	MG-NC	2.45	2.12	2.06
30	k	216	DD6	C35-C36	-2.45	1.47	1.51
25	d	314	CLA	C3B-C4B	2.45	1.48	1.42
25	g	214	CLA	C3B-C4B	2.45	1.48	1.42
25	f	606	CLA	C1D-ND	-2.45	1.34	1.37
25	k	206	CLA	C3B-C4B	2.45	1.48	1.42
25	o	609	CLA	C3B-C4B	2.45	1.48	1.42
25	d	313	CLA	C3B-C4B	2.45	1.48	1.42
25	i	210	CLA	C3B-C4B	2.45	1.48	1.42
25	e	217	CLA	CHC-C1C	2.45	1.43	1.38
25	f	607	CLA	CHC-C1C	2.45	1.43	1.38
25	b	207	CLA	C3B-C4B	2.45	1.48	1.42
25	f	609	CLA	C1D-ND	-2.45	1.34	1.37
25	B	823	CLA	C3B-C4B	2.44	1.48	1.42
25	n	207	CLA	C1D-ND	-2.44	1.34	1.37
25	k	210	CLA	C3B-C4B	2.44	1.48	1.42
25	A	808	CLA	C3B-C4B	2.44	1.48	1.42
25	c	312	CLA	C3B-C4B	2.44	1.48	1.42
25	c	315	CLA	C3B-C4B	2.44	1.48	1.42
25	l	609	CLA	C3B-C4B	2.44	1.48	1.42
25	f	612	CLA	C1D-ND	-2.44	1.34	1.37
25	p	601	CLA	CHC-C1C	2.44	1.43	1.38
25	B	810	CLA	C3B-C4B	2.44	1.48	1.42
25	e	204	CLA	C3B-C4B	2.44	1.48	1.42
25	e	215	CLA	C3B-C4B	2.44	1.48	1.42
25	h	206	CLA	C3B-C4B	2.44	1.48	1.42
25	i	208	CLA	C3B-C4B	2.44	1.48	1.42
25	b	210	CLA	C3B-C4B	2.44	1.48	1.42
25	m	203	CLA	CHC-C1C	2.44	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	203	CLA	C3B-C4B	2.44	1.48	1.42
25	A	840	CLA	C3B-C4B	2.44	1.48	1.42
25	f	602	CLA	CHC-C1C	2.44	1.43	1.38
25	k	204	CLA	C3B-C4B	2.44	1.48	1.42
25	f	611	CLA	C3B-C4B	2.44	1.48	1.42
25	f	604	CLA	CHC-C1C	2.44	1.43	1.38
25	l	611	CLA	C3B-C4B	2.44	1.48	1.42
25	g	206	CLA	C3B-C4B	2.44	1.48	1.42
25	b	205	CLA	C1D-ND	-2.44	1.34	1.37
25	d	305	CLA	C1D-ND	-2.44	1.34	1.37
25	c	309	CLA	C3B-C4B	2.44	1.48	1.42
25	p	605	CLA	C3B-C4B	2.43	1.48	1.42
25	f	601	CLA	C3B-C4B	2.43	1.48	1.42
25	f	603	CLA	MG-NC	2.43	2.12	2.06
25	n	204	CLA	C3B-C4B	2.43	1.48	1.42
25	B	840	CLA	C3B-C4B	2.43	1.48	1.42
25	B	812	CLA	CHC-C1C	2.43	1.43	1.38
25	m	211	CLA	C3B-C4B	2.43	1.48	1.42
25	e	217	CLA	C1D-ND	-2.43	1.34	1.37
25	n	211	CLA	CHC-C1C	2.43	1.43	1.38
30	d	319	DD6	O1-C20	-2.43	1.42	1.46
30	p	610	DD6	C35-C36	-2.43	1.47	1.51
25	n	208	CLA	C3B-C4B	2.43	1.48	1.42
25	p	607	CLA	C3B-C4B	2.43	1.48	1.42
25	B	838	CLA	CHC-C1C	2.43	1.43	1.38
25	m	205	CLA	C3B-C4B	2.43	1.48	1.42
25	a	210	CLA	C3B-C4B	2.43	1.48	1.42
35	d	307	CHL	MG-NB	2.43	2.10	2.05
25	B	816	CLA	C3B-C4B	2.43	1.48	1.42
25	a	204	CLA	C3B-C4B	2.43	1.48	1.42
25	B	840	CLA	CHC-C1C	2.43	1.43	1.38
25	m	204	CLA	C3B-C4B	2.43	1.48	1.42
30	A	855	DD6	C35-C36	-2.43	1.47	1.51
25	k	204	CLA	C1D-ND	-2.42	1.34	1.37
25	o	602	CLA	C3B-C4B	2.42	1.48	1.42
25	A	853	CLA	C3B-C4B	2.42	1.48	1.42
25	B	812	CLA	C3B-C4B	2.42	1.48	1.42
30	k	215	DD6	C35-C36	-2.42	1.47	1.51
25	i	211	CLA	C3B-C4B	2.42	1.48	1.42
25	b	204	CLA	C3B-C4B	2.42	1.48	1.42
25	A	809	CLA	C1B-NB	-2.42	1.34	1.37
25	A	804	CLA	CHC-C1C	2.42	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	602	CLA	MG-NB	2.42	2.10	2.05
25	h	203	CLA	C3B-C4B	2.42	1.48	1.42
25	n	210	CLA	C1D-ND	-2.42	1.34	1.37
25	h	215	CLA	C3B-C4B	2.42	1.48	1.42
25	B	810	CLA	CHC-C1C	2.42	1.43	1.38
30	e	220	DD6	C13-C11	-2.42	1.40	1.45
25	d	311	CLA	C3B-C4B	2.42	1.48	1.42
25	j	205	CLA	CHB-C1B	-2.42	1.34	1.39
25	k	210	CLA	CHB-C1B	-2.42	1.34	1.39
25	o	605	CLA	C3B-C4B	2.42	1.48	1.42
25	f	605	CLA	CHC-C1C	2.42	1.43	1.38
25	k	208	CLA	C3B-C4B	2.41	1.48	1.42
30	e	218	DD6	C25-C26	-2.41	1.36	1.43
25	A	825	CLA	CHB-C1B	-2.41	1.34	1.39
25	m	202	CLA	C3B-C4B	2.41	1.48	1.42
25	a	205	CLA	C3B-C4B	2.41	1.48	1.42
25	a	211	CLA	C3B-C4B	2.41	1.48	1.42
25	b	206	CLA	C3B-C4B	2.41	1.48	1.42
25	B	818	CLA	C3B-C4B	2.41	1.48	1.42
25	f	603	CLA	C1D-ND	-2.41	1.34	1.37
30	e	218	DD6	C26-C27	2.41	1.42	1.37
25	A	802	CLA	CHC-C1C	2.41	1.43	1.38
25	c	302	CLA	C3B-C4B	2.41	1.48	1.42
25	m	204	CLA	C1D-ND	-2.41	1.34	1.37
25	n	205	CLA	MG-NB	2.41	2.10	2.05
25	d	301	CLA	CHC-C1C	2.41	1.43	1.38
35	c	307	CHL	MG-NB	2.41	2.10	2.05
25	c	311	CLA	C3B-C4B	2.41	1.48	1.42
25	B	814	CLA	CHB-C1B	-2.41	1.34	1.39
25	B	838	CLA	CHB-C1B	-2.41	1.34	1.39
25	o	601	CLA	CHB-C1B	-2.41	1.34	1.39
25	A	830	CLA	CHC-C1C	2.41	1.43	1.38
25	n	205	CLA	MG-NC	2.41	2.12	2.06
25	A	831	CLA	C3B-C4B	2.40	1.48	1.42
25	e	208	CLA	C3B-C4B	2.40	1.48	1.42
25	i	212	CLA	C3B-C4B	2.40	1.48	1.42
25	A	852	CLA	CHC-C1C	2.40	1.43	1.38
25	B	837	CLA	C3B-C4B	2.40	1.48	1.42
25	f	609	CLA	CHB-C1B	-2.40	1.34	1.39
25	g	212	CLA	C3B-C4B	2.40	1.48	1.42
30	n	214	DD6	C24-C1	-2.40	1.40	1.45
35	d	308	CHL	MG-NB	2.40	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	309	CHL	MG-NB	2.40	2.10	2.05
25	A	852	CLA	CHB-C1B	-2.40	1.34	1.39
28	F	205	PQN	C2M-C2	-2.40	1.45	1.50
25	n	202	CLA	CHC-C1C	2.40	1.43	1.38
25	d	303	CLA	C3B-C4B	2.40	1.48	1.42
25	l	602	CLA	CHC-C1C	2.40	1.43	1.38
25	A	825	CLA	C3B-C4B	2.40	1.48	1.42
25	h	212	CLA	C3B-C4B	2.40	1.48	1.42
25	g	209	CLA	C3B-C4B	2.40	1.48	1.42
25	p	601	CLA	C1D-ND	-2.40	1.34	1.37
25	e	211	CLA	CHC-C1C	2.40	1.43	1.38
25	B	847	CLA	C3B-C4B	2.40	1.48	1.42
25	a	212	CLA	C3B-C4B	2.40	1.48	1.42
25	A	852	CLA	C1B-NB	-2.40	1.34	1.37
25	B	824	CLA	C3B-C4B	2.40	1.48	1.42
25	j	203	CLA	C3B-C4B	2.40	1.48	1.42
25	f	606	CLA	MG-NB	2.40	2.10	2.05
25	A	840	CLA	CHC-C1C	2.40	1.43	1.38
25	o	607	CLA	CHC-C1C	2.40	1.43	1.38
25	l	603	CLA	C1D-ND	-2.40	1.34	1.37
25	e	210	CLA	C3B-C4B	2.40	1.48	1.42
25	l	612	CLA	CHC-C1C	2.40	1.43	1.38
25	i	206	CLA	C3B-C4B	2.40	1.48	1.42
25	k	212	CLA	C3B-C4B	2.40	1.48	1.42
25	A	844	CLA	CHC-C1C	2.39	1.43	1.38
30	l	614	DD6	C35-C36	-2.39	1.47	1.51
25	n	210	CLA	CHC-C1C	2.39	1.43	1.38
25	e	204	CLA	MG-NB	2.39	2.10	2.05
25	o	604	CLA	CHC-C1C	2.39	1.43	1.38
25	i	204	CLA	CHB-C1B	-2.39	1.34	1.39
25	A	814	CLA	CHB-C1B	-2.39	1.34	1.39
25	e	215	CLA	CHB-C1B	-2.39	1.34	1.39
25	B	848	CLA	C3B-C4B	2.39	1.48	1.42
30	J	105	DD6	C25-C26	-2.39	1.36	1.43
25	B	844	CLA	CHC-C1C	2.39	1.43	1.38
30	f	614	DD6	O1-C20	-2.39	1.42	1.46
25	B	848	CLA	CHC-C1C	2.39	1.43	1.38
25	e	217	CLA	C3B-C4B	2.39	1.48	1.42
25	f	612	CLA	MG-NB	2.39	2.10	2.05
25	l	603	CLA	CHB-C1B	-2.39	1.34	1.39
25	h	209	CLA	CHC-C1C	2.39	1.43	1.38
25	l	610	CLA	C3B-C4B	2.39	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	826	CLA	C1B-NB	-2.39	1.34	1.37
25	B	809	CLA	C3B-C4B	2.39	1.48	1.42
25	h	213	CLA	C3B-C4B	2.39	1.48	1.42
25	n	205	CLA	C3B-C4B	2.39	1.48	1.42
25	p	602	CLA	C3B-C4B	2.39	1.48	1.42
25	h	205	CLA	CHC-C1C	2.39	1.43	1.38
25	l	607	CLA	CHC-C1C	2.39	1.43	1.38
25	g	207	CLA	CHC-C1C	2.39	1.43	1.38
25	h	214	CLA	C3B-C4B	2.39	1.48	1.42
25	k	203	CLA	C3B-C4B	2.39	1.48	1.42
25	d	316	CLA	C1D-ND	-2.39	1.34	1.37
25	m	207	CLA	CHB-C1B	-2.39	1.34	1.39
25	a	209	CLA	C3B-C4B	2.38	1.48	1.42
25	A	815	CLA	C1B-NB	-2.38	1.34	1.37
25	o	608	CLA	CHC-C1C	2.38	1.43	1.38
25	J	103	CLA	CHB-C1B	-2.38	1.34	1.39
25	B	842	CLA	C3B-C4B	2.38	1.48	1.42
25	k	213	CLA	C3B-C4B	2.38	1.48	1.42
25	c	308	CLA	C3B-C4B	2.38	1.48	1.42
25	m	206	CLA	C3B-C4B	2.38	1.48	1.42
25	f	606	CLA	CHC-C1C	2.38	1.43	1.38
25	c	303	CLA	C3B-C4B	2.38	1.48	1.42
25	g	213	CLA	C3B-C4B	2.38	1.48	1.42
25	b	203	CLA	MG-NB	2.38	2.10	2.05
25	B	819	CLA	C3B-C4B	2.38	1.48	1.42
25	j	213	CLA	C3B-C4B	2.38	1.48	1.42
25	A	806	CLA	C3B-C4B	2.38	1.48	1.42
25	j	211	CLA	C3B-C4B	2.38	1.48	1.42
25	k	205	CLA	C3B-C4B	2.38	1.48	1.42
25	l	608	CLA	CHC-C1C	2.38	1.43	1.38
25	b	206	CLA	CHC-C1C	2.38	1.43	1.38
25	h	207	CLA	CHC-C1C	2.38	1.43	1.38
25	p	602	CLA	CHC-C1C	2.38	1.43	1.38
25	b	208	CLA	C3B-C4B	2.38	1.48	1.42
35	d	308	CHL	CBA-CGA	2.38	1.56	1.50
25	A	847	CLA	CHC-C1C	2.38	1.43	1.38
25	B	805	CLA	CHC-C1C	2.38	1.43	1.38
25	m	202	CLA	CHB-C1B	-2.37	1.34	1.39
25	m	204	CLA	CHB-C1B	-2.37	1.34	1.39
25	B	839	CLA	C3B-C4B	2.37	1.48	1.42
25	l	605	CLA	C3B-C4B	2.37	1.48	1.42
25	B	844	CLA	CHB-C1B	-2.37	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	l	604	CLA	CHC-C1C	2.37	1.43	1.38
25	F	201	CLA	C3B-C4B	2.37	1.48	1.42
25	A	831	CLA	CHB-C1B	-2.37	1.34	1.39
25	a	208	CLA	CHB-C1B	-2.37	1.34	1.39
25	j	206	CLA	C3B-C4B	2.37	1.48	1.42
25	B	805	CLA	CHB-C1B	-2.37	1.34	1.39
25	F	202	CLA	MG-NB	2.37	2.10	2.05
25	A	827	CLA	C3B-C4B	2.37	1.48	1.42
25	A	842	CLA	C3B-C4B	2.37	1.48	1.42
25	A	848	CLA	C3B-C4B	2.37	1.48	1.42
25	A	842	CLA	CHB-C1B	-2.37	1.34	1.39
25	A	842	CLA	CHC-C1C	2.37	1.43	1.38
25	A	852	CLA	C3B-C4B	2.37	1.48	1.42
30	f	613	DD6	O1-C20	-2.37	1.42	1.46
25	A	850	CLA	C3B-C4B	2.37	1.48	1.42
25	A	843	CLA	CHC-C1C	2.37	1.43	1.38
25	b	212	CLA	CHB-C1B	-2.37	1.34	1.39
25	B	821	CLA	C3B-C4B	2.37	1.48	1.42
25	j	215	CLA	C3B-C4B	2.37	1.48	1.42
25	l	611	CLA	MG-NB	2.36	2.10	2.05
25	B	803	CLA	C1B-NB	-2.36	1.34	1.37
30	n	213	DD6	C25-C26	-2.36	1.36	1.43
25	j	204	CLA	CHC-C1C	2.36	1.43	1.38
25	i	202	CLA	C3B-C4B	2.36	1.48	1.42
25	o	608	CLA	C1D-ND	-2.36	1.34	1.37
25	o	603	CLA	CHB-C1B	-2.36	1.34	1.39
25	A	847	CLA	C3B-C4B	2.36	1.48	1.42
25	F	202	CLA	C3B-C4B	2.36	1.48	1.42
25	f	611	CLA	CHC-C1C	2.36	1.43	1.38
25	g	208	CLA	CHC-C1C	2.36	1.43	1.38
25	A	811	CLA	CHB-C1B	-2.36	1.34	1.39
25	a	207	CLA	C3B-C4B	2.36	1.48	1.42
25	B	817	CLA	CHB-C1B	-2.36	1.34	1.39
25	g	203	CLA	CHB-C1B	-2.36	1.34	1.39
35	e	209	CHL	CBA-CGA	2.36	1.56	1.50
25	i	208	CLA	CHC-C1C	2.36	1.43	1.38
25	A	821	CLA	C3B-C4B	2.36	1.48	1.42
25	d	303	CLA	CHC-C1C	2.36	1.43	1.38
25	k	203	CLA	CHC-C1C	2.36	1.43	1.38
25	A	822	CLA	C3B-C4B	2.36	1.48	1.42
30	n	214	DD6	C8-C6	-2.36	1.40	1.45
25	c	314	CLA	C3B-C4B	2.36	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	j	208	CLA	CHB-C1B	-2.36	1.34	1.39
25	m	210	CLA	C1D-ND	-2.36	1.34	1.37
25	A	826	CLA	CHB-C1B	-2.36	1.34	1.39
25	A	841	CLA	C3B-C4B	2.36	1.48	1.42
25	B	813	CLA	C3B-C4B	2.35	1.48	1.42
25	a	212	CLA	CHC-C1C	2.35	1.43	1.38
25	B	847	CLA	CHB-C1B	-2.35	1.34	1.39
25	e	205	CLA	C3B-C4B	2.35	1.48	1.42
25	g	211	CLA	CHB-C1B	-2.35	1.34	1.39
25	A	808	CLA	CHC-C1C	2.35	1.43	1.38
25	j	212	CLA	CHC-C1C	2.35	1.43	1.38
25	B	842	CLA	CHC-C1C	2.35	1.43	1.38
25	F	201	CLA	CHB-C1B	-2.35	1.34	1.39
25	b	209	CLA	C3B-C4B	2.35	1.48	1.42
25	k	206	CLA	CHB-C1B	-2.35	1.34	1.39
25	e	201	CLA	CHC-C1C	2.35	1.43	1.38
25	a	209	CLA	CHC-C1C	2.35	1.43	1.38
25	e	206	CLA	CHB-C1B	-2.35	1.34	1.39
25	m	205	CLA	CHC-C1C	2.35	1.43	1.38
25	A	832	CLA	C3B-C4B	2.35	1.48	1.42
25	B	846	CLA	C3B-C4B	2.35	1.48	1.42
25	d	314	CLA	CHC-C1C	2.35	1.43	1.38
25	e	207	CLA	C3B-C4B	2.35	1.48	1.42
25	m	210	CLA	CHB-C1B	-2.35	1.34	1.39
25	B	803	CLA	C3B-C4B	2.35	1.48	1.42
25	c	304	CLA	C3B-C4B	2.35	1.48	1.42
25	A	850	CLA	CHC-C1C	2.35	1.43	1.38
25	p	603	CLA	CHC-C1C	2.35	1.43	1.38
25	d	314	CLA	CHB-C1B	-2.35	1.34	1.39
29	B	828	BCR	C30-C25	-2.35	1.50	1.53
25	B	819	CLA	CHC-C1C	2.35	1.43	1.38
25	A	833	CLA	CHB-C1B	-2.35	1.34	1.39
25	h	211	CLA	CHB-C1B	-2.34	1.34	1.39
25	n	209	CLA	MG-NB	2.34	2.10	2.05
25	f	601	CLA	MG-NB	2.34	2.10	2.05
25	B	839	CLA	CHB-C1B	-2.34	1.34	1.39
25	i	209	CLA	C3B-C4B	2.34	1.48	1.42
25	i	204	CLA	MG-NB	2.34	2.10	2.05
25	A	817	CLA	CHB-C1B	-2.34	1.34	1.39
25	a	205	CLA	CHB-C1B	-2.34	1.34	1.39
25	k	211	CLA	C3B-C4B	2.34	1.48	1.42
29	J	101	BCR	C19-C18	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	203	CLA	CHC-C1C	2.34	1.43	1.38
25	B	807	CLA	C3B-C4B	2.34	1.48	1.42
25	J	103	CLA	C3B-C4B	2.34	1.48	1.42
25	g	207	CLA	MG-NB	2.34	2.10	2.05
25	j	207	CLA	CHC-C1C	2.34	1.43	1.38
25	c	305	CLA	C3B-C4B	2.34	1.48	1.42
25	i	205	CLA	C3B-C4B	2.34	1.48	1.42
35	d	310	CHL	MG-NB	2.34	2.10	2.05
25	c	312	CLA	CHC-C1C	2.34	1.43	1.38
25	p	607	CLA	CHB-C1B	-2.34	1.34	1.39
25	A	813	CLA	C3B-C4B	2.34	1.48	1.42
25	A	844	CLA	CHB-C1B	-2.34	1.34	1.39
25	c	313	CLA	CHB-C1B	-2.34	1.34	1.39
25	j	214	CLA	C3B-C4B	2.34	1.48	1.42
25	A	816	CLA	MG-NB	2.34	2.10	2.05
25	B	803	CLA	CHC-C1C	2.34	1.43	1.38
25	g	209	CLA	CHC-C1C	2.34	1.43	1.38
25	B	815	CLA	C3B-C4B	2.34	1.48	1.42
25	A	801	CLA	CHB-C1B	-2.34	1.34	1.39
25	B	841	CLA	CHB-C1B	-2.34	1.34	1.39
25	A	831	CLA	CHC-C1C	2.34	1.43	1.38
25	p	606	CLA	CHC-C1C	2.34	1.43	1.38
25	e	201	CLA	CHB-C1B	-2.34	1.34	1.39
25	h	206	CLA	CHB-C1B	-2.34	1.34	1.39
25	k	205	CLA	CHB-C1B	-2.34	1.34	1.39
30	o	612	DD6	C35-C36	-2.34	1.47	1.51
25	e	210	CLA	CHB-C1B	-2.34	1.34	1.39
25	j	205	CLA	MG-NB	2.34	2.10	2.05
25	n	202	CLA	MG-NB	2.34	2.10	2.05
25	g	212	CLA	CHB-C1B	-2.34	1.34	1.39
25	A	809	CLA	CHC-C1C	2.34	1.43	1.38
25	e	214	CLA	MG-NB	2.34	2.10	2.05
25	A	826	CLA	C3B-C4B	2.34	1.48	1.42
30	f	613	DD6	C35-C36	-2.34	1.47	1.51
25	B	846	CLA	C1B-NB	-2.34	1.34	1.37
25	o	606	CLA	C3B-C4B	2.33	1.48	1.42
25	p	606	CLA	CHB-C1B	-2.33	1.34	1.39
25	b	212	CLA	CHC-C1C	2.33	1.43	1.38
25	e	205	CLA	CHC-C1C	2.33	1.43	1.38
25	B	807	CLA	CHB-C1B	-2.33	1.34	1.39
25	d	311	CLA	CHB-C1B	-2.33	1.34	1.39
25	A	812	CLA	C3B-C4B	2.33	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	204	CLA	CHC-C1C	2.33	1.43	1.38
25	B	834	CLA	CHB-C1B	-2.33	1.34	1.39
25	B	816	CLA	C1B-NB	-2.33	1.34	1.37
25	B	826	CLA	CHB-C1B	-2.33	1.34	1.39
25	j	203	CLA	CHB-C1B	-2.33	1.34	1.39
35	d	310	CHL	CBA-CGA	2.33	1.56	1.50
25	l	610	CLA	CHC-C1C	2.33	1.43	1.38
25	g	205	CLA	C3B-C4B	2.33	1.48	1.42
25	d	304	CLA	C3B-C4B	2.33	1.48	1.42
25	b	211	CLA	MG-NB	2.33	2.10	2.05
25	d	312	CLA	C3B-C4B	2.33	1.48	1.42
25	i	204	CLA	C3B-C4B	2.33	1.48	1.42
25	d	305	CLA	CHB-C1B	-2.33	1.34	1.39
25	B	814	CLA	C3B-C4B	2.33	1.48	1.42
25	j	210	CLA	C3B-C4B	2.33	1.48	1.42
25	A	819	CLA	C3B-C4B	2.33	1.48	1.42
25	A	853	CLA	CHB-C1B	-2.33	1.34	1.39
25	e	208	CLA	CHC-C1C	2.33	1.43	1.38
25	p	602	CLA	MG-NC	2.33	2.11	2.06
25	B	804	CLA	C3B-C4B	2.33	1.48	1.42
30	e	220	DD6	C8-C6	-2.33	1.40	1.45
25	j	205	CLA	C1D-ND	-2.33	1.34	1.37
25	o	601	CLA	CHC-C1C	2.33	1.43	1.38
25	i	204	CLA	C1D-ND	-2.33	1.34	1.37
25	F	202	CLA	CHB-C1B	-2.33	1.34	1.39
25	i	202	CLA	CHB-C1B	-2.33	1.34	1.39
25	h	211	CLA	CHC-C1C	2.33	1.43	1.38
25	f	601	CLA	CHC-C1C	2.33	1.43	1.38
25	g	211	CLA	CHC-C1C	2.33	1.43	1.38
25	b	213	CLA	CHC-C1C	2.33	1.43	1.38
25	l	601	CLA	MG-NB	2.33	2.10	2.05
25	h	204	CLA	C3B-C4B	2.33	1.48	1.42
25	m	207	CLA	C3B-C4B	2.33	1.48	1.42
25	i	204	CLA	MG-NC	2.33	2.11	2.06
25	l	601	CLA	CHC-C1C	2.33	1.43	1.38
25	l	606	CLA	CHB-C1B	-2.33	1.34	1.39
25	j	212	CLA	C3B-C4B	2.32	1.48	1.42
25	B	836	CLA	CHB-C1B	-2.32	1.34	1.39
25	d	306	CLA	CHB-C1B	-2.32	1.34	1.39
25	g	207	CLA	CHB-C1B	-2.32	1.34	1.39
25	k	202	CLA	CHC-C1C	2.32	1.43	1.38
25	e	216	CLA	C3B-C4B	2.32	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	316	CLA	C3B-C4B	2.32	1.48	1.42
25	g	215	CLA	CHC-C1C	2.32	1.43	1.38
25	h	211	CLA	MG-NB	2.32	2.10	2.05
25	B	812	CLA	CHB-C1B	-2.32	1.34	1.39
25	i	207	CLA	C3B-C4B	2.32	1.48	1.42
25	a	213	CLA	CHC-C1C	2.32	1.43	1.38
25	h	206	CLA	CHC-C1C	2.32	1.43	1.38
25	h	210	CLA	C3B-C4B	2.32	1.48	1.42
25	l	611	CLA	CHB-C1B	-2.32	1.34	1.39
25	n	203	CLA	CHB-C1B	-2.32	1.34	1.39
25	A	841	CLA	CHC-C1C	2.32	1.43	1.38
25	B	845	CLA	C1B-NB	-2.32	1.34	1.37
25	B	805	CLA	C3B-C4B	2.32	1.48	1.42
25	B	834	CLA	C3B-C4B	2.32	1.48	1.42
25	A	817	CLA	C3B-C4B	2.32	1.48	1.42
25	j	213	CLA	CHB-C1B	-2.32	1.34	1.39
25	o	607	CLA	MG-NB	2.32	2.10	2.05
25	g	211	CLA	MG-NC	2.32	2.11	2.06
25	e	207	CLA	CHB-C1B	-2.32	1.34	1.39
25	n	206	CLA	CHC-C1C	2.32	1.43	1.38
25	B	808	CLA	CHB-C1B	-2.32	1.34	1.39
25	i	210	CLA	CHB-C1B	-2.32	1.34	1.39
25	k	210	CLA	CHC-C1C	2.32	1.43	1.38
25	o	604	CLA	CHB-C1B	-2.32	1.34	1.39
25	A	822	CLA	CHC-C1C	2.32	1.43	1.38
25	A	824	CLA	CHB-C1B	-2.32	1.34	1.39
25	l	603	CLA	MG-NB	2.32	2.10	2.05
25	c	312	CLA	CHB-C1B	-2.32	1.34	1.39
25	A	830	CLA	CHB-C1B	-2.32	1.34	1.39
25	i	211	CLA	CHC-C1C	2.32	1.43	1.38
25	o	606	CLA	CHC-C1C	2.32	1.43	1.38
25	a	203	CLA	CHB-C1B	-2.32	1.34	1.39
25	m	208	CLA	CHC-C1C	2.31	1.43	1.38
25	g	203	CLA	C3B-C4B	2.31	1.48	1.42
25	A	812	CLA	CHB-C1B	-2.31	1.34	1.39
25	c	309	CLA	CHC-C1C	2.31	1.43	1.38
25	B	807	CLA	MG-NB	2.31	2.10	2.05
25	g	213	CLA	MG-NB	2.31	2.10	2.05
25	b	204	CLA	CHC-C1C	2.31	1.43	1.38
25	g	206	CLA	CHC-C1C	2.31	1.43	1.38
25	A	828	CLA	C3B-C4B	2.31	1.48	1.42
25	a	208	CLA	C3B-C4B	2.31	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	m	209	CLA	MG-NB	2.31	2.10	2.05
25	B	815	CLA	CHB-C1B	-2.31	1.34	1.39
30	n	212	DD6	C35-C36	-2.31	1.47	1.51
25	a	208	CLA	C1B-NB	-2.31	1.34	1.37
25	j	208	CLA	C3B-C4B	2.31	1.48	1.42
25	j	210	CLA	C1B-NB	-2.31	1.34	1.37
25	p	606	CLA	MG-NB	2.31	2.10	2.05
25	h	203	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	811	CLA	C3B-C4B	2.31	1.48	1.42
25	B	818	CLA	CHB-C1B	-2.31	1.34	1.39
25	A	857	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	813	CLA	CHB-C1B	-2.31	1.34	1.39
25	c	309	CLA	CHB-C1B	-2.31	1.34	1.39
25	c	306	CLA	CHC-C1C	2.31	1.43	1.38
25	d	306	CLA	C3B-C4B	2.31	1.48	1.42
25	a	210	CLA	CHC-C1C	2.31	1.43	1.38
25	j	207	CLA	CHB-C1B	-2.31	1.34	1.39
25	A	833	CLA	C3B-C4B	2.31	1.48	1.42
25	e	215	CLA	CHC-C1C	2.31	1.43	1.38
25	m	206	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	844	CLA	MG-NB	2.31	2.10	2.05
25	n	204	CLA	MG-NB	2.31	2.10	2.05
25	A	857	CLA	C3B-C4B	2.31	1.48	1.42
25	d	305	CLA	C3B-C4B	2.31	1.48	1.42
25	B	843	CLA	CHB-C1B	-2.31	1.34	1.39
25	b	205	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	824	CLA	CHB-C1B	-2.31	1.34	1.39
25	p	602	CLA	CHD-C1D	2.31	1.42	1.38
25	A	832	CLA	CHC-C1C	2.31	1.43	1.38
25	o	602	CLA	CHC-C1C	2.31	1.43	1.38
25	g	210	CLA	CHB-C1B	-2.31	1.34	1.39
25	g	210	CLA	CHC-C1C	2.31	1.43	1.38
25	A	829	CLA	C1B-NB	-2.31	1.34	1.37
25	c	306	CLA	CHB-C1B	-2.31	1.34	1.39
25	B	806	CLA	C3B-C4B	2.30	1.48	1.42
25	i	206	CLA	CHB-C1B	-2.30	1.34	1.39
25	b	210	CLA	CHC-C1C	2.30	1.43	1.38
25	d	316	CLA	CHC-C1C	2.30	1.43	1.38
25	h	212	CLA	CHC-C1C	2.30	1.43	1.38
25	B	802	CLA	CHB-C1B	-2.30	1.34	1.39
25	g	214	CLA	CHC-C1C	2.30	1.43	1.38
25	B	845	CLA	CHB-C1B	-2.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	304	CLA	CHB-C1B	-2.30	1.34	1.39
25	B	822	CLA	C3B-C4B	2.30	1.48	1.42
32	b	202	DGD	C1E-C2E	2.30	1.59	1.52
25	j	205	CLA	MG-NC	2.30	2.11	2.06
25	A	827	CLA	CHB-C1B	-2.30	1.34	1.39
25	B	811	CLA	CHB-C1B	-2.30	1.34	1.39
25	A	851	CLA	CHC-C1C	2.30	1.43	1.38
25	m	211	CLA	CHC-C1C	2.30	1.43	1.38
25	g	212	CLA	CHC-C1C	2.30	1.43	1.38
25	i	210	CLA	CHC-C1C	2.30	1.43	1.38
25	p	605	CLA	MG-NB	2.30	2.10	2.05
25	B	817	CLA	CHC-C1C	2.30	1.43	1.38
25	a	203	CLA	CHC-C1C	2.30	1.43	1.38
25	p	609	CLA	CHC-C1C	2.30	1.43	1.38
25	n	202	CLA	CHB-C1B	-2.30	1.34	1.39
25	k	212	CLA	MG-NB	2.30	2.10	2.05
25	l	607	CLA	CHB-C1B	-2.30	1.34	1.39
25	e	214	CLA	CHC-C1C	2.30	1.43	1.38
25	h	214	CLA	CHB-C1B	-2.30	1.34	1.39
25	A	846	CLA	C3B-C4B	2.30	1.48	1.42
25	A	814	CLA	MG-NB	2.30	2.10	2.05
25	n	209	CLA	CHB-C1B	-2.30	1.34	1.39
25	j	204	CLA	C3B-C4B	2.30	1.48	1.42
25	b	209	CLA	CHB-C1B	-2.30	1.34	1.39
25	h	208	CLA	CHB-C1B	-2.30	1.34	1.39
25	i	209	CLA	CHC-C1C	2.30	1.43	1.38
25	e	212	CLA	C3B-C4B	2.30	1.48	1.42
25	A	840	CLA	CHB-C1B	-2.30	1.34	1.39
25	e	212	CLA	CHB-C1B	-2.30	1.34	1.39
25	B	841	CLA	CHC-C1C	2.30	1.43	1.38
25	d	311	CLA	CHC-C1C	2.30	1.43	1.38
25	f	610	CLA	CHC-C1C	2.30	1.43	1.38
25	A	846	CLA	CHC-C1C	2.30	1.43	1.38
25	l	609	CLA	CHC-C1C	2.30	1.43	1.38
25	n	206	CLA	MG-NB	2.30	2.10	2.05
25	m	210	CLA	CHC-C1C	2.30	1.43	1.38
25	A	810	CLA	CHC-C1C	2.29	1.43	1.38
25	b	203	CLA	CHC-C1C	2.29	1.43	1.38
25	j	206	CLA	CHC-C1C	2.29	1.43	1.38
25	c	313	CLA	C3B-C4B	2.29	1.48	1.42
25	A	828	CLA	CHB-C1B	-2.29	1.34	1.39
25	f	608	CLA	MG-NB	2.29	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	603	CLA	CHB-C1B	-2.29	1.34	1.39
25	f	608	CLA	CHC-C1C	2.29	1.43	1.38
25	h	204	CLA	C1B-NB	-2.29	1.35	1.37
30	m	212	DD6	C35-C36	-2.29	1.47	1.51
29	B	830	BCR	C1-C6	-2.29	1.50	1.53
25	l	605	CLA	CHB-C1B	-2.29	1.34	1.39
25	b	207	CLA	MG-NB	2.29	2.10	2.05
25	j	208	CLA	C1B-NB	-2.29	1.35	1.37
25	B	804	CLA	CHC-C1C	2.29	1.43	1.38
25	k	208	CLA	CHC-C1C	2.29	1.43	1.38
25	f	611	CLA	MG-NB	2.29	2.10	2.05
25	B	825	CLA	CHB-C1B	-2.29	1.34	1.39
25	A	814	CLA	C3B-C4B	2.29	1.48	1.42
25	B	816	CLA	CHC-C1C	2.29	1.43	1.38
25	c	305	CLA	CHB-C1B	-2.29	1.34	1.39
25	j	213	CLA	MG-NB	2.29	2.10	2.05
25	h	203	CLA	CHC-C1C	2.29	1.43	1.38
25	i	212	CLA	CHB-C1B	-2.29	1.34	1.39
25	e	215	CLA	MG-NB	2.29	2.10	2.05
25	d	313	CLA	CHB-C1B	-2.29	1.34	1.39
25	A	810	CLA	CHB-C1B	-2.29	1.34	1.39
25	k	209	CLA	CHC-C1C	2.29	1.43	1.38
25	o	609	CLA	CHC-C1C	2.29	1.43	1.38
25	g	208	CLA	CHB-C1B	-2.29	1.34	1.39
25	A	827	CLA	MG-NB	2.29	2.10	2.05
25	h	208	CLA	C3B-C4B	2.28	1.48	1.42
25	g	208	CLA	MG-NB	2.28	2.10	2.05
25	i	206	CLA	CHC-C1C	2.28	1.43	1.38
25	l	605	CLA	CHC-C1C	2.28	1.43	1.38
25	a	206	CLA	CHB-C1B	-2.28	1.34	1.39
25	c	310	CLA	CHB-C1B	-2.28	1.34	1.39
25	k	214	CLA	C3B-C4B	2.28	1.48	1.42
25	f	604	CLA	MG-NB	2.28	2.10	2.05
25	B	815	CLA	CHC-C1C	2.28	1.43	1.38
25	b	207	CLA	CHB-C1B	-2.28	1.34	1.39
25	k	202	CLA	MG-NB	2.28	2.10	2.05
35	e	209	CHL	MG-NB	2.28	2.10	2.05
30	l	613	DD6	C35-C36	-2.28	1.47	1.51
25	l	606	CLA	C3B-C4B	2.28	1.48	1.42
25	A	820	CLA	CHB-C1B	-2.28	1.34	1.39
25	a	210	CLA	CHB-C1B	-2.28	1.34	1.39
28	B	835	PQN	C2M-C2	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	824	CLA	C3B-C4B	2.28	1.48	1.42
25	c	314	CLA	CHB-C1B	-2.28	1.34	1.39
25	c	311	CLA	CHC-C1C	2.28	1.43	1.38
25	J	103	CLA	MG-NB	2.28	2.10	2.05
25	A	851	CLA	C3B-C4B	2.28	1.48	1.42
25	A	811	CLA	CHC-C1C	2.28	1.43	1.38
25	B	802	CLA	MG-NB	2.28	2.10	2.05
25	a	211	CLA	CHB-C1B	-2.28	1.34	1.39
25	h	207	CLA	CHB-C1B	-2.28	1.34	1.39
25	e	210	CLA	CHC-C1C	2.28	1.43	1.38
25	c	303	CLA	C1B-NB	-2.28	1.35	1.37
25	h	215	CLA	CHB-C1B	-2.28	1.34	1.39
25	A	825	CLA	CHC-C1C	2.28	1.43	1.38
25	A	807	CLA	C3B-C4B	2.28	1.48	1.42
25	d	312	CLA	CHB-C1B	-2.28	1.34	1.39
25	b	211	CLA	CHC-C1C	2.28	1.43	1.38
25	c	315	CLA	CHC-C1C	2.28	1.43	1.38
25	B	843	CLA	C3B-C4B	2.28	1.48	1.42
25	d	314	CLA	C1B-NB	-2.28	1.35	1.37
25	j	203	CLA	CHC-C1C	2.28	1.43	1.38
25	l	609	CLA	CHB-C1B	-2.28	1.34	1.39
25	f	605	CLA	MG-NB	2.28	2.10	2.05
25	j	211	CLA	MG-NC	2.27	2.11	2.06
25	n	203	CLA	MG-NB	2.27	2.10	2.05
34	a	202	LMG	O8-C28	2.27	1.40	1.33
25	d	313	CLA	CHC-C1C	2.27	1.43	1.38
25	A	818	CLA	MG-NB	2.27	2.10	2.05
25	B	804	CLA	C1B-NB	-2.27	1.35	1.37
25	A	816	CLA	CHB-C1B	-2.27	1.34	1.39
25	m	209	CLA	CHC-C1C	2.27	1.43	1.38
25	A	853	CLA	MG-NB	2.27	2.10	2.05
25	B	821	CLA	CHB-C1B	-2.27	1.34	1.39
25	b	205	CLA	CHC-C1C	2.27	1.43	1.38
25	B	818	CLA	MG-NB	2.27	2.10	2.05
25	B	809	CLA	CHB-C1B	-2.27	1.34	1.39
25	b	203	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	812	CLA	CHC-C1C	2.27	1.43	1.38
25	B	802	CLA	C3B-C4B	2.27	1.48	1.42
34	e	202	LMG	O8-C28	2.27	1.40	1.33
25	f	606	CLA	MG-NC	2.27	2.11	2.06
25	B	837	CLA	CHB-C1B	-2.27	1.34	1.39
25	n	206	CLA	CHB-C1B	-2.27	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	314	CLA	CHC-C1C	2.27	1.43	1.38
25	b	206	CLA	CHB-C1B	-2.27	1.34	1.39
25	e	204	CLA	CHB-C1B	-2.27	1.34	1.39
25	e	211	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	813	CLA	CHB-C1B	-2.27	1.34	1.39
25	g	214	CLA	CHB-C1B	-2.27	1.34	1.39
25	c	315	CLA	MG-NB	2.27	2.10	2.05
25	B	816	CLA	CHB-C1B	-2.27	1.34	1.39
25	k	214	CLA	CHB-C1B	-2.27	1.34	1.39
25	d	315	CLA	C3B-C4B	2.27	1.48	1.42
25	A	809	CLA	CHB-C1B	-2.27	1.34	1.39
25	h	212	CLA	CHB-C1B	-2.27	1.34	1.39
25	b	211	CLA	CHB-C1B	-2.27	1.34	1.39
25	j	214	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	849	CLA	C1B-NB	-2.27	1.35	1.37
30	o	611	DD6	C35-C36	-2.27	1.47	1.51
25	d	312	CLA	CHC-C1C	2.27	1.43	1.38
25	l	601	CLA	CHB-C1B	-2.27	1.34	1.39
25	c	308	CLA	CHB-C1B	-2.27	1.34	1.39
25	k	213	CLA	CHC-C1C	2.27	1.43	1.38
25	i	213	CLA	C3B-C4B	2.27	1.48	1.42
25	n	205	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	848	CLA	MG-NB	2.27	2.10	2.05
25	a	211	CLA	CHC-C1C	2.27	1.43	1.38
25	j	210	CLA	CHB-C1B	-2.27	1.34	1.39
25	A	802	CLA	CHB-C1B	-2.26	1.34	1.39
25	A	823	CLA	C1B-NB	-2.26	1.35	1.37
25	h	209	CLA	C1B-NB	-2.26	1.35	1.37
25	e	205	CLA	CHB-C1B	-2.26	1.34	1.39
25	i	203	CLA	CHB-C1B	-2.26	1.34	1.39
25	m	204	CLA	MG-NB	2.26	2.10	2.05
25	h	205	CLA	C1B-NB	-2.26	1.35	1.37
25	B	847	CLA	CHC-C1C	2.26	1.43	1.38
25	A	801	CLA	C3B-C4B	2.26	1.48	1.42
25	A	821	CLA	CHB-C1B	-2.26	1.34	1.39
25	d	303	CLA	CHB-C1B	-2.26	1.34	1.39
25	e	216	CLA	CHC-C1C	2.26	1.43	1.38
25	c	303	CLA	CHB-C1B	-2.26	1.34	1.39
25	A	848	CLA	CHC-C1C	2.26	1.43	1.38
25	d	304	CLA	CHC-C1C	2.26	1.43	1.38
25	j	204	CLA	C1B-NB	-2.26	1.35	1.37
25	i	213	CLA	CHB-C1B	-2.26	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	216	DD6	C35-C36	-2.26	1.47	1.51
25	B	834	CLA	MG-NB	2.26	2.10	2.05
25	B	822	CLA	C1B-NB	-2.26	1.35	1.37
25	b	208	CLA	CHB-C1B	-2.26	1.34	1.39
25	k	204	CLA	CHB-C1B	-2.26	1.34	1.39
25	c	308	CLA	CHC-C1C	2.26	1.43	1.38
30	i	215	DD6	C19-C20	-2.26	1.48	1.52
25	o	609	CLA	CHB-C1B	-2.26	1.34	1.39
25	h	210	CLA	CHC-C1C	2.26	1.43	1.38
25	f	612	CLA	CHC-C1C	2.26	1.43	1.38
25	f	607	CLA	CHB-C1B	-2.26	1.34	1.39
25	B	810	CLA	CHB-C1B	-2.26	1.34	1.39
25	e	216	CLA	CHB-C1B	-2.26	1.34	1.39
25	c	302	CLA	CHC-C1C	2.26	1.43	1.38
25	i	205	CLA	CHC-C1C	2.26	1.43	1.38
25	l	602	CLA	CHB-C1B	-2.26	1.34	1.39
25	l	603	CLA	C1B-NB	-2.26	1.35	1.37
25	B	839	CLA	CHC-C1C	2.26	1.43	1.38
25	o	609	CLA	MG-NB	2.26	2.10	2.05
25	a	213	CLA	CHB-C1B	-2.26	1.34	1.39
25	k	205	CLA	CHC-C1C	2.26	1.43	1.38
25	f	612	CLA	MG-NC	2.26	2.11	2.06
25	h	213	CLA	CHB-C1B	-2.26	1.34	1.39
25	l	603	CLA	MG-NC	2.26	2.11	2.06
25	m	208	CLA	CHB-C1B	-2.26	1.34	1.39
25	B	837	CLA	CHC-C1C	2.26	1.43	1.38
25	A	816	CLA	C3B-C4B	2.26	1.48	1.42
25	e	206	CLA	MG-NB	2.26	2.10	2.05
25	m	210	CLA	MG-NC	2.26	2.11	2.06
25	c	315	CLA	CHB-C1B	-2.25	1.34	1.39
25	k	212	CLA	CHB-C1B	-2.25	1.34	1.39
25	p	607	CLA	CHC-C1C	2.25	1.43	1.38
25	A	841	CLA	CHB-C1B	-2.25	1.34	1.39
25	f	611	CLA	CHB-C1B	-2.25	1.34	1.39
25	a	205	CLA	CHC-C1C	2.25	1.43	1.38
25	f	610	CLA	CHB-C1B	-2.25	1.34	1.39
25	h	215	CLA	CHC-C1C	2.25	1.43	1.38
25	k	207	CLA	C3B-C4B	2.25	1.48	1.42
25	h	204	CLA	CHB-C1B	-2.25	1.34	1.39
25	j	206	CLA	CHB-C1B	-2.25	1.34	1.39
25	n	211	CLA	CHB-C1B	-2.25	1.34	1.39
35	d	307	CHL	C2-C3	2.25	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	211	CLA	MG-NB	2.25	2.10	2.05
25	n	208	CLA	CHC-C1C	2.25	1.43	1.38
25	k	207	CLA	CHB-C1B	-2.25	1.34	1.39
25	c	305	CLA	MG-NB	2.25	2.10	2.05
25	n	204	CLA	CHC-C1C	2.25	1.43	1.38
25	a	205	CLA	MG-NB	2.25	2.10	2.05
25	j	215	CLA	CHB-C1B	-2.25	1.34	1.39
25	B	811	CLA	CHC-C1C	2.25	1.43	1.38
25	A	810	CLA	C1B-NB	-2.25	1.35	1.37
25	A	821	CLA	CHC-C1C	2.25	1.43	1.38
25	e	206	CLA	CHC-C1C	2.25	1.43	1.38
25	n	204	CLA	CHB-C1B	-2.25	1.34	1.39
25	m	204	CLA	MG-NC	2.25	2.11	2.06
25	B	808	CLA	C3B-C4B	2.25	1.48	1.42
25	m	210	CLA	MG-NB	2.25	2.10	2.05
25	g	207	CLA	MG-NC	2.25	2.11	2.06
25	A	824	CLA	MG-NB	2.25	2.10	2.05
25	l	604	CLA	CHB-C1B	-2.25	1.34	1.39
25	a	211	CLA	MG-NB	2.25	2.10	2.05
25	B	814	CLA	C1B-NB	-2.25	1.35	1.37
25	l	610	CLA	MG-NB	2.25	2.10	2.05
25	j	211	CLA	C1B-NB	-2.25	1.35	1.37
25	A	815	CLA	CHB-C1B	-2.25	1.34	1.39
25	c	311	CLA	CHB-C1B	-2.25	1.34	1.39
30	e	220	DD6	C25-C26	-2.25	1.36	1.43
25	o	607	CLA	CHB-C1B	-2.25	1.34	1.39
25	B	834	CLA	CHC-C1C	2.25	1.43	1.38
25	A	804	CLA	CHB-C1B	-2.25	1.34	1.39
25	c	304	CLA	MG-NB	2.25	2.10	2.05
25	B	821	CLA	CHC-C1C	2.25	1.43	1.38
25	i	205	CLA	CHB-C1B	-2.25	1.34	1.39
25	A	848	CLA	CHB-C1B	-2.25	1.34	1.39
25	a	206	CLA	CHC-C1C	2.25	1.43	1.38
25	l	611	CLA	CHC-C1C	2.25	1.43	1.38
25	l	608	CLA	MG-NB	2.25	2.10	2.05
25	d	301	CLA	CHB-C1B	-2.25	1.34	1.39
25	k	213	CLA	CHB-C1B	-2.25	1.34	1.39
25	k	211	CLA	CHB-C1B	-2.24	1.34	1.39
25	l	611	CLA	MG-NC	2.24	2.11	2.06
25	p	604	CLA	CHB-C1B	-2.24	1.34	1.39
25	B	820	CLA	C3B-C4B	2.24	1.48	1.42
25	o	603	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	847	CLA	MG-NB	2.24	2.10	2.05
25	A	831	CLA	MG-NB	2.24	2.10	2.05
25	a	203	CLA	MG-NB	2.24	2.10	2.05
25	e	213	CLA	CHB-C1B	-2.24	1.34	1.39
25	o	604	CLA	MG-NB	2.24	2.10	2.05
25	A	823	CLA	C3B-C4B	2.24	1.48	1.42
25	A	813	CLA	MG-NB	2.24	2.10	2.05
25	F	201	CLA	CHC-C1C	2.24	1.43	1.38
25	A	808	CLA	CHB-C1B	-2.24	1.34	1.39
25	B	806	CLA	CHB-C1B	-2.24	1.34	1.39
25	h	205	CLA	CHB-C1B	-2.24	1.34	1.39
25	e	208	CLA	CHB-C1B	-2.24	1.34	1.39
25	A	826	CLA	CHC-C1C	2.24	1.43	1.38
25	a	212	CLA	CHB-C1B	-2.24	1.34	1.39
25	A	819	CLA	C1B-NB	-2.24	1.35	1.37
25	b	208	CLA	CHC-C1C	2.24	1.43	1.38
25	n	208	CLA	CHB-C1B	-2.24	1.34	1.39
25	d	304	CLA	CHB-C1B	-2.24	1.34	1.39
25	B	820	CLA	C1B-NB	-2.24	1.35	1.37
25	A	847	CLA	CHB-C1B	-2.24	1.34	1.39
25	b	204	CLA	CHB-C1B	-2.24	1.34	1.39
25	m	211	CLA	MG-NB	2.24	2.10	2.05
25	j	215	CLA	CHC-C1C	2.24	1.43	1.38
25	A	810	CLA	C3B-C4B	2.24	1.48	1.42
25	b	204	CLA	C1B-NB	-2.24	1.35	1.37
25	k	207	CLA	CHC-C1C	2.24	1.43	1.38
25	p	607	CLA	MG-NC	2.24	2.11	2.06
25	B	839	CLA	C1B-NB	-2.24	1.35	1.37
25	i	208	CLA	CHB-C1B	-2.24	1.34	1.39
25	p	606	CLA	MG-NC	2.24	2.11	2.06
25	B	825	CLA	C3B-C4B	2.24	1.48	1.42
25	c	302	CLA	CHB-C1B	-2.24	1.34	1.39
25	f	606	CLA	CHB-C1B	-2.24	1.34	1.39
25	n	210	CLA	MG-NC	2.24	2.11	2.06
25	A	825	CLA	MG-NB	2.24	2.10	2.05
25	f	607	CLA	MG-NB	2.24	2.10	2.05
25	m	206	CLA	CHC-C1C	2.24	1.43	1.38
25	e	213	CLA	C3B-C4B	2.23	1.48	1.42
25	B	840	CLA	CHB-C1B	-2.23	1.34	1.39
25	k	209	CLA	CHB-C1B	-2.23	1.34	1.39
25	c	314	CLA	MG-NB	2.23	2.10	2.05
25	o	610	CLA	MG-NB	2.23	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	l	604	CLA	MG-NB	2.23	2.10	2.05
25	B	806	CLA	C1B-NB	-2.23	1.35	1.37
25	B	822	CLA	CHB-C1B	-2.23	1.34	1.39
25	g	213	CLA	CHB-C1B	-2.23	1.34	1.39
25	A	857	CLA	CHC-C1C	2.23	1.43	1.38
25	A	806	CLA	CHB-C1B	-2.23	1.34	1.39
25	A	851	CLA	CHB-C1B	-2.23	1.34	1.39
25	g	215	CLA	CHB-C1B	-2.23	1.34	1.39
25	o	606	CLA	CHB-C1B	-2.23	1.34	1.39
25	i	202	CLA	CHC-C1C	2.23	1.43	1.38
25	k	206	CLA	CHC-C1C	2.23	1.43	1.38
25	d	311	CLA	MG-NB	2.23	2.10	2.05
25	i	212	CLA	MG-NB	2.23	2.10	2.05
25	e	214	CLA	CHB-C1B	-2.23	1.34	1.39
25	B	806	CLA	CHC-C1C	2.23	1.43	1.38
25	e	207	CLA	CHC-C1C	2.23	1.43	1.38
25	k	209	CLA	MG-NB	2.23	2.10	2.05
25	n	208	CLA	MG-NB	2.23	2.10	2.05
25	c	306	CLA	MG-NB	2.23	2.10	2.05
25	b	206	CLA	C1B-NB	-2.23	1.35	1.37
25	d	312	CLA	C1B-NB	-2.23	1.35	1.37
25	n	210	CLA	CHB-C1B	-2.23	1.34	1.39
25	B	813	CLA	MG-NB	2.23	2.10	2.05
25	a	208	CLA	CHC-C1C	2.23	1.43	1.38
25	f	602	CLA	MG-NB	2.23	2.10	2.05
25	A	829	CLA	CHB-C1B	-2.23	1.34	1.39
25	n	210	CLA	MG-NB	2.23	2.10	2.05
25	n	203	CLA	MG-NC	2.23	2.11	2.06
25	A	845	CLA	C3B-C4B	2.23	1.48	1.42
25	A	831	CLA	MG-NC	2.23	2.11	2.06
25	A	832	CLA	CHB-C1B	-2.23	1.34	1.39
25	e	204	CLA	CHC-C1C	2.23	1.43	1.38
25	e	210	CLA	MG-NB	2.23	2.10	2.05
25	A	850	CLA	CHB-C1B	-2.23	1.34	1.39
25	A	806	CLA	CHC-C1C	2.23	1.43	1.38
25	c	310	CLA	CHC-C1C	2.23	1.43	1.38
25	A	811	CLA	MG-NB	2.23	2.10	2.05
25	A	817	CLA	CHC-C1C	2.22	1.43	1.38
25	B	814	CLA	CHC-C1C	2.22	1.43	1.38
25	A	801	CLA	C1B-NB	-2.22	1.35	1.37
25	m	207	CLA	CHC-C1C	2.22	1.43	1.38
25	o	605	CLA	CHC-C1C	2.22	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	848	CLA	CHB-C1B	-2.22	1.34	1.39
25	m	209	CLA	CHB-C1B	-2.22	1.34	1.39
25	A	840	CLA	MG-NB	2.22	2.10	2.05
25	i	207	CLA	CHB-C1B	-2.22	1.34	1.39
25	d	313	CLA	MG-NB	2.22	2.10	2.05
25	g	215	CLA	MG-NB	2.22	2.10	2.05
25	B	820	CLA	CHB-C1B	-2.22	1.34	1.39
25	c	303	CLA	CHC-C1C	2.22	1.43	1.38
25	a	213	CLA	MG-NB	2.22	2.10	2.05
25	n	202	CLA	MG-NC	2.22	2.11	2.06
25	l	609	CLA	MG-NB	2.22	2.10	2.05
25	A	806	CLA	C1B-NB	-2.22	1.35	1.37
25	B	819	CLA	CHB-C1B	-2.22	1.34	1.39
25	k	213	CLA	MG-NB	2.22	2.10	2.05
25	p	609	CLA	MG-NC	2.22	2.11	2.06
25	B	818	CLA	CHC-C1C	2.22	1.43	1.38
25	h	213	CLA	CHC-C1C	2.22	1.43	1.38
25	o	602	CLA	CHB-C1B	-2.22	1.34	1.39
25	A	818	CLA	CHC-C1C	2.22	1.43	1.38
25	j	210	CLA	CHC-C1C	2.22	1.43	1.38
25	f	612	CLA	CHB-C1B	-2.22	1.34	1.39
25	o	608	CLA	CHB-C1B	-2.22	1.34	1.39
30	c	317	DD6	C35-C36	-2.22	1.47	1.51
25	i	209	CLA	CHB-C1B	-2.22	1.34	1.39
25	c	309	CLA	MG-NB	2.22	2.10	2.05
25	k	210	CLA	MG-NC	2.22	2.11	2.06
25	a	207	CLA	CHC-C1C	2.22	1.43	1.38
25	A	846	CLA	CHB-C1B	-2.22	1.34	1.39
25	j	212	CLA	CHB-C1B	-2.22	1.34	1.39
25	A	833	CLA	CHC-C1C	2.22	1.43	1.38
25	A	813	CLA	CHC-C1C	2.22	1.43	1.38
25	e	201	CLA	MG-NB	2.22	2.10	2.05
25	i	205	CLA	C1B-NB	-2.22	1.35	1.37
25	i	207	CLA	CHC-C1C	2.22	1.43	1.38
25	f	603	CLA	CHC-C1C	2.22	1.43	1.38
25	p	605	CLA	CHB-C1B	-2.22	1.34	1.39
25	h	203	CLA	MG-NB	2.22	2.10	2.05
25	l	608	CLA	CHB-C1B	-2.22	1.34	1.39
25	k	211	CLA	CHC-C1C	2.21	1.43	1.38
25	n	207	CLA	CHB-C1B	-2.21	1.34	1.39
30	m	213	DD6	C35-C36	-2.21	1.47	1.51
25	n	208	CLA	MG-NC	2.21	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	205	CLA	C1D-ND	-2.21	1.35	1.37
25	b	212	CLA	MG-NB	2.21	2.10	2.05
25	h	207	CLA	MG-NB	2.21	2.10	2.05
25	n	211	CLA	MG-NB	2.21	2.10	2.05
25	m	205	CLA	MG-NB	2.21	2.10	2.05
25	i	212	CLA	CHC-C1C	2.21	1.43	1.38
25	k	212	CLA	CHC-C1C	2.21	1.43	1.38
25	B	846	CLA	CHB-C1B	-2.21	1.34	1.39
25	f	604	CLA	CHB-C1B	-2.21	1.34	1.39
25	g	206	CLA	CHB-C1B	-2.21	1.34	1.39
25	d	315	CLA	CHC-C1C	2.21	1.43	1.38
25	h	214	CLA	CHC-C1C	2.21	1.43	1.38
25	A	807	CLA	CHC-C1C	2.21	1.43	1.38
25	m	205	CLA	CHB-C1B	-2.21	1.34	1.39
25	A	806	CLA	MG-NB	2.21	2.10	2.05
25	A	820	CLA	C3B-C4B	2.21	1.47	1.42
25	h	204	CLA	CHC-C1C	2.21	1.43	1.38
25	i	210	CLA	MG-NB	2.21	2.10	2.05
25	e	215	CLA	C1B-NB	-2.21	1.35	1.37
25	a	211	CLA	MG-NC	2.21	2.11	2.06
25	d	305	CLA	MG-NC	2.21	2.11	2.06
25	e	213	CLA	CHC-C1C	2.21	1.43	1.38
25	o	606	CLA	MG-NB	2.21	2.10	2.05
25	p	601	CLA	MG-NC	2.21	2.11	2.06
25	B	823	CLA	CHB-C1B	-2.21	1.34	1.39
25	A	828	CLA	CHC-C1C	2.21	1.43	1.38
25	B	813	CLA	MG-NC	2.21	2.11	2.06
25	k	204	CLA	MG-NB	2.21	2.10	2.05
25	k	211	CLA	MG-NB	2.21	2.10	2.05
25	g	213	CLA	CHC-C1C	2.21	1.43	1.38
25	d	314	CLA	MG-NB	2.21	2.10	2.05
25	h	214	CLA	MG-NB	2.21	2.10	2.05
25	b	213	CLA	CHB-C1B	-2.21	1.34	1.39
25	j	214	CLA	C1B-NB	-2.21	1.35	1.37
25	k	204	CLA	CHC-C1C	2.21	1.43	1.38
25	B	813	CLA	CHC-C1C	2.21	1.43	1.38
25	B	822	CLA	CHC-C1C	2.21	1.43	1.38
25	A	845	CLA	C1B-NB	-2.21	1.35	1.37
25	e	208	CLA	MG-NB	2.21	2.10	2.05
25	j	207	CLA	MG-NC	2.21	2.11	2.06
25	b	207	CLA	CHC-C1C	2.21	1.43	1.38
25	B	817	CLA	MG-NB	2.20	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	602	CLA	CAA-C2A	2.20	1.58	1.54
25	p	604	CLA	MG-NB	2.20	2.10	2.05
25	j	205	CLA	C1B-NB	-2.20	1.35	1.37
25	k	214	CLA	CHC-C1C	2.20	1.43	1.38
25	B	836	CLA	C1B-NB	-2.20	1.35	1.37
25	h	212	CLA	C1B-NB	-2.20	1.35	1.37
25	l	609	CLA	MG-NC	2.20	2.11	2.06
25	A	849	CLA	CHB-C1B	-2.20	1.34	1.39
25	F	202	CLA	MG-NC	2.20	2.11	2.06
25	f	608	CLA	CHB-C1B	-2.20	1.34	1.39
34	j	201	LMG	O8-C28	2.20	1.39	1.33
25	k	210	CLA	MG-NB	2.20	2.10	2.05
25	d	316	CLA	MG-NC	2.20	2.11	2.06
25	l	612	CLA	MG-NB	2.20	2.10	2.05
25	B	808	CLA	C1B-NB	-2.20	1.35	1.37
25	A	814	CLA	CHC-C1C	2.20	1.43	1.38
25	B	825	CLA	CHC-C1C	2.20	1.43	1.38
25	a	207	CLA	MG-NB	2.20	2.10	2.05
25	A	843	CLA	CHB-C1B	-2.20	1.34	1.39
25	B	846	CLA	CHC-C1C	2.20	1.43	1.38
25	m	208	CLA	MG-NB	2.20	2.10	2.05
25	e	217	CLA	CHB-C1B	-2.20	1.34	1.39
25	j	214	CLA	MG-NB	2.20	2.10	2.05
25	A	818	CLA	C1B-NB	-2.20	1.35	1.37
25	A	815	CLA	C3B-C4B	2.20	1.47	1.42
25	B	836	CLA	CHC-C1C	2.20	1.43	1.38
25	B	821	CLA	C1B-NB	-2.20	1.35	1.37
25	B	826	CLA	MG-NC	2.20	2.11	2.06
25	e	214	CLA	MG-NC	2.20	2.11	2.06
25	h	211	CLA	MG-NC	2.20	2.11	2.06
25	B	837	CLA	MG-NB	2.20	2.10	2.05
25	n	207	CLA	MG-NC	2.19	2.11	2.06
25	b	208	CLA	C1B-NB	-2.19	1.35	1.37
25	j	206	CLA	C1B-NB	-2.19	1.35	1.37
30	g	217	DD6	C19-C20	-2.19	1.48	1.52
25	m	211	CLA	CHB-C1B	-2.19	1.34	1.39
25	B	836	CLA	C3B-C4B	2.19	1.47	1.42
25	l	612	CLA	CHB-C1B	-2.19	1.34	1.39
25	m	203	CLA	CHB-C1B	-2.19	1.34	1.39
25	k	207	CLA	C1B-NB	-2.19	1.35	1.37
25	g	214	CLA	MG-NB	2.19	2.10	2.05
33	J	102	SQD	O9-S	2.19	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	605	CLA	CHC-C1C	2.19	1.43	1.38
25	A	821	CLA	MG-NC	2.19	2.11	2.06
25	c	311	CLA	MG-NC	2.19	2.11	2.06
25	b	212	CLA	MG-NC	2.19	2.11	2.06
25	d	314	CLA	MG-NC	2.19	2.11	2.06
25	A	825	CLA	C1B-NB	-2.19	1.35	1.37
25	B	838	CLA	C1B-NB	-2.19	1.35	1.37
25	o	610	CLA	MG-NC	2.19	2.11	2.06
25	A	823	CLA	CHC-C1C	2.19	1.43	1.38
25	o	605	CLA	CHB-C1B	-2.19	1.34	1.39
25	c	310	CLA	C1B-NB	-2.19	1.35	1.37
25	b	210	CLA	CHB-C1B	-2.19	1.34	1.39
25	f	602	CLA	CHB-C1B	-2.19	1.34	1.39
25	b	209	CLA	CHC-C1C	2.19	1.43	1.38
25	e	204	CLA	MG-NC	2.19	2.11	2.06
25	l	601	CLA	MG-NC	2.19	2.11	2.06
25	A	828	CLA	MG-NB	2.19	2.10	2.05
30	e	219	DD6	C19-C20	-2.19	1.49	1.52
25	c	313	CLA	CHC-C1C	2.19	1.43	1.38
25	A	823	CLA	MG-NC	2.19	2.11	2.06
25	o	605	CLA	MG-NB	2.19	2.10	2.05
25	j	209	CLA	C3B-C4B	2.19	1.47	1.42
25	B	824	CLA	C1B-NB	-2.19	1.35	1.37
25	A	801	CLA	CHC-C1C	2.19	1.43	1.38
25	d	306	CLA	MG-NC	2.19	2.11	2.06
25	A	804	CLA	MG-NB	2.19	2.10	2.05
25	F	201	CLA	MG-NB	2.19	2.10	2.05
25	i	213	CLA	MG-NB	2.19	2.10	2.05
25	B	811	CLA	C1B-NB	-2.19	1.35	1.37
25	i	208	CLA	C1B-NB	-2.19	1.35	1.37
25	j	208	CLA	CHC-C1C	2.19	1.43	1.38
25	c	311	CLA	MG-NB	2.19	2.10	2.05
25	p	609	CLA	MG-NB	2.19	2.10	2.05
25	A	823	CLA	CHB-C1B	-2.19	1.34	1.39
25	a	210	CLA	MG-NB	2.19	2.10	2.05
25	j	209	CLA	CHC-C1C	2.18	1.43	1.38
25	k	210	CLA	C1B-NB	-2.18	1.35	1.37
25	m	203	CLA	MG-NB	2.18	2.10	2.05
25	A	821	CLA	C1B-NB	-2.18	1.35	1.37
25	B	812	CLA	MG-NB	2.18	2.10	2.05
25	b	213	CLA	MG-NB	2.18	2.10	2.05
25	o	608	CLA	MG-NB	2.18	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	842	CLA	C1B-NB	-2.18	1.35	1.37
25	A	816	CLA	MG-NC	2.18	2.11	2.06
25	A	845	CLA	CHB-C1B	-2.18	1.34	1.39
25	i	210	CLA	MG-NC	2.18	2.11	2.06
25	B	812	CLA	C1B-NB	-2.18	1.35	1.37
25	h	214	CLA	C1B-NB	-2.18	1.35	1.37
25	e	212	CLA	MG-NC	2.18	2.11	2.06
25	n	204	CLA	MG-NC	2.18	2.11	2.06
25	j	209	CLA	CHB-C1B	-2.18	1.34	1.39
25	B	824	CLA	CHC-C1C	2.18	1.43	1.38
25	A	811	CLA	MG-NC	2.18	2.11	2.06
25	a	207	CLA	CHB-C1B	-2.18	1.34	1.39
25	k	203	CLA	CHB-C1B	-2.18	1.34	1.39
25	b	205	CLA	MG-NB	2.18	2.10	2.05
25	A	819	CLA	CHB-C1B	-2.18	1.34	1.39
25	i	211	CLA	CHB-C1B	-2.18	1.34	1.39
32	b	202	DGD	C3D-C2D	2.18	1.57	1.52
25	a	203	CLA	MG-NC	2.18	2.11	2.06
25	c	315	CLA	MG-NC	2.18	2.11	2.06
25	h	210	CLA	CHB-C1B	-2.18	1.34	1.39
25	c	313	CLA	C1B-NB	-2.18	1.35	1.37
25	n	206	CLA	MG-NC	2.18	2.11	2.06
25	p	602	CLA	C1B-NB	-2.18	1.35	1.37
25	d	306	CLA	MG-NB	2.18	2.10	2.05
25	m	204	CLA	CHC-C1C	2.18	1.42	1.38
25	b	203	CLA	MG-NC	2.18	2.11	2.06
25	e	216	CLA	C1B-NB	-2.18	1.35	1.37
25	c	305	CLA	MG-NC	2.18	2.11	2.06
25	c	304	CLA	C1B-NB	-2.18	1.35	1.37
25	e	206	CLA	MG-NC	2.18	2.11	2.06
25	e	211	CLA	MG-NB	2.18	2.10	2.05
25	l	606	CLA	CHC-C1C	2.18	1.42	1.38
25	A	807	CLA	CHB-C1B	-2.18	1.34	1.39
25	p	605	CLA	MG-NC	2.18	2.11	2.06
25	d	306	CLA	C1B-NB	-2.18	1.35	1.37
25	f	601	CLA	MG-NC	2.17	2.11	2.06
25	g	206	CLA	MG-NB	2.17	2.10	2.05
25	c	304	CLA	MG-NC	2.17	2.11	2.06
25	f	605	CLA	CHB-C1B	-2.17	1.34	1.39
25	A	819	CLA	CHC-C1C	2.17	1.42	1.38
25	A	824	CLA	MG-NC	2.17	2.11	2.06
25	j	207	CLA	MG-NB	2.17	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	840	CLA	C1B-NB	-2.17	1.35	1.37
25	d	303	CLA	C1B-NB	-2.17	1.35	1.37
25	A	849	CLA	MG-NC	2.17	2.11	2.06
33	F	204	SQD	O9-S	2.17	1.51	1.45
25	l	605	CLA	C1B-NB	-2.17	1.35	1.37
25	f	601	CLA	CHB-C1B	-2.17	1.34	1.39
25	f	607	CLA	MG-NC	2.17	2.11	2.06
30	g	216	DD6	C35-C36	-2.17	1.47	1.51
25	d	316	CLA	CHB-C1B	-2.17	1.34	1.39
25	c	312	CLA	MG-NC	2.17	2.11	2.06
25	A	822	CLA	CHB-C1B	-2.17	1.34	1.39
25	B	817	CLA	C1B-NB	-2.17	1.35	1.37
25	h	208	CLA	C1B-NB	-2.17	1.35	1.37
25	m	207	CLA	C1B-NB	-2.17	1.35	1.37
25	j	203	CLA	MG-NB	2.17	2.10	2.05
29	B	833	BCR	C30-C25	-2.17	1.50	1.53
25	B	804	CLA	CHB-C1B	-2.17	1.34	1.39
25	m	205	CLA	MG-NC	2.17	2.11	2.06
25	d	306	CLA	CHC-C1C	2.17	1.42	1.38
25	h	207	CLA	MG-NC	2.17	2.11	2.06
25	g	203	CLA	MG-NC	2.17	2.11	2.06
25	j	214	CLA	CHC-C1C	2.17	1.42	1.38
25	A	813	CLA	MG-NC	2.17	2.11	2.06
25	B	820	CLA	MG-NC	2.17	2.11	2.06
25	c	305	CLA	CHC-C1C	2.17	1.42	1.38
25	B	843	CLA	MG-NB	2.17	2.10	2.05
28	A	834	PQN	C11-C12	-2.17	1.47	1.50
25	B	842	CLA	CHB-C1B	-2.17	1.34	1.39
25	b	211	CLA	MG-NC	2.17	2.11	2.06
35	d	308	CHL	MG-NC	2.17	2.11	2.06
25	k	208	CLA	CHB-C1B	-2.17	1.34	1.39
25	m	206	CLA	C1B-NB	-2.17	1.35	1.37
25	e	215	CLA	MG-NC	2.17	2.11	2.06
33	g	202	SQD	O9-S	2.17	1.51	1.45
25	l	603	CLA	CHC-C1C	2.17	1.42	1.38
25	n	205	CLA	CHC-C1C	2.17	1.42	1.38
25	A	820	CLA	C1B-NB	-2.17	1.35	1.37
25	B	834	CLA	MG-NC	2.16	2.11	2.06
25	k	202	CLA	CHB-C1B	-2.16	1.34	1.39
25	A	809	CLA	C3B-C4B	2.16	1.47	1.42
25	B	846	CLA	MG-NC	2.16	2.11	2.06
25	a	205	CLA	MG-NC	2.16	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	601	CLA	MG-NC	2.16	2.11	2.06
25	a	211	CLA	C1B-NB	-2.16	1.35	1.37
25	h	207	CLA	C1B-NB	-2.16	1.35	1.37
25	A	825	CLA	MG-NC	2.16	2.11	2.06
25	j	206	CLA	MG-NC	2.16	2.11	2.06
25	B	841	CLA	MG-NB	2.16	2.10	2.05
25	c	312	CLA	MG-NB	2.16	2.10	2.05
25	A	852	CLA	MG-NC	2.16	2.11	2.06
25	b	209	CLA	C1B-NB	-2.16	1.35	1.37
25	l	610	CLA	CHB-C1B	-2.16	1.34	1.39
25	d	316	CLA	MG-NB	2.16	2.10	2.05
25	j	211	CLA	MG-NB	2.16	2.10	2.05
25	A	827	CLA	CHC-C1C	2.16	1.42	1.38
25	g	205	CLA	C1B-NB	-2.16	1.35	1.37
25	p	601	CLA	MG-NB	2.16	2.10	2.05
25	d	305	CLA	C1B-NB	-2.16	1.35	1.37
25	n	211	CLA	C1B-NB	-2.16	1.35	1.37
25	a	206	CLA	MG-NB	2.16	2.10	2.05
25	f	610	CLA	MG-NB	2.16	2.10	2.05
25	b	207	CLA	MG-NC	2.16	2.11	2.06
25	i	213	CLA	CHC-C1C	2.16	1.42	1.38
25	e	212	CLA	MG-NB	2.16	2.10	2.05
25	B	805	CLA	C1B-NB	-2.16	1.35	1.37
25	B	841	CLA	C1B-NB	-2.16	1.35	1.37
25	c	310	CLA	MG-NB	2.16	2.10	2.05
25	g	204	CLA	MG-NB	2.16	2.10	2.05
25	A	812	CLA	C1B-NB	-2.16	1.35	1.37
25	m	202	CLA	C1D-ND	-2.16	1.35	1.37
25	f	608	CLA	MG-NC	2.16	2.11	2.06
25	p	609	CLA	CHB-C1B	-2.16	1.34	1.39
25	c	308	CLA	MG-NB	2.16	2.10	2.05
25	m	207	CLA	MG-NB	2.16	2.10	2.05
25	a	209	CLA	CHB-C1B	-2.16	1.34	1.39
25	A	853	CLA	C1B-NB	-2.16	1.35	1.37
25	B	826	CLA	C1B-NB	-2.16	1.35	1.37
25	a	210	CLA	MG-NC	2.16	2.11	2.06
25	j	213	CLA	CHC-C1C	2.16	1.42	1.38
30	j	217	DD6	C19-C20	-2.16	1.49	1.52
25	B	807	CLA	MG-NC	2.16	2.11	2.06
25	F	201	CLA	MG-NC	2.16	2.11	2.06
25	k	206	CLA	MG-NC	2.16	2.11	2.06
25	o	602	CLA	MG-NC	2.16	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	304	CLA	C1B-NB	-2.16	1.35	1.37
33	J	102	SQD	O7-S	2.16	1.51	1.45
25	h	213	CLA	MG-NB	2.16	2.10	2.05
25	m	209	CLA	MG-NC	2.16	2.11	2.06
25	B	810	CLA	C1B-NB	-2.16	1.35	1.37
25	A	849	CLA	C3B-C4B	2.16	1.47	1.42
25	f	610	CLA	MG-NC	2.16	2.11	2.06
25	A	829	CLA	CHC-C1C	2.15	1.42	1.38
25	d	301	CLA	MG-NC	2.15	2.11	2.06
25	e	216	CLA	MG-NC	2.15	2.11	2.06
25	l	612	CLA	MG-NC	2.15	2.11	2.06
25	o	608	CLA	MG-NC	2.15	2.11	2.06
25	A	801	CLA	MG-NB	2.15	2.10	2.05
25	n	211	CLA	MG-NC	2.15	2.11	2.06
25	A	807	CLA	C1B-NB	-2.15	1.35	1.37
25	A	811	CLA	C1B-NB	-2.15	1.35	1.37
25	c	314	CLA	MG-NC	2.15	2.11	2.06
25	B	826	CLA	MG-NB	2.15	2.10	2.05
25	b	207	CLA	C1B-NB	-2.15	1.35	1.37
25	j	203	CLA	C1B-NB	-2.15	1.35	1.37
25	j	205	CLA	CHC-C1C	2.15	1.42	1.38
25	k	209	CLA	MG-NC	2.15	2.11	2.06
25	B	836	CLA	MG-NC	2.15	2.11	2.06
25	k	206	CLA	MG-NB	2.15	2.10	2.05
25	e	212	CLA	CHC-C1C	2.15	1.42	1.38
35	e	209	CHL	MG-NC	2.15	2.11	2.06
25	b	209	CLA	MG-NB	2.15	2.10	2.05
25	j	213	CLA	MG-NC	2.15	2.11	2.06
25	l	602	CLA	C1B-NB	-2.15	1.35	1.37
25	o	608	CLA	C1B-NB	-2.15	1.35	1.37
25	A	831	CLA	C1B-NB	-2.15	1.35	1.37
25	n	201	CLA	C1B-NB	-2.15	1.35	1.37
25	a	204	CLA	CHB-C1B	-2.15	1.34	1.39
25	l	607	CLA	MG-NB	2.15	2.10	2.05
25	B	819	CLA	C1B-NB	-2.14	1.35	1.37
25	e	206	CLA	C1B-NB	-2.14	1.35	1.37
25	A	857	CLA	MG-NB	2.14	2.10	2.05
25	f	605	CLA	MG-NC	2.14	2.11	2.06
25	j	209	CLA	C1B-NB	-2.14	1.35	1.37
25	A	824	CLA	CHC-C1C	2.14	1.42	1.38
25	A	804	CLA	C1B-NB	-2.14	1.35	1.37
25	B	802	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	203	CLA	MG-NB	2.14	2.10	2.05
25	k	202	CLA	MG-NC	2.14	2.11	2.06
25	A	850	CLA	C1B-NB	-2.14	1.35	1.37
25	i	204	CLA	C1B-NB	-2.14	1.35	1.37
25	B	808	CLA	CHC-C1C	2.14	1.42	1.38
25	J	103	CLA	MG-NC	2.14	2.11	2.06
25	A	853	CLA	CHC-C1C	2.14	1.42	1.38
25	e	217	CLA	MG-NC	2.14	2.11	2.06
25	h	208	CLA	CHC-C1C	2.14	1.42	1.38
25	a	206	CLA	C1B-NB	-2.14	1.35	1.37
25	i	202	CLA	C1B-NB	-2.14	1.35	1.37
25	f	604	CLA	MG-NC	2.14	2.11	2.06
25	f	611	CLA	MG-NC	2.14	2.11	2.06
25	o	606	CLA	MG-NC	2.14	2.11	2.06
25	o	602	CLA	MG-NB	2.14	2.10	2.05
25	B	843	CLA	CHC-C1C	2.14	1.42	1.38
25	h	206	CLA	MG-NC	2.14	2.11	2.06
25	g	203	CLA	C1B-NB	-2.14	1.35	1.37
25	d	305	CLA	CHC-C1C	2.14	1.42	1.38
25	A	814	CLA	MG-NC	2.14	2.11	2.06
25	l	605	CLA	MG-NC	2.14	2.11	2.06
25	m	211	CLA	MG-NC	2.14	2.11	2.06
25	p	601	CLA	CHB-C1B	-2.14	1.34	1.39
25	i	211	CLA	C1B-NB	-2.14	1.35	1.37
30	j	216	DD6	C19-C20	-2.14	1.49	1.52
25	b	210	CLA	MG-NB	2.14	2.10	2.05
25	B	843	CLA	MG-NC	2.14	2.11	2.06
25	p	604	CLA	MG-NC	2.14	2.11	2.06
25	h	206	CLA	C1B-NB	-2.14	1.35	1.37
25	B	837	CLA	MG-NC	2.14	2.11	2.06
25	l	602	CLA	MG-NB	2.14	2.10	2.05
30	i	214	DD6	C19-C20	-2.14	1.49	1.52
25	k	206	CLA	C1B-NB	-2.14	1.35	1.37
25	j	211	CLA	CHC-C1C	2.14	1.42	1.38
25	k	212	CLA	MG-NC	2.14	2.11	2.06
25	A	829	CLA	C3B-C4B	2.13	1.47	1.42
25	B	820	CLA	CHC-C1C	2.13	1.42	1.38
25	i	206	CLA	C1B-NB	-2.13	1.35	1.37
25	A	857	CLA	MG-NC	2.13	2.11	2.06
25	g	209	CLA	CHB-C1B	-2.13	1.34	1.39
25	k	214	CLA	MG-NB	2.13	2.10	2.05
25	k	205	CLA	MG-NB	2.13	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	301	CLA	MG-NB	2.13	2.10	2.05
25	d	305	CLA	MG-NB	2.13	2.10	2.05
33	D	200	SQD	O9-S	2.13	1.51	1.45
25	m	206	CLA	MG-NC	2.13	2.11	2.06
25	A	816	CLA	C1B-NB	-2.13	1.35	1.37
25	B	842	CLA	MG-NC	2.13	2.11	2.06
25	i	202	CLA	MG-NB	2.13	2.10	2.05
25	A	846	CLA	C1B-NB	-2.13	1.35	1.37
25	A	851	CLA	C1B-NB	-2.13	1.35	1.37
25	b	205	CLA	MG-NC	2.13	2.11	2.06
25	l	610	CLA	MG-NC	2.13	2.11	2.06
25	d	313	CLA	MG-NC	2.13	2.11	2.06
25	l	604	CLA	MG-NC	2.13	2.11	2.06
25	e	205	CLA	C1B-NB	-2.13	1.35	1.37
25	A	815	CLA	CHC-C1C	2.13	1.42	1.38
25	e	207	CLA	MG-NB	2.13	2.10	2.05
25	l	608	CLA	MG-NC	2.13	2.11	2.06
25	l	606	CLA	MG-NB	2.13	2.10	2.05
32	b	202	DGD	O2G-C1B	2.13	1.40	1.34
25	a	205	CLA	C1B-NB	-2.13	1.35	1.37
25	e	201	CLA	C1B-NB	-2.13	1.35	1.37
25	B	811	CLA	MG-NB	2.13	2.10	2.05
25	i	209	CLA	MG-NB	2.13	2.10	2.05
25	A	827	CLA	MG-NC	2.13	2.11	2.06
25	A	829	CLA	MG-NC	2.13	2.11	2.06
25	b	208	CLA	MG-NC	2.13	2.11	2.06
25	b	213	CLA	MG-NC	2.13	2.11	2.06
32	b	202	DGD	C3E-C2E	2.13	1.57	1.52
25	A	833	CLA	MG-NB	2.13	2.10	2.05
25	i	213	CLA	MG-NC	2.13	2.11	2.06
25	B	809	CLA	C1B-NB	-2.13	1.35	1.37
25	d	315	CLA	CHB-C1B	-2.13	1.34	1.39
25	j	204	CLA	CHB-C1B	-2.13	1.34	1.39
25	o	604	CLA	MG-NC	2.13	2.11	2.06
25	a	206	CLA	MG-NC	2.13	2.11	2.06
30	f	614	DD6	C35-C36	-2.13	1.47	1.51
25	g	214	CLA	MG-NC	2.12	2.11	2.06
25	B	803	CLA	CHB-C1B	-2.12	1.34	1.39
25	p	608	CLA	CHB-C1B	-2.12	1.34	1.39
35	d	309	CHL	MG-NC	2.12	2.11	2.06
25	k	213	CLA	MG-NC	2.12	2.11	2.06
25	e	217	CLA	MG-NB	2.12	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	808	CLA	MG-NC	2.12	2.11	2.06
25	A	830	CLA	C1B-NB	-2.12	1.35	1.37
25	B	836	CLA	MG-NB	2.12	2.10	2.05
25	B	823	CLA	MG-NB	2.12	2.10	2.05
25	a	213	CLA	MG-NC	2.12	2.11	2.06
25	c	308	CLA	C1B-NB	-2.12	1.35	1.37
25	j	215	CLA	C1B-NB	-2.12	1.35	1.37
25	c	306	CLA	MG-NC	2.12	2.11	2.06
25	g	204	CLA	CHB-C1B	-2.12	1.34	1.39
25	o	610	CLA	CHB-C1B	-2.12	1.34	1.39
25	b	210	CLA	MG-NC	2.12	2.11	2.06
25	g	210	CLA	MG-NB	2.12	2.10	2.05
25	g	213	CLA	MG-NC	2.12	2.11	2.06
25	B	847	CLA	C1B-NB	-2.12	1.35	1.37
25	B	814	CLA	MG-NB	2.12	2.10	2.05
25	A	845	CLA	MG-NC	2.12	2.11	2.06
25	o	609	CLA	MG-NC	2.12	2.11	2.06
25	b	209	CLA	MG-NC	2.12	2.11	2.06
25	B	824	CLA	MG-NB	2.12	2.10	2.05
25	A	841	CLA	C1B-NB	-2.11	1.35	1.37
25	A	847	CLA	C1B-NB	-2.11	1.35	1.37
25	B	840	CLA	C1B-NB	-2.11	1.35	1.37
30	n	212	DD6	O1-C20	-2.11	1.43	1.46
35	d	310	CHL	MG-NC	2.11	2.11	2.06
25	A	822	CLA	C1B-NB	-2.11	1.35	1.37
25	a	212	CLA	C1B-NB	-2.11	1.35	1.37
25	g	215	CLA	MG-NC	2.11	2.11	2.06
25	h	211	CLA	C1B-NB	-2.11	1.35	1.37
25	B	841	CLA	MG-NC	2.11	2.11	2.06
25	B	815	CLA	MG-NB	2.11	2.10	2.05
25	B	826	CLA	C3B-C4B	2.11	1.47	1.42
25	h	214	CLA	MG-NC	2.11	2.11	2.06
25	B	802	CLA	MG-NC	2.11	2.11	2.06
25	h	205	CLA	MG-NB	2.11	2.10	2.05
25	A	827	CLA	C1B-NB	-2.11	1.35	1.37
25	k	211	CLA	C1B-NB	-2.11	1.35	1.37
25	i	212	CLA	MG-NC	2.11	2.11	2.06
25	B	809	CLA	MG-NC	2.11	2.11	2.06
25	J	103	CLA	C1B-NB	-2.11	1.35	1.37
25	k	204	CLA	C1B-NB	-2.11	1.35	1.37
25	g	212	CLA	C1B-NB	-2.11	1.35	1.37
25	h	215	CLA	MG-NB	2.11	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	k	204	CLA	MG-NC	2.11	2.11	2.06
25	B	807	CLA	CHC-C1C	2.11	1.42	1.38
25	m	208	CLA	MG-NC	2.11	2.11	2.06
25	c	302	CLA	MG-NB	2.11	2.10	2.05
25	B	844	CLA	MG-NC	2.11	2.11	2.06
25	B	847	CLA	MG-NC	2.11	2.11	2.06
25	B	808	CLA	MG-NB	2.11	2.10	2.05
25	B	842	CLA	C1B-NB	-2.11	1.35	1.37
25	b	212	CLA	C1B-NB	-2.11	1.35	1.37
25	A	806	CLA	MG-NC	2.11	2.11	2.06
25	h	206	CLA	MG-NB	2.11	2.10	2.05
25	A	826	CLA	MG-NC	2.11	2.11	2.06
25	g	211	CLA	C1B-NB	-2.11	1.35	1.37
25	n	209	CLA	MG-NC	2.11	2.11	2.06
25	c	302	CLA	C1B-NB	-2.11	1.35	1.37
34	k	201	LMG	O8-C28	2.10	1.39	1.33
25	p	603	CLA	CHB-C1B	-2.10	1.34	1.39
25	e	207	CLA	MG-NC	2.10	2.11	2.06
25	j	207	CLA	C1B-NB	-2.10	1.35	1.37
25	k	213	CLA	C1B-NB	-2.10	1.35	1.37
25	f	609	CLA	CHC-C1C	2.10	1.42	1.38
25	B	821	CLA	MG-NB	2.10	2.10	2.05
25	g	212	CLA	MG-NC	2.10	2.11	2.06
25	A	842	CLA	MG-NB	2.10	2.10	2.05
25	h	210	CLA	MG-NC	2.10	2.11	2.06
25	i	206	CLA	MG-NB	2.10	2.10	2.05
25	A	853	CLA	MG-NC	2.10	2.11	2.06
25	c	309	CLA	MG-NC	2.10	2.11	2.06
25	p	607	CLA	CAA-C2A	2.10	1.58	1.54
25	d	303	CLA	MG-NC	2.10	2.11	2.06
25	e	207	CLA	C1B-NB	-2.10	1.35	1.37
25	B	812	CLA	MG-NC	2.10	2.11	2.06
25	F	202	CLA	CHC-C1C	2.10	1.42	1.38
25	e	208	CLA	MG-NC	2.10	2.11	2.06
25	i	205	CLA	MG-NC	2.10	2.11	2.06
25	A	822	CLA	MG-NB	2.10	2.09	2.05
25	g	206	CLA	C1B-NB	-2.10	1.35	1.37
25	B	825	CLA	MG-NC	2.10	2.11	2.06
25	A	832	CLA	MG-NB	2.10	2.09	2.05
25	h	209	CLA	CHB-C1B	-2.10	1.34	1.39
25	A	828	CLA	MG-NC	2.10	2.11	2.06
25	h	215	CLA	C1B-NB	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	m	204	CLA	C1B-NB	-2.10	1.35	1.37
25	i	213	CLA	C1B-NB	-2.10	1.35	1.37
25	o	605	CLA	MG-NC	2.10	2.11	2.06
25	c	304	CLA	CHC-C1C	2.10	1.42	1.38
25	j	206	CLA	MG-NB	2.10	2.09	2.05
35	d	307	CHL	MG-NC	2.10	2.11	2.06
30	c	316	DD6	C19-C20	-2.09	1.49	1.52
25	d	315	CLA	MG-NC	2.09	2.11	2.06
25	k	211	CLA	MG-NC	2.09	2.11	2.06
25	g	206	CLA	MG-NC	2.09	2.11	2.06
28	B	827	PQN	C11-C3	-2.09	1.48	1.51
25	B	844	CLA	C1B-NB	-2.09	1.35	1.37
25	b	204	CLA	MG-NB	2.09	2.09	2.05
25	i	202	CLA	MG-NC	2.09	2.11	2.06
25	B	815	CLA	MG-NC	2.09	2.11	2.06
25	A	814	CLA	C1B-NB	-2.09	1.35	1.37
25	a	207	CLA	MG-NC	2.09	2.11	2.06
25	B	825	CLA	C1B-NB	-2.09	1.35	1.37
25	j	212	CLA	MG-NB	2.09	2.09	2.05
25	g	212	CLA	MG-NB	2.09	2.09	2.05
25	g	203	CLA	CHC-C1C	2.09	1.42	1.38
25	i	207	CLA	MG-NC	2.09	2.11	2.06
25	B	837	CLA	C1B-NB	-2.09	1.35	1.37
25	c	313	CLA	MG-NB	2.09	2.09	2.05
25	h	210	CLA	MG-NB	2.09	2.09	2.05
25	A	801	CLA	MG-NC	2.09	2.11	2.06
25	A	817	CLA	C1B-NB	-2.09	1.35	1.37
25	B	848	CLA	C1B-NB	-2.09	1.35	1.37
25	A	804	CLA	MG-NC	2.09	2.11	2.06
25	k	203	CLA	MG-NB	2.09	2.09	2.05
25	b	204	CLA	MG-NC	2.09	2.11	2.06
25	c	312	CLA	C1B-NB	-2.09	1.35	1.37
25	h	208	CLA	MG-NB	2.09	2.09	2.05
32	b	202	DGD	C4E-C3E	2.09	1.57	1.52
25	A	857	CLA	C1B-NB	-2.09	1.35	1.37
25	B	820	CLA	MG-NB	2.09	2.09	2.05
25	B	813	CLA	C1B-NB	-2.09	1.35	1.37
25	k	214	CLA	MG-NC	2.09	2.11	2.06
25	d	312	CLA	MG-NC	2.09	2.11	2.06
25	i	209	CLA	MG-NC	2.09	2.11	2.06
25	J	103	CLA	CHC-C1C	2.09	1.42	1.38
33	D	200	SQD	O7-S	2.09	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	207	CLA	MG-NB	2.09	2.09	2.05
25	h	205	CLA	MG-NC	2.08	2.11	2.06
25	k	205	CLA	MG-NC	2.08	2.11	2.06
30	c	318	DD6	O1-C20	-2.08	1.43	1.46
25	i	210	CLA	C1B-NB	-2.08	1.35	1.37
25	j	214	CLA	MG-NC	2.08	2.11	2.06
25	j	215	CLA	MG-NC	2.08	2.11	2.06
25	d	315	CLA	C1B-NB	-2.08	1.35	1.37
25	n	208	CLA	C1B-NB	-2.08	1.35	1.37
25	A	830	CLA	MG-NB	2.08	2.09	2.05
25	k	208	CLA	MG-NB	2.08	2.09	2.05
25	i	203	CLA	MG-NB	2.08	2.09	2.05
25	d	313	CLA	C1B-NB	-2.08	1.35	1.37
33	g	202	SQD	O7-S	2.08	1.51	1.45
25	b	205	CLA	C1B-NB	-2.08	1.35	1.37
25	o	607	CLA	MG-NC	2.08	2.11	2.06
33	F	204	SQD	C8-C7	2.08	1.56	1.50
25	c	302	CLA	MG-NC	2.08	2.11	2.06
25	c	314	CLA	C1B-NB	-2.08	1.35	1.37
25	B	814	CLA	MG-NC	2.08	2.11	2.06
25	i	211	CLA	MG-NB	2.08	2.09	2.05
25	l	606	CLA	C1B-NB	-2.08	1.35	1.37
25	o	605	CLA	C1B-NB	-2.08	1.35	1.37
25	B	818	CLA	MG-NC	2.08	2.11	2.06
25	B	819	CLA	MG-NC	2.08	2.11	2.06
25	A	843	CLA	MG-NC	2.08	2.11	2.06
25	d	303	CLA	MG-NB	2.08	2.09	2.05
25	j	210	CLA	MG-NB	2.08	2.09	2.05
29	A	836	BCR	C1-C6	-2.08	1.50	1.53
25	g	209	CLA	MG-NB	2.08	2.09	2.05
25	o	601	CLA	C1B-NB	-2.08	1.35	1.37
25	p	608	CLA	MG-NC	2.08	2.11	2.06
25	h	208	CLA	MG-NC	2.08	2.11	2.06
25	a	204	CLA	C1B-NB	-2.08	1.35	1.37
25	B	804	CLA	MG-NC	2.08	2.11	2.06
25	i	206	CLA	MG-NC	2.08	2.11	2.06
25	B	839	CLA	MG-NB	2.07	2.09	2.05
25	h	204	CLA	MG-NC	2.07	2.11	2.06
25	A	820	CLA	MG-NB	2.07	2.09	2.05
25	A	819	CLA	MG-NB	2.07	2.09	2.05
25	A	849	CLA	CHC-C1C	2.07	1.42	1.38
25	j	203	CLA	MG-NC	2.07	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	203	CLA	C1B-NB	-2.07	1.35	1.37
25	B	839	CLA	MG-NC	2.07	2.11	2.06
25	c	313	CLA	MG-NC	2.07	2.11	2.06
25	B	810	CLA	MG-NC	2.07	2.11	2.06
25	B	815	CLA	C1B-NB	-2.07	1.35	1.37
25	B	806	CLA	MG-NC	2.07	2.11	2.06
25	A	844	CLA	C1B-NB	-2.07	1.35	1.37
25	A	812	CLA	MG-NB	2.07	2.09	2.05
25	A	844	CLA	MG-NB	2.07	2.09	2.05
25	c	309	CLA	C1B-NB	-2.07	1.35	1.37
25	h	203	CLA	C1B-NB	-2.07	1.35	1.37
25	b	208	CLA	MG-NB	2.07	2.09	2.05
25	A	845	CLA	CHC-C1C	2.07	1.42	1.38
25	a	209	CLA	MG-NB	2.07	2.09	2.05
32	e	203	DGD	O2G-C2G	-2.07	1.41	1.46
25	A	848	CLA	MG-NC	2.07	2.11	2.06
25	m	207	CLA	MG-NC	2.07	2.11	2.06
25	l	605	CLA	MG-NB	2.07	2.09	2.05
25	A	810	CLA	MG-NC	2.07	2.11	2.06
25	b	206	CLA	MG-NC	2.07	2.11	2.06
25	A	808	CLA	C1B-NB	-2.07	1.35	1.37
25	A	828	CLA	C1B-NB	-2.07	1.35	1.37
25	e	210	CLA	C1B-NB	-2.07	1.35	1.37
25	F	201	CLA	C1B-NB	-2.07	1.35	1.37
25	l	609	CLA	C1B-NB	-2.07	1.35	1.37
25	A	808	CLA	MG-NC	2.07	2.11	2.06
25	B	822	CLA	MG-NB	2.06	2.09	2.05
25	B	838	CLA	MG-NB	2.06	2.09	2.05
25	k	208	CLA	C1B-NB	-2.06	1.35	1.37
25	d	311	CLA	MG-NC	2.06	2.11	2.06
25	b	206	CLA	MG-NB	2.06	2.09	2.05
25	A	815	CLA	MG-NC	2.06	2.11	2.06
34	e	202	LMG	O7-C8	-2.06	1.41	1.46
25	A	816	CLA	CHC-C1C	2.06	1.42	1.38
25	i	209	CLA	C1B-NB	-2.06	1.35	1.37
25	a	208	CLA	MG-NB	2.06	2.09	2.05
25	j	208	CLA	MG-NC	2.06	2.11	2.06
25	e	208	CLA	C1B-NB	-2.06	1.35	1.37
25	a	213	CLA	C1B-NB	-2.06	1.35	1.37
25	c	306	CLA	C1B-NB	-2.06	1.35	1.37
25	n	207	CLA	C1B-NB	-2.06	1.35	1.37
25	e	201	CLA	MG-NC	2.06	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	201	CLA	CHB-C1B	-2.06	1.34	1.39
25	A	822	CLA	MG-NC	2.06	2.11	2.06
25	n	207	CLA	MG-NB	2.06	2.09	2.05
25	A	840	CLA	MG-NC	2.06	2.11	2.06
25	g	208	CLA	MG-NC	2.06	2.11	2.06
25	k	207	CLA	MG-NB	2.06	2.09	2.05
25	e	205	CLA	MG-NC	2.06	2.11	2.06
25	l	602	CLA	MG-NC	2.06	2.11	2.06
25	h	215	CLA	MG-NC	2.06	2.11	2.06
25	i	207	CLA	C1B-NB	-2.05	1.35	1.37
25	A	846	CLA	MG-NB	2.05	2.09	2.05
25	e	213	CLA	MG-NB	2.05	2.09	2.05
25	k	207	CLA	MG-NC	2.05	2.11	2.06
25	e	213	CLA	MG-NC	2.05	2.11	2.06
25	h	210	CLA	C1B-NB	-2.05	1.35	1.37
25	A	808	CLA	MG-NB	2.05	2.09	2.05
25	B	811	CLA	MG-NC	2.05	2.11	2.06
25	p	603	CLA	C1D-ND	-2.05	1.35	1.37
25	B	821	CLA	MG-NC	2.05	2.11	2.06
25	e	210	CLA	MG-NC	2.05	2.11	2.06
25	a	208	CLA	MG-NC	2.05	2.11	2.06
25	e	211	CLA	MG-NC	2.05	2.11	2.06
25	p	605	CLA	C1B-NB	-2.05	1.35	1.37
25	A	820	CLA	CHC-C1C	2.05	1.42	1.38
25	B	842	CLA	MG-NB	2.05	2.09	2.05
25	i	204	CLA	CHC-C1C	2.05	1.42	1.38
25	b	213	CLA	C1B-NB	-2.05	1.35	1.37
25	c	315	CLA	C1B-NB	-2.05	1.35	1.37
29	A	837	BCR	C15-C14	-2.05	1.37	1.43
25	k	208	CLA	MG-NC	2.05	2.11	2.06
25	k	203	CLA	C1B-NB	-2.05	1.35	1.37
25	e	211	CLA	C1B-NB	-2.04	1.35	1.37
29	B	830	BCR	C30-C25	-2.04	1.51	1.53
25	h	209	CLA	MG-NB	2.04	2.09	2.05
25	c	308	CLA	MG-NC	2.04	2.11	2.06
25	A	821	CLA	MG-NB	2.04	2.09	2.05
25	j	208	CLA	MG-NB	2.04	2.09	2.05
25	A	818	CLA	MG-NC	2.04	2.11	2.06
25	g	209	CLA	MG-NC	2.04	2.11	2.06
25	o	603	CLA	C1B-NB	-2.04	1.35	1.37
25	m	206	CLA	MG-NB	2.04	2.09	2.05
25	d	315	CLA	MG-NB	2.04	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	210	CLA	C1B-NB	-2.04	1.35	1.37
25	B	840	CLA	MG-NC	2.04	2.11	2.06
25	B	845	CLA	MG-NC	2.04	2.11	2.06
25	h	213	CLA	MG-NC	2.04	2.11	2.06
25	e	212	CLA	C1B-NB	-2.04	1.35	1.37
25	A	820	CLA	MG-NC	2.04	2.11	2.06
25	c	303	CLA	C3D-C4D	-2.04	1.39	1.44
25	j	210	CLA	MG-NC	2.04	2.11	2.06
25	B	824	CLA	MG-NC	2.04	2.11	2.06
25	A	819	CLA	MG-NC	2.03	2.11	2.06
25	g	210	CLA	MG-NC	2.03	2.11	2.06
25	A	845	CLA	MG-NB	2.03	2.09	2.05
25	l	606	CLA	MG-NC	2.03	2.11	2.06
25	m	210	CLA	C1B-NB	-2.03	1.35	1.37
25	c	310	CLA	MG-NC	2.03	2.11	2.06
25	a	207	CLA	C1B-NB	-2.03	1.35	1.37
25	g	208	CLA	C1B-NB	-2.03	1.35	1.37
25	h	212	CLA	MG-NB	2.03	2.09	2.05
25	A	817	CLA	MG-NC	2.03	2.11	2.06
25	A	832	CLA	C1B-NB	-2.03	1.35	1.37
25	a	209	CLA	C1B-NB	-2.03	1.35	1.37
25	e	216	CLA	MG-NB	2.03	2.09	2.05
33	F	204	SQD	O7-S	2.03	1.51	1.45
30	m	213	DD6	C19-C20	-2.03	1.49	1.52
25	B	805	CLA	MG-NC	2.03	2.11	2.06
25	m	203	CLA	C1B-NB	-2.03	1.35	1.37
25	m	205	CLA	C1B-NB	-2.03	1.35	1.37
25	A	833	CLA	MG-NC	2.03	2.11	2.06
25	n	210	CLA	C1B-NB	-2.03	1.35	1.37
25	p	608	CLA	C1B-NB	-2.03	1.35	1.37
25	A	817	CLA	MG-NB	2.03	2.09	2.05
25	h	213	CLA	C1B-NB	-2.03	1.35	1.37
25	A	817	CLA	C3D-C4D	-2.03	1.39	1.44
25	k	203	CLA	MG-NC	2.03	2.11	2.06
25	k	205	CLA	C1B-NB	-2.02	1.35	1.37
25	B	818	CLA	C1B-NB	-2.02	1.35	1.37
25	l	604	CLA	C1B-NB	-2.02	1.35	1.37
25	d	311	CLA	C1B-NB	-2.02	1.35	1.37
25	B	810	CLA	MG-NB	2.02	2.09	2.05
25	c	303	CLA	MG-NC	2.02	2.11	2.06
25	d	304	CLA	MG-NB	2.02	2.09	2.05
25	A	807	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	846	CLA	MG-NC	2.02	2.11	2.06
25	g	214	CLA	C1B-NB	-2.02	1.35	1.37
25	B	806	CLA	MG-NB	2.02	2.09	2.05
25	B	848	CLA	MG-NC	2.02	2.11	2.06
29	A	837	BCR	C20-C21	-2.02	1.37	1.43
25	B	822	CLA	MG-NC	2.02	2.11	2.06
25	m	202	CLA	CHC-C1C	2.02	1.42	1.38
25	A	826	CLA	MG-NB	2.02	2.09	2.05
25	A	832	CLA	MG-NC	2.02	2.11	2.06
25	i	211	CLA	MG-NC	2.02	2.11	2.06
25	f	602	CLA	MG-NC	2.02	2.11	2.06
25	B	802	CLA	C1B-NB	-2.02	1.35	1.37
25	A	844	CLA	MG-NC	2.02	2.11	2.06
25	g	204	CLA	MG-NC	2.02	2.11	2.06
25	B	848	CLA	MG-NB	2.02	2.09	2.05
25	B	825	CLA	MG-NB	2.02	2.09	2.05
25	A	841	CLA	MG-NB	2.01	2.09	2.05
25	A	851	CLA	MG-NB	2.01	2.09	2.05
25	n	207	CLA	CAA-C2A	2.01	1.57	1.53
25	c	305	CLA	C1B-NB	-2.01	1.35	1.37
25	A	851	CLA	MG-NC	2.01	2.11	2.06
25	A	841	CLA	MG-NC	2.01	2.11	2.06
25	A	809	CLA	C3D-C4D	-2.01	1.39	1.44
25	A	850	CLA	MG-NB	2.01	2.09	2.05
25	h	204	CLA	MG-NB	2.01	2.09	2.05
25	p	604	CLA	C1B-NB	-2.01	1.35	1.37
25	B	819	CLA	MG-NB	2.01	2.09	2.05
25	B	816	CLA	MG-NB	2.01	2.09	2.05
25	f	610	CLA	C1B-NB	-2.01	1.35	1.37
25	o	601	CLA	CAA-C2A	2.01	1.57	1.53
35	c	307	CHL	MG-NC	2.01	2.11	2.06
25	j	213	CLA	C1B-NB	-2.01	1.35	1.37
25	B	838	CLA	MG-NC	2.01	2.11	2.06
25	A	807	CLA	MG-NB	2.01	2.09	2.05
25	h	203	CLA	MG-NC	2.01	2.11	2.06
32	b	202	DGD	O1G-C1A	2.00	1.39	1.33
25	n	202	CLA	C1B-NB	-2.00	1.35	1.37
25	i	205	CLA	MG-NB	2.00	2.09	2.05
25	i	203	CLA	C3D-C4D	-2.00	1.39	1.44
25	f	603	CLA	C1B-NB	-2.00	1.35	1.37
25	e	205	CLA	MG-NB	2.00	2.09	2.05
25	j	215	CLA	MG-NB	2.00	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	301	CLA	CAA-C2A	2.00	1.57	1.53

All (3426) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	823	CLA	C4A-NA-C1A	11.56	111.90	106.71
25	k	204	CLA	C4A-NA-C1A	11.50	111.88	106.71
25	B	803	CLA	C4A-NA-C1A	11.20	111.74	106.71
25	o	608	CLA	C4A-NA-C1A	11.17	111.73	106.71
25	A	826	CLA	C4A-NA-C1A	11.10	111.70	106.71
35	e	209	CHL	C4A-NA-C1A	11.10	111.70	106.71
25	l	612	CLA	C4A-NA-C1A	11.01	111.66	106.71
25	A	815	CLA	C4A-NA-C1A	10.97	111.64	106.71
35	c	307	CHL	C4A-NA-C1A	10.96	111.63	106.71
25	B	846	CLA	C4A-NA-C1A	10.95	111.63	106.71
35	d	308	CHL	C4A-NA-C1A	10.89	111.60	106.71
25	p	602	CLA	C4A-NA-C1A	10.83	111.58	106.71
25	A	810	CLA	C4A-NA-C1A	10.79	111.56	106.71
25	B	811	CLA	C4A-NA-C1A	10.78	111.55	106.71
25	d	301	CLA	C4A-NA-C1A	10.75	111.54	106.71
35	d	307	CHL	C4A-NA-C1A	10.72	111.53	106.71
25	A	852	CLA	C4A-NA-C1A	10.71	111.52	106.71
25	h	205	CLA	C4A-NA-C1A	10.68	111.51	106.71
25	A	853	CLA	C4A-NA-C1A	10.66	111.50	106.71
25	d	303	CLA	C4A-NA-C1A	10.65	111.50	106.71
25	n	210	CLA	C4A-NA-C1A	10.64	111.49	106.71
25	B	804	CLA	C4A-NA-C1A	10.59	111.47	106.71
25	f	605	CLA	C4A-NA-C1A	10.59	111.47	106.71
25	d	305	CLA	C4A-NA-C1A	10.57	111.46	106.71
25	m	205	CLA	C4A-NA-C1A	10.56	111.45	106.71
25	f	608	CLA	C4A-NA-C1A	10.53	111.44	106.71
25	B	807	CLA	C4A-NA-C1A	10.53	111.44	106.71
25	e	215	CLA	C4A-NA-C1A	10.50	111.42	106.71
25	A	843	CLA	C4A-NA-C1A	10.48	111.42	106.71
25	h	214	CLA	C4A-NA-C1A	10.44	111.40	106.71
25	A	806	CLA	C4A-NA-C1A	10.44	111.40	106.71
25	A	846	CLA	C4A-NA-C1A	10.41	111.39	106.71
25	A	820	CLA	C4A-NA-C1A	10.38	111.37	106.71
25	j	207	CLA	C4A-NA-C1A	10.38	111.37	106.71
25	n	208	CLA	C4A-NA-C1A	10.38	111.37	106.71
25	k	206	CLA	C4A-NA-C1A	10.36	111.36	106.71
25	a	211	CLA	C4A-NA-C1A	10.35	111.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	i	206	CLA	C4A-NA-C1A	10.34	111.35	106.71
25	F	201	CLA	C4A-NA-C1A	10.33	111.35	106.71
25	B	845	CLA	C4A-NA-C1A	10.32	111.34	106.71
25	B	837	CLA	C4A-NA-C1A	10.31	111.34	106.71
25	B	848	CLA	C4A-NA-C1A	10.31	111.34	106.71
25	l	611	CLA	C4A-NA-C1A	10.30	111.34	106.71
25	j	206	CLA	C4A-NA-C1A	10.30	111.34	106.71
25	d	314	CLA	C4A-NA-C1A	10.29	111.33	106.71
25	j	215	CLA	C4A-NA-C1A	10.29	111.33	106.71
25	B	839	CLA	C4A-NA-C1A	10.28	111.33	106.71
25	j	214	CLA	C4A-NA-C1A	10.26	111.32	106.71
25	k	213	CLA	C4A-NA-C1A	10.26	111.32	106.71
25	l	603	CLA	C4A-NA-C1A	10.26	111.32	106.71
25	A	808	CLA	C4A-NA-C1A	10.25	111.31	106.71
25	n	201	CLA	C4A-NA-C1A	10.23	111.31	106.71
25	e	201	CLA	C4A-NA-C1A	10.23	111.30	106.71
25	B	844	CLA	C4A-NA-C1A	10.22	111.30	106.71
25	c	312	CLA	C4A-NA-C1A	10.21	111.30	106.71
25	i	207	CLA	C4A-NA-C1A	10.21	111.29	106.71
25	g	211	CLA	C4A-NA-C1A	10.20	111.29	106.71
25	d	311	CLA	C4A-NA-C1A	10.18	111.28	106.71
35	d	309	CHL	C4A-NA-C1A	10.18	111.28	106.71
25	k	211	CLA	C4A-NA-C1A	10.17	111.28	106.71
25	i	213	CLA	C4A-NA-C1A	10.16	111.28	106.71
25	B	822	CLA	C4A-NA-C1A	10.15	111.27	106.71
25	g	212	CLA	C4A-NA-C1A	10.15	111.27	106.71
25	f	603	CLA	C4A-NA-C1A	10.15	111.27	106.71
25	l	606	CLA	C4A-NA-C1A	10.15	111.27	106.71
25	b	205	CLA	C4A-NA-C1A	10.14	111.26	106.71
25	f	612	CLA	C4A-NA-C1A	10.13	111.26	106.71
25	g	207	CLA	C4A-NA-C1A	10.12	111.26	106.71
25	m	210	CLA	C4A-NA-C1A	10.12	111.25	106.71
25	e	208	CLA	C4A-NA-C1A	10.11	111.25	106.71
25	i	209	CLA	C4A-NA-C1A	10.11	111.25	106.71
25	B	847	CLA	C4A-NA-C1A	10.11	111.25	106.71
25	i	210	CLA	C4A-NA-C1A	10.10	111.25	106.71
25	B	826	CLA	C4A-NA-C1A	10.09	111.24	106.71
25	g	214	CLA	C4A-NA-C1A	10.09	111.24	106.71
25	b	207	CLA	C4A-NA-C1A	10.08	111.24	106.71
25	h	207	CLA	C4A-NA-C1A	10.08	111.24	106.71
25	A	816	CLA	C4A-NA-C1A	10.08	111.24	106.71
25	B	812	CLA	C4A-NA-C1A	10.07	111.23	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	848	CLA	C4A-NA-C1A	10.07	111.23	106.71
25	J	103	CLA	C4A-NA-C1A	10.06	111.23	106.71
25	A	827	CLA	C4A-NA-C1A	10.06	111.23	106.71
25	A	809	CLA	C4A-NA-C1A	10.06	111.23	106.71
25	h	206	CLA	C4A-NA-C1A	10.05	111.22	106.71
25	n	202	CLA	C4A-NA-C1A	10.05	111.22	106.71
25	o	606	CLA	C4A-NA-C1A	10.05	111.22	106.71
25	l	609	CLA	C4A-NA-C1A	10.03	111.22	106.71
25	A	828	CLA	C4A-NA-C1A	10.03	111.22	106.71
25	A	811	CLA	C4A-NA-C1A	10.02	111.21	106.71
25	e	210	CLA	C4A-NA-C1A	10.01	111.21	106.71
25	b	212	CLA	C4A-NA-C1A	10.01	111.21	106.71
25	o	609	CLA	C4A-NA-C1A	10.01	111.20	106.71
35	d	310	CHL	C4A-NA-C1A	10.00	111.20	106.71
25	g	213	CLA	C4A-NA-C1A	9.99	111.20	106.71
25	B	805	CLA	C4A-NA-C1A	9.99	111.20	106.71
25	c	309	CLA	C4A-NA-C1A	9.98	111.19	106.71
25	o	605	CLA	C4A-NA-C1A	9.98	111.19	106.71
25	B	841	CLA	C4A-NA-C1A	9.97	111.19	106.71
25	a	209	CLA	C4A-NA-C1A	9.97	111.19	106.71
25	A	807	CLA	C4A-NA-C1A	9.97	111.19	106.71
25	B	816	CLA	C4A-NA-C1A	9.96	111.18	106.71
25	p	605	CLA	C4A-NA-C1A	9.95	111.18	106.71
25	j	205	CLA	C4A-NA-C1A	9.94	111.18	106.71
25	d	315	CLA	C4A-NA-C1A	9.94	111.17	106.71
25	e	204	CLA	C4A-NA-C1A	9.94	111.17	106.71
25	l	608	CLA	C4A-NA-C1A	9.94	111.17	106.71
25	A	804	CLA	C4A-NA-C1A	9.93	111.17	106.71
25	d	304	CLA	C4A-NA-C1A	9.92	111.17	106.71
25	A	814	CLA	C4A-NA-C1A	9.92	111.17	106.71
25	a	210	CLA	C4A-NA-C1A	9.91	111.16	106.71
25	b	206	CLA	C4A-NA-C1A	9.91	111.16	106.71
25	B	820	CLA	C4A-NA-C1A	9.91	111.16	106.71
25	k	210	CLA	C4A-NA-C1A	9.90	111.16	106.71
25	o	603	CLA	C4A-NA-C1A	9.90	111.16	106.71
25	j	213	CLA	C4A-NA-C1A	9.89	111.15	106.71
25	k	214	CLA	C4A-NA-C1A	9.89	111.15	106.71
25	B	818	CLA	C4A-NA-C1A	9.89	111.15	106.71
25	e	212	CLA	C4A-NA-C1A	9.88	111.15	106.71
25	h	203	CLA	C4A-NA-C1A	9.88	111.15	106.71
25	B	834	CLA	C4A-NA-C1A	9.88	111.15	106.71
25	j	208	CLA	C4A-NA-C1A	9.87	111.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	205	CLA	C4A-NA-C1A	9.87	111.14	106.71
25	m	206	CLA	C4A-NA-C1A	9.86	111.14	106.71
25	A	831	CLA	C4A-NA-C1A	9.85	111.14	106.71
25	e	206	CLA	C4A-NA-C1A	9.85	111.13	106.71
25	b	203	CLA	C4A-NA-C1A	9.85	111.13	106.71
25	a	213	CLA	C4A-NA-C1A	9.84	111.13	106.71
25	h	211	CLA	C4A-NA-C1A	9.84	111.13	106.71
25	b	211	CLA	C4A-NA-C1A	9.84	111.13	106.71
25	j	210	CLA	C4A-NA-C1A	9.83	111.13	106.71
25	a	205	CLA	C4A-NA-C1A	9.82	111.12	106.71
25	A	842	CLA	C4A-NA-C1A	9.82	111.12	106.71
25	B	838	CLA	C4A-NA-C1A	9.80	111.11	106.71
25	n	203	CLA	C4A-NA-C1A	9.80	111.11	106.71
25	j	204	CLA	C4A-NA-C1A	9.80	111.11	106.71
25	B	821	CLA	C4A-NA-C1A	9.79	111.11	106.71
25	o	602	CLA	C4A-NA-C1A	9.78	111.10	106.71
25	n	204	CLA	C4A-NA-C1A	9.78	111.10	106.71
25	d	312	CLA	C4A-NA-C1A	9.78	111.10	106.71
25	B	809	CLA	C4A-NA-C1A	9.77	111.10	106.71
25	p	604	CLA	C4A-NA-C1A	9.77	111.10	106.71
25	g	210	CLA	C4A-NA-C1A	9.77	111.10	106.71
25	i	202	CLA	C4A-NA-C1A	9.76	111.10	106.71
25	b	213	CLA	C4A-NA-C1A	9.72	111.08	106.71
25	l	605	CLA	C4A-NA-C1A	9.72	111.08	106.71
25	B	808	CLA	C4A-NA-C1A	9.72	111.08	106.71
25	m	207	CLA	C4A-NA-C1A	9.72	111.08	106.71
25	c	304	CLA	C4A-NA-C1A	9.72	111.07	106.71
25	d	313	CLA	C4A-NA-C1A	9.71	111.07	106.71
25	f	607	CLA	C4A-NA-C1A	9.66	111.05	106.71
25	c	306	CLA	C4A-NA-C1A	9.66	111.05	106.71
25	e	207	CLA	C4A-NA-C1A	9.66	111.05	106.71
25	c	305	CLA	C4A-NA-C1A	9.65	111.05	106.71
25	a	208	CLA	C4A-NA-C1A	9.64	111.04	106.71
25	A	813	CLA	C4A-NA-C1A	9.63	111.04	106.71
25	A	822	CLA	C4A-NA-C1A	9.63	111.03	106.71
25	a	212	CLA	C4A-NA-C1A	9.62	111.03	106.71
25	h	208	CLA	C4A-NA-C1A	9.62	111.03	106.71
25	k	212	CLA	C4A-NA-C1A	9.60	111.02	106.71
25	c	311	CLA	C4A-NA-C1A	9.59	111.02	106.71
25	A	844	CLA	C4A-NA-C1A	9.59	111.02	106.71
25	A	851	CLA	C4A-NA-C1A	9.57	111.01	106.71
25	p	606	CLA	C4A-NA-C1A	9.57	111.01	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	210	CLA	C4A-NA-C1A	9.57	111.01	106.71
25	g	215	CLA	C4A-NA-C1A	9.56	111.00	106.71
25	p	609	CLA	C4A-NA-C1A	9.56	111.00	106.71
25	B	814	CLA	C4A-NA-C1A	9.55	111.00	106.71
25	B	836	CLA	C4A-NA-C1A	9.54	111.00	106.71
25	b	209	CLA	C4A-NA-C1A	9.54	110.99	106.71
25	n	206	CLA	C4A-NA-C1A	9.52	110.98	106.71
25	g	203	CLA	C4A-NA-C1A	9.51	110.98	106.71
25	A	812	CLA	C4A-NA-C1A	9.50	110.98	106.71
25	A	857	CLA	C4A-NA-C1A	9.50	110.98	106.71
25	A	849	CLA	C4A-NA-C1A	9.49	110.97	106.71
25	j	211	CLA	C4A-NA-C1A	9.49	110.97	106.71
25	e	213	CLA	C4A-NA-C1A	9.49	110.97	106.71
25	b	208	CLA	C4A-NA-C1A	9.49	110.97	106.71
25	B	806	CLA	C4A-NA-C1A	9.48	110.97	106.71
25	e	216	CLA	C4A-NA-C1A	9.45	110.95	106.71
25	h	215	CLA	C4A-NA-C1A	9.44	110.95	106.71
25	b	204	CLA	C4A-NA-C1A	9.44	110.95	106.71
25	k	205	CLA	C4A-NA-C1A	9.44	110.95	106.71
25	e	217	CLA	C4A-NA-C1A	9.43	110.95	106.71
25	B	810	CLA	C4A-NA-C1A	9.43	110.94	106.71
25	l	610	CLA	C4A-NA-C1A	9.42	110.94	106.71
25	A	829	CLA	C4A-NA-C1A	9.41	110.94	106.71
25	B	813	CLA	C4A-NA-C1A	9.40	110.93	106.71
25	A	817	CLA	C4A-NA-C1A	9.39	110.93	106.71
25	d	306	CLA	C4A-NA-C1A	9.39	110.93	106.71
25	f	604	CLA	C4A-NA-C1A	9.39	110.93	106.71
25	m	211	CLA	C4A-NA-C1A	9.38	110.92	106.71
25	c	315	CLA	C4A-NA-C1A	9.37	110.92	106.71
25	g	208	CLA	C4A-NA-C1A	9.36	110.91	106.71
25	A	824	CLA	C4A-NA-C1A	9.36	110.91	106.71
25	k	209	CLA	C4A-NA-C1A	9.35	110.91	106.71
25	h	204	CLA	C4A-NA-C1A	9.34	110.91	106.71
25	k	207	CLA	C4A-NA-C1A	9.32	110.90	106.71
25	o	604	CLA	C4A-NA-C1A	9.31	110.89	106.71
25	b	210	CLA	C4A-NA-C1A	9.30	110.89	106.71
25	c	313	CLA	C4A-NA-C1A	9.30	110.89	106.71
25	A	821	CLA	C4A-NA-C1A	9.29	110.88	106.71
25	c	310	CLA	C4A-NA-C1A	9.29	110.88	106.71
25	i	203	CLA	C4A-NA-C1A	9.27	110.87	106.71
25	k	202	CLA	C4A-NA-C1A	9.27	110.87	106.71
25	f	606	CLA	C4A-NA-C1A	9.26	110.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	203	CLA	C4A-NA-C1A	9.26	110.87	106.71
25	i	205	CLA	C4A-NA-C1A	9.25	110.86	106.71
25	i	211	CLA	C4A-NA-C1A	9.22	110.85	106.71
25	a	207	CLA	C4A-NA-C1A	9.22	110.85	106.71
25	A	845	CLA	C4A-NA-C1A	9.21	110.85	106.71
25	a	206	CLA	C4A-NA-C1A	9.21	110.85	106.71
25	o	610	CLA	C4A-NA-C1A	9.21	110.85	106.71
25	h	212	CLA	C4A-NA-C1A	9.21	110.85	106.71
25	B	815	CLA	C4A-NA-C1A	9.21	110.84	106.71
25	A	825	CLA	C4A-NA-C1A	9.20	110.84	106.71
25	n	207	CLA	C4A-NA-C1A	9.20	110.84	106.71
25	c	314	CLA	C4A-NA-C1A	9.20	110.84	106.71
25	A	841	CLA	C4A-NA-C1A	9.19	110.84	106.71
25	F	202	CLA	C4A-NA-C1A	9.18	110.83	106.71
25	B	824	CLA	C4A-NA-C1A	9.18	110.83	106.71
25	i	204	CLA	C4A-NA-C1A	9.15	110.82	106.71
25	f	610	CLA	C4A-NA-C1A	9.14	110.81	106.71
25	A	801	CLA	C4A-NA-C1A	9.11	110.80	106.71
25	g	205	CLA	C4A-NA-C1A	9.10	110.80	106.71
25	e	205	CLA	C4A-NA-C1A	9.09	110.79	106.71
25	j	212	CLA	C4A-NA-C1A	9.07	110.78	106.71
25	h	213	CLA	C4A-NA-C1A	9.06	110.78	106.71
25	g	209	CLA	C4A-NA-C1A	9.05	110.78	106.71
25	l	601	CLA	C4A-NA-C1A	9.05	110.77	106.71
25	c	302	CLA	C4A-NA-C1A	9.04	110.77	106.71
25	m	204	CLA	C4A-NA-C1A	9.03	110.76	106.71
25	c	308	CLA	C4A-NA-C1A	9.01	110.76	106.71
25	f	611	CLA	C4A-NA-C1A	9.00	110.75	106.71
25	j	203	CLA	C4A-NA-C1A	8.99	110.75	106.71
25	l	602	CLA	C4A-NA-C1A	8.98	110.74	106.71
25	A	819	CLA	C4A-NA-C1A	8.98	110.74	106.71
25	d	316	CLA	C4A-NA-C1A	8.97	110.74	106.71
25	A	802	CLA	C4A-NA-C1A	8.97	110.74	106.71
25	B	843	CLA	C4A-NA-C1A	8.97	110.74	106.71
25	m	209	CLA	C4A-NA-C1A	8.96	110.74	106.71
25	e	211	CLA	C4A-NA-C1A	8.96	110.73	106.71
25	i	212	CLA	C4A-NA-C1A	8.94	110.72	106.71
25	k	208	CLA	C4A-NA-C1A	8.94	110.72	106.71
25	l	604	CLA	C4A-NA-C1A	8.90	110.71	106.71
25	A	818	CLA	C4A-NA-C1A	8.88	110.70	106.71
25	f	601	CLA	C4A-NA-C1A	8.88	110.70	106.71
25	B	802	CLA	C4A-NA-C1A	8.86	110.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	206	CLA	C4A-NA-C1A	8.84	110.68	106.71
25	p	607	CLA	C4A-NA-C1A	8.81	110.67	106.71
25	A	840	CLA	C4A-NA-C1A	8.80	110.66	106.71
25	f	602	CLA	C4A-NA-C1A	8.78	110.65	106.71
25	B	817	CLA	C4A-NA-C1A	8.77	110.65	106.71
25	c	303	CLA	C4A-NA-C1A	8.77	110.65	106.71
25	a	203	CLA	C4A-NA-C1A	8.76	110.65	106.71
25	m	208	CLA	C4A-NA-C1A	8.76	110.65	106.71
30	J	104	DD6	C14-C13-C11	8.76	139.13	125.53
25	n	211	CLA	C4A-NA-C1A	8.73	110.63	106.71
25	e	214	CLA	C4A-NA-C1A	8.64	110.59	106.71
25	g	204	CLA	C4A-NA-C1A	8.63	110.59	106.71
30	j	216	DD6	C14-C13-C11	8.63	138.92	125.53
25	A	847	CLA	C4A-NA-C1A	8.61	110.58	106.71
25	i	208	CLA	C4A-NA-C1A	8.60	110.57	106.71
30	g	217	DD6	C14-C13-C11	8.56	138.81	125.53
25	l	607	CLA	C4A-NA-C1A	8.50	110.53	106.71
25	B	842	CLA	C4A-NA-C1A	8.49	110.53	106.71
30	k	215	DD6	C14-C13-C11	8.46	138.66	125.53
25	j	209	CLA	C4A-NA-C1A	8.45	110.50	106.71
30	i	214	DD6	C14-C13-C11	8.43	138.61	125.53
25	o	601	CLA	C4A-NA-C1A	8.39	110.48	106.71
25	B	819	CLA	C4A-NA-C1A	8.39	110.48	106.71
25	m	202	CLA	C4A-NA-C1A	8.37	110.47	106.71
30	n	212	DD6	O1-C20-C19	8.36	119.67	113.38
30	A	855	DD6	C14-C13-C11	8.36	138.50	125.53
30	g	216	DD6	C14-C13-C11	8.34	138.47	125.53
25	B	825	CLA	C4A-NA-C1A	8.24	110.41	106.71
30	h	216	DD6	C14-C13-C11	8.23	138.30	125.53
25	n	209	CLA	C4A-NA-C1A	8.23	110.40	106.71
25	p	603	CLA	C4A-NA-C1A	8.22	110.40	106.71
30	m	213	DD6	C14-C13-C11	8.17	138.21	125.53
25	h	209	CLA	C4A-NA-C1A	8.17	110.38	106.71
25	p	601	CLA	C4A-NA-C1A	8.16	110.38	106.71
25	A	830	CLA	C4A-NA-C1A	8.13	110.36	106.71
30	a	214	DD6	C15-C14-C13	8.12	143.17	125.99
25	A	833	CLA	C4A-NA-C1A	8.12	110.36	106.71
25	B	840	CLA	C4A-NA-C1A	8.12	110.36	106.71
25	f	609	CLA	C4A-NA-C1A	8.10	110.35	106.71
30	c	316	DD6	C14-C13-C11	8.09	138.09	125.53
25	A	832	CLA	C4A-NA-C1A	8.07	110.33	106.71
30	l	613	DD6	C14-C13-C11	8.04	138.00	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	o	607	CLA	C4A-NA-C1A	8.03	110.32	106.71
30	e	219	DD6	C14-C13-C11	8.03	137.98	125.53
30	j	217	DD6	C14-C13-C11	7.97	137.89	125.53
30	d	317	DD6	C14-C13-C11	7.93	137.83	125.53
25	p	608	CLA	C4A-NA-C1A	7.93	110.27	106.71
30	a	215	DD6	C14-C13-C11	7.93	137.83	125.53
30	d	318	DD6	C14-C13-C11	7.84	137.70	125.53
30	b	215	DD6	C14-C13-C11	7.81	137.65	125.53
25	a	204	CLA	C4A-NA-C1A	7.73	110.18	106.71
30	l	614	DD6	C14-C13-C11	7.69	137.46	125.53
30	o	612	DD6	C14-C13-C11	7.63	137.37	125.53
30	b	214	DD6	C15-C14-C13	7.63	142.12	125.99
30	p	610	DD6	C14-C13-C11	7.62	137.35	125.53
25	m	203	CLA	C4A-NA-C1A	7.60	110.12	106.71
30	h	217	DD6	C14-C13-C11	7.60	137.32	125.53
25	A	850	CLA	C4A-NA-C1A	7.57	110.11	106.71
30	f	614	DD6	O1-C20-C19	7.54	119.05	113.38
30	i	215	DD6	C14-C13-C11	7.50	137.17	125.53
30	c	318	DD6	O1-C20-C19	7.49	119.01	113.38
30	n	212	DD6	C15-C14-C13	7.49	141.83	125.99
30	c	317	DD6	C14-C13-C11	7.43	137.06	125.53
30	n	212	DD6	C14-C13-C11	7.39	137.00	125.53
30	f	613	DD6	O1-C20-C19	7.39	118.93	113.38
30	o	611	DD6	C14-C13-C11	7.33	136.90	125.53
25	B	823	CLA	C4A-NA-C1A	7.31	109.99	106.71
30	k	216	DD6	C14-C13-C11	7.30	136.85	125.53
30	m	212	DD6	C14-C13-C11	7.30	136.85	125.53
30	c	318	DD6	C15-C14-C13	7.19	141.20	125.99
30	f	614	DD6	C15-C14-C13	7.09	140.98	125.99
30	d	319	DD6	O1-C20-C19	6.90	118.57	113.38
30	d	319	DD6	C14-C13-C11	6.80	136.08	125.53
28	B	835	PQN	C14-C13-C15	6.56	126.30	115.27
30	A	854	DD6	C15-C14-C13	6.54	139.82	125.99
28	A	834	PQN	C14-C13-C15	6.43	126.08	115.27
28	F	205	PQN	C14-C13-C15	6.40	126.04	115.27
28	B	827	PQN	C14-C13-C15	6.40	126.03	115.27
30	i	216	DD6	C14-C13-C11	6.36	135.40	125.53
30	A	854	DD6	O1-C20-C19	6.35	118.15	113.38
30	f	613	DD6	C14-C13-C11	6.32	135.33	125.53
30	f	613	DD6	C15-C14-C13	6.22	139.14	125.99
30	i	216	DD6	C15-C14-C13	5.97	138.62	125.99
30	f	614	DD6	C14-C13-C11	5.95	134.76	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	214	DD6	O1-C20-C19	5.90	117.81	113.38
30	d	319	DD6	C15-C14-C13	5.85	138.36	125.99
30	p	610	DD6	O1-C20-C19	5.81	117.75	113.38
25	A	801	CLA	O2D-CGD-CBD	5.75	121.49	111.27
30	i	216	DD6	O1-C20-C19	5.44	117.47	113.38
30	A	854	DD6	C14-C13-C11	5.40	133.90	125.53
30	A	854	DD6	C25-C26-C27	-5.36	111.01	126.58
30	b	214	DD6	C14-C13-C11	5.19	133.58	125.53
30	o	611	DD6	C15-C14-C13	5.18	136.95	125.99
30	m	212	DD6	O1-C20-C19	5.14	117.24	113.38
30	m	212	DD6	C15-C14-C13	5.13	136.84	125.99
30	c	318	DD6	C14-C13-C11	5.09	133.43	125.53
30	p	610	DD6	C15-C14-C13	5.07	136.71	125.99
30	A	855	DD6	O1-C20-C19	5.06	117.18	113.38
30	a	214	DD6	C14-C13-C11	5.05	133.36	125.53
30	k	216	DD6	C15-C14-C13	5.01	136.59	125.99
30	A	855	DD6	C15-C14-C13	4.90	136.35	125.99
30	h	217	DD6	C15-C14-C13	4.82	136.18	125.99
30	c	317	DD6	C15-C14-C13	4.80	136.15	125.99
30	o	612	DD6	C15-C14-C13	4.78	136.10	125.99
30	i	215	DD6	C15-C14-C13	4.77	136.09	125.99
30	d	318	DD6	C15-C14-C13	4.76	136.05	125.99
30	g	216	DD6	C25-C26-C27	-4.63	113.13	126.58
30	b	215	DD6	C15-C14-C13	4.60	135.72	125.99
30	j	217	DD6	C15-C14-C13	4.56	135.63	125.99
28	B	827	PQN	C15-C13-C12	-4.53	111.95	121.12
28	B	835	PQN	C15-C13-C12	-4.52	111.98	121.12
30	i	215	DD6	C32-C31-C36	4.51	129.01	122.63
30	A	854	DD6	C32-C31-C36	4.49	128.97	122.63
30	p	610	DD6	C25-C26-C27	-4.49	113.55	126.58
30	e	220	DD6	C4-C3-C2	4.45	132.59	123.47
27	j	202	LHG	C25-C24-C23	4.42	129.71	113.62
28	A	834	PQN	C15-C13-C12	-4.41	112.19	121.12
28	F	205	PQN	C15-C13-C12	-4.40	112.20	121.12
25	A	808	CLA	O2D-CGD-CBD	4.40	119.09	111.27
33	F	204	SQD	O47-C7-C8	4.38	120.94	111.50
25	p	609	CLA	O2D-CGD-CBD	4.37	119.03	111.27
30	g	216	DD6	C15-C14-C13	4.37	135.22	125.99
25	m	209	CLA	O2D-CGD-CBD	4.37	119.03	111.27
27	i	201	LHG	C25-C24-C23	4.36	129.47	113.62
25	c	310	CLA	O2D-CGD-CBD	4.36	119.01	111.27
30	e	219	DD6	C15-C14-C13	4.35	135.20	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	h	202	LHG	C25-C24-C23	4.35	129.45	113.62
30	d	319	DD6	C25-C26-C27	-4.35	113.94	126.58
25	d	311	CLA	O2D-CGD-CBD	4.35	118.99	111.27
25	A	804	CLA	O2D-CGD-CBD	4.35	118.99	111.27
30	k	216	DD6	O1-C20-C19	4.34	116.65	113.38
30	g	217	DD6	C25-C26-C27	-4.32	114.04	126.58
25	i	207	CLA	O2D-CGD-CBD	4.31	118.92	111.27
30	l	614	DD6	C15-C14-C13	4.31	135.10	125.99
25	a	209	CLA	O2D-CGD-CBD	4.29	118.90	111.27
25	l	603	CLA	O2D-CGD-CBD	4.29	118.89	111.27
25	h	209	CLA	O2D-CGD-CBD	4.28	118.88	111.27
30	b	215	DD6	C32-C31-C36	4.28	128.68	122.63
30	d	317	DD6	C15-C14-C13	4.28	135.04	125.99
30	a	214	DD6	O1-C20-C19	4.28	116.60	113.38
30	d	318	DD6	C32-C31-C36	4.28	128.68	122.63
25	j	212	CLA	O2D-CGD-CBD	4.28	118.87	111.27
35	d	309	CHL	CAA-C2A-C3A	-4.28	103.57	114.26
27	m	201	LHG	C25-C24-C23	4.28	129.17	113.62
30	e	220	DD6	C12-C11-C10	-4.27	116.94	122.92
27	g	201	LHG	C25-C24-C23	4.27	129.15	113.62
30	n	214	DD6	C3-C4-C5	4.27	132.21	123.47
27	b	201	LHG	C25-C24-C23	4.27	129.13	113.62
25	e	208	CLA	O2D-CGD-CBD	4.26	118.84	111.27
25	B	844	CLA	O2D-CGD-CBD	4.26	118.83	111.27
30	n	212	DD6	C25-C26-C27	-4.26	114.22	126.58
27	A	835	LHG	C25-C24-C23	4.25	129.09	113.62
25	j	204	CLA	O2D-CGD-CBD	4.25	118.83	111.27
25	c	309	CLA	O2D-CGD-CBD	4.25	118.81	111.27
25	A	825	CLA	O2D-CGD-CBD	4.24	118.81	111.27
30	l	613	DD6	C15-C14-C13	4.24	134.96	125.99
25	m	206	CLA	O2D-CGD-CBD	4.23	118.79	111.27
25	l	607	CLA	O2D-CGD-CBD	4.23	118.79	111.27
25	n	201	CLA	O2D-CGD-CBD	4.22	118.76	111.27
25	b	208	CLA	O2D-CGD-CBD	4.21	118.74	111.27
25	B	848	CLA	O2D-CGD-CBD	4.20	118.74	111.27
25	h	211	CLA	O2D-CGD-CBD	4.20	118.74	111.27
27	a	201	LHG	C25-C24-C23	4.20	128.89	113.62
33	g	202	SQD	O7-S-C6	4.20	111.93	106.94
25	p	606	CLA	O2D-CGD-CBD	4.20	118.73	111.27
25	j	207	CLA	O2D-CGD-CBD	4.20	118.73	111.27
25	A	823	CLA	O2D-CGD-CBD	4.20	118.73	111.27
30	f	614	DD6	C25-C26-C27	-4.20	114.40	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	214	CLA	O2D-CGD-CBD	4.19	118.72	111.27
25	m	208	CLA	O2D-CGD-CBD	4.19	118.72	111.27
27	c	301	LHG	C25-C24-C23	4.19	128.87	113.62
25	B	810	CLA	O2D-CGD-CBD	4.19	118.72	111.27
25	g	209	CLA	O2D-CGD-CBD	4.19	118.72	111.27
30	e	219	DD6	C25-C26-C27	-4.18	114.45	126.58
25	B	845	CLA	O2D-CGD-CBD	4.18	118.69	111.27
30	J	105	DD6	C12-C11-C10	-4.17	117.08	122.92
25	B	847	CLA	O2D-CGD-CBD	4.17	118.68	111.27
25	A	830	CLA	O2D-CGD-CBD	4.17	118.68	111.27
30	J	104	DD6	C25-C26-C27	-4.17	114.47	126.58
30	g	217	DD6	C15-C14-C13	4.17	134.81	125.99
30	J	104	DD6	C32-C31-C36	4.16	128.51	122.63
25	i	208	CLA	O2D-CGD-CBD	4.16	118.67	111.27
25	n	209	CLA	O2D-CGD-CBD	4.16	118.66	111.27
30	n	214	DD6	C24-C1-C2	4.16	125.32	118.94
25	i	211	CLA	O2D-CGD-CBD	4.16	118.66	111.27
25	h	208	CLA	O2D-CGD-CBD	4.16	118.65	111.27
25	i	205	CLA	O2D-CGD-CBD	4.16	118.65	111.27
25	f	605	CLA	O2D-CGD-CBD	4.16	118.65	111.27
27	A	805	LHG	C25-C24-C23	4.15	128.71	113.62
30	n	213	DD6	C12-C11-C10	-4.15	117.11	122.92
30	a	215	DD6	C15-C14-C13	4.14	134.75	125.99
30	i	215	DD6	O1-C20-C19	4.14	116.49	113.38
25	f	606	CLA	O2D-CGD-CBD	4.13	118.61	111.27
30	o	611	DD6	O1-C20-C19	4.13	116.49	113.38
25	m	207	CLA	O2D-CGD-CBD	4.13	118.61	111.27
25	k	209	CLA	O2D-CGD-CBD	4.13	118.60	111.27
25	b	203	CLA	O2D-CGD-CBD	4.13	118.60	111.27
25	l	605	CLA	O2D-CGD-CBD	4.13	118.60	111.27
25	n	208	CLA	O2D-CGD-CBD	4.13	118.60	111.27
33	g	202	SQD	O47-C7-C8	4.12	120.39	111.50
25	b	211	CLA	O2D-CGD-CBD	4.12	118.58	111.27
25	B	838	CLA	O2D-CGD-CBD	4.12	118.58	111.27
30	e	218	DD6	C12-C11-C10	-4.11	117.16	122.92
25	g	210	CLA	O2D-CGD-CBD	4.11	118.57	111.27
25	g	211	CLA	O2D-CGD-CBD	4.11	118.57	111.27
25	B	809	CLA	O2D-CGD-CBD	4.11	118.56	111.27
30	m	213	DD6	C15-C14-C13	4.11	134.67	125.99
25	o	609	CLA	O2D-CGD-CBD	4.10	118.56	111.27
30	h	216	DD6	C15-C14-C13	4.10	134.66	125.99
25	k	207	CLA	O2D-CGD-CBD	4.09	118.53	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	212	CLA	O2D-CGD-CBD	4.08	118.52	111.27
25	B	808	CLA	O2D-CGD-CBD	4.08	118.51	111.27
25	B	812	CLA	O2D-CGD-CBD	4.08	118.51	111.27
30	g	216	DD6	C32-C31-C36	4.08	128.39	122.63
25	A	845	CLA	O2D-CGD-CBD	4.08	118.51	111.27
29	J	101	BCR	C34-C9-C10	-4.07	117.22	122.92
25	B	819	CLA	O2D-CGD-CBD	4.07	118.49	111.27
25	g	205	CLA	O2D-CGD-CBD	4.07	118.49	111.27
25	l	608	CLA	O2D-CGD-CBD	4.06	118.49	111.27
30	d	319	DD6	C32-C31-C36	4.06	128.37	122.63
25	B	804	CLA	O2D-CGD-CBD	4.06	118.48	111.27
25	f	607	CLA	O2D-CGD-CBD	4.05	118.47	111.27
30	c	318	DD6	C25-C26-C27	-4.05	114.81	126.58
25	b	206	CLA	O2D-CGD-CBD	4.05	118.47	111.27
25	d	315	CLA	O2D-CGD-CBD	4.05	118.47	111.27
25	i	206	CLA	O2D-CGD-CBD	4.05	118.46	111.27
29	J	101	BCR	C37-C22-C21	-4.05	117.25	122.92
25	F	201	CLA	O2D-CGD-CBD	4.05	118.46	111.27
25	o	610	CLA	O2D-CGD-CBD	4.05	118.46	111.27
25	e	213	CLA	O2D-CGD-CBD	4.04	118.45	111.27
30	a	214	DD6	C32-C31-C36	4.04	128.34	122.63
25	j	209	CLA	O2D-CGD-CBD	4.03	118.43	111.27
25	n	205	CLA	O2D-CGD-CBD	4.03	118.43	111.27
25	B	803	CLA	O2D-CGD-CBD	4.03	118.43	111.27
25	k	204	CLA	O2D-CGD-CBD	4.03	118.43	111.27
30	d	318	DD6	C25-C26-C27	-4.03	114.89	126.58
25	j	208	CLA	O2D-CGD-CBD	4.03	118.42	111.27
25	b	210	CLA	O2D-CGD-CBD	4.03	118.42	111.27
30	n	214	DD6	C12-C11-C10	-4.02	117.28	122.92
30	F	203	DD6	C12-C11-C10	-4.02	117.29	122.92
25	A	832	CLA	O2D-CGD-CBD	4.02	118.40	111.27
25	e	210	CLA	O2D-CGD-CBD	4.01	118.40	111.27
25	A	816	CLA	O2D-CGD-CBD	4.01	118.40	111.27
25	g	207	CLA	O2D-CGD-CBD	4.01	118.39	111.27
25	A	842	CLA	O2D-CGD-CBD	4.01	118.39	111.27
25	j	214	CLA	O2D-CGD-CBD	4.01	118.39	111.27
25	g	206	CLA	O2D-CGD-CBD	4.01	118.39	111.27
25	n	203	CLA	O2D-CGD-CBD	4.00	118.38	111.27
29	B	832	BCR	C34-C9-C10	-4.00	117.31	122.92
25	f	610	CLA	O2D-CGD-CBD	4.00	118.38	111.27
25	g	214	CLA	O2D-CGD-CBD	4.00	118.38	111.27
25	B	817	CLA	O2D-CGD-CBD	4.00	118.37	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	826	CLA	O2D-CGD-CBD	4.00	118.37	111.27
25	o	607	CLA	O2D-CGD-CBD	4.00	118.37	111.27
25	g	215	CLA	O2D-CGD-CBD	3.99	118.37	111.27
25	A	850	CLA	O2D-CGD-CBD	3.99	118.37	111.27
25	B	807	CLA	O2D-CGD-CBD	3.99	118.36	111.27
25	B	821	CLA	O2D-CGD-CBD	3.99	118.36	111.27
29	B	831	BCR	C34-C9-C10	-3.99	117.34	122.92
25	B	841	CLA	O2D-CGD-CBD	3.99	118.35	111.27
25	A	822	CLA	O2D-CGD-CBD	3.99	118.35	111.27
25	o	601	CLA	O2D-CGD-CBD	3.99	118.35	111.27
29	J	101	BCR	C16-C15-C14	3.98	131.63	123.47
29	A	837	BCR	C37-C22-C21	-3.98	117.34	122.92
25	B	825	CLA	O2D-CGD-CBD	3.98	118.34	111.27
25	A	850	CLA	O2A-CGA-CBA	3.98	124.39	111.91
25	h	209	CLA	O2A-CGA-CBA	3.98	124.39	111.91
29	B	831	BCR	C37-C22-C21	-3.97	117.36	122.92
25	b	205	CLA	O2D-CGD-CBD	3.97	118.33	111.27
25	A	821	CLA	O2D-CGD-CBD	3.97	118.32	111.27
25	a	205	CLA	O2D-CGD-CBD	3.97	118.32	111.27
33	F	204	SQD	O7-S-C6	3.96	111.65	106.94
25	n	201	CLA	C3B-C4B-NB	-3.96	106.84	110.52
25	n	211	CLA	O2D-CGD-CBD	3.96	118.31	111.27
25	d	312	CLA	O2D-CGD-CBD	3.96	118.30	111.27
25	i	209	CLA	O2D-CGD-CBD	3.96	118.30	111.27
25	n	210	CLA	O2D-CGD-CBD	3.95	118.29	111.27
30	k	215	DD6	C15-C14-C13	3.95	134.34	125.99
30	e	220	DD6	C24-C1-C2	3.95	125.00	118.94
25	n	206	CLA	O2D-CGD-CBD	3.95	118.28	111.27
25	l	606	CLA	O2D-CGD-CBD	3.95	118.28	111.27
25	b	207	CLA	O2D-CGD-CBD	3.94	118.28	111.27
25	p	608	CLA	O2D-CGD-CBD	3.94	118.28	111.27
25	B	837	CLA	O2D-CGD-CBD	3.94	118.27	111.27
25	A	811	CLA	O2D-CGD-CBD	3.94	118.27	111.27
25	A	813	CLA	O2D-CGD-CBD	3.94	118.27	111.27
25	A	812	CLA	O2D-CGD-CBD	3.94	118.27	111.27
30	c	318	DD6	C32-C31-C36	3.94	128.19	122.63
25	g	212	CLA	O2D-CGD-CBD	3.93	118.26	111.27
25	k	213	CLA	O2D-CGD-CBD	3.93	118.26	111.27
25	p	605	CLA	O2D-CGD-CBD	3.93	118.25	111.27
25	g	213	CLA	O2D-CGD-CBD	3.93	118.25	111.27
30	n	214	DD6	C4-C3-C2	3.92	131.51	123.47
25	p	603	CLA	O2D-CGD-CBD	3.92	118.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	F	202	CLA	O2D-CGD-CBD	3.92	118.24	111.27
25	a	207	CLA	O2D-CGD-CBD	3.92	118.24	111.27
25	o	605	CLA	O2D-CGD-CBD	3.92	118.23	111.27
25	h	206	CLA	O2D-CGD-CBD	3.92	118.23	111.27
25	p	607	CLA	O2D-CGD-CBD	3.91	118.22	111.27
30	j	217	DD6	O1-C20-C19	3.91	116.32	113.38
25	j	212	CLA	O2A-CGA-CBA	3.91	124.17	111.91
25	e	212	CLA	O2D-CGD-CBD	3.91	118.21	111.27
25	d	303	CLA	O2D-CGD-CBD	3.91	118.21	111.27
29	B	832	BCR	C37-C22-C21	-3.90	117.45	122.92
25	k	214	CLA	O2D-CGD-CBD	3.90	118.20	111.27
29	A	837	BCR	C34-C9-C10	-3.90	117.46	122.92
25	A	829	CLA	O2D-CGD-CBD	3.90	118.20	111.27
30	e	220	DD6	C-C1-C2	-3.90	117.46	122.92
30	l	613	DD6	C32-C31-C36	3.90	128.14	122.63
25	a	208	CLA	O2D-CGD-CBD	3.90	118.19	111.27
25	B	824	CLA	O2D-CGD-CBD	3.90	118.19	111.27
25	i	213	CLA	O2D-CGD-CBD	3.90	118.19	111.27
25	c	305	CLA	O2D-CGD-CBD	3.90	118.19	111.27
25	k	208	CLA	O2D-CGD-CBD	3.90	118.19	111.27
25	B	834	CLA	O2D-CGD-CBD	3.89	118.19	111.27
25	a	212	CLA	O2D-CGD-CBD	3.89	118.18	111.27
25	J	103	CLA	O2D-CGD-CBD	3.89	118.18	111.27
25	d	313	CLA	O2D-CGD-CBD	3.89	118.17	111.27
33	D	200	SQD	O47-C7-C8	3.89	119.87	111.50
25	B	813	CLA	O2D-CGD-CBD	3.88	118.17	111.27
25	A	826	CLA	O2D-CGD-CBD	3.88	118.17	111.27
25	B	816	CLA	O2D-CGD-CBD	3.88	118.17	111.27
30	l	613	DD6	C25-C26-C27	-3.88	115.31	126.58
25	b	213	CLA	O2D-CGD-CBD	3.88	118.17	111.27
30	g	217	DD6	C32-C31-C36	3.88	128.11	122.63
25	e	217	CLA	O2D-CGD-CBD	3.88	118.16	111.27
25	j	204	CLA	C3B-C4B-NB	-3.88	106.92	110.52
25	p	601	CLA	O2D-CGD-CBD	3.87	118.15	111.27
25	e	216	CLA	O2D-CGD-CBD	3.87	118.15	111.27
25	A	817	CLA	O2D-CGD-CBD	3.87	118.15	111.27
25	o	603	CLA	O2D-CGD-CBD	3.87	118.14	111.27
25	k	212	CLA	O2D-CGD-CBD	3.87	118.14	111.27
30	i	214	DD6	C32-C31-C36	3.87	128.09	122.63
25	p	608	CLA	C3B-C4B-NB	-3.86	106.93	110.52
25	d	306	CLA	O2D-CGD-CBD	3.86	118.13	111.27
35	e	209	CHL	O2D-CGD-CBD	3.86	118.13	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	f	601	CLA	O2D-CGD-CBD	3.86	118.13	111.27
25	h	207	CLA	O2D-CGD-CBD	3.86	118.12	111.27
25	j	215	CLA	O2D-CGD-CBD	3.86	118.12	111.27
25	d	305	CLA	O2D-CGD-CBD	3.85	118.12	111.27
25	e	204	CLA	O2D-CGD-CBD	3.85	118.12	111.27
25	c	311	CLA	O2D-CGD-CBD	3.85	118.11	111.27
30	a	215	DD6	C32-C31-C36	3.85	128.07	122.63
30	n	214	DD6	C-C1-C2	-3.85	117.53	122.92
25	i	203	CLA	O2D-CGD-CBD	3.85	118.11	111.27
33	J	102	SQD	O9-S-O7	-3.85	100.62	113.95
25	A	857	CLA	O2D-CGD-CBD	3.85	118.11	111.27
25	n	204	CLA	O2D-CGD-CBD	3.85	118.10	111.27
25	c	308	CLA	O2D-CGD-CBD	3.84	118.10	111.27
25	B	818	CLA	O2D-CGD-CBD	3.84	118.09	111.27
25	f	602	CLA	O2D-CGD-CBD	3.84	118.09	111.27
25	k	205	CLA	O2D-CGD-CBD	3.84	118.09	111.27
25	j	205	CLA	O2D-CGD-CBD	3.84	118.09	111.27
25	b	209	CLA	O2D-CGD-CBD	3.84	118.08	111.27
25	o	604	CLA	O2D-CGD-CBD	3.84	118.08	111.27
25	h	215	CLA	O2D-CGD-CBD	3.83	118.08	111.27
25	n	202	CLA	O2D-CGD-CBD	3.83	118.08	111.27
25	a	211	CLA	O2D-CGD-CBD	3.83	118.08	111.27
25	e	206	CLA	O2D-CGD-CBD	3.83	118.07	111.27
30	i	216	DD6	C25-C26-C27	-3.82	115.47	126.58
25	A	849	CLA	O2D-CGD-CBD	3.82	118.06	111.27
25	A	853	CLA	O2D-CGD-CBD	3.82	118.06	111.27
25	m	202	CLA	O2D-CGD-CBD	3.82	118.06	111.27
25	c	315	CLA	O2D-CGD-CBD	3.82	118.05	111.27
35	d	308	CHL	O2D-CGD-CBD	3.82	118.05	111.27
28	B	827	PQN	C9-C10-C5	3.82	123.51	119.26
25	A	807	CLA	O2D-CGD-CBD	3.82	118.05	111.27
30	b	214	DD6	C25-C26-C27	-3.81	115.52	126.58
25	l	612	CLA	O2D-CGD-CBD	3.81	118.03	111.27
30	j	216	DD6	C32-C31-C36	3.81	128.01	122.63
25	p	604	CLA	O2D-CGD-CBD	3.81	118.03	111.27
25	j	210	CLA	O2D-CGD-CBD	3.81	118.03	111.27
35	d	310	CHL	O2D-CGD-CBD	3.80	118.03	111.27
25	B	845	CLA	C3B-C4B-NB	-3.80	106.99	110.52
25	A	833	CLA	O2D-CGD-CBD	3.80	118.03	111.27
30	a	214	DD6	C25-C26-C27	-3.80	115.54	126.58
35	d	309	CHL	O2D-CGD-CBD	3.80	118.02	111.27
25	k	203	CLA	O2D-CGD-CBD	3.80	118.02	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	217	DD6	C25-C26-C27	-3.80	115.55	126.58
25	l	611	CLA	O2D-CGD-CBD	3.80	118.01	111.27
25	i	211	CLA	O2A-CGA-CBA	3.80	123.82	111.91
30	f	613	DD6	C25-C26-C27	-3.79	115.57	126.58
25	j	213	CLA	O2D-CGD-CBD	3.79	118.01	111.27
25	d	314	CLA	O2D-CGD-CBD	3.79	118.00	111.27
30	c	316	DD6	C15-C14-C13	3.79	134.00	125.99
30	c	316	DD6	C25-C26-C27	-3.78	115.60	126.58
25	p	604	CLA	CHD-C1D-ND	-3.78	120.98	124.45
33	g	202	SQD	O9-S-O7	-3.78	100.87	113.95
35	d	307	CHL	O2D-CGD-CBD	3.78	117.98	111.27
25	A	841	CLA	O2D-CGD-CBD	3.77	117.97	111.27
30	o	611	DD6	C25-C26-C27	-3.77	115.63	126.58
33	F	204	SQD	O9-S-O7	-3.76	100.92	113.95
35	c	307	CHL	CAA-C2A-C3A	-3.76	102.47	112.78
25	B	806	CLA	O2D-CGD-CBD	3.76	117.95	111.27
30	a	215	DD6	C25-C26-C27	-3.76	115.67	126.58
25	g	208	CLA	O2D-CGD-CBD	3.76	117.94	111.27
25	A	852	CLA	C3B-C4B-NB	-3.75	107.03	110.52
30	n	212	DD6	C41-C32-C31	3.75	116.43	110.47
30	c	316	DD6	C32-C31-C36	3.75	127.93	122.63
30	d	317	DD6	C32-C31-C36	3.75	127.93	122.63
25	o	608	CLA	O2D-CGD-CBD	3.75	117.75	111.49
35	c	307	CHL	O2D-CGD-CBD	3.75	117.92	111.27
25	B	843	CLA	O2D-CGD-CBD	3.74	117.92	111.27
25	f	608	CLA	O2D-CGD-CBD	3.74	117.92	111.27
30	i	216	DD6	C32-C31-C36	3.74	127.92	122.63
25	m	205	CLA	O2D-CGD-CBD	3.74	117.91	111.27
25	A	809	CLA	O2D-CGD-CBD	3.74	117.91	111.27
33	D	200	SQD	O9-S-C6	3.74	111.38	106.94
30	d	317	DD6	C25-C26-C27	-3.73	115.74	126.58
25	B	840	CLA	C3B-C4B-NB	-3.73	107.05	110.52
30	j	216	DD6	C15-C14-C13	3.73	133.88	125.99
30	A	855	DD6	C25-C26-C27	-3.73	115.76	126.58
25	f	603	CLA	O2D-CGD-CBD	3.72	117.88	111.27
30	f	614	DD6	C32-C31-C36	3.72	127.89	122.63
25	d	304	CLA	O2D-CGD-CBD	3.72	117.88	111.27
30	h	217	DD6	C32-C31-C36	3.72	127.89	122.63
25	A	848	CLA	O2D-CGD-CBD	3.72	117.88	111.27
30	c	317	DD6	C32-C31-C36	3.72	127.88	122.63
25	c	306	CLA	O2D-CGD-CBD	3.72	117.87	111.27
25	A	851	CLA	O2D-CGD-CBD	3.72	117.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	o	606	CLA	O2D-CGD-CBD	3.71	117.87	111.27
25	n	207	CLA	C3B-C4B-NB	-3.71	107.07	110.52
25	h	213	CLA	O2D-CGD-CBD	3.71	117.85	111.27
25	A	843	CLA	O2D-CGD-CBD	3.71	117.85	111.27
25	a	213	CLA	O2D-CGD-CBD	3.71	117.85	111.27
30	i	214	DD6	C15-C14-C13	3.71	133.83	125.99
25	A	802	CLA	O2D-CGD-CBD	3.70	117.84	111.27
25	A	827	CLA	O2D-CGD-CBD	3.70	117.84	111.27
25	d	316	CLA	O2D-CGD-CBD	3.70	117.83	111.27
25	A	842	CLA	C3B-C4B-NB	-3.69	107.09	110.52
30	m	212	DD6	C32-C31-C36	3.69	127.85	122.63
25	e	211	CLA	O2D-CGD-CBD	3.69	117.83	111.27
25	B	838	CLA	C3B-C4B-NB	-3.69	107.09	110.52
30	i	214	DD6	C25-C26-C27	-3.69	115.88	126.58
30	o	611	DD6	C32-C31-C36	3.68	127.84	122.63
30	c	317	DD6	C41-C32-C31	3.68	116.32	110.47
30	p	610	DD6	C32-C31-C36	3.68	127.83	122.63
30	g	217	DD6	O1-C20-C19	3.68	116.14	113.38
25	l	609	CLA	O2D-CGD-CBD	3.68	117.80	111.27
30	e	219	DD6	C32-C31-C36	3.68	127.83	122.63
25	e	215	CLA	O2D-CGD-CBD	3.68	117.80	111.27
33	D	200	SQD	O7-S-C6	3.67	111.31	106.94
25	A	814	CLA	O2D-CGD-CBD	3.67	117.80	111.27
25	k	206	CLA	O2D-CGD-CBD	3.67	117.79	111.27
30	f	614	DD6	C41-C32-C31	3.67	116.30	110.47
30	d	318	DD6	C37-C36-C31	-3.67	119.36	124.35
25	b	212	CLA	O2D-CGD-CBD	3.66	117.77	111.27
33	D	200	SQD	O9-S-O7	-3.66	101.28	113.95
25	d	301	CLA	O2D-CGD-CBD	3.66	117.77	111.27
25	i	212	CLA	O2D-CGD-CBD	3.66	117.77	111.27
25	A	828	CLA	O2D-CGD-CBD	3.66	117.77	111.27
25	k	202	CLA	O2D-CGD-CBD	3.66	117.76	111.27
30	J	104	DD6	C15-C14-C13	3.65	133.72	125.99
30	f	613	DD6	C41-C32-C31	3.65	116.27	110.47
25	p	609	CLA	CHD-C1D-ND	-3.65	121.10	124.45
25	A	844	CLA	O2D-CGD-CBD	3.65	117.75	111.27
25	B	823	CLA	O2D-CGD-CBD	3.65	117.75	111.27
25	p	609	CLA	C3B-C4B-NB	-3.64	107.14	110.52
30	d	319	DD6	C41-C32-C31	3.64	116.25	110.47
28	F	205	PQN	C9-C10-C5	3.64	123.31	119.26
25	A	810	CLA	O2D-CGD-CBD	3.64	117.73	111.27
25	f	612	CLA	O2D-CGD-CBD	3.63	117.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	314	CLA	O2D-CGD-CBD	3.63	117.72	111.27
30	J	104	DD6	C41-C32-C31	3.63	116.24	110.47
30	o	611	DD6	C41-C32-C31	3.63	116.24	110.47
30	j	217	DD6	C32-C31-C36	3.63	127.76	122.63
28	B	835	PQN	C9-C10-C5	3.63	123.30	119.26
30	j	217	DD6	C41-C32-C31	3.62	116.22	110.47
25	l	607	CLA	C3B-C4B-NB	-3.62	107.16	110.52
30	p	610	DD6	C41-C32-C31	3.62	116.22	110.47
25	c	313	CLA	O2D-CGD-CBD	3.62	117.70	111.27
25	h	210	CLA	O2D-CGD-CBD	3.62	117.70	111.27
25	g	204	CLA	C3B-C4B-NB	-3.62	107.16	110.52
25	A	802	CLA	C3B-C4B-NB	-3.62	107.16	110.52
25	m	203	CLA	C3B-C4B-NB	-3.61	107.16	110.52
30	b	215	DD6	O1-C20-C19	3.61	116.10	113.38
28	A	834	PQN	C9-C10-C5	3.61	123.28	119.26
25	B	814	CLA	O2D-CGD-CBD	3.61	117.69	111.27
25	h	204	CLA	O2A-CGA-CBA	3.61	123.24	111.91
25	h	212	CLA	O2A-CGA-CBA	3.61	123.24	111.91
30	d	318	DD6	C41-C32-C31	3.61	116.20	110.47
25	B	846	CLA	O2D-CGD-CBD	3.61	117.68	111.27
27	d	302	LHG	C25-C24-C23	3.60	129.15	114.34
25	l	601	CLA	O2D-CGD-CBD	3.60	117.67	111.27
25	A	809	CLA	C3B-C4B-NB	-3.60	107.17	110.52
25	A	844	CLA	C3B-C4B-NB	-3.60	107.17	110.52
30	A	854	DD6	C41-C32-C31	3.60	116.19	110.47
25	B	810	CLA	C3B-C4B-NB	-3.60	107.17	110.52
30	e	219	DD6	C41-C32-C31	3.60	116.19	110.47
25	B	844	CLA	CHD-C1D-ND	-3.60	121.15	124.45
25	A	806	CLA	O2D-CGD-CBD	3.60	117.66	111.27
30	m	213	DD6	C41-C32-C31	3.60	116.18	110.47
25	p	602	CLA	O2D-CGD-CBD	3.60	117.66	111.27
25	f	604	CLA	O2D-CGD-CBD	3.60	117.66	111.27
30	k	215	DD6	C41-C32-C31	3.60	116.18	110.47
25	e	207	CLA	O2D-CGD-CBD	3.59	117.65	111.27
33	J	102	SQD	O9-S-C6	3.59	111.20	106.94
25	m	204	CLA	O2D-CGD-CBD	3.59	117.64	111.27
25	k	210	CLA	O2D-CGD-CBD	3.59	117.64	111.27
30	m	212	DD6	C25-C26-C27	-3.59	116.17	126.58
25	i	204	CLA	O2D-CGD-CBD	3.58	117.64	111.27
25	A	804	CLA	C3B-C4B-NB	-3.58	107.19	110.52
30	b	214	DD6	C32-C31-C36	3.58	127.69	122.63
30	k	215	DD6	C25-C26-C27	-3.58	116.19	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	204	CLA	O2A-CGA-CBA	3.58	123.13	111.91
33	J	102	SQD	O7-S-C6	3.58	111.19	106.94
30	h	216	DD6	C41-C32-C31	3.58	116.15	110.47
30	g	216	DD6	C41-C32-C31	3.57	116.14	110.47
25	i	203	CLA	C3B-C4B-NB	-3.57	107.20	110.52
30	o	612	DD6	C32-C31-C36	3.57	127.68	122.63
30	A	855	DD6	C41-C32-C31	3.57	116.14	110.47
25	A	840	CLA	C3B-C4B-NB	-3.57	107.20	110.52
25	e	217	CLA	C3B-C4B-NB	-3.57	107.20	110.52
25	A	824	CLA	O2D-CGD-CBD	3.57	117.61	111.27
25	j	203	CLA	O2D-CGD-CBD	3.57	117.61	111.27
25	B	803	CLA	C3B-C4B-NB	-3.57	107.20	110.52
30	l	613	DD6	C41-C32-C31	3.57	116.14	110.47
25	h	204	CLA	O2D-CGD-CBD	3.57	117.60	111.27
25	j	211	CLA	O2D-CGD-CBD	3.57	117.60	111.27
25	A	847	CLA	C3B-C4B-NB	-3.56	107.21	110.52
30	h	216	DD6	C32-C31-C36	3.56	127.67	122.63
30	e	218	DD6	C-C1-C2	-3.56	117.93	122.92
30	k	216	DD6	C25-C26-C27	-3.56	116.24	126.58
30	g	216	DD6	O1-C20-C19	3.56	116.06	113.38
30	l	614	DD6	C25-C26-C27	-3.56	116.24	126.58
30	o	612	DD6	C25-C26-C27	-3.56	116.25	126.58
30	o	612	DD6	C41-C32-C31	3.56	116.12	110.47
25	f	611	CLA	O2D-CGD-CBD	3.55	117.58	111.27
25	B	812	CLA	C3B-C4B-NB	-3.55	107.22	110.52
25	n	207	CLA	O2D-CGD-CBD	3.55	117.58	111.27
25	p	604	CLA	C3B-C4B-NB	-3.55	107.22	110.52
25	p	602	CLA	C3B-C4B-NB	-3.55	107.23	110.52
25	b	204	CLA	O2D-CGD-CBD	3.54	117.56	111.27
25	A	840	CLA	O2D-CGD-CBD	3.54	117.56	111.27
30	J	105	DD6	C3-C4-C5	3.54	130.73	123.47
25	A	847	CLA	O2D-CGD-CBD	3.54	117.56	111.27
25	A	830	CLA	C3B-C4B-NB	-3.54	107.23	110.52
30	a	214	DD6	C41-C32-C31	3.54	116.09	110.47
25	A	852	CLA	O2D-CGD-CBD	3.54	117.56	111.27
30	c	316	DD6	C41-C32-C31	3.54	116.09	110.47
25	h	212	CLA	C3B-C4B-NB	-3.54	107.23	110.52
25	k	211	CLA	O2D-CGD-CBD	3.53	117.55	111.27
30	A	854	DD6	C37-C36-C31	-3.53	119.55	124.35
25	j	212	CLA	C3B-C4B-NB	-3.53	107.24	110.52
29	A	837	BCR	C16-C15-C14	3.53	130.71	123.47
30	k	216	DD6	C41-C32-C31	3.53	116.08	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	301	CLA	C3B-C4B-NB	-3.53	107.24	110.52
30	l	614	DD6	C41-C32-C31	3.53	116.08	110.47
25	A	832	CLA	C3B-C4B-NB	-3.53	107.24	110.52
25	j	207	CLA	C3B-C4B-NB	-3.53	107.24	110.52
25	B	848	CLA	C3B-C4B-NB	-3.52	107.25	110.52
25	l	604	CLA	O2D-CGD-CBD	3.52	117.53	111.27
25	B	809	CLA	C3B-C4B-NB	-3.52	107.25	110.52
25	B	805	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	A	807	CLA	CHD-C1D-ND	-3.52	121.22	124.45
30	i	215	DD6	C41-C32-C31	3.52	116.06	110.47
25	j	206	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	c	302	CLA	O2D-CGD-CBD	3.51	117.51	111.27
30	i	216	DD6	C41-C32-C31	3.51	116.05	110.47
25	i	211	CLA	C3B-C4B-NB	-3.51	107.26	110.52
25	B	836	CLA	O2D-CGD-CBD	3.51	117.50	111.27
25	a	204	CLA	C3B-C4B-NB	-3.51	107.26	110.52
25	e	211	CLA	C3B-C4B-NB	-3.51	107.26	110.52
25	a	212	CLA	C3B-C4B-NB	-3.51	107.26	110.52
30	j	216	DD6	C41-C32-C31	3.51	116.04	110.47
25	A	817	CLA	C3B-C4B-NB	-3.50	107.27	110.52
30	m	212	DD6	C41-C32-C31	3.50	116.03	110.47
25	m	210	CLA	O2D-CGD-CBD	3.50	117.49	111.27
25	B	805	CLA	C3B-C4B-NB	-3.50	107.27	110.52
25	i	202	CLA	O2D-CGD-CBD	3.50	117.49	111.27
25	g	209	CLA	C3B-C4B-NB	-3.50	107.27	110.52
30	l	614	DD6	C32-C31-C36	3.50	127.57	122.63
30	J	105	DD6	C-C1-C2	-3.50	118.03	122.92
30	d	317	DD6	C41-C32-C31	3.50	116.02	110.47
25	c	304	CLA	O2D-CGD-CBD	3.50	117.48	111.27
25	h	207	CLA	C3B-C4B-NB	-3.49	107.27	110.52
30	o	612	DD6	O1-C20-C19	3.49	116.01	113.38
25	o	607	CLA	C3B-C4B-NB	-3.49	107.27	110.52
30	n	214	DD6	C7-C6-C5	-3.49	118.03	122.92
25	B	811	CLA	O2D-CGD-CBD	3.49	117.47	111.27
30	g	217	DD6	C41-C32-C31	3.49	116.02	110.47
25	A	801	CLA	O1D-CGD-CBD	-3.49	117.34	124.48
25	A	844	CLA	CHD-C1D-ND	-3.49	121.25	124.45
25	a	210	CLA	O2D-CGD-CBD	3.49	117.47	111.27
25	B	804	CLA	C3B-C4B-NB	-3.48	107.28	110.52
25	B	822	CLA	O2D-CGD-CBD	3.48	117.45	111.27
25	A	841	CLA	C3B-C4B-NB	-3.48	107.28	110.52
25	h	209	CLA	CMB-C2B-C1B	-3.48	120.07	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	215	DD6	C41-C32-C31	3.48	115.99	110.47
25	e	214	CLA	O2D-CGD-CBD	3.47	117.44	111.27
25	B	820	CLA	O2D-CGD-CBD	3.47	117.44	111.27
30	k	215	DD6	C32-C31-C36	3.47	127.54	122.63
30	i	214	DD6	C41-C32-C31	3.47	115.99	110.47
25	B	802	CLA	O2D-CGD-CBD	3.47	117.44	111.27
25	e	201	CLA	O2D-CGD-CBD	3.47	117.44	111.27
25	A	815	CLA	O2D-CGD-CBD	3.47	117.44	111.27
25	B	839	CLA	O2D-CGD-CBD	3.47	117.43	111.27
30	J	105	DD6	C24-C1-C2	3.46	124.25	118.94
25	A	851	CLA	C3B-C4B-NB	-3.46	107.31	110.52
25	i	210	CLA	O2D-CGD-CBD	3.45	117.41	111.27
25	B	819	CLA	C3B-C4B-NB	-3.45	107.31	110.52
25	d	303	CLA	C3B-C4B-NB	-3.45	107.31	110.52
25	A	819	CLA	O2D-CGD-CBD	3.45	117.40	111.27
25	m	211	CLA	O2D-CGD-CBD	3.45	117.40	111.27
30	n	213	DD6	C-C1-C2	-3.45	118.09	122.92
25	l	607	CLA	CHD-C1D-ND	-3.45	121.28	124.45
25	A	801	CLA	CHD-C1D-ND	-3.45	121.28	124.45
25	B	815	CLA	O2D-CGD-CBD	3.45	117.40	111.27
25	B	823	CLA	C3B-C4B-NB	-3.45	107.32	110.52
25	o	602	CLA	O2D-CGD-CBD	3.45	117.39	111.27
25	A	808	CLA	C3B-C4B-NB	-3.45	107.32	110.52
30	h	217	DD6	C41-C32-C31	3.45	115.94	110.47
33	F	204	SQD	O9-S-C6	3.44	111.03	106.94
25	a	206	CLA	O2D-CGD-CBD	3.44	117.39	111.27
25	e	210	CLA	C3B-C4B-NB	-3.44	107.32	110.52
25	A	831	CLA	O2D-CGD-CBD	3.44	117.38	111.27
25	g	204	CLA	O2D-CGD-CBD	3.44	117.38	111.27
30	h	216	DD6	C25-C26-C27	-3.44	116.60	126.58
25	f	607	CLA	C3B-C4B-NB	-3.44	107.33	110.52
35	d	308	CHL	CAA-C2A-C3A	-3.44	103.37	112.78
30	c	317	DD6	C40-C32-C31	-3.43	105.01	110.47
30	e	220	DD6	C7-C6-C5	-3.43	118.11	122.92
30	f	613	DD6	C32-C31-C36	3.43	127.48	122.63
25	l	612	CLA	C3B-C4B-NB	-3.43	107.33	110.52
25	B	842	CLA	C3B-C4B-NB	-3.42	107.34	110.52
25	e	216	CLA	C3B-C4B-NB	-3.42	107.34	110.52
25	B	839	CLA	C3B-C4B-NB	-3.42	107.34	110.52
25	a	209	CLA	C3B-C4B-NB	-3.42	107.34	110.52
25	d	311	CLA	C3B-C4B-NB	-3.42	107.34	110.52
25	a	203	CLA	O2D-CGD-CBD	3.42	117.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	318	DD6	C41-C32-C31	3.42	115.90	110.47
25	d	301	CLA	CHD-C1D-ND	-3.42	121.31	124.45
25	m	205	CLA	CHD-C1D-ND	-3.42	121.31	124.45
30	A	855	DD6	C32-C31-C36	3.41	127.45	122.63
25	l	612	CLA	CHD-C1D-ND	-3.41	121.32	124.45
25	B	803	CLA	CHD-C1D-ND	-3.40	121.33	124.45
29	J	101	BCR	C36-C18-C17	-3.40	118.16	122.92
25	A	826	CLA	C3B-C4B-NB	-3.40	107.36	110.52
25	B	842	CLA	O2D-CGD-CBD	3.40	117.30	111.27
25	A	840	CLA	CHD-C1D-ND	-3.40	121.33	124.45
25	l	602	CLA	C3B-C4B-NB	-3.40	107.36	110.52
25	e	201	CLA	C3B-C4B-NB	-3.39	107.37	110.52
25	o	610	CLA	C3B-C4B-NB	-3.39	107.37	110.52
30	e	218	DD6	C24-C1-C2	3.39	124.14	118.94
25	j	215	CLA	C3B-C4B-NB	-3.38	107.38	110.52
25	f	604	CLA	C3B-C4B-NB	-3.38	107.38	110.52
25	A	846	CLA	O2D-CGD-CBD	3.38	117.28	111.27
25	o	604	CLA	C3B-C4B-NB	-3.38	107.38	110.52
25	A	829	CLA	C3B-C4B-NB	-3.38	107.38	110.52
25	e	213	CLA	C3B-C4B-NB	-3.37	107.39	110.52
25	A	810	CLA	C3B-C4B-NB	-3.37	107.39	110.52
30	b	214	DD6	C41-C32-C31	3.37	115.82	110.47
25	A	801	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
25	j	209	CLA	C3B-C4B-NB	-3.37	107.39	110.52
25	k	205	CLA	C3B-C4B-NB	-3.37	107.39	110.52
30	k	216	DD6	C32-C31-C36	3.36	127.38	122.63
25	i	205	CLA	C3B-C4B-NB	-3.36	107.40	110.52
35	d	307	CHL	CAA-C2A-C3A	-3.36	103.58	112.78
25	B	823	CLA	CHD-C1D-ND	-3.36	121.37	124.45
30	J	105	DD6	C7-C6-C5	-3.36	118.22	122.92
25	i	209	CLA	C3B-C4B-NB	-3.36	107.40	110.52
25	B	844	CLA	C3B-C4B-NB	-3.35	107.40	110.52
25	e	205	CLA	C3B-C4B-NB	-3.35	107.41	110.52
25	A	826	CLA	O2A-CGA-CBA	3.35	122.42	111.91
25	h	205	CLA	O2D-CGD-CBD	3.35	117.22	111.27
25	A	815	CLA	C3B-C4B-NB	-3.34	107.41	110.52
25	n	209	CLA	C3B-C4B-NB	-3.34	107.41	110.52
25	g	204	CLA	O2A-CGA-CBA	3.34	122.40	111.91
30	n	212	DD6	C32-C31-C36	3.34	127.35	122.63
30	j	216	DD6	C25-C26-C27	-3.34	116.88	126.58
25	o	610	CLA	CHD-C1D-ND	-3.34	121.38	124.45
30	j	217	DD6	C25-C26-C27	-3.34	116.88	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	J	101	BCR	C35-C13-C14	-3.34	118.25	122.92
30	m	213	DD6	C21-C20-C15	-3.34	116.67	122.26
25	k	203	CLA	C3B-C4B-NB	-3.33	107.42	110.52
25	g	210	CLA	C3B-C4B-NB	-3.33	107.42	110.52
25	p	601	CLA	C3B-C4B-NB	-3.33	107.42	110.52
30	n	214	DD6	C8-C6-C5	3.33	124.06	118.94
25	B	825	CLA	C3B-C4B-NB	-3.33	107.42	110.52
25	A	807	CLA	C3B-C4B-NB	-3.33	107.42	110.52
33	J	102	SQD	O47-C7-C8	3.33	120.08	110.80
30	d	317	DD6	O1-C20-C19	3.32	115.88	113.38
25	i	208	CLA	CHD-C1D-ND	-3.32	121.40	124.45
30	m	213	DD6	C32-C31-C36	3.32	127.32	122.63
25	B	841	CLA	C3B-C4B-NB	-3.32	107.44	110.52
25	h	206	CLA	C3B-C4B-NB	-3.32	107.44	110.52
25	h	205	CLA	C3B-C4B-NB	-3.32	107.44	110.52
25	A	811	CLA	C3B-C4B-NB	-3.32	107.44	110.52
25	k	206	CLA	C3B-C4B-NB	-3.31	107.44	110.52
25	B	840	CLA	O2D-CGD-CBD	3.31	117.16	111.27
25	a	204	CLA	O2D-CGD-CBD	3.31	117.15	111.27
25	a	212	CLA	O2A-CGA-CBA	3.31	122.29	111.91
35	e	209	CHL	CAA-C2A-C3A	-3.31	103.72	112.78
30	j	216	DD6	C40-C32-C31	-3.31	105.21	110.47
25	A	843	CLA	C3B-C4B-NB	-3.31	107.45	110.52
25	A	846	CLA	C3B-C4B-NB	-3.30	107.45	110.52
30	m	213	DD6	C25-C26-C27	-3.30	116.99	126.58
25	A	831	CLA	C3B-C4B-NB	-3.30	107.45	110.52
25	B	834	CLA	O2A-CGA-CBA	3.30	122.25	111.91
25	f	605	CLA	C3B-C4B-NB	-3.30	107.46	110.52
25	a	209	CLA	CHD-C1D-ND	-3.29	121.43	124.45
25	k	209	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	B	814	CLA	CHD-C1D-ND	-3.29	121.43	124.45
25	c	312	CLA	O2D-CGD-CBD	3.29	117.12	111.27
25	B	815	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	m	208	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	g	212	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	A	815	CLA	C1-C2-C3	3.29	131.74	126.04
30	F	203	DD6	C4-C3-C2	3.29	130.22	123.47
30	h	217	DD6	C40-C32-C31	-3.29	105.24	110.47
25	B	803	CLA	O2A-CGA-CBA	3.29	122.24	111.91
25	A	822	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	l	604	CLA	C3B-C4B-NB	-3.29	107.46	110.52
25	d	312	CLA	O2A-CGA-CBA	3.29	122.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	l	610	CLA	O2D-CGD-CBD	3.29	117.11	111.27
25	B	817	CLA	C3B-C4B-NB	-3.29	107.47	110.52
29	A	837	BCR	C35-C13-C14	-3.29	118.32	122.92
25	e	207	CLA	C3B-C4B-NB	-3.29	107.47	110.52
25	g	207	CLA	C3B-C4B-NB	-3.29	107.47	110.52
30	j	217	DD6	C37-C36-C31	-3.29	119.89	124.35
25	b	213	CLA	C3B-C4B-NB	-3.28	107.47	110.52
30	J	104	DD6	C37-C36-C35	3.28	120.44	114.36
35	d	310	CHL	CAA-C2A-C3A	-3.28	103.79	112.78
25	j	206	CLA	C3B-C4B-NB	-3.28	107.47	110.52
25	f	602	CLA	C3B-C4B-NB	-3.28	107.47	110.52
25	a	206	CLA	C3B-C4B-NB	-3.28	107.47	110.52
25	a	208	CLA	C3B-C4B-NB	-3.28	107.47	110.52
25	o	604	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	B	831	BCR	C35-C13-C14	-3.28	118.33	122.92
30	n	213	DD6	C4-C3-C2	3.28	130.19	123.47
25	d	311	CLA	O2A-CGA-CBA	3.28	122.19	111.91
25	B	814	CLA	C3B-C4B-NB	-3.28	107.48	110.52
25	o	607	CLA	CMA-C3A-C2A	-3.28	108.45	116.10
25	l	605	CLA	C3B-C4B-NB	-3.27	107.48	110.52
25	B	816	CLA	C3B-C4B-NB	-3.27	107.48	110.52
30	J	104	DD6	C40-C32-C31	-3.27	105.27	110.47
25	c	302	CLA	C3B-C4B-NB	-3.27	107.48	110.52
25	c	308	CLA	C3B-C4B-NB	-3.27	107.48	110.52
25	k	205	CLA	O2A-CGA-CBA	3.27	122.16	111.91
25	f	610	CLA	C3B-C4B-NB	-3.27	107.49	110.52
25	B	836	CLA	C3B-C4B-NB	-3.26	107.49	110.52
25	f	602	CLA	CHD-C1D-ND	-3.26	121.46	124.45
25	A	812	CLA	C3B-C4B-NB	-3.26	107.49	110.52
25	m	211	CLA	C3B-C4B-NB	-3.26	107.49	110.52
25	A	824	CLA	C3B-C4B-NB	-3.26	107.49	110.52
25	a	210	CLA	C3B-C4B-NB	-3.26	107.49	110.52
25	c	309	CLA	O2A-CGA-CBA	3.26	122.13	111.91
30	i	214	DD6	C40-C32-C31	-3.26	105.29	110.47
25	e	208	CLA	C3B-C4B-NB	-3.25	107.50	110.52
30	p	610	DD6	C37-C36-C35	3.25	120.38	114.36
30	e	218	DD6	C7-C6-C5	-3.25	118.36	122.92
25	m	211	CLA	CHD-C1D-ND	-3.25	121.46	124.45
25	c	306	CLA	C3B-C4B-NB	-3.25	107.50	110.52
25	e	201	CLA	CHD-C1D-ND	-3.25	121.47	124.45
25	f	604	CLA	CHD-C1D-ND	-3.25	121.47	124.45
25	o	607	CLA	CHD-C1D-ND	-3.25	121.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	811	CLA	C3B-C4B-NB	-3.25	107.50	110.52
25	c	303	CLA	O2D-CGD-CBD	3.25	117.04	111.27
30	e	220	DD6	C3-C4-C5	3.25	130.13	123.47
25	p	606	CLA	O2A-CGA-CBA	3.25	122.10	111.91
25	A	833	CLA	C3B-C4B-NB	-3.25	107.50	110.52
25	e	210	CLA	CHD-C1D-ND	-3.24	121.47	124.45
30	n	214	DD6	C32-C31-C36	-3.24	118.06	122.63
25	B	802	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	g	206	CLA	C3B-C4B-NB	-3.24	107.51	110.52
25	j	207	CLA	O2A-CGA-CBA	3.24	122.07	111.91
25	n	203	CLA	C3B-C4B-NB	-3.24	107.51	110.52
29	B	832	BCR	C35-C13-C14	-3.24	118.39	122.92
25	A	825	CLA	C3B-C4B-NB	-3.24	107.51	110.52
25	k	207	CLA	C3B-C4B-NB	-3.24	107.51	110.52
25	A	820	CLA	O2D-CGD-CBD	3.24	117.02	111.27
25	B	806	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	j	210	CLA	C3B-C4B-NB	-3.24	107.51	110.52
25	c	310	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	n	203	CLA	O2A-CGA-CBA	3.23	122.06	111.91
25	B	806	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	j	215	CLA	O2A-CGA-CBA	3.23	122.06	111.91
25	i	208	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	A	801	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	g	214	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	B	817	CLA	CHD-C1D-ND	-3.23	121.49	124.45
25	A	850	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	h	204	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	a	203	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	m	205	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	l	607	CLA	O2A-CGA-CBA	3.22	122.02	111.91
25	B	838	CLA	C1-C2-C3	3.22	131.61	126.04
25	e	213	CLA	O2A-CGA-CBA	3.22	122.01	111.91
25	o	602	CLA	C3B-C4B-NB	-3.22	107.53	110.52
30	n	213	DD6	C24-C1-C2	3.22	123.88	118.94
25	c	303	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	n	210	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	a	213	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	m	206	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	B	839	CLA	O2A-CGA-CBA	3.21	122.00	111.91
25	e	205	CLA	O2D-CGD-CBD	3.21	116.98	111.27
25	g	208	CLA	O2A-CGA-CBA	3.21	122.00	111.91
33	D	200	SQD	C3-C4-C5	3.21	115.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	817	CLA	O2A-CGA-CBA	3.21	121.99	111.91
25	b	204	CLA	O2A-CGA-CBA	3.21	121.99	111.91
25	A	812	CLA	CHD-C1D-ND	-3.21	121.50	124.45
25	d	314	CLA	C3B-C4B-NB	-3.21	107.53	110.52
30	g	217	DD6	C37-C36-C35	3.21	120.31	114.36
25	b	208	CLA	C3B-C4B-NB	-3.21	107.54	110.52
25	o	602	CLA	O2A-CGA-CBA	3.21	121.98	111.91
25	A	814	CLA	CHD-C1D-ND	-3.21	121.50	124.45
25	b	210	CLA	C3B-C4B-NB	-3.21	107.54	110.52
25	c	303	CLA	C12-C11-C10	-3.21	102.27	113.62
30	F	203	DD6	C7-C6-C5	-3.21	118.43	122.92
25	a	213	CLA	CHD-C1D-ND	-3.21	121.51	124.45
25	A	848	CLA	C4-C3-C5	-3.21	112.32	115.98
30	i	215	DD6	C25-C26-C27	-3.21	117.27	126.58
25	B	847	CLA	C3B-C4B-NB	-3.20	107.54	110.52
30	d	319	DD6	C37-C36-C31	-3.20	120.00	124.35
25	A	820	CLA	O2A-CGA-CBA	3.20	121.96	111.91
25	d	315	CLA	C3B-C4B-NB	-3.20	107.55	110.52
25	i	206	CLA	C3B-C4B-NB	-3.20	107.55	110.52
25	k	202	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	i	202	CLA	O2A-CGA-CBA	3.20	121.95	111.91
30	f	614	DD6	C21-C20-C15	-3.20	116.90	122.26
30	m	212	DD6	C37-C36-C35	3.20	120.28	114.36
25	j	208	CLA	C3B-C4B-NB	-3.20	107.55	110.52
30	o	611	DD6	C37-C36-C35	3.20	120.28	114.36
30	b	214	DD6	C40-C32-C31	-3.20	105.39	110.47
25	A	851	CLA	CHD-C1D-ND	-3.19	121.52	124.45
25	l	608	CLA	C3B-C4B-NB	-3.19	107.55	110.52
25	m	203	CLA	O2D-CGD-CBD	3.19	116.94	111.27
25	f	607	CLA	CHD-C1D-ND	-3.19	121.52	124.45
25	a	213	CLA	O2A-CGA-CBA	3.19	121.92	111.91
30	o	612	DD6	C40-C32-C31	-3.19	105.40	110.47
25	h	210	CLA	C3B-C4B-NB	-3.19	107.56	110.52
25	n	211	CLA	C3B-C4B-NB	-3.19	107.56	110.52
25	i	203	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
30	c	316	DD6	C40-C32-C31	-3.19	105.40	110.47
30	f	614	DD6	C37-C36-C35	3.19	120.26	114.36
25	k	214	CLA	C3B-C4B-NB	-3.19	107.56	110.52
30	g	217	DD6	C40-C32-C31	-3.19	105.40	110.47
25	b	203	CLA	CHD-C1D-ND	-3.19	121.53	124.45
25	d	312	CLA	C3B-C4B-NB	-3.19	107.56	110.52
25	g	213	CLA	C3B-C4B-NB	-3.19	107.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	841	CLA	CHD-C1D-ND	-3.19	121.53	124.45
25	c	311	CLA	C3B-C4B-NB	-3.19	107.56	110.52
25	g	209	CLA	O2A-CGA-CBA	3.19	121.90	111.91
25	c	309	CLA	C3B-C4B-NB	-3.18	107.56	110.52
30	m	212	DD6	C40-C32-C31	-3.18	105.41	110.47
25	A	857	CLA	C3B-C4B-NB	-3.18	107.56	110.52
25	e	206	CLA	C3B-C4B-NB	-3.18	107.56	110.52
25	l	608	CLA	CHD-C1D-ND	-3.18	121.53	124.45
33	D	200	SQD	O6-C1-C2	3.18	113.27	108.30
25	h	208	CLA	C3B-C4B-NB	-3.18	107.57	110.52
25	A	814	CLA	C3B-C4B-NB	-3.18	107.57	110.52
25	B	845	CLA	O2A-CGA-CBA	3.18	121.87	111.91
25	A	821	CLA	C3B-C4B-NB	-3.17	107.57	110.52
25	f	610	CLA	C12-C11-C10	-3.17	102.40	113.62
25	A	833	CLA	O2A-CGA-CBA	3.17	121.87	111.91
25	l	610	CLA	C3B-C4B-NB	-3.17	107.57	110.52
30	b	215	DD6	C41-C32-C31	3.17	115.51	110.47
25	o	608	CLA	C3B-C4B-NB	-3.17	107.57	110.52
30	d	319	DD6	C21-C20-C15	-3.17	116.94	122.26
25	a	212	CLA	CHD-C1D-ND	-3.17	121.54	124.45
25	f	608	CLA	C3B-C4B-NB	-3.17	107.57	110.52
25	n	206	CLA	C3B-C4B-NB	-3.17	107.57	110.52
30	A	855	DD6	C37-C36-C35	3.17	120.23	114.36
25	g	213	CLA	CHD-C1D-ND	-3.17	121.54	124.45
25	d	304	CLA	C3B-C4B-NB	-3.17	107.57	110.52
25	k	202	CLA	C3B-C4B-NB	-3.17	107.57	110.52
25	f	609	CLA	O2D-CGD-CBD	3.17	116.90	111.27
30	j	217	DD6	C40-C32-C31	-3.17	105.43	110.47
25	A	842	CLA	CHD-C1D-ND	-3.17	121.54	124.45
25	f	606	CLA	CHD-C1D-ND	-3.17	121.54	124.45
25	A	807	CLA	O2A-CGA-CBA	3.17	121.85	111.91
30	f	613	DD6	C37-C36-C35	3.17	120.23	114.36
25	h	215	CLA	C3B-C4B-NB	-3.17	107.58	110.52
25	h	206	CLA	O2A-CGA-CBA	3.17	121.84	111.91
25	c	308	CLA	O2A-CGA-CBA	3.16	121.84	111.91
25	A	823	CLA	C3B-C4B-NB	-3.16	107.58	110.52
25	c	312	CLA	C3B-C4B-NB	-3.16	107.58	110.52
25	g	210	CLA	CHD-C1D-ND	-3.16	121.55	124.45
30	A	854	DD6	C21-C20-C15	-3.16	116.96	122.26
25	f	602	CLA	O2A-CGA-CBA	3.16	121.83	111.91
30	n	214	DD6	C13-C11-C10	3.16	123.79	118.94
30	c	317	DD6	C25-C26-C27	-3.16	117.41	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	212	DD6	C37-C36-C35	3.16	120.20	114.36
30	j	216	DD6	C37-C36-C35	3.15	120.20	114.36
25	B	808	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	i	210	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	i	207	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	o	606	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	f	606	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	p	606	CLA	C3B-C4B-NB	-3.15	107.59	110.52
29	B	831	BCR	C16-C15-C14	3.15	129.93	123.47
30	l	614	DD6	C40-C32-C31	-3.15	105.46	110.47
25	b	204	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	c	315	CLA	O2A-CGA-CBA	3.15	121.79	111.91
30	i	215	DD6	C37-C36-C35	3.15	120.19	114.36
25	B	841	CLA	C12-C11-C10	-3.15	102.49	113.62
25	l	610	CLA	O2A-CGA-CBA	3.15	121.78	111.91
30	n	213	DD6	C7-C6-C5	-3.15	118.52	122.92
25	m	209	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	m	207	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	k	211	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	g	208	CLA	CHD-C1D-ND	-3.14	121.57	124.45
25	n	201	CLA	C12-C11-C10	-3.14	102.51	113.62
25	g	208	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	h	213	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	o	609	CLA	C3B-C4B-NB	-3.14	107.60	110.52
35	d	310	CHL	C3B-C4B-NB	-3.14	107.60	110.52
25	A	844	CLA	O2A-CGA-CBA	3.14	121.76	111.91
25	f	602	CLA	C12-C11-C10	-3.14	102.52	113.62
25	A	830	CLA	O2A-CGA-CBA	3.14	121.75	111.91
25	B	843	CLA	O2A-CGA-CBA	3.14	121.75	111.91
30	b	214	DD6	C37-C36-C35	3.14	120.16	114.36
30	b	215	DD6	C40-C32-C31	-3.13	105.49	110.47
30	e	219	DD6	C37-C36-C35	3.13	120.16	114.36
30	i	215	DD6	C40-C32-C31	-3.13	105.49	110.47
29	B	828	BCR	C15-C14-C13	-3.13	122.84	127.31
25	A	848	CLA	O2A-CGA-CBA	3.13	121.73	111.91
30	c	317	DD6	O1-C20-C19	3.13	115.73	113.38
25	B	822	CLA	C3B-C4B-NB	-3.13	107.61	110.52
30	o	612	DD6	C37-C36-C35	3.13	120.15	114.36
30	n	212	DD6	O1-C20-C21	-3.13	111.31	115.06
30	h	216	DD6	C40-C32-C31	-3.13	105.50	110.47
25	A	813	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	b	211	CLA	C3B-C4B-NB	-3.12	107.62	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	l	606	CLA	C3B-C4B-NB	-3.12	107.62	110.52
30	J	104	DD6	C21-C20-C15	-3.12	117.03	122.26
25	h	207	CLA	O2A-CGA-CBA	3.12	121.71	111.91
25	B	824	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	d	313	CLA	C3B-C4B-NB	-3.12	107.62	110.52
30	k	215	DD6	C40-C32-C31	-3.12	105.50	110.47
25	A	823	CLA	O2A-CGA-CBA	3.12	121.71	111.91
30	h	217	DD6	O1-C20-C19	3.12	115.73	113.38
25	B	823	CLA	O2A-CGA-CBA	3.12	121.70	111.91
30	h	216	DD6	C21-C20-C15	-3.12	117.03	122.26
25	k	214	CLA	O2A-CGA-CBA	3.12	121.70	111.91
25	d	316	CLA	C3B-C4B-NB	-3.12	107.62	110.52
30	f	613	DD6	C40-C32-C31	-3.12	105.51	110.47
25	A	802	CLA	O2A-CGA-CBA	3.12	121.69	111.91
25	a	207	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	i	208	CLA	O2A-CGA-CBA	3.12	121.69	111.91
25	d	312	CLA	C12-C11-C10	-3.12	102.60	113.62
30	h	217	DD6	C37-C36-C35	3.12	120.13	114.36
25	B	843	CLA	C3B-C4B-NB	-3.12	107.62	110.52
29	A	837	BCR	C36-C18-C17	-3.12	118.56	122.92
25	e	201	CLA	O2A-CGA-CBA	3.11	121.68	111.91
25	f	610	CLA	O2A-CGA-CBA	3.11	121.68	111.91
30	g	216	DD6	C37-C36-C35	3.11	120.12	114.36
25	A	802	CLA	CHD-C1D-ND	-3.11	121.59	124.45
30	l	613	DD6	C21-C20-C15	-3.11	117.04	122.26
25	d	306	CLA	C3B-C4B-NB	-3.11	107.63	110.52
35	e	209	CHL	C3B-C4B-NB	-3.11	107.63	110.52
25	B	837	CLA	C3B-C4B-NB	-3.11	107.63	110.52
30	g	216	DD6	C21-C20-C15	-3.11	117.05	122.26
25	i	213	CLA	C3B-C4B-NB	-3.11	107.63	110.52
25	k	211	CLA	CHD-C1D-ND	-3.11	121.60	124.45
33	J	102	SQD	O8-S-C6	3.10	110.69	105.74
30	k	216	DD6	C37-C36-C35	3.10	120.11	114.36
25	a	208	CLA	O2A-CGA-CBA	3.10	121.65	111.91
25	b	212	CLA	C3B-C4B-NB	-3.10	107.64	110.52
25	A	818	CLA	O2D-CGD-CBD	3.10	116.78	111.27
25	m	209	CLA	CHD-C1D-ND	-3.10	121.60	124.45
30	i	216	DD6	C37-C36-C35	3.10	120.10	114.36
25	o	601	CLA	CHD-C1D-ND	-3.10	121.61	124.45
25	h	211	CLA	C3B-C4B-NB	-3.10	107.64	110.52
25	a	204	CLA	CHD-C1D-ND	-3.10	121.61	124.45
25	c	305	CLA	C3B-C4B-NB	-3.10	107.64	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	m	213	DD6	C40-C32-C31	-3.10	105.54	110.47
25	f	611	CLA	C3B-C4B-NB	-3.10	107.64	110.52
25	A	840	CLA	O2A-CGA-CBA	3.10	121.62	111.91
25	g	203	CLA	O2D-CGD-CBD	3.10	116.77	111.27
25	k	208	CLA	O2A-CGA-CBA	3.09	121.62	111.91
25	n	202	CLA	C3B-C4B-NB	-3.09	107.64	110.52
25	g	212	CLA	O2A-CGA-CBA	3.09	121.61	111.91
25	a	213	CLA	C1-C2-C3	3.09	131.39	126.04
25	B	834	CLA	C3B-C4B-NB	-3.09	107.65	110.52
25	B	822	CLA	O2A-CGA-CBA	3.09	121.61	111.91
35	d	307	CHL	C3B-C4B-NB	-3.09	107.65	110.52
25	n	206	CLA	CHD-C1D-ND	-3.09	121.62	124.45
25	c	313	CLA	C3B-C4B-NB	-3.09	107.65	110.52
30	c	318	DD6	C37-C36-C35	3.09	120.07	114.36
25	e	214	CLA	C3B-C4B-NB	-3.09	107.65	110.52
30	c	318	DD6	C40-C32-C31	-3.09	105.56	110.47
25	b	205	CLA	C3B-C4B-NB	-3.08	107.65	110.52
25	c	315	CLA	C3B-C4B-NB	-3.08	107.65	110.52
25	h	203	CLA	C3B-C4B-NB	-3.08	107.65	110.52
25	A	822	CLA	CHD-C1D-ND	-3.08	121.62	124.45
25	l	602	CLA	C12-C11-C10	-3.08	102.72	113.62
25	l	609	CLA	C3B-C4B-NB	-3.08	107.66	110.52
25	g	211	CLA	C3B-C4B-NB	-3.08	107.66	110.52
25	e	216	CLA	O2A-CGA-CBA	3.08	121.58	111.91
25	d	311	CLA	CHD-C1D-ND	-3.08	121.63	124.45
30	a	215	DD6	C37-C36-C35	3.08	120.05	114.36
25	k	206	CLA	O2A-CGA-CBA	3.07	121.55	111.91
25	n	207	CLA	CHD-C1D-ND	-3.07	121.63	124.45
25	f	608	CLA	CHD-C1D-ND	-3.07	121.63	124.45
25	j	204	CLA	O2A-CGA-CBA	3.07	121.54	111.91
30	J	104	DD6	O1-C20-C19	3.07	115.69	113.38
25	h	203	CLA	O2A-CGA-CBA	3.07	121.53	111.91
30	e	218	DD6	C4-C3-C2	3.07	129.76	123.47
25	e	208	CLA	CHD-C1D-ND	-3.07	121.64	124.45
29	B	801	BCR	C29-C30-C25	3.07	115.20	110.48
25	j	209	CLA	O2A-CGA-CBA	3.07	121.53	111.91
25	b	209	CLA	C3B-C4B-NB	-3.07	107.67	110.52
30	e	220	DD6	C8-C6-C5	3.06	123.64	118.94
25	B	814	CLA	C12-C11-C10	-3.06	102.78	113.62
25	l	601	CLA	C3B-C4B-NB	-3.06	107.67	110.52
25	B	820	CLA	C3B-C4B-NB	-3.06	107.67	110.52
30	i	214	DD6	C21-C20-C15	-3.06	117.13	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	p	610	DD6	C21-C20-C15	-3.06	117.13	122.26
33	F	204	SQD	O8-S-C6	3.06	110.62	105.74
25	k	210	CLA	C3B-C4B-NB	-3.06	107.67	110.52
30	a	215	DD6	C40-C32-C31	-3.06	105.60	110.47
25	e	215	CLA	C3B-C4B-NB	-3.06	107.68	110.52
25	i	202	CLA	C3B-C4B-NB	-3.06	107.68	110.52
30	k	215	DD6	C21-C20-C15	-3.06	117.13	122.26
29	B	832	BCR	C15-C16-C17	3.06	129.74	123.47
25	m	204	CLA	O2A-CGA-CBA	3.06	121.50	111.91
25	p	602	CLA	CHD-C1D-ND	-3.06	121.65	124.45
30	c	317	DD6	C37-C36-C31	-3.06	120.20	124.35
25	B	812	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	k	209	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	c	316	DD6	C37-C36-C35	3.05	120.01	114.36
25	B	818	CLA	C3B-C4B-NB	-3.05	107.68	110.52
25	l	602	CLA	C1-C2-C3	3.05	131.32	126.04
25	c	309	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	d	312	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	e	214	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	i	203	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	f	601	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	A	855	DD6	C40-C32-C31	-3.05	105.62	110.47
25	h	209	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	i	214	DD6	C37-C36-C35	3.05	120.01	114.36
25	e	207	CLA	O2A-CGA-CBA	3.05	121.48	111.91
25	b	210	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	b	206	CLA	C3B-C4B-NB	-3.05	107.69	110.52
25	n	208	CLA	C3B-C4B-NB	-3.05	107.69	110.52
25	l	602	CLA	O2D-CGD-CBD	3.04	116.68	111.27
30	o	611	DD6	C40-C32-C31	-3.04	105.63	110.47
25	i	212	CLA	C3B-C4B-NB	-3.04	107.69	110.52
25	b	203	CLA	C3B-C4B-NB	-3.04	107.69	110.52
25	A	829	CLA	O2A-CGA-CBA	3.04	121.45	111.91
25	j	208	CLA	O2A-CGA-CBA	3.04	121.45	111.91
25	b	211	CLA	CHD-C1D-ND	-3.04	121.66	124.45
30	h	216	DD6	C37-C36-C35	3.04	119.98	114.36
25	J	103	CLA	C3B-C4B-NB	-3.04	107.70	110.52
30	a	214	DD6	C37-C36-C35	3.04	119.98	114.36
25	A	828	CLA	CHD-C1D-ND	-3.04	121.66	124.45
25	a	211	CLA	C3B-C4B-NB	-3.04	107.70	110.52
25	k	208	CLA	C3B-C4B-NB	-3.04	107.70	110.52
25	d	303	CLA	O2A-CGA-CBA	3.03	121.43	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	202	CLA	O2A-CGA-CBA	3.03	121.43	111.91
30	A	855	DD6	C21-C20-C15	-3.03	117.18	122.26
25	F	201	CLA	C3B-C4B-NB	-3.03	107.70	110.52
25	A	845	CLA	C3B-C4B-NB	-3.03	107.70	110.52
25	A	848	CLA	C3B-C4B-NB	-3.03	107.70	110.52
30	d	319	DD6	C40-C32-C31	-3.03	105.65	110.47
25	l	610	CLA	CHD-C1D-ND	-3.03	121.67	124.45
28	B	827	PQN	C2M-C2-C1	-3.03	111.25	116.27
25	A	847	CLA	CHD-C1D-ND	-3.03	121.67	124.45
25	B	821	CLA	C3B-C4B-NB	-3.03	107.71	110.52
25	A	831	CLA	O2A-CGA-CBA	3.03	121.41	111.91
30	e	219	DD6	C40-C32-C31	-3.03	105.66	110.47
35	d	309	CHL	C3B-C4B-NB	-3.03	107.71	110.52
25	h	208	CLA	O2A-CGA-CBA	3.03	121.40	111.91
25	A	818	CLA	C3B-C4B-NB	-3.02	107.71	110.52
29	B	831	BCR	C36-C18-C17	-3.02	118.69	122.92
25	n	204	CLA	C3B-C4B-NB	-3.02	107.71	110.52
30	k	216	DD6	C40-C32-C31	-3.02	105.67	110.47
25	e	205	CLA	O2A-CGA-CBA	3.02	121.39	111.91
25	j	208	CLA	CHD-C1D-ND	-3.02	121.68	124.45
25	B	837	CLA	O2A-CGA-CBA	3.02	121.39	111.91
25	a	205	CLA	C3B-C4B-NB	-3.02	107.71	110.52
25	c	305	CLA	O2A-CGA-CBA	3.02	121.38	111.91
25	A	828	CLA	C3B-C4B-NB	-3.02	107.72	110.52
25	a	207	CLA	O2A-CGA-CBA	3.02	121.37	111.91
25	l	606	CLA	O2A-CGA-CBA	3.01	121.36	111.91
25	k	205	CLA	CHD-C1D-ND	-3.01	121.69	124.45
30	k	215	DD6	C37-C36-C35	3.01	119.93	114.36
25	l	604	CLA	CHD-C1D-ND	-3.01	121.69	124.45
25	B	841	CLA	O2A-CGA-CBA	3.01	121.36	111.91
25	B	842	CLA	O2A-CGA-CBA	3.01	121.36	111.91
25	A	825	CLA	O2A-CGA-CBA	3.01	121.35	111.91
25	b	212	CLA	CHD-C1D-ND	-3.01	121.69	124.45
25	g	205	CLA	C2D-C1D-ND	3.01	112.32	110.10
30	g	216	DD6	C37-C36-C31	-3.01	120.26	124.35
25	A	820	CLA	CHD-C1D-ND	-3.01	121.69	124.45
25	A	844	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
35	d	307	CHL	C1-C2-C3	3.01	131.62	126.75
25	k	204	CLA	C3B-C4B-NB	-3.01	107.73	110.52
33	g	202	SQD	O8-S-C6	3.01	110.53	105.74
25	B	837	CLA	CHD-C1D-ND	-3.01	121.69	124.45
30	b	215	DD6	C37-C36-C35	3.00	119.92	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	310	CLA	C3B-C4B-NB	-3.00	107.73	110.52
25	A	843	CLA	O2A-CGA-CBA	3.00	121.33	111.91
25	k	208	CLA	CHD-C1D-ND	-3.00	121.69	124.45
30	o	611	DD6	C21-C20-C15	-3.00	117.23	122.26
30	d	317	DD6	C37-C36-C35	3.00	119.92	114.36
25	j	210	CLA	O2A-CGA-CBA	3.00	121.33	111.91
25	o	606	CLA	CHD-C1D-ND	-3.00	121.70	124.45
30	b	215	DD6	C25-C26-C27	-3.00	117.88	126.58
25	g	215	CLA	C3B-C4B-NB	-3.00	107.74	110.52
30	l	614	DD6	C37-C36-C35	3.00	119.90	114.36
25	B	814	CLA	O2A-CGA-CBA	2.99	121.31	111.91
25	p	607	CLA	CHD-C1D-ND	-2.99	121.70	124.45
25	j	203	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	b	213	CLA	CHD-C1D-ND	-2.99	121.70	124.45
25	l	611	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	k	213	CLA	C3B-C4B-NB	-2.99	107.74	110.52
30	n	212	DD6	C21-C20-C15	-2.99	117.25	122.26
25	B	812	CLA	O2A-CGA-CBA	2.99	121.28	111.91
30	e	220	DD6	C13-C11-C10	2.99	123.53	118.94
25	B	818	CLA	O2A-CGA-CBA	2.99	121.28	111.91
30	d	317	DD6	C40-C32-C31	-2.98	105.72	110.47
25	B	802	CLA	C3B-C4B-NB	-2.98	107.75	110.52
30	l	613	DD6	C37-C36-C31	-2.98	120.30	124.35
25	B	805	CLA	C1-C2-C3	2.98	131.20	126.04
29	J	101	BCR	C12-C13-C14	2.98	123.51	118.94
25	c	314	CLA	C3B-C4B-NB	-2.98	107.75	110.52
30	f	614	DD6	C37-C36-C31	-2.98	120.30	124.35
25	A	801	CLA	O2A-CGA-CBA	2.98	121.25	111.91
30	c	318	DD6	C37-C36-C31	-2.98	120.31	124.35
30	A	854	DD6	C28-C27-C29	-2.97	110.95	116.84
25	A	827	CLA	C3B-C4B-NB	-2.97	107.76	110.52
30	a	214	DD6	C40-C32-C31	-2.97	105.74	110.47
30	j	216	DD6	C21-C20-C15	-2.97	117.28	122.26
25	m	207	CLA	O2A-CGA-CBA	2.97	121.23	111.91
25	m	210	CLA	C3B-C4B-NB	-2.97	107.76	110.52
25	A	810	CLA	O2A-CGA-CBA	2.97	121.23	111.91
25	h	212	CLA	CHD-C1D-ND	-2.97	121.72	124.45
25	B	819	CLA	O2A-CGA-CBA	2.97	121.23	111.91
25	A	818	CLA	CHD-C1D-ND	-2.97	121.73	124.45
25	c	304	CLA	O2A-CGA-CBA	2.97	121.22	111.91
30	g	217	DD6	C37-C36-C31	-2.97	120.32	124.35
25	h	203	CLA	O1D-CGD-CBD	-2.97	118.41	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	e	219	DD6	C37-C36-C31	-2.97	120.32	124.35
30	d	318	DD6	C21-C20-C15	-2.97	117.29	122.26
25	e	212	CLA	C3B-C4B-NB	-2.97	107.76	110.52
25	o	605	CLA	C3B-C4B-NB	-2.97	107.76	110.52
25	f	601	CLA	C3B-C4B-NB	-2.97	107.76	110.52
25	d	305	CLA	C3B-C4B-NB	-2.96	107.77	110.52
25	l	602	CLA	O2A-CGA-CBA	2.96	121.21	111.91
30	g	216	DD6	C3-C2-C1	-2.96	123.08	127.31
25	f	610	CLA	CHD-C1D-ND	-2.96	121.73	124.45
25	i	209	CLA	CHD-C1D-ND	-2.96	121.73	124.45
25	m	203	CLA	CHD-C1D-ND	-2.96	121.73	124.45
25	m	207	CLA	CHD-C1D-ND	-2.96	121.73	124.45
30	l	613	DD6	C40-C32-C31	-2.96	105.76	110.47
25	o	602	CLA	O1D-CGD-CBD	-2.96	118.43	124.48
30	J	105	DD6	C8-C6-C5	2.96	123.48	118.94
30	d	319	DD6	C37-C36-C35	2.96	119.84	114.36
25	i	207	CLA	CHD-C1D-ND	-2.96	121.74	124.45
25	d	304	CLA	O2A-CGA-CBA	2.96	121.19	111.91
30	A	854	DD6	C40-C32-C31	-2.96	105.77	110.47
25	A	849	CLA	C3B-C4B-NB	-2.96	107.77	110.52
25	A	814	CLA	O2A-CGA-CBA	2.96	121.18	111.91
25	A	827	CLA	CHD-C1D-ND	-2.96	121.74	124.45
30	d	317	DD6	C37-C36-C31	-2.95	120.33	124.35
25	j	211	CLA	C1-C2-C3	2.95	131.15	126.04
30	o	612	DD6	C21-C20-C15	-2.95	117.31	122.26
30	h	217	DD6	C21-C20-C15	-2.95	117.31	122.26
25	B	807	CLA	C3B-C4B-NB	-2.95	107.78	110.52
27	h	201	LHG	O7-C7-C8	2.95	117.86	111.50
30	b	215	DD6	C21-C20-C15	-2.95	117.32	122.26
25	c	304	CLA	C1-C2-C3	2.95	131.14	126.04
25	A	812	CLA	O2A-CGA-CBA	2.95	121.16	111.91
30	p	610	DD6	C40-C32-C31	-2.94	105.79	110.47
25	B	838	CLA	O2A-CGA-CBA	2.94	121.15	111.91
30	d	317	DD6	C21-C20-C15	-2.94	117.33	122.26
25	h	209	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
35	c	307	CHL	C2A-C1A-CHA	2.94	129.00	123.86
25	A	842	CLA	O2A-CGA-CBA	2.94	121.14	111.91
25	i	213	CLA	O2A-CGA-CBA	2.94	121.14	111.91
25	a	208	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	e	204	CLA	C3B-C4B-NB	-2.94	107.79	110.52
25	c	306	CLA	CHD-C1D-ND	-2.94	121.75	124.45
30	f	614	DD6	C40-C32-C31	-2.94	105.80	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	813	CLA	C3B-C4B-NB	-2.94	107.79	110.52
30	l	614	DD6	C21-C20-C15	-2.94	117.34	122.26
25	A	813	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	c	318	DD6	O1-C20-C21	-2.93	111.54	115.06
25	A	841	CLA	O2A-CGA-CBA	2.93	121.12	111.91
30	A	855	DD6	C37-C36-C31	-2.93	120.36	124.35
30	g	216	DD6	C40-C32-C31	-2.93	105.81	110.47
25	c	303	CLA	O2A-CGA-CBA	2.93	121.11	111.91
30	j	217	DD6	C21-C20-C15	-2.93	117.34	122.26
30	m	213	DD6	C37-C36-C31	-2.93	120.36	124.35
30	a	214	DD6	C37-C36-C31	-2.93	120.37	124.35
30	l	613	DD6	C37-C36-C35	2.93	119.78	114.36
25	B	816	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	o	609	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	A	818	CLA	CHB-C1B-NB	2.93	127.36	124.26
25	k	211	CLA	O2A-CGA-CBA	2.93	121.10	111.91
25	n	209	CLA	CMA-C3A-C2A	-2.93	109.27	116.10
25	B	815	CLA	O2A-CGA-CBA	2.93	121.10	111.91
33	D	200	SQD	O8-S-C6	2.93	110.41	105.74
25	B	840	CLA	O2A-CGA-CBA	2.93	121.09	111.91
25	A	824	CLA	CHD-C1D-ND	-2.93	121.77	124.45
25	A	852	CLA	O2A-CGA-CBA	2.93	121.09	111.91
25	j	211	CLA	O2A-CGA-CBA	2.92	121.08	111.91
25	j	206	CLA	O2A-CGA-CBA	2.92	121.08	111.91
25	g	203	CLA	C3B-C4B-NB	-2.92	107.81	110.52
25	B	805	CLA	CHD-C1D-ND	-2.92	121.77	124.45
25	c	310	CLA	O2A-CGA-CBA	2.92	121.07	111.91
25	k	207	CLA	O2A-CGA-CBA	2.92	121.07	111.91
30	e	218	DD6	C3-C4-C5	2.92	129.45	123.47
25	a	203	CLA	CHD-C1D-ND	-2.92	121.77	124.45
25	A	819	CLA	C3B-C4B-NB	-2.92	107.81	110.52
25	b	207	CLA	C3B-C4B-NB	-2.92	107.81	110.52
30	g	217	DD6	C21-C20-C15	-2.91	117.38	122.26
25	b	204	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
33	D	200	SQD	C1-O5-C5	-2.91	107.98	113.69
25	g	209	CLA	CHD-C1D-ND	-2.91	121.78	124.45
25	B	846	CLA	O2A-CGA-CBA	2.91	121.03	111.91
30	b	215	DD6	C37-C36-C31	-2.91	120.40	124.35
25	n	209	CLA	CHD-C1D-ND	-2.91	121.78	124.45
25	p	606	CLA	CHD-C1D-ND	-2.91	121.78	124.45
25	m	204	CLA	C3B-C4B-NB	-2.91	107.82	110.52
25	A	849	CLA	O2A-CGA-CBA	2.90	121.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	e	211	CLA	O2A-CGA-CBA	2.90	121.02	111.91
25	l	603	CLA	C3B-C4B-NB	-2.90	107.82	110.52
25	f	612	CLA	C3B-C4B-NB	-2.90	107.82	110.52
35	c	307	CHL	C3B-C4B-NB	-2.90	107.82	110.52
25	A	830	CLA	CHD-C1D-ND	-2.90	121.79	124.45
30	d	318	DD6	C40-C32-C31	-2.90	105.86	110.47
30	a	214	DD6	C21-C20-C15	-2.90	117.40	122.26
29	B	832	BCR	C36-C18-C17	-2.90	118.86	122.92
25	A	811	CLA	CHD-C1D-ND	-2.90	121.79	124.45
25	g	212	CLA	CHD-C1D-ND	-2.90	121.79	124.45
25	B	847	CLA	O2A-CGA-CBA	2.90	121.00	111.91
29	J	101	BCR	C15-C16-C17	2.90	129.41	123.47
25	a	209	CLA	O2A-CGA-CBA	2.90	121.00	111.91
25	F	202	CLA	CHD-C1D-ND	-2.90	121.79	124.45
25	A	811	CLA	O2A-CGA-CBA	2.90	121.00	111.91
25	h	206	CLA	CHD-C1D-ND	-2.89	121.79	124.45
30	m	213	DD6	C37-C36-C35	2.89	119.71	114.36
25	A	848	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	a	206	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	m	208	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	A	817	CLA	O2A-CGA-CBA	2.89	120.98	111.91
25	a	210	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	l	611	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	A	814	CLA	C1-C2-C3	2.89	131.04	126.04
25	B	821	CLA	O2A-CGA-CBA	2.89	120.98	111.91
30	i	216	DD6	C40-C32-C31	-2.89	105.88	110.47
25	k	207	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	m	203	CLA	O2A-CGA-CBA	2.89	120.97	111.91
25	A	824	CLA	O2A-CGA-CBA	2.89	120.97	111.91
30	f	613	DD6	C21-C20-C15	-2.89	117.42	122.26
25	c	305	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	e	216	CLA	CHD-C1D-ND	-2.89	121.80	124.45
28	B	827	PQN	C6-C5-C4	-2.89	115.87	120.10
27	g	201	LHG	O7-C7-C8	2.88	117.72	111.50
30	n	212	DD6	C40-C32-C31	-2.88	105.88	110.47
25	f	607	CLA	O2A-CGA-CBA	2.88	120.96	111.91
30	g	216	DD6	C28-C27-C29	-2.88	111.13	116.84
25	c	313	CLA	CHD-C1D-ND	-2.88	121.81	124.45
25	c	313	CLA	O2A-CGA-CBA	2.88	120.95	111.91
25	h	214	CLA	C3B-C4B-NB	-2.88	107.84	110.52
25	h	203	CLA	O2D-CGD-CBD	2.88	116.38	111.27
25	b	212	CLA	O2A-CGA-CBA	2.88	120.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	J	101	BCR	C19-C18-C17	2.88	123.36	118.94
25	i	203	CLA	O2A-CGA-CBA	2.88	120.94	111.91
25	B	824	CLA	O2A-CGA-CBA	2.87	120.93	111.91
25	k	203	CLA	CHD-C1D-ND	-2.87	121.81	124.45
29	A	837	BCR	C12-C13-C14	2.87	123.35	118.94
25	A	819	CLA	O2A-CGA-CBA	2.87	120.92	111.91
25	J	103	CLA	O2A-CGA-CBA	2.87	120.91	111.91
30	c	316	DD6	C21-C20-C15	-2.87	117.45	122.26
25	F	202	CLA	C3B-C4B-NB	-2.87	107.85	110.52
33	g	202	SQD	O9-S-C6	2.87	110.35	106.94
30	c	317	DD6	C37-C36-C35	2.87	119.67	114.36
25	A	853	CLA	O2A-CGA-CBA	2.87	120.91	111.91
25	g	203	CLA	O1D-CGD-CBD	-2.87	118.62	124.48
25	d	306	CLA	O2A-CGA-CBA	2.87	120.91	111.91
25	k	213	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	B	807	CLA	O2A-CGA-CBA	2.87	120.90	111.91
25	d	304	CLA	CHD-C1D-ND	-2.86	121.82	124.45
25	c	303	CLA	CHD-C1D-ND	-2.86	121.83	124.45
30	b	214	DD6	O1-C20-C21	-2.86	111.63	115.06
25	j	205	CLA	C3B-C4B-NB	-2.86	107.86	110.52
25	o	601	CLA	C3B-C4B-NB	-2.86	107.86	110.52
25	c	314	CLA	CHD-C1D-ND	-2.86	121.83	124.45
25	b	208	CLA	CMA-C3A-C2A	-2.86	109.43	116.10
25	g	203	CLA	CHD-C1D-ND	-2.86	121.83	124.45
27	m	201	LHG	O7-C7-C8	2.86	117.66	111.50
25	A	804	CLA	CHD-C1D-ND	-2.86	121.83	124.45
25	A	804	CLA	C1-C2-C3	2.85	130.98	126.04
25	A	806	CLA	C3B-C4B-NB	-2.85	107.87	110.52
25	A	820	CLA	C3B-C4B-NB	-2.85	107.87	110.52
25	f	612	CLA	CHD-C1D-ND	-2.85	121.83	124.45
30	j	217	DD6	C37-C36-C35	2.85	119.64	114.36
29	B	831	BCR	C12-C13-C14	2.85	123.31	118.94
25	l	606	CLA	C1-C2-C3	2.85	130.97	126.04
30	m	212	DD6	C21-C20-C15	-2.85	117.49	122.26
25	F	201	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	j	204	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	A	808	CLA	O2A-CGA-CBA	2.85	120.84	111.91
25	b	207	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	A	832	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	B	838	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	A	833	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	B	824	CLA	CHD-C1D-ND	-2.84	121.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	805	CLA	O2A-CGA-CBA	2.84	120.83	111.91
25	c	313	CLA	C1-C2-C3	2.84	130.96	126.04
35	d	307	CHL	O2A-CGA-CBA	2.84	120.83	111.91
25	h	215	CLA	CHD-C1D-ND	-2.84	121.84	124.45
25	l	606	CLA	CHD-C1D-ND	-2.84	121.84	124.45
25	h	203	CLA	CHD-C1D-ND	-2.84	121.84	124.45
30	d	318	DD6	C37-C36-C35	2.84	119.61	114.36
25	j	203	CLA	CHD-C1D-ND	-2.84	121.85	124.45
33	J	102	SQD	O6-C1-C2	2.84	112.73	108.30
27	h	202	LHG	O7-C7-C8	2.84	117.61	111.50
25	a	203	CLA	O2A-CGA-CBA	2.84	120.81	111.91
25	m	202	CLA	C2D-C1D-ND	2.83	112.19	110.10
32	e	203	DGD	O6D-C1D-O3G	-2.83	103.27	109.97
25	i	211	CLA	CHD-C1D-ND	-2.83	121.85	124.45
25	j	214	CLA	C3B-C4B-NB	-2.83	107.89	110.52
30	f	614	DD6	O1-C20-C21	-2.83	111.67	115.06
25	A	844	CLA	O1D-CGD-CBD	-2.83	118.70	124.48
25	A	814	CLA	C12-C11-C10	-2.83	103.63	113.62
25	p	607	CLA	C3B-C4B-NB	-2.83	107.89	110.52
25	h	211	CLA	O2A-CGA-CBA	2.82	120.77	111.91
25	B	846	CLA	CHD-C1D-ND	-2.82	121.86	124.45
25	A	857	CLA	O2A-CGA-CBA	2.82	120.77	111.91
30	k	215	DD6	O1-C20-C19	2.82	115.50	113.38
25	j	210	CLA	CHD-C1D-ND	-2.82	121.86	124.45
25	j	203	CLA	O2A-CGA-CBA	2.82	120.76	111.91
25	c	304	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	B	836	CLA	O2A-CGA-CBA	2.82	120.76	111.91
30	i	216	DD6	C37-C36-C31	-2.82	120.52	124.35
25	a	207	CLA	CHD-C1D-ND	-2.82	121.86	124.45
25	d	306	CLA	C1-C2-C3	2.82	130.92	126.04
30	l	613	DD6	O1-C20-C19	2.82	115.50	113.38
25	e	212	CLA	O2A-CGA-CBA	2.82	120.75	111.91
25	A	853	CLA	CHD-C1D-ND	-2.82	121.86	124.45
25	B	846	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	B	844	CLA	O2A-CGA-CBA	2.82	120.74	111.91
25	i	205	CLA	CHD-C1D-ND	-2.82	121.87	124.45
25	A	804	CLA	O2A-CGA-CBA	2.81	120.74	111.91
25	j	213	CLA	C3B-C4B-NB	-2.81	107.90	110.52
25	B	834	CLA	CHD-C1D-ND	-2.81	121.87	124.45
27	A	835	LHG	O7-C7-C8	2.81	117.56	111.50
27	i	201	LHG	O7-C7-C8	2.81	117.56	111.50
25	h	210	CLA	CHD-C1D-ND	-2.81	121.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	205	PQN	C6-C5-C4	-2.81	115.98	120.10
29	B	831	BCR	C15-C16-C17	2.81	129.23	123.47
30	i	215	DD6	C37-C36-C31	-2.81	120.53	124.35
25	b	209	CLA	CHD-C1D-ND	-2.81	121.87	124.45
25	A	826	CLA	CHD-C1D-ND	-2.81	121.87	124.45
25	k	212	CLA	C3B-C4B-NB	-2.81	107.91	110.52
35	d	308	CHL	C3B-C4B-NB	-2.81	107.91	110.52
30	c	316	DD6	C37-C36-C31	-2.81	120.53	124.35
25	J	103	CLA	CHD-C1D-ND	-2.81	121.88	124.45
25	h	209	CLA	C3B-C4B-NB	-2.81	107.91	110.52
25	g	214	CLA	CHD-C1D-ND	-2.80	121.88	124.45
27	d	302	LHG	O7-C7-C8	2.80	117.54	111.50
25	p	605	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	B	839	CLA	CHD-C1D-ND	-2.80	121.88	124.45
33	D	200	SQD	O48-C23-C24	2.80	120.69	111.91
25	p	603	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	A	846	CLA	O2A-CGA-CBA	2.80	120.68	111.91
25	h	204	CLA	CHD-C1D-ND	-2.80	121.89	124.45
30	o	612	DD6	C37-C36-C31	-2.79	120.55	124.35
25	i	211	CLA	C12-C11-C10	-2.79	103.74	113.62
25	A	832	CLA	O2A-CGA-CBA	2.79	120.68	111.91
25	f	603	CLA	C3B-C4B-NB	-2.79	107.92	110.52
25	A	850	CLA	C2A-C1A-CHA	2.79	128.74	123.86
29	B	828	BCR	C2-C1-C6	2.79	114.78	110.48
30	J	104	DD6	C28-C27-C29	-2.79	111.31	116.84
25	h	211	CLA	C2D-C1D-ND	2.79	112.16	110.10
25	g	206	CLA	CHD-C1D-ND	-2.79	121.89	124.45
30	i	214	DD6	C37-C36-C31	-2.79	120.56	124.35
25	A	853	CLA	C1-C2-C3	2.79	130.86	126.04
25	b	206	CLA	CHD-C1D-ND	-2.78	121.89	124.45
30	g	216	DD6	C32-C33-C34	-2.78	107.36	113.64
35	d	310	CHL	CHD-C1D-ND	-2.78	121.90	124.45
25	h	211	CLA	CHD-C1D-ND	-2.78	121.90	124.45
25	B	816	CLA	O2A-CGA-CBA	2.78	120.63	111.91
27	c	301	LHG	O7-C7-C8	2.78	117.49	111.50
29	A	837	BCR	C1-C6-C5	-2.78	118.70	122.61
25	e	212	CLA	CHD-C1D-ND	-2.78	121.90	124.45
25	d	303	CLA	CHD-C1D-ND	-2.78	121.90	124.45
30	a	215	DD6	C37-C36-C31	-2.78	120.58	124.35
25	c	308	CLA	CHD-C1D-ND	-2.78	121.90	124.45
28	B	827	PQN	C9-C10-C1	-2.78	116.03	120.10
30	e	219	DD6	C21-C20-C15	-2.77	117.61	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	303	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
25	e	205	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	f	603	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	l	602	CLA	CHD-C1D-ND	-2.76	121.92	124.45
30	d	319	DD6	C28-C27-C29	-2.76	111.37	116.84
25	b	204	CLA	CHD-C1D-ND	-2.76	121.92	124.45
27	A	805	LHG	O7-C7-C8	2.76	117.45	111.50
25	A	849	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	h	208	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	A	857	CLA	CHD-C1D-ND	-2.76	121.92	124.45
30	A	854	DD6	C37-C36-C35	2.76	119.46	114.36
28	A	834	PQN	C6-C5-C4	-2.76	116.06	120.10
25	B	822	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	f	611	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	A	819	CLA	CHD-C1D-ND	-2.76	121.92	124.45
29	B	801	BCR	C2-C1-C6	2.75	114.72	110.48
25	k	210	CLA	CHD-C1D-ND	-2.75	121.92	124.45
25	g	204	CLA	CHD-C1D-ND	-2.75	121.92	124.45
30	m	212	DD6	C37-C36-C31	-2.75	120.61	124.35
25	i	202	CLA	CHD-C1D-ND	-2.75	121.93	124.45
25	B	836	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	k	215	DD6	C37-C36-C31	-2.75	120.61	124.35
25	A	846	CLA	CHD-C1D-ND	-2.75	121.93	124.45
25	B	843	CLA	CHD-C1D-ND	-2.75	121.93	124.45
30	a	215	DD6	C21-C20-C15	-2.75	117.66	122.26
25	n	203	CLA	CHD-C1D-ND	-2.75	121.93	124.45
25	A	815	CLA	O2A-CGA-CBA	2.75	120.53	111.91
30	d	319	DD6	O1-C20-C21	-2.74	111.77	115.06
25	e	213	CLA	CHD-C1D-ND	-2.74	121.93	124.45
25	g	215	CLA	CHD-C1D-ND	-2.74	121.93	124.45
25	i	206	CLA	O2A-CGA-CBA	2.74	120.52	111.91
28	F	205	PQN	C10-C5-C4	2.74	123.65	120.68
25	A	809	CLA	O2A-CGA-CBA	2.74	120.52	111.91
25	e	216	CLA	C1-C2-C3	2.74	130.78	126.04
33	g	202	SQD	O48-C23-C24	2.74	120.51	111.91
30	f	613	DD6	O1-C20-C21	-2.74	111.77	115.06
25	j	213	CLA	CHD-C1D-ND	-2.74	121.94	124.45
30	h	216	DD6	C37-C36-C31	-2.74	120.62	124.35
25	i	203	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
25	A	853	CLA	C3B-C4B-NB	-2.74	107.98	110.52
25	B	836	CLA	C1-C2-C3	2.74	130.78	126.04
27	j	202	LHG	O7-C7-C8	2.74	117.40	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	843	CLA	CHD-C1D-ND	-2.74	121.94	124.45
25	j	211	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	F	203	DD6	C3-C4-C5	2.73	129.07	123.47
30	l	614	DD6	C37-C36-C31	-2.73	120.64	124.35
25	b	212	CLA	C1-C2-C3	2.73	130.76	126.04
34	a	202	LMG	O1-C7-C8	-2.73	104.31	110.90
25	k	212	CLA	CHD-C1D-ND	-2.73	121.95	124.45
30	A	855	DD6	C9-C8-C6	2.73	134.08	126.42
30	p	610	DD6	C37-C36-C31	-2.73	120.64	124.35
25	d	316	CLA	CHD-C1D-ND	-2.73	121.95	124.45
25	e	212	CLA	C1-C2-C3	2.73	130.76	126.04
30	i	214	DD6	C32-C33-C34	-2.73	107.49	113.64
25	p	601	CLA	CHD-C1D-ND	-2.72	121.95	124.45
25	A	824	CLA	C1-C2-C3	2.72	130.75	126.04
25	d	306	CLA	CHB-C1B-NB	2.72	127.14	124.26
25	j	212	CLA	CHD-C1D-ND	-2.72	121.95	124.45
28	B	835	PQN	C6-C5-C4	-2.72	116.11	120.10
25	k	214	CLA	CHD-C1D-ND	-2.72	121.95	124.45
25	A	831	CLA	CHD-C1D-ND	-2.72	121.95	124.45
25	A	832	CLA	C1-C2-C3	2.72	130.74	126.04
25	j	214	CLA	CHD-C1D-ND	-2.71	121.96	124.45
25	A	813	CLA	O2A-CGA-CBA	2.71	120.42	111.91
25	n	201	CLA	O2A-CGA-CBA	2.71	120.42	111.91
25	B	804	CLA	O2A-CGA-CBA	2.71	120.42	111.91
25	n	205	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	A	821	CLA	CHD-C1D-ND	-2.71	121.96	124.45
25	o	602	CLA	CHD-C1D-ND	-2.71	121.97	124.45
25	o	603	CLA	CHD-C1D-ND	-2.71	121.97	124.45
25	B	811	CLA	O2A-CGA-CBA	2.70	120.39	111.91
27	a	201	LHG	O7-C7-C8	2.70	117.33	111.50
30	k	216	DD6	C21-C20-C15	-2.70	117.73	122.26
25	f	608	CLA	O1D-CGD-CBD	-2.70	118.95	124.48
25	a	205	CLA	O2A-CGA-CBA	2.70	120.39	111.91
25	k	203	CLA	O2A-CGA-CBA	2.70	120.38	111.91
25	A	806	CLA	CHD-C1D-ND	-2.70	121.97	124.45
25	B	824	CLA	C4-C3-C5	-2.70	110.73	115.27
25	e	206	CLA	CHD-C1D-ND	-2.70	121.97	124.45
25	h	213	CLA	CHD-C1D-ND	-2.70	121.97	124.45
25	B	811	CLA	CHD-C1D-ND	-2.70	121.98	124.45
25	a	205	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	c	304	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	e	204	CLA	CHD-C1D-ND	-2.69	121.98	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	212	DD6	C37-C36-C31	-2.69	120.69	124.35
30	c	317	DD6	C21-C20-C15	-2.69	117.75	122.26
25	B	840	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	d	306	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	l	605	CLA	CHD-C1D-ND	-2.69	121.98	124.45
30	e	219	DD6	C32-C33-C34	-2.69	107.58	113.64
25	e	207	CLA	CHD-C1D-ND	-2.69	121.99	124.45
30	i	216	DD6	C21-C20-C15	-2.69	117.76	122.26
25	n	207	CLA	CMA-C3A-C2A	-2.69	109.83	116.10
25	B	810	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	l	601	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	A	817	CLA	CHD-C1D-ND	-2.68	121.99	124.45
30	A	855	DD6	C4-C5-C6	-2.68	123.48	127.31
35	c	307	CHL	O2A-CGA-CBA	2.68	120.33	111.91
25	e	217	CLA	CHD-C1D-ND	-2.68	121.99	124.45
30	F	203	DD6	C-C1-C2	-2.68	119.17	122.92
25	i	212	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	B	848	CLA	O2A-CGA-CBA	2.68	120.31	111.91
25	m	204	CLA	O1D-CGD-CBD	-2.68	119.01	124.48
25	d	314	CLA	C2D-C1D-ND	2.68	112.08	110.10
25	d	315	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	h	204	CLA	C1-C2-C3	2.67	130.67	126.04
30	A	855	DD6	C7-C6-C5	-2.67	119.18	122.92
30	J	104	DD6	C37-C36-C31	-2.67	120.72	124.35
25	B	808	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	e	207	CLA	CHB-C1B-NB	2.67	127.08	124.26
25	h	205	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
25	n	208	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	l	603	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	B	826	CLA	C3B-C4B-NB	-2.67	108.04	110.52
30	a	215	DD6	O1-C20-C15	-2.67	56.75	58.96
28	B	835	PQN	C2M-C2-C1	-2.67	111.85	116.27
25	i	208	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
25	c	302	CLA	CHD-C1D-ND	-2.66	122.00	124.45
30	e	218	DD6	C8-C6-C5	2.66	123.03	118.94
25	B	813	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	B	841	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	B	823	CLA	C1-C2-C3	2.66	130.65	126.04
25	A	825	CLA	C4-C3-C5	-2.66	110.79	115.27
25	B	836	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
25	A	809	CLA	C1-C2-C3	2.66	130.65	126.04
33	F	204	SQD	O48-C23-C24	2.66	120.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	i	210	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	l	602	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
30	o	611	DD6	C37-C36-C31	-2.66	120.74	124.35
25	e	217	CLA	C2D-C1D-ND	2.66	112.06	110.10
25	B	836	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	d	316	CLA	C2D-C1D-ND	2.65	112.06	110.10
25	e	211	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	A	850	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	A	852	CLA	CHD-C1D-ND	-2.65	122.02	124.45
29	J	101	BCR	C29-C30-C25	2.65	114.56	110.48
25	i	204	CLA	C2D-C1D-ND	2.65	112.06	110.10
25	B	847	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	n	205	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	d	314	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	d	301	CLA	CMA-C3A-C2A	-2.65	109.92	116.10
25	m	206	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	b	212	CLA	C2D-C1D-ND	2.65	112.05	110.10
25	o	605	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	n	202	CLA	CHD-C1D-ND	-2.64	122.02	124.45
34	j	201	LMG	O6-C1-O1	-2.64	103.72	109.97
25	A	845	CLA	O2A-CGA-CBA	2.64	120.20	111.91
25	B	822	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
25	B	809	CLA	CHD-C1D-ND	-2.64	122.03	124.45
25	d	312	CLA	C1-C2-C3	2.64	130.61	126.04
25	h	207	CLA	CHD-C1D-ND	-2.64	122.03	124.45
30	d	318	DD6	C21-C20-C19	2.64	117.25	114.28
25	e	205	CLA	C1-C2-C3	2.64	130.61	126.04
25	l	609	CLA	CHD-C1D-ND	-2.64	122.03	124.45
25	n	211	CLA	CHD-C1D-ND	-2.64	122.03	124.45
35	d	309	CHL	CHD-C1D-ND	-2.64	122.03	124.45
25	e	206	CLA	C2D-C1D-ND	2.64	112.05	110.10
25	n	205	CLA	C2D-C1D-ND	2.63	112.05	110.10
28	B	827	PQN	C10-C5-C4	2.63	123.53	120.68
29	B	828	BCR	C29-C30-C25	2.63	114.53	110.48
30	d	318	DD6	C28-C27-C29	-2.63	111.63	116.84
25	g	209	CLA	C1-C2-C3	2.63	130.59	126.04
25	B	842	CLA	CHD-C1D-ND	-2.63	122.04	124.45
30	j	216	DD6	C37-C36-C31	-2.63	120.78	124.35
30	n	213	DD6	C3-C4-C5	2.63	128.86	123.47
25	m	207	CLA	CHB-C1B-NB	2.63	127.04	124.26
30	j	216	DD6	C32-C33-C34	-2.63	107.71	113.64
30	a	214	DD6	C32-C33-C34	-2.63	107.71	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	827	PQN	C11-C3-C4	-2.63	115.69	118.50
25	A	817	CLA	C1-C2-C3	2.63	130.58	126.04
29	B	828	BCR	C11-C10-C9	-2.62	123.56	127.31
25	j	209	CLA	CHD-C1D-ND	-2.62	122.05	124.45
25	o	603	CLA	C3B-C4B-NB	-2.62	108.08	110.52
30	A	855	DD6	C32-C33-C34	-2.62	107.73	113.64
25	f	603	CLA	C2D-C1D-ND	2.62	112.03	110.10
25	A	845	CLA	CHD-C1D-ND	-2.62	122.05	124.45
30	i	215	DD6	C21-C20-C15	-2.61	117.88	122.26
30	n	213	DD6	C8-C6-C5	2.61	122.95	118.94
25	B	819	CLA	CHD-C1D-ND	-2.61	122.05	124.45
28	B	835	PQN	C10-C5-C4	2.61	123.50	120.68
25	l	603	CLA	C2D-C1D-ND	2.61	112.03	110.10
25	n	204	CLA	CHD-C1D-ND	-2.61	122.06	124.45
25	A	808	CLA	CHD-C1D-ND	-2.61	122.06	124.45
25	e	205	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
30	o	611	DD6	C32-C33-C34	-2.61	107.75	113.64
28	F	205	PQN	C9-C10-C1	-2.61	116.28	120.10
30	F	203	DD6	C8-C6-C5	2.61	122.94	118.94
30	e	219	DD6	C28-C27-C29	-2.60	111.68	116.84
25	k	202	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
28	B	835	PQN	C9-C10-C1	-2.60	116.29	120.10
25	g	204	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
25	B	838	CLA	CHB-C1B-NB	2.60	127.01	124.26
25	f	609	CLA	C3B-C4B-NB	-2.60	108.10	110.52
25	d	313	CLA	CHD-C1D-ND	-2.60	122.06	124.45
30	A	855	DD6	C28-C27-C29	-2.60	111.69	116.84
30	k	215	DD6	C32-C33-C34	-2.60	107.77	113.64
29	B	832	BCR	C12-C13-C14	2.60	122.93	118.94
25	A	818	CLA	O1D-CGD-CBD	-2.60	119.17	124.48
25	n	202	CLA	C1-C2-C3	2.59	130.53	126.04
25	A	816	CLA	CHD-C1D-ND	-2.59	122.07	124.45
25	k	206	CLA	CHD-C1D-ND	-2.59	122.07	124.45
28	F	205	PQN	C2M-C2-C1	-2.59	111.98	116.27
30	m	213	DD6	O1-C20-C19	2.59	115.33	113.38
30	d	318	DD6	C32-C33-C34	-2.59	107.80	113.64
25	A	840	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
25	B	807	CLA	CHD-C1D-ND	-2.59	122.08	124.45
25	j	211	CLA	CHD-C1D-ND	-2.59	122.08	124.45
25	h	212	CLA	CHB-C1B-NB	2.59	127.00	124.26
25	i	206	CLA	O2A-CGA-O1A	-2.59	117.07	123.59
30	h	217	DD6	C32-C33-C34	-2.58	107.81	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	211	CLA	C2D-C1D-ND	2.58	112.01	110.10
25	B	820	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	p	608	CLA	CHD-C1D-ND	-2.58	122.08	124.45
35	d	307	CHL	CHD-C1D-ND	-2.58	122.08	124.45
29	A	836	BCR	C2-C1-C6	2.58	114.45	110.48
29	A	837	BCR	C19-C18-C17	2.58	122.90	118.94
25	e	213	CLA	C1-C2-C3	2.58	130.50	126.04
35	c	307	CHL	CHD-C1D-ND	-2.58	122.08	124.45
25	A	844	CLA	C4-C3-C5	-2.58	110.93	115.27
30	f	614	DD6	C13-C11-C10	2.58	122.89	118.94
25	m	207	CLA	C1-C2-C3	2.58	130.92	126.75
30	c	318	DD6	C21-C20-C15	-2.58	117.94	122.26
25	m	203	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
25	e	215	CLA	CHD-C1D-ND	-2.58	122.09	124.45
29	A	839	BCR	C2-C1-C6	2.58	114.45	110.48
25	A	832	CLA	C12-C11-C10	-2.57	101.41	113.24
25	A	841	CLA	C1-C2-C3	2.57	130.50	126.04
30	a	215	DD6	O1-C20-C19	2.57	115.31	113.38
28	A	834	PQN	C2M-C2-C1	-2.57	112.00	116.27
25	A	840	CLA	CHB-C1B-NB	2.57	126.98	124.26
25	h	213	CLA	CHB-C1B-NB	2.57	126.98	124.26
30	g	217	DD6	C32-C33-C34	-2.57	107.83	113.64
25	k	210	CLA	C2D-C1D-ND	2.57	112.00	110.10
25	g	207	CLA	CHD-C1D-ND	-2.57	122.09	124.45
25	B	802	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
28	A	834	PQN	C9-C10-C1	-2.57	116.34	120.10
25	f	611	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
25	m	203	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
25	B	808	CLA	CHB-C1B-NB	2.56	126.97	124.26
25	b	209	CLA	CHB-C1B-NB	2.56	126.97	124.26
25	p	607	CLA	CHB-C1B-NB	2.56	126.97	124.26
25	A	814	CLA	C2D-C1D-ND	2.56	111.99	110.10
30	b	214	DD6	C37-C36-C31	-2.56	120.87	124.35
35	e	209	CHL	CHD-C1D-ND	-2.56	122.10	124.45
30	J	105	DD6	C4-C3-C2	2.56	128.72	123.47
30	f	614	DD6	C28-C27-C29	-2.56	111.77	116.84
30	i	214	DD6	C21-C20-C19	2.56	117.16	114.28
30	c	317	DD6	C32-C33-C34	-2.56	107.87	113.64
25	g	211	CLA	C2D-C1D-ND	2.56	111.99	110.10
28	A	834	PQN	C10-C5-C4	2.56	123.44	120.68
25	e	210	CLA	CMD-C2D-C1D	2.56	129.22	124.71
30	g	217	DD6	C28-C27-C29	-2.55	111.78	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	310	CLA	CMB-C2B-C1B	-2.55	121.48	125.37
25	a	208	CLA	CHB-C1B-NB	2.55	126.96	124.26
25	A	823	CLA	C1-C2-C3	2.55	130.46	126.04
25	m	211	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
35	d	310	CHL	C3C-C4C-NC	-2.55	107.71	110.57
25	b	204	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
30	k	216	DD6	C37-C36-C31	-2.55	120.88	124.35
27	A	835	LHG	O8-C23-C24	2.55	119.91	111.91
30	a	215	DD6	C32-C33-C34	-2.55	107.88	113.64
25	a	203	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
25	A	816	CLA	C3B-C4B-NB	-2.55	108.15	110.52
25	A	825	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	B	821	CLA	CHD-C1D-ND	-2.55	122.11	124.45
30	A	854	DD6	C32-C33-C34	-2.55	107.89	113.64
25	o	601	CLA	CMA-C3A-C2A	-2.54	110.16	116.10
25	B	821	CLA	C1-C2-C3	2.54	130.44	126.04
25	A	824	CLA	CHB-C1B-NB	2.54	126.95	124.26
25	A	809	CLA	C12-C11-C10	-2.54	101.56	113.24
25	e	211	CLA	CHB-C1B-NB	2.54	126.95	124.26
25	n	209	CLA	CHB-C1B-NB	2.54	126.95	124.26
25	j	203	CLA	C1-C2-C3	2.54	130.86	126.75
25	A	821	CLA	C1-C2-C3	2.54	130.44	126.04
25	B	825	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	m	204	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	h	203	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	l	613	DD6	C21-C20-C19	2.54	117.14	114.28
29	B	832	BCR	C29-C30-C25	2.54	114.39	110.48
30	F	203	DD6	C28-C27-C29	2.54	121.86	116.84
25	A	811	CLA	C1-C2-C3	2.54	130.85	126.75
25	B	817	CLA	CHB-C1B-NB	2.53	126.94	124.26
27	d	302	LHG	O8-C23-C24	2.53	119.86	111.91
30	p	610	DD6	C32-C33-C34	-2.53	107.92	113.64
25	B	815	CLA	CHD-C1D-ND	-2.53	122.13	124.45
30	h	216	DD6	C32-C33-C34	-2.53	107.93	113.64
29	A	838	BCR	C20-C21-C22	-2.53	123.70	127.31
30	d	319	DD6	C7-C6-C5	-2.53	119.38	122.92
25	d	303	CLA	C1-C2-C3	2.53	130.84	126.75
25	B	841	CLA	C1-C2-C3	2.53	130.42	126.04
25	A	832	CLA	C2A-C1A-CHA	2.53	128.28	123.86
30	f	614	DD6	C32-C33-C34	-2.53	107.93	113.64
27	b	201	LHG	O8-C23-C24	2.53	119.84	111.91
30	m	212	DD6	C32-C33-C34	-2.53	107.94	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	l	614	DD6	C21-C20-C19	2.53	117.12	114.28
25	B	834	CLA	C1-C2-C3	2.53	130.41	126.04
25	B	821	CLA	C4-C3-C5	-2.53	111.02	115.27
25	A	821	CLA	O1D-CGD-CBD	-2.53	119.32	124.48
28	B	835	PQN	C11-C3-C4	-2.52	115.80	118.50
25	B	826	CLA	CHD-C1D-ND	-2.52	122.13	124.45
25	j	212	CLA	C2A-C1A-CHA	2.52	128.27	123.86
25	a	204	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
28	A	834	PQN	C11-C3-C4	-2.52	115.80	118.50
25	j	205	CLA	C2D-C1D-ND	2.52	111.96	110.10
30	f	613	DD6	C33-C34-C35	2.52	113.76	110.30
27	h	202	LHG	O8-C23-C24	2.52	119.83	111.91
30	k	216	DD6	C32-C33-C34	-2.52	107.94	113.64
25	a	211	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	e	201	CLA	C1-C2-C3	2.52	130.41	126.04
25	A	810	CLA	C12-C11-C10	-2.52	101.65	113.24
25	i	212	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
27	g	201	LHG	O8-C23-C24	2.52	119.82	111.91
25	f	607	CLA	C1-C2-C3	2.52	130.41	126.04
25	B	820	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
30	e	219	DD6	O1-C20-C19	2.52	115.28	113.38
30	f	614	DD6	C9-C10-C11	-2.52	123.71	127.31
30	m	213	DD6	O1-C20-C15	-2.52	56.87	58.96
25	p	609	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
25	B	804	CLA	C12-C11-C10	-2.52	101.66	113.24
25	A	829	CLA	CHB-C1B-NB	2.52	126.92	124.26
25	j	212	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
35	d	308	CHL	CHD-C1D-ND	-2.52	122.14	124.45
30	e	219	DD6	O1-C20-C15	-2.52	56.87	58.96
25	A	818	CLA	O2A-CGA-CBA	2.52	119.81	111.91
25	h	210	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
25	B	842	CLA	C1-C2-C3	2.52	130.40	126.04
30	A	854	DD6	C3-C2-C1	-2.51	123.72	127.31
25	e	214	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
25	B	804	CLA	CHD-C1D-ND	-2.51	122.14	124.45
25	B	814	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	l	609	CLA	C2D-C1D-ND	2.51	111.95	110.10
25	p	606	CLA	CHB-C1B-NB	2.51	126.92	124.26
25	h	206	CLA	C4-C3-C5	-2.51	111.05	115.27
25	B	813	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
30	A	855	DD6	C8-C6-C5	2.51	122.79	118.94
25	d	305	CLA	C2D-C1D-ND	2.51	111.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	318	DD6	C4-C5-C6	-2.51	123.73	127.31
25	A	804	CLA	C4-C3-C5	-2.51	111.05	115.27
25	k	205	CLA	C1-C2-C3	2.51	130.38	126.04
25	c	315	CLA	CHD-C1D-ND	-2.51	122.15	124.45
30	f	614	DD6	C7-C6-C5	-2.51	119.41	122.92
30	n	212	DD6	C32-C33-C34	-2.51	107.98	113.64
25	B	818	CLA	CHD-C1D-ND	-2.50	122.15	124.45
25	c	311	CLA	CHD-C1D-ND	-2.50	122.15	124.45
25	m	210	CLA	CHD-C1D-ND	-2.50	122.15	124.45
25	k	211	CLA	C1-C2-C3	2.50	130.37	126.04
25	a	211	CLA	C2D-C1D-ND	2.50	111.95	110.10
30	c	318	DD6	C7-C6-C5	-2.50	119.42	122.92
30	g	216	DD6	O1-C20-C15	-2.50	56.89	58.96
25	A	819	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
35	d	309	CHL	C2A-C3A-C4A	2.50	105.90	101.87
25	B	814	CLA	CHB-C1B-NB	2.49	126.90	124.26
27	c	301	LHG	O8-C23-C24	2.49	119.74	111.91
30	c	316	DD6	O1-C20-C19	2.49	115.25	113.38
25	p	605	CLA	CHD-C1D-ND	-2.49	122.16	124.45
30	n	212	DD6	C28-C27-C29	-2.49	111.90	116.84
25	B	823	CLA	C3C-C4C-NC	-2.49	107.78	110.57
30	a	215	DD6	C28-C27-C29	-2.49	111.91	116.84
25	B	846	CLA	C1-C2-C3	2.49	130.78	126.75
25	A	822	CLA	O2A-CGA-CBA	2.49	119.72	111.91
25	o	610	CLA	C3C-C4C-NC	-2.49	107.78	110.57
25	A	819	CLA	C1-C2-C3	2.49	130.34	126.04
25	A	849	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
25	l	606	CLA	CHB-C1B-NB	2.49	126.89	124.26
25	b	208	CLA	CHD-C1D-ND	-2.49	122.17	124.45
25	g	207	CLA	O2A-CGA-CBA	2.49	122.02	114.03
25	A	829	CLA	C1-C2-C3	2.49	130.34	126.04
30	l	614	DD6	C32-C33-C34	-2.48	108.03	113.64
25	f	611	CLA	CHB-C1B-NB	2.48	126.89	124.26
30	j	217	DD6	C32-C33-C34	-2.48	108.04	113.64
25	f	602	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
25	B	848	CLA	CHD-C1D-ND	-2.48	122.17	124.45
34	k	201	LMG	O1-C7-C8	-2.48	104.91	110.90
29	B	830	BCR	C2-C1-C6	2.48	114.30	110.48
25	A	829	CLA	C4-C3-C5	-2.48	111.10	115.27
25	h	205	CLA	CHD-C1D-ND	-2.48	122.17	124.45
25	i	213	CLA	CHD-C1D-ND	-2.48	122.17	124.45
25	A	846	CLA	C4-C3-C5	-2.48	111.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	216	DD6	C21-C20-C19	2.48	117.07	114.28
25	A	810	CLA	CHD-C1D-ND	-2.48	122.18	124.45
25	B	802	CLA	O2A-CGA-CBA	2.48	119.69	111.91
25	k	208	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
30	h	217	DD6	C37-C36-C31	-2.48	120.98	124.35
25	F	202	CLA	CHB-C1B-NB	2.48	126.88	124.26
25	A	845	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	a	213	CLA	C4-C3-C5	-2.48	111.10	115.27
25	A	809	CLA	CHD-C1D-ND	-2.48	122.18	124.45
25	h	214	CLA	CHD-C1D-ND	-2.47	122.18	124.45
25	a	210	CLA	O2A-CGA-CBA	2.47	121.98	114.03
25	j	205	CLA	CHD-C1D-ND	-2.47	122.18	124.45
30	a	214	DD6	C28-C27-C29	-2.47	111.94	116.84
25	A	821	CLA	C2D-C1D-ND	2.47	111.92	110.10
25	A	850	CLA	C3C-C4C-NC	-2.47	107.80	110.57
25	d	313	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
25	j	206	CLA	CHD-C1D-ND	-2.47	122.19	124.45
27	j	202	LHG	O8-C23-C24	2.47	119.65	111.91
25	m	202	CLA	C3B-C4B-NB	-2.47	108.23	110.52
25	B	839	CLA	C1-C2-C3	2.47	130.31	126.04
25	l	607	CLA	C1-C2-C3	2.46	130.31	126.04
25	n	201	CLA	CHD-C1D-ND	-2.46	122.19	124.45
30	c	318	DD6	C28-C27-C29	-2.46	111.96	116.84
30	m	213	DD6	C21-C20-C19	2.46	117.05	114.28
25	A	843	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
25	A	808	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
25	l	608	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
30	b	215	DD6	C26-C25-C24	-2.46	115.54	123.22
30	d	317	DD6	C32-C33-C34	-2.46	108.09	113.64
25	b	204	CLA	C4-C3-C5	-2.46	111.13	115.27
25	B	822	CLA	C12-C11-C10	-2.46	101.94	113.24
27	b	201	LHG	O7-C7-C8	2.46	117.66	110.80
25	A	821	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
27	i	201	LHG	O8-C23-C24	2.46	119.62	111.91
30	l	613	DD6	C32-C33-C34	-2.46	108.09	113.64
30	A	854	DD6	O1-C20-C21	-2.46	112.11	115.06
25	B	845	CLA	CHD-C1D-ND	-2.46	122.20	124.45
25	i	210	CLA	C2D-C1D-ND	2.45	111.91	110.10
25	o	608	CLA	O1D-CGD-CBD	-2.45	119.94	124.51
25	a	212	CLA	C1-C2-C3	2.45	130.29	126.04
30	b	214	DD6	C32-C33-C34	-2.45	108.11	113.64
35	d	308	CHL	C2A-C3A-C4A	2.45	105.83	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	215	DD6	C32-C33-C34	-2.45	108.11	113.64
25	e	215	CLA	C2D-C1D-ND	2.45	111.91	110.10
25	c	303	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
25	f	609	CLA	CHD-C1D-ND	-2.45	122.20	124.45
30	d	319	DD6	C33-C34-C35	2.45	113.65	110.30
25	a	208	CLA	C1-C2-C3	2.45	130.71	126.75
25	m	210	CLA	C2D-C1D-ND	2.45	111.91	110.10
25	A	853	CLA	CHB-C1B-NB	2.45	126.85	124.26
25	o	602	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
25	c	304	CLA	C2D-C1D-ND	2.45	111.91	110.10
25	B	806	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
30	c	316	DD6	C32-C33-C34	-2.44	108.12	113.64
25	A	830	CLA	CHB-C1B-NB	2.44	126.84	124.26
25	B	802	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
25	h	211	CLA	C1-C2-C3	2.44	130.27	126.04
25	p	602	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
30	n	212	DD6	C33-C34-C35	2.44	113.65	110.30
25	d	305	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	B	814	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
25	j	207	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	A	843	CLA	C1-C2-C3	2.44	130.26	126.04
25	A	820	CLA	C3C-C4C-NC	-2.44	107.83	110.57
25	g	207	CLA	CHB-C1B-NB	2.44	126.84	124.26
25	B	803	CLA	C3C-C4C-NC	-2.44	107.83	110.57
25	A	846	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
35	d	310	CHL	C2B-C1B-NB	-2.44	108.60	110.23
30	F	203	DD6	C24-C1-C2	2.44	122.68	118.94
25	a	205	CLA	C2A-C1A-CHA	2.44	128.12	123.86
25	i	212	CLA	CHB-C1B-NB	2.44	126.84	124.26
25	i	204	CLA	CHD-C1D-ND	-2.44	122.22	124.45
25	B	844	CLA	C1-C2-C3	2.44	130.26	126.04
25	i	204	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
34	e	202	LMG	C1-C2-C3	-2.43	104.92	110.00
25	l	607	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
35	d	307	CHL	OMC-CMC-C2C	-2.43	120.18	125.69
25	k	204	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	k	207	CLA	C1-C2-C3	2.43	130.69	126.75
25	B	843	CLA	C1-C2-C3	2.43	130.25	126.04
25	l	602	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
30	d	318	DD6	O1-C20-C15	-2.43	56.95	58.96
25	A	815	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	i	206	CLA	CHD-C1D-ND	-2.43	122.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	d	307	CHL	O2A-CGA-O1A	-2.43	117.46	123.59
25	e	210	CLA	CHB-C1B-NB	2.43	126.83	124.26
25	B	821	CLA	C12-C11-C10	-2.43	102.08	113.24
25	A	814	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
25	g	208	CLA	C1-C2-C3	2.43	130.68	126.75
25	a	204	CLA	C12-C11-C10	-2.43	102.09	113.24
30	d	317	DD6	O1-C20-C15	-2.43	56.95	58.96
25	g	215	CLA	O2A-CGA-CBA	2.43	121.83	114.03
25	A	846	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
29	A	838	BCR	C29-C30-C25	2.42	114.21	110.48
25	j	203	CLA	O1D-CGD-CBD	-2.42	119.52	124.48
30	f	613	DD6	C37-C36-C31	-2.42	121.06	124.35
25	g	208	CLA	CHB-C1B-NB	2.42	126.82	124.26
25	B	838	CLA	C12-C11-C10	-2.42	102.11	113.24
30	m	213	DD6	C32-C33-C34	-2.42	108.17	113.64
30	o	612	DD6	C32-C33-C34	-2.42	108.17	113.64
25	a	204	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
25	j	212	CLA	CHB-C1B-NB	2.42	126.82	124.26
25	A	801	CLA	C4D-C3D-CAD	-2.42	105.25	108.10
29	B	831	BCR	C19-C18-C17	2.42	122.65	118.94
25	B	811	CLA	C2D-C1D-ND	2.42	111.89	110.10
29	B	829	BCR	C2-C1-C6	2.41	114.20	110.48
25	e	206	CLA	O2A-CGA-CBA	2.41	121.78	114.03
25	f	611	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	B	815	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	c	305	CLA	CHB-C1B-NB	2.41	126.81	124.26
25	l	606	CLA	C12-C11-C10	-2.41	102.16	113.24
30	c	316	DD6	C21-C20-C19	2.41	116.99	114.28
25	B	844	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
30	p	610	DD6	C28-C27-C29	-2.41	112.07	116.84
25	g	205	CLA	C3B-C4B-NB	-2.41	108.28	110.52
25	a	204	CLA	C3C-C4C-NC	-2.41	107.87	110.57
25	j	215	CLA	C1-C2-C3	2.41	130.65	126.75
30	b	214	DD6	C21-C20-C15	-2.40	118.23	122.26
25	a	203	CLA	CHB-C1B-NB	2.40	126.80	124.26
25	j	215	CLA	CHB-C1B-NB	2.40	126.80	124.26
25	B	812	CLA	C1-C2-C3	2.40	130.20	126.04
25	g	208	CLA	C3C-C4C-NC	-2.40	107.88	110.57
25	i	209	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
25	e	214	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
35	d	307	CHL	C2A-C3A-C4A	2.40	105.75	101.87
25	d	311	CLA	CHB-C1B-NB	2.40	126.80	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	e	217	CLA	CHB-C1B-NB	2.40	126.80	124.26
25	A	846	CLA	C12-C11-C10	-2.40	102.21	113.24
30	m	213	DD6	C33-C34-C35	2.40	113.59	110.30
25	j	215	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	h	206	CLA	C12-C11-C10	-2.40	102.21	113.24
25	B	848	CLA	C4-C3-C5	-2.40	111.23	115.27
25	e	205	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
30	p	610	DD6	C3-C2-C1	-2.40	123.89	127.31
25	l	607	CLA	C3C-C4C-NC	-2.40	107.88	110.57
25	m	204	CLA	C1-C2-C3	2.40	130.19	126.04
25	f	602	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
29	B	832	BCR	C23-C22-C21	2.40	122.62	118.94
25	j	207	CLA	CHB-C1B-NB	2.40	126.80	124.26
25	k	203	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
25	l	607	CLA	CHB-C1B-NB	2.40	126.79	124.26
25	A	850	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
25	i	204	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	a	207	CLA	C1-C2-C3	2.40	130.19	126.04
25	k	205	CLA	C12-C11-C10	-2.40	102.23	113.24
25	i	202	CLA	C1-C2-C3	2.40	130.19	126.04
25	B	816	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
25	k	212	CLA	CHB-C1B-NB	2.39	126.79	124.26
25	k	206	CLA	C1-C2-C3	2.39	130.62	126.75
25	A	806	CLA	O2A-CGA-CBA	2.39	121.72	114.03
25	g	211	CLA	CHD-C1D-ND	-2.39	122.25	124.45
25	A	845	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
25	c	303	CLA	C3C-C4C-NC	-2.39	107.89	110.57
30	n	213	DD6	C28-C27-C29	2.39	121.58	116.84
25	B	822	CLA	C1-C2-C3	2.39	130.18	126.04
25	i	203	CLA	C1-C2-C3	2.39	130.18	126.04
25	n	210	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	j	204	CLA	C1-C2-C3	2.39	130.18	126.04
25	d	304	CLA	C1-C2-C3	2.39	130.18	126.04
25	j	209	CLA	C1-C2-C3	2.39	130.17	126.04
25	b	205	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	b	203	CLA	CHB-C1B-NB	2.39	126.78	124.26
25	A	830	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
25	A	832	CLA	C4-C3-C5	-2.39	111.26	115.27
25	A	850	CLA	CHB-C1B-NB	2.39	126.78	124.26
30	i	216	DD6	C32-C33-C34	-2.39	108.25	113.64
25	B	843	CLA	C12-C11-C10	-2.39	102.28	113.24
25	B	846	CLA	CMB-C2B-C1B	-2.39	121.74	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	m	202	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	B	847	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	b	210	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	a	206	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
30	p	610	DD6	O1-C20-C21	-2.38	112.20	115.06
25	f	609	CLA	C2D-C1D-ND	2.38	111.86	110.10
25	h	209	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	B	804	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
34	a	202	LMG	C1-C2-C3	-2.38	105.04	110.00
25	n	210	CLA	C2D-C1D-ND	2.38	111.86	110.10
29	A	836	BCR	C37-C22-C23	2.38	121.83	118.08
30	g	217	DD6	O1-C20-C15	-2.38	56.99	58.96
25	A	847	CLA	C3C-C4C-NC	-2.38	107.90	110.57
25	g	203	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
25	A	820	CLA	C1-C2-C3	2.38	130.16	126.04
25	c	314	CLA	CHB-C1B-NB	2.38	126.77	124.26
29	A	837	BCR	C8-C9-C10	2.38	122.59	118.94
25	k	203	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
25	c	314	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
25	l	604	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
34	j	201	LMG	C1-C2-C3	-2.38	105.05	110.00
25	b	208	CLA	CAA-C2A-C3A	-2.37	110.56	116.10
25	B	840	CLA	O1D-CGD-CBD	-2.37	119.62	124.48
25	A	812	CLA	C12-C11-C10	-2.37	102.33	113.24
25	A	818	CLA	C3C-C4C-NC	-2.37	107.91	110.57
25	i	208	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
25	d	316	CLA	CHB-C1B-NB	2.37	126.77	124.26
25	A	831	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
30	A	855	DD6	O1-C20-C21	-2.37	112.21	115.06
25	B	839	CLA	C12-C11-C10	-2.37	102.34	113.24
25	A	850	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	B	805	CLA	C3C-C4C-NC	-2.37	107.91	110.57
25	o	607	CLA	CHB-C1B-NB	2.37	126.77	124.26
25	B	818	CLA	CHB-C1B-NB	2.37	126.76	124.26
25	A	808	CLA	C2D-C1D-ND	2.37	111.85	110.10
25	o	601	CLA	CAA-C2A-C3A	-2.37	110.57	116.10
25	c	313	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
30	h	217	DD6	C21-C20-C19	2.37	116.94	114.28
29	A	837	BCR	C15-C16-C17	2.37	128.32	123.47
25	m	204	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
27	m	201	LHG	O8-C23-C24	2.36	119.33	111.91
25	A	804	CLA	C12-C11-C10	-2.36	102.37	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	i	208	CLA	C1-C2-C3	2.36	130.13	126.04
25	k	206	CLA	CHB-C1B-NB	2.36	126.76	124.26
35	e	209	CHL	C2A-C3A-C4A	2.36	105.69	101.87
25	A	820	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	j	213	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	f	609	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	e	214	CLA	CHB-C1B-NB	2.36	126.75	124.26
25	i	202	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
25	e	204	CLA	CHB-C1B-NB	2.36	126.75	124.26
30	d	319	DD6	C32-C33-C34	-2.36	108.32	113.64
25	A	825	CLA	CHB-C1B-NB	2.36	126.75	124.26
25	B	807	CLA	C12-C11-C10	-2.35	102.42	113.24
25	A	844	CLA	C3C-C4C-NC	-2.35	107.93	110.57
25	l	601	CLA	CHB-C1B-NB	2.35	126.75	124.26
25	d	304	CLA	C3C-C4C-NC	-2.35	107.93	110.57
28	A	834	PQN	C17-C16-C15	-2.35	106.97	113.36
25	A	840	CLA	C12-C11-C10	-2.35	102.43	113.24
25	A	809	CLA	C3C-C4C-NC	-2.35	107.93	110.57
25	A	808	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
25	f	612	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
35	c	307	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
27	A	805	LHG	O8-C23-C24	2.35	119.28	111.91
30	b	215	DD6	C32-C33-C34	-2.35	108.34	113.64
25	g	204	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
30	j	216	DD6	C21-C20-C19	2.35	116.92	114.28
25	f	605	CLA	CHD-C1D-ND	-2.35	122.30	124.45
25	A	843	CLA	C4-C3-C5	-2.35	111.32	115.27
25	n	201	CLA	C2B-C1B-NB	-2.35	108.66	110.23
34	k	201	LMG	C1-C2-C3	-2.35	105.11	110.00
27	i	201	LHG	O8-C23-O10	-2.35	117.67	123.59
30	l	613	DD6	C28-C27-C29	-2.35	112.19	116.84
25	A	825	CLA	C1-C2-C3	2.35	130.10	126.04
30	i	216	DD6	C33-C34-C35	2.35	113.52	110.30
25	B	805	CLA	CHB-C1B-NB	2.35	126.74	124.26
30	b	214	DD6	C28-C27-C29	-2.34	112.19	116.84
25	c	302	CLA	CHB-C1B-NB	2.34	126.74	124.26
25	A	808	CLA	C12-C11-C10	-2.34	102.47	113.24
25	j	211	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
25	B	821	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
25	c	312	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
25	B	817	CLA	C3C-C4C-NC	-2.34	107.94	110.57
25	k	203	CLA	O2D-CGD-O1D	-2.34	119.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	208	CLA	CHB-C1B-NB	2.34	126.74	124.26
25	m	203	CLA	CHB-C1B-NB	2.34	126.74	124.26
25	a	212	CLA	C3C-C4C-NC	-2.34	107.94	110.57
30	k	215	DD6	C21-C20-C19	2.34	116.91	114.28
25	b	210	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
29	B	829	BCR	C29-C30-C25	2.34	114.08	110.48
25	A	848	CLA	CHB-C1B-NB	2.34	126.73	124.26
25	d	303	CLA	C2D-C1D-ND	2.34	111.83	110.10
25	h	209	CLA	CMB-C2B-C3B	2.34	132.25	126.59
30	h	216	DD6	C28-C27-C29	-2.34	112.21	116.84
25	d	315	CLA	CBA-CAA-C2A	2.34	118.67	113.47
25	c	302	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
25	i	212	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
35	d	310	CHL	C4D-CHA-C1A	2.34	124.09	121.25
25	A	807	CLA	C1-C2-C3	2.34	130.08	126.04
25	A	848	CLA	C1-C2-C3	2.34	130.08	126.04
25	B	822	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
30	c	318	DD6	C33-C34-C35	2.34	113.50	110.30
25	j	209	CLA	C3C-C4C-NC	-2.34	107.95	110.57
25	j	206	CLA	C1-C2-C3	2.33	130.08	126.04
25	k	208	CLA	C1-C2-C3	2.33	130.08	126.04
30	f	613	DD6	C32-C33-C34	-2.33	108.37	113.64
25	B	811	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	p	608	CLA	CHB-C1B-NB	2.33	126.73	124.26
28	B	827	PQN	C17-C16-C15	-2.33	107.02	113.36
30	J	105	DD6	C13-C11-C10	2.33	122.52	118.94
25	h	203	CLA	CHB-C1B-NB	2.33	126.73	124.26
27	a	201	LHG	O8-C23-C24	2.33	119.23	111.91
25	m	205	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
30	f	614	DD6	C33-C34-C35	2.33	113.49	110.30
25	m	204	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	c	309	CLA	C4-C3-C5	-2.33	111.35	115.27
25	B	820	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	p	601	CLA	C2D-C1D-ND	2.33	111.82	110.10
25	e	206	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	i	208	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	i	211	CLA	C3C-C4C-NC	-2.33	107.96	110.57
25	b	205	CLA	C2D-C1D-ND	2.33	111.82	110.10
25	m	204	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	B	831	BCR	C23-C22-C21	2.33	122.51	118.94
30	d	318	DD6	C33-C34-C35	2.33	113.49	110.30
25	c	303	CLA	CHB-C1B-NB	2.33	126.72	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	207	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	h	209	CLA	C3C-C4C-NC	-2.33	107.96	110.57
25	A	842	CLA	CHB-C1B-NB	2.32	126.72	124.26
25	j	208	CLA	C1-C2-C3	2.32	130.51	126.75
25	j	211	CLA	CHB-C1B-NB	2.32	126.72	124.26
25	A	851	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
25	B	841	CLA	CHB-C1B-NB	2.32	126.72	124.26
25	A	801	CLA	C1-C2-C3	2.32	130.06	126.04
25	A	821	CLA	C4-C3-C5	-2.32	111.36	115.27
25	a	210	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
25	B	814	CLA	C3C-C4C-NC	-2.32	107.97	110.57
25	j	208	CLA	C3C-C4C-NC	-2.32	107.97	110.57
25	A	851	CLA	C3C-C4C-NC	-2.32	107.97	110.57
25	g	204	CLA	CHB-C1B-NB	2.32	126.71	124.26
25	B	819	CLA	C12-C11-C10	-2.32	102.58	113.24
30	c	317	DD6	C21-C20-C19	2.32	116.89	114.28
30	c	316	DD6	C28-C27-C29	-2.32	112.25	116.84
25	p	609	CLA	CED-O2D-CGD	2.32	121.18	115.94
25	A	817	CLA	CHB-C1B-NB	2.32	126.71	124.26
30	J	104	DD6	C21-C20-C19	2.32	116.89	114.28
25	c	311	CLA	O1D-CGD-CBD	-2.32	119.75	124.48
25	B	802	CLA	C2D-C1D-ND	2.31	111.81	110.10
25	h	212	CLA	C3C-C4C-NC	-2.31	107.97	110.57
25	a	208	CLA	C3C-C4C-NC	-2.31	107.98	110.57
25	p	608	CLA	C3C-C4C-NC	-2.31	107.98	110.57
29	M	201	BCR	C24-C23-C22	-2.31	122.74	126.23
30	j	216	DD6	O1-C20-C15	-2.31	57.04	58.96
30	d	317	DD6	C28-C27-C29	-2.31	112.26	116.84
30	A	855	DD6	C10-C9-C8	-2.31	116.00	123.22
30	c	318	DD6	C32-C33-C34	-2.31	108.42	113.64
25	B	848	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
25	B	811	CLA	C12-C11-C10	-2.31	102.62	113.24
25	c	312	CLA	CHD-C1D-ND	-2.31	122.33	124.45
29	B	829	BCR	C37-C22-C23	2.31	121.72	118.08
25	c	313	CLA	C3C-C4C-NC	-2.31	107.98	110.57
25	i	206	CLA	C12-C11-C10	-2.31	102.63	113.24
25	h	212	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
30	o	612	DD6	O1-C20-C15	-2.31	57.05	58.96
30	c	317	DD6	C33-C34-C35	2.31	113.46	110.30
25	p	606	CLA	C1-C2-C3	2.31	130.48	126.75
25	k	204	CLA	C3C-C4C-NC	-2.31	107.98	110.57
30	e	220	DD6	C20-C19-C18	-2.31	108.19	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	812	CLA	C1-C2-C3	2.31	130.03	126.04
27	b	201	LHG	O8-C23-O10	-2.30	117.78	123.59
25	h	205	CLA	CHB-C1B-NB	2.30	126.70	124.26
25	e	211	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
25	A	848	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
35	d	307	CHL	O1D-CGD-CBD	-2.30	119.77	124.48
29	M	201	BCR	C2-C1-C6	2.30	114.03	110.48
35	d	308	CHL	C2B-C1B-NB	-2.30	108.69	110.23
25	A	813	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	B	821	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	c	315	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	i	206	CLA	C1-C2-C3	2.30	130.02	126.04
30	J	104	DD6	C32-C33-C34	-2.30	108.45	113.64
25	j	212	CLA	C3C-C4C-NC	-2.30	107.99	110.57
25	p	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
35	e	209	CHL	C2B-C1B-NB	-2.30	108.69	110.23
25	B	803	CLA	C2C-C1C-NC	-2.30	107.82	109.97
25	A	813	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
25	B	813	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	A	829	CLA	CHD-C1D-ND	-2.30	122.34	124.45
25	B	805	CLA	C4-C3-C5	-2.30	111.41	115.27
25	a	209	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	c	310	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	f	605	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	B	812	CLA	C3C-C4C-NC	-2.30	108.00	110.57
29	B	833	BCR	C2-C1-C6	2.29	114.01	110.48
25	d	313	CLA	CHB-C1B-NB	2.29	126.69	124.26
30	l	614	DD6	O1-C20-C15	-2.29	57.06	58.96
29	A	837	BCR	C23-C22-C21	2.29	122.46	118.94
29	B	832	BCR	C19-C18-C17	2.29	122.46	118.94
25	j	210	CLA	C1-C2-C3	2.29	130.46	126.75
25	m	208	CLA	CHB-C1B-NB	2.29	126.68	124.26
25	j	215	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
25	i	211	CLA	C4-C3-C5	-2.29	111.42	115.27
35	c	307	CHL	O2A-CGA-O1A	-2.29	117.81	123.59
25	c	308	CLA	CHB-C1B-NB	2.29	126.68	124.26
25	A	852	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
29	A	836	BCR	C29-C30-C25	2.29	114.00	110.48
25	B	816	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
25	f	606	CLA	CHB-C1B-NB	2.28	126.68	124.26
35	d	310	CHL	C2A-C3A-C4A	2.28	105.56	101.87
25	a	207	CLA	CHB-C1B-NB	2.28	126.67	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	f	607	CLA	CHB-C1B-NB	2.28	126.67	124.26
25	J	103	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
25	A	829	CLA	C2B-C1B-NB	-2.28	108.70	110.23
25	A	825	CLA	C12-C11-C10	-2.28	102.75	113.24
25	A	812	CLA	C3C-C4C-NC	-2.28	108.01	110.57
25	A	846	CLA	C3C-C4C-NC	-2.28	108.01	110.57
25	m	207	CLA	C3C-C4C-NC	-2.28	108.01	110.57
30	k	216	DD6	O1-C20-C21	-2.28	112.32	115.06
25	A	844	CLA	C12-C11-C10	-2.28	102.76	113.24
25	A	815	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
25	A	845	CLA	C3C-C4C-NC	-2.28	108.01	110.57
30	k	215	DD6	C28-C27-C29	-2.28	112.33	116.84
25	o	608	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	A	807	CLA	CHB-C1B-NB	2.28	126.67	124.26
25	B	844	CLA	C12-C11-C10	-2.28	102.77	113.24
25	B	844	CLA	C4-C3-C5	-2.28	111.44	115.27
25	b	204	CLA	C3C-C4C-NC	-2.28	108.02	110.57
29	B	801	BCR	C20-C21-C22	-2.28	124.06	127.31
30	c	316	DD6	O1-C20-C15	-2.28	57.07	58.96
30	f	613	DD6	C28-C27-C29	-2.28	112.33	116.84
25	p	603	CLA	C2D-C1D-ND	2.28	111.78	110.10
25	e	205	CLA	C3C-C4C-NC	-2.28	108.02	110.57
30	i	214	DD6	O1-C20-C15	-2.28	57.08	58.96
25	A	817	CLA	C3C-C4C-NC	-2.27	108.02	110.57
25	B	812	CLA	C12-C11-C10	-2.27	102.79	113.24
32	b	202	DGD	O6D-C1D-O3G	-2.27	104.59	109.97
25	B	816	CLA	C1-C2-C3	2.27	129.98	126.04
25	h	205	CLA	C3C-C4C-NC	-2.27	108.02	110.57
25	B	815	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
25	a	204	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
25	b	208	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
25	h	205	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
25	m	203	CLA	C12-C11-C10	-2.27	102.80	113.24
27	d	302	LHG	O8-C23-O10	-2.27	117.86	123.59
25	n	203	CLA	C2D-C1D-ND	2.27	111.78	110.10
30	k	216	DD6	O1-C20-C15	-2.27	57.08	58.96
25	d	303	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
25	B	807	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	B	843	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	e	207	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
30	j	217	DD6	C28-C27-C29	-2.27	112.34	116.84
25	l	611	CLA	CHB-C1B-NB	2.27	126.66	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	211	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
25	g	213	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
27	j	202	LHG	O8-C23-O10	-2.27	117.87	123.59
25	i	208	CLA	C3C-C4C-NC	-2.27	108.03	110.57
25	B	839	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
25	k	213	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
25	n	202	CLA	C2D-C1D-ND	2.27	111.77	110.10
25	j	203	CLA	CHB-C1B-NB	2.27	126.66	124.26
27	g	201	LHG	O8-C23-O10	-2.27	117.88	123.59
25	B	848	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	k	207	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	o	601	CLA	CHB-C1B-NB	2.26	126.65	124.26
30	i	214	DD6	C28-C27-C29	-2.26	112.36	116.84
25	g	213	CLA	C2D-C1D-ND	2.26	111.77	110.10
35	d	308	CHL	C4D-CHA-C1A	2.26	124.00	121.25
25	A	831	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	c	302	CLA	C3C-C4C-NC	-2.26	108.03	110.57
25	i	205	CLA	C3C-C4C-NC	-2.26	108.03	110.57
25	A	846	CLA	C1-C2-C3	2.26	129.95	126.04
25	p	603	CLA	CMD-C2D-C1D	2.26	128.70	124.71
25	m	202	CLA	C4B-CHC-C1C	-2.26	120.98	126.34
25	o	606	CLA	O2A-CGA-CBA	2.26	121.29	114.03
25	p	609	CLA	CMD-C2D-C1D	2.26	128.69	124.71
29	J	101	BCR	C23-C22-C21	2.26	122.41	118.94
25	o	608	CLA	C2D-C1D-ND	2.26	111.77	110.10
25	A	826	CLA	C1-C2-C3	2.26	129.95	126.04
25	A	853	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
25	b	209	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
25	A	844	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	c	311	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	n	203	CLA	CHB-C1B-NB	2.26	126.65	124.26
30	o	612	DD6	C33-C34-C35	2.26	113.39	110.30
25	o	601	CLA	C2D-C1D-ND	2.26	111.77	110.10
25	A	802	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
25	B	838	CLA	C3C-C4C-NC	-2.26	108.04	110.57
25	h	203	CLA	C3C-C4C-NC	-2.26	108.04	110.57
25	A	830	CLA	C2A-C1A-CHA	2.25	127.80	123.86
25	d	304	CLA	C12-C11-C10	-2.25	102.41	113.29
25	B	839	CLA	C3C-C4C-NC	-2.25	108.04	110.57
30	i	216	DD6	C28-C27-C29	-2.25	112.38	116.84
25	m	204	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	B	818	CLA	O1D-CGD-CBD	-2.25	119.87	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	l	614	DD6	C7-C6-C5	-2.25	119.77	122.92
25	A	833	CLA	C1-C2-C3	2.25	129.94	126.04
25	i	210	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
25	B	811	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
30	j	216	DD6	O1-C20-C19	2.25	115.07	113.38
25	A	832	CLA	C3C-C4C-NC	-2.25	108.05	110.57
25	B	824	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	l	608	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	j	212	CLA	C12-C11-C10	-2.25	102.90	113.24
25	f	610	CLA	C1-C2-C3	2.25	129.94	126.04
25	a	203	CLA	C1-C2-C3	2.25	130.39	126.75
25	g	212	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
25	A	822	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
29	A	839	BCR	C15-C16-C17	-2.25	118.87	123.47
27	g	201	LHG	O4-P-O5	2.25	123.35	112.24
25	p	607	CLA	O2A-CGA-CBA	2.25	121.25	114.03
25	n	202	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	a	209	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
25	B	819	CLA	C3C-C4C-NC	-2.25	108.05	110.57
25	a	209	CLA	C3C-C4C-NC	-2.25	108.05	110.57
25	c	303	CLA	C1-C2-C3	2.25	129.93	126.04
25	B	823	CLA	C12-C11-C10	-2.24	102.93	113.24
25	B	817	CLA	C1-C2-C3	2.24	130.38	126.75
25	A	819	CLA	C3C-C4C-NC	-2.24	108.06	110.57
25	a	206	CLA	O2A-CGA-CBA	2.24	121.24	114.03
25	B	823	CLA	C4-C3-C5	-2.24	111.50	115.27
25	A	811	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
25	A	830	CLA	C3C-C4C-NC	-2.24	108.06	110.57
25	h	206	CLA	C1-C2-C3	2.24	129.92	126.04
25	f	602	CLA	C1-C2-C3	2.24	129.92	126.04
25	a	205	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	j	208	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	B	803	CLA	C1-C2-C3	2.24	129.92	126.04
25	k	208	CLA	C3C-C4C-NC	-2.24	108.06	110.57
25	A	809	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
27	A	805	LHG	O4-P-O5	2.24	123.31	112.24
25	k	207	CLA	C3C-C4C-NC	-2.24	108.06	110.57
25	A	845	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	b	208	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	B	826	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
25	k	208	CLA	C4-C3-C5	-2.24	111.50	115.27
30	h	216	DD6	O1-C20-C15	-2.24	57.11	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	215	DD6	O1-C20-C15	-2.24	57.11	58.96
30	j	216	DD6	C28-C27-C29	-2.24	112.41	116.84
27	i	201	LHG	O4-P-O5	2.24	123.31	112.24
25	a	204	CLA	C4-C3-C5	-2.24	111.51	115.27
30	c	316	DD6	C4-C3-C2	-2.24	118.89	123.47
25	n	201	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
25	h	210	CLA	C3C-C4C-NC	-2.24	108.06	110.57
25	i	203	CLA	C12-C11-C10	-2.24	102.97	113.24
25	B	815	CLA	CHB-C1B-NB	2.23	126.62	124.26
25	o	606	CLA	CHB-C1B-NB	2.23	126.62	124.26
25	A	831	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
25	c	310	CLA	C3C-C4C-NC	-2.23	108.06	110.57
25	c	305	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
25	l	602	CLA	C4-C3-C5	-2.23	111.51	115.27
30	b	215	DD6	C21-C20-C19	2.23	116.79	114.28
25	B	825	CLA	C3C-C4C-NC	-2.23	108.07	110.57
30	b	214	DD6	O1-C20-C15	-2.23	57.11	58.96
25	d	313	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
25	h	215	CLA	CHB-C1B-NB	2.23	126.62	124.26
25	k	202	CLA	CHB-C1B-NB	2.23	126.62	124.26
25	B	834	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
25	l	601	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
30	o	611	DD6	C28-C27-C29	-2.23	112.42	116.84
25	d	313	CLA	O2A-CGA-CBA	2.23	121.20	114.03
25	j	209	CLA	CHB-C1B-NB	2.23	126.62	124.26
30	o	611	DD6	O1-C20-C15	-2.23	57.11	58.96
35	c	307	CHL	C2B-C1B-NB	-2.23	108.74	110.23
25	A	824	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
30	A	854	DD6	C33-C34-C35	2.23	113.36	110.30
25	B	816	CLA	C2D-C1D-ND	2.23	111.75	110.10
25	B	805	CLA	C12-C11-C10	-2.23	103.00	113.24
25	f	607	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
25	j	213	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
27	m	201	LHG	O8-C23-O10	-2.23	117.97	123.59
29	B	801	BCR	C34-C9-C10	-2.23	119.80	122.92
25	A	849	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
30	h	217	DD6	C28-C27-C29	-2.23	112.43	116.84
25	p	601	CLA	CHB-C1B-NB	2.23	126.61	124.26
25	c	309	CLA	C12-C11-C10	-2.23	103.00	113.24
25	c	308	CLA	C3C-C4C-NC	-2.23	108.07	110.57
25	n	208	CLA	O2A-CGA-CBA	2.23	121.18	114.03
25	a	212	CLA	O1D-CGD-CBD	-2.23	119.93	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	209	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
27	c	301	LHG	O4-P-O5	2.23	123.24	112.24
25	A	848	CLA	C3C-C4C-NC	-2.23	108.08	110.57
25	k	209	CLA	CHB-C1B-NB	2.23	126.61	124.26
25	n	205	CLA	CHB-C1B-NB	2.23	126.61	124.26
25	A	819	CLA	C12-C11-C10	-2.23	103.01	113.24
25	f	608	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
25	i	213	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
25	n	209	CLA	CAA-C2A-C3A	-2.22	110.91	116.10
25	f	606	CLA	CMD-C2D-C1D	2.22	128.63	124.71
25	A	826	CLA	C12-C11-C10	-2.22	103.02	113.24
25	A	824	CLA	C2A-C1A-CHA	2.22	127.75	123.86
30	e	219	DD6	C21-C20-C19	2.22	116.78	114.28
25	A	849	CLA	C1-C2-C3	2.22	130.35	126.75
27	A	805	LHG	O8-C23-O10	-2.22	117.98	123.59
25	o	604	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
30	m	212	DD6	C28-C27-C29	-2.22	112.44	116.84
25	A	827	CLA	CHB-C1B-NB	2.22	126.61	124.26
25	B	813	CLA	C1-C2-C3	2.22	130.35	126.75
25	A	801	CLA	C2A-C1A-CHA	2.22	127.74	123.86
30	i	214	DD6	O1-C20-C19	2.22	115.05	113.38
25	a	213	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
25	i	211	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	B	845	CLA	C12-C11-C10	-2.22	103.04	113.24
25	i	206	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
25	A	818	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
25	l	606	CLA	C3C-C4C-NC	-2.22	108.08	110.57
25	m	203	CLA	C3C-C4C-NC	-2.22	108.08	110.57
25	m	209	CLA	CHB-C1B-NB	2.22	126.60	124.26
25	i	204	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
25	B	823	CLA	CMD-C2D-C1D	2.22	128.62	124.71
25	A	810	CLA	C2D-C1D-ND	2.22	111.74	110.10
25	B	824	CLA	C3C-C4C-NC	-2.22	108.09	110.57
30	b	215	DD6	C33-C34-C35	2.22	113.34	110.30
25	B	805	CLA	CMD-C2D-C1D	2.22	128.62	124.71
25	l	605	CLA	CHB-C1B-NB	2.22	126.60	124.26
25	e	215	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
25	j	209	CLA	C12-C11-C10	-2.21	103.06	113.24
25	b	207	CLA	O2A-CGA-CBA	2.21	121.14	114.03
25	i	213	CLA	CHB-C1B-NB	2.21	126.60	124.26
25	j	206	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
25	l	610	CLA	O2D-CGD-O1D	-2.21	119.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	204	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
25	A	810	CLA	CHB-C1B-NB	2.21	126.60	124.26
25	a	210	CLA	CHB-C1B-NB	2.21	126.60	124.26
27	h	202	LHG	O8-C23-O10	-2.21	118.01	123.59
25	A	806	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
25	g	213	CLA	CHB-C1B-NB	2.21	126.60	124.26
25	A	810	CLA	C1-C2-C3	2.21	129.87	126.04
25	A	823	CLA	C12-C11-C10	-2.21	103.09	113.24
25	b	206	CLA	C3C-C4C-NC	-2.21	108.09	110.57
25	g	210	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
25	B	840	CLA	C3C-C4C-NC	-2.21	108.09	110.57
25	k	203	CLA	C3C-C4C-NC	-2.21	108.09	110.57
25	B	842	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
25	f	601	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
25	A	828	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
25	k	205	CLA	CHB-C1B-NB	2.21	126.59	124.26
30	c	318	DD6	O4-C34-C33	-2.21	105.42	109.80
25	o	602	CLA	C3C-C4C-NC	-2.21	108.10	110.57
35	d	309	CHL	OMC-CMC-C2C	-2.21	120.70	125.69
25	B	816	CLA	CHB-C1B-NB	2.21	126.59	124.26
25	a	204	CLA	CHB-C1B-NB	2.21	126.59	124.26
25	b	209	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
25	h	208	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
25	e	211	CLA	C3C-C4C-NC	-2.21	108.10	110.57
25	B	836	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
25	h	207	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
27	j	202	LHG	O4-P-O5	2.21	123.14	112.24
25	c	306	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
30	A	855	DD6	C25-C24-C1	-2.20	120.22	126.42
25	d	301	CLA	CAA-C2A-C3A	-2.20	110.95	116.10
25	k	214	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
25	B	812	CLA	CMD-C2D-C1D	2.20	128.60	124.71
25	o	610	CLA	C2C-C1C-NC	-2.20	107.91	109.97
25	B	803	CLA	C4-C3-C5	-2.20	111.56	115.27
25	f	602	CLA	C4-C3-C5	-2.20	111.56	115.27
25	c	311	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
25	g	203	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	n	201	CLA	C3C-C4C-NC	-2.20	108.10	110.57
25	A	822	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
27	b	201	LHG	O4-P-O5	2.20	123.13	112.24
30	n	212	DD6	O4-C34-C33	-2.20	105.43	109.80
25	e	204	CLA	O1D-CGD-CBD	-2.20	119.98	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	848	CLA	C3C-C4C-NC	-2.20	108.10	110.57
30	F	203	DD6	C26-C25-C24	2.20	130.09	123.22
25	h	211	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	m	204	CLA	CMD-C2D-C1D	2.20	128.59	124.71
25	B	839	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	k	206	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
25	B	806	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
25	B	823	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	a	207	CLA	C3C-C4C-NC	-2.20	108.10	110.57
30	k	215	DD6	O1-C20-C15	-2.20	57.14	58.96
25	n	201	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	A	821	CLA	CHB-C1B-NB	2.20	126.58	124.26
25	c	304	CLA	CHB-C1B-NB	2.20	126.58	124.26
25	e	213	CLA	CHB-C1B-NB	2.20	126.58	124.26
25	a	207	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
25	g	212	CLA	CHB-C1B-NB	2.20	126.58	124.26
25	F	202	CLA	CMD-C2D-C1D	2.20	128.59	124.71
35	d	309	CHL	C2A-C1A-CHA	2.20	127.70	123.86
27	a	201	LHG	O4-P-O5	2.20	123.10	112.24
25	A	815	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
29	B	830	BCR	C29-C30-C25	2.20	113.86	110.48
25	b	210	CLA	C3C-C4C-NC	-2.20	108.11	110.57
25	c	313	CLA	C4-C3-C5	-2.20	111.58	115.27
35	d	307	CHL	C2B-C1B-NB	-2.20	108.76	110.23
25	B	804	CLA	C2D-C1D-ND	2.20	111.72	110.10
25	A	833	CLA	C2A-C1A-CHA	2.20	127.70	123.86
30	h	217	DD6	O1-C20-C15	-2.20	57.14	58.96
25	A	851	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
25	k	208	CLA	C12-C11-C10	-2.19	102.69	113.29
25	c	309	CLA	C3C-C4C-NC	-2.19	108.11	110.57
25	n	211	CLA	C3C-C4C-NC	-2.19	108.11	110.57
25	B	824	CLA	C12-C11-C10	-2.19	103.17	113.24
27	h	201	LHG	O4-P-O5	2.19	123.07	112.24
30	n	213	DD6	C13-C11-C10	2.19	122.30	118.94
25	B	815	CLA	C3C-C4C-NC	-2.19	108.11	110.57
30	J	104	DD6	O4-C34-C33	-2.19	105.45	109.80
30	e	218	DD6	C15-C14-C13	-2.19	121.36	125.99
25	p	609	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	A	827	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
30	p	610	DD6	C33-C34-C35	2.19	113.30	110.30
29	M	201	BCR	C29-C30-C25	2.19	113.85	110.48
27	h	202	LHG	O4-P-O5	2.19	123.06	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	857	CLA	CHB-C1B-NB	2.19	126.57	124.26
30	c	317	DD6	O1-C20-C15	-2.19	57.15	58.96
25	f	612	CLA	C2D-C1D-ND	2.19	111.72	110.10
25	n	209	CLA	C2D-C1D-ND	2.19	111.72	110.10
25	B	824	CLA	C1-C2-C3	2.19	129.83	126.04
30	o	611	DD6	C33-C34-C35	2.19	113.30	110.30
25	B	813	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	i	206	CLA	CHB-C1B-NB	2.19	126.57	124.26
25	B	825	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
35	d	307	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
25	d	316	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
25	A	811	CLA	CHB-C1B-NB	2.19	126.57	124.26
25	h	203	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
25	B	808	CLA	C3C-C4C-NC	-2.19	108.12	110.57
25	A	853	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
35	d	309	CHL	C4D-CHA-C1A	2.18	123.91	121.25
25	A	801	CLA	C2D-C1D-ND	2.18	111.71	110.10
25	A	833	CLA	C2D-C1D-ND	2.18	111.71	110.10
25	f	602	CLA	C3C-C4C-NC	-2.18	108.12	110.57
25	e	216	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
27	d	302	LHG	O4-P-O5	2.18	123.04	112.24
25	p	602	CLA	CMD-C2D-C1D	2.18	128.56	124.71
25	c	310	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
25	A	819	CLA	CHB-C1B-NB	2.18	126.57	124.26
25	e	210	CLA	C3C-C4C-NC	-2.18	108.12	110.57
32	b	202	DGD	O2D-C2D-C1D	-2.18	104.75	110.05
25	m	209	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
30	l	613	DD6	C33-C34-C35	2.18	113.29	110.30
25	j	211	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
30	c	316	DD6	O4-C34-C33	-2.18	105.47	109.80
25	l	604	CLA	CHB-C1B-NB	2.18	126.56	124.26
25	n	207	CLA	CHB-C1B-NB	2.18	126.56	124.26
27	c	301	LHG	O8-C23-O10	-2.18	118.09	123.59
27	m	201	LHG	O4-P-O5	2.18	123.02	112.24
25	A	825	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
25	A	821	CLA	C12-C11-C10	-2.18	103.22	113.24
25	A	802	CLA	C1-C2-C3	2.18	129.81	126.04
25	g	211	CLA	CHB-C1B-NB	2.18	126.56	124.26
25	o	604	CLA	CHB-C1B-NB	2.18	126.56	124.26
35	c	307	CHL	C2A-C3A-C4A	2.18	105.39	101.87
25	B	838	CLA	C2C-C1C-NC	-2.18	107.93	109.97
25	a	210	CLA	O2D-CGD-O1D	-2.18	119.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	811	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
25	B	816	CLA	C3C-C4C-NC	-2.18	108.13	110.57
25	e	201	CLA	C3C-C4C-NC	-2.18	108.13	110.57
32	B	849	DGD	O6D-C1D-O3G	-2.18	104.82	109.97
25	i	211	CLA	CHB-C1B-NB	2.18	126.56	124.26
25	n	207	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
25	g	210	CLA	C3C-C4C-NC	-2.17	108.13	110.57
25	B	840	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	e	201	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
25	j	205	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
29	B	833	BCR	C29-C30-C25	2.17	113.83	110.48
25	g	209	CLA	C3C-C4C-NC	-2.17	108.13	110.57
25	n	207	CLA	C2D-C1D-ND	2.17	111.71	110.10
25	B	809	CLA	CHB-C1B-NB	2.17	126.56	124.26
25	n	201	CLA	CHB-C1B-NB	2.17	126.56	124.26
29	A	837	BCR	C24-C23-C22	-2.17	122.95	126.23
35	e	209	CHL	O2A-CGA-CBA	2.17	121.01	114.03
25	A	808	CLA	CHB-C1B-NB	2.17	126.56	124.26
25	A	802	CLA	C3C-C4C-NC	-2.17	108.14	110.57
25	h	208	CLA	C3C-C4C-NC	-2.17	108.14	110.57
25	b	212	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
25	A	840	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	A	814	CLA	C4-C3-C5	-2.17	111.62	115.27
25	l	610	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
25	l	603	CLA	CHB-C1B-NB	2.17	126.55	124.26
25	A	844	CLA	CMD-C2D-C1D	2.17	128.53	124.71
25	d	312	CLA	C3C-C4C-NC	-2.17	108.14	110.57
25	F	201	CLA	C2D-C1D-ND	2.17	111.70	110.10
25	A	815	CLA	CHB-C1B-NB	2.17	126.55	124.26
25	B	845	CLA	CHB-C1B-NB	2.17	126.55	124.26
25	o	602	CLA	CHB-C1B-NB	2.17	126.55	124.26
25	j	210	CLA	C3C-C4C-NC	-2.17	108.14	110.57
25	B	802	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	B	816	CLA	C12-C11-C10	-2.17	103.28	113.24
25	a	206	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	c	315	CLA	C2D-C1D-ND	2.17	111.70	110.10
30	J	105	DD6	C34-C35-C36	2.17	116.17	111.85
25	b	205	CLA	CHB-C1B-NB	2.17	126.55	124.26
25	A	801	CLA	C3C-C4C-NC	-2.17	108.14	110.57
25	A	833	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
25	B	818	CLA	C12-C11-C10	-2.17	103.29	113.24
25	B	826	CLA	CHB-C1B-NB	2.17	126.55	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	l	614	DD6	C19-C18-C17	-2.16	106.59	110.77
25	B	848	CLA	C12-C11-C10	-2.16	103.29	113.24
25	b	210	CLA	CBA-CAA-C2A	2.16	118.28	113.47
25	A	852	CLA	CHB-C1B-NB	2.16	126.55	124.26
25	c	306	CLA	CHB-C1B-NB	2.16	126.55	124.26
25	p	606	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
25	A	811	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
35	d	310	CHL	O2A-CGA-CBA	2.16	120.98	114.03
30	k	216	DD6	C28-C27-C29	-2.16	112.56	116.84
25	e	207	CLA	C1-C2-C3	2.16	130.25	126.75
25	A	808	CLA	C1-C2-C3	2.16	129.78	126.04
25	a	205	CLA	C3C-C4C-NC	-2.16	108.15	110.57
25	d	305	CLA	CHB-C1B-NB	2.16	126.55	124.26
25	k	205	CLA	C4-C3-C5	-2.16	111.64	115.27
35	e	209	CHL	C2A-C1A-CHA	2.16	127.64	123.86
25	B	826	CLA	C3C-C4C-NC	-2.16	108.15	110.57
25	A	853	CLA	C2D-C1D-ND	2.16	111.70	110.10
25	A	844	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
25	B	846	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
25	f	604	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
25	A	852	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	m	210	CLA	CHB-C1B-NB	2.16	126.54	124.26
25	f	601	CLA	CHB-C1B-NB	2.16	126.54	124.26
25	A	830	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
33	D	200	SQD	O5-C5-C4	2.16	113.61	109.69
28	B	835	PQN	C17-C16-C15	-2.16	107.50	113.36
25	A	828	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	i	211	CLA	C2A-C1A-CHA	2.16	127.63	123.86
25	j	206	CLA	C12-C11-C10	-2.16	102.88	113.29
25	h	212	CLA	C1-C2-C3	2.16	129.77	126.04
30	m	212	DD6	O1-C20-C15	-2.16	57.17	58.96
25	f	605	CLA	CMD-C2D-C1D	2.16	128.51	124.71
25	A	846	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
29	A	839	BCR	C29-C30-C25	2.15	113.80	110.48
25	j	205	CLA	CHB-C1B-NB	2.15	126.54	124.26
33	F	204	SQD	O5-C5-C4	2.15	113.61	109.69
25	B	822	CLA	C3C-C4C-NC	-2.15	108.16	110.57
30	l	614	DD6	C28-C27-C29	-2.15	112.58	116.84
25	A	833	CLA	C12-C11-C10	-2.15	103.35	113.24
25	c	306	CLA	C3C-C4C-NC	-2.15	108.16	110.57
25	a	211	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
25	A	828	CLA	C3C-C4C-NC	-2.15	108.16	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	j	217	DD6	O1-C20-C15	-2.15	57.18	58.96
25	g	215	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	n	204	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	B	807	CLA	C2D-C1D-ND	2.15	111.69	110.10
25	B	834	CLA	C2D-C1D-ND	2.15	111.69	110.10
25	B	818	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
25	A	820	CLA	C12-C11-C10	-2.15	102.91	113.29
25	B	803	CLA	C4D-CHA-C1A	2.15	123.87	121.25
25	b	213	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
25	j	203	CLA	C3C-C4C-NC	-2.15	108.16	110.57
25	h	215	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
25	B	813	CLA	O2A-CGA-CBA	2.15	121.56	110.26
25	a	206	CLA	C3C-C4C-NC	-2.15	108.16	110.57
27	A	835	LHG	O8-C23-O10	-2.15	118.17	123.59
25	B	813	CLA	C2D-C1D-ND	2.15	111.69	110.10
25	a	206	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	n	201	CLA	C1-C2-C3	2.15	129.76	126.04
35	d	310	CHL	OMC-CMC-C2C	-2.15	120.83	125.69
25	A	802	CLA	C2D-C1D-ND	2.15	111.69	110.10
25	B	846	CLA	C2D-C1D-ND	2.15	111.69	110.10
25	l	611	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
25	A	845	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
25	i	203	CLA	C3C-C4C-NC	-2.15	108.17	110.57
30	l	613	DD6	O4-C34-C33	-2.15	105.54	109.80
27	A	835	LHG	O4-P-O5	2.14	122.84	112.24
25	J	103	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
25	A	821	CLA	O2A-CGA-CBA	2.14	121.53	110.26
30	d	319	DD6	O4-C34-C33	-2.14	105.54	109.80
25	g	212	CLA	C3C-C4C-NC	-2.14	108.17	110.57
30	i	216	DD6	O1-C20-C15	-2.14	57.18	58.96
25	B	819	CLA	CHB-C1B-NB	2.14	126.53	124.26
25	B	816	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
25	k	212	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
25	B	806	CLA	C3C-C4C-NC	-2.14	108.17	110.57
25	k	205	CLA	C3C-C4C-NC	-2.14	108.17	110.57
25	e	201	CLA	CHB-C1B-NB	2.14	126.53	124.26
25	B	841	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
25	B	844	CLA	C3C-C4C-NC	-2.14	108.17	110.57
25	f	611	CLA	C3C-C4C-NC	-2.14	108.17	110.57
25	o	606	CLA	C3C-C4C-NC	-2.14	108.17	110.57
30	A	854	DD6	O4-C34-C33	-2.14	105.55	109.80
30	a	215	DD6	C21-C20-C19	2.14	116.69	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	l	611	CLA	C2D-C1D-ND	2.14	111.68	110.10
25	e	212	CLA	C4-C3-C5	-2.14	111.67	115.27
25	o	604	CLA	C3C-C4C-NC	-2.14	108.17	110.57
35	d	308	CHL	O2A-CGA-CBA	2.14	120.91	114.03
25	j	205	CLA	CMD-C2D-C1D	2.14	128.49	124.71
25	A	831	CLA	C2D-C1D-ND	2.14	111.68	110.10
29	A	838	BCR	C28-C27-C26	-2.14	110.26	114.08
30	l	614	DD6	C33-C34-C35	2.14	113.23	110.30
30	c	317	DD6	O4-C34-C33	-2.14	105.55	109.80
25	A	809	CLA	C2B-C1B-NB	-2.14	108.80	110.23
25	d	312	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
25	B	844	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	j	214	CLA	C3C-C4C-NC	-2.14	108.17	110.57
25	A	827	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
25	i	203	CLA	CHB-C1B-NB	2.14	126.52	124.26
30	o	612	DD6	O4-C34-C33	-2.14	105.56	109.80
27	a	201	LHG	O8-C23-O10	-2.14	118.20	123.59
25	d	315	CLA	C3C-C4C-NC	-2.14	108.17	110.57
25	e	216	CLA	C3C-C4C-NC	-2.14	108.17	110.57
30	o	612	DD6	C28-C27-C29	-2.14	112.61	116.84
25	A	804	CLA	C3C-C4C-NC	-2.14	108.18	110.57
25	A	807	CLA	C12-C11-C10	-2.14	103.43	113.24
25	l	609	CLA	CHB-C1B-NB	2.13	126.52	124.26
25	f	605	CLA	C3C-C4C-NC	-2.13	108.18	110.57
30	m	213	DD6	C7-C6-C5	-2.13	119.93	122.92
30	i	216	DD6	O1-C20-C21	-2.13	112.50	115.06
25	A	847	CLA	CHB-C1B-NB	2.13	126.52	124.26
25	b	207	CLA	C3C-C4C-NC	-2.13	108.18	110.57
25	m	211	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
25	n	208	CLA	C2D-C1D-ND	2.13	111.68	110.10
25	h	210	CLA	CHB-C1B-NB	2.13	126.52	124.26
25	g	205	CLA	CHD-C1D-ND	-2.13	122.49	124.45
25	A	810	CLA	CED-O2D-CGD	2.13	120.76	115.94
25	B	825	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	B	845	CLA	C2C-C1C-NC	-2.13	107.97	109.97
30	d	317	DD6	C21-C20-C19	2.13	116.68	114.28
30	e	218	DD6	C33-C32-C31	2.13	113.94	109.62
25	l	610	CLA	C3C-C4C-NC	-2.13	108.18	110.57
25	e	208	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	J	103	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
25	B	844	CLA	C4D-CHA-C1A	2.13	123.84	121.25
25	B	816	CLA	CMD-C2D-C1D	2.13	128.47	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	204	CLA	C3C-C4C-NC	-2.13	108.18	110.57
25	J	103	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	B	805	CLA	C2D-C1D-ND	2.13	111.67	110.10
25	c	310	CLA	C1-C2-C3	2.13	129.72	126.04
25	c	303	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
25	A	822	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	A	833	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	a	205	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
25	A	828	CLA	CMD-C2D-C1D	2.13	128.46	124.71
25	b	209	CLA	O2A-CGA-CBA	2.13	120.87	114.03
25	i	209	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
25	n	204	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
25	i	210	CLA	CMD-C2D-C1D	2.13	128.46	124.71
25	B	814	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	l	603	CLA	CMD-C2D-C1D	2.13	128.46	124.71
25	p	604	CLA	C3C-C4C-NC	-2.13	108.19	110.57
30	i	215	DD6	O1-C20-C21	-2.13	112.51	115.06
25	A	818	CLA	C12-C11-C10	-2.13	103.47	113.24
25	b	211	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	h	211	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	F	202	CLA	O2A-CGA-CBA	2.13	120.86	114.03
29	B	831	BCR	C8-C9-C10	2.13	122.20	118.94
25	o	609	CLA	C2D-C1D-ND	2.13	111.67	110.10
30	b	215	DD6	O1-C20-C15	-2.12	57.20	58.96
30	h	216	DD6	O1-C20-C19	2.12	114.98	113.38
25	c	315	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
30	a	215	DD6	C19-C18-C17	-2.12	106.67	110.77
25	c	308	CLA	CMD-C2D-C1D	2.12	128.46	124.71
25	j	203	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
25	B	838	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
25	d	301	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
25	p	605	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	c	305	CLA	C2D-C1D-ND	2.12	111.67	110.10
25	c	303	CLA	CMD-C2D-C1D	2.12	128.45	124.71
25	B	818	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
25	A	841	CLA	C12-C11-C10	-2.12	103.05	113.29
25	k	210	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
25	A	824	CLA	C4-C3-C5	-2.12	111.70	115.27
25	n	203	CLA	CMD-C2D-C1D	2.12	128.45	124.71
25	A	833	CLA	C3C-C4C-NC	-2.12	108.19	110.57
25	A	857	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
30	f	614	DD6	C8-C6-C5	2.12	122.19	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	o	606	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
25	c	313	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
25	c	314	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
25	A	810	CLA	C3C-C4C-NC	-2.12	108.20	110.57
25	i	212	CLA	C3C-C4C-NC	-2.12	108.20	110.57
25	h	212	CLA	C2A-C1A-CHA	2.12	127.56	123.86
25	A	823	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	j	211	CLA	CMB-C2B-C1B	-2.12	122.15	125.37
25	e	208	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	m	209	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	B	810	CLA	CHB-C1B-NB	2.11	126.50	124.26
25	A	802	CLA	C12-C11-C10	-2.11	103.53	113.24
25	j	213	CLA	C2D-C1D-ND	2.11	111.66	110.10
25	o	609	CLA	CBA-CAA-C2A	2.11	118.17	113.47
25	j	208	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
25	a	213	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	c	309	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	g	206	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	A	857	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	B	842	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	o	608	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	j	214	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	k	211	CLA	C3C-C4C-NC	-2.11	108.20	110.57
25	g	214	CLA	CMD-C2D-C1D	2.11	128.43	124.71
25	A	812	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
25	A	801	CLA	C12-C11-C10	-2.11	103.55	113.24
30	m	213	DD6	O4-C34-C33	-2.11	105.61	109.80
25	a	212	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	b	208	CLA	C3C-C4C-NC	-2.11	108.21	110.57
25	d	303	CLA	C3C-C4C-NC	-2.11	108.21	110.57
29	B	830	BCR	C37-C22-C23	2.11	121.40	118.08
25	e	213	CLA	C3C-C4C-NC	-2.11	108.21	110.57
25	m	208	CLA	C3C-C4C-NC	-2.11	108.21	110.57
25	b	206	CLA	O2A-CGA-CBA	2.11	120.80	114.03
25	A	832	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	A	802	CLA	C2C-C1C-NC	-2.11	108.00	109.97
25	B	844	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
30	J	104	DD6	O1-C20-C15	-2.11	57.22	58.96
25	k	214	CLA	CHB-C1B-NB	2.11	126.49	124.26
25	p	604	CLA	O1D-CGD-CBD	-2.11	120.18	124.48
25	f	603	CLA	CMD-C2D-C1D	2.11	128.42	124.71
30	m	213	DD6	C28-C27-C29	-2.10	112.67	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	204	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
25	c	302	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
30	d	319	DD6	C4-C5-C6	-2.10	124.31	127.31
29	B	833	BCR	C24-C25-C26	2.10	126.56	121.46
25	a	207	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
25	k	202	CLA	C3C-C4C-NC	-2.10	108.21	110.57
25	B	844	CLA	C2D-C1D-ND	2.10	111.65	110.10
25	e	205	CLA	C12-C11-C10	-2.10	103.58	113.24
25	f	609	CLA	CHB-C1B-NB	2.10	126.48	124.26
25	h	210	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
25	A	801	CLA	CHB-C1B-NB	2.10	126.48	124.26
28	B	827	PQN	C10-C1-C2	-2.10	115.95	118.95
25	a	209	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
29	B	833	BCR	C37-C22-C23	2.10	121.39	118.08
25	e	213	CLA	CMD-C2D-C1D	2.10	128.41	124.71
30	a	214	DD6	O1-C20-C21	-2.10	112.54	115.06
30	i	216	DD6	O4-C34-C33	-2.10	105.63	109.80
25	k	204	CLA	CMD-C2D-C1D	2.10	128.41	124.71
30	c	318	DD6	O1-C20-C15	-2.10	57.22	58.96
33	J	102	SQD	C44-O6-C1	2.10	117.84	113.74
25	a	213	CLA	C12-C11-C10	-2.10	103.59	113.24
25	B	810	CLA	C3C-C4C-NC	-2.10	108.22	110.57
25	d	311	CLA	C3C-C4C-NC	-2.10	108.22	110.57
25	h	213	CLA	C3C-C4C-NC	-2.10	108.22	110.57
25	g	215	CLA	C3C-C4C-NC	-2.10	108.22	110.57
25	j	209	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	B	842	CLA	CHB-C1B-NB	2.10	126.48	124.26
25	A	840	CLA	C2D-C1D-ND	2.10	111.65	110.10
25	A	842	CLA	C3C-C4C-NC	-2.10	108.22	110.57
25	b	207	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	l	613	DD6	O1-C20-C15	-2.10	57.22	58.96
25	A	813	CLA	C1-C2-C3	2.10	129.67	126.04
25	A	815	CLA	C2D-C1D-ND	2.10	111.65	110.10
30	p	610	DD6	O4-C34-C33	-2.10	105.64	109.80
25	l	602	CLA	CHB-C1B-NB	2.10	126.48	124.26
25	B	844	CLA	CMD-C2D-C1D	2.10	128.41	124.71
25	h	205	CLA	CMD-C2D-C1D	2.10	128.41	124.71
30	A	855	DD6	O1-C20-C15	-2.10	57.22	58.96
25	h	215	CLA	C3C-C4C-NC	-2.10	108.22	110.57
25	j	206	CLA	C3C-C4C-NC	-2.10	108.22	110.57
29	B	801	BCR	C11-C10-C9	-2.10	124.32	127.31
25	j	204	CLA	C2B-C1B-NB	-2.09	108.83	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	810	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
30	m	212	DD6	O1-C20-C21	-2.09	112.55	115.06
25	A	852	CLA	C3C-C4C-NC	-2.09	108.22	110.57
25	B	841	CLA	C3C-C4C-NC	-2.09	108.22	110.57
25	A	853	CLA	C4-C3-C5	-2.09	111.75	115.27
25	a	205	CLA	C2D-C1D-ND	2.09	111.65	110.10
25	o	607	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
25	B	842	CLA	CED-O2D-CGD	2.09	120.67	115.94
25	A	851	CLA	O2A-CGA-CBA	2.09	120.75	114.03
25	B	837	CLA	C1-C2-C3	2.09	130.13	126.75
25	l	608	CLA	C3C-C4C-NC	-2.09	108.23	110.57
25	h	213	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
25	o	603	CLA	C2D-C1D-ND	2.09	111.64	110.10
25	c	304	CLA	CMD-C2D-C1D	2.09	128.40	124.71
25	b	209	CLA	C3C-C4C-NC	-2.09	108.23	110.57
29	A	836	BCR	C16-C17-C18	-2.09	124.33	127.31
25	m	210	CLA	CMD-C2D-C1D	2.09	128.39	124.71
25	c	312	CLA	C2D-C1D-ND	2.09	111.64	110.10
25	B	810	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
25	c	304	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
25	j	210	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	l	614	DD6	O4-C34-C33	-2.09	105.65	109.80
25	B	845	CLA	CMD-C2D-C1D	2.09	128.39	124.71
28	F	205	PQN	C10-C1-C2	-2.09	115.98	118.95
25	A	822	CLA	C3C-C4C-NC	-2.09	108.23	110.57
25	F	202	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
25	A	818	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	A	852	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	j	206	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
25	B	821	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
25	B	819	CLA	C2A-C1A-CHA	2.08	127.50	123.86
25	b	213	CLA	C3C-C4C-NC	-2.08	108.23	110.57
30	c	316	DD6	C33-C34-C35	2.08	113.16	110.30
30	f	613	DD6	O1-C20-C15	-2.08	57.24	58.96
25	k	214	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	B	834	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	i	213	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	l	604	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	j	213	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	k	210	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	n	206	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	a	209	CLA	C1-C2-C3	2.08	129.64	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	820	CLA	CED-O2D-CGD	2.08	120.64	115.94
25	c	312	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	o	603	CLA	CMD-C2D-C1D	2.08	128.38	124.71
25	e	214	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	f	604	CLA	C2D-C1D-ND	2.08	111.64	110.10
25	B	807	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
25	B	821	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	k	206	CLA	CMD-C2D-C1D	2.08	128.38	124.71
30	b	215	DD6	O4-C34-C33	-2.08	105.67	109.80
25	j	212	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
25	B	834	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	A	830	CLA	C1-C2-C3	2.08	129.64	126.04
25	J	103	CLA	CMD-C2D-C1D	2.08	128.38	124.71
25	m	205	CLA	C3C-C4C-NC	-2.08	108.24	110.57
30	d	318	DD6	O4-C34-C33	-2.08	105.67	109.80
25	f	606	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
25	g	214	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	p	605	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	e	204	CLA	C3C-C4C-NC	-2.08	108.31	110.57
25	A	841	CLA	C3C-C4C-NC	-2.07	108.24	110.57
25	A	823	CLA	C2D-C1D-ND	2.07	111.63	110.10
35	d	307	CHL	C4D-CHA-C1A	2.07	123.77	121.25
25	g	209	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	i	202	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
25	f	610	CLA	CMD-C2D-C1D	2.07	128.37	124.71
25	A	816	CLA	C2D-C1D-ND	2.07	111.63	110.10
25	p	605	CLA	CMD-C2D-C1D	2.07	128.37	124.71
25	B	809	CLA	C3C-C4C-NC	-2.07	108.25	110.57
30	a	215	DD6	O4-C34-C33	-2.07	105.68	109.80
25	B	802	CLA	C1-C2-C3	2.07	129.63	126.04
25	A	811	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
25	e	212	CLA	CHB-C1B-NB	2.07	126.45	124.26
29	B	828	BCR	C34-C9-C10	-2.07	120.02	122.92
25	B	813	CLA	C3C-C4C-NC	-2.07	108.25	110.57
25	l	605	CLA	CMD-C2D-C1D	2.07	128.37	124.71
25	e	204	CLA	CMD-C2D-C1D	2.07	128.36	124.71
25	g	210	CLA	CHB-C1B-NB	2.07	126.45	124.26
29	B	828	BCR	C37-C22-C23	2.07	121.34	118.08
29	M	201	BCR	C30-C25-C24	-2.07	109.92	115.78
25	h	204	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
25	i	210	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	p	607	CLA	C3C-C4C-NC	-2.07	108.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	840	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	i	213	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
25	B	824	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	B	835	PQN	C10-C1-C2	-2.07	116.00	118.95
25	f	610	CLA	C5-C3-C2	2.07	125.30	121.12
25	A	806	CLA	C3C-C4C-NC	-2.07	108.25	110.57
25	g	204	CLA	C3C-C4C-NC	-2.07	108.25	110.57
25	o	601	CLA	C3C-C4C-NC	-2.07	108.25	110.57
25	A	814	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	k	209	CLA	C3C-C4C-NC	-2.07	108.25	110.57
25	n	206	CLA	C3C-C4C-NC	-2.07	108.25	110.57
25	A	846	CLA	CHB-C1B-NB	2.07	126.44	124.26
25	e	215	CLA	CHB-C1B-NB	2.07	126.44	124.26
25	b	207	CLA	C2D-C1D-ND	2.07	111.63	110.10
30	j	217	DD6	O4-C34-C33	-2.07	105.70	109.80
25	A	804	CLA	CHB-C1B-NB	2.07	126.44	124.26
25	b	213	CLA	CHB-C1B-NB	2.07	126.44	124.26
25	i	202	CLA	CHB-C1B-NB	2.07	126.44	124.26
30	j	216	DD6	C19-C18-C17	-2.07	106.78	110.77
25	p	605	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
25	k	211	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
30	d	318	DD6	C23-C16-C17	-2.06	105.39	108.98
30	c	316	DD6	C19-C18-C17	-2.06	106.79	110.77
25	B	805	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
30	b	214	DD6	O4-C34-C33	-2.06	105.70	109.80
25	A	808	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
25	a	203	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
25	a	210	CLA	C2D-C1D-ND	2.06	111.62	110.10
25	i	206	CLA	C3C-C4C-NC	-2.06	108.26	110.57
25	l	602	CLA	C3C-C4C-NC	-2.06	108.26	110.57
25	n	204	CLA	C3C-C4C-NC	-2.06	108.26	110.57
35	d	309	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
29	M	201	BCR	C24-C25-C26	2.06	126.46	121.46
25	A	813	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
25	c	314	CLA	C3C-C4C-NC	-2.06	108.26	110.57
25	e	215	CLA	CMD-C2D-C1D	2.06	128.35	124.71
25	i	202	CLA	C2D-C1D-ND	2.06	111.62	110.10
30	F	203	DD6	C40-C32-C31	-2.06	107.19	110.47
30	A	854	DD6	O1-C20-C15	-2.06	57.25	58.96
25	g	212	CLA	C4-C3-C5	-2.06	111.81	115.27
35	d	308	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
35	c	307	CHL	O2D-CGD-O1D	-2.06	119.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	308	CLA	C1-C2-C3	2.06	130.08	126.75
25	h	203	CLA	C1-C2-C3	2.06	130.08	126.75
25	f	608	CLA	CHB-C1B-NB	2.06	126.44	124.26
30	n	214	DD6	C25-C26-C27	-2.06	120.60	126.58
25	o	607	CLA	C3C-C4C-NC	-2.06	108.26	110.57
25	h	204	CLA	C5-C3-C2	2.06	125.28	121.12
25	A	814	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
25	b	203	CLA	C2D-C1D-ND	2.06	111.62	110.10
25	a	205	CLA	C1-C2-C3	2.06	129.60	126.04
25	A	819	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
25	A	843	CLA	C3C-C4C-NC	-2.06	108.26	110.57
25	n	207	CLA	C3C-C4C-NC	-2.06	108.26	110.57
25	a	207	CLA	C5-C3-C2	2.06	125.28	121.12
30	k	216	DD6	C21-C20-C19	2.06	116.59	114.28
25	g	212	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	d	304	CLA	CHB-C1B-NB	2.06	126.43	124.26
25	o	601	CLA	CMD-C2D-C1D	2.06	128.34	124.71
25	B	809	CLA	C2D-C1D-ND	2.06	111.62	110.10
25	g	213	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
25	b	211	CLA	C3C-C4C-NC	-2.06	108.27	110.57
25	h	204	CLA	C4D-CHA-C1A	2.06	123.75	121.25
25	A	822	CLA	C1-C2-C3	2.05	129.60	126.04
25	h	214	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	B	837	CLA	C2D-C1D-ND	2.05	111.62	110.10
25	o	604	CLA	CMD-C2D-C1D	2.05	128.33	124.71
25	A	851	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
25	l	603	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
25	c	315	CLA	C3C-C4C-NC	-2.05	108.27	110.57
25	f	607	CLA	C3C-C4C-NC	-2.05	108.27	110.57
30	d	319	DD6	O1-C20-C15	-2.05	57.26	58.96
25	A	819	CLA	CED-O2D-CGD	2.05	120.58	115.94
25	A	816	CLA	C3C-C4C-NC	-2.05	108.27	110.57
25	j	204	CLA	C3C-C4C-NC	-2.05	108.27	110.57
25	j	215	CLA	C3C-C4C-NC	-2.05	108.27	110.57
25	k	202	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
25	j	213	CLA	C3C-C4C-NC	-2.05	108.27	110.57
35	d	310	CHL	C2A-C1A-CHA	2.05	127.44	123.86
25	A	813	CLA	C2D-C1D-ND	2.05	111.61	110.10
30	h	216	DD6	C19-C18-C17	-2.05	106.81	110.77
30	o	611	DD6	O4-C34-C33	-2.05	105.73	109.80
25	e	212	CLA	C3C-C4C-NC	-2.05	108.27	110.57
25	l	612	CLA	C3C-C4C-NC	-2.05	108.27	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	215	DD6	C21-C20-C19	2.05	116.59	114.28
25	A	841	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	g	214	CLA	CHB-C1B-NB	2.05	126.43	124.26
35	c	307	CHL	O1D-CGD-CBD	-2.05	120.29	124.48
25	e	207	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	B	801	BCR	C24-C23-C22	-2.05	123.14	126.23
35	d	309	CHL	C2B-C1B-NB	-2.05	108.86	110.23
29	A	838	BCR	C2-C1-C6	2.05	113.64	110.48
25	n	209	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
25	k	203	CLA	C1-C2-C3	2.05	129.59	126.04
25	h	214	CLA	C3C-C4C-NC	-2.05	108.27	110.57
25	p	602	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	o	601	CLA	CED-O2D-CGD	2.05	120.57	115.94
25	b	203	CLA	CMD-C2D-C1D	2.05	128.32	124.71
30	i	215	DD6	O4-C34-C33	-2.05	105.73	109.80
25	l	612	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
25	n	207	CLA	CAA-C2A-C3A	-2.05	111.32	116.10
25	g	207	CLA	C3C-C4C-NC	-2.05	108.28	110.57
25	a	204	CLA	CMD-C2D-C1D	2.05	128.32	124.71
25	B	802	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	f	612	CLA	CHB-C1B-NB	2.05	126.42	124.26
34	e	202	LMG	O1-C7-C8	-2.05	105.96	110.90
25	h	214	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
25	i	209	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	o	608	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	A	813	CLA	C3C-C4C-NC	-2.04	108.28	110.57
25	l	611	CLA	CMD-C2D-C1D	2.04	128.32	124.71
25	m	202	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
25	B	839	CLA	CED-O2D-CGD	2.04	120.56	115.94
25	B	840	CLA	C1-C2-C3	2.04	130.06	126.75
25	n	209	CLA	C3C-C4C-NC	-2.04	108.28	110.57
32	b	202	DGD	O5D-C6D-C5D	-2.04	105.27	109.05
25	i	203	CLA	C2C-C1C-NC	-2.04	108.06	109.97
25	j	204	CLA	CMD-C2D-C1D	2.04	128.31	124.71
25	m	207	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	B	818	CLA	C3C-C4C-NC	-2.04	108.28	110.57
25	e	207	CLA	C3C-C4C-NC	-2.04	108.28	110.57
25	k	213	CLA	C3C-C4C-NC	-2.04	108.28	110.57
25	A	826	CLA	C2D-C1D-ND	2.04	111.61	110.10
25	B	838	CLA	C4-C3-C5	-2.04	111.84	115.27
25	h	212	CLA	C4-C3-C5	-2.04	111.84	115.27
29	A	839	BCR	C37-C22-C23	2.04	121.29	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	p	608	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
29	B	829	BCR	C21-C20-C19	-2.04	116.85	123.22
25	c	305	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	o	605	CLA	C3C-C4C-NC	-2.04	108.28	110.57
25	d	304	CLA	CMD-C2D-C1D	2.04	128.31	124.71
25	l	608	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	d	306	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
32	B	849	DGD	O5D-C6D-C5D	-2.04	105.27	109.05
30	d	317	DD6	O4-C34-C33	-2.04	105.75	109.80
30	k	216	DD6	O4-C34-C33	-2.04	105.75	109.80
25	f	607	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	l	610	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	c	312	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	d	304	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
25	p	602	CLA	CED-O2D-CGD	2.04	120.55	115.94
25	B	807	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	o	607	CLA	C2D-C1D-ND	2.04	111.61	110.10
25	A	849	CLA	C3C-C4C-NC	-2.04	108.29	110.57
25	p	601	CLA	C3C-C4C-NC	-2.04	108.29	110.57
35	d	308	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
25	b	209	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
25	m	210	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
30	g	216	DD6	C7-C6-C5	-2.04	120.07	122.92
30	h	216	DD6	O4-C34-C33	-2.04	105.76	109.80
25	b	205	CLA	CMD-C2D-C1D	2.04	128.30	124.71
25	c	305	CLA	C3C-C4C-NC	-2.04	108.29	110.57
25	B	845	CLA	C2D-C1D-ND	2.04	111.60	110.10
25	d	303	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	B	817	CLA	CMD-C2D-C1D	2.04	128.30	124.71
25	n	204	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
30	f	614	DD6	O4-C34-C33	-2.03	105.76	109.80
25	f	610	CLA	C3C-C4C-NC	-2.03	108.29	110.57
25	A	801	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	k	214	CLA	C1-C2-C3	2.03	130.04	126.75
30	n	212	DD6	C7-C6-C5	-2.03	120.07	122.92
25	A	833	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
25	j	203	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
25	e	213	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	B	843	CLA	CED-O2D-CGD	2.03	120.53	115.94
25	e	207	CLA	CMD-C2D-C1D	2.03	128.29	124.71
25	p	608	CLA	CBA-CAA-C2A	2.03	118.30	114.02
29	J	101	BCR	C8-C9-C10	2.03	122.06	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	811	CLA	C3C-C4C-NC	-2.03	108.29	110.57
25	B	846	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	o	605	CLA	C2D-C1D-ND	2.03	111.60	110.10
25	f	610	CLA	CHB-C1B-NB	2.03	126.41	124.26
25	d	303	CLA	CMD-C2D-C1D	2.03	128.29	124.71
25	a	204	CLA	C4D-CHA-C1A	2.03	123.72	121.25
25	p	609	CLA	C3C-C4C-NC	-2.03	108.30	110.57
25	e	205	CLA	CMD-C2D-C1D	2.03	128.29	124.71
25	B	843	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
25	B	836	CLA	C3C-C4C-NC	-2.03	108.30	110.57
25	j	207	CLA	C3C-C4C-NC	-2.03	108.30	110.57
35	d	307	CHL	C3C-C4C-NC	-2.03	108.30	110.57
25	A	806	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
30	a	214	DD6	O1-C20-C15	-2.03	57.28	58.96
25	k	203	CLA	CHB-C1B-NB	2.03	126.40	124.26
25	g	206	CLA	CHB-C1B-NB	2.03	126.40	124.26
25	o	608	CLA	CMD-C2D-C1D	2.03	128.29	124.71
25	B	843	CLA	C2D-C1D-ND	2.03	111.60	110.10
25	e	206	CLA	CED-O2D-CGD	2.03	120.52	115.94
25	A	826	CLA	C3C-C4C-NC	-2.03	108.30	110.57
25	A	827	CLA	C3C-C4C-NC	-2.03	108.30	110.57
30	g	216	DD6	C21-C20-C19	2.03	116.56	114.28
25	B	840	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
30	p	610	DD6	O1-C20-C15	-2.03	57.28	58.96
25	o	605	CLA	CED-O2D-CGD	2.03	120.52	115.94
32	b	202	DGD	C4E-C3E-C2E	2.03	114.36	110.82
25	A	830	CLA	C4-C3-C5	-2.03	111.86	115.27
35	d	307	CHL	C2C-C3C-C4C	2.03	107.93	106.49
25	c	306	CLA	CMD-C2D-C1D	2.03	128.28	124.71
25	o	606	CLA	CMD-C2D-C1D	2.03	128.28	124.71
25	A	818	CLA	C5-C3-C2	2.03	125.22	121.12
33	J	102	SQD	O5-C5-C4	2.02	113.37	109.69
30	d	319	DD6	C8-C6-C5	2.02	122.05	118.94
30	c	317	DD6	C33-C32-C31	-2.02	105.51	109.62
25	h	206	CLA	CHB-C1B-NB	2.02	126.40	124.26
25	n	210	CLA	CHB-C1B-NB	2.02	126.40	124.26
25	B	823	CLA	C2C-C1C-NC	-2.02	108.08	109.97
25	n	201	CLA	C2C-C1C-NC	-2.02	108.08	109.97
30	F	203	DD6	C20-C19-C18	2.02	116.75	112.75
25	f	607	CLA	CMD-C2D-C1D	2.02	128.28	124.71
25	n	207	CLA	CMD-C2D-C1D	2.02	128.28	124.71
25	A	815	CLA	O2D-CGD-O1D	-2.02	119.88	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	304	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
25	B	802	CLA	C12-C11-C10	-2.02	103.95	113.24
25	p	604	CLA	CMD-C2D-C1D	2.02	128.28	124.71
25	n	202	CLA	CMD-C2D-C1D	2.02	128.28	124.71
25	B	815	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	b	213	CLA	CBA-CAA-C2A	2.02	117.97	113.47
25	m	202	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	p	601	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	j	204	CLA	C2D-C1D-ND	2.02	111.59	110.10
25	k	209	CLA	C2D-C1D-ND	2.02	111.59	110.10
25	n	203	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
25	B	842	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	A	857	CLA	CED-O2D-CGD	2.02	120.50	115.94
25	b	212	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
25	p	602	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
34	e	202	LMG	O6-C1-O1	-2.02	105.19	109.97
25	k	206	CLA	CED-O2D-CGD	2.02	120.50	115.94
25	d	311	CLA	C2D-C1D-ND	2.02	111.59	110.10
25	p	601	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
25	d	301	CLA	C3C-C4C-NC	-2.02	108.31	110.57
25	B	846	CLA	CED-O2D-CGD	2.02	120.50	115.94
25	a	204	CLA	C1-C2-C3	2.02	129.53	126.04
30	o	612	DD6	C7-C6-C5	-2.02	120.10	122.92
25	A	817	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	c	315	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	f	611	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	f	603	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
29	B	801	BCR	C28-C27-C26	-2.02	110.47	114.08
25	A	848	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	e	213	CLA	C4-C3-C5	-2.02	111.88	115.27
25	n	211	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
25	A	819	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	B	848	CLA	CMD-C2D-C1D	2.02	128.27	124.71
25	o	607	CLA	CAA-C2A-C3A	-2.02	111.39	116.10
25	A	853	CLA	C3C-C4C-NC	-2.02	108.31	110.57
25	f	601	CLA	C3C-C4C-NC	-2.02	108.31	110.57
30	j	217	DD6	C7-C6-C5	-2.02	120.10	122.92
25	A	843	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
25	d	305	CLA	CMD-C2D-C1D	2.02	128.26	124.71
25	A	818	CLA	CED-O2D-CGD	2.02	120.50	115.94
25	J	103	CLA	C3C-C4C-NC	-2.02	108.31	110.57
25	k	211	CLA	CHB-C1B-NB	2.01	126.39	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	820	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
35	e	209	CHL	C2C-C3C-C4C	2.01	107.92	106.49
25	A	849	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	A	842	CLA	CMD-C2D-C1D	2.01	128.26	124.71
25	k	210	CLA	CMD-C2D-C1D	2.01	128.26	124.71
25	c	311	CLA	C3C-C4C-NC	-2.01	108.31	110.57
25	k	213	CLA	CHB-C1B-NB	2.01	126.39	124.26
30	c	318	DD6	C8-C6-C5	2.01	122.03	118.94
25	A	825	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	B	845	CLA	C3C-C4C-NC	-2.01	108.31	110.57
25	h	208	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
28	A	834	PQN	C10-C1-C2	-2.01	116.08	118.95
25	A	807	CLA	C3C-C4C-NC	-2.01	108.31	110.57
25	A	853	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
25	B	847	CLA	C1-C2-C3	2.01	130.01	126.75
25	e	208	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
25	B	822	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	p	604	CLA	CHB-C1B-NB	2.01	126.39	124.26
25	e	204	CLA	C2D-C1D-ND	2.01	111.59	110.10
25	k	211	CLA	C2D-C1D-ND	2.01	111.59	110.10
30	g	217	DD6	O4-C34-C33	-2.01	105.81	109.80
25	m	208	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
25	f	606	CLA	C3C-C4C-NC	-2.01	108.32	110.57
25	a	213	CLA	CMD-C2D-C1D	2.01	128.25	124.71
25	g	212	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
35	c	307	CHL	C3C-C4C-NC	-2.01	108.32	110.57
35	d	310	CHL	C2C-C3C-C4C	2.01	107.92	106.49
25	A	807	CLA	CMD-C2D-C1D	2.01	128.25	124.71
25	A	830	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
25	j	207	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
25	i	204	CLA	CMD-C2D-C1D	2.01	128.25	124.71
25	m	203	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
25	h	208	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	l	606	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
25	A	841	CLA	C2D-C1D-ND	2.01	111.58	110.10
25	n	204	CLA	C2D-C1D-ND	2.01	111.58	110.10
25	f	612	CLA	CMD-C2D-C1D	2.01	128.25	124.71
25	n	210	CLA	CMD-C2D-C1D	2.01	128.25	124.71
25	b	205	CLA	C3C-C4C-NC	-2.01	108.32	110.57
30	b	214	DD6	C8-C6-C5	2.01	122.02	118.94
25	a	208	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
25	g	215	CLA	O1D-CGD-CBD	-2.01	120.38	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	o	610	CLA	CED-O2D-CGD	2.01	120.47	115.94
25	d	313	CLA	C3C-C4C-NC	-2.00	108.32	110.57
25	e	216	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	l	609	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
25	i	212	CLA	C2D-C1D-ND	2.00	111.58	110.10
25	g	203	CLA	C2D-C1D-ND	2.00	111.58	110.10
25	A	827	CLA	CMD-C2D-C1D	2.00	128.25	124.71
25	B	847	CLA	CED-O2D-CGD	2.00	120.47	115.94
25	l	609	CLA	CMD-C2D-C1D	2.00	128.24	124.71
28	F	205	PQN	C17-C16-C15	-2.00	107.92	113.36
30	l	614	DD6	C4-C5-C6	-2.00	124.45	127.31
25	c	309	CLA	CMD-C2D-C1D	2.00	128.24	124.71
30	a	214	DD6	O4-C34-C33	-2.00	105.82	109.80
34	k	201	LMG	O6-C1-O1	-2.00	105.23	109.97
25	B	812	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
25	c	312	CLA	CMD-C2D-C1D	2.00	128.24	124.71
25	e	206	CLA	CMD-C2D-C1D	2.00	128.24	124.71
25	f	602	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	o	603	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	o	605	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	B	847	CLA	C2D-C1D-ND	2.00	111.58	110.10
25	o	610	CLA	C2D-C1D-ND	2.00	111.58	110.10
25	A	829	CLA	C12-C11-C10	-2.00	102.15	114.64
25	m	211	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	h	212	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
25	p	607	CLA	C2D-C1D-ND	2.00	111.58	110.10
25	g	209	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	A	811	CLA	CED-O2D-CGD	2.00	120.46	115.94
25	g	210	CLA	C4D-CHA-C1A	2.00	123.68	121.25

There are no chirality outliers.

All (2949) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CHA-CBD-CGD-O2D
25	A	802	CLA	C1-C2-C3-C4
25	A	802	CLA	C1-C2-C3-C5
25	A	806	CLA	C2B-C3B-CAB-CBB
25	A	806	CLA	C4B-C3B-CAB-CBB
25	A	808	CLA	CHA-CBD-CGD-O2D
25	A	809	CLA	C2B-C3B-CAB-CBB
25	A	809	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	809	CLA	CHA-CBD-CGD-O1D
25	A	809	CLA	CAD-CBD-CGD-O1D
25	A	809	CLA	O2A-C1-C2-C3
25	A	809	CLA	C1-C2-C3-C4
25	A	809	CLA	C1-C2-C3-C5
25	A	810	CLA	C2B-C3B-CAB-CBB
25	A	810	CLA	C4B-C3B-CAB-CBB
25	A	810	CLA	C12-C13-C15-C16
25	A	812	CLA	CHA-CBD-CGD-O2D
25	A	813	CLA	CBD-CGD-O2D-CED
25	A	814	CLA	C1A-C2A-CAA-CBA
25	A	814	CLA	C4-C3-C5-C6
25	A	815	CLA	C2B-C3B-CAB-CBB
25	A	815	CLA	C4B-C3B-CAB-CBB
25	A	815	CLA	C1-C2-C3-C4
25	A	815	CLA	C1-C2-C3-C5
25	A	816	CLA	C1A-C2A-CAA-CBA
25	A	816	CLA	C2B-C3B-CAB-CBB
25	A	816	CLA	C4B-C3B-CAB-CBB
25	A	817	CLA	C3A-C2A-CAA-CBA
25	A	818	CLA	C4B-C3B-CAB-CBB
25	A	819	CLA	C2B-C3B-CAB-CBB
25	A	819	CLA	C4B-C3B-CAB-CBB
25	A	820	CLA	C1A-C2A-CAA-CBA
25	A	821	CLA	C2B-C3B-CAB-CBB
25	A	821	CLA	C1-C2-C3-C5
25	A	822	CLA	C2B-C3B-CAB-CBB
25	A	822	CLA	C4B-C3B-CAB-CBB
25	A	822	CLA	C4-C3-C5-C6
25	A	823	CLA	C2B-C3B-CAB-CBB
25	A	823	CLA	C4B-C3B-CAB-CBB
25	A	824	CLA	C2B-C3B-CAB-CBB
25	A	824	CLA	C4B-C3B-CAB-CBB
25	A	824	CLA	C1-C2-C3-C5
25	A	826	CLA	C2-C3-C5-C6
25	A	828	CLA	C1A-C2A-CAA-CBA
25	A	828	CLA	C2B-C3B-CAB-CBB
25	A	828	CLA	C4B-C3B-CAB-CBB
25	A	828	CLA	CBD-CGD-O2D-CED
25	A	829	CLA	C1-C2-C3-C5
25	A	830	CLA	C1-C2-C3-C4
25	A	831	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	A	831	CLA	CBD-CGD-O2D-CED
25	A	832	CLA	C1-C2-C3-C4
25	A	832	CLA	C1-C2-C3-C5
25	A	833	CLA	C1-C2-C3-C4
25	A	833	CLA	C1-C2-C3-C5
25	A	833	CLA	C4-C3-C5-C6
25	A	840	CLA	C2B-C3B-CAB-CBB
25	A	840	CLA	C4B-C3B-CAB-CBB
25	A	840	CLA	C1-C2-C3-C4
25	A	842	CLA	C1A-C2A-CAA-CBA
25	A	842	CLA	C3A-C2A-CAA-CBA
25	A	842	CLA	C2B-C3B-CAB-CBB
25	A	842	CLA	C4B-C3B-CAB-CBB
25	A	843	CLA	C1-C2-C3-C4
25	A	843	CLA	C1-C2-C3-C5
25	A	843	CLA	C2-C3-C5-C6
25	A	844	CLA	C1A-C2A-CAA-CBA
25	A	844	CLA	C3A-C2A-CAA-CBA
25	A	844	CLA	C4B-C3B-CAB-CBB
25	A	844	CLA	CHA-CBD-CGD-O2D
25	A	844	CLA	C1-C2-C3-C4
25	A	844	CLA	C1-C2-C3-C5
25	A	845	CLA	C1A-C2A-CAA-CBA
25	A	845	CLA	C3A-C2A-CAA-CBA
25	A	846	CLA	C3A-C2A-CAA-CBA
25	A	846	CLA	C11-C12-C13-C14
25	A	847	CLA	C1A-C2A-CAA-CBA
25	A	847	CLA	C2B-C3B-CAB-CBB
25	A	847	CLA	C4B-C3B-CAB-CBB
25	A	848	CLA	C1-C2-C3-C5
25	A	848	CLA	C4-C3-C5-C6
25	A	849	CLA	C1A-C2A-CAA-CBA
25	A	849	CLA	C3A-C2A-CAA-CBA
25	A	849	CLA	C2B-C3B-CAB-CBB
25	A	849	CLA	C4B-C3B-CAB-CBB
25	A	850	CLA	C2B-C3B-CAB-CBB
25	A	850	CLA	C4B-C3B-CAB-CBB
25	A	851	CLA	CHA-CBD-CGD-O2D
25	B	802	CLA	CHA-CBD-CGD-O1D
25	B	803	CLA	C2B-C3B-CAB-CBB
25	B	803	CLA	C4B-C3B-CAB-CBB
25	B	803	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	803	CLA	C1-C2-C3-C5
25	B	804	CLA	C2B-C3B-CAB-CBB
25	B	804	CLA	C4B-C3B-CAB-CBB
25	B	805	CLA	C4-C3-C5-C6
25	B	805	CLA	C11-C10-C8-C9
25	B	806	CLA	C1A-C2A-CAA-CBA
25	B	807	CLA	CHA-CBD-CGD-O2D
25	B	808	CLA	C2B-C3B-CAB-CBB
25	B	808	CLA	C4B-C3B-CAB-CBB
25	B	811	CLA	C3A-C2A-CAA-CBA
25	B	813	CLA	C2B-C3B-CAB-CBB
25	B	813	CLA	C4B-C3B-CAB-CBB
25	B	814	CLA	C1A-C2A-CAA-CBA
25	B	814	CLA	C3A-C2A-CAA-CBA
25	B	814	CLA	C4-C3-C5-C6
25	B	815	CLA	C1A-C2A-CAA-CBA
25	B	815	CLA	C3A-C2A-CAA-CBA
25	B	816	CLA	C2B-C3B-CAB-CBB
25	B	816	CLA	C4B-C3B-CAB-CBB
25	B	816	CLA	O2A-C1-C2-C3
25	B	817	CLA	C2B-C3B-CAB-CBB
25	B	817	CLA	C4B-C3B-CAB-CBB
25	B	817	CLA	CHA-CBD-CGD-O1D
25	B	817	CLA	CHA-CBD-CGD-O2D
25	B	818	CLA	C1-C2-C3-C4
25	B	819	CLA	C2B-C3B-CAB-CBB
25	B	819	CLA	C4B-C3B-CAB-CBB
25	B	820	CLA	C1A-C2A-CAA-CBA
25	B	820	CLA	C3A-C2A-CAA-CBA
25	B	820	CLA	C2B-C3B-CAB-CBB
25	B	820	CLA	C4B-C3B-CAB-CBB
25	B	821	CLA	C1A-C2A-CAA-CBA
25	B	821	CLA	C2B-C3B-CAB-CBB
25	B	822	CLA	C2B-C3B-CAB-CBB
25	B	822	CLA	C4B-C3B-CAB-CBB
25	B	823	CLA	C1A-C2A-CAA-CBA
25	B	823	CLA	C1-C2-C3-C4
25	B	824	CLA	C1A-C2A-CAA-CBA
25	B	824	CLA	C2B-C3B-CAB-CBB
25	B	824	CLA	C4B-C3B-CAB-CBB
25	B	824	CLA	C1-C2-C3-C4
25	B	825	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	825	CLA	C3A-C2A-CAA-CBA
25	B	825	CLA	C2A-CAA-CBA-CGA
25	B	826	CLA	C1A-C2A-CAA-CBA
25	B	826	CLA	C3A-C2A-CAA-CBA
25	B	834	CLA	C1-C2-C3-C4
25	B	836	CLA	C2B-C3B-CAB-CBB
25	B	836	CLA	C4B-C3B-CAB-CBB
25	B	837	CLA	C2B-C3B-CAB-CBB
25	B	837	CLA	C4B-C3B-CAB-CBB
25	B	839	CLA	C1A-C2A-CAA-CBA
25	B	839	CLA	C3A-C2A-CAA-CBA
25	B	839	CLA	C1-C2-C3-C4
25	B	839	CLA	C4-C3-C5-C6
25	B	840	CLA	C1A-C2A-CAA-CBA
25	B	841	CLA	C1A-C2A-CAA-CBA
25	B	842	CLA	C2B-C3B-CAB-CBB
25	B	842	CLA	C4B-C3B-CAB-CBB
25	B	842	CLA	C1-C2-C3-C4
25	B	843	CLA	C1A-C2A-CAA-CBA
25	B	843	CLA	C3A-C2A-CAA-CBA
25	B	843	CLA	C2B-C3B-CAB-CBB
25	B	843	CLA	C4B-C3B-CAB-CBB
25	B	845	CLA	C1A-C2A-CAA-CBA
25	B	847	CLA	C1-C2-C3-C4
25	B	847	CLA	C1-C2-C3-C5
25	B	848	CLA	C1A-C2A-CAA-CBA
25	F	202	CLA	C1A-C2A-CAA-CBA
25	F	202	CLA	C3A-C2A-CAA-CBA
25	F	202	CLA	CHA-CBD-CGD-O1D
25	F	202	CLA	CHA-CBD-CGD-O2D
25	J	103	CLA	C3A-C2A-CAA-CBA
25	J	103	CLA	C2B-C3B-CAB-CBB
25	J	103	CLA	C4B-C3B-CAB-CBB
25	J	103	CLA	CHA-CBD-CGD-O1D
25	J	103	CLA	C1-C2-C3-C4
25	a	203	CLA	C1A-C2A-CAA-CBA
25	a	203	CLA	CHA-CBD-CGD-O2D
25	a	204	CLA	C1A-C2A-CAA-CBA
25	a	204	CLA	C3A-C2A-CAA-CBA
25	a	204	CLA	C2B-C3B-CAB-CBB
25	a	204	CLA	C4B-C3B-CAB-CBB
25	a	204	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	a	204	CLA	C1-C2-C3-C5
25	a	204	CLA	C4-C3-C5-C6
25	a	205	CLA	CBA-CGA-O2A-C1
25	a	205	CLA	O1A-CGA-O2A-C1
25	a	206	CLA	CHA-CBD-CGD-O2D
25	a	207	CLA	C1A-C2A-CAA-CBA
25	a	207	CLA	C3A-C2A-CAA-CBA
25	a	207	CLA	C2B-C3B-CAB-CBB
25	a	207	CLA	C4B-C3B-CAB-CBB
25	a	207	CLA	CBD-CGD-O2D-CED
25	a	208	CLA	C1A-C2A-CAA-CBA
25	a	208	CLA	C1-C2-C3-C4
25	a	208	CLA	C1-C2-C3-C5
25	a	209	CLA	C1A-C2A-CAA-CBA
25	a	209	CLA	C3A-C2A-CAA-CBA
25	a	210	CLA	C1A-C2A-CAA-CBA
25	a	210	CLA	C3A-C2A-CAA-CBA
25	a	211	CLA	C2A-CAA-CBA-CGA
25	a	212	CLA	C1A-C2A-CAA-CBA
25	a	212	CLA	CBA-CGA-O2A-C1
25	a	212	CLA	O1A-CGA-O2A-C1
25	a	212	CLA	C4-C3-C5-C6
25	a	213	CLA	CBA-CGA-O2A-C1
25	a	213	CLA	O1A-CGA-O2A-C1
25	a	213	CLA	CBD-CGD-O2D-CED
25	a	213	CLA	O1D-CGD-O2D-CED
25	a	213	CLA	C1-C2-C3-C4
25	a	213	CLA	C1-C2-C3-C5
25	a	213	CLA	C4-C3-C5-C6
25	b	204	CLA	C1A-C2A-CAA-CBA
25	b	204	CLA	C3A-C2A-CAA-CBA
25	b	204	CLA	C2B-C3B-CAB-CBB
25	b	204	CLA	C4B-C3B-CAB-CBB
25	b	204	CLA	CHA-CBD-CGD-O1D
25	b	204	CLA	CBD-CGD-O2D-CED
25	b	205	CLA	C1A-C2A-CAA-CBA
25	b	205	CLA	C3A-C2A-CAA-CBA
25	b	207	CLA	C2B-C3B-CAB-CBB
25	b	207	CLA	C4B-C3B-CAB-CBB
25	b	208	CLA	C2B-C3B-CAB-CBB
25	b	208	CLA	C4B-C3B-CAB-CBB
25	b	210	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	b	210	CLA	C2B-C3B-CAB-CBB
25	b	210	CLA	C4B-C3B-CAB-CBB
25	b	211	CLA	CHA-CBD-CGD-O2D
25	b	212	CLA	CBA-CGA-O2A-C1
25	b	212	CLA	O1A-CGA-O2A-C1
25	b	212	CLA	C1-C2-C3-C4
25	b	212	CLA	C2-C3-C5-C6
25	b	213	CLA	C1A-C2A-CAA-CBA
25	b	213	CLA	C3A-C2A-CAA-CBA
25	c	302	CLA	C1A-C2A-CAA-CBA
25	c	302	CLA	C3A-C2A-CAA-CBA
25	c	303	CLA	C1A-C2A-CAA-CBA
25	c	303	CLA	C3A-C2A-CAA-CBA
25	c	304	CLA	CBA-CGA-O2A-C1
25	c	304	CLA	O1A-CGA-O2A-C1
25	c	304	CLA	C4-C3-C5-C6
25	c	305	CLA	C2B-C3B-CAB-CBB
25	c	305	CLA	C4B-C3B-CAB-CBB
25	c	306	CLA	C1A-C2A-CAA-CBA
25	c	308	CLA	C1-C2-C3-C4
25	c	308	CLA	C1-C2-C3-C5
25	c	309	CLA	C1A-C2A-CAA-CBA
25	c	309	CLA	C3A-C2A-CAA-CBA
25	c	310	CLA	C3A-C2A-CAA-CBA
25	c	313	CLA	C1-C2-C3-C5
25	c	314	CLA	C1A-C2A-CAA-CBA
25	c	314	CLA	C3A-C2A-CAA-CBA
25	c	315	CLA	CHA-CBD-CGD-O1D
25	c	315	CLA	CHA-CBD-CGD-O2D
25	c	315	CLA	CAD-CBD-CGD-O1D
25	c	315	CLA	CAD-CBD-CGD-O2D
25	d	301	CLA	CHA-CBD-CGD-O1D
25	d	301	CLA	CAD-CBD-CGD-O1D
25	d	301	CLA	CBD-CGD-O2D-CED
25	d	304	CLA	C2B-C3B-CAB-CBB
25	d	304	CLA	C4B-C3B-CAB-CBB
25	d	304	CLA	CHA-CBD-CGD-O2D
25	d	311	CLA	C1-C2-C3-C4
25	d	312	CLA	C1A-C2A-CAA-CBA
25	d	312	CLA	C3A-C2A-CAA-CBA
25	d	313	CLA	C1A-C2A-CAA-CBA
25	d	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	d	315	CLA	C1A-C2A-CAA-CBA
25	d	315	CLA	C3A-C2A-CAA-CBA
25	d	315	CLA	CBD-CGD-O2D-CED
25	d	316	CLA	C1A-C2A-CAA-CBA
25	d	316	CLA	CBD-CGD-O2D-CED
25	e	204	CLA	C3A-C2A-CAA-CBA
25	e	205	CLA	C1A-C2A-CAA-CBA
25	e	205	CLA	C3A-C2A-CAA-CBA
25	e	205	CLA	C2B-C3B-CAB-CBB
25	e	205	CLA	C4B-C3B-CAB-CBB
25	e	205	CLA	CBD-CGD-O2D-CED
25	e	205	CLA	C1-C2-C3-C4
25	e	205	CLA	C2-C3-C5-C6
25	e	208	CLA	C1A-C2A-CAA-CBA
25	e	212	CLA	C1A-C2A-CAA-CBA
25	e	212	CLA	C3A-C2A-CAA-CBA
25	e	212	CLA	C2B-C3B-CAB-CBB
25	e	212	CLA	C4B-C3B-CAB-CBB
25	e	213	CLA	C1A-C2A-CAA-CBA
25	e	213	CLA	C3A-C2A-CAA-CBA
25	e	213	CLA	C2B-C3B-CAB-CBB
25	e	213	CLA	C4B-C3B-CAB-CBB
25	e	214	CLA	C1A-C2A-CAA-CBA
25	e	214	CLA	C3A-C2A-CAA-CBA
25	e	217	CLA	C1A-C2A-CAA-CBA
25	h	203	CLA	C1A-C2A-CAA-CBA
25	h	203	CLA	C3A-C2A-CAA-CBA
25	h	203	CLA	CHA-CBD-CGD-O2D
25	h	204	CLA	C2B-C3B-CAB-CBB
25	h	204	CLA	C4B-C3B-CAB-CBB
25	h	204	CLA	CHA-CBD-CGD-O2D
25	h	204	CLA	C1-C2-C3-C4
25	h	205	CLA	C1A-C2A-CAA-CBA
25	h	205	CLA	C3A-C2A-CAA-CBA
25	h	206	CLA	C1A-C2A-CAA-CBA
25	h	206	CLA	C3A-C2A-CAA-CBA
25	h	206	CLA	CBA-CGA-O2A-C1
25	h	206	CLA	O1A-CGA-O2A-C1
25	h	206	CLA	C1-C2-C3-C4
25	h	207	CLA	C1A-C2A-CAA-CBA
25	h	207	CLA	C3A-C2A-CAA-CBA
25	h	208	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	h	208	CLA	C3A-C2A-CAA-CBA
25	h	209	CLA	C1A-C2A-CAA-CBA
25	h	209	CLA	C1-C2-C3-C5
25	h	210	CLA	C2B-C3B-CAB-CBB
25	h	210	CLA	C4B-C3B-CAB-CBB
25	h	211	CLA	C1-C2-C3-C4
25	h	211	CLA	C1-C2-C3-C5
25	h	212	CLA	C1-C2-C3-C4
25	h	212	CLA	C4-C3-C5-C6
25	h	213	CLA	C1A-C2A-CAA-CBA
25	h	214	CLA	C1A-C2A-CAA-CBA
25	h	214	CLA	C3A-C2A-CAA-CBA
25	h	214	CLA	C2B-C3B-CAB-CBB
25	h	214	CLA	C4B-C3B-CAB-CBB
25	i	202	CLA	C1A-C2A-CAA-CBA
25	i	202	CLA	C3A-C2A-CAA-CBA
25	i	202	CLA	C2B-C3B-CAB-CBB
25	i	202	CLA	C4B-C3B-CAB-CBB
25	i	202	CLA	CBD-CGD-O2D-CED
25	i	203	CLA	C1A-C2A-CAA-CBA
25	i	203	CLA	C3A-C2A-CAA-CBA
25	i	203	CLA	O1A-CGA-O2A-C1
25	i	205	CLA	C2B-C3B-CAB-CBB
25	i	205	CLA	C4B-C3B-CAB-CBB
25	i	206	CLA	C1-C2-C3-C4
25	i	207	CLA	C2B-C3B-CAB-CBB
25	i	207	CLA	C4B-C3B-CAB-CBB
25	i	208	CLA	C3A-C2A-CAA-CBA
25	i	209	CLA	C1A-C2A-CAA-CBA
25	i	209	CLA	C3A-C2A-CAA-CBA
25	i	210	CLA	C1A-C2A-CAA-CBA
25	i	211	CLA	C11-C10-C8-C9
25	i	212	CLA	C1A-C2A-CAA-CBA
25	i	212	CLA	C3A-C2A-CAA-CBA
25	j	203	CLA	C1A-C2A-CAA-CBA
25	j	203	CLA	C2B-C3B-CAB-CBB
25	j	203	CLA	C4B-C3B-CAB-CBB
25	j	203	CLA	CBD-CGD-O2D-CED
25	j	203	CLA	C1-C2-C3-C5
25	j	204	CLA	C4B-C3B-CAB-CBB
25	j	206	CLA	CBD-CGD-O2D-CED
25	j	206	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	j	207	CLA	C1A-C2A-CAA-CBA
25	j	207	CLA	CBA-CGA-O2A-C1
25	j	208	CLA	C1-C2-C3-C4
25	j	208	CLA	C1-C2-C3-C5
25	j	209	CLA	C3A-C2A-CAA-CBA
25	j	209	CLA	C2B-C3B-CAB-CBB
25	j	209	CLA	C4B-C3B-CAB-CBB
25	j	209	CLA	C4-C3-C5-C6
25	j	209	CLA	C11-C10-C8-C9
25	j	210	CLA	C1A-C2A-CAA-CBA
25	j	210	CLA	C2B-C3B-CAB-CBB
25	j	210	CLA	C4B-C3B-CAB-CBB
25	j	210	CLA	C1-C2-C3-C5
25	j	211	CLA	C1-C2-C3-C4
25	j	211	CLA	C1-C2-C3-C5
25	j	212	CLA	C1-C2-C3-C5
25	j	213	CLA	C2B-C3B-CAB-CBB
25	j	213	CLA	C4B-C3B-CAB-CBB
25	j	214	CLA	C1A-C2A-CAA-CBA
25	j	214	CLA	C3A-C2A-CAA-CBA
25	j	214	CLA	C2B-C3B-CAB-CBB
25	j	214	CLA	C4B-C3B-CAB-CBB
25	j	215	CLA	C1A-C2A-CAA-CBA
25	j	215	CLA	C3A-C2A-CAA-CBA
25	j	215	CLA	C1-C2-C3-C5
25	k	202	CLA	C1A-C2A-CAA-CBA
25	k	203	CLA	C1A-C2A-CAA-CBA
25	k	203	CLA	C3A-C2A-CAA-CBA
25	k	203	CLA	C2B-C3B-CAB-CBB
25	k	203	CLA	C4B-C3B-CAB-CBB
25	k	203	CLA	C1-C2-C3-C4
25	k	203	CLA	C1-C2-C3-C5
25	k	204	CLA	C1A-C2A-CAA-CBA
25	k	204	CLA	C3A-C2A-CAA-CBA
25	k	205	CLA	C1A-C2A-CAA-CBA
25	k	205	CLA	C1-C2-C3-C5
25	k	205	CLA	C11-C10-C8-C9
25	k	208	CLA	C3A-C2A-CAA-CBA
25	k	209	CLA	C1A-C2A-CAA-CBA
25	k	209	CLA	C3A-C2A-CAA-CBA
25	k	209	CLA	CHA-CBD-CGD-O1D
25	k	211	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	k	211	CLA	C2-C3-C5-C6
25	k	211	CLA	C4-C3-C5-C6
25	k	212	CLA	C1A-C2A-CAA-CBA
25	k	212	CLA	CBD-CGD-O2D-CED
25	k	212	CLA	O1D-CGD-O2D-CED
25	k	213	CLA	C1A-C2A-CAA-CBA
25	k	213	CLA	C2B-C3B-CAB-CBB
25	k	213	CLA	C4B-C3B-CAB-CBB
25	l	601	CLA	C1A-C2A-CAA-CBA
25	l	602	CLA	C1A-C2A-CAA-CBA
25	l	602	CLA	C3A-C2A-CAA-CBA
25	l	602	CLA	C1-C2-C3-C4
25	l	602	CLA	C1-C2-C3-C5
25	l	602	CLA	C2-C3-C5-C6
25	l	604	CLA	CHA-CBD-CGD-O1D
25	l	605	CLA	C1A-C2A-CAA-CBA
25	l	605	CLA	C2A-CAA-CBA-CGA
25	l	605	CLA	C2B-C3B-CAB-CBB
25	l	605	CLA	C4B-C3B-CAB-CBB
25	l	606	CLA	C1A-C2A-CAA-CBA
25	l	606	CLA	C1-C2-C3-C4
25	l	607	CLA	C3A-C2A-CAA-CBA
25	l	607	CLA	C2B-C3B-CAB-CBB
25	l	607	CLA	C4B-C3B-CAB-CBB
25	l	607	CLA	C2-C3-C5-C6
25	l	611	CLA	C3A-C2A-CAA-CBA
25	l	611	CLA	CBD-CGD-O2D-CED
25	l	612	CLA	C1A-C2A-CAA-CBA
25	l	612	CLA	C3A-C2A-CAA-CBA
25	l	612	CLA	CHA-CBD-CGD-O1D
25	m	202	CLA	C1A-C2A-CAA-CBA
25	m	202	CLA	C3A-C2A-CAA-CBA
25	m	202	CLA	CBD-CGD-O2D-CED
25	m	203	CLA	C1A-C2A-CAA-CBA
25	m	203	CLA	C1-C2-C3-C4
25	m	203	CLA	C1-C2-C3-C5
25	m	203	CLA	C4-C3-C5-C6
25	m	206	CLA	C2B-C3B-CAB-CBB
25	m	206	CLA	C4B-C3B-CAB-CBB
25	m	207	CLA	C1-C2-C3-C4
25	m	207	CLA	C1-C2-C3-C5
25	m	208	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	m	208	CLA	C2B-C3B-CAB-CBB
25	m	208	CLA	C4B-C3B-CAB-CBB
25	m	209	CLA	C1A-C2A-CAA-CBA
25	m	209	CLA	C3A-C2A-CAA-CBA
25	m	211	CLA	C3A-C2A-CAA-CBA
25	f	601	CLA	C1A-C2A-CAA-CBA
25	f	601	CLA	C2B-C3B-CAB-CBB
25	f	601	CLA	C4B-C3B-CAB-CBB
25	f	601	CLA	CBD-CGD-O2D-CED
25	f	601	CLA	O1D-CGD-O2D-CED
25	f	602	CLA	C1A-C2A-CAA-CBA
25	f	602	CLA	C3A-C2A-CAA-CBA
25	f	604	CLA	C1A-C2A-CAA-CBA
25	f	604	CLA	C3A-C2A-CAA-CBA
25	f	604	CLA	CHA-CBD-CGD-O2D
25	f	605	CLA	CBD-CGD-O2D-CED
25	f	605	CLA	O1D-CGD-O2D-CED
25	f	606	CLA	C1A-C2A-CAA-CBA
25	f	606	CLA	C3A-C2A-CAA-CBA
25	f	606	CLA	CBD-CGD-O2D-CED
25	f	607	CLA	CHA-CBD-CGD-O1D
25	f	607	CLA	CBD-CGD-O2D-CED
25	f	607	CLA	C2-C3-C5-C6
25	f	607	CLA	C4-C3-C5-C6
25	f	608	CLA	C3A-C2A-CAA-CBA
25	f	609	CLA	C1A-C2A-CAA-CBA
25	f	609	CLA	C3A-C2A-CAA-CBA
25	f	609	CLA	CBD-CGD-O2D-CED
25	f	611	CLA	C1A-C2A-CAA-CBA
25	f	611	CLA	CBD-CGD-O2D-CED
25	f	612	CLA	C1A-C2A-CAA-CBA
25	f	612	CLA	C3A-C2A-CAA-CBA
25	f	612	CLA	C2B-C3B-CAB-CBB
25	f	612	CLA	C4B-C3B-CAB-CBB
25	f	612	CLA	CHA-CBD-CGD-O1D
25	f	612	CLA	CAD-CBD-CGD-O1D
25	g	203	CLA	C1A-C2A-CAA-CBA
25	g	203	CLA	C3A-C2A-CAA-CBA
25	g	203	CLA	C2B-C3B-CAB-CBB
25	g	203	CLA	C4B-C3B-CAB-CBB
25	g	203	CLA	CHA-CBD-CGD-O2D
25	g	204	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	g	204	CLA	C2B-C3B-CAB-CBB
25	g	204	CLA	C4B-C3B-CAB-CBB
25	g	204	CLA	CBD-CGD-O2D-CED
25	g	204	CLA	C2-C3-C5-C6
25	g	205	CLA	C1A-C2A-CAA-CBA
25	g	205	CLA	C3A-C2A-CAA-CBA
25	g	206	CLA	CBD-CGD-O2D-CED
25	g	207	CLA	C1A-C2A-CAA-CBA
25	g	207	CLA	C3A-C2A-CAA-CBA
25	g	207	CLA	C2A-CAA-CBA-CGA
25	g	209	CLA	C3A-C2A-CAA-CBA
25	g	209	CLA	C2B-C3B-CAB-CBB
25	g	209	CLA	C4B-C3B-CAB-CBB
25	g	210	CLA	C3A-C2A-CAA-CBA
25	g	211	CLA	CBD-CGD-O2D-CED
25	g	212	CLA	C1-C2-C3-C4
25	g	212	CLA	C1-C2-C3-C5
25	g	212	CLA	C2-C3-C5-C6
25	g	213	CLA	C1A-C2A-CAA-CBA
25	g	215	CLA	C1A-C2A-CAA-CBA
25	g	215	CLA	C2B-C3B-CAB-CBB
25	g	215	CLA	C4B-C3B-CAB-CBB
25	n	201	CLA	C1A-C2A-CAA-CBA
25	n	201	CLA	C3A-C2A-CAA-CBA
25	n	201	CLA	C1-C2-C3-C5
25	n	202	CLA	C4-C3-C5-C6
25	n	203	CLA	CHA-CBD-CGD-O1D
25	n	203	CLA	CHA-CBD-CGD-O2D
25	n	204	CLA	C1A-C2A-CAA-CBA
25	n	204	CLA	C3A-C2A-CAA-CBA
25	n	205	CLA	C1A-C2A-CAA-CBA
25	n	205	CLA	C3A-C2A-CAA-CBA
25	n	205	CLA	C2B-C3B-CAB-CBB
25	n	205	CLA	C4B-C3B-CAB-CBB
25	n	206	CLA	C1A-C2A-CAA-CBA
25	n	206	CLA	C3A-C2A-CAA-CBA
25	n	208	CLA	C2B-C3B-CAB-CBB
25	n	208	CLA	C4B-C3B-CAB-CBB
25	n	209	CLA	C2B-C3B-CAB-CBB
25	n	209	CLA	C4B-C3B-CAB-CBB
25	n	210	CLA	C1A-C2A-CAA-CBA
25	n	210	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	n	211	CLA	C1A-C2A-CAA-CBA
25	n	211	CLA	C3A-C2A-CAA-CBA
25	o	601	CLA	CBD-CGD-O2D-CED
25	o	602	CLA	C1A-C2A-CAA-CBA
25	o	602	CLA	C3A-C2A-CAA-CBA
25	o	602	CLA	C2B-C3B-CAB-CBB
25	o	602	CLA	C4B-C3B-CAB-CBB
25	o	602	CLA	CHA-CBD-CGD-O1D
25	o	602	CLA	CBD-CGD-O2D-CED
25	o	604	CLA	C1A-C2A-CAA-CBA
25	o	604	CLA	C3A-C2A-CAA-CBA
25	o	605	CLA	C2A-CAA-CBA-CGA
25	o	605	CLA	C2B-C3B-CAB-CBB
25	o	605	CLA	C4B-C3B-CAB-CBB
25	o	606	CLA	C1A-C2A-CAA-CBA
25	o	606	CLA	C3A-C2A-CAA-CBA
25	o	607	CLA	C2B-C3B-CAB-CBB
25	o	607	CLA	C4B-C3B-CAB-CBB
25	o	609	CLA	C1A-C2A-CAA-CBA
25	o	609	CLA	C3A-C2A-CAA-CBA
25	o	609	CLA	CHA-CBD-CGD-O1D
25	o	609	CLA	CHA-CBD-CGD-O2D
25	o	609	CLA	CAD-CBD-CGD-O1D
25	o	609	CLA	CAD-CBD-CGD-O2D
25	o	609	CLA	CBD-CGD-O2D-CED
25	p	602	CLA	C1A-C2A-CAA-CBA
25	p	602	CLA	C3A-C2A-CAA-CBA
25	p	603	CLA	CBD-CGD-O2D-CED
25	p	603	CLA	O1D-CGD-O2D-CED
25	p	605	CLA	C2B-C3B-CAB-CBB
25	p	605	CLA	C4B-C3B-CAB-CBB
25	p	606	CLA	C1A-C2A-CAA-CBA
25	p	606	CLA	C3A-C2A-CAA-CBA
25	p	606	CLA	CBD-CGD-O2D-CED
25	p	606	CLA	O1D-CGD-O2D-CED
25	p	606	CLA	C1-C2-C3-C5
25	p	607	CLA	C1A-C2A-CAA-CBA
25	p	607	CLA	C3A-C2A-CAA-CBA
25	p	607	CLA	C2B-C3B-CAB-CBB
25	p	607	CLA	C4B-C3B-CAB-CBB
25	p	607	CLA	CBD-CGD-O2D-CED
25	p	608	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	p	609	CLA	C1A-C2A-CAA-CBA
25	p	609	CLA	C3A-C2A-CAA-CBA
25	p	609	CLA	CBD-CGD-O2D-CED
26	A	803	LMT	C2-C1-O1'-C1'
27	a	201	LHG	C4-O6-P-O5
27	b	201	LHG	C3-O3-P-O5
27	b	201	LHG	C4-O6-P-O3
27	b	201	LHG	C4-O6-P-O5
27	b	201	LHG	C8-C7-O7-C5
27	c	301	LHG	C1-C2-C3-O3
27	d	302	LHG	C8-C7-O7-C5
27	h	201	LHG	O2-C2-C3-O3
27	h	201	LHG	C3-O3-P-O5
27	h	201	LHG	C4-O6-P-O3
27	h	201	LHG	C4-O6-P-O5
27	h	202	LHG	C1-C2-C3-O3
27	h	202	LHG	C8-C7-O7-C5
27	i	201	LHG	C3-O3-P-O4
27	j	202	LHG	O2-C2-C3-O3
27	j	202	LHG	C4-O6-P-O5
27	m	201	LHG	O9-C7-O7-C5
27	g	201	LHG	C3-O3-P-O5
27	g	201	LHG	C4-O6-P-O3
27	g	201	LHG	C8-C7-O7-C5
28	B	835	PQN	C12-C13-C15-C16
28	B	835	PQN	C14-C13-C15-C16
28	F	205	PQN	C16-C17-C18-C19
29	A	836	BCR	C17-C18-C19-C20
29	A	836	BCR	C36-C18-C19-C20
29	A	837	BCR	C6-C7-C8-C9
29	A	837	BCR	C7-C8-C9-C10
29	A	837	BCR	C7-C8-C9-C34
29	A	837	BCR	C12-C13-C14-C15
29	A	837	BCR	C35-C13-C14-C15
29	A	837	BCR	C14-C15-C16-C17
29	A	838	BCR	C23-C24-C25-C26
29	A	839	BCR	C7-C8-C9-C10
29	A	839	BCR	C7-C8-C9-C34
29	A	839	BCR	C21-C22-C23-C24
29	A	839	BCR	C37-C22-C23-C24
29	B	801	BCR	C23-C24-C25-C26
29	B	828	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	B	828	BCR	C7-C8-C9-C34
29	B	831	BCR	C11-C10-C9-C8
29	B	831	BCR	C11-C10-C9-C34
29	B	831	BCR	C10-C11-C12-C13
29	B	831	BCR	C36-C18-C19-C20
29	B	831	BCR	C18-C19-C20-C21
29	B	832	BCR	C11-C10-C9-C8
29	B	832	BCR	C11-C10-C9-C34
29	B	832	BCR	C10-C11-C12-C13
29	B	832	BCR	C21-C22-C23-C24
29	B	832	BCR	C37-C22-C23-C24
29	B	832	BCR	C22-C23-C24-C25
29	B	833	BCR	C37-C22-C23-C24
29	B	833	BCR	C23-C24-C25-C26
29	J	101	BCR	C7-C8-C9-C34
29	J	101	BCR	C11-C10-C9-C8
29	J	101	BCR	C11-C10-C9-C34
29	J	101	BCR	C11-C12-C13-C35
29	J	101	BCR	C12-C13-C14-C15
29	J	101	BCR	C35-C13-C14-C15
29	J	101	BCR	C16-C17-C18-C19
29	J	101	BCR	C16-C17-C18-C36
29	M	201	BCR	C21-C22-C23-C24
29	M	201	BCR	C37-C22-C23-C24
29	M	201	BCR	C23-C24-C25-C26
30	A	854	DD6	C13-C14-C15-O1
30	A	855	DD6	C13-C14-C15-O1
30	A	855	DD6	C24-C25-C26-C27
30	A	855	DD6	C5-C6-C8-C9
30	A	855	DD6	C7-C6-C8-C9
30	F	203	DD6	C-C1-C2-C3
30	F	203	DD6	C24-C1-C2-C3
30	F	203	DD6	C-C1-C24-C25
30	F	203	DD6	C2-C1-C24-C25
30	F	203	DD6	C25-C26-C27-C29
30	F	203	DD6	C2-C3-C4-C5
30	F	203	DD6	C5-C6-C8-C9
30	F	203	DD6	C7-C6-C8-C9
30	J	104	DD6	C13-C14-C15-O1
30	J	105	DD6	C10-C11-C13-C14
30	J	105	DD6	C12-C11-C13-C14
30	J	105	DD6	C1-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	J	105	DD6	C25-C26-C27-C29
30	a	214	DD6	C-C1-C24-C25
30	a	214	DD6	C2-C1-C24-C25
30	a	214	DD6	C10-C11-C13-C14
30	a	214	DD6	C12-C11-C13-C14
30	c	316	DD6	C-C1-C24-C25
30	c	316	DD6	C2-C1-C24-C25
30	c	318	DD6	C-C1-C24-C25
30	c	318	DD6	C2-C1-C24-C25
30	d	317	DD6	C-C1-C24-C25
30	d	317	DD6	C2-C1-C24-C25
30	d	318	DD6	C10-C11-C13-C14
30	d	318	DD6	C12-C11-C13-C14
30	d	319	DD6	C10-C11-C13-C14
30	d	319	DD6	C13-C14-C15-O1
30	e	218	DD6	C9-C10-C11-C12
30	e	218	DD6	C9-C10-C11-C13
30	e	218	DD6	C25-C26-C27-C29
30	e	219	DD6	C-C1-C24-C25
30	e	219	DD6	C2-C1-C24-C25
30	e	219	DD6	C10-C11-C13-C14
30	e	219	DD6	C12-C11-C13-C14
30	e	220	DD6	C11-C13-C14-C15
30	e	220	DD6	C24-C25-C26-C27
30	e	220	DD6	C25-C26-C27-C28
30	e	220	DD6	C25-C26-C27-C29
30	h	216	DD6	C-C1-C24-C25
30	h	216	DD6	C2-C1-C24-C25
30	i	214	DD6	C-C1-C24-C25
30	i	214	DD6	C2-C1-C24-C25
30	i	215	DD6	C-C1-C24-C25
30	i	215	DD6	C2-C1-C24-C25
30	j	216	DD6	C-C1-C24-C25
30	j	216	DD6	C2-C1-C24-C25
30	j	217	DD6	C-C1-C24-C25
30	j	217	DD6	C2-C1-C24-C25
30	j	217	DD6	C24-C25-C26-C27
30	k	215	DD6	C-C1-C24-C25
30	k	216	DD6	C-C1-C24-C25
30	k	216	DD6	C2-C1-C24-C25
30	l	613	DD6	C10-C11-C13-C14
30	l	613	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
30	l	614	DD6	C-C1-C24-C25
30	l	614	DD6	C2-C1-C24-C25
30	m	212	DD6	C10-C11-C13-C14
30	m	212	DD6	C12-C11-C13-C14
30	m	213	DD6	C-C1-C24-C25
30	m	213	DD6	C2-C1-C24-C25
30	m	213	DD6	C10-C11-C13-C14
30	m	213	DD6	C12-C11-C13-C14
30	f	613	DD6	C-C1-C24-C25
30	f	613	DD6	C10-C11-C13-C14
30	f	613	DD6	C12-C11-C13-C14
30	f	614	DD6	C-C1-C24-C25
30	f	614	DD6	C2-C1-C24-C25
30	f	614	DD6	C10-C11-C13-C14
30	f	614	DD6	C12-C11-C13-C14
30	f	614	DD6	C13-C14-C15-C20
30	f	614	DD6	C13-C14-C15-O1
30	n	212	DD6	C13-C14-C15-O1
30	n	213	DD6	C12-C11-C13-C14
30	n	213	DD6	C11-C13-C14-C15
30	n	213	DD6	C1-C24-C25-C26
30	n	213	DD6	C25-C26-C27-C28
30	n	213	DD6	C25-C26-C27-C29
30	n	213	DD6	C3-C4-C5-C6
30	n	214	DD6	C1-C24-C25-C26
30	n	214	DD6	C3-C4-C5-C6
30	o	611	DD6	C-C1-C24-C25
30	o	611	DD6	C2-C1-C24-C25
30	o	611	DD6	C10-C11-C13-C14
30	o	611	DD6	C12-C11-C13-C14
30	o	612	DD6	C-C1-C24-C25
30	o	612	DD6	C2-C1-C24-C25
30	o	612	DD6	C24-C25-C26-C27
30	p	610	DD6	C-C1-C24-C25
30	p	610	DD6	C2-C1-C24-C25
32	b	202	DGD	O1B-C1B-O2G-C2G
32	b	202	DGD	O1G-C1G-C2G-O2G
32	b	202	DGD	C2D-C1D-O3G-C3G
32	b	202	DGD	O6D-C1D-O3G-C3G
33	F	204	SQD	C2-C1-O6-C44
33	F	204	SQD	O5-C1-O6-C44
33	F	204	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
33	F	204	SQD	C8-C7-O47-C45
33	F	204	SQD	C5-C6-S-O7
33	F	204	SQD	C5-C6-S-O8
33	F	204	SQD	C5-C6-S-O9
33	J	102	SQD	O5-C5-C6-S
33	J	102	SQD	C5-C6-S-O7
33	J	102	SQD	C5-C6-S-O8
33	J	102	SQD	C5-C6-S-O9
33	g	202	SQD	C2-C1-O6-C44
33	g	202	SQD	O5-C1-O6-C44
33	g	202	SQD	O47-C45-C46-O48
33	g	202	SQD	O5-C5-C6-S
34	a	202	LMG	O9-C10-O7-C8
34	a	202	LMG	C11-C10-O7-C8
34	j	201	LMG	C2-C1-O1-C7
34	j	201	LMG	O6-C1-O1-C7
35	c	307	CHL	C3C-C2C-CMC-OMC
35	d	307	CHL	C1A-C2A-CAA-CBA
35	d	307	CHL	C3A-C2A-CAA-CBA
35	d	307	CHL	C3C-C2C-CMC-OMC
35	d	307	CHL	O2A-C1-C2-C3
35	d	308	CHL	C1A-C2A-CAA-CBA
35	d	308	CHL	C2B-C3B-CAB-CBB
35	d	308	CHL	C4B-C3B-CAB-CBB
35	d	309	CHL	C1A-C2A-CAA-CBA
35	d	309	CHL	C3A-C2A-CAA-CBA
35	d	310	CHL	C1A-C2A-CAA-CBA
35	d	310	CHL	C2B-C3B-CAB-CBB
35	d	310	CHL	C4B-C3B-CAB-CBB
35	e	209	CHL	C2B-C3B-CAB-CBB
35	e	209	CHL	C4B-C3B-CAB-CBB
25	e	210	CLA	O1D-CGD-O2D-CED
25	o	610	CLA	O1D-CGD-O2D-CED
25	p	607	CLA	O1D-CGD-O2D-CED
25	A	813	CLA	O1D-CGD-O2D-CED
25	b	203	CLA	O1D-CGD-O2D-CED
25	l	611	CLA	O1D-CGD-O2D-CED
25	g	206	CLA	O1D-CGD-O2D-CED
25	n	210	CLA	O1D-CGD-O2D-CED
25	A	820	CLA	CBD-CGD-O2D-CED
25	B	812	CLA	CBD-CGD-O2D-CED
25	B	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	840	CLA	CBD-CGD-O2D-CED
25	B	842	CLA	CBD-CGD-O2D-CED
25	b	203	CLA	CBD-CGD-O2D-CED
25	c	302	CLA	CBD-CGD-O2D-CED
25	c	308	CLA	CBD-CGD-O2D-CED
25	c	314	CLA	CBD-CGD-O2D-CED
25	d	305	CLA	CBD-CGD-O2D-CED
25	e	210	CLA	CBD-CGD-O2D-CED
25	e	217	CLA	CBD-CGD-O2D-CED
25	k	213	CLA	CBD-CGD-O2D-CED
25	l	602	CLA	CBD-CGD-O2D-CED
25	l	609	CLA	CBD-CGD-O2D-CED
25	l	610	CLA	CBD-CGD-O2D-CED
25	l	612	CLA	CBD-CGD-O2D-CED
25	m	203	CLA	CBD-CGD-O2D-CED
25	m	205	CLA	CBD-CGD-O2D-CED
25	m	211	CLA	CBD-CGD-O2D-CED
25	n	204	CLA	CBD-CGD-O2D-CED
25	n	207	CLA	CBD-CGD-O2D-CED
25	o	610	CLA	CBD-CGD-O2D-CED
25	p	602	CLA	CBD-CGD-O2D-CED
25	p	605	CLA	CBD-CGD-O2D-CED
35	d	310	CHL	CBD-CGD-O2D-CED
25	B	824	CLA	O1A-CGA-O2A-C1
25	B	834	CLA	O1A-CGA-O2A-C1
25	c	303	CLA	O1A-CGA-O2A-C1
25	h	207	CLA	O1A-CGA-O2A-C1
25	j	207	CLA	O1A-CGA-O2A-C1
25	f	602	CLA	O1A-CGA-O2A-C1
25	a	207	CLA	O1D-CGD-O2D-CED
25	l	612	CLA	O1D-CGD-O2D-CED
25	A	827	CLA	O1D-CGD-O2D-CED
25	h	203	CLA	O1D-CGD-O2D-CED
25	m	202	CLA	O1D-CGD-O2D-CED
25	f	609	CLA	O1D-CGD-O2D-CED
25	g	211	CLA	O1D-CGD-O2D-CED
25	n	204	CLA	O1D-CGD-O2D-CED
25	n	207	CLA	O1D-CGD-O2D-CED
25	o	601	CLA	O1D-CGD-O2D-CED
25	p	609	CLA	O1D-CGD-O2D-CED
25	A	810	CLA	CBA-CGA-O2A-C1
25	a	207	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	i	203	CLA	CBA-CGA-O2A-C1
25	f	602	CLA	CBA-CGA-O2A-C1
25	A	806	CLA	CBD-CGD-O2D-CED
25	A	827	CLA	CBD-CGD-O2D-CED
25	A	832	CLA	CBD-CGD-O2D-CED
25	A	848	CLA	CBD-CGD-O2D-CED
25	B	822	CLA	CBD-CGD-O2D-CED
25	B	836	CLA	CBD-CGD-O2D-CED
25	a	204	CLA	CBD-CGD-O2D-CED
25	e	201	CLA	CBD-CGD-O2D-CED
25	j	212	CLA	CBD-CGD-O2D-CED
25	f	612	CLA	CBD-CGD-O2D-CED
25	n	202	CLA	CBD-CGD-O2D-CED
25	n	205	CLA	CBD-CGD-O2D-CED
25	p	604	CLA	CBD-CGD-O2D-CED
25	A	809	CLA	O1A-CGA-O2A-C1
25	A	810	CLA	O1A-CGA-O2A-C1
25	A	848	CLA	O1A-CGA-O2A-C1
25	A	853	CLA	O1A-CGA-O2A-C1
25	A	857	CLA	O1A-CGA-O2A-C1
25	B	804	CLA	O1A-CGA-O2A-C1
25	B	818	CLA	O1A-CGA-O2A-C1
25	a	207	CLA	O1A-CGA-O2A-C1
25	j	215	CLA	O1A-CGA-O2A-C1
25	k	214	CLA	O1A-CGA-O2A-C1
25	f	607	CLA	O1A-CGA-O2A-C1
25	o	602	CLA	O1A-CGA-O2A-C1
27	b	201	LHG	O10-C23-O8-C6
27	c	301	LHG	O10-C23-O8-C6
27	m	201	LHG	O10-C23-O8-C6
27	g	201	LHG	O10-C23-O8-C6
34	a	202	LMG	O10-C28-O8-C9
25	c	308	CLA	O1D-CGD-O2D-CED
25	d	315	CLA	O1D-CGD-O2D-CED
25	A	846	CLA	C15-C16-C17-C18
25	f	612	CLA	C2A-CAA-CBA-CGA
25	c	312	CLA	CBD-CGD-O2D-CED
25	g	213	CLA	CBD-CGD-O2D-CED
25	n	211	CLA	CBD-CGD-O2D-CED
25	p	608	CLA	CBD-CGD-O2D-CED
25	e	201	CLA	O1D-CGD-O2D-CED
25	m	211	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	d	302	LHG	O9-C7-O7-C5
27	h	201	LHG	O9-C7-O7-C5
27	h	202	LHG	O9-C7-O7-C5
27	g	201	LHG	O9-C7-O7-C5
32	e	203	DGD	O1B-C1B-O2G-C2G
33	F	204	SQD	O49-C7-O47-C45
25	d	312	CLA	C3-C5-C6-C7
25	j	209	CLA	C3-C5-C6-C7
25	k	208	CLA	C3-C5-C6-C7
25	g	209	CLA	C3-C5-C6-C7
28	F	205	PQN	C13-C15-C16-C17
25	A	809	CLA	CBA-CGA-O2A-C1
25	A	846	CLA	CBA-CGA-O2A-C1
25	A	848	CLA	CBA-CGA-O2A-C1
25	A	857	CLA	CBA-CGA-O2A-C1
25	B	811	CLA	CBA-CGA-O2A-C1
25	B	834	CLA	CBA-CGA-O2A-C1
25	c	303	CLA	CBA-CGA-O2A-C1
25	j	215	CLA	CBA-CGA-O2A-C1
27	c	301	LHG	C24-C23-O8-C6
27	g	201	LHG	C24-C23-O8-C6
34	a	202	LMG	C29-C28-O8-C9
27	h	201	LHG	C8-C7-O7-C5
27	m	201	LHG	C8-C7-O7-C5
32	b	202	DGD	C2B-C1B-O2G-C2G
32	e	203	DGD	C2B-C1B-O2G-C2G
25	o	609	CLA	O1D-CGD-O2D-CED
25	d	314	CLA	CBD-CGD-O2D-CED
25	f	610	CLA	CBD-CGD-O2D-CED
25	A	804	CLA	C4-C3-C5-C6
25	a	209	CLA	C4-C3-C5-C6
25	b	204	CLA	C4-C3-C5-C6
25	h	204	CLA	C4-C3-C5-C6
25	A	824	CLA	C2-C3-C5-C6
25	a	209	CLA	C2-C3-C5-C6
25	h	204	CLA	C2-C3-C5-C6
25	k	208	CLA	C2-C3-C5-C6
25	A	817	CLA	CBD-CGD-O2D-CED
35	d	308	CHL	CBD-CGD-O2D-CED
25	A	812	CLA	C2A-CAA-CBA-CGA
25	A	825	CLA	C2A-CAA-CBA-CGA
25	a	207	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	c	309	CLA	C2A-CAA-CBA-CGA
25	h	208	CLA	C2A-CAA-CBA-CGA
25	h	209	CLA	C2A-CAA-CBA-CGA
25	i	213	CLA	C2A-CAA-CBA-CGA
25	j	206	CLA	C2A-CAA-CBA-CGA
25	k	208	CLA	C2A-CAA-CBA-CGA
25	l	607	CLA	C2A-CAA-CBA-CGA
25	m	204	CLA	C2A-CAA-CBA-CGA
25	f	602	CLA	C2A-CAA-CBA-CGA
35	e	209	CHL	C2A-CAA-CBA-CGA
25	j	208	CLA	O1A-CGA-O2A-C1
25	A	821	CLA	C3-C5-C6-C7
25	A	853	CLA	C3-C5-C6-C7
25	B	807	CLA	C3-C5-C6-C7
25	k	203	CLA	C3-C5-C6-C7
25	n	202	CLA	C3-C5-C6-C7
28	B	827	PQN	C13-C15-C16-C17
25	c	306	CLA	C2A-CAA-CBA-CGA
25	j	214	CLA	C2A-CAA-CBA-CGA
25	o	610	CLA	C2A-CAA-CBA-CGA
25	p	609	CLA	C2A-CAA-CBA-CGA
25	A	802	CLA	CBA-CGA-O2A-C1
25	A	853	CLA	CBA-CGA-O2A-C1
25	B	804	CLA	CBA-CGA-O2A-C1
25	B	818	CLA	CBA-CGA-O2A-C1
25	B	824	CLA	CBA-CGA-O2A-C1
25	B	838	CLA	CBA-CGA-O2A-C1
25	d	312	CLA	CBA-CGA-O2A-C1
25	h	207	CLA	CBA-CGA-O2A-C1
25	i	206	CLA	CBA-CGA-O2A-C1
25	j	208	CLA	CBA-CGA-O2A-C1
25	k	205	CLA	CBA-CGA-O2A-C1
25	k	211	CLA	CBA-CGA-O2A-C1
25	f	607	CLA	CBA-CGA-O2A-C1
25	o	602	CLA	CBA-CGA-O2A-C1
25	p	606	CLA	CBA-CGA-O2A-C1
27	b	201	LHG	C24-C23-O8-C6
27	m	201	LHG	C24-C23-O8-C6
34	k	201	LMG	C29-C28-O8-C9
25	A	814	CLA	C1-C2-C3-C5
25	A	840	CLA	C1-C2-C3-C5
25	B	823	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
25	B	824	CLA	C1-C2-C3-C5
25	B	842	CLA	C1-C2-C3-C5
25	b	212	CLA	C1-C2-C3-C5
25	d	306	CLA	C1-C2-C3-C5
25	h	204	CLA	C1-C2-C3-C5
25	h	206	CLA	C1-C2-C3-C5
25	h	212	CLA	C1-C2-C3-C5
25	B	803	CLA	O1D-CGD-O2D-CED
25	B	837	CLA	O1D-CGD-O2D-CED
25	d	305	CLA	O1D-CGD-O2D-CED
25	l	610	CLA	O1D-CGD-O2D-CED
25	f	606	CLA	O1D-CGD-O2D-CED
35	d	308	CHL	O1D-CGD-O2D-CED
27	b	201	LHG	O9-C7-O7-C5
25	A	802	CLA	O1A-CGA-O2A-C1
25	A	844	CLA	O1A-CGA-O2A-C1
25	B	811	CLA	O1A-CGA-O2A-C1
25	c	310	CLA	O1A-CGA-O2A-C1
25	d	312	CLA	O1A-CGA-O2A-C1
25	k	203	CLA	O1A-CGA-O2A-C1
25	p	606	CLA	O1A-CGA-O2A-C1
30	A	855	DD6	C11-C10-C9-C8
30	n	213	DD6	C1-C2-C3-C4
30	p	610	DD6	C24-C25-C26-C27
25	A	812	CLA	CBD-CGD-O2D-CED
25	A	829	CLA	CBD-CGD-O2D-CED
25	A	833	CLA	CBD-CGD-O2D-CED
25	B	805	CLA	CBD-CGD-O2D-CED
25	B	817	CLA	CBD-CGD-O2D-CED
25	B	819	CLA	CBD-CGD-O2D-CED
25	B	820	CLA	CBD-CGD-O2D-CED
25	b	205	CLA	CBD-CGD-O2D-CED
25	c	303	CLA	CBD-CGD-O2D-CED
25	c	304	CLA	CBD-CGD-O2D-CED
25	e	211	CLA	CBD-CGD-O2D-CED
25	h	203	CLA	CBD-CGD-O2D-CED
25	k	202	CLA	CBD-CGD-O2D-CED
25	k	204	CLA	CBD-CGD-O2D-CED
25	l	601	CLA	CBD-CGD-O2D-CED
25	m	210	CLA	CBD-CGD-O2D-CED
25	p	601	CLA	CBD-CGD-O2D-CED
25	j	212	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	c	301	LHG	O2-C2-C3-O3
27	i	201	LHG	O2-C2-C3-O3
25	A	829	CLA	C3-C5-C6-C7
25	A	840	CLA	C3-C5-C6-C7
25	B	838	CLA	O1A-CGA-O2A-C1
25	e	213	CLA	O1A-CGA-O2A-C1
25	e	207	CLA	O1D-CGD-O2D-CED
33	J	102	SQD	C8-C7-O47-C45
25	A	824	CLA	CBD-CGD-O2D-CED
25	A	844	CLA	CBD-CGD-O2D-CED
25	B	846	CLA	CBD-CGD-O2D-CED
25	b	211	CLA	CBD-CGD-O2D-CED
25	i	203	CLA	CBD-CGD-O2D-CED
25	j	210	CLA	CBD-CGD-O2D-CED
25	m	204	CLA	CBD-CGD-O2D-CED
25	o	603	CLA	CBD-CGD-O2D-CED
25	h	205	CLA	C2A-CAA-CBA-CGA
25	a	209	CLA	O1A-CGA-O2A-C1
25	i	202	CLA	O1A-CGA-O2A-C1
25	i	206	CLA	O1A-CGA-O2A-C1
25	n	201	CLA	O1A-CGA-O2A-C1
34	e	202	LMG	O6-C5-C6-O5
25	A	817	CLA	O1D-CGD-O2D-CED
25	i	210	CLA	CBD-CGD-O2D-CED
25	n	208	CLA	CBD-CGD-O2D-CED
25	A	804	CLA	C3-C5-C6-C7
25	A	815	CLA	C3-C5-C6-C7
25	k	214	CLA	CBA-CGA-O2A-C1
25	n	205	CLA	O1D-CGD-O2D-CED
27	g	201	LHG	C5-C4-O6-P
25	J	103	CLA	O1A-CGA-O2A-C1
25	k	205	CLA	O1A-CGA-O2A-C1
25	l	607	CLA	O1A-CGA-O2A-C1
25	g	204	CLA	O1A-CGA-O2A-C1
25	g	209	CLA	O1A-CGA-O2A-C1
34	k	201	LMG	O10-C28-O8-C9
25	B	822	CLA	C5-C6-C7-C8
25	A	815	CLA	C4-C3-C5-C6
25	A	824	CLA	C4-C3-C5-C6
25	b	212	CLA	C4-C3-C5-C6
25	e	201	CLA	C4-C3-C5-C6
25	e	205	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	804	CLA	C2-C3-C5-C6
25	A	814	CLA	C2-C3-C5-C6
25	A	815	CLA	C2-C3-C5-C6
25	A	822	CLA	C2-C3-C5-C6
25	A	833	CLA	C2-C3-C5-C6
25	B	805	CLA	C2-C3-C5-C6
25	B	814	CLA	C2-C3-C5-C6
25	e	201	CLA	C2-C3-C5-C6
25	h	212	CLA	C2-C3-C5-C6
25	j	209	CLA	C2-C3-C5-C6
25	d	303	CLA	CBD-CGD-O2D-CED
32	e	203	DGD	O1A-C1A-O1G-C1G
25	A	820	CLA	C2A-CAA-CBA-CGA
25	B	838	CLA	C2A-CAA-CBA-CGA
25	a	210	CLA	C2A-CAA-CBA-CGA
25	i	208	CLA	C2A-CAA-CBA-CGA
25	j	209	CLA	C2A-CAA-CBA-CGA
32	B	849	DGD	O6E-C5E-C6E-O5E
25	A	813	CLA	O1A-CGA-O2A-C1
25	B	840	CLA	O1A-CGA-O2A-C1
32	B	849	DGD	O6D-C1D-O3G-C3G
25	h	211	CLA	CBA-CGA-O2A-C1
25	g	212	CLA	CBA-CGA-O2A-C1
25	B	826	CLA	O1D-CGD-O2D-CED
25	c	313	CLA	O1D-CGD-O2D-CED
25	f	611	CLA	O1D-CGD-O2D-CED
25	A	830	CLA	C1-C2-C3-C5
25	B	805	CLA	C1-C2-C3-C5
25	e	212	CLA	C1-C2-C3-C5
25	l	606	CLA	C1-C2-C3-C5
25	f	607	CLA	C1-C2-C3-C5
27	b	201	LHG	C25-C26-C27-C28
25	b	213	CLA	O1D-CGD-O2D-CED
25	d	301	CLA	O1D-CGD-O2D-CED
25	g	204	CLA	O1D-CGD-O2D-CED
27	h	201	LHG	C24-C23-O8-C6
32	e	203	DGD	C2A-C1A-O1G-C1G
25	A	801	CLA	CBD-CGD-O2D-CED
25	d	316	CLA	O1D-CGD-O2D-CED
27	A	835	LHG	C1-C2-C3-O3
27	h	201	LHG	C1-C2-C3-O3
27	i	201	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	g	201	LHG	C1-C2-C3-O3
25	i	202	CLA	O1D-CGD-O2D-CED
25	A	801	CLA	CBA-CGA-O2A-C1
25	A	826	CLA	CBA-CGA-O2A-C1
25	A	841	CLA	CBA-CGA-O2A-C1
25	A	844	CLA	CBA-CGA-O2A-C1
25	B	821	CLA	CBA-CGA-O2A-C1
25	B	843	CLA	CBA-CGA-O2A-C1
25	c	310	CLA	CBA-CGA-O2A-C1
25	e	213	CLA	CBA-CGA-O2A-C1
25	i	202	CLA	CBA-CGA-O2A-C1
25	j	211	CLA	CBA-CGA-O2A-C1
25	k	203	CLA	CBA-CGA-O2A-C1
25	l	607	CLA	CBA-CGA-O2A-C1
25	g	204	CLA	CBA-CGA-O2A-C1
25	g	209	CLA	CBA-CGA-O2A-C1
32	B	849	DGD	C2A-C1A-O1G-C1G
32	b	202	DGD	C2A-C1A-O1G-C1G
25	A	833	CLA	C10-C11-C12-C13
25	B	826	CLA	CBD-CGD-O2D-CED
25	c	309	CLA	CBD-CGD-O2D-CED
25	d	304	CLA	CBD-CGD-O2D-CED
25	g	203	CLA	CBD-CGD-O2D-CED
25	f	607	CLA	O1D-CGD-O2D-CED
30	J	105	DD6	C3-C4-C5-C6
30	n	213	DD6	C11-C10-C9-C8
30	n	214	DD6	C1-C2-C3-C4
25	A	801	CLA	C15-C16-C17-C18
34	a	202	LMG	O6-C5-C6-O5
25	B	843	CLA	O1A-CGA-O2A-C1
32	B	849	DGD	C4E-C5E-C6E-O5E
25	A	810	CLA	C8-C10-C11-C12
25	B	821	CLA	C5-C6-C7-C8
25	a	212	CLA	C5-C6-C7-C8
25	i	206	CLA	C8-C10-C11-C12
25	n	202	CLA	C5-C6-C7-C8
27	h	202	LHG	O2-C2-C3-O3
32	B	849	DGD	C2D-C1D-O3G-C3G
33	J	102	SQD	C2-C1-O6-C44
25	A	830	CLA	O1A-CGA-O2A-C1
25	A	826	CLA	C4-C3-C5-C6
34	e	202	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
25	i	208	CLA	C2-C3-C5-C6
25	f	602	CLA	C2-C3-C5-C6
25	A	808	CLA	C6-C7-C8-C9
25	A	809	CLA	C11-C10-C8-C9
25	A	813	CLA	C11-C10-C8-C9
25	A	824	CLA	C11-C10-C8-C9
25	A	829	CLA	C11-C10-C8-C9
25	A	833	CLA	C11-C12-C13-C14
25	B	804	CLA	C11-C10-C8-C9
25	B	807	CLA	C11-C12-C13-C14
25	B	818	CLA	C14-C13-C15-C16
25	B	819	CLA	C11-C10-C8-C9
25	B	819	CLA	C11-C12-C13-C14
25	B	821	CLA	C11-C10-C8-C9
25	B	839	CLA	C11-C10-C8-C9
25	B	841	CLA	C11-C10-C8-C9
25	B	843	CLA	C11-C10-C8-C9
25	c	303	CLA	C6-C7-C8-C9
25	c	303	CLA	C11-C10-C8-C9
25	d	312	CLA	C11-C10-C8-C9
25	j	212	CLA	C6-C7-C8-C9
25	l	606	CLA	C11-C10-C8-C9
25	f	602	CLA	C6-C7-C8-C9
28	A	834	PQN	C16-C17-C18-C19
25	A	831	CLA	O1D-CGD-O2D-CED
25	F	202	CLA	O1D-CGD-O2D-CED
25	j	203	CLA	O1D-CGD-O2D-CED
25	p	605	CLA	O1D-CGD-O2D-CED
35	d	310	CHL	O1D-CGD-O2D-CED
25	B	809	CLA	CBD-CGD-O2D-CED
27	h	201	LHG	C10-C11-C12-C13
25	A	857	CLA	C2A-CAA-CBA-CGA
25	i	202	CLA	C2A-CAA-CBA-CGA
29	A	839	BCR	C36-C18-C19-C20
29	B	801	BCR	C11-C12-C13-C35
29	B	828	BCR	C37-C22-C23-C24
29	B	832	BCR	C36-C18-C19-C20
30	A	854	DD6	C12-C11-C13-C14
30	A	855	DD6	C-C1-C24-C25
30	J	105	DD6	C-C1-C24-C25
30	J	105	DD6	C7-C6-C8-C9
30	b	214	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
30	b	214	DD6	C12-C11-C13-C14
30	c	318	DD6	C12-C11-C13-C14
30	c	318	DD6	C7-C6-C8-C9
30	d	319	DD6	C12-C11-C13-C14
30	g	216	DD6	C12-C11-C13-C14
30	g	217	DD6	C-C1-C24-C25
29	B	801	BCR	C11-C12-C13-C14
29	B	831	BCR	C17-C18-C19-C20
29	B	832	BCR	C17-C18-C19-C20
29	J	101	BCR	C7-C8-C9-C10
29	J	101	BCR	C11-C12-C13-C14
30	A	855	DD6	C2-C1-C24-C25
30	A	855	DD6	C10-C11-C13-C14
30	J	105	DD6	C5-C6-C8-C9
30	c	318	DD6	C10-C11-C13-C14
30	c	318	DD6	C5-C6-C8-C9
30	e	220	DD6	C5-C6-C8-C9
30	n	212	DD6	C10-C11-C13-C14
25	f	610	CLA	O1D-CGD-O2D-CED
27	c	301	LHG	C7-C8-C9-C10
27	h	202	LHG	C7-C8-C9-C10
25	h	204	CLA	O1A-CGA-O2A-C1
25	i	208	CLA	O1A-CGA-O2A-C1
25	A	812	CLA	C15-C16-C17-C18
25	A	825	CLA	C13-C15-C16-C17
25	A	840	CLA	C10-C11-C12-C13
25	B	843	CLA	C8-C10-C11-C12
25	k	205	CLA	C10-C11-C12-C13
28	B	827	PQN	C25-C26-C27-C28
28	B	835	PQN	C15-C16-C17-C18
25	A	828	CLA	O1D-CGD-O2D-CED
25	B	812	CLA	O1D-CGD-O2D-CED
25	h	215	CLA	O1D-CGD-O2D-CED
34	a	202	LMG	C29-C30-C31-C32
25	e	207	CLA	CBD-CGD-O2D-CED
25	A	810	CLA	C3-C5-C6-C7
25	i	210	CLA	C2A-CAA-CBA-CGA
25	p	602	CLA	C2A-CAA-CBA-CGA
25	B	837	CLA	CBA-CGA-O2A-C1
25	J	103	CLA	CBA-CGA-O2A-C1
25	a	209	CLA	CBA-CGA-O2A-C1
25	n	201	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	d	302	LHG	C24-C23-O8-C6
25	B	819	CLA	C5-C6-C7-C8
25	B	824	CLA	C15-C16-C17-C18
28	A	834	PQN	C25-C26-C27-C28
25	A	804	CLA	C10-C11-C12-C13
25	A	810	CLA	C15-C16-C17-C18
25	A	812	CLA	C13-C15-C16-C17
25	A	815	CLA	C8-C10-C11-C12
25	A	821	CLA	C5-C6-C7-C8
25	B	848	CLA	C13-C15-C16-C17
25	c	310	CLA	C5-C6-C7-C8
25	e	205	CLA	C5-C6-C7-C8
25	i	203	CLA	C10-C11-C12-C13
25	k	205	CLA	C15-C16-C17-C18
25	i	211	CLA	C1-C2-C3-C5
27	g	201	LHG	C7-C8-C9-C10
33	F	204	SQD	C23-C24-C25-C26
34	j	201	LMG	C28-C29-C30-C31
25	h	214	CLA	CBD-CGD-O2D-CED
25	A	818	CLA	C10-C11-C12-C13
25	B	843	CLA	C10-C11-C12-C13
25	A	845	CLA	CBA-CGA-O2A-C1
25	f	604	CLA	O1D-CGD-O2D-CED
33	J	102	SQD	O49-C7-O47-C45
25	A	801	CLA	C8-C10-C11-C12
25	B	814	CLA	C5-C6-C7-C8
25	B	844	CLA	C15-C16-C17-C18
25	B	848	CLA	C15-C16-C17-C18
25	A	816	CLA	C2A-CAA-CBA-CGA
25	b	205	CLA	C2A-CAA-CBA-CGA
25	c	310	CLA	C4-C3-C5-C6
25	A	801	CLA	C11-C12-C13-C15
25	A	807	CLA	C11-C10-C8-C7
25	A	818	CLA	C11-C10-C8-C7
25	A	823	CLA	C11-C10-C8-C7
25	A	823	CLA	C11-C12-C13-C15
25	B	816	CLA	C11-C10-C8-C7
25	B	822	CLA	C11-C10-C8-C7
25	B	843	CLA	C11-C10-C8-C7
25	a	213	CLA	C11-C10-C8-C7
25	h	206	CLA	C11-C10-C8-C7
25	j	209	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	k	205	CLA	C12-C13-C15-C16
25	f	602	CLA	C11-C10-C8-C7
25	B	803	CLA	C3-C5-C6-C7
28	B	835	PQN	C13-C15-C16-C17
25	A	826	CLA	O1A-CGA-O2A-C1
25	j	211	CLA	O1A-CGA-O2A-C1
32	B	849	DGD	O1A-C1A-O1G-C1G
29	B	832	BCR	C19-C20-C21-C22
30	J	105	DD6	C11-C10-C9-C8
30	e	219	DD6	C24-C25-C26-C27
30	e	220	DD6	C3-C4-C5-C6
25	A	810	CLA	C2A-CAA-CBA-CGA
25	A	853	CLA	C2A-CAA-CBA-CGA
25	B	816	CLA	C2A-CAA-CBA-CGA
25	B	821	CLA	C2A-CAA-CBA-CGA
25	e	216	CLA	C2A-CAA-CBA-CGA
25	f	607	CLA	C2A-CAA-CBA-CGA
25	A	829	CLA	O1D-CGD-O2D-CED
25	A	843	CLA	O1D-CGD-O2D-CED
25	e	217	CLA	O1D-CGD-O2D-CED
25	h	205	CLA	O1D-CGD-O2D-CED
25	A	826	CLA	C5-C6-C7-C8
25	B	819	CLA	C10-C11-C12-C13
25	j	212	CLA	C5-C6-C7-C8
25	A	846	CLA	O1A-CGA-O2A-C1
25	k	211	CLA	O1A-CGA-O2A-C1
25	A	849	CLA	CBD-CGD-O2D-CED
25	F	202	CLA	CBD-CGD-O2D-CED
25	e	214	CLA	CBD-CGD-O2D-CED
34	a	202	LMG	C4-C5-C6-O5
32	b	202	DGD	O6E-C1E-O5D-C6D
34	a	202	LMG	O6-C1-O1-C7
25	A	826	CLA	C13-C15-C16-C17
25	B	811	CLA	C8-C10-C11-C12
25	B	848	CLA	C8-C10-C11-C12
25	h	213	CLA	O1D-CGD-O2D-CED
29	B	832	BCR	C18-C19-C20-C21
30	F	203	DD6	C1-C24-C25-C26
30	F	203	DD6	C6-C8-C9-C10
30	e	218	DD6	C1-C24-C25-C26
30	e	218	DD6	C6-C8-C9-C10
30	e	220	DD6	C1-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	e	220	DD6	C6-C8-C9-C10
27	d	302	LHG	C10-C11-C12-C13
27	A	835	LHG	O2-C2-C3-O3
27	m	201	LHG	O2-C2-C3-O3
27	g	201	LHG	O2-C2-C3-O3
25	A	814	CLA	C3-C5-C6-C7
25	B	810	CLA	C2A-CAA-CBA-CGA
25	p	604	CLA	C2A-CAA-CBA-CGA
25	B	804	CLA	C10-C11-C12-C13
25	B	807	CLA	C8-C10-C11-C12
25	B	818	CLA	C8-C10-C11-C12
25	B	848	CLA	C5-C6-C7-C8
25	m	203	CLA	C10-C11-C12-C13
25	i	204	CLA	O1D-CGD-O2D-CED
25	A	832	CLA	O1A-CGA-O2A-C1
25	k	208	CLA	O1A-CGA-O2A-C1
27	d	302	LHG	O10-C23-O8-C6
32	b	202	DGD	O1A-C1A-O1G-C1G
27	d	302	LHG	C7-C8-C9-C10
25	B	823	CLA	C8-C10-C11-C12
25	B	838	CLA	C10-C11-C12-C13
25	B	844	CLA	C5-C6-C7-C8
25	l	606	CLA	C5-C6-C7-C8
28	B	827	PQN	C20-C21-C22-C23
25	B	823	CLA	O1D-CGD-O2D-CED
25	A	822	CLA	O1A-CGA-O2A-C1
25	B	824	CLA	C5-C6-C7-C8
25	B	844	CLA	C10-C11-C12-C13
25	i	211	CLA	C8-C10-C11-C12
25	m	203	CLA	C5-C6-C7-C8
27	A	805	LHG	C4-O6-P-O3
27	a	201	LHG	C4-O6-P-O3
27	b	201	LHG	C3-O3-P-O6
27	h	201	LHG	C3-O3-P-O6
27	i	201	LHG	C3-O3-P-O6
27	j	202	LHG	C4-O6-P-O3
27	m	201	LHG	C3-O3-P-O6
27	g	201	LHG	C3-O3-P-O6
25	B	844	CLA	C3-C5-C6-C7
25	c	313	CLA	C3-C5-C6-C7
25	A	814	CLA	CBA-CGA-O2A-C1
25	A	842	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	840	CLA	CBA-CGA-O2A-C1
25	e	205	CLA	CBA-CGA-O2A-C1
25	i	208	CLA	CBA-CGA-O2A-C1
25	A	815	CLA	O1D-CGD-O2D-CED
25	B	807	CLA	C10-C11-C12-C13
25	e	211	CLA	O2A-C1-C2-C3
25	o	606	CLA	O1D-CGD-O2D-CED
25	i	204	CLA	C2A-CAA-CBA-CGA
25	i	205	CLA	C2A-CAA-CBA-CGA
25	g	206	CLA	C2A-CAA-CBA-CGA
25	h	214	CLA	O1D-CGD-O2D-CED
25	o	608	CLA	O1D-CGD-O2D-CED
27	j	202	LHG	C1-C2-C3-O3
27	m	201	LHG	C1-C2-C3-O3
25	k	208	CLA	C4-C3-C5-C6
25	g	204	CLA	C4-C3-C5-C6
25	l	606	CLA	C10-C11-C12-C13
27	A	805	LHG	C34-C35-C36-C37
25	A	848	CLA	C2A-CAA-CBA-CGA
25	B	839	CLA	C2A-CAA-CBA-CGA
25	J	103	CLA	C2A-CAA-CBA-CGA
25	c	310	CLA	C2A-CAA-CBA-CGA
25	h	203	CLA	C2A-CAA-CBA-CGA
35	c	307	CHL	C2A-CAA-CBA-CGA
25	A	818	CLA	C16-C17-C18-C19
25	A	813	CLA	CBA-CGA-O2A-C1
30	e	218	DD6	C25-C26-C27-C28
30	J	105	DD6	C1-C2-C3-C4
30	e	220	DD6	C1-C2-C3-C4
27	b	201	LHG	C26-C27-C28-C29
27	h	202	LHG	C10-C11-C12-C13
25	k	213	CLA	O1D-CGD-O2D-CED
25	h	210	CLA	CBD-CGD-O2D-CED
29	A	837	BCR	C11-C10-C9-C34
29	B	832	BCR	C35-C13-C14-C15
30	F	203	DD6	C9-C10-C11-C12
30	e	220	DD6	C4-C5-C6-C7
30	n	213	DD6	C9-C10-C11-C12
30	n	213	DD6	C4-C5-C6-C7
30	n	214	DD6	C4-C5-C6-C7
25	o	603	CLA	C2A-CAA-CBA-CGA
25	i	203	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	f	610	CLA	C10-C11-C12-C13
27	A	805	LHG	C26-C27-C28-C29
34	j	201	LMG	C34-C35-C36-C37
25	p	602	CLA	O1D-CGD-O2D-CED
25	A	846	CLA	C16-C17-C18-C20
25	A	850	CLA	C6-C7-C8-C9
25	a	212	CLA	C6-C7-C8-C9
25	g	212	CLA	C6-C7-C8-C9
25	A	830	CLA	CBA-CGA-O2A-C1
25	d	311	CLA	CBA-CGA-O2A-C1
27	h	201	LHG	O10-C23-O8-C6
27	i	201	LHG	C26-C27-C28-C29
27	j	202	LHG	C28-C29-C30-C31
27	g	201	LHG	C10-C11-C12-C13
25	m	205	CLA	O1D-CGD-O2D-CED
25	B	837	CLA	C1-C2-C3-C5
25	J	103	CLA	C1-C2-C3-C5
25	h	208	CLA	C1-C2-C3-C5
25	j	210	CLA	C1-C2-C3-C4
25	j	215	CLA	C1-C2-C3-C4
25	p	606	CLA	C1-C2-C3-C4
25	B	816	CLA	CBD-CGD-O2D-CED
25	a	209	CLA	C5-C6-C7-C8
34	e	202	LMG	C31-C32-C33-C34
25	g	212	CLA	O1A-CGA-O2A-C1
25	h	209	CLA	C5-C6-C7-C8
27	g	201	LHG	C9-C10-C11-C12
33	F	204	SQD	C12-C13-C14-C15
34	e	202	LMG	C41-C42-C43-C44
25	e	205	CLA	O1D-CGD-O2D-CED
25	B	811	CLA	C10-C11-C12-C13
25	B	841	CLA	C3-C5-C6-C7
28	A	834	PQN	C13-C15-C16-C17
25	c	309	CLA	O1D-CGD-O2D-CED
25	l	609	CLA	O1D-CGD-O2D-CED
26	A	803	LMT	C2'-C1'-O1'-C1
29	A	837	BCR	C11-C10-C9-C8
29	B	832	BCR	C12-C13-C14-C15
30	F	203	DD6	C9-C10-C11-C13
30	e	220	DD6	C4-C5-C6-C8
30	n	213	DD6	C9-C10-C11-C13
30	n	213	DD6	C4-C5-C6-C8

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Mol	Chain	Res	Type	Atoms
30	n	214	DD6	C4-C5-C6-C8
32	b	202	DGD	C2E-C1E-O5D-C6D
34	a	202	LMG	C2-C1-O1-C7
34	k	201	LMG	C2-C1-O1-C7
27	j	202	LHG	C24-C23-O8-C6
25	B	841	CLA	C10-C11-C12-C13
33	D	200	SQD	C24-C25-C26-C27
34	j	201	LMG	C12-C13-C14-C15
34	k	201	LMG	C30-C31-C32-C33
25	A	844	CLA	C10-C11-C12-C13
25	j	206	CLA	C5-C6-C7-C8
25	f	610	CLA	C8-C10-C11-C12
25	h	208	CLA	O1A-CGA-O2A-C1
25	j	209	CLA	O1A-CGA-O2A-C1
25	B	824	CLA	C16-C17-C18-C20
25	B	844	CLA	C16-C17-C18-C20
25	g	212	CLA	C6-C7-C8-C10
25	A	832	CLA	O1D-CGD-O2D-CED
32	b	202	DGD	C3A-C4A-C5A-C6A
25	a	212	CLA	C2-C3-C5-C6
25	A	801	CLA	C11-C12-C13-C14
25	A	807	CLA	C11-C10-C8-C9
25	A	809	CLA	C6-C7-C8-C9
25	B	824	CLA	C6-C7-C8-C9
25	B	824	CLA	C11-C12-C13-C14
25	h	206	CLA	C11-C10-C8-C9
25	e	204	CLA	O1D-CGD-O2D-CED
25	k	204	CLA	O1D-CGD-O2D-CED
25	m	210	CLA	C2A-CAA-CBA-CGA
33	D	200	SQD	C23-C24-C25-C26
25	j	209	CLA	C15-C16-C17-C18
27	A	805	LHG	C28-C29-C30-C31
27	h	201	LHG	C9-C10-C11-C12
27	i	201	LHG	C11-C12-C13-C14
32	b	202	DGD	C4B-C5B-C6B-C7B
33	F	204	SQD	C11-C12-C13-C14
25	j	209	CLA	C10-C11-C12-C13
25	A	824	CLA	C2A-CAA-CBA-CGA
35	d	307	CHL	C2A-CAA-CBA-CGA
29	A	838	BCR	C37-C22-C23-C24
30	A	855	DD6	C12-C11-C13-C14
30	e	220	DD6	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
30	n	212	DD6	C12-C11-C13-C14
27	b	201	LHG	O1-C1-C2-C3
27	j	202	LHG	O1-C1-C2-C3
29	A	838	BCR	C21-C22-C23-C24
29	B	833	BCR	C21-C22-C23-C24
30	A	854	DD6	C10-C11-C13-C14
30	k	215	DD6	C2-C1-C24-C25
30	f	613	DD6	C2-C1-C24-C25
30	n	213	DD6	C10-C11-C13-C14
25	e	201	CLA	C3-C5-C6-C7
25	h	212	CLA	C3-C5-C6-C7
25	j	206	CLA	C3-C5-C6-C7
25	B	818	CLA	C5-C6-C7-C8
25	a	203	CLA	CBA-CGA-O2A-C1
25	A	810	CLA	O1D-CGD-O2D-CED
25	b	205	CLA	O1D-CGD-O2D-CED
25	f	602	CLA	C10-C11-C12-C13
27	A	805	LHG	C30-C31-C32-C33
27	b	201	LHG	C28-C29-C30-C31
27	i	201	LHG	C9-C10-C11-C12
27	j	202	LHG	C9-C10-C11-C12
33	D	200	SQD	C25-C26-C27-C28
25	A	802	CLA	C4B-C3B-CAB-CBB
25	A	807	CLA	C4B-C3B-CAB-CBB
25	A	821	CLA	C4B-C3B-CAB-CBB
25	A	826	CLA	C4B-C3B-CAB-CBB
25	A	843	CLA	C4B-C3B-CAB-CBB
25	A	853	CLA	C4B-C3B-CAB-CBB
25	B	821	CLA	C4B-C3B-CAB-CBB
25	a	209	CLA	C4B-C3B-CAB-CBB
25	b	206	CLA	C4B-C3B-CAB-CBB
25	c	303	CLA	C4B-C3B-CAB-CBB
25	d	306	CLA	C4B-C3B-CAB-CBB
25	d	312	CLA	C4B-C3B-CAB-CBB
25	i	204	CLA	C4B-C3B-CAB-CBB
25	A	809	CLA	C16-C17-C18-C19
25	A	809	CLA	C16-C17-C18-C20
25	A	846	CLA	C16-C17-C18-C19
25	A	850	CLA	C6-C7-C8-C10
25	B	844	CLA	C16-C17-C18-C19
25	B	845	CLA	C16-C17-C18-C20
25	e	205	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	e	205	CLA	C16-C17-C18-C20
25	k	205	CLA	C16-C17-C18-C19
25	k	205	CLA	C16-C17-C18-C20
25	g	209	CLA	C6-C7-C8-C9
25	g	209	CLA	C6-C7-C8-C10
26	A	803	LMT	O5'-C1'-O1'-C1
34	k	201	LMG	O6-C1-O1-C7
25	B	819	CLA	C15-C16-C17-C18
25	B	848	CLA	C10-C11-C12-C13
27	A	805	LHG	C24-C25-C26-C27
25	B	811	CLA	CBD-CGD-O2D-CED
25	j	205	CLA	CBD-CGD-O2D-CED
25	B	838	CLA	O1D-CGD-O2D-CED
25	o	602	CLA	O1D-CGD-O2D-CED
25	B	842	CLA	O1A-CGA-O2A-C1
25	h	211	CLA	O1A-CGA-O2A-C1
27	j	202	LHG	C10-C11-C12-C13
25	B	848	CLA	C3-C5-C6-C7
25	A	817	CLA	CBA-CGA-O2A-C1
33	D	200	SQD	C24-C23-O48-C46
25	B	802	CLA	O1D-CGD-O2D-CED
25	A	814	CLA	C3A-C2A-CAA-CBA
25	A	841	CLA	C3A-C2A-CAA-CBA
25	A	847	CLA	C3A-C2A-CAA-CBA
25	B	822	CLA	C3A-C2A-CAA-CBA
25	B	824	CLA	C3A-C2A-CAA-CBA
25	B	840	CLA	C3A-C2A-CAA-CBA
25	B	841	CLA	C3A-C2A-CAA-CBA
25	B	845	CLA	C3A-C2A-CAA-CBA
25	a	208	CLA	C3A-C2A-CAA-CBA
25	b	206	CLA	C3A-C2A-CAA-CBA
25	c	306	CLA	C3A-C2A-CAA-CBA
25	i	204	CLA	C3A-C2A-CAA-CBA
25	i	210	CLA	C3A-C2A-CAA-CBA
25	j	203	CLA	C3A-C2A-CAA-CBA
25	j	207	CLA	C3A-C2A-CAA-CBA
25	k	205	CLA	C3A-C2A-CAA-CBA
25	l	604	CLA	C3A-C2A-CAA-CBA
25	l	605	CLA	C3A-C2A-CAA-CBA
25	l	609	CLA	C3A-C2A-CAA-CBA
25	m	204	CLA	C3A-C2A-CAA-CBA
25	o	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	o	605	CLA	C3A-C2A-CAA-CBA
25	p	604	CLA	C3A-C2A-CAA-CBA
35	c	307	CHL	C3A-C2A-CAA-CBA
35	e	209	CHL	C3A-C2A-CAA-CBA
25	B	807	CLA	C15-C16-C17-C18
30	i	215	DD6	C24-C25-C26-C27
33	F	204	SQD	C9-C10-C11-C12
25	B	817	CLA	O1D-CGD-O2D-CED
25	c	302	CLA	O1D-CGD-O2D-CED
25	A	801	CLA	O1A-CGA-O2A-C1
25	a	212	CLA	C6-C7-C8-C10
34	k	201	LMG	O1-C7-C8-C9
25	b	213	CLA	CBD-CGD-O2D-CED
25	A	823	CLA	C15-C16-C17-C18
27	A	805	LHG	C32-C33-C34-C35
34	e	202	LMG	C12-C13-C14-C15
25	B	838	CLA	O2A-C1-C2-C3
25	f	602	CLA	C3-C5-C6-C7
25	A	841	CLA	O1A-CGA-O2A-C1
25	A	843	CLA	O1A-CGA-O2A-C1
25	A	819	CLA	C4-C3-C5-C6
25	k	205	CLA	C4-C3-C5-C6
25	e	216	CLA	CBA-CGA-O2A-C1
25	h	204	CLA	CBA-CGA-O2A-C1
25	A	819	CLA	C2-C3-C5-C6
25	A	825	CLA	C2-C3-C5-C6
27	i	201	LHG	C27-C28-C29-C30
25	e	213	CLA	C1-C2-C3-C5
27	j	202	LHG	O1-C1-C2-O2
27	A	805	LHG	C27-C28-C29-C30
27	A	835	LHG	C10-C11-C12-C13
27	m	201	LHG	C9-C10-C11-C12
32	B	849	DGD	C6A-C7A-C8A-C9A
34	k	201	LMG	C31-C32-C33-C34
33	g	202	SQD	C23-C24-C25-C26
25	n	202	CLA	O1D-CGD-O2D-CED
25	e	211	CLA	O1A-CGA-O2A-C1
25	B	824	CLA	C16-C17-C18-C19
25	A	802	CLA	C2B-C3B-CAB-CBB
25	A	807	CLA	C2B-C3B-CAB-CBB
25	A	818	CLA	C2B-C3B-CAB-CBB
25	A	826	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	843	CLA	C2B-C3B-CAB-CBB
25	A	844	CLA	C2B-C3B-CAB-CBB
25	A	853	CLA	C2B-C3B-CAB-CBB
25	a	209	CLA	C2B-C3B-CAB-CBB
25	b	206	CLA	C2B-C3B-CAB-CBB
25	c	303	CLA	C2B-C3B-CAB-CBB
25	d	306	CLA	C2B-C3B-CAB-CBB
25	d	312	CLA	C2B-C3B-CAB-CBB
25	i	204	CLA	C2B-C3B-CAB-CBB
25	j	204	CLA	C2B-C3B-CAB-CBB
25	j	211	CLA	C2B-C3B-CAB-CBB
25	A	808	CLA	C5-C6-C7-C8
27	d	302	LHG	C9-C10-C11-C12
25	A	857	CLA	C3-C5-C6-C7
33	F	204	SQD	C24-C23-O48-C46
25	n	206	CLA	O1D-CGD-O2D-CED
27	j	202	LHG	O10-C23-O8-C6
34	k	201	LMG	C28-C29-C30-C31
25	B	814	CLA	CBD-CGD-O2D-CED
25	B	842	CLA	C2-C1-O2A-CGA
27	i	201	LHG	C10-C11-C12-C13
25	j	212	CLA	C10-C11-C12-C13
25	A	823	CLA	O1A-CGA-O2A-C1
25	c	309	CLA	O1A-CGA-O2A-C1
27	A	835	LHG	C11-C12-C13-C14
25	f	610	CLA	C3-C5-C6-C7
29	A	836	BCR	C23-C24-C25-C26
29	A	837	BCR	C23-C24-C25-C26
29	A	837	BCR	C23-C24-C25-C30
29	A	838	BCR	C23-C24-C25-C30
29	B	801	BCR	C5-C6-C7-C8
29	B	829	BCR	C23-C24-C25-C26
29	J	101	BCR	C23-C24-C25-C26
29	J	101	BCR	C23-C24-C25-C30
29	M	201	BCR	C23-C24-C25-C30
25	B	814	CLA	C10-C11-C12-C13
25	A	825	CLA	CBA-CGA-O2A-C1
25	l	602	CLA	CBA-CGA-O2A-C1
25	f	610	CLA	CBA-CGA-O2A-C1
25	A	825	CLA	C15-C16-C17-C18
25	A	844	CLA	C8-C10-C11-C12
25	B	807	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B	834	CLA	C5-C6-C7-C8
25	a	205	CLA	C5-C6-C7-C8
27	h	201	LHG	C11-C10-C9-C8
34	e	202	LMG	C32-C33-C34-C35
25	A	845	CLA	O2A-C1-C2-C3
25	f	610	CLA	O1A-CGA-O2A-C1
34	a	202	LMG	C10-C11-C12-C13
27	A	835	LHG	C18-C19-C20-C21
25	A	832	CLA	C10-C11-C12-C13
25	A	833	CLA	C5-C6-C7-C8
27	j	202	LHG	C27-C28-C29-C30
25	A	821	CLA	C2-C1-O2A-CGA
25	B	812	CLA	C4-C3-C5-C6
25	B	842	CLA	C4-C3-C5-C6
25	A	809	CLA	C6-C7-C8-C10
25	A	824	CLA	C11-C10-C8-C7
25	B	824	CLA	C6-C7-C8-C10
25	B	824	CLA	C11-C12-C13-C15
25	c	303	CLA	C11-C10-C8-C7
25	c	309	CLA	C11-C10-C8-C7
28	F	205	PQN	C16-C17-C18-C20
25	A	809	CLA	C3-C5-C6-C7
25	B	815	CLA	O1A-CGA-O2A-C1
25	B	822	CLA	O1A-CGA-O2A-C1
25	B	837	CLA	O1A-CGA-O2A-C1
25	c	305	CLA	O1A-CGA-O2A-C1
33	D	200	SQD	O10-C23-O48-C46
33	F	204	SQD	O10-C23-O48-C46
26	A	803	LMT	C2-C3-C4-C5
30	F	203	DD6	C1-C2-C3-C4
30	c	318	DD6	C24-C25-C26-C27
30	d	319	DD6	C24-C25-C26-C27
30	l	614	DD6	C24-C25-C26-C27
30	m	213	DD6	C24-C25-C26-C27
25	h	204	CLA	C6-C7-C8-C9
25	B	824	CLA	O1D-CGD-O2D-CED
27	A	835	LHG	O9-C7-O7-C5
27	A	835	LHG	C23-C24-C25-C26
27	b	201	LHG	C23-C24-C25-C26
25	b	204	CLA	CBA-CGA-O2A-C1
25	c	313	CLA	CBA-CGA-O2A-C1
34	e	202	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	h	207	CLA	C2A-CAA-CBA-CGA
25	k	211	CLA	C2A-CAA-CBA-CGA
25	A	823	CLA	C10-C11-C12-C13
28	B	827	PQN	C18-C20-C21-C22
34	e	202	LMG	C37-C38-C39-C40
25	l	609	CLA	C2A-CAA-CBA-CGA
25	B	843	CLA	C1-C2-C3-C5
27	m	201	LHG	C10-C11-C12-C13
34	k	201	LMG	C12-C13-C14-C15
25	m	208	CLA	O1D-CGD-O2D-CED
27	g	201	LHG	C24-C25-C26-C27
34	k	201	LMG	C34-C35-C36-C37
32	B	849	DGD	C4A-C5A-C6A-C7A
25	B	844	CLA	O1D-CGD-O2D-CED
33	F	204	SQD	C10-C11-C12-C13
27	A	835	LHG	C8-C7-O7-C5
27	j	202	LHG	C8-C7-O7-C5
25	a	204	CLA	C10-C11-C12-C13
27	A	805	LHG	C33-C34-C35-C36
27	j	202	LHG	O9-C7-O7-C5
33	D	200	SQD	O49-C7-O47-C45
25	B	805	CLA	C3-C5-C6-C7
25	h	204	CLA	C3-C5-C6-C7
25	k	210	CLA	C2A-CAA-CBA-CGA
25	A	833	CLA	C15-C16-C17-C18
27	i	201	LHG	C23-C24-C25-C26
25	n	202	CLA	C2-C3-C5-C6
25	A	823	CLA	C11-C10-C8-C9
25	B	811	CLA	C11-C12-C13-C14
25	B	811	CLA	C14-C13-C15-C16
25	B	822	CLA	C6-C7-C8-C9
25	B	848	CLA	C6-C7-C8-C9
25	i	211	CLA	C6-C7-C8-C9
25	j	209	CLA	C11-C12-C13-C14
25	k	208	CLA	C6-C7-C8-C9
25	c	303	CLA	C3-C5-C6-C7
25	A	846	CLA	C2A-CAA-CBA-CGA
25	B	845	CLA	C2A-CAA-CBA-CGA
25	b	212	CLA	C2A-CAA-CBA-CGA
32	b	202	DGD	C2A-C3A-C4A-C5A
34	j	201	LMG	O6-C5-C6-O5
25	k	208	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	801	BCR	C7-C8-C9-C34
25	b	204	CLA	O1D-CGD-O2D-CED
25	A	809	CLA	C10-C11-C12-C13
25	a	204	CLA	C5-C6-C7-C8
25	m	208	CLA	CBD-CGD-O2D-CED
27	A	835	LHG	C16-C17-C18-C19
29	B	801	BCR	C7-C8-C9-C10
30	b	214	DD6	C10-C11-C13-C14
25	d	311	CLA	O1A-CGA-O2A-C1
25	d	314	CLA	O1D-CGD-O2D-CED
25	A	811	CLA	C1A-C2A-CAA-CBA
25	A	813	CLA	C1A-C2A-CAA-CBA
25	A	817	CLA	C1A-C2A-CAA-CBA
25	A	829	CLA	C1A-C2A-CAA-CBA
25	A	841	CLA	C1A-C2A-CAA-CBA
25	A	846	CLA	C1A-C2A-CAA-CBA
25	B	811	CLA	C1A-C2A-CAA-CBA
25	B	822	CLA	C1A-C2A-CAA-CBA
25	B	844	CLA	C1A-C2A-CAA-CBA
25	J	103	CLA	C1A-C2A-CAA-CBA
25	b	206	CLA	C1A-C2A-CAA-CBA
25	c	308	CLA	C1A-C2A-CAA-CBA
25	c	310	CLA	C1A-C2A-CAA-CBA
25	c	311	CLA	C1A-C2A-CAA-CBA
25	d	306	CLA	C1A-C2A-CAA-CBA
25	d	311	CLA	C1A-C2A-CAA-CBA
25	h	204	CLA	C1A-C2A-CAA-CBA
25	h	210	CLA	C1A-C2A-CAA-CBA
25	i	204	CLA	C1A-C2A-CAA-CBA
25	i	208	CLA	C1A-C2A-CAA-CBA
25	j	209	CLA	C1A-C2A-CAA-CBA
25	k	208	CLA	C1A-C2A-CAA-CBA
25	l	604	CLA	C1A-C2A-CAA-CBA
25	l	607	CLA	C1A-C2A-CAA-CBA
25	l	608	CLA	C1A-C2A-CAA-CBA
25	l	609	CLA	C1A-C2A-CAA-CBA
25	m	204	CLA	C1A-C2A-CAA-CBA
25	g	204	CLA	C1A-C2A-CAA-CBA
25	g	209	CLA	C1A-C2A-CAA-CBA
25	o	603	CLA	C1A-C2A-CAA-CBA
25	o	605	CLA	C1A-C2A-CAA-CBA
25	p	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	c	307	CHL	C1A-C2A-CAA-CBA
35	e	209	CHL	C1A-C2A-CAA-CBA
25	h	204	CLA	C6-C7-C8-C10
33	D	200	SQD	C8-C7-O47-C45
33	g	202	SQD	C8-C7-O47-C45
34	e	202	LMG	C11-C10-O7-C8
27	g	201	LHG	C25-C26-C27-C28
32	B	849	DGD	C3A-C4A-C5A-C6A
30	k	216	DD6	C24-C25-C26-C27
30	n	214	DD6	C11-C10-C9-C8
27	h	202	LHG	C3-O3-P-O6
27	m	201	LHG	C4-O6-P-O3
27	g	201	LHG	O6-C4-C5-C6
34	k	201	LMG	C33-C34-C35-C36
33	g	202	SQD	C24-C23-O48-C46
25	B	821	CLA	C4-C3-C5-C6
25	a	205	CLA	C4-C3-C5-C6
25	c	309	CLA	C4-C3-C5-C6
25	l	607	CLA	C4-C3-C5-C6
25	n	201	CLA	C4-C3-C5-C6
25	A	809	CLA	C2-C3-C5-C6
25	B	806	CLA	C3A-C2A-CAA-CBA
25	b	203	CLA	C3A-C2A-CAA-CBA
25	d	316	CLA	C3A-C2A-CAA-CBA
25	e	217	CLA	C3A-C2A-CAA-CBA
25	f	601	CLA	C3A-C2A-CAA-CBA
25	f	611	CLA	C3A-C2A-CAA-CBA
25	n	210	CLA	C3A-C2A-CAA-CBA
25	p	601	CLA	C3A-C2A-CAA-CBA
26	A	803	LMT	O1'-C1-C2-C3
25	A	840	CLA	C5-C6-C7-C8
25	i	206	CLA	C5-C6-C7-C8
33	F	204	SQD	C24-C25-C26-C27
25	k	207	CLA	O1A-CGA-O2A-C1
25	A	840	CLA	C2A-CAA-CBA-CGA
25	c	308	CLA	C2A-CAA-CBA-CGA
25	p	607	CLA	C2A-CAA-CBA-CGA
25	h	212	CLA	O1D-CGD-O2D-CED
25	A	815	CLA	C10-C11-C12-C13
33	D	200	SQD	C44-C45-C46-O48
33	F	204	SQD	O6-C44-C45-C46
33	g	202	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
34	a	202	LMG	O1-C7-C8-C9
25	a	213	CLA	C15-C16-C17-C18
25	m	203	CLA	O1A-CGA-O2A-C1
34	j	201	LMG	C8-C7-O1-C1
25	A	829	CLA	C10-C11-C12-C13
25	g	208	CLA	CBD-CGD-O2D-CED
27	c	301	LHG	C24-C25-C26-C27
33	F	204	SQD	C25-C26-C27-C28
30	J	105	DD6	C25-C26-C27-C28
27	i	201	LHG	O8-C23-C24-C25
27	i	201	LHG	C11-C10-C9-C8
27	b	201	LHG	O1-C1-C2-O2
25	h	207	CLA	O2A-C1-C2-C3
25	l	610	CLA	O2A-C1-C2-C3
27	h	201	LHG	C12-C13-C14-C15
27	i	201	LHG	C28-C29-C30-C31
32	B	849	DGD	C8A-C9A-CAA-CBA
25	A	813	CLA	C5-C6-C7-C8
26	A	803	LMT	C3-C4-C5-C6
25	A	829	CLA	C5-C6-C7-C8
25	A	821	CLA	C2A-CAA-CBA-CGA
29	B	831	BCR	C20-C21-C22-C37
30	J	105	DD6	C4-C5-C6-C7
30	e	220	DD6	C-C1-C2-C3
30	n	214	DD6	C9-C10-C11-C12
32	b	202	DGD	O6E-C5E-C6E-O5E
25	A	825	CLA	C4-C3-C5-C6
25	j	206	CLA	C4-C3-C5-C6
33	F	204	SQD	C11-C10-C9-C8
25	j	206	CLA	C2-C3-C5-C6
25	A	829	CLA	CBA-CGA-O2A-C1
25	j	206	CLA	CBA-CGA-O2A-C1
35	c	307	CHL	CBA-CGA-O2A-C1
25	A	840	CLA	CBD-CGD-O2D-CED
25	B	805	CLA	C10-C11-C12-C13
28	B	827	PQN	C15-C16-C17-C18
28	B	835	PQN	C18-C20-C21-C22
25	g	204	CLA	C5-C6-C7-C8
27	j	202	LHG	C30-C31-C32-C33
33	D	200	SQD	C10-C11-C12-C13
25	e	211	CLA	C2A-CAA-CBA-CGA
25	c	309	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	A	811	CLA	C1-C2-C3-C4
25	B	834	CLA	C2-C1-O2A-CGA
25	B	844	CLA	C2-C1-O2A-CGA
25	B	846	CLA	C1-C2-C3-C5
25	a	203	CLA	C1-C2-C3-C4
25	d	303	CLA	C1-C2-C3-C4
25	d	303	CLA	C1-C2-C3-C5
25	e	207	CLA	C1-C2-C3-C4
25	k	203	CLA	C2-C1-O2A-CGA
25	k	206	CLA	C1-C2-C3-C5
25	k	207	CLA	C1-C2-C3-C4
25	B	811	CLA	C15-C16-C17-C18
27	h	202	LHG	C12-C13-C14-C15
25	p	604	CLA	O1D-CGD-O2D-CED
25	f	607	CLA	C3-C5-C6-C7
25	o	608	CLA	CHA-CBD-CGD-O1D
32	B	849	DGD	C5A-C6A-C7A-C8A
32	B	849	DGD	C3B-C4B-C5B-C6B
25	B	817	CLA	CBA-CGA-O2A-C1
25	B	842	CLA	CBA-CGA-O2A-C1
25	c	309	CLA	CBA-CGA-O2A-C1
27	i	201	LHG	C24-C23-O8-C6
27	b	201	LHG	O6-C4-C5-O7
27	A	835	LHG	C25-C26-C27-C28
25	e	212	CLA	O1A-CGA-O2A-C1
25	B	842	CLA	C5-C6-C7-C8
25	A	812	CLA	C8-C10-C11-C12
25	B	803	CLA	C5-C6-C7-C8
25	B	824	CLA	C13-C15-C16-C17
25	f	610	CLA	C5-C6-C7-C8
29	B	831	BCR	C20-C21-C22-C23
25	a	212	CLA	C1-C2-C3-C5
27	m	201	LHG	C24-C25-C26-C27
32	B	849	DGD	C6B-C7B-C8B-C9B
33	g	202	SQD	O10-C23-O48-C46
25	n	201	CLA	C10-C11-C12-C13
25	A	850	CLA	O1D-CGD-O2D-CED
25	A	801	CLA	C11-C10-C8-C7
25	A	802	CLA	C11-C10-C8-C7
25	A	804	CLA	C11-C10-C8-C7
25	A	813	CLA	C11-C10-C8-C7
25	A	824	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	A	826	CLA	C11-C10-C8-C7
25	A	832	CLA	C11-C10-C8-C7
25	A	844	CLA	C11-C10-C8-C7
25	A	846	CLA	C12-C13-C15-C16
25	B	811	CLA	C12-C13-C15-C16
25	B	812	CLA	C11-C10-C8-C7
25	B	818	CLA	C6-C7-C8-C10
25	B	819	CLA	C11-C10-C8-C7
25	B	821	CLA	C11-C10-C8-C7
25	B	822	CLA	C2-C3-C5-C6
25	B	822	CLA	C6-C7-C8-C10
25	B	823	CLA	C11-C10-C8-C7
25	B	848	CLA	C6-C7-C8-C10
25	h	211	CLA	C6-C7-C8-C10
25	i	211	CLA	C6-C7-C8-C10
25	i	211	CLA	C11-C10-C8-C7
25	k	208	CLA	C6-C7-C8-C10
25	f	602	CLA	C6-C7-C8-C10
28	A	834	PQN	C16-C17-C18-C20
25	a	205	CLA	C3-C5-C6-C7
25	A	840	CLA	C15-C16-C17-C18
25	A	801	CLA	C11-C10-C8-C9
25	A	812	CLA	C11-C12-C13-C14
25	A	818	CLA	C11-C10-C8-C9
25	A	840	CLA	C11-C12-C13-C14
25	A	844	CLA	C11-C10-C8-C9
25	B	805	CLA	C6-C7-C8-C9
25	B	812	CLA	C11-C10-C8-C9
25	B	822	CLA	C11-C10-C8-C9
25	B	823	CLA	C11-C10-C8-C9
25	d	312	CLA	C6-C7-C8-C9
25	h	211	CLA	C6-C7-C8-C9
25	i	206	CLA	C6-C7-C8-C9
28	A	834	PQN	C19-C18-C20-C21
25	A	827	CLA	C2A-CAA-CBA-CGA
32	b	202	DGD	C5B-C6B-C7B-C8B
34	e	202	LMG	C38-C39-C40-C41
25	n	202	CLA	CBA-CGA-O2A-C1
25	B	816	CLA	C10-C11-C12-C13
25	A	807	CLA	C2A-CAA-CBA-CGA
25	m	203	CLA	C2A-CAA-CBA-CGA
25	d	312	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	b	201	LHG	C24-C25-C26-C27
30	e	218	DD6	C12-C11-C13-C14
30	m	212	DD6	C-C1-C24-C25
25	A	808	CLA	C11-C12-C13-C14
25	B	822	CLA	C11-C12-C13-C14
30	J	105	DD6	C2-C1-C24-C25
30	g	217	DD6	C2-C1-C24-C25
25	A	819	CLA	C13-C15-C16-C17
25	n	208	CLA	O1D-CGD-O2D-CED
25	B	846	CLA	C4B-C3B-CAB-CBB
25	c	310	CLA	C4B-C3B-CAB-CBB
25	j	211	CLA	C4B-C3B-CAB-CBB
25	k	208	CLA	C4B-C3B-CAB-CBB
25	A	809	CLA	C15-C16-C17-C18
27	c	301	LHG	O6-C4-C5-C6
27	d	302	LHG	O6-C4-C5-C6
25	B	821	CLA	C8-C10-C11-C12
25	a	212	CLA	O1D-CGD-O2D-CED
25	A	820	CLA	C4-C3-C5-C6
25	B	845	CLA	C4-C3-C5-C6
25	A	818	CLA	C2-C3-C5-C6
25	A	821	CLA	C15-C16-C17-C18
33	g	202	SQD	O49-C7-O47-C45
25	g	207	CLA	C2C-C3C-CAC-CBC
27	A	835	LHG	C30-C31-C32-C33
27	A	835	LHG	C32-C33-C34-C35
27	h	202	LHG	C24-C25-C26-C27
25	A	823	CLA	CBA-CGA-O2A-C1
25	A	843	CLA	CBA-CGA-O2A-C1
25	a	204	CLA	CBA-CGA-O2A-C1
25	A	833	CLA	CAA-CBA-CGA-O2A
27	h	202	LHG	C2-C3-O3-P
25	l	606	CLA	O1D-CGD-O2D-CED
25	p	608	CLA	O1D-CGD-O2D-CED
25	A	816	CLA	C3A-C2A-CAA-CBA
25	B	810	CLA	C3A-C2A-CAA-CBA
25	B	836	CLA	C3A-C2A-CAA-CBA
25	c	308	CLA	C3A-C2A-CAA-CBA
25	d	306	CLA	C3A-C2A-CAA-CBA
25	d	311	CLA	C3A-C2A-CAA-CBA
25	h	209	CLA	C3A-C2A-CAA-CBA
25	j	210	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	l	606	CLA	C3A-C2A-CAA-CBA
25	l	608	CLA	C3A-C2A-CAA-CBA
25	m	203	CLA	C3A-C2A-CAA-CBA
25	g	212	CLA	C3A-C2A-CAA-CBA
35	d	309	CHL	C4C-C3C-CAC-CBC
25	k	211	CLA	O1D-CGD-O2D-CED
29	B	801	BCR	C9-C10-C11-C12
30	J	104	DD6	C1-C2-C3-C4
25	A	853	CLA	C5-C6-C7-C8
25	B	812	CLA	C16-C17-C18-C19
25	B	841	CLA	O1D-CGD-O2D-CED
25	n	203	CLA	O2A-C1-C2-C3
27	b	201	LHG	C4-C5-C6-O8
32	b	202	DGD	O1G-C1G-C2G-C3G
33	g	202	SQD	O6-C44-C45-C46
34	e	202	LMG	O9-C10-O7-C8
27	A	805	LHG	C7-C8-C9-C10
25	c	312	CLA	C2A-CAA-CBA-CGA
25	l	607	CLA	C5-C6-C7-C8
25	B	841	CLA	O2A-C1-C2-C3
25	j	211	CLA	O2A-C1-C2-C3
27	A	805	LHG	O8-C23-C24-C25
25	A	808	CLA	C3-C5-C6-C7
25	A	846	CLA	C3-C5-C6-C7
25	l	606	CLA	C4-C3-C5-C6
32	b	202	DGD	C6A-C7A-C8A-C9A
34	j	201	LMG	C32-C33-C34-C35
25	o	608	CLA	CAD-CBD-CGD-O2D
35	d	308	CHL	C3C-C2C-CMC-OMC
35	e	209	CHL	C3C-C2C-CMC-OMC
25	B	805	CLA	O1A-CGA-O2A-C1
27	i	201	LHG	O10-C23-O8-C6
25	l	602	CLA	C10-C11-C12-C13
25	m	203	CLA	O1D-CGD-O2D-CED
25	B	815	CLA	C2A-CAA-CBA-CGA
34	k	201	LMG	C11-C12-C13-C14
27	A	835	LHG	O6-C4-C5-O7
27	c	301	LHG	O6-C4-C5-O7
25	j	209	CLA	CBA-CGA-O2A-C1
25	n	211	CLA	O1D-CGD-O2D-CED
25	A	833	CLA	O1A-CGA-O2A-C1
32	B	849	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
33	D	200	SQD	O47-C45-C46-O48
33	g	202	SQD	O6-C44-C45-O47
34	a	202	LMG	O1-C7-C8-O7
25	A	818	CLA	CBA-CGA-O2A-C1
25	A	824	CLA	C5-C6-C7-C8
25	i	211	CLA	CAA-CBA-CGA-O2A
25	A	808	CLA	C11-C12-C13-C15
25	A	826	CLA	C16-C17-C18-C20
27	d	302	LHG	C1-C2-C3-O3
25	A	823	CLA	C16-C17-C18-C19
25	J	103	CLA	C2-C1-O2A-CGA
25	b	204	CLA	C2-C1-O2A-CGA
25	i	208	CLA	C2-C1-O2A-CGA
25	j	211	CLA	C2-C1-O2A-CGA
25	k	208	CLA	C2-C1-O2A-CGA
25	A	812	CLA	O1A-CGA-O2A-C1
25	A	819	CLA	C5-C6-C7-C8
25	A	802	CLA	C11-C10-C8-C9
25	A	812	CLA	C11-C10-C8-C9
25	B	816	CLA	C11-C10-C8-C9
25	B	818	CLA	C6-C7-C8-C9
25	B	848	CLA	C11-C12-C13-C14
25	e	205	CLA	C14-C13-C15-C16
25	j	212	CLA	C14-C13-C15-C16
25	k	205	CLA	C6-C7-C8-C9
25	h	215	CLA	CBD-CGD-O2D-CED
34	a	202	LMG	C14-C15-C16-C17
25	A	804	CLA	C2A-CAA-CBA-CGA
25	A	817	CLA	C2A-CAA-CBA-CGA
25	l	602	CLA	C2A-CAA-CBA-CGA
25	l	610	CLA	C2A-CAA-CBA-CGA
25	A	818	CLA	C16-C17-C18-C20
25	B	821	CLA	C11-C12-C13-C14
25	B	822	CLA	C11-C12-C13-C15
25	B	845	CLA	C16-C17-C18-C19
25	B	821	CLA	C1-C2-C3-C5
25	B	848	CLA	C1-C2-C3-C5
29	B	801	BCR	C23-C24-C25-C30
29	B	828	BCR	C5-C6-C7-C8
29	B	831	BCR	C23-C24-C25-C26
29	B	831	BCR	C23-C24-C25-C30
29	J	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	J	101	BCR	C5-C6-C7-C8
30	c	316	DD6	C12-C11-C13-C14
25	h	209	CLA	C6-C7-C8-C9
25	i	202	CLA	C5-C6-C7-C8
34	a	202	LMG	C11-C12-C13-C14
25	b	203	CLA	C1A-C2A-CAA-CBA
25	b	210	CLA	C1A-C2A-CAA-CBA
25	e	204	CLA	C1A-C2A-CAA-CBA
25	f	608	CLA	C1A-C2A-CAA-CBA
25	g	210	CLA	C1A-C2A-CAA-CBA
25	p	601	CLA	C1A-C2A-CAA-CBA
25	p	603	CLA	C1A-C2A-CAA-CBA
29	B	828	BCR	C21-C22-C23-C24
30	b	214	DD6	C2-C1-C24-C25
30	g	216	DD6	C10-C11-C13-C14
25	A	846	CLA	C8-C10-C11-C12
25	b	206	CLA	O1D-CGD-O2D-CED
25	A	817	CLA	C11-C10-C8-C9
30	F	203	DD6	C25-C26-C27-C28
25	i	209	CLA	CBD-CGD-O2D-CED
25	B	813	CLA	C2-C1-O2A-CGA
27	A	805	LHG	O6-C4-C5-C6
27	b	201	LHG	O6-C4-C5-C6
25	A	846	CLA	C4-C3-C5-C6
25	A	801	CLA	C12-C13-C15-C16
25	A	807	CLA	C12-C13-C15-C16
25	A	808	CLA	C6-C7-C8-C10
25	A	809	CLA	C11-C10-C8-C7
25	A	820	CLA	C11-C10-C8-C7
25	A	829	CLA	C11-C10-C8-C7
25	A	846	CLA	C11-C10-C8-C7
25	A	846	CLA	C11-C12-C13-C15
25	B	804	CLA	C11-C10-C8-C7
25	B	805	CLA	C11-C10-C8-C7
25	B	824	CLA	C12-C13-C15-C16
25	B	841	CLA	C11-C10-C8-C7
25	d	312	CLA	C6-C7-C8-C10
25	e	205	CLA	C12-C13-C15-C16
25	i	206	CLA	C6-C7-C8-C10
25	i	211	CLA	C2-C3-C5-C6
25	j	209	CLA	C11-C10-C8-C7
25	j	212	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	k	205	CLA	C11-C10-C8-C7
28	A	834	PQN	C17-C18-C20-C21
25	B	843	CLA	C1-C2-C3-C4
29	A	837	BCR	C15-C16-C17-C18
30	f	614	DD6	C24-C25-C26-C27
25	A	830	CLA	O1D-CGD-O2D-CED
25	B	812	CLA	C15-C16-C17-C18
27	A	805	LHG	C23-C24-C25-C26
25	j	208	CLA	O1D-CGD-O2D-CED
25	A	819	CLA	C15-C16-C17-C18
25	B	812	CLA	C2A-CAA-CBA-CGA
25	B	837	CLA	C2A-CAA-CBA-CGA
29	J	101	BCR	C20-C21-C22-C37
30	e	218	DD6	C-C1-C2-C3
25	B	814	CLA	C11-C12-C13-C14
25	e	211	CLA	CBA-CGA-O2A-C1
25	h	208	CLA	CBA-CGA-O2A-C1
25	A	801	CLA	CAD-CBD-CGD-O2D
25	A	821	CLA	CAD-CBD-CGD-O2D
25	A	852	CLA	CAD-CBD-CGD-O2D
25	B	840	CLA	CAD-CBD-CGD-O2D
25	c	310	CLA	CAD-CBD-CGD-O2D
25	e	205	CLA	CAD-CBD-CGD-O2D
25	i	204	CLA	CAD-CBD-CGD-O2D
25	i	206	CLA	CAD-CBD-CGD-O2D
25	i	209	CLA	CAD-CBD-CGD-O2D
25	j	205	CLA	CAD-CBD-CGD-O2D
25	m	209	CLA	CAD-CBD-CGD-O2D
25	g	210	CLA	CAD-CBD-CGD-O2D
35	d	310	CHL	CAD-CBD-CGD-O2D
35	e	209	CHL	CAD-CBD-CGD-O2D
25	l	606	CLA	C11-C12-C13-C14
32	b	202	DGD	C4A-C5A-C6A-C7A
27	c	301	LHG	C4-C5-C6-O8
32	B	849	DGD	C1G-C2G-C3G-O3G
25	A	821	CLA	CBD-CGD-O2D-CED
27	d	302	LHG	O6-C4-C5-O7
27	m	201	LHG	O6-C4-C5-O7
27	g	201	LHG	O6-C4-C5-O7
25	A	846	CLA	C5-C6-C7-C8
25	B	819	CLA	C8-C10-C11-C12
25	B	843	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	f	610	CLA	C2A-CAA-CBA-CGA
25	B	804	CLA	C16-C17-C18-C19
25	A	806	CLA	CHA-CBD-CGD-O1D
25	A	808	CLA	CHA-CBD-CGD-O1D
25	A	809	CLA	CHA-CBD-CGD-O2D
25	A	812	CLA	CHA-CBD-CGD-O1D
25	A	815	CLA	CHA-CBD-CGD-O1D
25	A	821	CLA	CHA-CBD-CGD-O1D
25	A	823	CLA	CHA-CBD-CGD-O1D
25	A	826	CLA	CHA-CBD-CGD-O1D
25	A	842	CLA	CHA-CBD-CGD-O2D
25	A	847	CLA	CHA-CBD-CGD-O2D
25	A	849	CLA	CHA-CBD-CGD-O1D
25	A	853	CLA	CHA-CBD-CGD-O1D
25	B	804	CLA	CHA-CBD-CGD-O1D
25	B	804	CLA	CHA-CBD-CGD-O2D
25	B	807	CLA	CHA-CBD-CGD-O1D
25	B	809	CLA	CHA-CBD-CGD-O1D
25	B	811	CLA	CHA-CBD-CGD-O1D
25	B	816	CLA	CHA-CBD-CGD-O1D
25	B	842	CLA	CHA-CBD-CGD-O2D
25	B	846	CLA	CHA-CBD-CGD-O1D
25	B	848	CLA	CHA-CBD-CGD-O1D
25	a	205	CLA	CHA-CBD-CGD-O1D
25	b	204	CLA	CHA-CBD-CGD-O2D
25	b	209	CLA	CHA-CBD-CGD-O1D
25	b	211	CLA	CHA-CBD-CGD-O1D
25	b	213	CLA	CHA-CBD-CGD-O2D
25	c	312	CLA	CHA-CBD-CGD-O1D
25	d	303	CLA	CHA-CBD-CGD-O1D
25	e	204	CLA	CHA-CBD-CGD-O1D
25	e	206	CLA	CHA-CBD-CGD-O1D
25	h	204	CLA	CHA-CBD-CGD-O1D
25	i	204	CLA	CHA-CBD-CGD-O1D
25	j	204	CLA	CHA-CBD-CGD-O1D
25	j	213	CLA	CHA-CBD-CGD-O2D
25	k	209	CLA	CHA-CBD-CGD-O2D
25	k	211	CLA	CHA-CBD-CGD-O2D
25	l	604	CLA	CHA-CBD-CGD-O2D
25	l	612	CLA	CHA-CBD-CGD-O2D
25	m	204	CLA	CHA-CBD-CGD-O1D
25	f	601	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	f	607	CLA	CHA-CBD-CGD-O2D
25	g	204	CLA	CHA-CBD-CGD-O1D
25	g	208	CLA	CHA-CBD-CGD-O1D
25	n	201	CLA	CHA-CBD-CGD-O1D
25	n	202	CLA	CHA-CBD-CGD-O1D
25	o	602	CLA	CHA-CBD-CGD-O2D
25	o	603	CLA	CHA-CBD-CGD-O1D
25	p	607	CLA	CHA-CBD-CGD-O1D
25	p	607	CLA	CHA-CBD-CGD-O2D
25	l	607	CLA	C3-C5-C6-C7
25	a	211	CLA	CBD-CGD-O2D-CED
25	A	842	CLA	O1A-CGA-O2A-C1
25	B	821	CLA	O1A-CGA-O2A-C1
25	B	848	CLA	O1A-CGA-O2A-C1
25	d	303	CLA	O1A-CGA-O2A-C1
25	e	216	CLA	O1A-CGA-O2A-C1
30	J	105	DD6	C4-C5-C6-C8
30	e	220	DD6	C24-C1-C2-C3
30	n	214	DD6	C9-C10-C11-C13
25	B	808	CLA	C2A-CAA-CBA-CGA
27	g	201	LHG	O7-C5-C6-O8
33	J	102	SQD	O6-C44-C45-O47
25	B	812	CLA	O1A-CGA-O2A-C1
27	c	301	LHG	C11-C10-C9-C8
25	f	607	CLA	C6-C7-C8-C9
25	B	812	CLA	C3-C5-C6-C7
25	A	810	CLA	C14-C13-C15-C16
25	B	819	CLA	C6-C7-C8-C9
25	a	213	CLA	C11-C10-C8-C9
25	b	207	CLA	O1D-CGD-O2D-CED
25	c	314	CLA	O1D-CGD-O2D-CED
25	a	204	CLA	O1A-CGA-O2A-C1
25	B	842	CLA	O1D-CGD-O2D-CED
25	f	603	CLA	O1D-CGD-O2D-CED
25	A	843	CLA	C2A-CAA-CBA-CGA
25	j	207	CLA	C2A-CAA-CBA-CGA
25	f	602	CLA	CBD-CGD-O2D-CED
25	A	852	CLA	O2A-C1-C2-C3
25	B	843	CLA	C15-C16-C17-C18
29	A	839	BCR	C17-C18-C19-C20
30	c	316	DD6	C10-C11-C13-C14
25	o	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	810	CLA	C1A-C2A-CAA-CBA
25	A	844	CLA	C11-C12-C13-C14
25	B	845	CLA	C13-C15-C16-C17
25	B	802	CLA	C2-C1-O2A-CGA
34	e	202	LMG	C30-C31-C32-C33
30	F	203	DD6	C11-C10-C9-C8
30	J	105	DD6	C24-C25-C26-C27
30	n	212	DD6	C24-C25-C26-C27
27	a	201	LHG	O2-C2-C3-O3
27	c	301	LHG	C2-C3-O3-P
27	d	302	LHG	C2-C3-O3-P
25	A	813	CLA	C4B-C3B-CAB-CBB
25	A	832	CLA	C4B-C3B-CAB-CBB
25	B	802	CLA	C4B-C3B-CAB-CBB
25	B	812	CLA	C4B-C3B-CAB-CBB
25	B	839	CLA	C4B-C3B-CAB-CBB
25	c	314	CLA	C4B-C3B-CAB-CBB
25	e	210	CLA	C4B-C3B-CAB-CBB
25	h	213	CLA	C4B-C3B-CAB-CBB
25	k	205	CLA	C4B-C3B-CAB-CBB
25	n	203	CLA	C4B-C3B-CAB-CBB
25	p	602	CLA	C4B-C3B-CAB-CBB
27	b	201	LHG	C3-O3-P-O4
27	b	201	LHG	C4-O6-P-O4
27	j	202	LHG	C4-O6-P-O4
27	m	201	LHG	C3-O3-P-O5
27	g	201	LHG	C3-O3-P-O4
27	g	201	LHG	C4-O6-P-O5
25	A	826	CLA	C16-C17-C18-C19
25	A	832	CLA	CBA-CGA-O2A-C1
25	B	847	CLA	CBA-CGA-O2A-C1
25	c	315	CLA	CBD-CGD-O2D-CED
27	h	202	LHG	O6-C4-C5-C6
25	e	215	CLA	C2A-CAA-CBA-CGA
25	c	305	CLA	O2A-C1-C2-C3
25	i	203	CLA	C16-C17-C18-C20
25	k	206	CLA	O1D-CGD-O2D-CED
25	A	801	CLA	CAD-CBD-CGD-O1D
25	A	806	CLA	CAD-CBD-CGD-O1D
25	A	815	CLA	CAD-CBD-CGD-O1D
25	A	823	CLA	CAD-CBD-CGD-O1D
25	A	848	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	849	CLA	CAD-CBD-CGD-O1D
25	A	853	CLA	CAD-CBD-CGD-O1D
25	B	804	CLA	CAD-CBD-CGD-O1D
25	B	809	CLA	CAD-CBD-CGD-O1D
25	B	811	CLA	CAD-CBD-CGD-O1D
25	B	846	CLA	CAD-CBD-CGD-O1D
25	B	848	CLA	CAD-CBD-CGD-O1D
25	c	302	CLA	CAD-CBD-CGD-O1D
25	d	303	CLA	CAD-CBD-CGD-O1D
25	e	206	CLA	CAD-CBD-CGD-O1D
25	e	210	CLA	CAD-CBD-CGD-O1D
25	l	609	CLA	CAD-CBD-CGD-O1D
25	f	611	CLA	CAD-CBD-CGD-O1D
25	g	204	CLA	CAD-CBD-CGD-O1D
25	g	211	CLA	CAD-CBD-CGD-O1D
25	n	202	CLA	CAD-CBD-CGD-O1D
25	p	602	CLA	CAD-CBD-CGD-O1D
25	A	830	CLA	CAA-CBA-CGA-O2A
28	F	205	PQN	C15-C16-C17-C18
27	i	201	LHG	C24-C25-C26-C27
27	j	202	LHG	C25-C26-C27-C28
25	B	822	CLA	CBA-CGA-O2A-C1
27	a	201	LHG	C1-C2-C3-O3
25	A	810	CLA	C11-C12-C13-C15
25	A	812	CLA	C12-C13-C15-C16
25	A	815	CLA	C11-C10-C8-C7
25	A	819	CLA	C12-C13-C15-C16
25	B	805	CLA	C6-C7-C8-C10
25	B	807	CLA	C11-C12-C13-C15
25	B	814	CLA	C11-C10-C8-C7
25	B	819	CLA	C6-C7-C8-C10
25	B	839	CLA	C11-C10-C8-C7
25	c	303	CLA	C6-C7-C8-C10
25	d	305	CLA	C3A-C2A-CAA-CBA
25	d	312	CLA	C11-C10-C8-C7
25	i	206	CLA	C12-C13-C15-C16
25	k	205	CLA	C6-C7-C8-C10
25	k	212	CLA	C3A-C2A-CAA-CBA
25	m	208	CLA	C3A-C2A-CAA-CBA
25	p	603	CLA	C3A-C2A-CAA-CBA
35	d	308	CHL	C3A-C2A-CAA-CBA
32	B	849	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
25	g	204	CLA	C3-C5-C6-C7
25	a	206	CLA	CBD-CGD-O2D-CED
25	d	312	CLA	C5-C6-C7-C8
25	A	814	CLA	C10-C11-C12-C13
32	e	203	DGD	C1G-C2G-C3G-O3G
33	J	102	SQD	O6-C44-C45-C46
35	c	307	CHL	C1C-C2C-CMC-OMC
35	d	307	CHL	C1C-C2C-CMC-OMC
35	d	309	CHL	C1C-C2C-CMC-OMC
35	e	209	CHL	C1C-C2C-CMC-OMC
34	k	201	LMG	O1-C7-C8-O7
27	j	202	LHG	C12-C13-C14-C15
25	e	205	CLA	O1A-CGA-O2A-C1
25	A	818	CLA	C15-C16-C17-C18
25	B	802	CLA	C13-C15-C16-C17
27	j	202	LHG	C26-C27-C28-C29
25	e	210	CLA	C2A-CAA-CBA-CGA
25	a	203	CLA	O1A-CGA-O2A-C1
25	B	822	CLA	C4-C3-C5-C6
25	A	801	CLA	C14-C13-C15-C16
25	A	804	CLA	C11-C10-C8-C9
25	A	807	CLA	C14-C13-C15-C16
25	A	819	CLA	C14-C13-C15-C16
25	A	820	CLA	C11-C10-C8-C9
25	A	823	CLA	C11-C12-C13-C14
25	A	824	CLA	C6-C7-C8-C9
25	A	846	CLA	C11-C10-C8-C9
25	B	824	CLA	C14-C13-C15-C16
25	a	204	CLA	C11-C10-C8-C9
25	A	849	CLA	O1A-CGA-O2A-C1
25	l	606	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	O1A-CGA-O2A-C1
29	J	101	BCR	C9-C10-C11-C12
25	l	602	CLA	O1D-CGD-O2D-CED
25	A	812	CLA	C2B-C3B-CAB-CBB
25	A	832	CLA	C2B-C3B-CAB-CBB
25	B	812	CLA	C2B-C3B-CAB-CBB
25	B	846	CLA	C2B-C3B-CAB-CBB
25	c	310	CLA	C2B-C3B-CAB-CBB
25	e	210	CLA	C2B-C3B-CAB-CBB
25	i	208	CLA	C2B-C3B-CAB-CBB
25	k	205	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	k	208	CLA	C2B-C3B-CAB-CBB
25	n	203	CLA	C2B-C3B-CAB-CBB
25	p	602	CLA	C2B-C3B-CAB-CBB
25	d	312	CLA	C8-C10-C11-C12
25	A	845	CLA	O1A-CGA-O2A-C1
25	i	206	CLA	C16-C17-C18-C20
34	k	201	LMG	O6-C5-C6-O5
25	B	815	CLA	C1-C2-C3-C4
34	a	202	LMG	C30-C31-C32-C33
25	A	841	CLA	C3-C5-C6-C7
27	A	835	LHG	O6-C4-C5-C6
25	A	833	CLA	C2A-CAA-CBA-CGA
25	a	212	CLA	C2A-CAA-CBA-CGA
25	k	211	CLA	C1-C2-C3-C5
25	A	822	CLA	CBA-CGA-O2A-C1
25	A	807	CLA	C2-C1-O2A-CGA
25	A	824	CLA	C2-C1-O2A-CGA
25	a	203	CLA	C2-C1-O2A-CGA
25	a	208	CLA	C2-C1-O2A-CGA
25	k	214	CLA	C2-C1-O2A-CGA
25	g	212	CLA	C2-C1-O2A-CGA
25	n	201	CLA	C2-C1-O2A-CGA
25	h	211	CLA	C10-C11-C12-C13
25	h	209	CLA	CAA-CBA-CGA-O2A
25	m	203	CLA	CAA-CBA-CGA-O2A
25	A	825	CLA	C10-C11-C12-C13
25	B	839	CLA	C3-C5-C6-C7
25	i	202	CLA	C3-C5-C6-C7
34	e	202	LMG	C11-C12-C13-C14
27	j	202	LHG	C5-C4-O6-P
27	A	805	LHG	O6-C4-C5-O7
25	A	820	CLA	O1D-CGD-O2D-CED
29	A	838	BCR	C1-C6-C7-C8
25	B	845	CLA	C2-C3-C5-C6
25	B	840	CLA	O1D-CGD-O2D-CED
25	B	803	CLA	C2C-C3C-CAC-CBC
25	B	821	CLA	C11-C12-C13-C15
32	B	849	DGD	C4B-C5B-C6B-C7B
27	A	805	LHG	C3-O3-P-O6
27	d	302	LHG	C3-O3-P-O6
27	m	201	LHG	C26-C27-C28-C29
25	B	818	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	A	812	CLA	C11-C12-C13-C15
25	B	818	CLA	C12-C13-C15-C16
25	B	848	CLA	CAA-CBA-CGA-O2A
25	A	815	CLA	C11-C10-C8-C9
25	B	814	CLA	C11-C10-C8-C9
25	f	602	CLA	C11-C10-C8-C9
29	B	828	BCR	C13-C14-C15-C16
30	d	318	DD6	C24-C25-C26-C27
25	B	839	CLA	C11-C12-C13-C15
27	g	201	LHG	C11-C12-C13-C14
27	A	835	LHG	C24-C25-C26-C27
25	B	813	CLA	CBA-CGA-O2A-C1
27	A	835	LHG	C19-C20-C21-C22
34	e	202	LMG	C36-C37-C38-C39
25	g	208	CLA	CBA-CGA-O2A-C1
27	j	202	LHG	C2-C3-O3-P
27	m	201	LHG	C2-C3-O3-P
30	m	212	DD6	C2-C1-C24-C25
25	A	817	CLA	C11-C10-C8-C7
34	e	202	LMG	C33-C34-C35-C36
25	i	206	CLA	C4-C3-C5-C6
25	A	825	CLA	O1A-CGA-O2A-C1
25	c	313	CLA	CBD-CGD-O2D-CED
25	c	309	CLA	C2-C3-C5-C6
25	e	213	CLA	C2-C3-C5-C6
25	i	206	CLA	C16-C17-C18-C19
25	c	305	CLA	CBA-CGA-O2A-C1
25	B	813	CLA	CBD-CGD-O2D-CED
25	e	206	CLA	CBD-CGD-O2D-CED
25	j	209	CLA	O1D-CGD-O2D-CED
25	A	812	CLA	C4B-C3B-CAB-CBB
25	i	208	CLA	C4B-C3B-CAB-CBB
35	e	209	CHL	CAA-CBA-CGA-O2A
29	A	836	BCR	C9-C10-C11-C12
29	B	829	BCR	C9-C10-C11-C12
29	M	201	BCR	C13-C14-C15-C16
30	c	318	DD6	C11-C10-C9-C8
30	e	220	DD6	C11-C10-C9-C8
30	g	217	DD6	C3-C4-C5-C6
27	a	201	LHG	C24-C25-C26-C27
25	A	817	CLA	O1A-CGA-O2A-C1
25	A	823	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B	845	CLA	C5-C6-C7-C8
26	A	803	LMT	C5-C6-C7-C8
25	o	606	CLA	CAA-CBA-CGA-O2A
25	n	202	CLA	O1A-CGA-O2A-C1
27	i	201	LHG	O10-C23-C24-C25
25	B	804	CLA	C4-C3-C5-C6
25	B	836	CLA	C4-C3-C5-C6
25	i	208	CLA	C4-C3-C5-C6
25	B	802	CLA	C15-C16-C17-C18
25	h	211	CLA	C2-C3-C5-C6
34	e	202	LMG	C21-C22-C23-C24
25	B	817	CLA	C2-C1-O2A-CGA
25	c	308	CLA	C2-C1-O2A-CGA
25	c	310	CLA	C2-C1-O2A-CGA
25	h	203	CLA	C2-C1-O2A-CGA
25	j	210	CLA	C2-C1-O2A-CGA
25	l	603	CLA	C2A-CAA-CBA-CGA
25	A	818	CLA	C2A-CAA-CBA-CGA
25	c	313	CLA	C2A-CAA-CBA-CGA
25	g	212	CLA	C2A-CAA-CBA-CGA
25	m	204	CLA	C6-C7-C8-C9
34	j	201	LMG	C37-C38-C39-C40
25	A	819	CLA	C3A-C2A-CAA-CBA
25	A	824	CLA	C3A-C2A-CAA-CBA
25	A	828	CLA	C3A-C2A-CAA-CBA
25	A	830	CLA	C3A-C2A-CAA-CBA
25	B	823	CLA	C3A-C2A-CAA-CBA
25	b	207	CLA	C3A-C2A-CAA-CBA
25	e	211	CLA	C3A-C2A-CAA-CBA
25	i	207	CLA	C3A-C2A-CAA-CBA
25	m	207	CLA	C3A-C2A-CAA-CBA
25	g	215	CLA	C3A-C2A-CAA-CBA
29	B	828	BCR	C9-C10-C11-C12
25	a	206	CLA	CAA-CBA-CGA-O2A
25	B	844	CLA	C2-C3-C5-C6
25	A	832	CLA	C11-C12-C13-C14
25	B	804	CLA	C11-C12-C13-C14
25	B	807	CLA	C14-C13-C15-C16
25	m	203	CLA	C6-C7-C8-C9
28	A	834	PQN	C21-C22-C23-C24
25	c	309	CLA	C11-C12-C13-C14
25	n	203	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	i	201	LHG	C4-C5-C6-O8
29	A	839	BCR	C11-C10-C9-C34
29	A	839	BCR	C16-C17-C18-C36
29	B	830	BCR	C11-C10-C9-C34
29	B	830	BCR	C20-C21-C22-C37
30	F	203	DD6	C4-C5-C6-C7
30	g	216	DD6	C4-C5-C6-C7
25	A	841	CLA	C8-C10-C11-C12
25	d	306	CLA	C2A-CAA-CBA-CGA
25	d	313	CLA	C2A-CAA-CBA-CGA
25	A	849	CLA	O2A-C1-C2-C3
25	B	836	CLA	O2A-C1-C2-C3
25	m	204	CLA	O2A-C1-C2-C3
25	n	202	CLA	O2A-C1-C2-C3
25	d	313	CLA	CAA-CBA-CGA-O1A
30	j	216	DD6	C12-C11-C13-C14
25	B	848	CLA	CAA-CBA-CGA-O1A
25	B	818	CLA	C13-C15-C16-C17
30	e	218	DD6	C10-C11-C13-C14
34	j	201	LMG	C30-C31-C32-C33
27	j	202	LHG	C4-C5-O7-C7
27	j	202	LHG	C6-C5-O7-C7
27	g	201	LHG	C6-C5-O7-C7
25	A	807	CLA	C1A-C2A-CAA-CBA
25	A	853	CLA	C1A-C2A-CAA-CBA
25	B	804	CLA	C1A-C2A-CAA-CBA
25	B	836	CLA	C1A-C2A-CAA-CBA
25	a	211	CLA	C1A-C2A-CAA-CBA
25	i	207	CLA	C1A-C2A-CAA-CBA
25	g	212	CLA	C1A-C2A-CAA-CBA
25	o	610	CLA	C1A-C2A-CAA-CBA
25	e	212	CLA	CBA-CGA-O2A-C1
25	A	833	CLA	C11-C12-C13-C15
25	B	811	CLA	C11-C10-C8-C7
25	i	203	CLA	C12-C13-C15-C16
25	l	606	CLA	C11-C10-C8-C7
25	B	840	CLA	C1-C2-C3-C5
25	A	853	CLA	O1D-CGD-O2D-CED
25	B	815	CLA	CBA-CGA-O2A-C1
35	e	209	CHL	CAA-CBA-CGA-O1A
25	n	201	CLA	C11-C12-C13-C14
25	c	303	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	k	205	CLA	C5-C6-C7-C8
25	A	820	CLA	O1A-CGA-O2A-C1
34	k	201	LMG	C4-C5-C6-O5
25	p	607	CLA	CAA-CBA-CGA-O1A
32	e	203	DGD	C1B-C2B-C3B-C4B
35	d	307	CHL	CBA-CGA-O2A-C1
25	g	207	CLA	CAA-CBA-CGA-O2A
25	o	606	CLA	CAA-CBA-CGA-O1A
25	p	607	CLA	CAA-CBA-CGA-O2A
25	B	807	CLA	C4-C3-C5-C6
25	f	610	CLA	C4-C3-C5-C6
25	A	813	CLA	C2B-C3B-CAB-CBB
25	B	802	CLA	C2B-C3B-CAB-CBB
25	B	839	CLA	C2B-C3B-CAB-CBB
25	c	314	CLA	C2B-C3B-CAB-CBB
25	h	213	CLA	C2B-C3B-CAB-CBB
25	F	202	CLA	CAA-CBA-CGA-O1A
25	A	814	CLA	O1A-CGA-O2A-C1
25	B	809	CLA	O1D-CGD-O2D-CED
25	B	821	CLA	O1D-CGD-O2D-CED
29	A	839	BCR	C11-C10-C9-C8
29	A	839	BCR	C16-C17-C18-C19
29	B	830	BCR	C11-C10-C9-C8
29	B	830	BCR	C20-C21-C22-C23
29	J	101	BCR	C20-C21-C22-C23
30	F	203	DD6	C4-C5-C6-C8
30	g	216	DD6	C4-C5-C6-C8
25	e	206	CLA	CAA-CBA-CGA-O1A
27	A	835	LHG	C9-C10-C11-C12
33	D	200	SQD	O6-C44-C45-O47
25	B	804	CLA	C16-C17-C18-C20
25	B	844	CLA	O1A-CGA-O2A-C1
27	A	835	LHG	C33-C34-C35-C36
25	A	815	CLA	C2-C1-O2A-CGA
25	B	811	CLA	C2-C1-O2A-CGA
25	a	212	CLA	C2-C1-O2A-CGA
25	j	209	CLA	C2-C1-O2A-CGA
25	p	605	CLA	C3A-C2A-CAA-CBA
25	d	313	CLA	CAA-CBA-CGA-O2A
25	b	211	CLA	O1D-CGD-O2D-CED
25	A	832	CLA	CAA-CBA-CGA-O2A
25	c	310	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	k	205	CLA	C14-C13-C15-C16
25	A	815	CLA	O1A-CGA-O2A-C1
25	A	822	CLA	C5-C6-C7-C8
34	e	202	LMG	C14-C15-C16-C17
25	e	206	CLA	CAA-CBA-CGA-O2A
25	A	802	CLA	C15-C16-C17-C18
27	j	202	LHG	C24-C25-C26-C27
25	h	212	CLA	C5-C6-C7-C8
25	A	814	CLA	C2A-CAA-CBA-CGA
25	A	815	CLA	C2A-CAA-CBA-CGA
25	A	844	CLA	C2A-CAA-CBA-CGA
25	g	209	CLA	C2A-CAA-CBA-CGA
25	f	607	CLA	C6-C7-C8-C10
27	d	302	LHG	C11-C10-C9-C8
29	A	839	BCR	C5-C6-C7-C8
29	B	801	BCR	C1-C6-C7-C8
29	B	830	BCR	C1-C6-C7-C8
29	B	832	BCR	C23-C24-C25-C30
29	B	833	BCR	C1-C6-C7-C8
29	B	833	BCR	C23-C24-C25-C30
25	A	808	CLA	C8-C10-C11-C12
25	A	801	CLA	CAA-CBA-CGA-O2A
25	a	204	CLA	CAA-CBA-CGA-O2A
27	g	201	LHG	O1-C1-C2-C3
25	m	203	CLA	CAA-CBA-CGA-O1A
29	A	836	BCR	C15-C16-C17-C18
30	F	203	DD6	C24-C25-C26-C27
30	f	613	DD6	C11-C10-C9-C8
30	o	611	DD6	C24-C25-C26-C27
25	B	811	CLA	C4-C3-C5-C6
25	e	216	CLA	C4-C3-C5-C6
28	F	205	PQN	C14-C13-C15-C16
25	d	305	CLA	C1A-C2A-CAA-CBA
25	l	611	CLA	C1A-C2A-CAA-CBA
25	B	839	CLA	C11-C12-C13-C14
25	e	205	CLA	C8-C10-C11-C12
25	B	804	CLA	C2-C3-C5-C6
25	j	212	CLA	CAA-CBA-CGA-O2A
25	B	811	CLA	C3-C5-C6-C7
25	a	206	CLA	CAA-CBA-CGA-O1A
25	p	606	CLA	C2C-C3C-CAC-CBC
34	a	202	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	B	818	CLA	C16-C17-C18-C20
25	m	211	CLA	C2C-C3C-CAC-CBC
25	l	607	CLA	C6-C7-C8-C9
25	n	208	CLA	CAA-CBA-CGA-O1A
25	B	836	CLA	C2A-CAA-CBA-CGA
25	h	212	CLA	CAA-CBA-CGA-O2A
25	A	857	CLA	C4-C3-C5-C6
25	A	824	CLA	C10-C11-C12-C13
25	A	840	CLA	C2-C3-C5-C6
25	B	805	CLA	C11-C12-C13-C15
25	B	807	CLA	C11-C10-C8-C7
25	B	814	CLA	C6-C7-C8-C10
25	B	848	CLA	C11-C12-C13-C15
25	n	201	CLA	C11-C10-C8-C7
25	B	841	CLA	CBA-CGA-O2A-C1
25	B	823	CLA	CBD-CGD-O2D-CED
25	A	821	CLA	C1-C2-C3-C4
25	A	824	CLA	C1-C2-C3-C4
25	A	829	CLA	C1-C2-C3-C4
25	A	848	CLA	C1-C2-C3-C4
25	A	857	CLA	C1-C2-C3-C4
25	B	802	CLA	C1-C2-C3-C4
25	B	822	CLA	C1-C2-C3-C4
25	B	836	CLA	C1-C2-C3-C4
25	B	844	CLA	C1-C2-C3-C4
25	a	209	CLA	C1-C2-C3-C4
25	a	212	CLA	C1-C2-C3-C4
25	d	306	CLA	C1-C2-C3-C4
25	h	209	CLA	C1-C2-C3-C4
25	j	212	CLA	C1-C2-C3-C4
25	k	205	CLA	C1-C2-C3-C4
25	n	201	CLA	C1-C2-C3-C4
30	a	214	DD6	C11-C10-C9-C8
30	m	212	DD6	C3-C4-C5-C6
25	l	610	CLA	CAA-CBA-CGA-O2A
34	e	202	LMG	O7-C8-C9-O8
34	e	202	LMG	C40-C41-C42-C43
25	B	820	CLA	C2A-CAA-CBA-CGA
27	A	805	LHG	O10-C23-C24-C25
25	A	842	CLA	O2A-C1-C2-C3
25	A	810	CLA	CAA-CBA-CGA-O2A
25	g	207	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	B	831	BCR	C35-C13-C14-C15
29	B	832	BCR	C20-C21-C22-C37
25	l	607	CLA	CAA-CBA-CGA-O2A
25	h	209	CLA	CAA-CBA-CGA-O1A
25	c	313	CLA	C4-C3-C5-C6
25	g	212	CLA	C4-C3-C5-C6
28	B	827	PQN	C14-C13-C15-C16
25	A	818	CLA	C8-C10-C11-C12
25	B	807	CLA	C2-C3-C5-C6
25	B	821	CLA	C2-C3-C5-C6
25	a	207	CLA	C2-C3-C5-C6
25	f	610	CLA	C2-C3-C5-C6
25	B	804	CLA	CAA-CBA-CGA-O2A
25	A	810	CLA	C11-C12-C13-C14
25	A	821	CLA	C6-C7-C8-C9
25	A	833	CLA	C6-C7-C8-C9
25	A	846	CLA	C14-C13-C15-C16
25	B	807	CLA	C11-C10-C8-C9
25	a	204	CLA	C6-C7-C8-C9
25	i	206	CLA	C14-C13-C15-C16
25	A	807	CLA	C3A-C2A-CAA-CBA
25	A	853	CLA	C3A-C2A-CAA-CBA
25	A	857	CLA	C3A-C2A-CAA-CBA
25	B	804	CLA	C3A-C2A-CAA-CBA
25	B	821	CLA	C3A-C2A-CAA-CBA
25	B	837	CLA	C3A-C2A-CAA-CBA
25	a	206	CLA	C3A-C2A-CAA-CBA
25	a	211	CLA	C3A-C2A-CAA-CBA
25	a	212	CLA	C3A-C2A-CAA-CBA
25	m	205	CLA	C3A-C2A-CAA-CBA
25	f	610	CLA	C3A-C2A-CAA-CBA
25	n	208	CLA	C3A-C2A-CAA-CBA
25	o	610	CLA	C3A-C2A-CAA-CBA
35	d	310	CHL	C3A-C2A-CAA-CBA
27	A	805	LHG	O10-C23-O8-C6
25	c	310	CLA	CAA-CBA-CGA-O2A
27	A	835	LHG	O8-C23-C24-C25
33	F	204	SQD	O48-C23-C24-C25
25	b	209	CLA	CAA-CBA-CGA-O1A
25	A	816	CLA	CAD-CBD-CGD-O2D
25	A	822	CLA	CAD-CBD-CGD-O2D
25	A	833	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	A	849	CLA	CAD-CBD-CGD-O2D
25	B	811	CLA	CAD-CBD-CGD-O2D
25	B	812	CLA	CAD-CBD-CGD-O2D
25	B	819	CLA	CAD-CBD-CGD-O2D
25	B	820	CLA	CAD-CBD-CGD-O2D
25	B	825	CLA	CAD-CBD-CGD-O2D
25	J	103	CLA	CAD-CBD-CGD-O2D
25	a	205	CLA	CAD-CBD-CGD-O2D
25	b	212	CLA	CAD-CBD-CGD-O2D
25	c	305	CLA	CAD-CBD-CGD-O2D
25	c	309	CLA	CAD-CBD-CGD-O2D
25	c	312	CLA	CAD-CBD-CGD-O2D
25	e	201	CLA	CAD-CBD-CGD-O2D
25	e	208	CLA	CAD-CBD-CGD-O2D
25	e	215	CLA	CAD-CBD-CGD-O2D
25	i	210	CLA	CAD-CBD-CGD-O2D
25	j	211	CLA	CAD-CBD-CGD-O2D
25	k	209	CLA	CAD-CBD-CGD-O2D
25	k	210	CLA	CAD-CBD-CGD-O2D
25	l	605	CLA	CAD-CBD-CGD-O2D
25	m	204	CLA	CAD-CBD-CGD-O2D
25	f	611	CLA	CAD-CBD-CGD-O2D
25	g	205	CLA	CAD-CBD-CGD-O2D
25	g	207	CLA	CAD-CBD-CGD-O2D
25	n	204	CLA	CAD-CBD-CGD-O2D
25	n	209	CLA	CAD-CBD-CGD-O2D
25	p	602	CLA	CAD-CBD-CGD-O2D
30	b	215	DD6	C24-C25-C26-C27
25	A	851	CLA	CAA-CBA-CGA-O1A
25	n	203	CLA	C4C-C3C-CAC-CBC
25	a	205	CLA	CAA-CBA-CGA-O2A
25	B	824	CLA	C4-C3-C5-C6
25	F	202	CLA	CAA-CBA-CGA-O2A
25	m	203	CLA	C2-C3-C5-C6
25	A	850	CLA	CAA-CBA-CGA-O2A
25	i	208	CLA	CAA-CBA-CGA-O2A
29	M	201	BCR	C11-C12-C13-C14
30	h	216	DD6	C10-C11-C13-C14
30	i	216	DD6	C10-C11-C13-C14
30	j	216	DD6	C10-C11-C13-C14
30	b	214	DD6	C13-C14-C15-O1
30	m	213	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
32	b	202	DGD	C1G-C2G-C3G-O3G
25	a	210	CLA	CAA-CBA-CGA-O1A
25	A	808	CLA	CAA-CBA-CGA-O2A
25	B	815	CLA	CAA-CBA-CGA-O2A
27	m	201	LHG	O8-C23-C24-C25
25	A	829	CLA	O2A-C1-C2-C3
25	c	308	CLA	O2A-C1-C2-C3
25	e	201	CLA	O2A-C1-C2-C3
25	g	208	CLA	O2A-C1-C2-C3
25	A	829	CLA	O1A-CGA-O2A-C1
25	i	211	CLA	C2A-CAA-CBA-CGA
25	l	608	CLA	C2A-CAA-CBA-CGA
25	A	815	CLA	CAA-CBA-CGA-O2A
25	A	843	CLA	CAA-CBA-CGA-O2A
25	a	210	CLA	CAA-CBA-CGA-O2A
25	A	801	CLA	CHA-CBD-CGD-O1D
25	A	818	CLA	CHA-CBD-CGD-O2D
25	A	820	CLA	CHA-CBD-CGD-O2D
25	A	823	CLA	CHA-CBD-CGD-O2D
25	A	826	CLA	CHA-CBD-CGD-O2D
25	A	828	CLA	CHA-CBD-CGD-O2D
25	A	842	CLA	CHA-CBD-CGD-O1D
25	A	847	CLA	CHA-CBD-CGD-O1D
25	B	815	CLA	CHA-CBD-CGD-O2D
25	B	816	CLA	CHA-CBD-CGD-O2D
25	B	822	CLA	CHA-CBD-CGD-O2D
25	B	824	CLA	CHA-CBD-CGD-O2D
25	B	837	CLA	CHA-CBD-CGD-O1D
25	B	837	CLA	CHA-CBD-CGD-O2D
25	B	845	CLA	CHA-CBD-CGD-O1D
25	B	845	CLA	CHA-CBD-CGD-O2D
25	J	103	CLA	CHA-CBD-CGD-O2D
25	a	204	CLA	CHA-CBD-CGD-O2D
25	a	206	CLA	CHA-CBD-CGD-O1D
25	a	210	CLA	CHA-CBD-CGD-O2D
25	b	212	CLA	CHA-CBD-CGD-O1D
25	c	302	CLA	CHA-CBD-CGD-O1D
25	c	303	CLA	CHA-CBD-CGD-O2D
25	c	306	CLA	CHA-CBD-CGD-O2D
25	d	301	CLA	CHA-CBD-CGD-O2D
25	d	304	CLA	CHA-CBD-CGD-O1D
25	d	314	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	e	204	CLA	CHA-CBD-CGD-O2D
25	e	210	CLA	CHA-CBD-CGD-O1D
25	h	205	CLA	CHA-CBD-CGD-O1D
25	h	210	CLA	CHA-CBD-CGD-O2D
25	h	212	CLA	CHA-CBD-CGD-O2D
25	i	202	CLA	CHA-CBD-CGD-O2D
25	i	212	CLA	CHA-CBD-CGD-O2D
25	j	203	CLA	CHA-CBD-CGD-O2D
25	j	204	CLA	CHA-CBD-CGD-O2D
25	j	206	CLA	CHA-CBD-CGD-O2D
25	l	601	CLA	CHA-CBD-CGD-O2D
25	l	602	CLA	CHA-CBD-CGD-O2D
25	l	611	CLA	CHA-CBD-CGD-O2D
25	m	202	CLA	CHA-CBD-CGD-O2D
25	m	203	CLA	CHA-CBD-CGD-O2D
25	m	205	CLA	CHA-CBD-CGD-O2D
25	f	604	CLA	CHA-CBD-CGD-O1D
25	f	612	CLA	CHA-CBD-CGD-O2D
25	g	204	CLA	CHA-CBD-CGD-O2D
25	g	206	CLA	CHA-CBD-CGD-O2D
25	g	211	CLA	CHA-CBD-CGD-O2D
25	n	201	CLA	CHA-CBD-CGD-O2D
25	n	202	CLA	CHA-CBD-CGD-O2D
25	n	204	CLA	CHA-CBD-CGD-O2D
25	p	605	CLA	CHA-CBD-CGD-O1D
25	p	608	CLA	CHA-CBD-CGD-O1D
25	B	819	CLA	CAA-CBA-CGA-O2A
25	n	202	CLA	CAA-CBA-CGA-O2A
25	A	819	CLA	C3-C5-C6-C7
27	m	201	LHG	O6-C4-C5-C6
25	c	309	CLA	CAA-CBA-CGA-O2A
25	k	208	CLA	CAA-CBA-CGA-O2A
34	k	201	LMG	O7-C8-C9-O8
25	A	809	CLA	CAA-CBA-CGA-O2A
25	f	607	CLA	CAA-CBA-CGA-O2A
25	e	207	CLA	C2A-CAA-CBA-CGA
25	e	212	CLA	C2A-CAA-CBA-CGA
27	g	201	LHG	O1-C1-C2-O2
27	A	805	LHG	C24-C23-O8-C6
32	B	849	DGD	O2G-C1B-C2B-C3B
25	B	839	CLA	C6-C7-C8-C10
25	B	844	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	B	814	CLA	C6-C7-C8-C9
25	B	839	CLA	C6-C7-C8-C9
25	i	203	CLA	C14-C13-C15-C16
28	A	834	PQN	C24-C23-C25-C26
30	g	217	DD6	C24-C25-C26-C27
35	d	310	CHL	CAA-CBA-CGA-O2A
25	A	852	CLA	CBA-CGA-O2A-C1
25	A	817	CLA	CAA-CBA-CGA-O2A
25	i	202	CLA	CAA-CBA-CGA-O2A
33	J	102	SQD	C4-C5-C6-S
33	g	202	SQD	C4-C5-C6-S
25	B	807	CLA	CBD-CGD-O2D-CED
25	j	206	CLA	C1-C2-C3-C5
27	b	201	LHG	C30-C31-C32-C33
25	i	213	CLA	CAA-CBA-CGA-O1A
25	h	204	CLA	CAA-CBA-CGA-O2A
27	a	201	LHG	O8-C23-C24-C25
29	B	830	BCR	C7-C8-C9-C34
25	j	209	CLA	C8-C10-C11-C12
27	i	201	LHG	O1-C1-C2-C3
25	i	202	CLA	CAA-CBA-CGA-O1A
25	n	202	CLA	CAA-CBA-CGA-O1A
29	B	830	BCR	C7-C8-C9-C10
25	A	806	CLA	C1A-C2A-CAA-CBA
25	A	819	CLA	C1A-C2A-CAA-CBA
25	A	850	CLA	C1A-C2A-CAA-CBA
25	A	857	CLA	C1A-C2A-CAA-CBA
25	B	837	CLA	C1A-C2A-CAA-CBA
25	B	842	CLA	C1A-C2A-CAA-CBA
25	a	206	CLA	C1A-C2A-CAA-CBA
25	b	207	CLA	C1A-C2A-CAA-CBA
25	i	213	CLA	C1A-C2A-CAA-CBA
25	l	610	CLA	C1A-C2A-CAA-CBA
25	m	205	CLA	C1A-C2A-CAA-CBA
25	m	207	CLA	C1A-C2A-CAA-CBA
25	m	210	CLA	C1A-C2A-CAA-CBA
25	f	610	CLA	C1A-C2A-CAA-CBA
25	n	208	CLA	C1A-C2A-CAA-CBA
25	o	608	CLA	C1A-C2A-CAA-CBA
25	b	212	CLA	CAA-CBA-CGA-O1A
25	m	204	CLA	CAA-CBA-CGA-O1A
25	l	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	k	211	CLA	C2-C1-O2A-CGA
25	c	308	CLA	CAA-CBA-CGA-O1A
25	f	607	CLA	CAA-CBA-CGA-O1A
27	m	201	LHG	O10-C23-C24-C25
27	g	201	LHG	C4-C5-C6-O8
25	A	830	CLA	C2A-CAA-CBA-CGA
25	F	202	CLA	C2A-CAA-CBA-CGA
25	e	205	CLA	C2A-CAA-CBA-CGA
25	g	204	CLA	C2A-CAA-CBA-CGA
25	A	843	CLA	CBD-CGD-O2D-CED
25	B	834	CLA	CBD-CGD-O2D-CED
25	l	607	CLA	CAA-CBA-CGA-O1A
27	a	201	LHG	O10-C23-C24-C25
25	B	844	CLA	C4-C3-C5-C6
25	B	811	CLA	C13-C15-C16-C17
25	B	805	CLA	CAA-CBA-CGA-O1A
25	h	208	CLA	CAA-CBA-CGA-O1A
25	j	211	CLA	CAA-CBA-CGA-O1A
27	A	835	LHG	O10-C23-C24-C25
25	A	831	CLA	O2A-C1-C2-C3
25	f	602	CLA	C11-C12-C13-C14
25	B	825	CLA	C4B-C3B-CAB-CBB
25	i	211	CLA	C4B-C3B-CAB-CBB
25	o	604	CLA	C4B-C3B-CAB-CBB
27	A	805	LHG	C4-O6-P-O5
27	a	201	LHG	C4-O6-P-O4
27	m	201	LHG	C4-O6-P-O5
25	A	812	CLA	C16-C17-C18-C19
25	m	211	CLA	C4C-C3C-CAC-CBC
34	a	202	LMG	O7-C10-C11-C12
29	A	839	BCR	C23-C24-C25-C26
25	A	813	CLA	C10-C11-C12-C13
25	i	203	CLA	C5-C6-C7-C8
30	n	212	DD6	C11-C13-C14-C15
25	a	207	CLA	CAA-CBA-CGA-O1A
25	B	802	CLA	CAA-CBA-CGA-O1A
25	c	304	CLA	CAA-CBA-CGA-O1A
25	b	207	CLA	CAA-CBA-CGA-O1A
25	c	308	CLA	CAA-CBA-CGA-O2A
27	A	835	LHG	O7-C7-C8-C9
25	J	103	CLA	CAA-CBA-CGA-O1A
25	A	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	844	CLA	CAD-CBD-CGD-O1D
25	A	852	CLA	CAD-CBD-CGD-O1D
25	B	841	CLA	CAD-CBD-CGD-O1D
25	a	211	CLA	CAD-CBD-CGD-O1D
25	b	205	CLA	CAD-CBD-CGD-O1D
25	d	305	CLA	CAD-CBD-CGD-O1D
25	h	203	CLA	CAD-CBD-CGD-O1D
25	h	212	CLA	CAD-CBD-CGD-O1D
25	k	204	CLA	CAD-CBD-CGD-O1D
25	l	603	CLA	CAD-CBD-CGD-O1D
25	g	205	CLA	CAD-CBD-CGD-O1D
25	g	206	CLA	CAD-CBD-CGD-O1D
25	c	313	CLA	O1A-CGA-O2A-C1
33	F	204	SQD	O10-C23-C24-C25
25	p	606	CLA	C4C-C3C-CAC-CBC
25	A	818	CLA	C14-C13-C15-C16
25	B	844	CLA	C11-C12-C13-C14
25	c	309	CLA	C11-C10-C8-C9
34	j	201	LMG	C31-C32-C33-C34
25	A	801	CLA	C10-C11-C12-C13
25	A	809	CLA	C8-C10-C11-C12
25	g	208	CLA	C1-C2-C3-C5
25	A	801	CLA	CAA-CBA-CGA-O1A
25	A	809	CLA	CAA-CBA-CGA-O1A
25	h	203	CLA	CAA-CBA-CGA-O1A
25	l	606	CLA	C11-C12-C13-C15
25	A	804	CLA	CAA-CBA-CGA-O2A
25	a	213	CLA	CAA-CBA-CGA-O2A
25	m	204	CLA	CAA-CBA-CGA-O2A
25	n	201	CLA	CAA-CBA-CGA-O2A
27	b	201	LHG	O8-C23-C24-C25
35	d	308	CHL	CAA-CBA-CGA-O1A
32	B	849	DGD	O1B-C1B-C2B-C3B
28	B	827	PQN	C23-C25-C26-C27
25	A	818	CLA	CBD-CGD-O2D-CED
33	D	200	SQD	C26-C27-C28-C29
25	A	823	CLA	CAA-CBA-CGA-O2A
25	c	304	CLA	CAA-CBA-CGA-O2A
27	m	201	LHG	O7-C7-C8-C9
25	b	209	CLA	CAA-CBA-CGA-O2A
27	a	201	LHG	C5-C4-O6-P
25	A	802	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	A	806	CLA	C3A-C2A-CAA-CBA
25	A	820	CLA	C3A-C2A-CAA-CBA
25	A	841	CLA	C6-C7-C8-C10
25	A	850	CLA	C3A-C2A-CAA-CBA
25	B	818	CLA	C2-C3-C5-C6
25	B	848	CLA	C3A-C2A-CAA-CBA
25	a	204	CLA	C6-C7-C8-C10
25	e	205	CLA	C11-C10-C8-C7
25	e	208	CLA	C3A-C2A-CAA-CBA
25	k	202	CLA	C3A-C2A-CAA-CBA
25	l	601	CLA	C3A-C2A-CAA-CBA
25	l	610	CLA	C3A-C2A-CAA-CBA
25	f	610	CLA	C11-C10-C8-C7
25	g	213	CLA	C3A-C2A-CAA-CBA
25	p	608	CLA	C3A-C2A-CAA-CBA
25	B	819	CLA	CAA-CBA-CGA-O1A
25	j	206	CLA	CAA-CBA-CGA-O1A
27	b	201	LHG	O10-C23-C24-C25
25	B	803	CLA	CAA-CBA-CGA-O2A
25	b	212	CLA	CAA-CBA-CGA-O2A
25	i	213	CLA	CAA-CBA-CGA-O2A
25	j	209	CLA	CAA-CBA-CGA-O2A
25	j	211	CLA	CAA-CBA-CGA-O2A
25	B	839	CLA	C1-C2-C3-C5
25	A	852	CLA	C2C-C3C-CAC-CBC
25	A	843	CLA	CAA-CBA-CGA-O1A
25	h	209	CLA	O1D-CGD-O2D-CED
25	c	309	CLA	CAA-CBA-CGA-O1A
25	i	208	CLA	CAA-CBA-CGA-O1A
27	b	201	LHG	O2-C2-C3-O3
27	d	302	LHG	O2-C2-C3-O3
25	B	802	CLA	CAA-CBA-CGA-O2A
25	h	207	CLA	CAA-CBA-CGA-O1A
34	a	202	LMG	O9-C10-C11-C12
25	n	203	CLA	C2A-CAA-CBA-CGA
25	A	812	CLA	CBA-CGA-O2A-C1
25	A	841	CLA	CAA-CBA-CGA-O1A
25	a	213	CLA	CAA-CBA-CGA-O1A
27	A	835	LHG	O9-C7-C8-C9
35	d	307	CHL	CAA-CBA-CGA-O1A
25	a	207	CLA	C4-C3-C5-C6
25	a	207	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	h	208	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

259 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	j	206	CLA	2	0
25	e	215	CLA	3	0
25	m	203	CLA	5	0
25	d	312	CLA	4	0
25	k	210	CLA	1	0
25	A	801	CLA	7	0
25	h	206	CLA	2	0
25	B	840	CLA	5	0
25	o	608	CLA	1	0
25	l	603	CLA	1	0
25	h	204	CLA	1	0
25	A	820	CLA	2	0
25	l	604	CLA	1	0
25	n	203	CLA	2	0
25	B	819	CLA	6	0
25	i	210	CLA	1	0
25	a	203	CLA	1	0
27	a	201	LHG	1	0
25	g	205	CLA	1	0
25	f	605	CLA	1	0
25	m	208	CLA	3	0
30	a	215	DD6	1	0
25	b	208	CLA	1	0
25	d	304	CLA	1	0
25	B	841	CLA	4	0
25	A	814	CLA	3	0
25	B	802	CLA	9	0
25	b	210	CLA	2	0
25	n	208	CLA	1	0
25	k	206	CLA	3	0
25	e	207	CLA	1	0
25	B	816	CLA	4	0
25	c	309	CLA	2	0
25	B	823	CLA	2	0
25	a	208	CLA	1	0
30	m	213	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	c	301	LHG	3	0
25	B	803	CLA	4	0
27	b	201	LHG	3	0
25	a	205	CLA	1	0
25	A	804	CLA	2	0
25	l	610	CLA	1	0
25	g	203	CLA	2	0
25	p	605	CLA	1	0
30	n	213	DD6	1	0
25	l	602	CLA	4	0
25	a	204	CLA	7	0
35	d	309	CHL	2	0
25	B	839	CLA	5	0
35	d	308	CHL	2	0
25	g	209	CLA	7	0
25	B	845	CLA	9	0
25	g	212	CLA	3	0
25	c	306	CLA	1	0
29	A	839	BCR	2	0
25	l	606	CLA	3	0
25	n	210	CLA	1	0
25	A	810	CLA	3	0
25	m	211	CLA	1	0
25	p	609	CLA	1	0
25	A	806	CLA	1	0
25	B	826	CLA	3	0
25	h	209	CLA	9	0
25	k	203	CLA	1	0
25	e	208	CLA	1	0
25	A	846	CLA	1	0
25	A	841	CLA	3	0
25	J	103	CLA	2	0
25	n	205	CLA	2	0
27	m	201	LHG	2	0
35	d	307	CHL	1	0
27	i	201	LHG	2	0
25	B	821	CLA	2	0
28	B	827	PQN	2	0
25	i	212	CLA	1	0
25	i	204	CLA	2	0
25	k	207	CLA	1	0
25	l	611	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	e	214	CLA	1	0
30	d	319	DD6	1	0
25	j	208	CLA	2	0
25	a	207	CLA	3	0
25	b	209	CLA	2	0
25	A	823	CLA	3	0
25	i	207	CLA	1	0
25	j	212	CLA	4	0
25	b	207	CLA	1	0
25	A	829	CLA	3	0
25	B	837	CLA	3	0
34	e	202	LMG	5	0
30	i	215	DD6	1	0
25	n	201	CLA	2	0
25	o	610	CLA	4	0
25	h	203	CLA	3	0
25	F	201	CLA	3	0
25	c	311	CLA	3	0
25	B	848	CLA	2	0
25	d	313	CLA	1	0
25	m	204	CLA	1	0
27	A	805	LHG	2	0
25	g	204	CLA	3	0
25	A	821	CLA	4	0
25	d	316	CLA	1	0
25	A	826	CLA	4	0
25	A	817	CLA	3	0
29	B	828	BCR	2	0
25	e	206	CLA	1	0
25	g	207	CLA	4	0
25	i	203	CLA	2	0
25	B	807	CLA	3	0
29	M	201	BCR	2	0
25	A	832	CLA	5	0
25	p	602	CLA	3	0
25	i	206	CLA	2	0
25	B	842	CLA	5	0
25	d	306	CLA	2	0
25	n	209	CLA	1	0
25	b	203	CLA	1	0
25	A	816	CLA	3	0
35	c	307	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	j	210	CLA	2	0
25	c	314	CLA	1	0
25	B	814	CLA	1	0
25	o	601	CLA	1	0
25	B	811	CLA	3	0
25	m	202	CLA	5	0
25	A	815	CLA	5	0
25	a	213	CLA	5	0
29	B	829	BCR	2	0
25	i	208	CLA	3	0
25	B	822	CLA	4	0
25	i	202	CLA	2	0
25	B	846	CLA	4	0
25	B	808	CLA	1	0
25	B	815	CLA	1	0
25	k	205	CLA	1	0
25	o	607	CLA	3	0
25	h	214	CLA	2	0
25	A	843	CLA	3	0
25	A	849	CLA	2	0
33	g	202	SQD	2	0
25	j	215	CLA	1	0
25	e	201	CLA	2	0
25	A	813	CLA	1	0
25	A	807	CLA	6	0
32	e	203	DGD	2	0
28	A	834	PQN	5	0
25	h	211	CLA	2	0
25	A	842	CLA	2	0
25	B	844	CLA	2	0
25	k	211	CLA	2	0
25	h	210	CLA	1	0
25	B	836	CLA	3	0
25	e	211	CLA	3	0
35	d	310	CHL	2	0
25	A	822	CLA	3	0
25	k	214	CLA	2	0
25	B	847	CLA	3	0
25	e	216	CLA	1	0
25	c	310	CLA	3	0
25	l	605	CLA	1	0
25	k	208	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	825	CLA	1	0
25	A	845	CLA	2	0
25	B	818	CLA	6	0
29	B	832	BCR	8	0
25	A	812	CLA	3	0
25	g	211	CLA	1	0
25	p	607	CLA	1	0
32	b	202	DGD	3	0
25	e	213	CLA	4	0
25	f	610	CLA	3	0
25	B	824	CLA	5	0
25	f	602	CLA	2	0
25	i	213	CLA	2	0
25	A	844	CLA	5	0
25	k	204	CLA	1	0
32	B	849	DGD	2	0
25	A	840	CLA	6	0
29	J	101	BCR	3	0
25	j	209	CLA	3	0
25	b	204	CLA	1	0
25	A	825	CLA	3	0
25	B	843	CLA	7	0
25	j	203	CLA	4	0
25	A	850	CLA	2	0
25	o	606	CLA	1	0
25	d	305	CLA	2	0
25	A	830	CLA	2	0
25	j	207	CLA	1	0
29	A	837	BCR	3	0
25	A	824	CLA	7	0
25	c	303	CLA	2	0
27	A	835	LHG	5	0
25	A	802	CLA	7	0
25	A	857	CLA	1	0
25	h	205	CLA	1	0
25	c	302	CLA	1	0
30	m	212	DD6	1	0
25	B	817	CLA	4	0
27	h	202	LHG	2	0
25	f	607	CLA	1	0
25	g	208	CLA	3	0
25	i	205	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	210	CLA	1	0
25	A	853	CLA	2	0
27	d	302	LHG	3	0
25	B	810	CLA	1	0
25	c	313	CLA	2	0
29	A	838	BCR	1	0
27	h	201	LHG	1	0
25	g	214	CLA	1	0
25	n	206	CLA	1	0
25	A	809	CLA	6	0
29	B	831	BCR	4	0
25	B	812	CLA	3	0
25	d	315	CLA	1	0
25	a	206	CLA	1	0
25	f	612	CLA	1	0
25	A	819	CLA	4	0
25	A	818	CLA	5	0
25	A	831	CLA	2	0
25	f	611	CLA	1	0
25	B	805	CLA	5	0
25	h	207	CLA	3	0
25	A	833	CLA	7	0
25	l	607	CLA	4	0
25	c	312	CLA	3	0
25	B	813	CLA	4	0
25	o	602	CLA	2	0
29	B	833	BCR	3	0
25	m	206	CLA	1	0
25	n	202	CLA	3	0
25	l	612	CLA	1	0
25	p	608	CLA	1	0
25	B	838	CLA	5	0
25	b	212	CLA	4	0
25	c	308	CLA	3	0
25	h	212	CLA	3	0
29	B	830	BCR	5	0
25	p	603	CLA	4	0
25	b	206	CLA	3	0
25	o	605	CLA	1	0
27	j	202	LHG	4	0
25	a	209	CLA	3	0
25	a	212	CLA	2	0

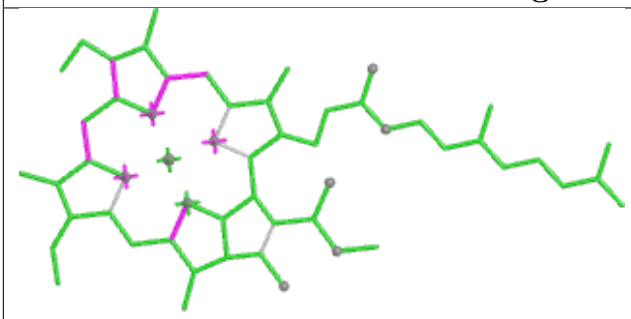
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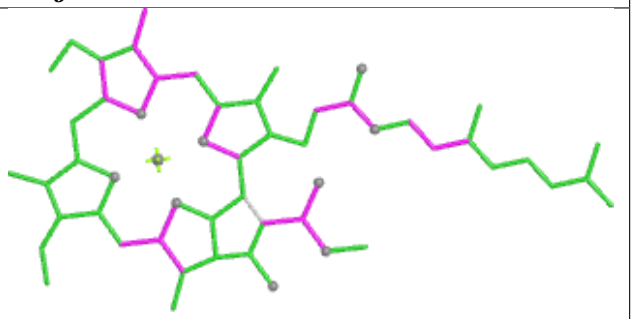
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	f	604	CLA	1	0
29	A	836	BCR	3	0
29	B	801	BCR	2	0
25	p	606	CLA	1	0
25	c	304	CLA	4	0
25	i	211	CLA	2	0
25	d	303	CLA	1	0
25	F	202	CLA	3	0
25	n	207	CLA	3	0
25	B	804	CLA	3	0
25	e	205	CLA	4	0
25	h	208	CLA	2	0
34	k	201	LMG	3	0

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

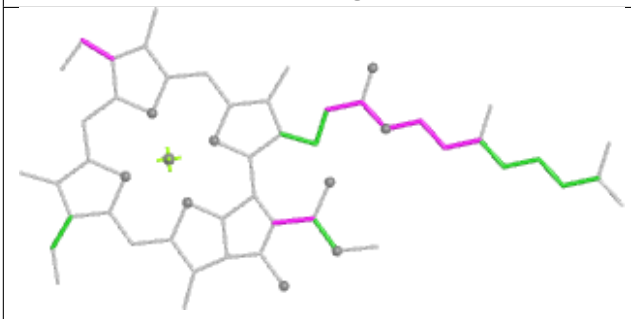
Ligand CLA j 211



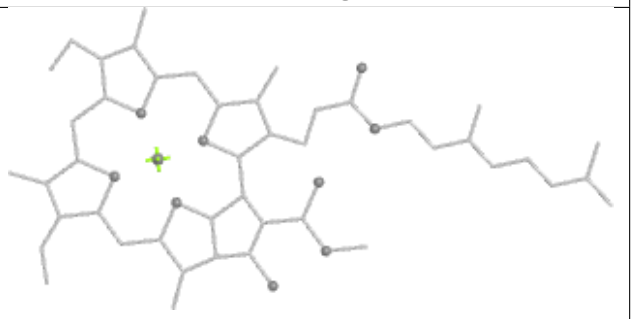
Bond lengths



Bond angles

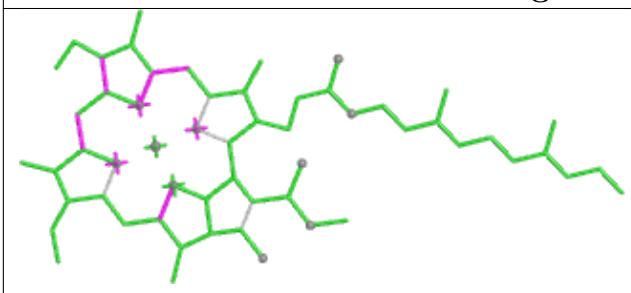


Torsions

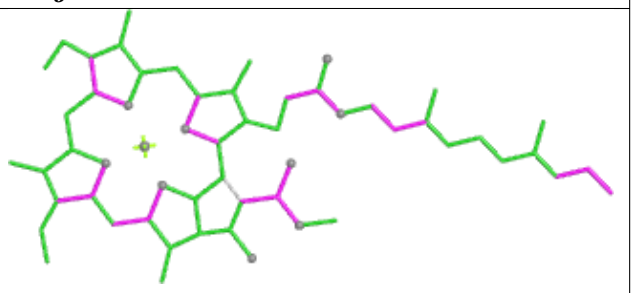


Rings

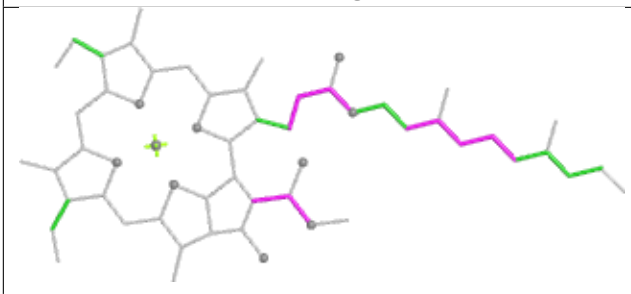
Ligand CLA j 206



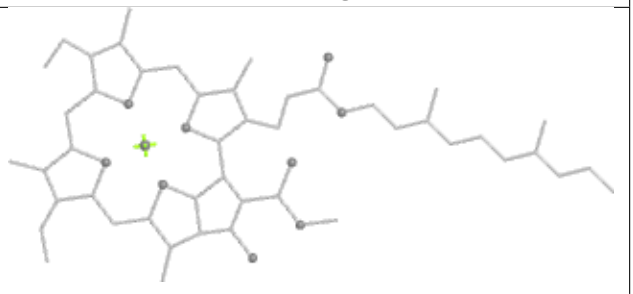
Bond lengths



Bond angles

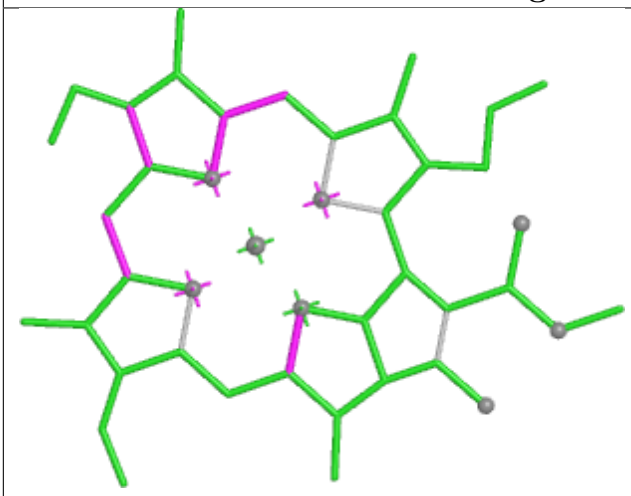


Torsions

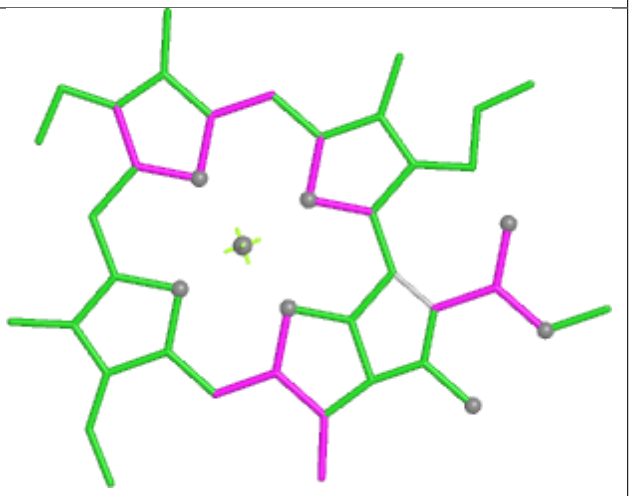


Rings

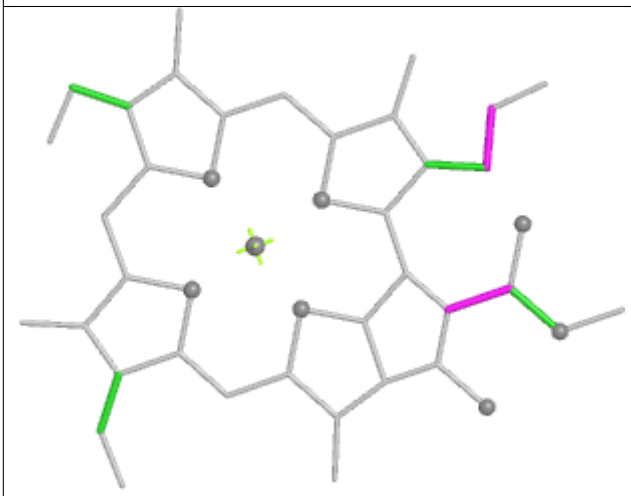
Ligand CLA e 215



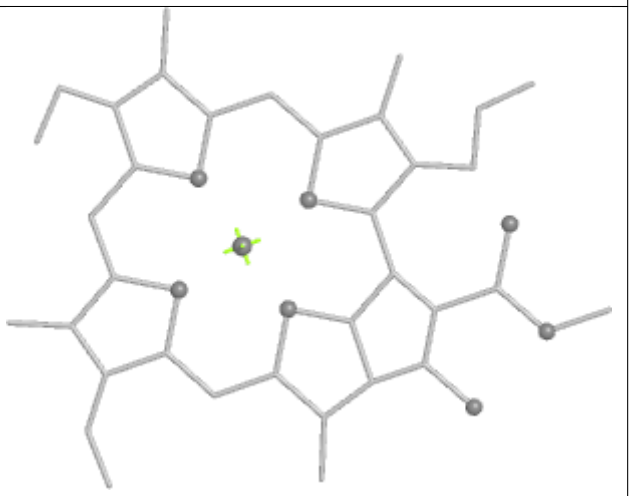
Bond lengths



Bond angles

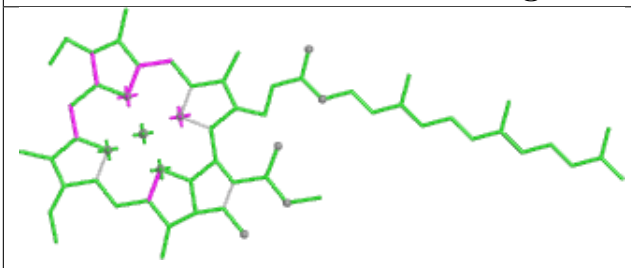


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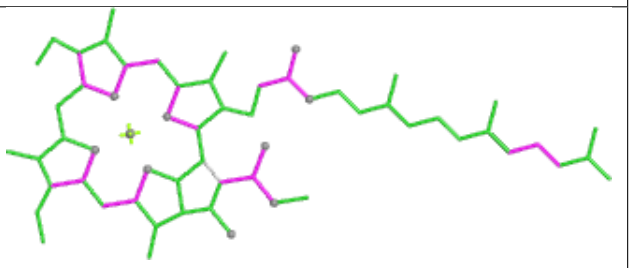


Rings

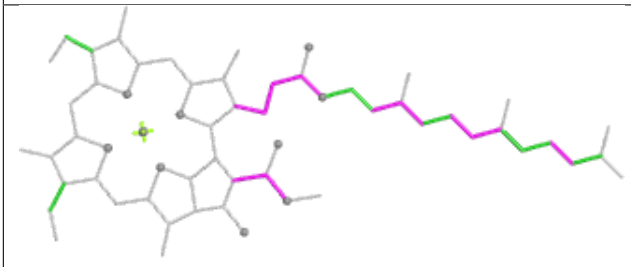
Ligand CLA m 203



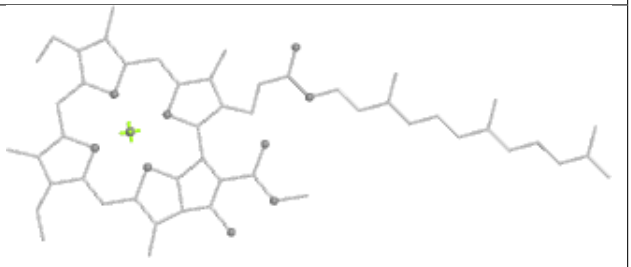
Bond lengths



Bond angles

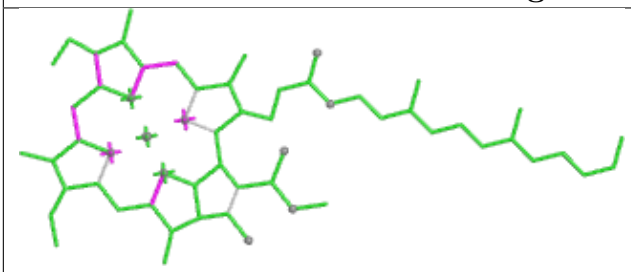


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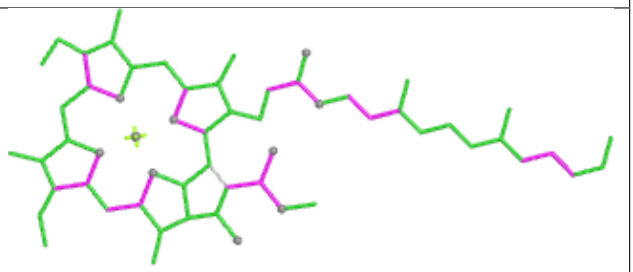


Rings

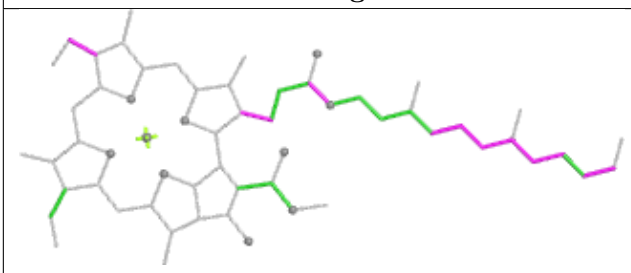
Ligand CLA d 312



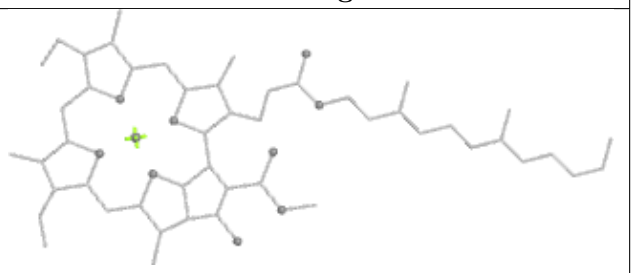
Bond lengths



Bond angles

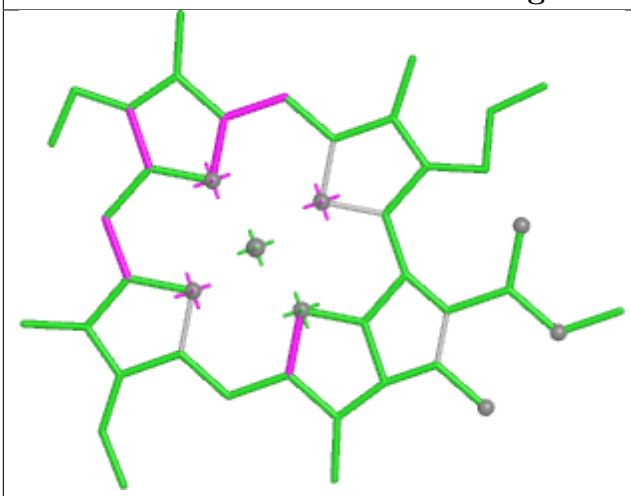


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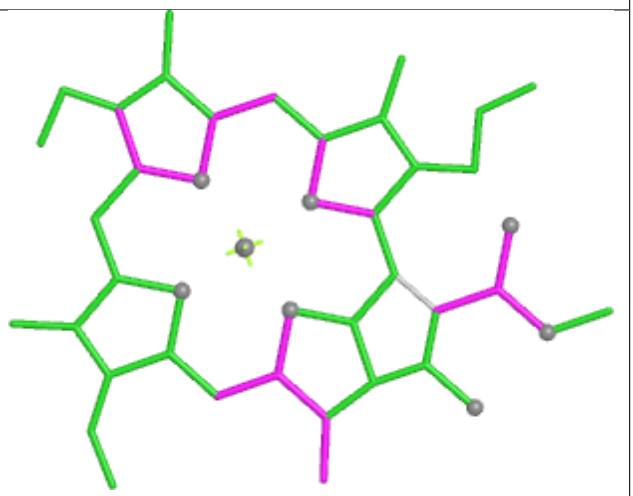


Rings

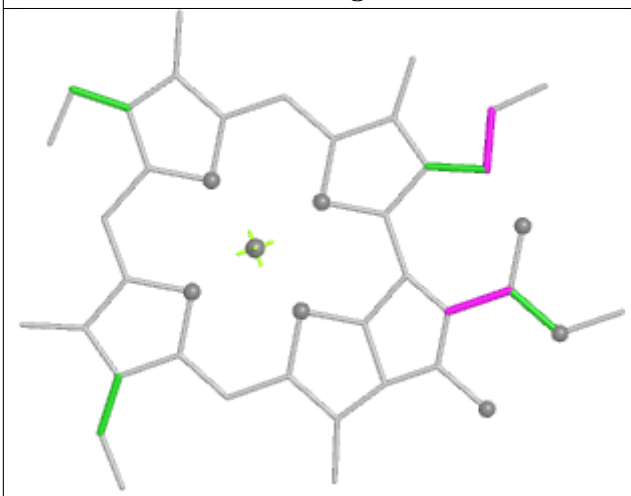
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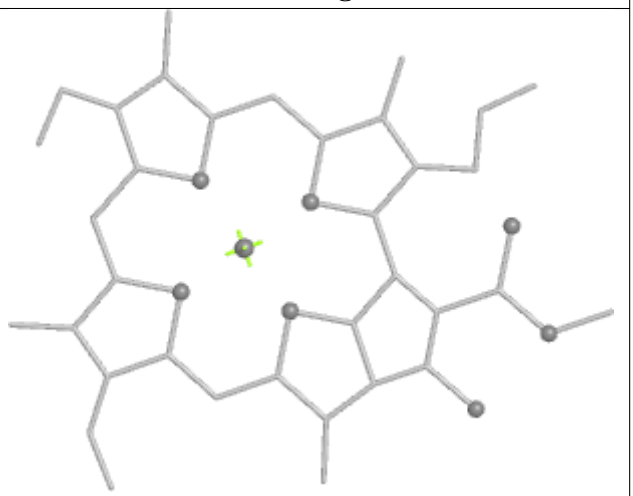
Bond lengths



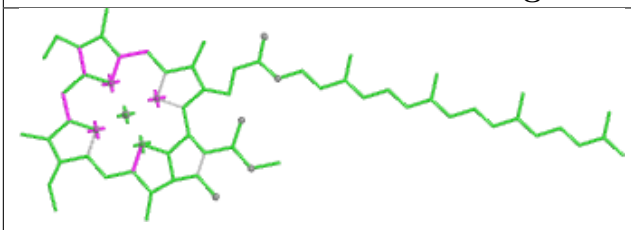
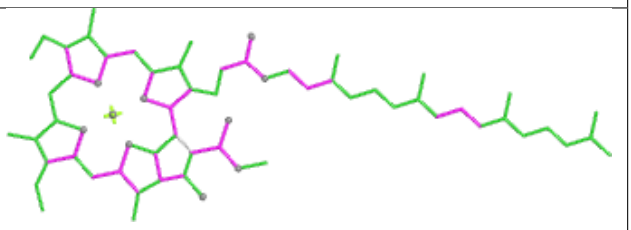
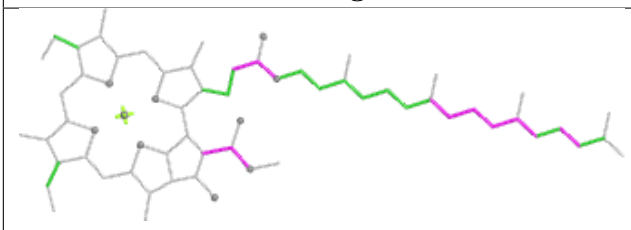
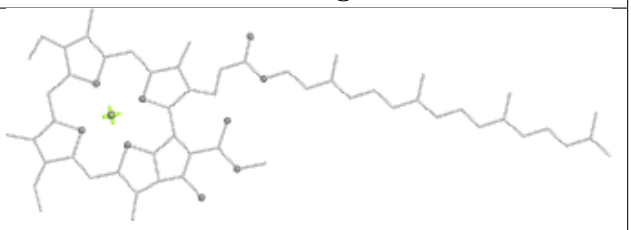
Bond angles

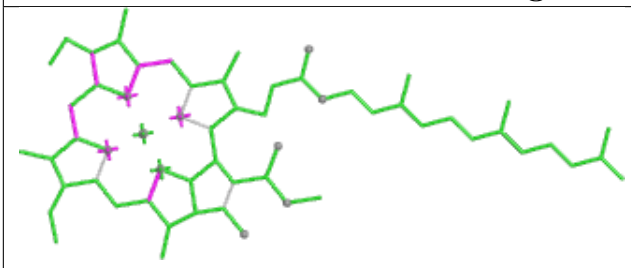
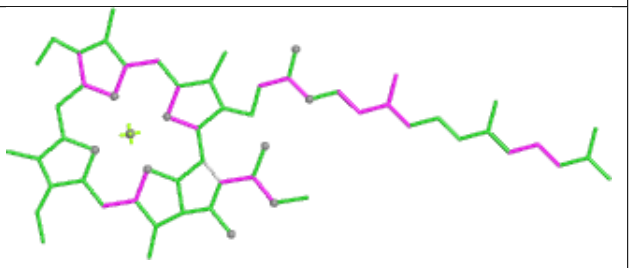
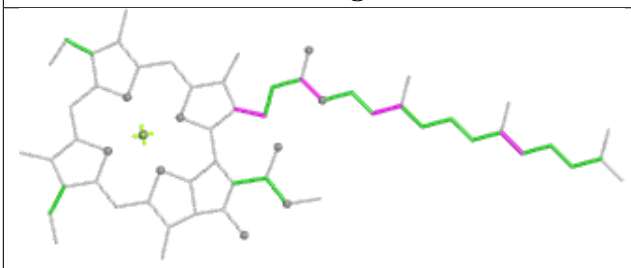
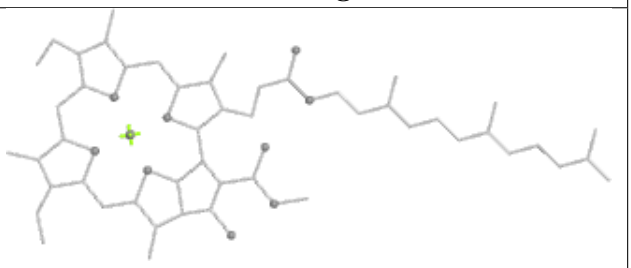


Torsions

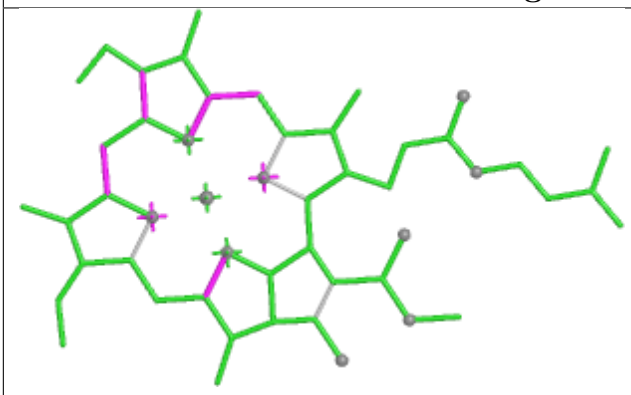


Rings

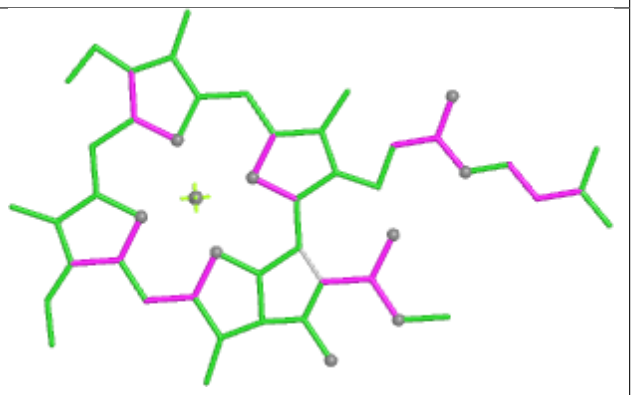
Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA h 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

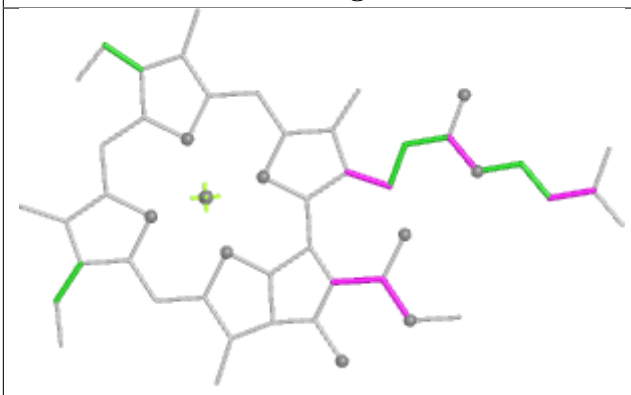
Ligand CLA B 840



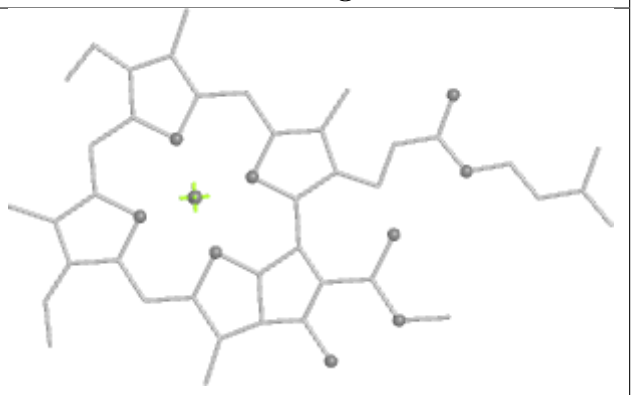
Bond lengths



Bond angles

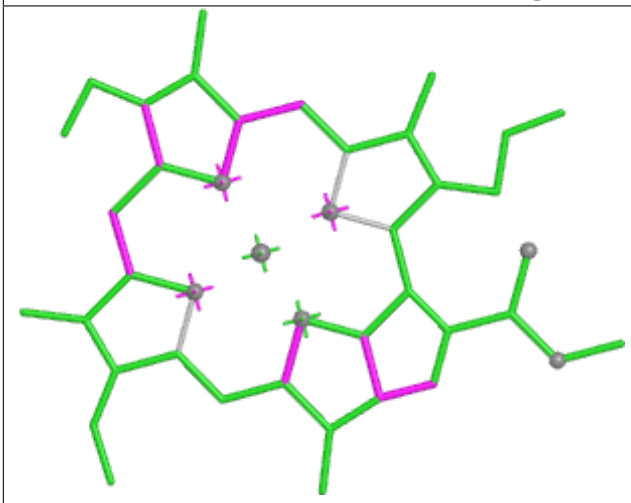


Torsions

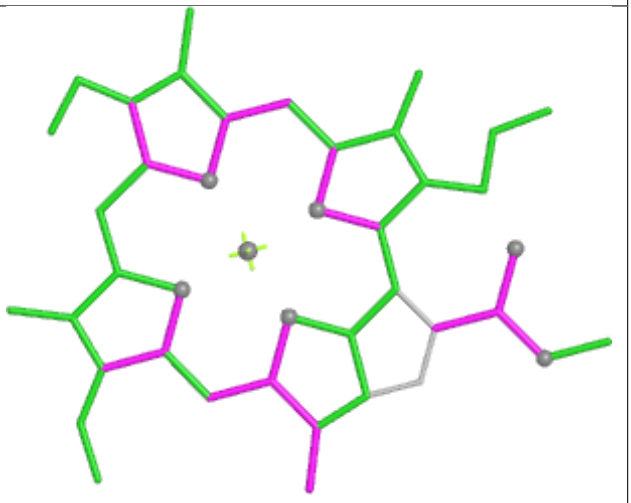


Rings

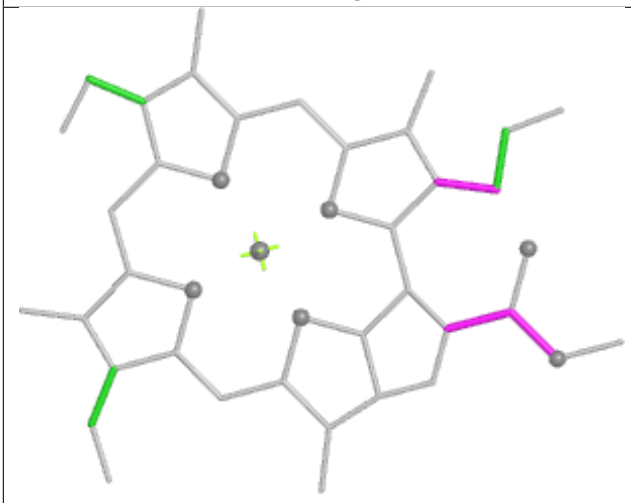
Ligand CLA o 608



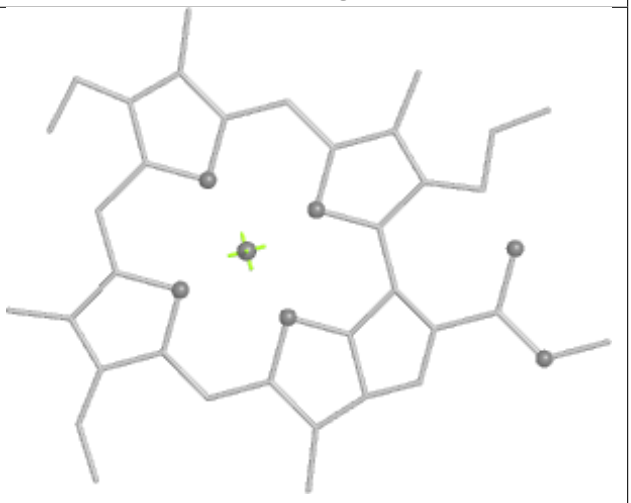
Bond lengths



Bond angles

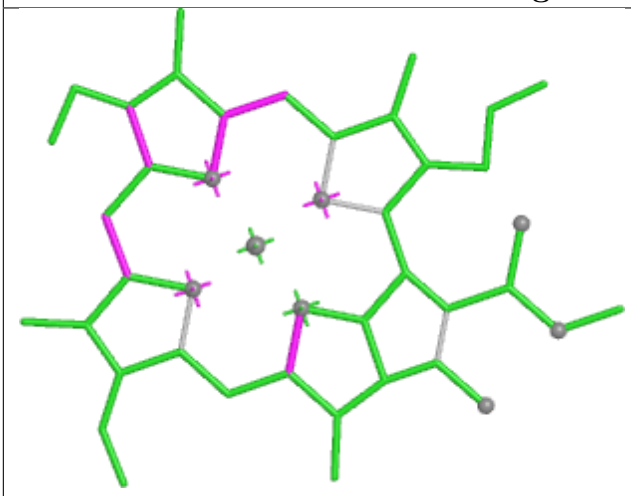


Torsions

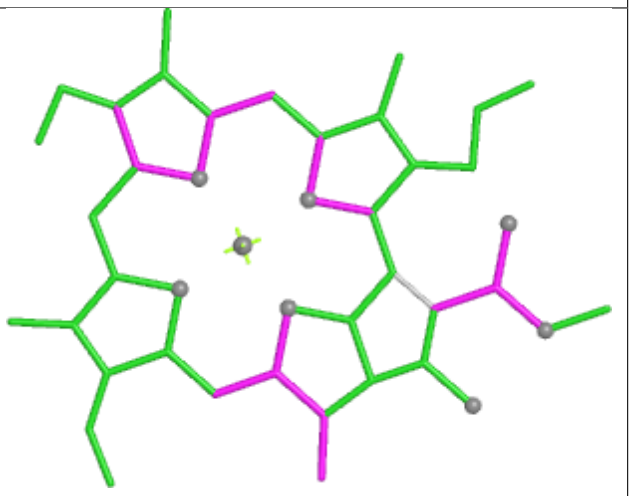


Rings

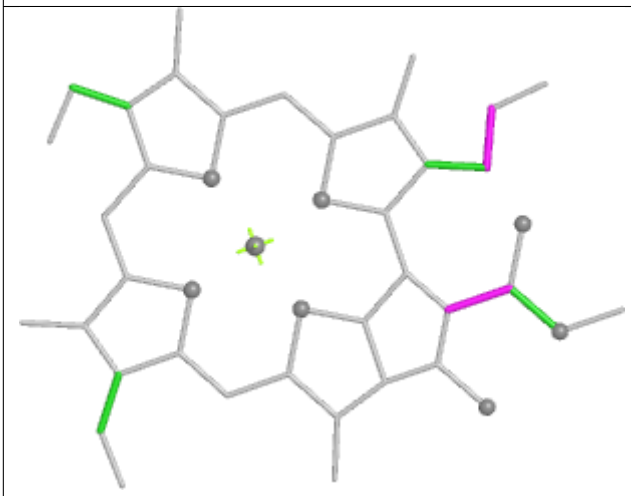
Ligand CLA l 603



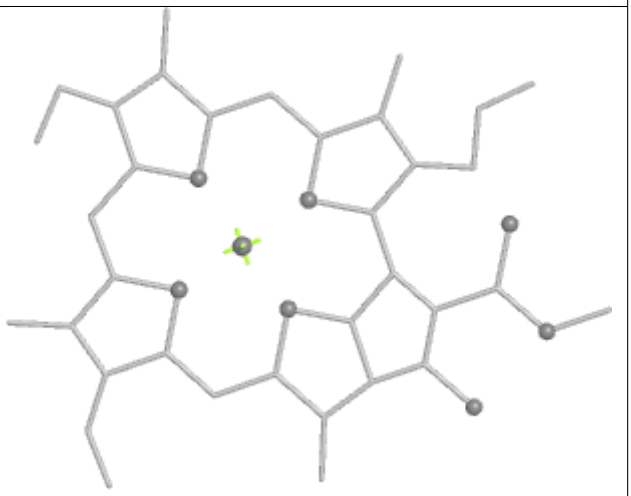
Bond lengths



Bond angles

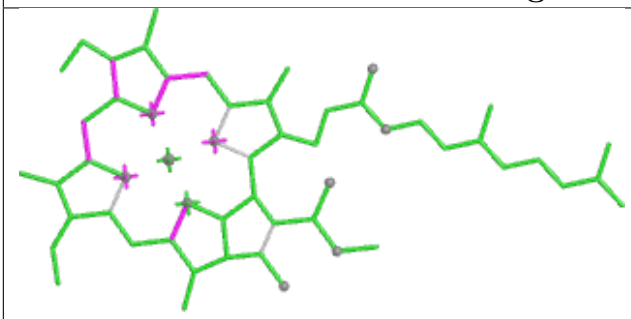


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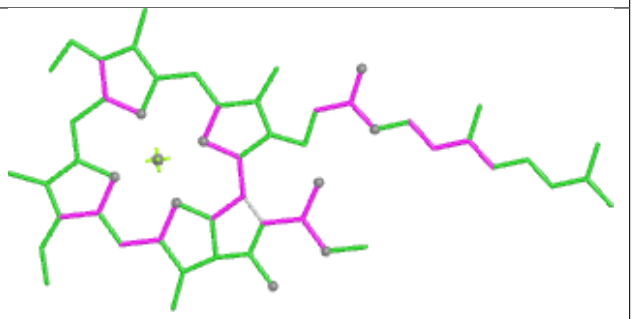


Rings

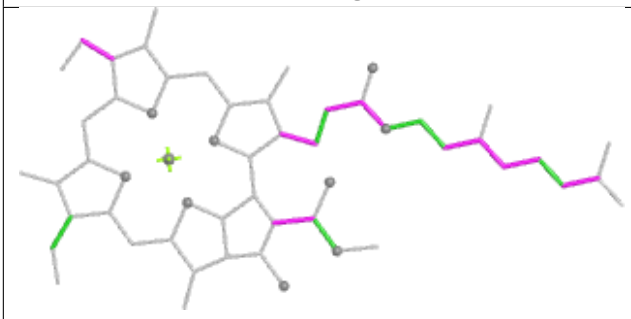
Ligand CLA h 204



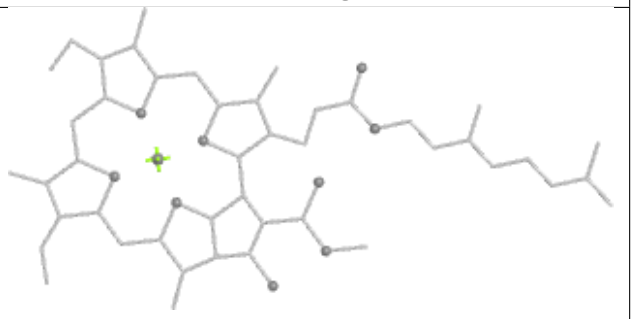
Bond lengths



Bond angles

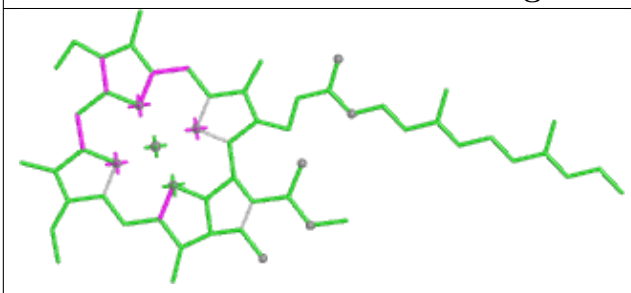


Torsions

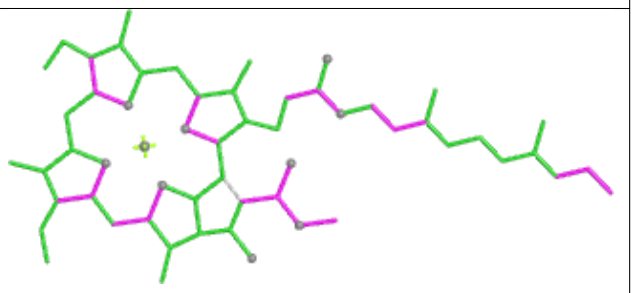


Rings

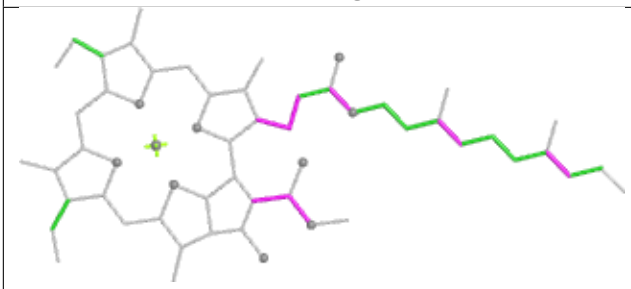
Ligand CLA A 820



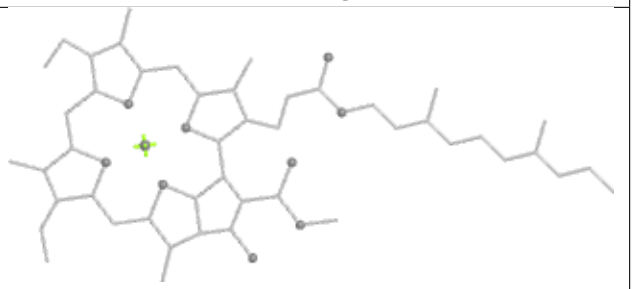
Bond lengths



Bond angles

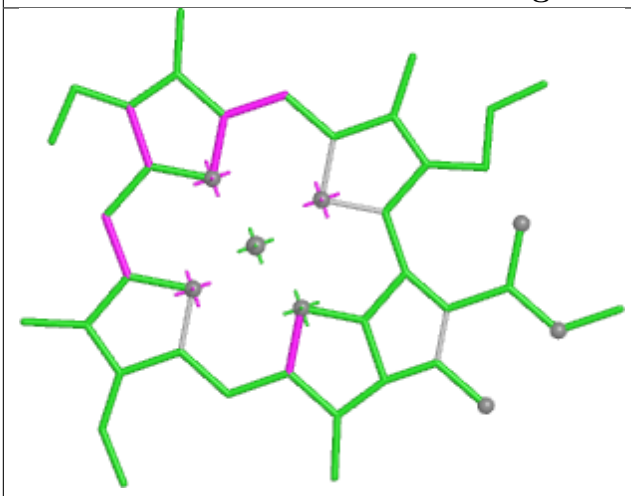


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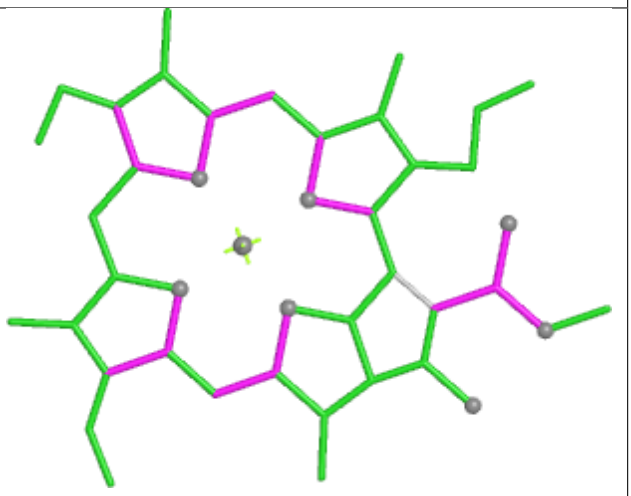


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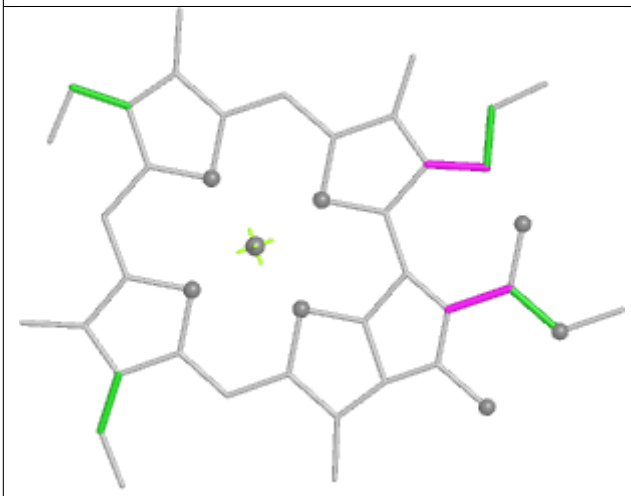
Ligand CLA l 604



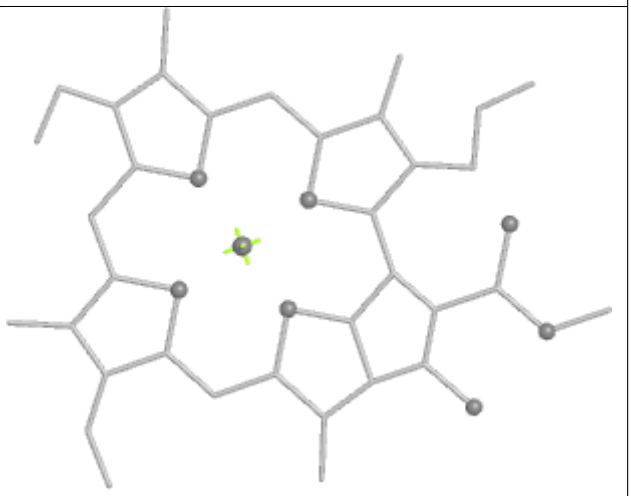
Bond lengths



Bond angles

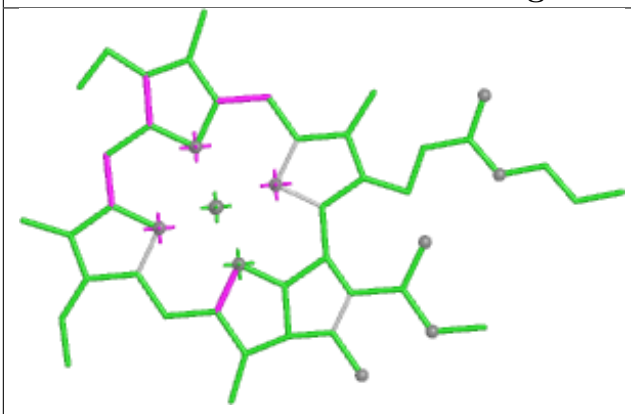


Torsions

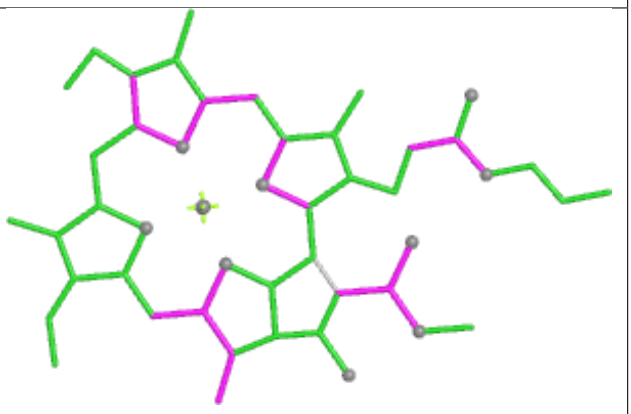


Rings

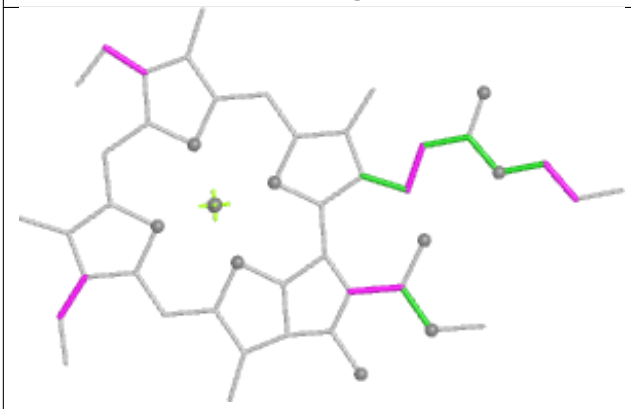
Ligand CLA n 203



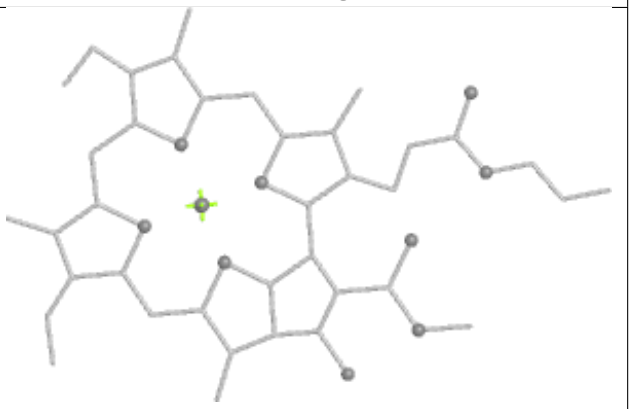
Bond lengths



Bond angles

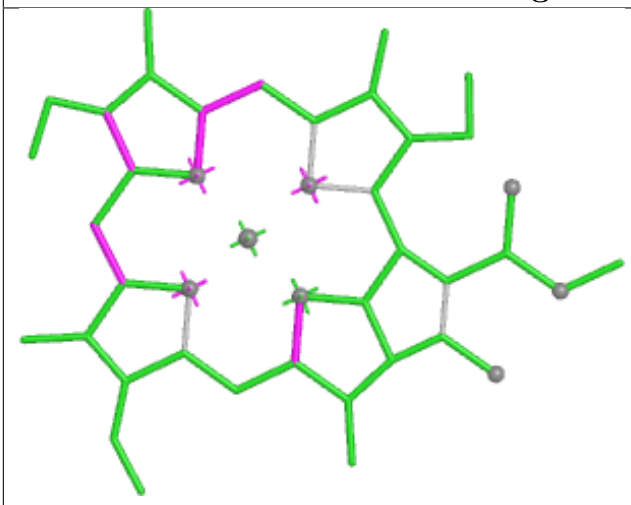


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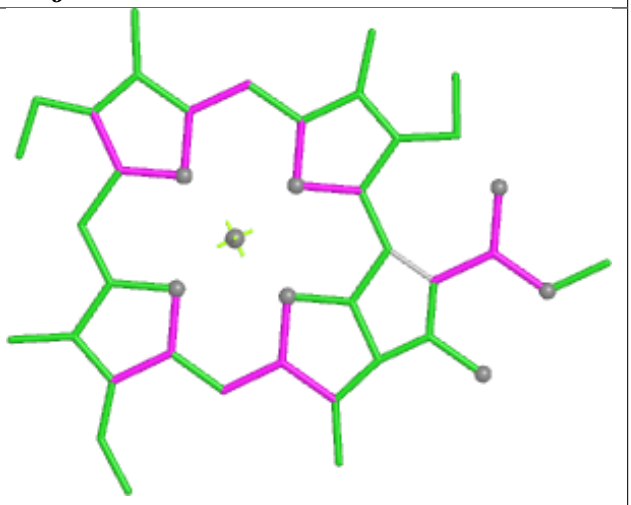


Rings

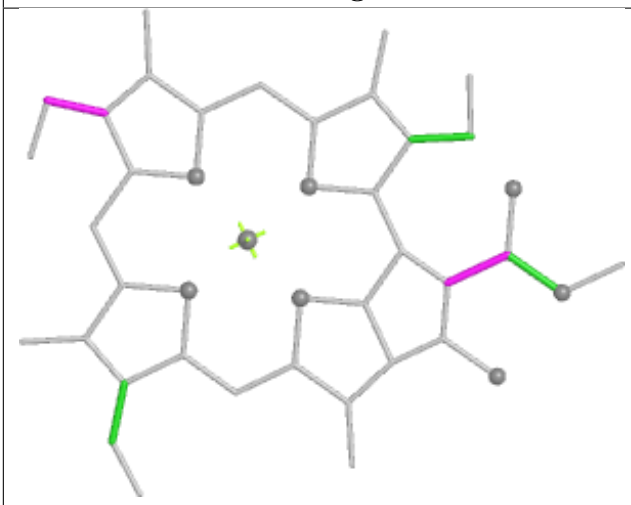
Ligand CLA j 213



Bond lengths



Bond angles

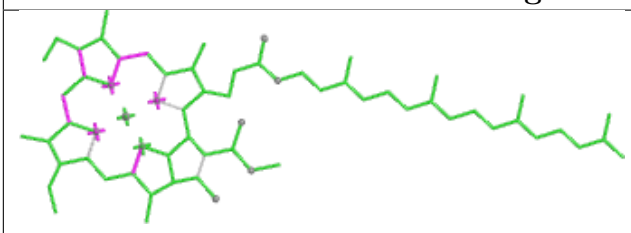


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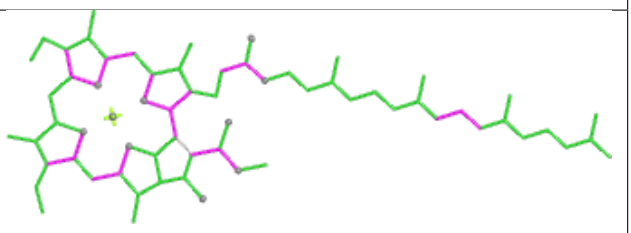


Rings

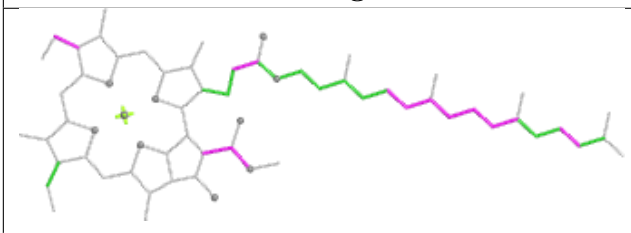
Ligand CLA B 819



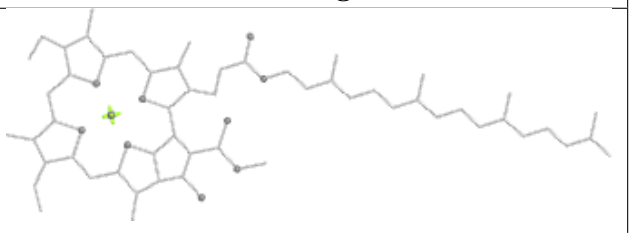
Bond lengths



Bond angles

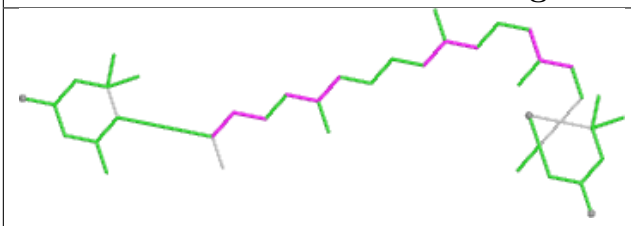


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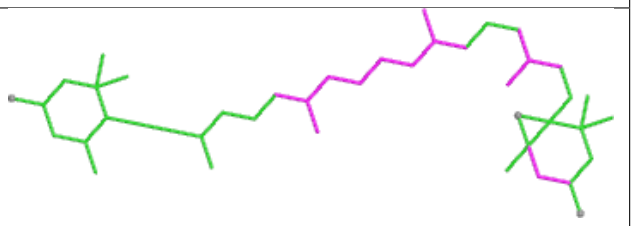


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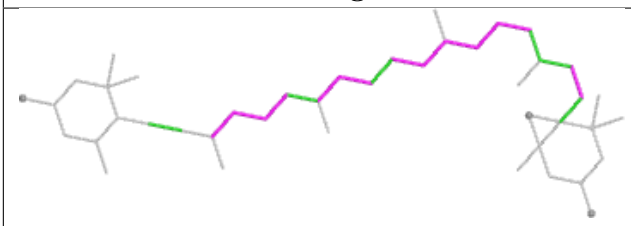
Ligand DD6 e 220



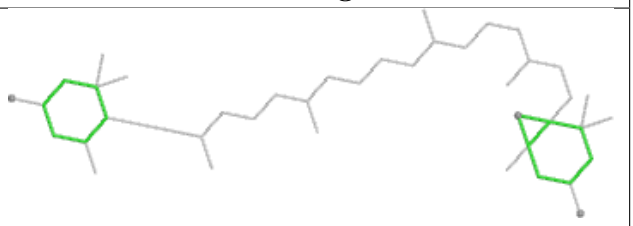
Bond lengths



Bond angles

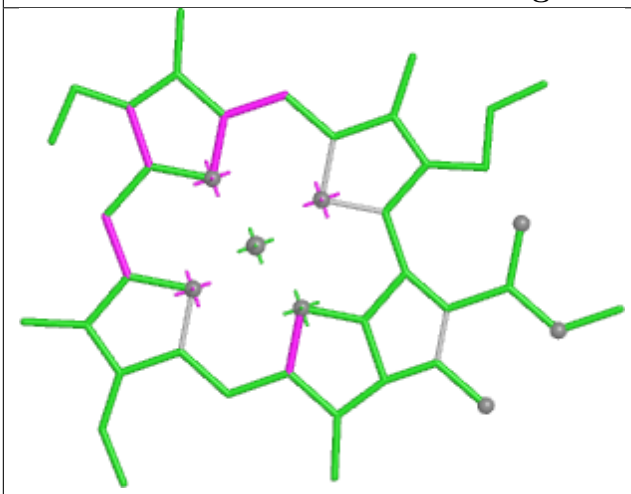


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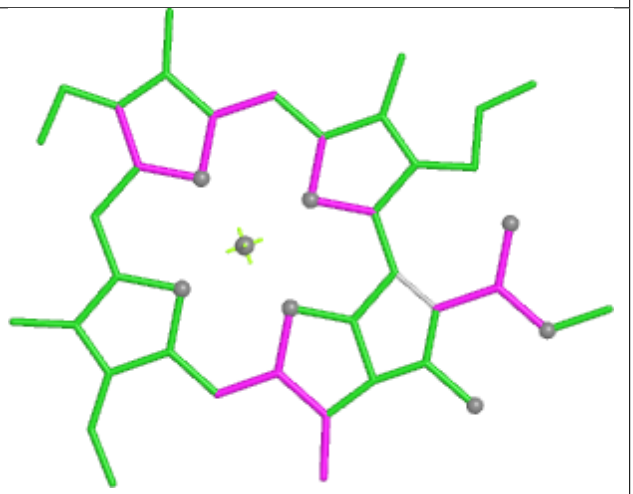


Rings

Ligand CLA i 210



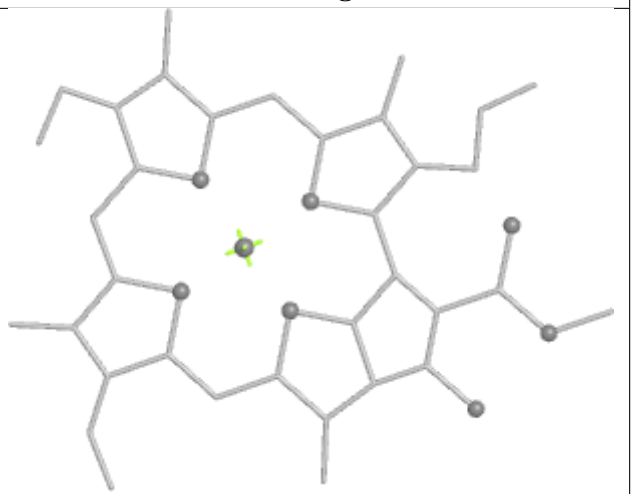
Bond lengths



Bond angles

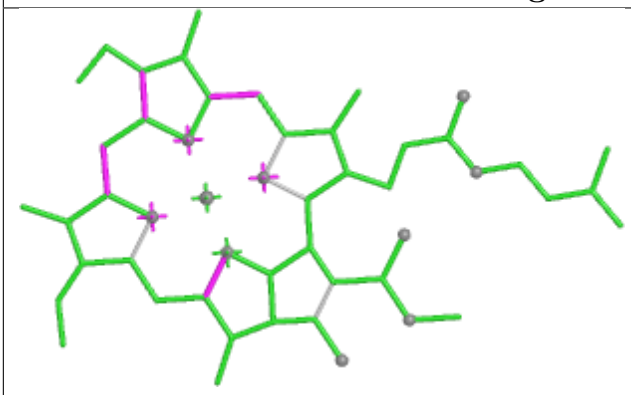


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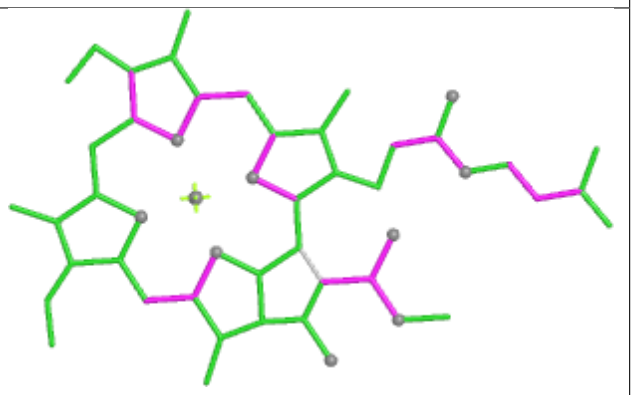


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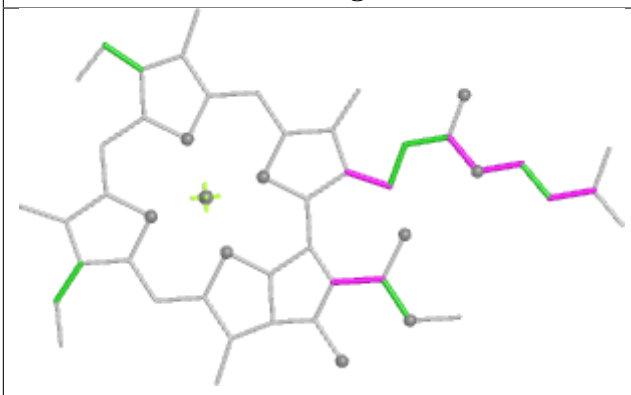
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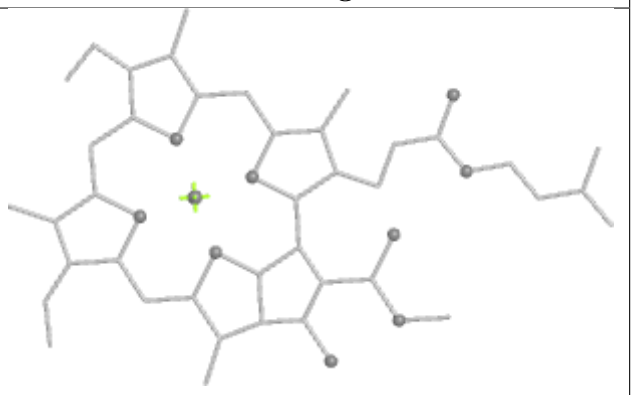
Bond lengths



Bond angles

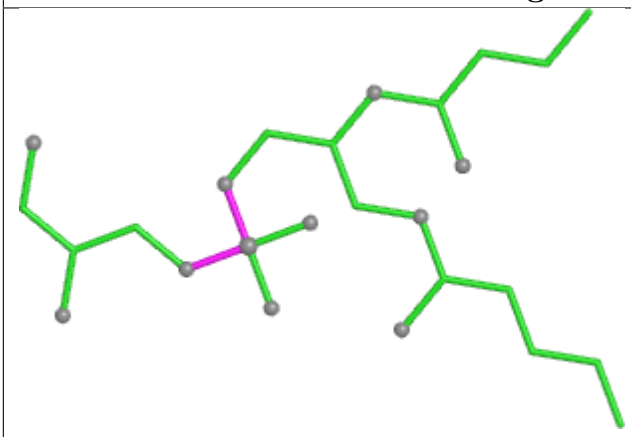


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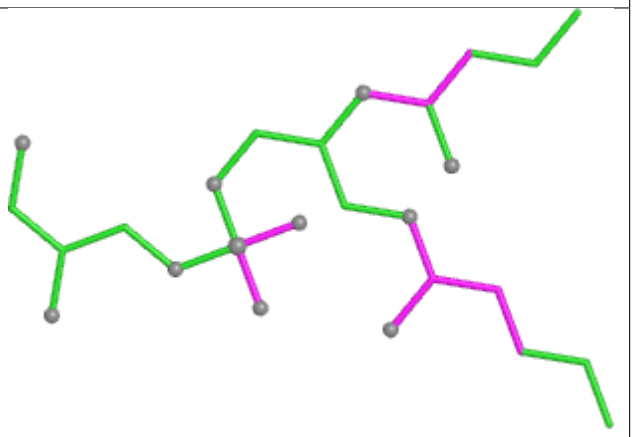


Rings

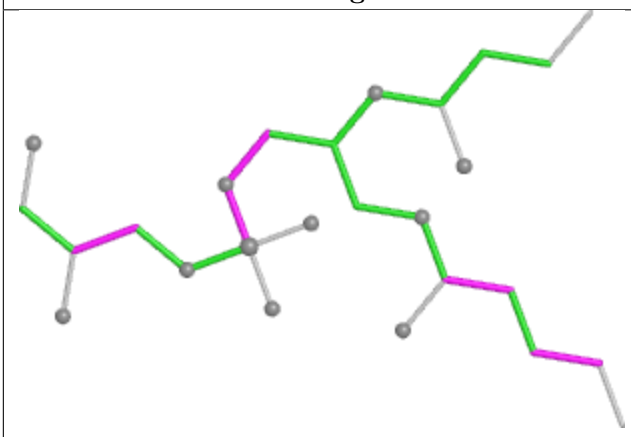
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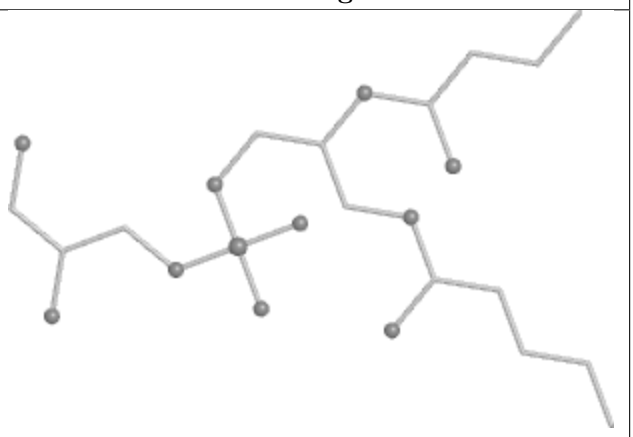
Bond lengths



Bond angles

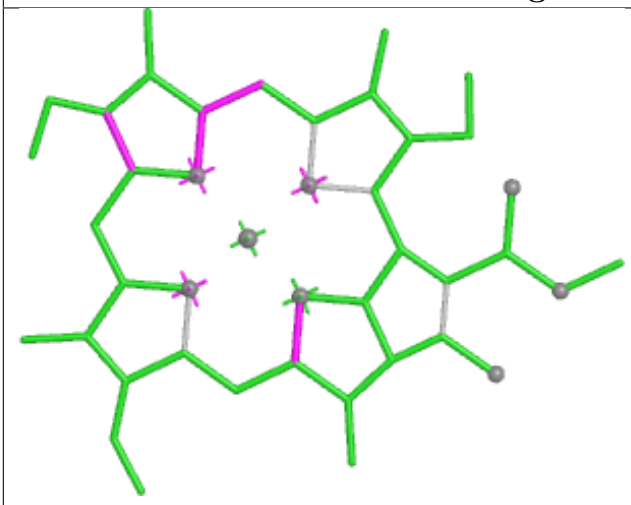


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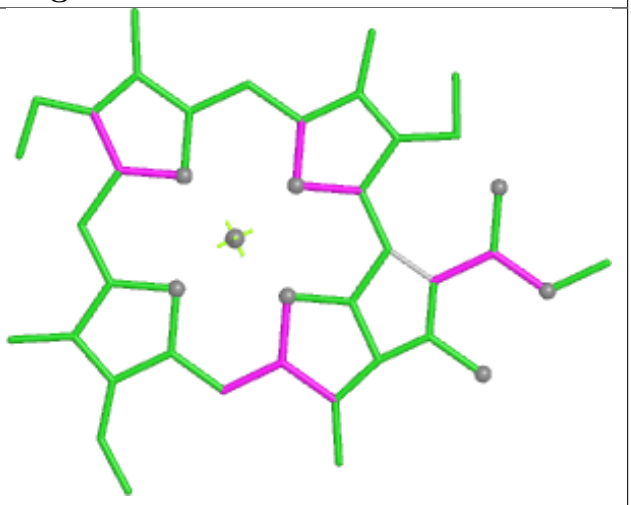


Rings

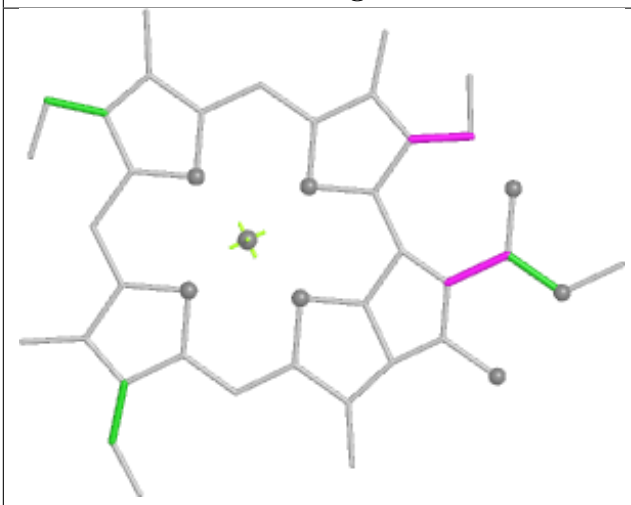
Ligand CLA g 205



Bond lengths



Bond angles

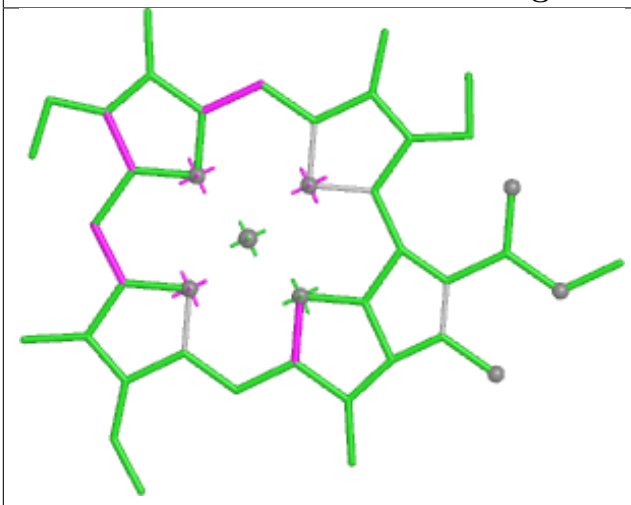


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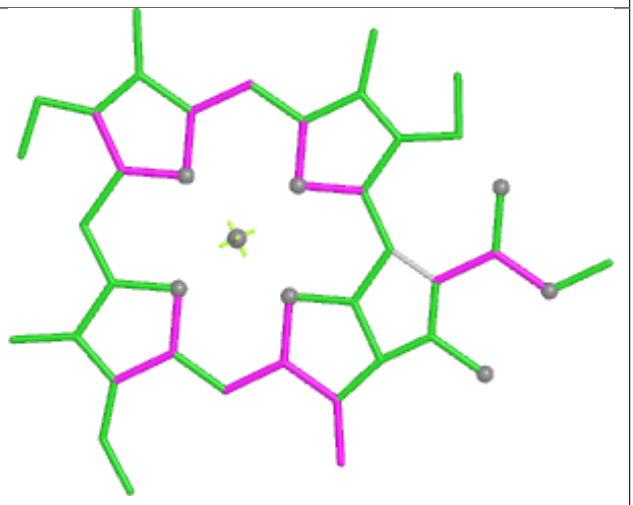


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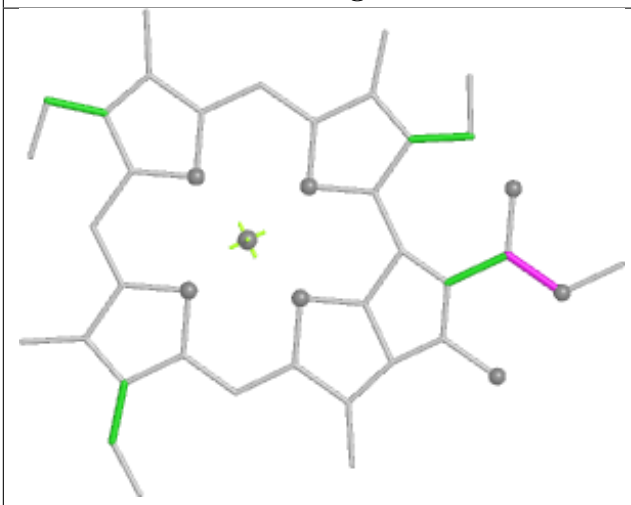
Ligand CLA f 605



Bond lengths



Bond angles

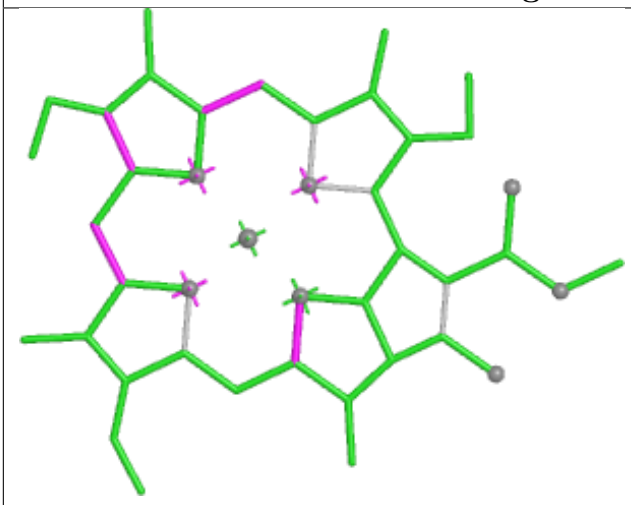


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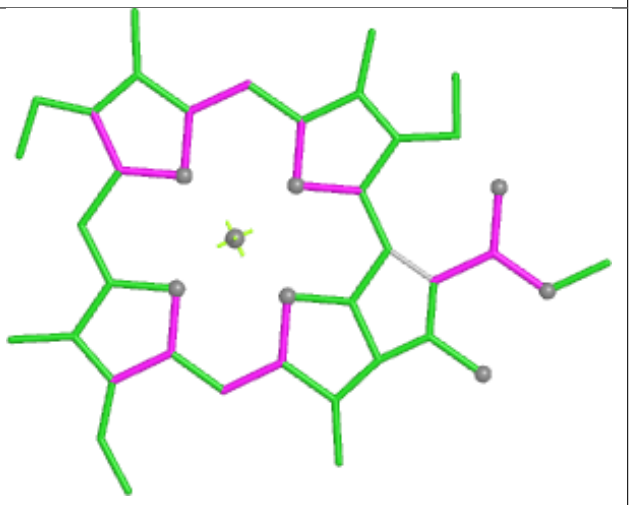


Rings

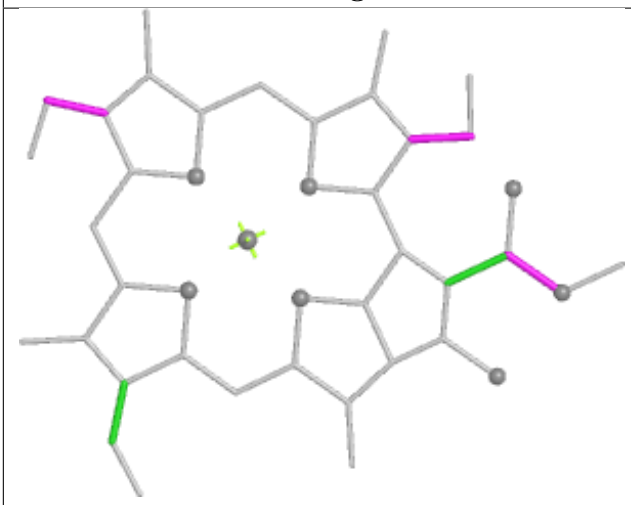
Ligand CLA m 208



Bond lengths



Bond angles

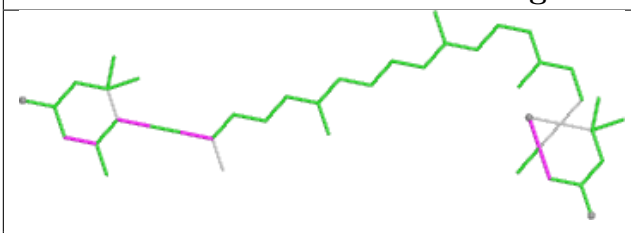


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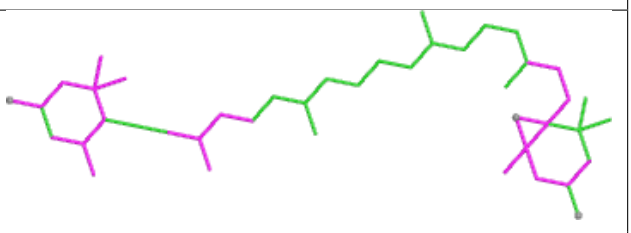


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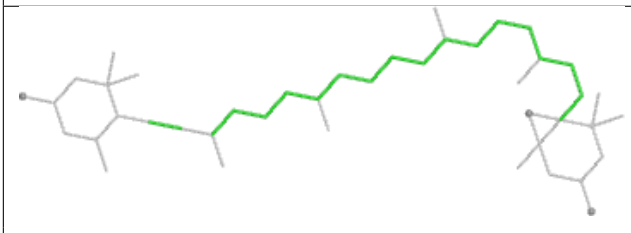
Ligand DD6 a 215



Bond lengths



Bond angles

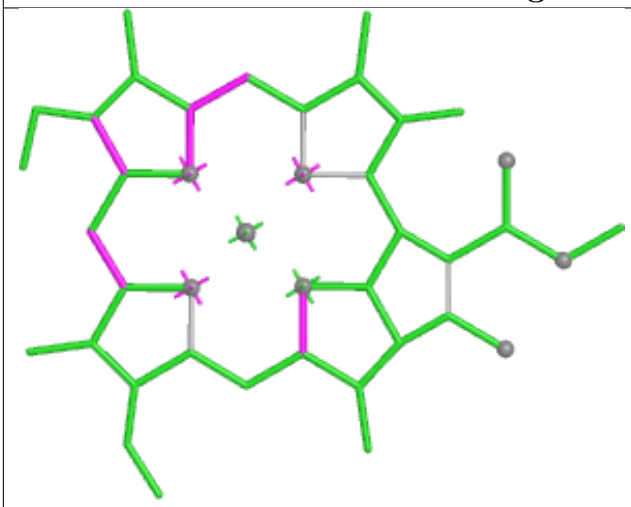


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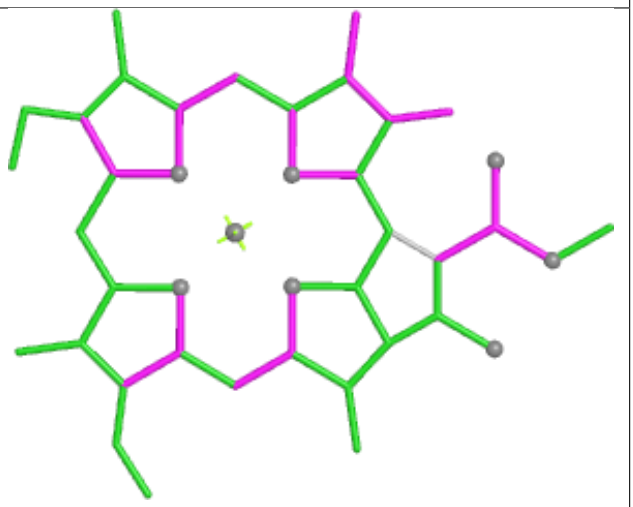


Rings

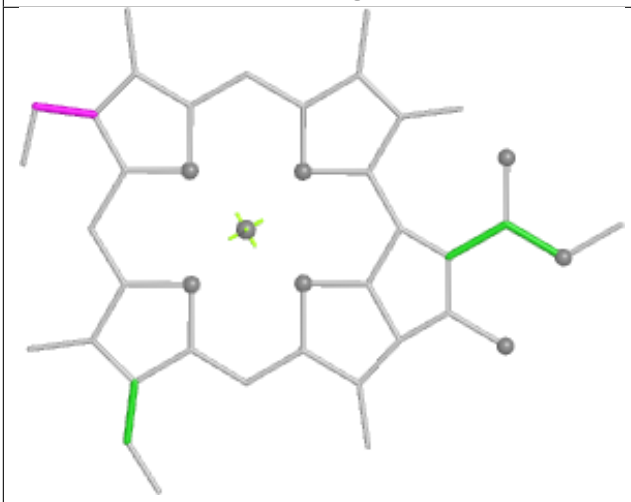
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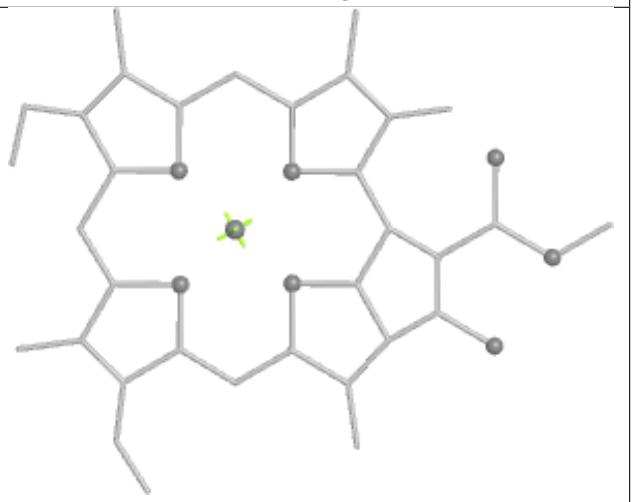
Bond lengths



Bond angles

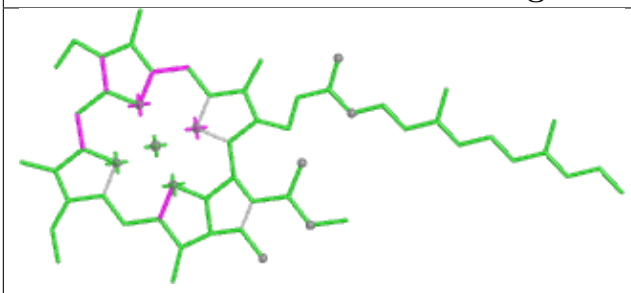


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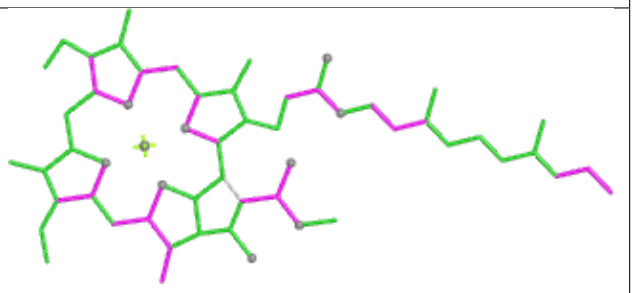


Rings

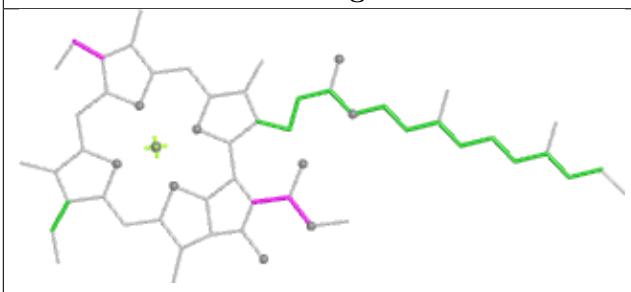
Ligand CLA d 304



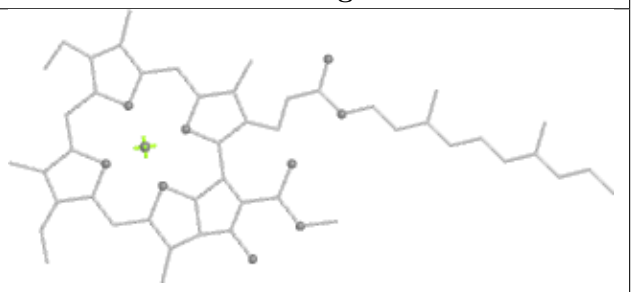
Bond lengths



Bond angles

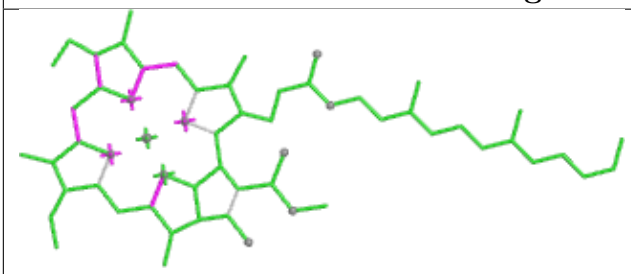


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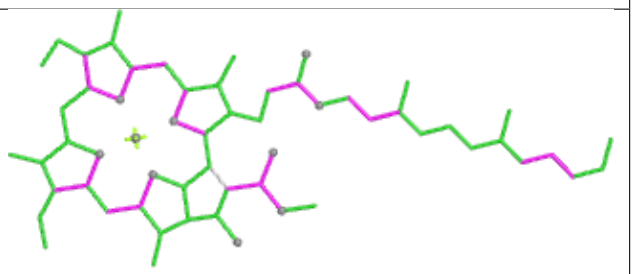


Rings

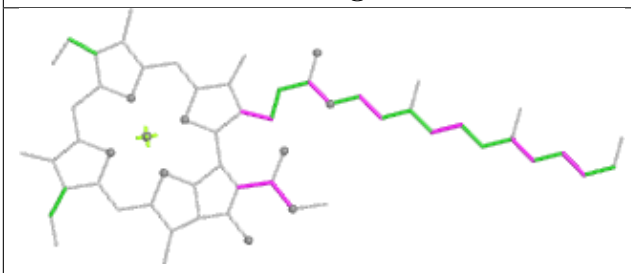
Ligand CLA B 841



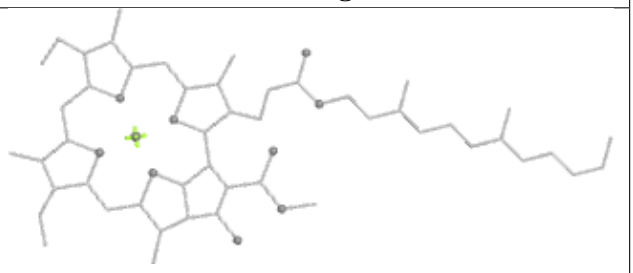
Bond lengths



Bond angles

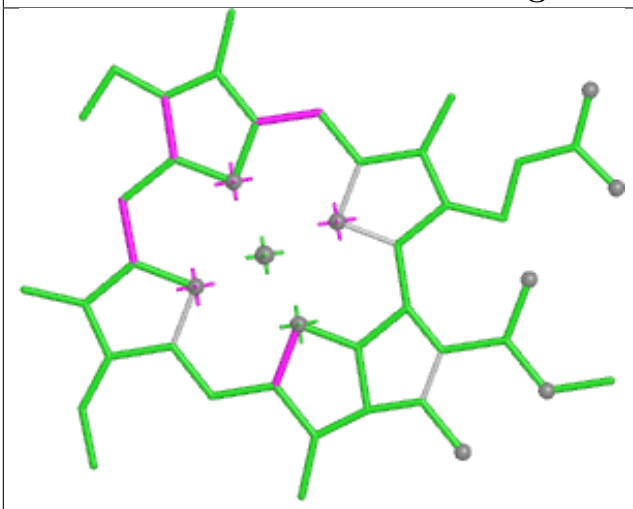


Torsions

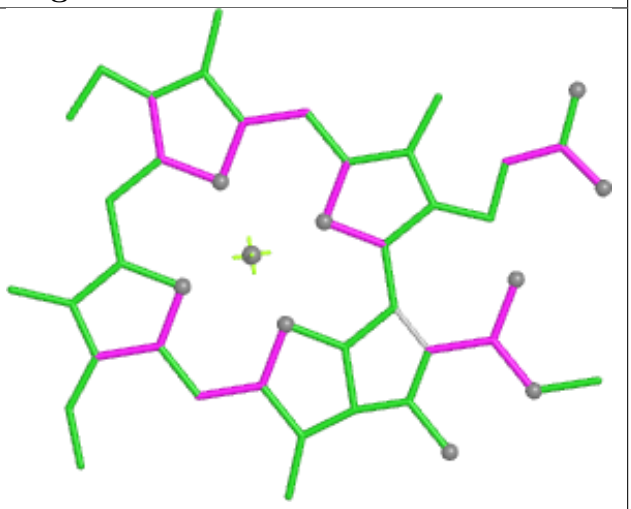


Rings

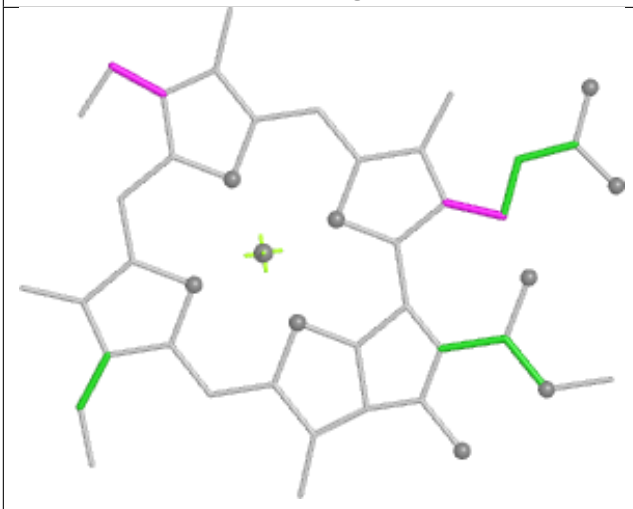
Ligand CLA g 215



Bond lengths



Bond angles

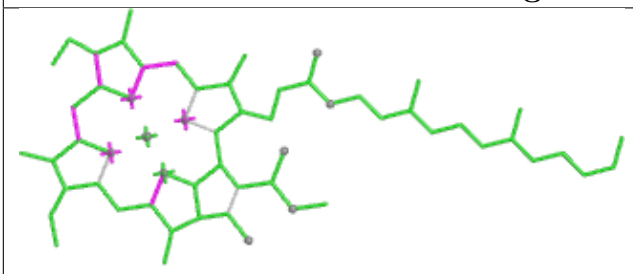


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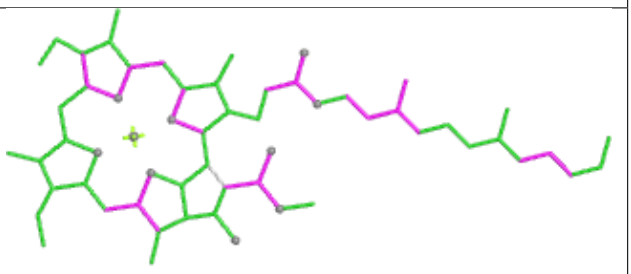


Rings

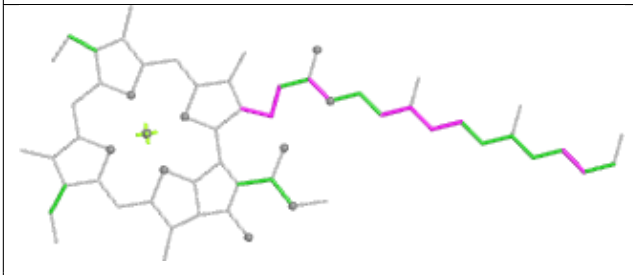
Ligand CLA A 814



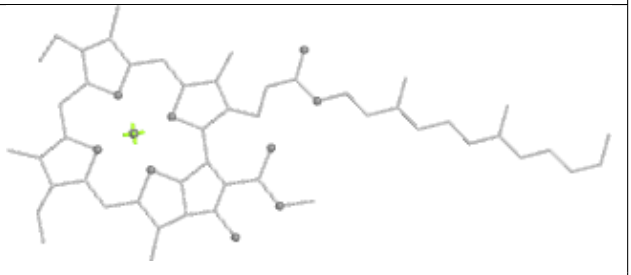
Bond lengths



Bond angles

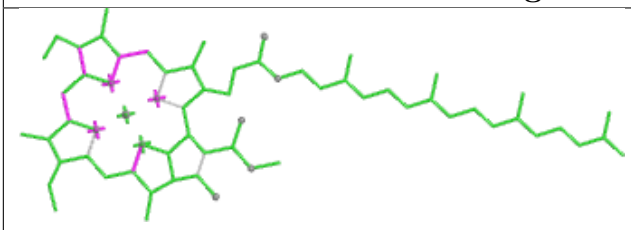


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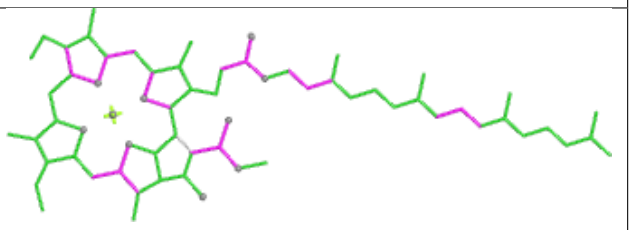


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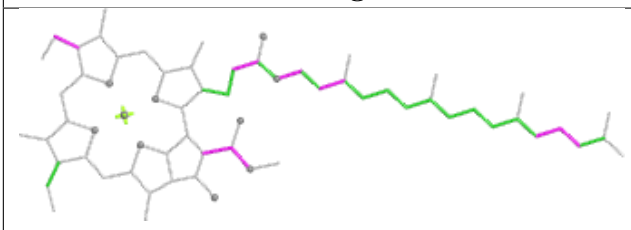
Ligand CLA B 802



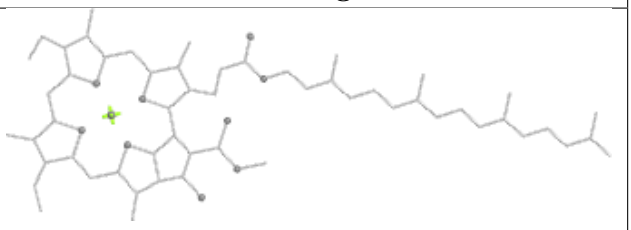
Bond lengths



Bond angles

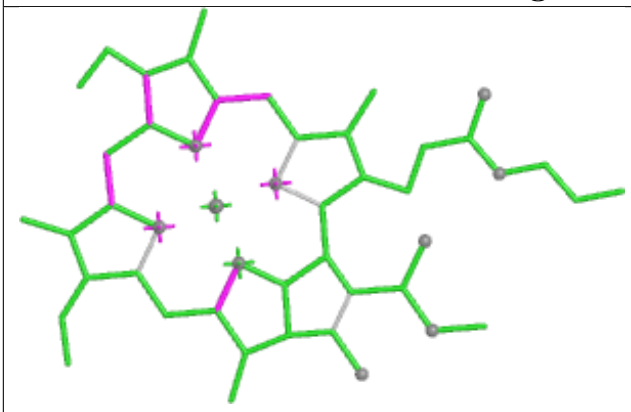


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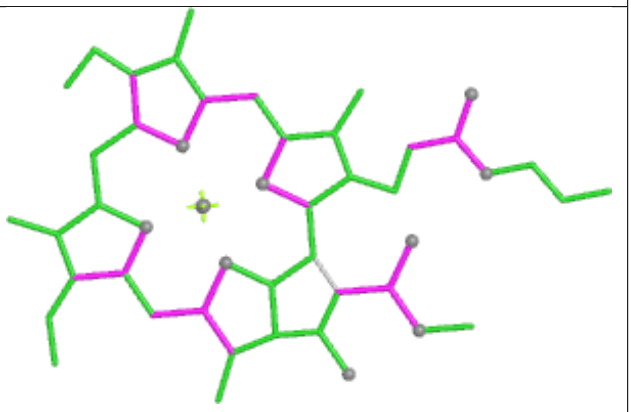


Rings

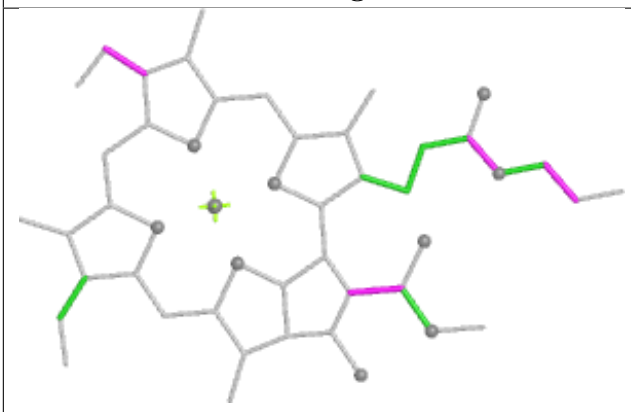
Ligand CLA c 305



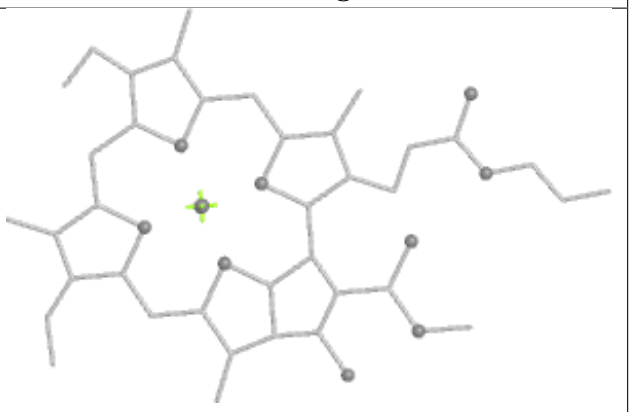
Bond lengths



Bond angles

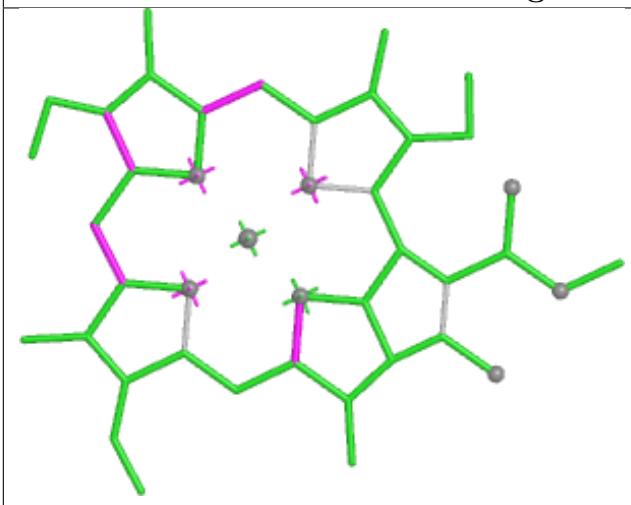


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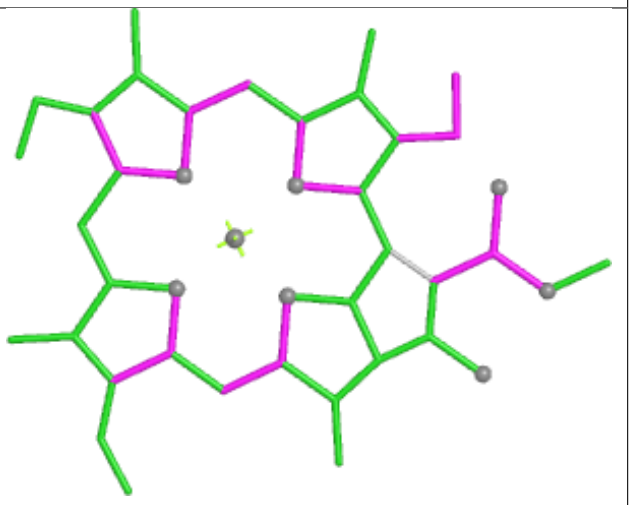


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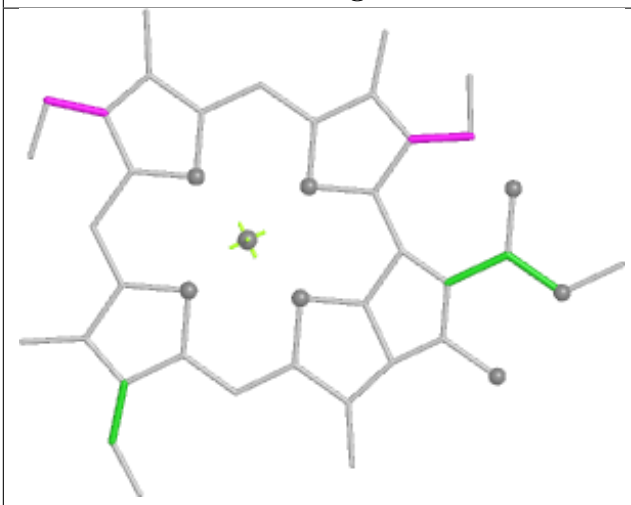
Ligand CLA b 210



Bond lengths



Bond angles

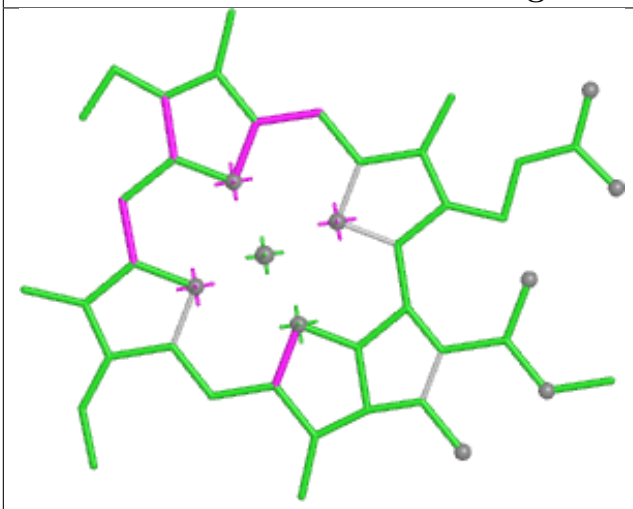


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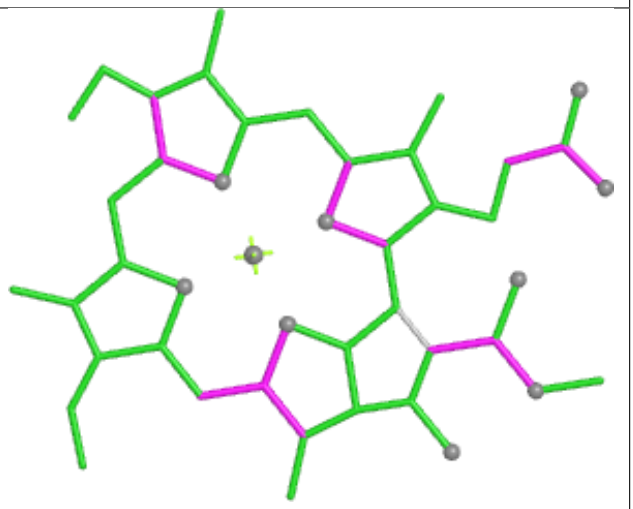


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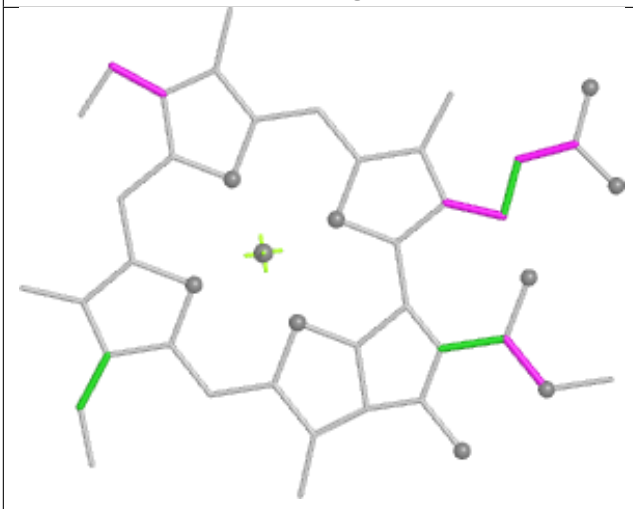
Ligand CLA n 208



Bond lengths



Bond angles

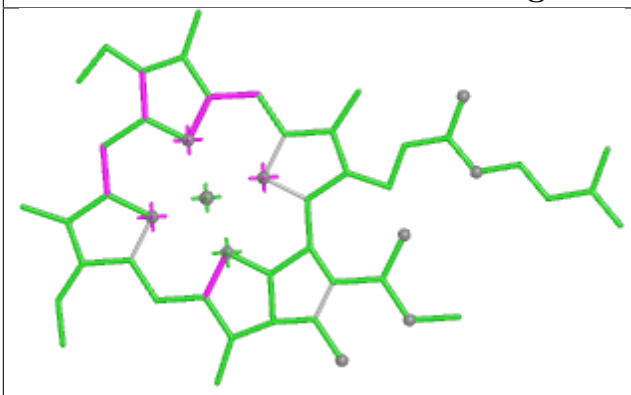


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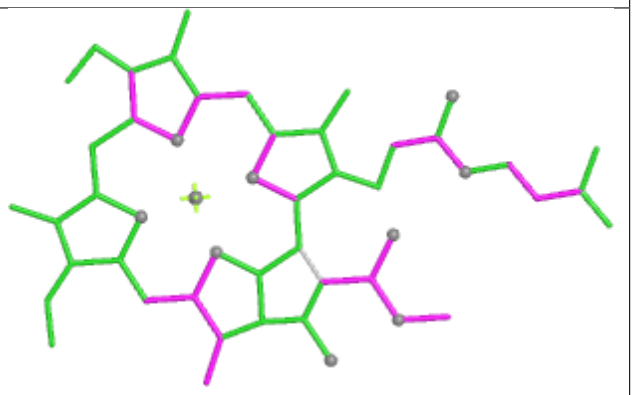


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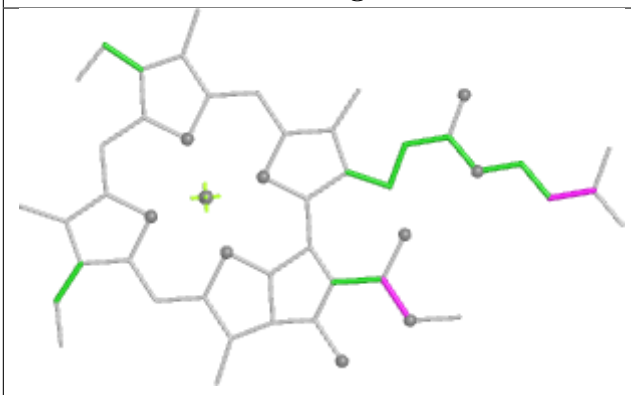
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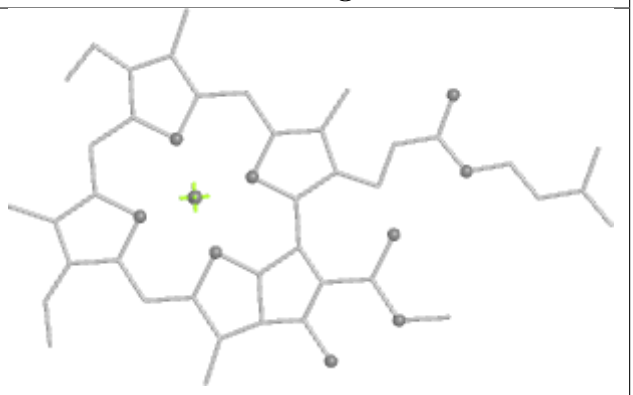
Bond lengths



Bond angles

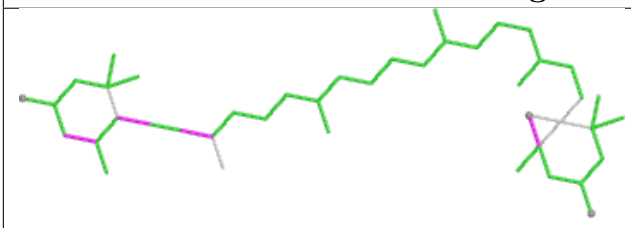


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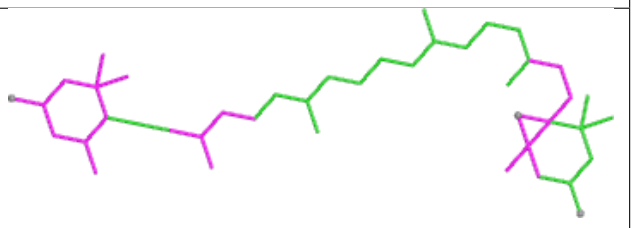


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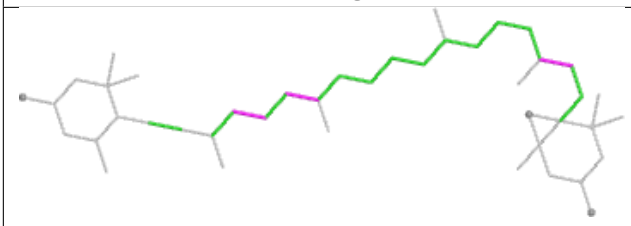
Ligand DD6 o 611



Bond lengths



Bond angles

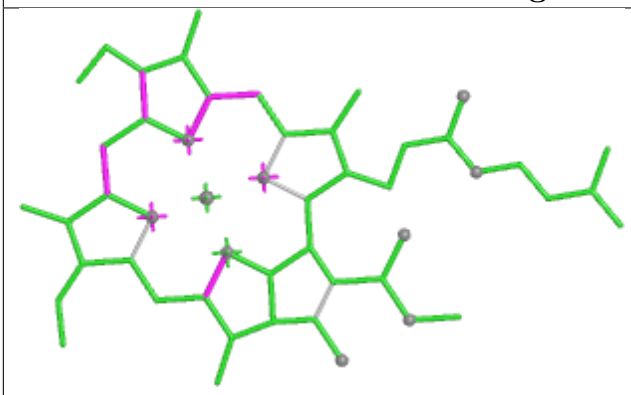


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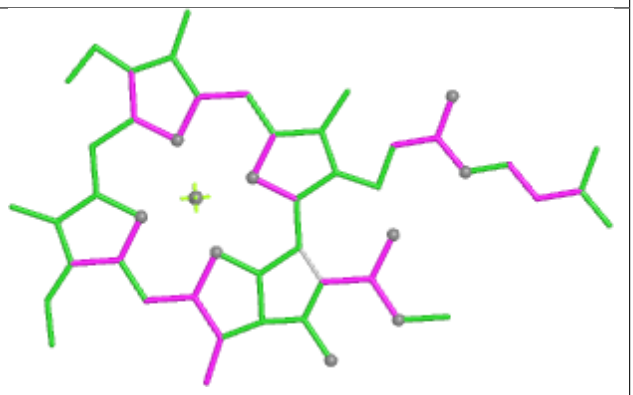


Rings

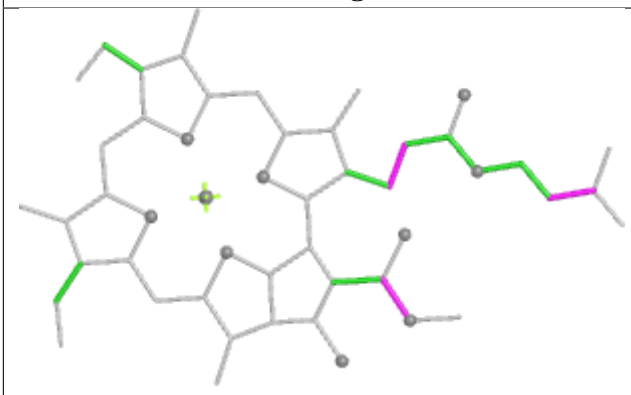
Ligand CLA e 207



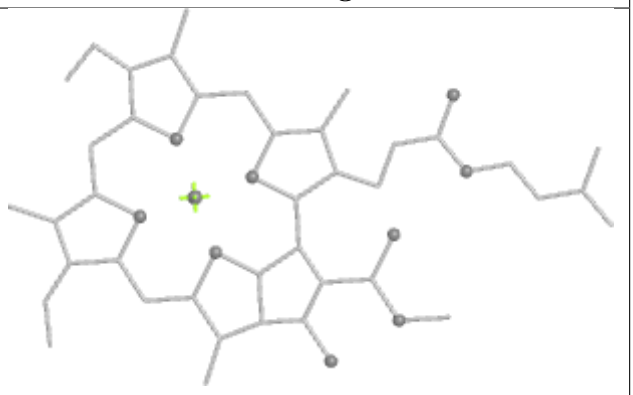
Bond lengths



Bond angles

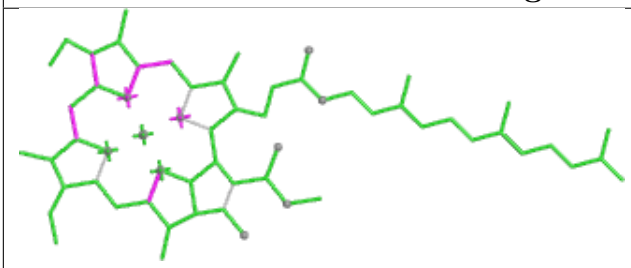


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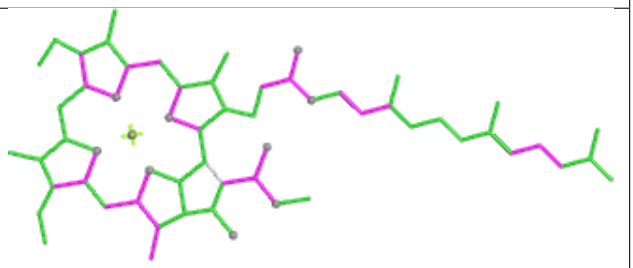


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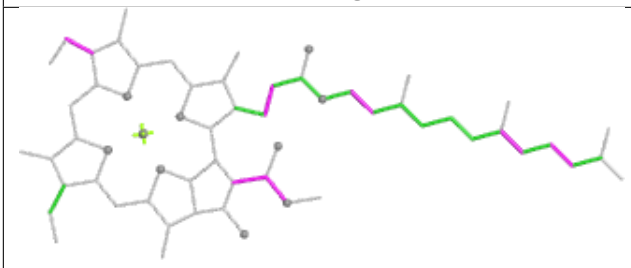
Ligand CLA B 816



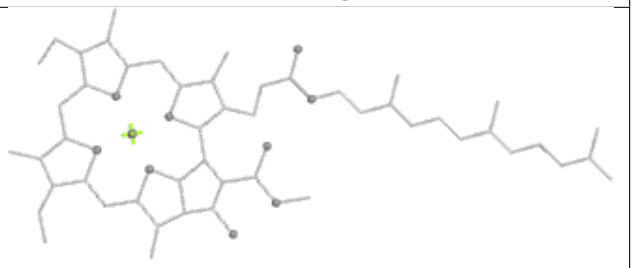
Bond lengths



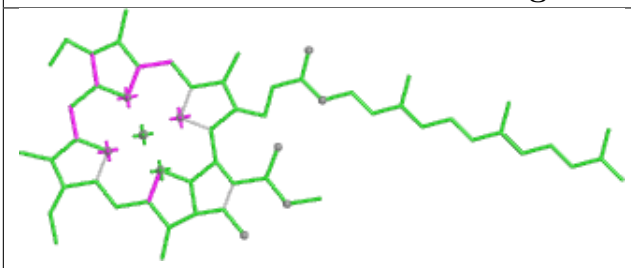
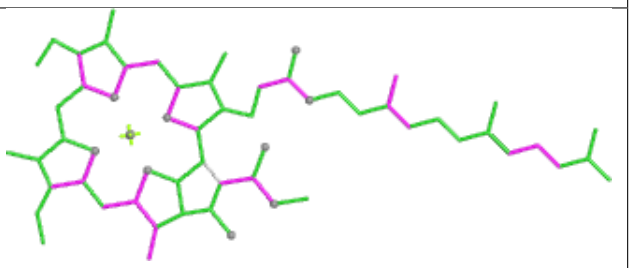
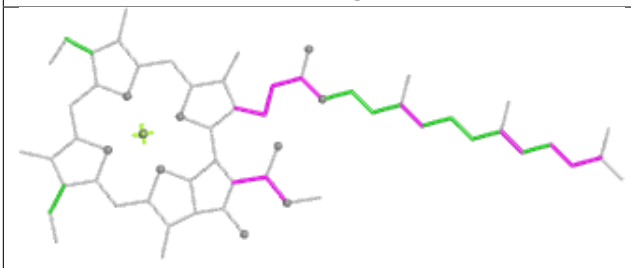
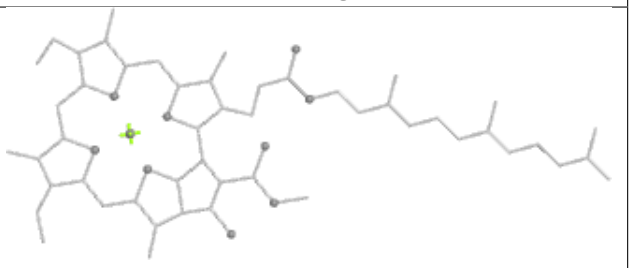
Bond angles

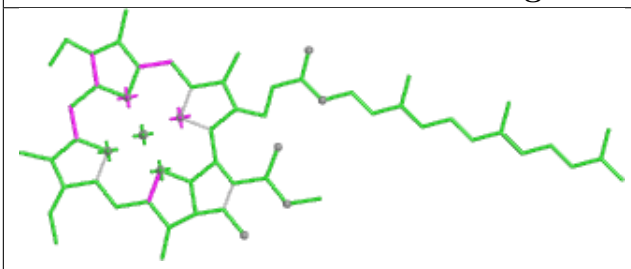
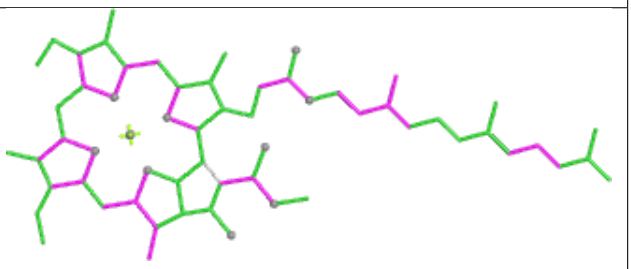
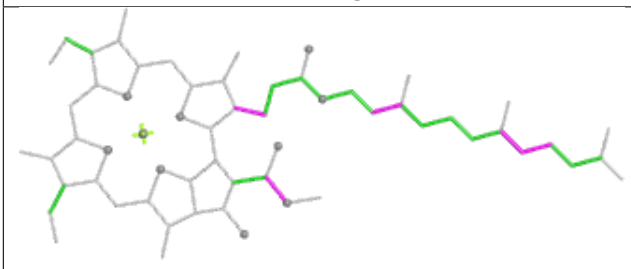
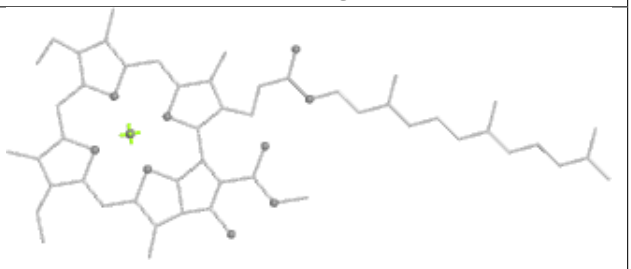


Torsions

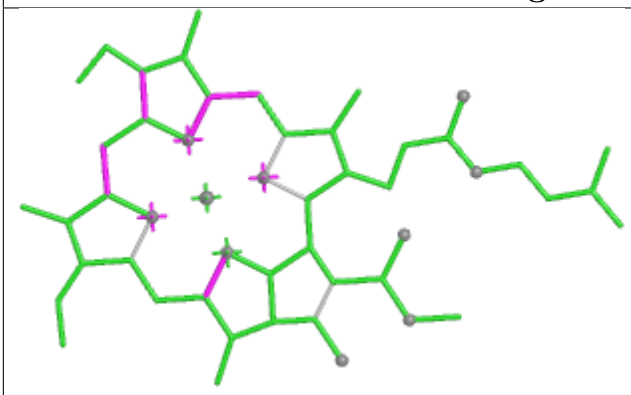


Rings

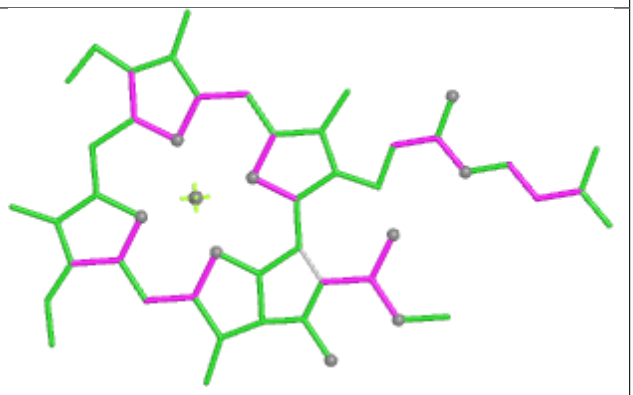
Ligand CLA c 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

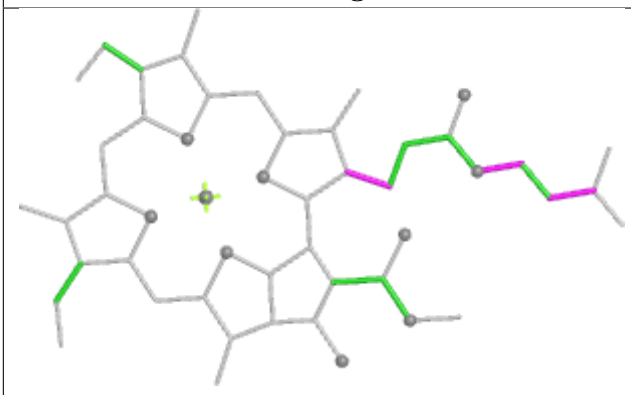
Ligand CLA a 208



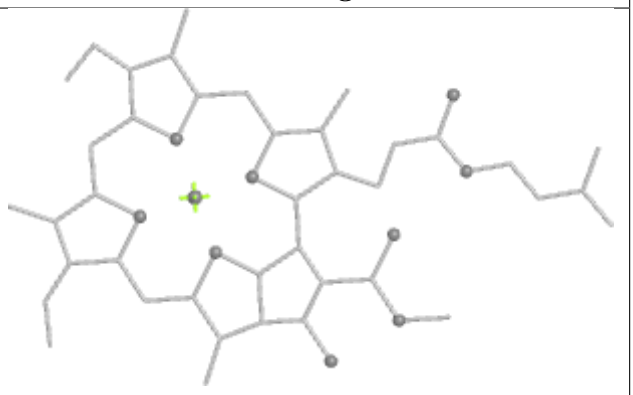
Bond lengths



Bond angles

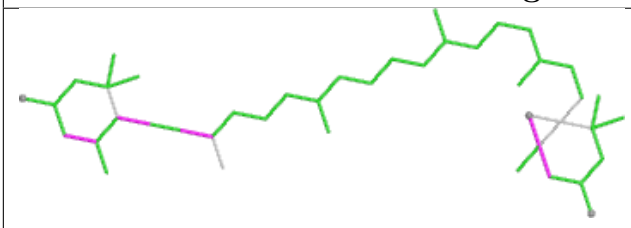


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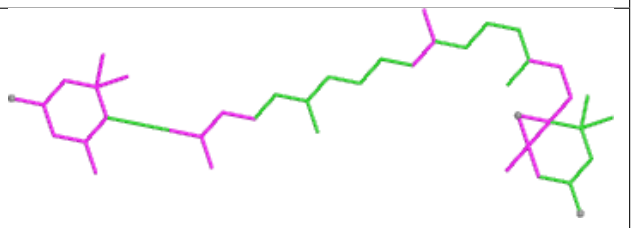


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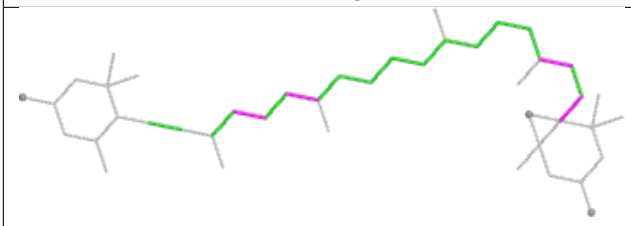
Ligand DD6 m 213



Bond lengths



Bond angles

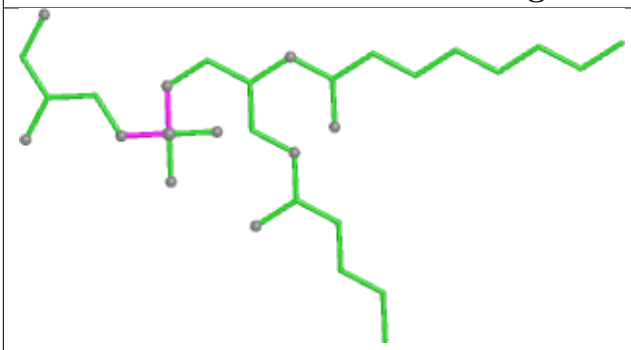


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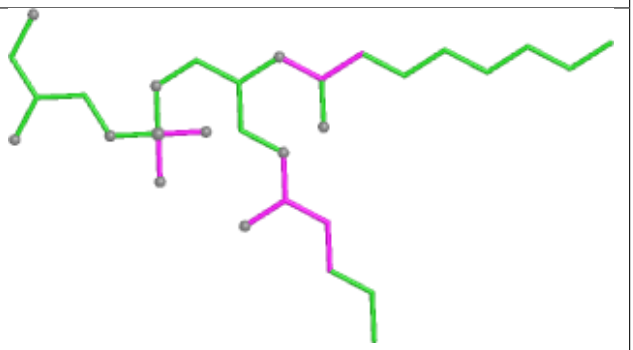


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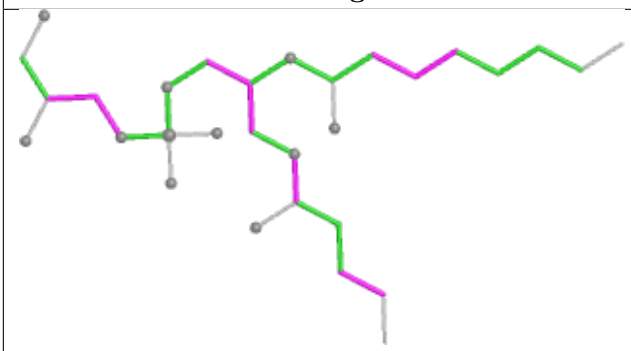
Ligand LHG c 301



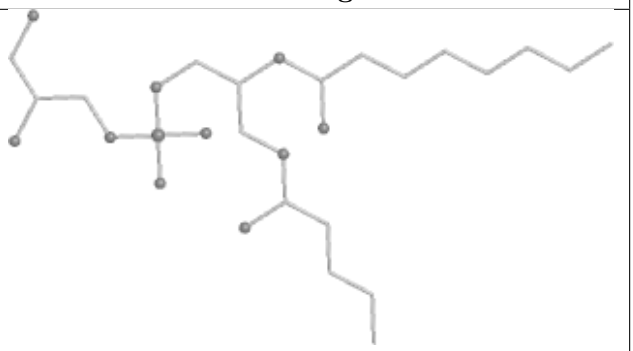
Bond lengths



Bond angles

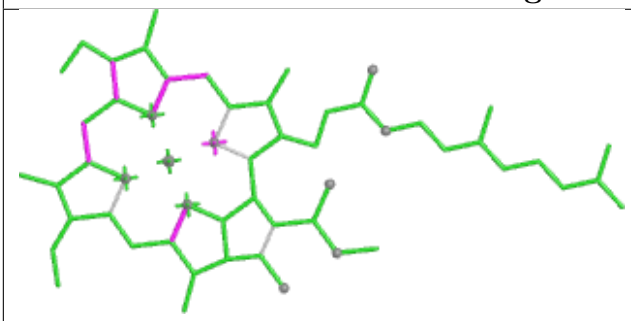


Torsions

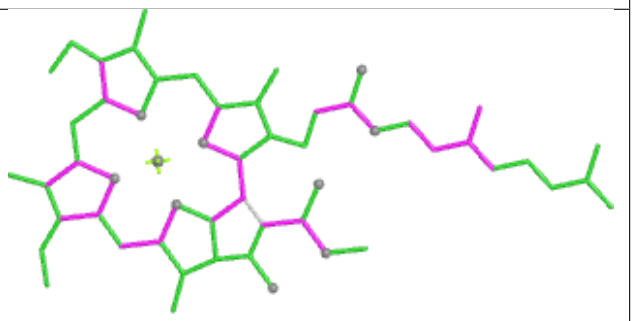


Rings

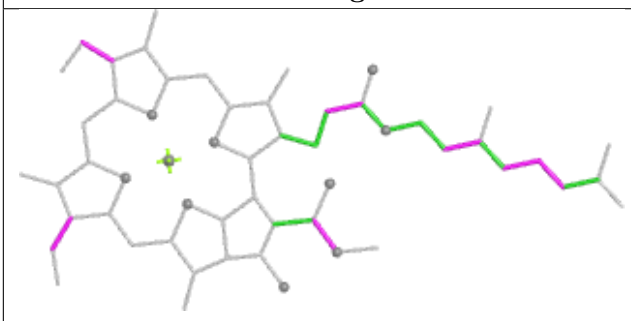
Ligand CLA B 803



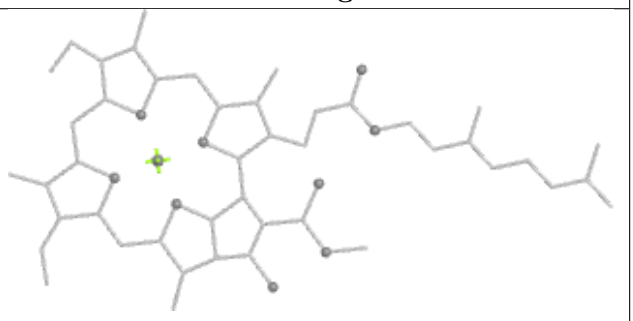
Bond lengths



Bond angles

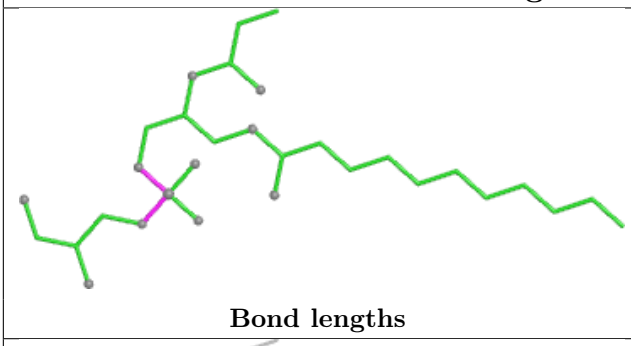


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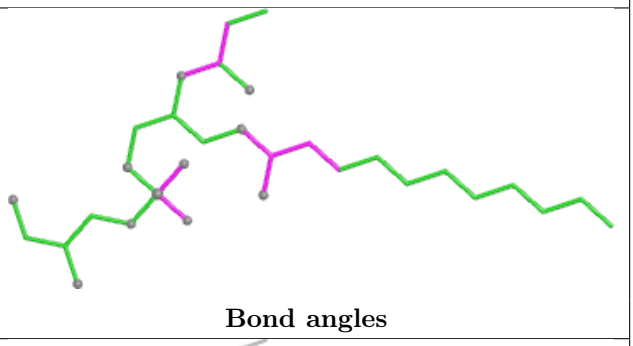


Rings

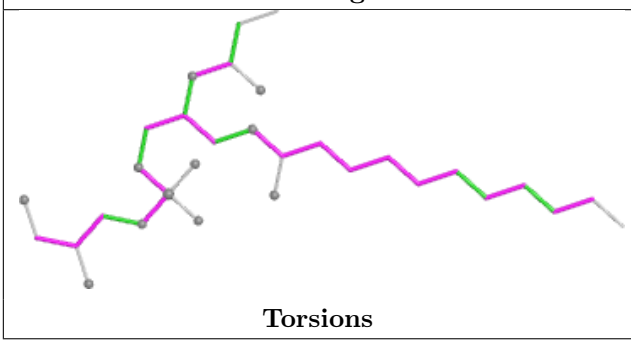
Ligand LHG b 201



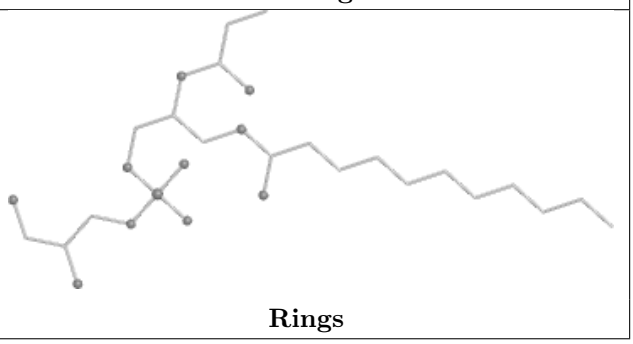
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Bond angles

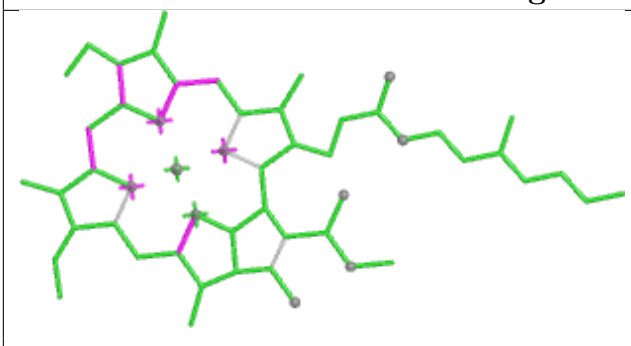


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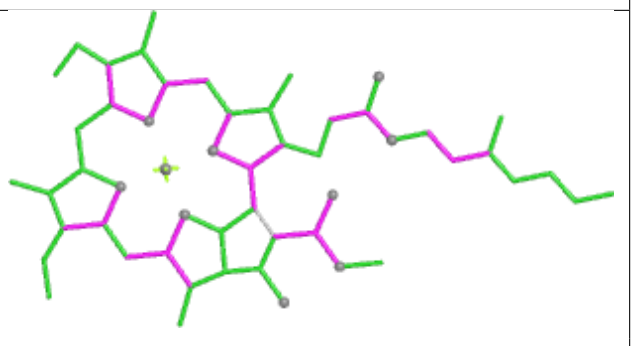


Rings

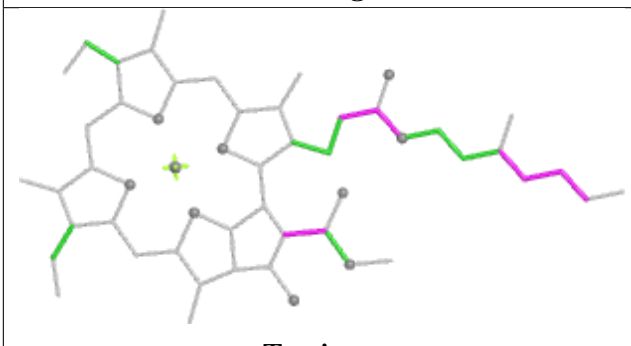
Ligand CLA a 205



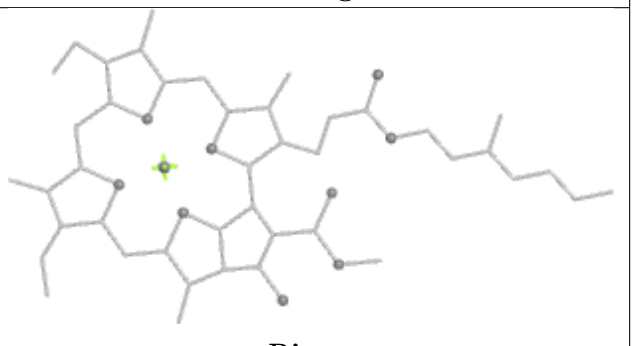
Bond lengths



Bond angles

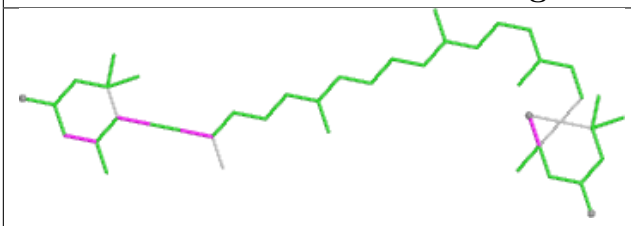


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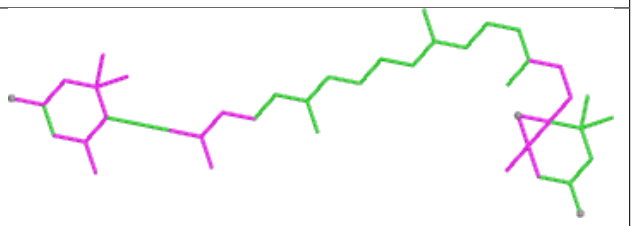


Rings

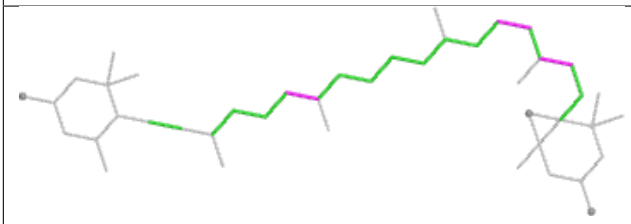
Ligand DD6 a 214



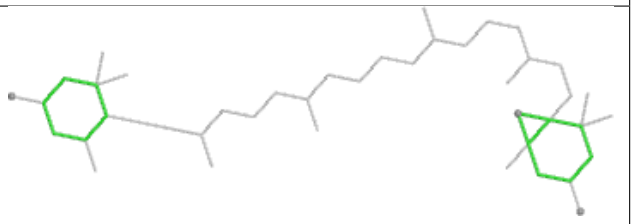
Bond lengths



Bond angles

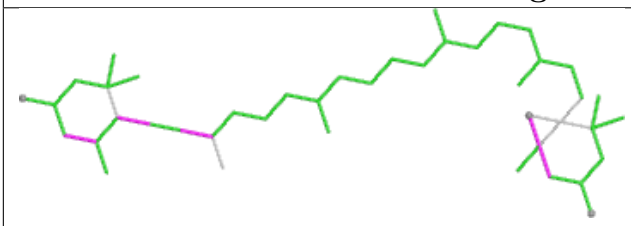


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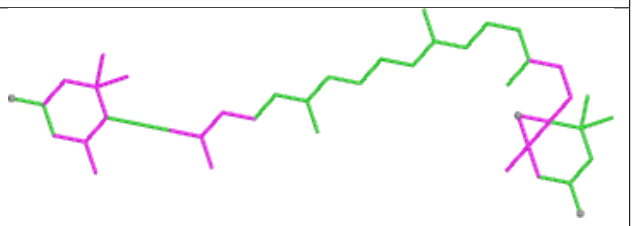


Rings

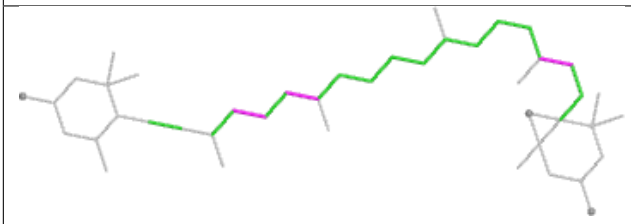
Ligand DD6 e 219



Bond lengths



Bond angles

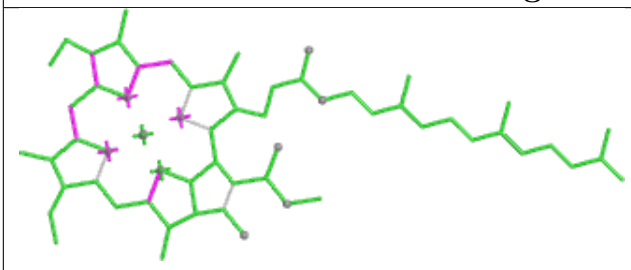


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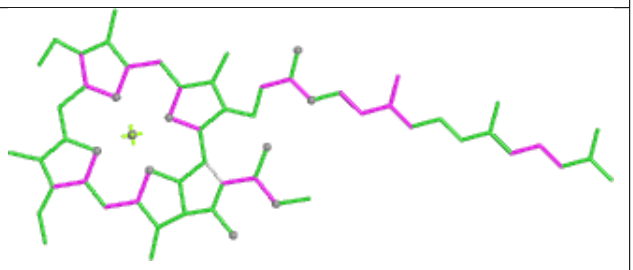


Rings

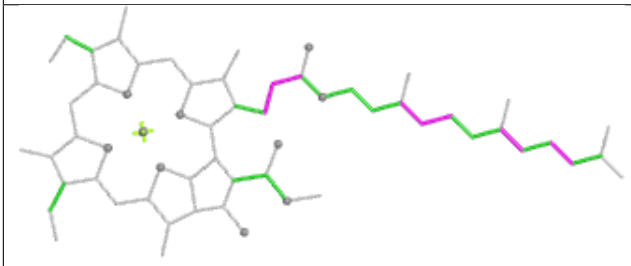
Ligand CLA A 804



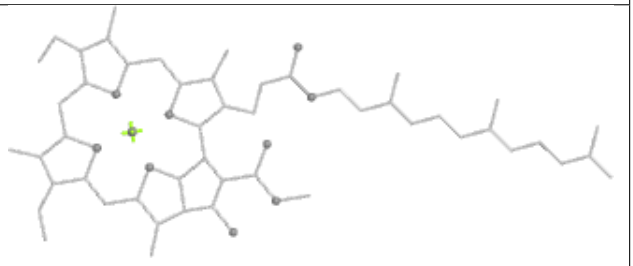
Bond lengths



Bond angles

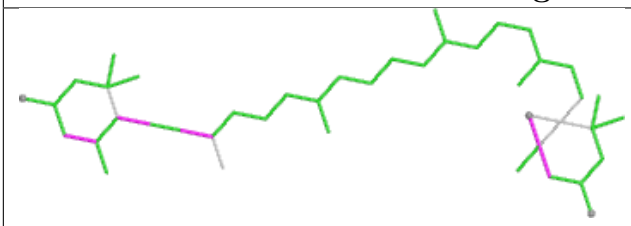


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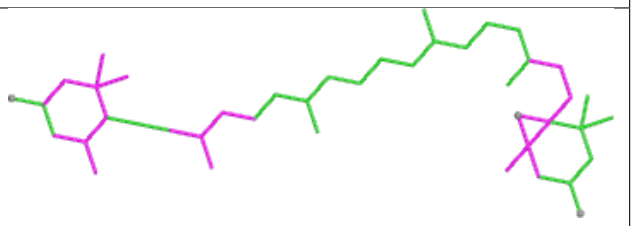


Rings

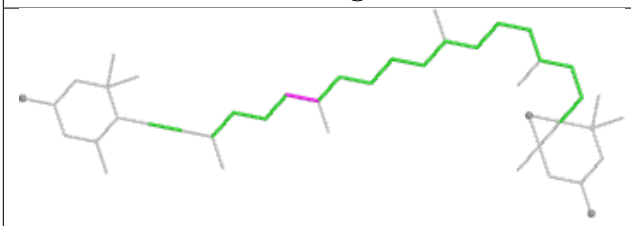
Ligand DD6 i 214



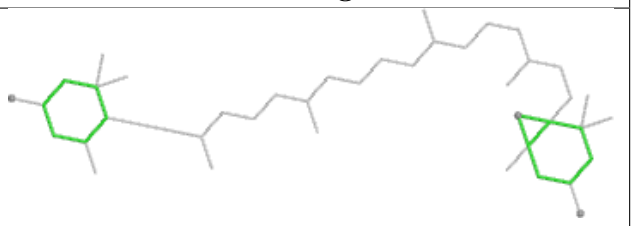
Bond lengths



Bond angles

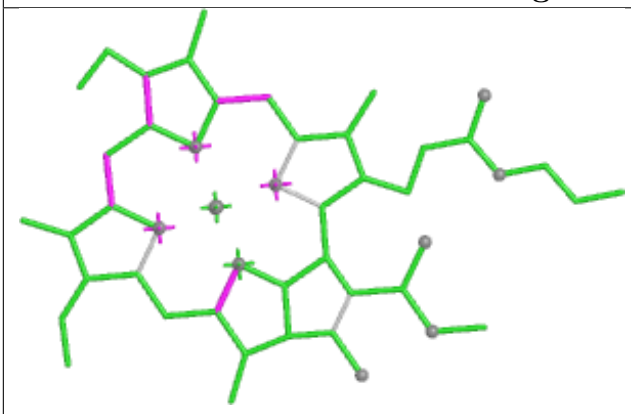


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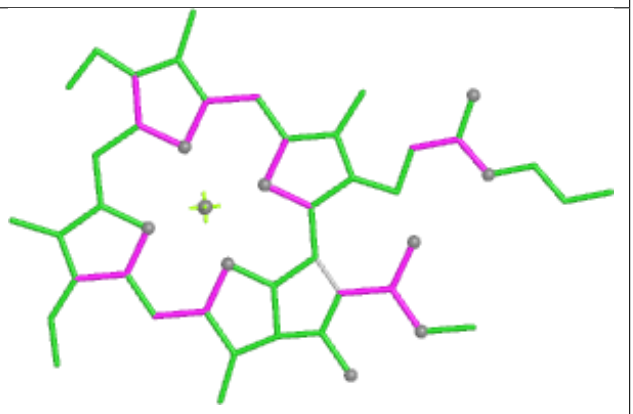


Rings

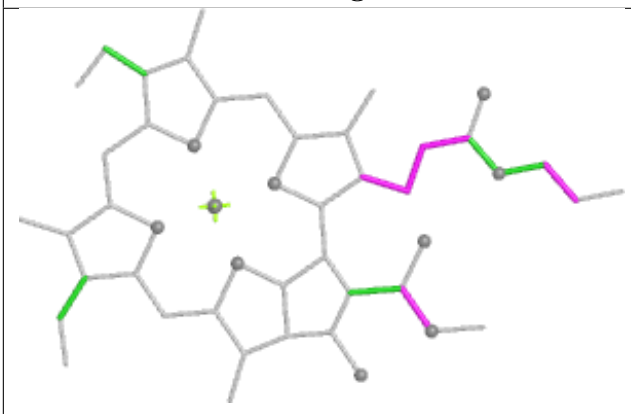
Ligand CLA l 610



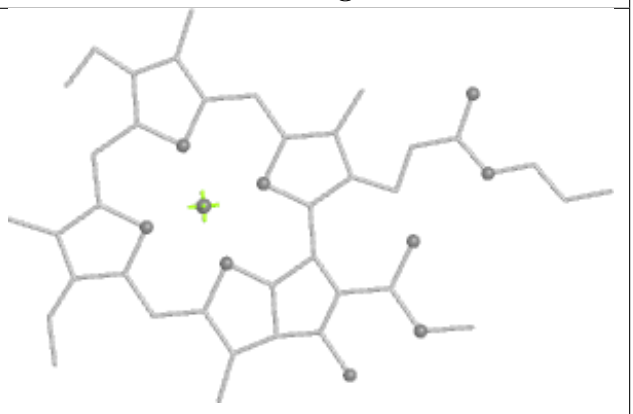
Bond lengths



Bond angles

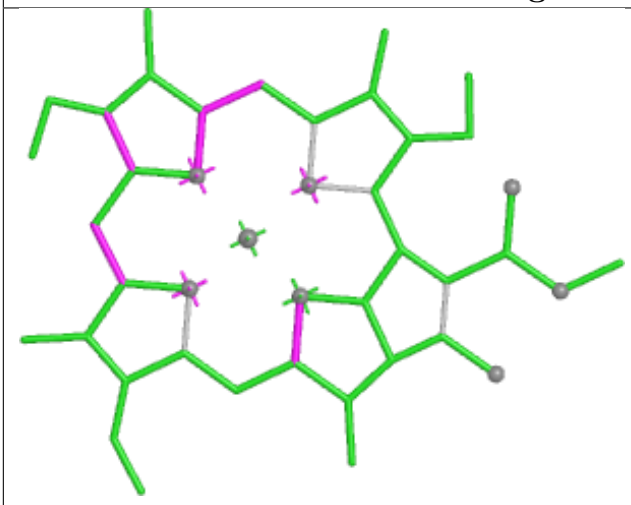


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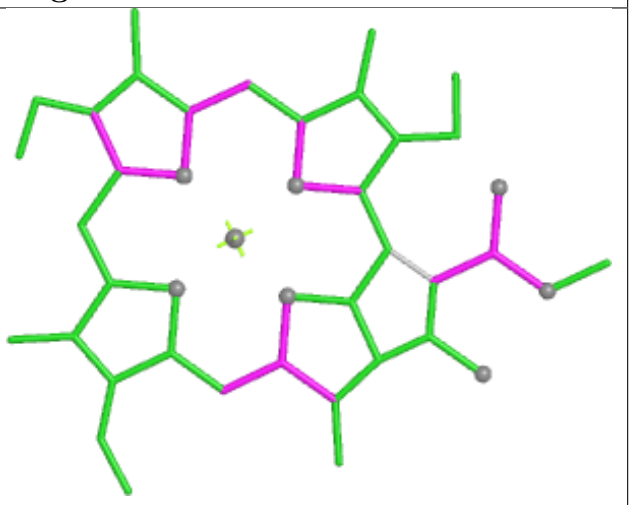


Rings

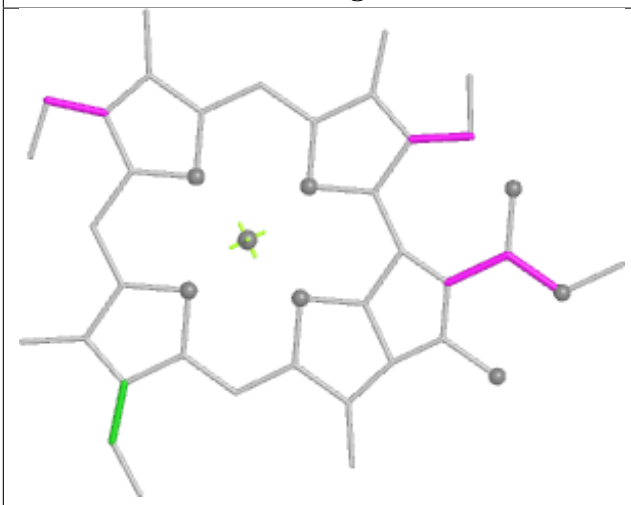
Ligand CLA g 203



Bond lengths



Bond angles

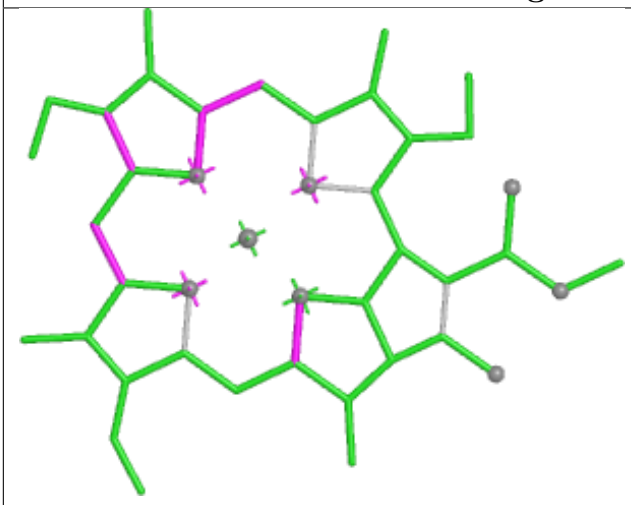


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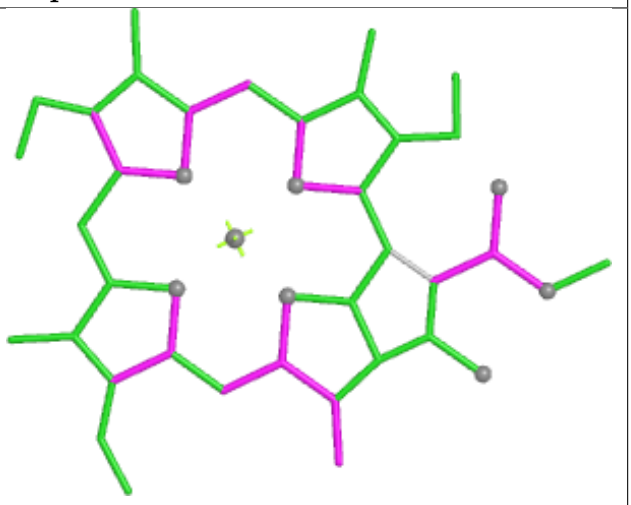


Rings

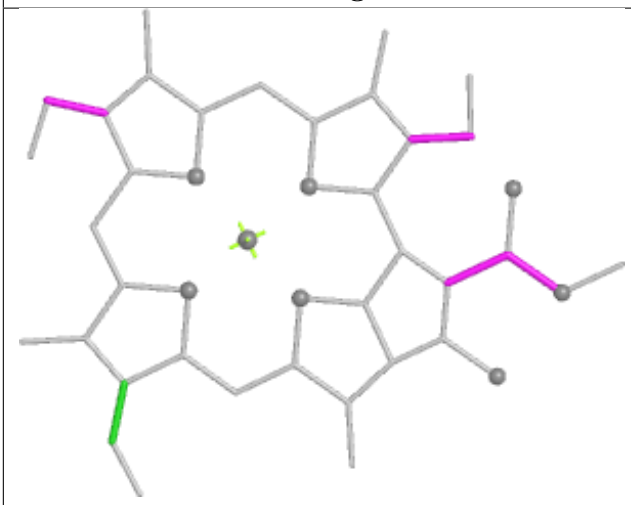
Ligand CLA p 605



Bond lengths



Bond angles

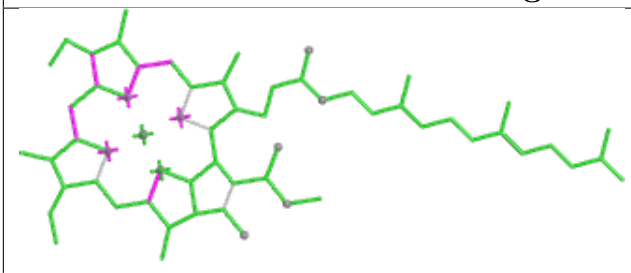


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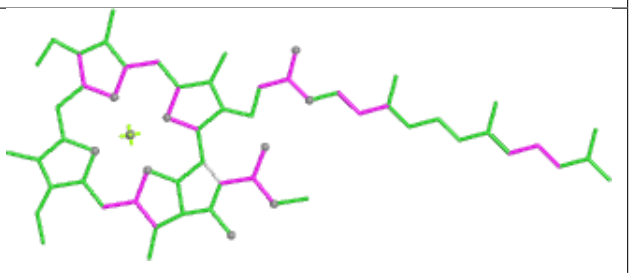


Rings

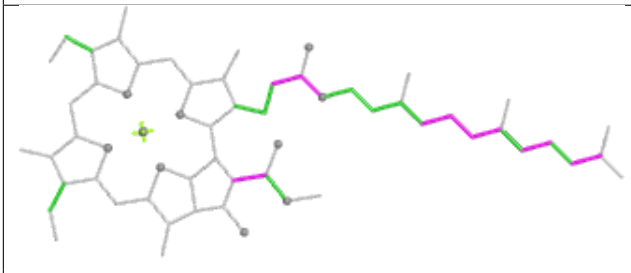
Ligand CLA A 808



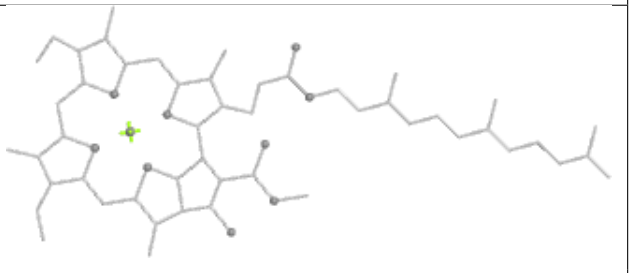
Bond lengths



Bond angles

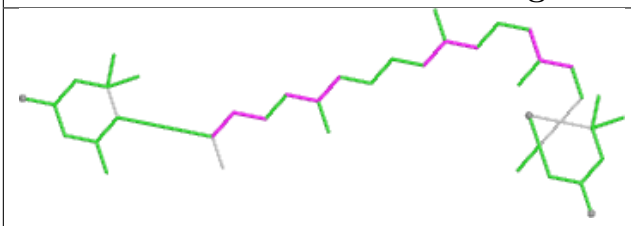


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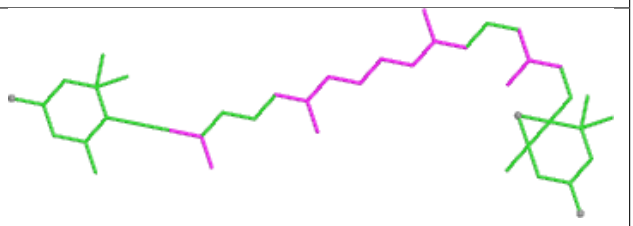


Rings

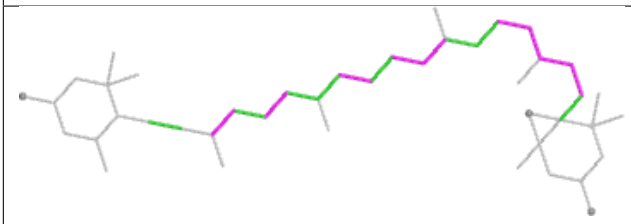
Ligand DD6 n 213



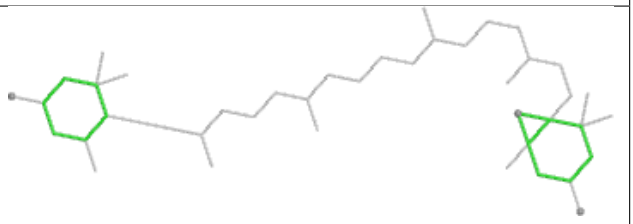
Bond lengths



Bond angles

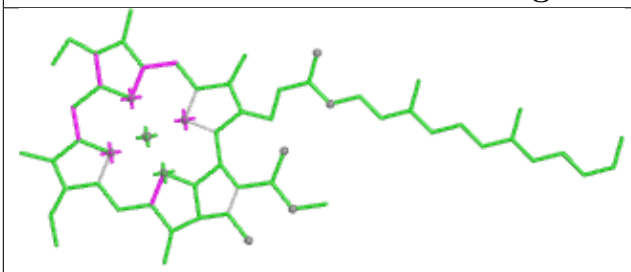


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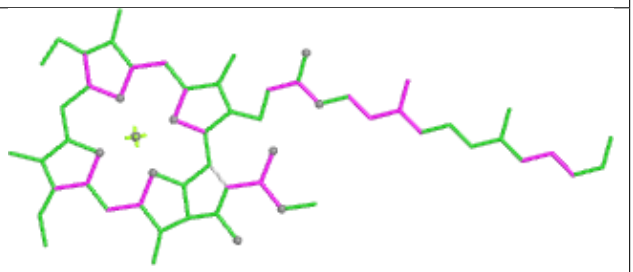


Rings

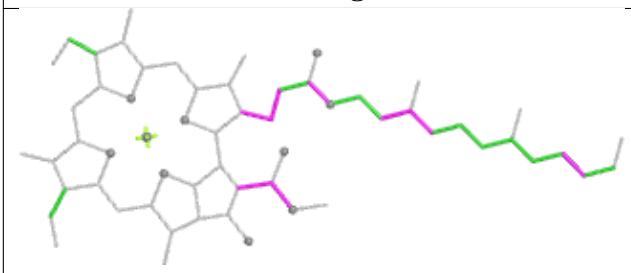
Ligand CLA l 602



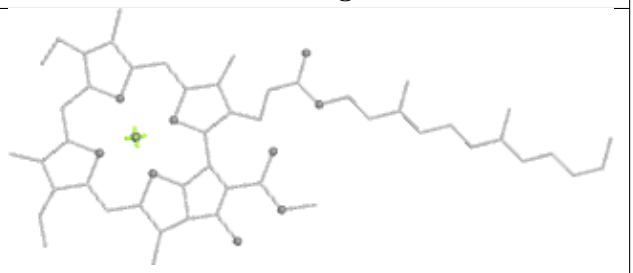
Bond lengths



Bond angles

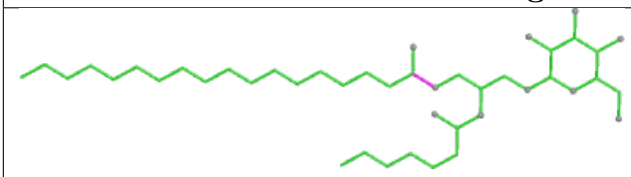


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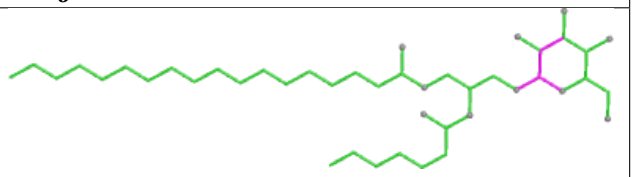


Rings

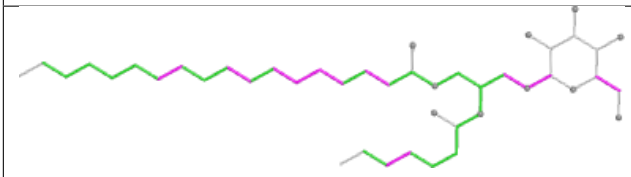
Ligand LMG j 201



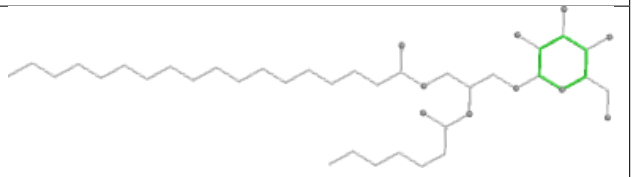
Bond lengths



Bond angles

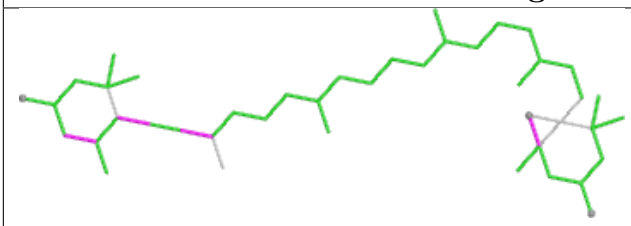


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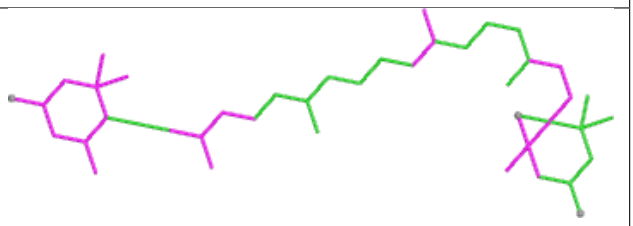


Rings

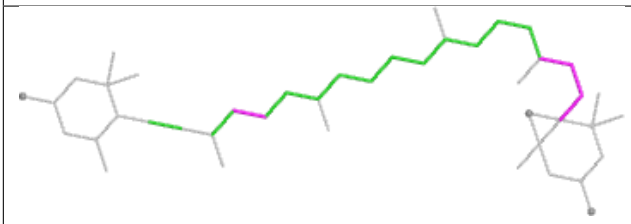
Ligand DD6 n 212



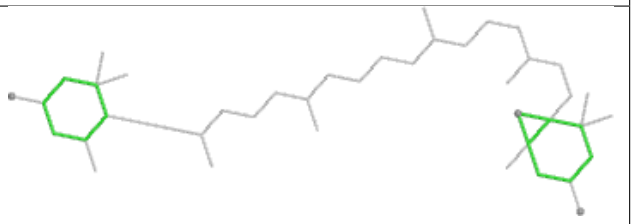
Bond lengths



Bond angles

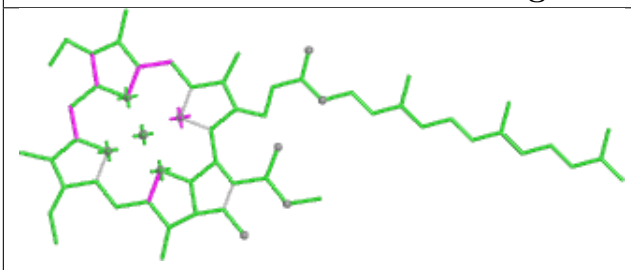


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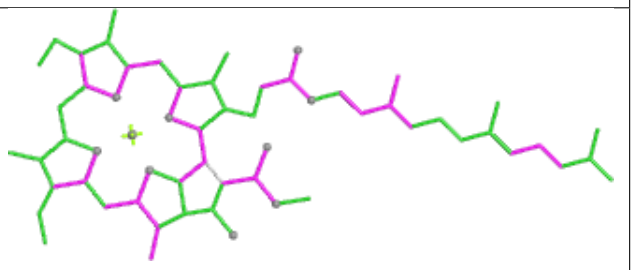


Rings

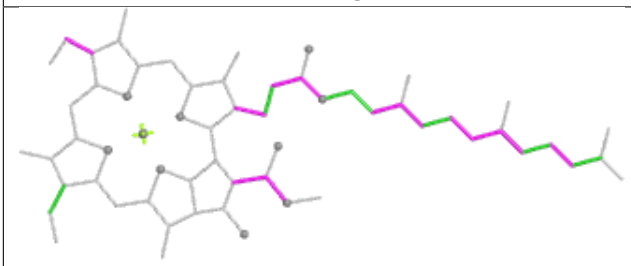
Ligand CLA a 204



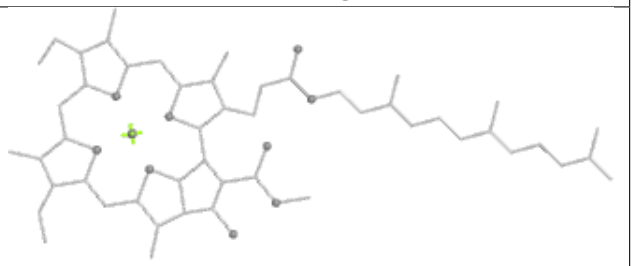
Bond lengths



Bond angles

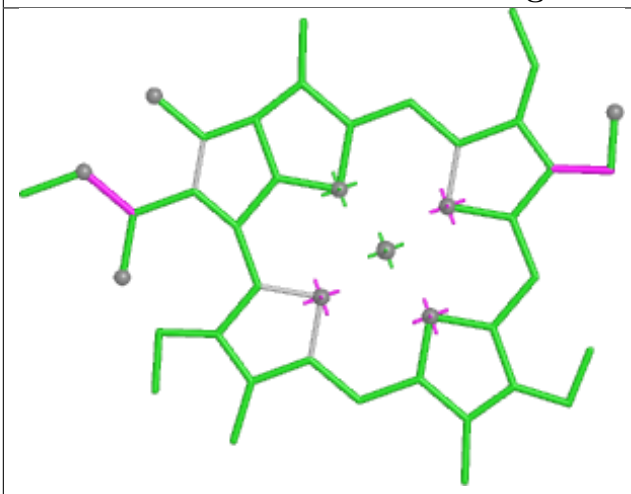


Torsions

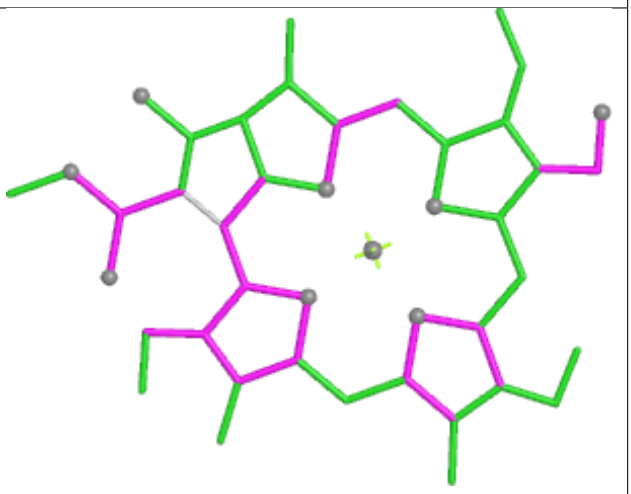


Rings

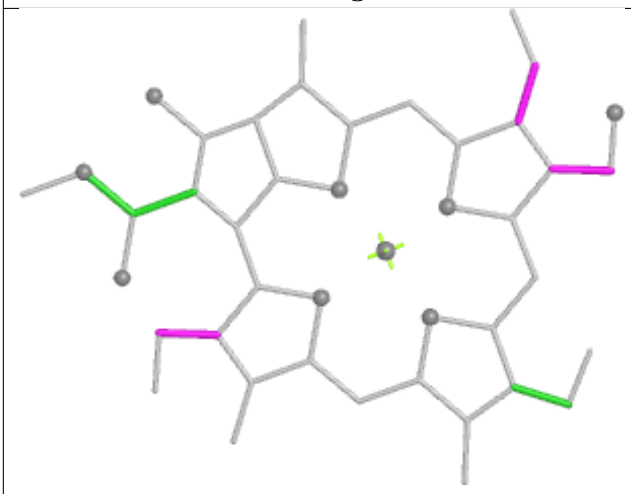
Ligand CHL d 309



Bond lengths



Bond angles

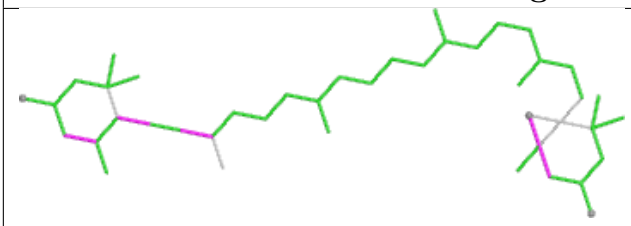


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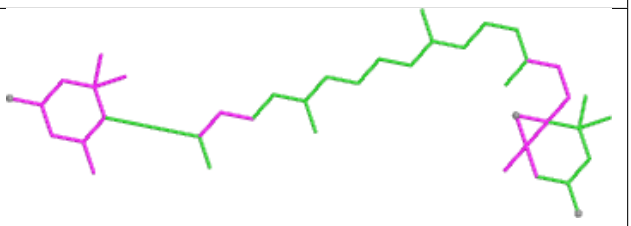


Rings

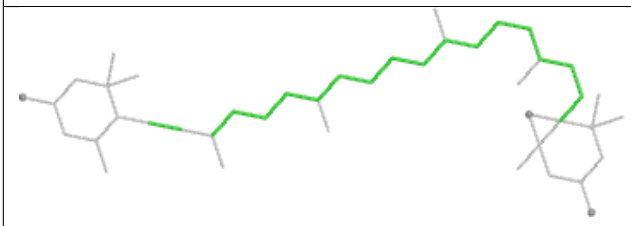
Ligand DD6 c 317



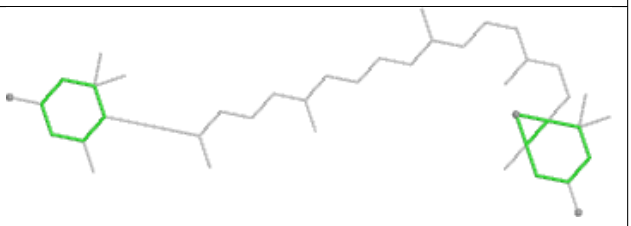
Bond lengths



Bond angles

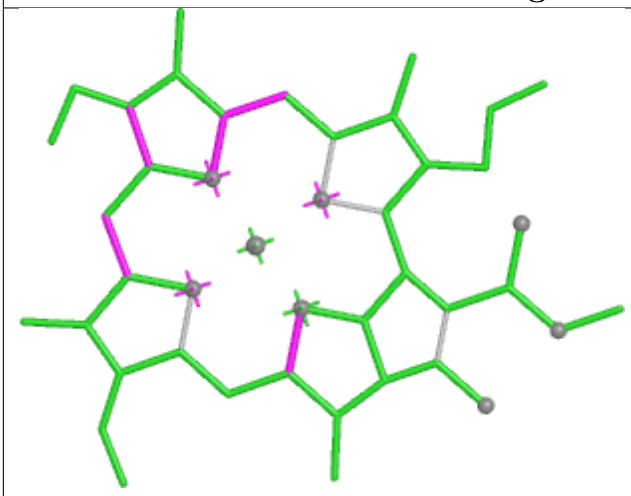


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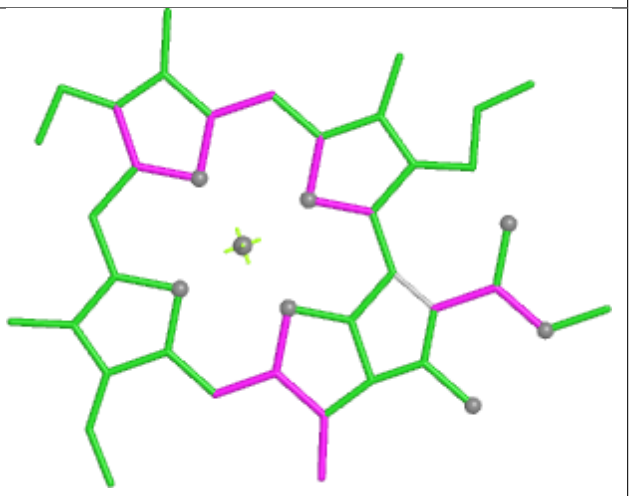


Rings

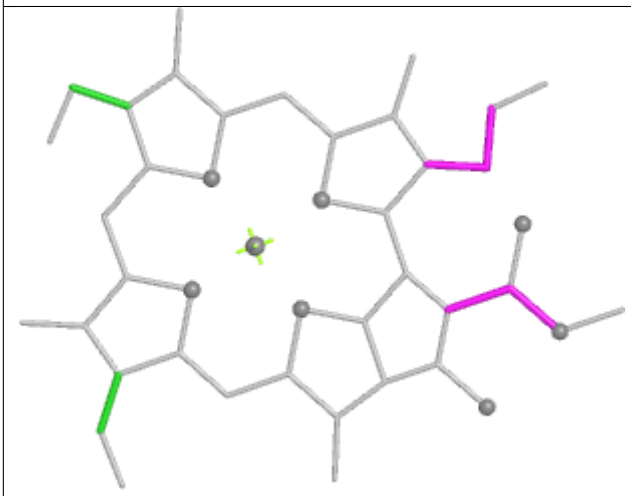
Ligand CLA o 603



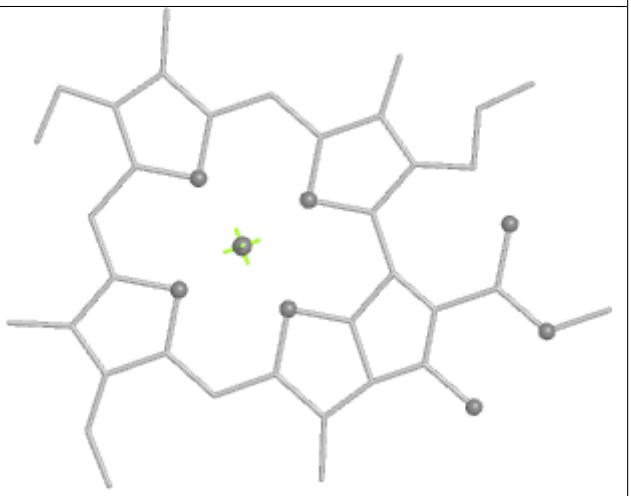
Bond lengths



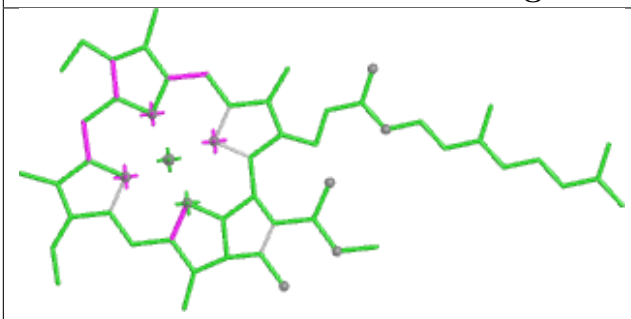
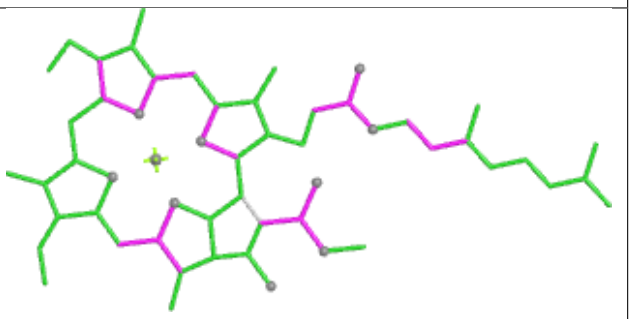
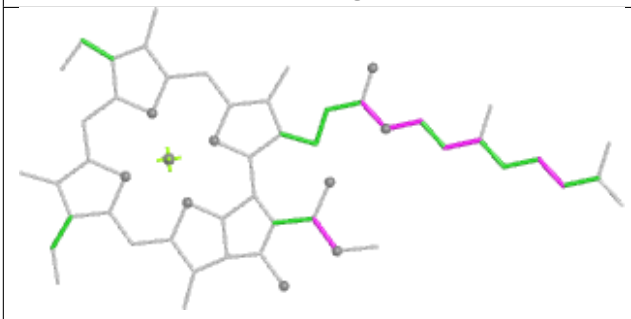
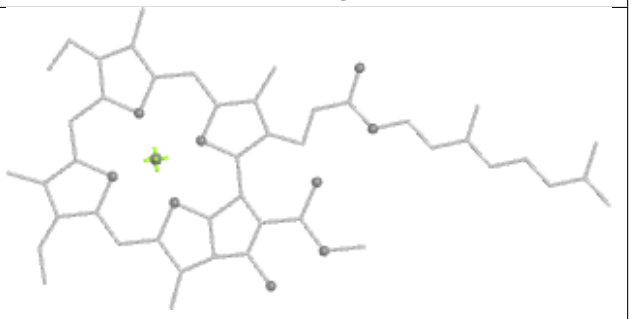
Bond angles

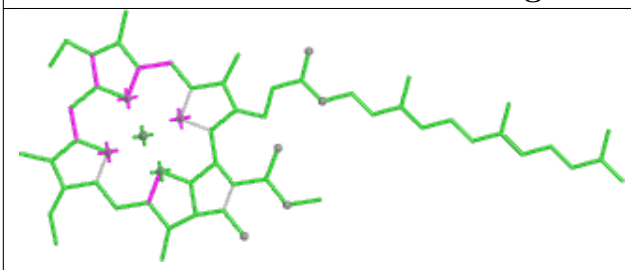
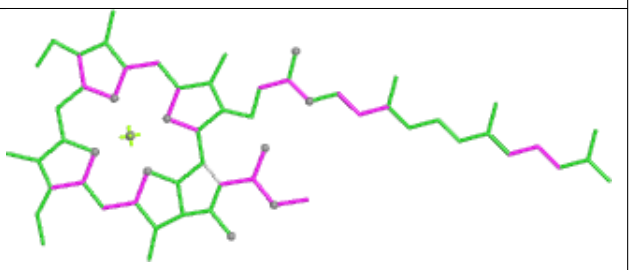
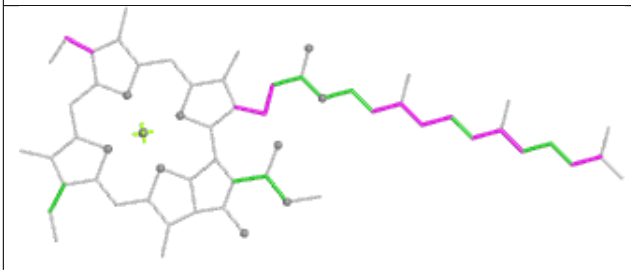
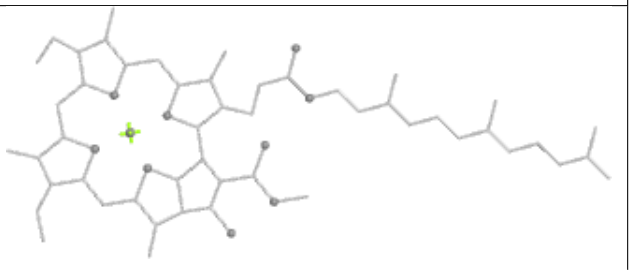


Torsions

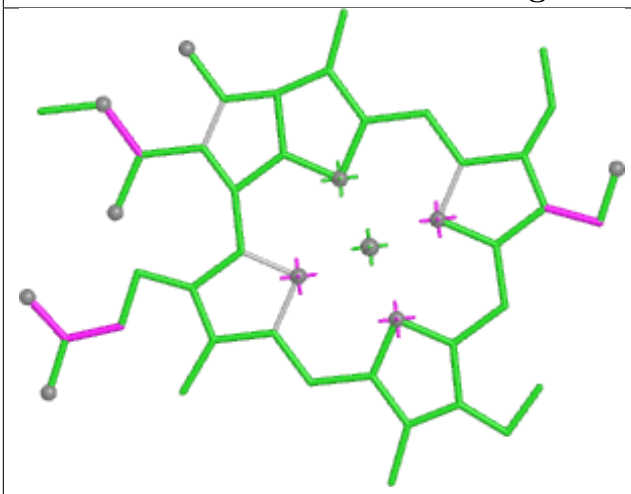


Rings

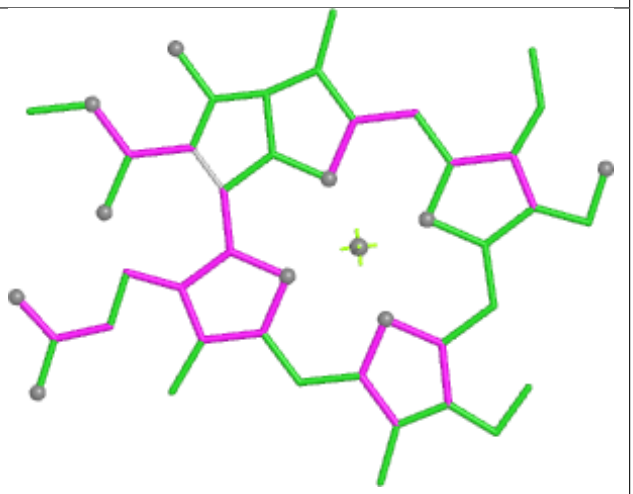
Ligand CLA B 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

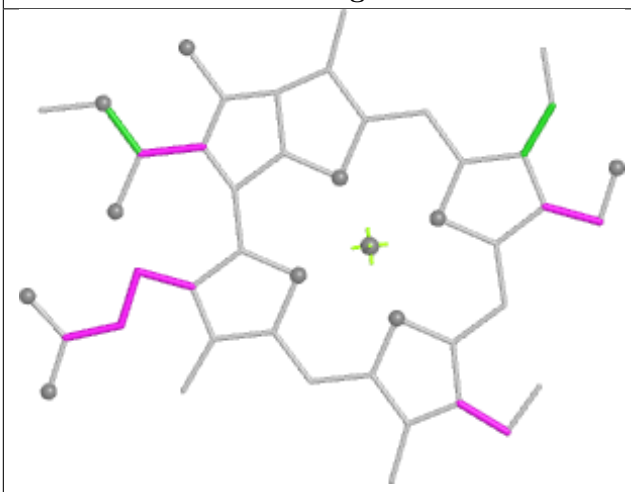
Ligand CHL e 209



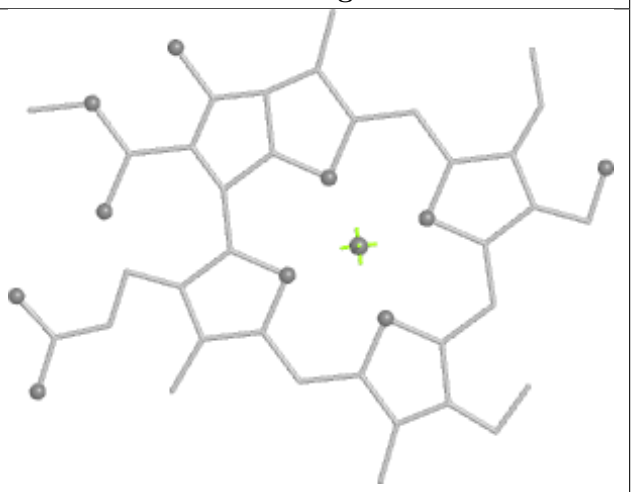
Bond lengths



Bond angles

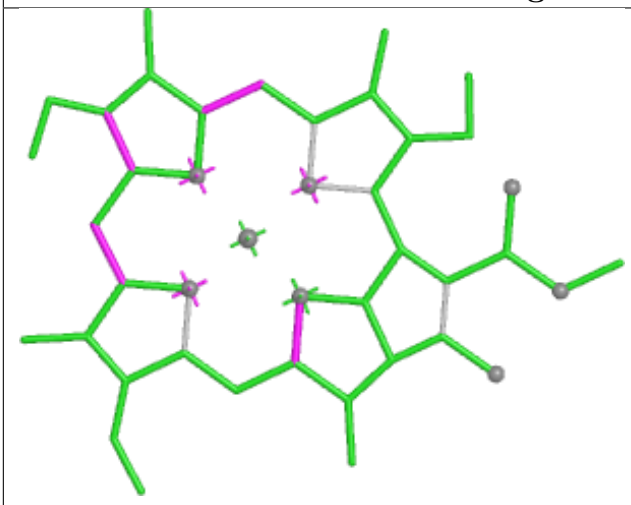


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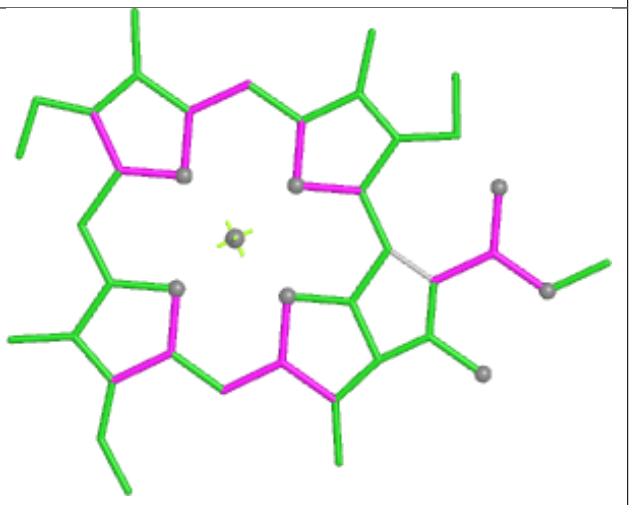


Rings

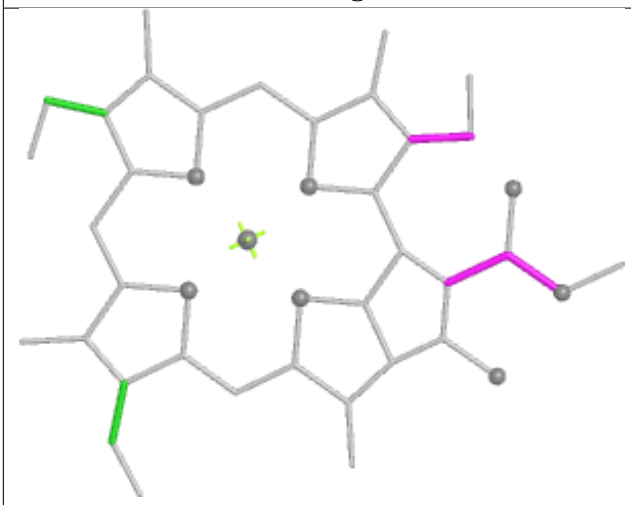
Ligand CLA n 204



Bond lengths



Bond angles

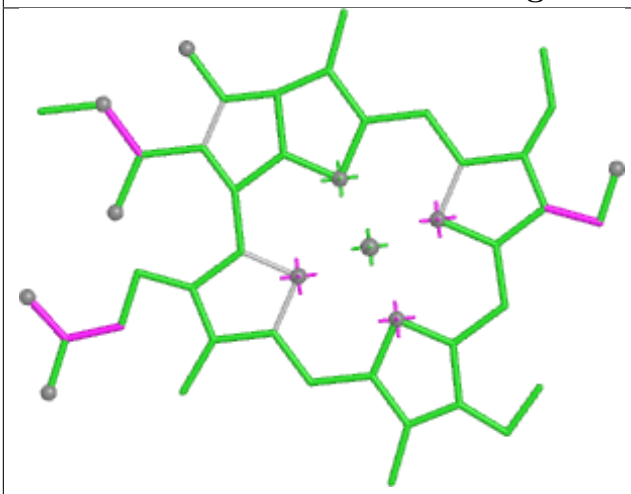


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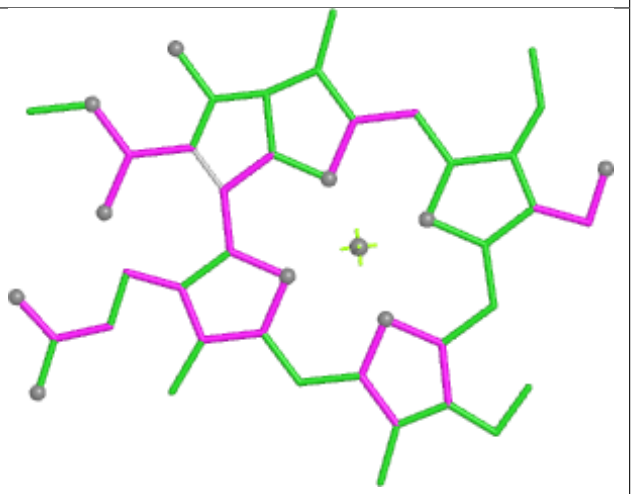


Rings

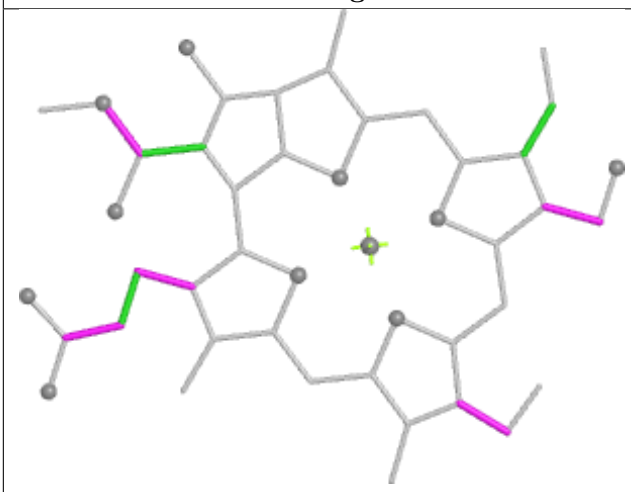
Ligand CHL d 308



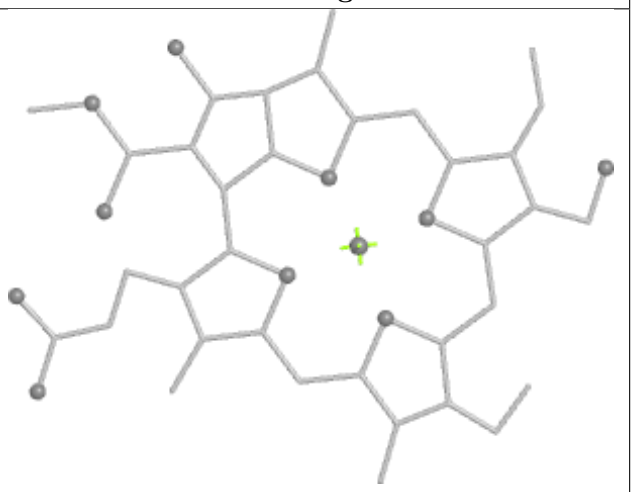
Bond lengths



Bond angles

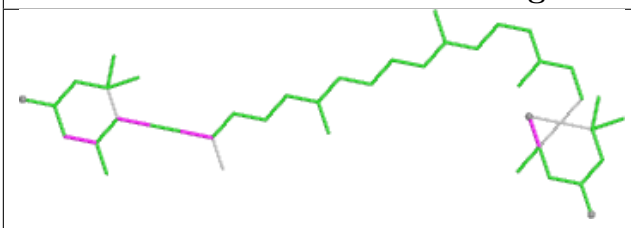


Torsions

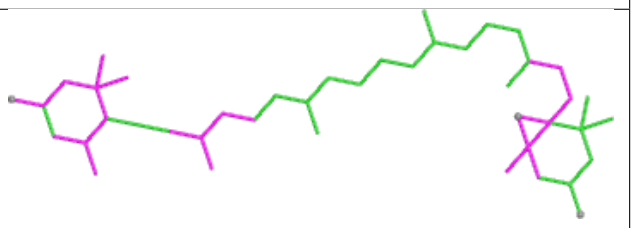


Rings

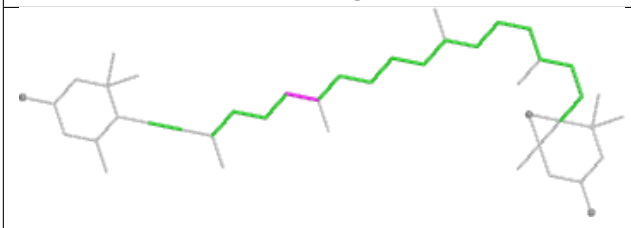
Ligand DD6 d 317



Bond lengths



Bond angles

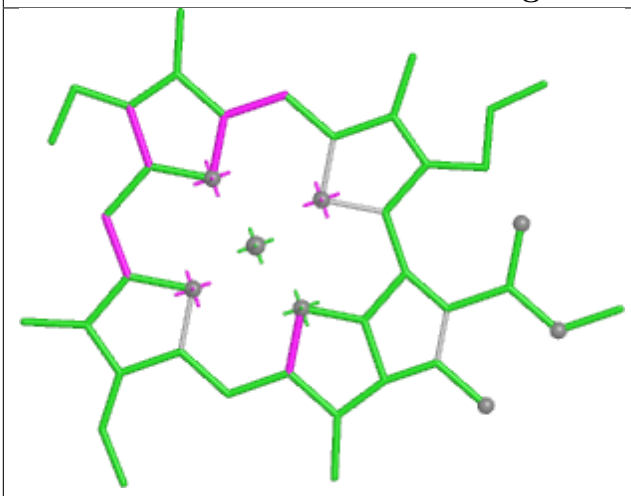


Torsions

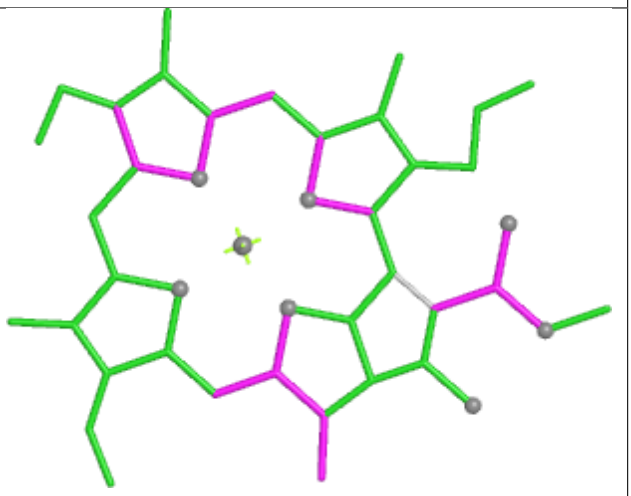


Rings

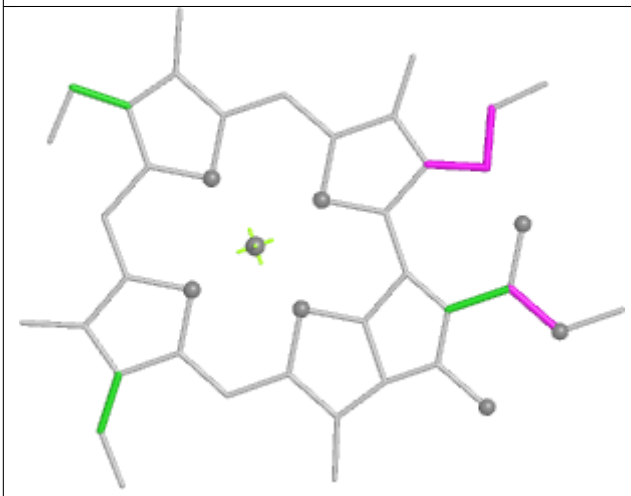
Ligand CLA m 210



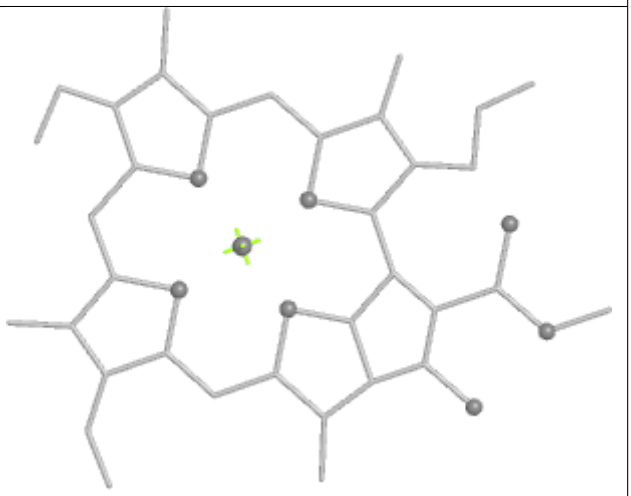
Bond lengths



Bond angles

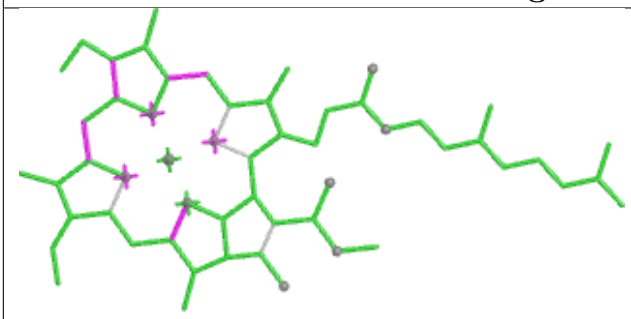


Torsions

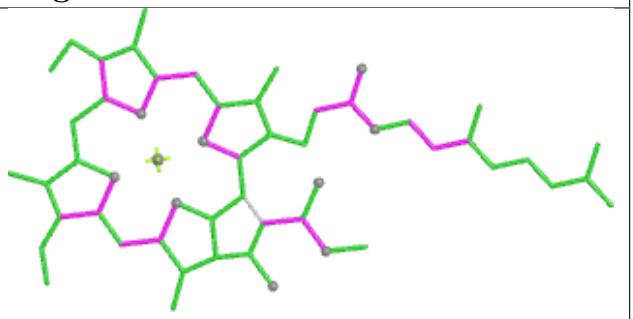


Rings

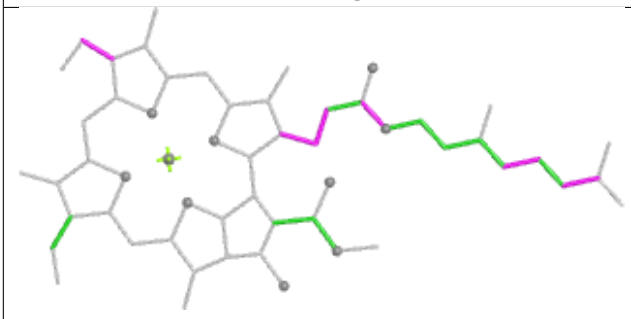
Ligand CLA g 209



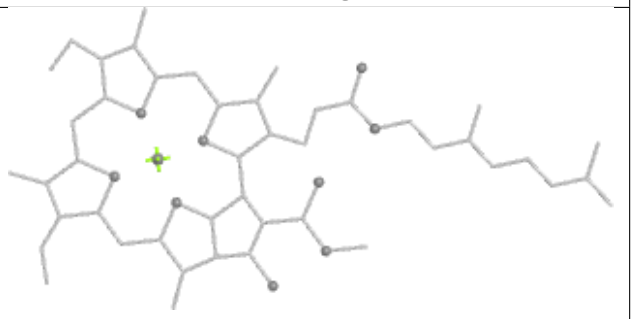
Bond lengths



Bond angles

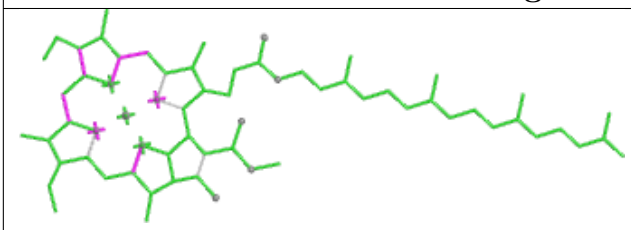


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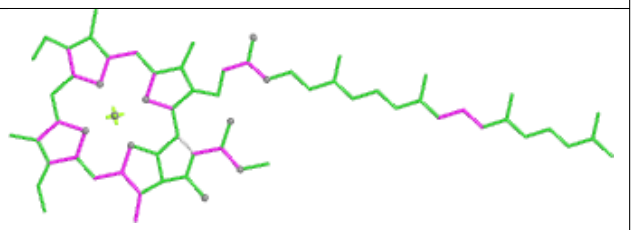


Rings

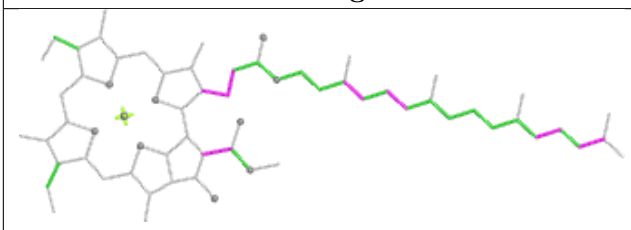
Ligand CLA B 845



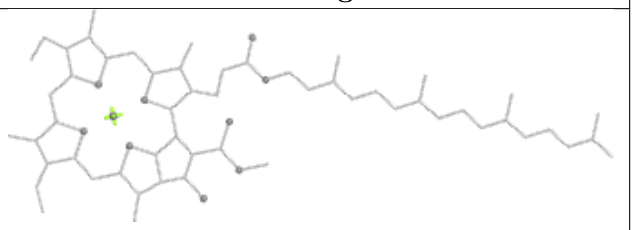
Bond lengths



Bond angles

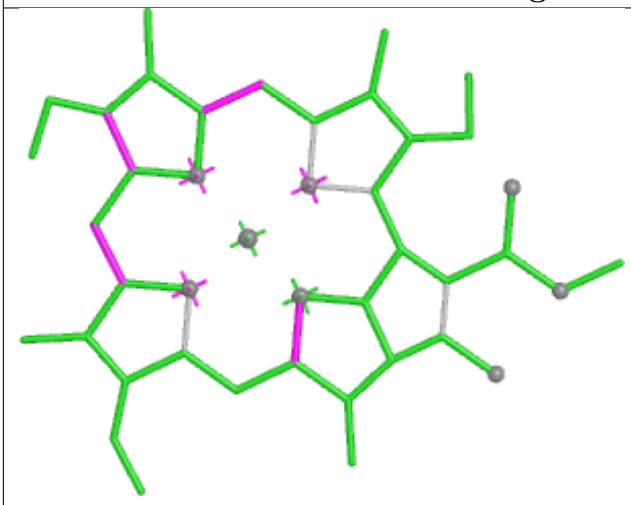


Torsions

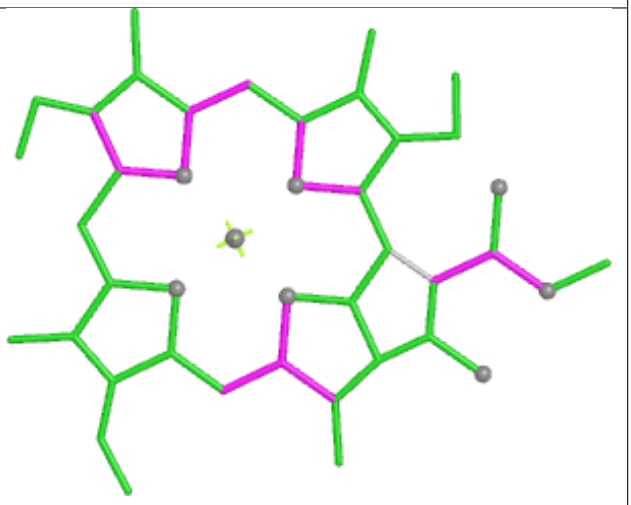


Rings

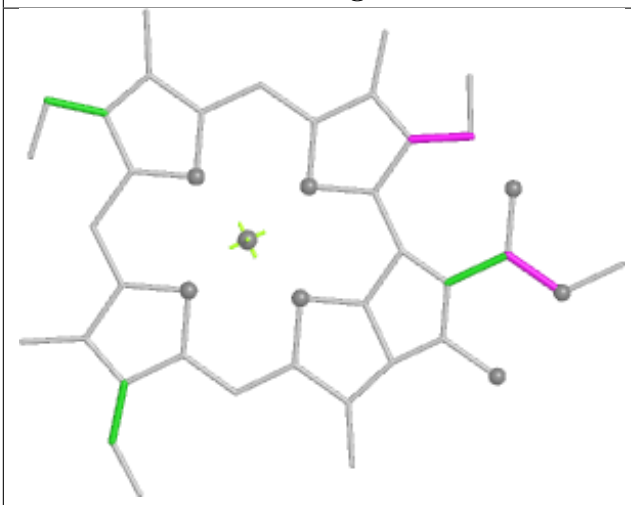
Ligand CLA e 217



Bond lengths



Bond angles

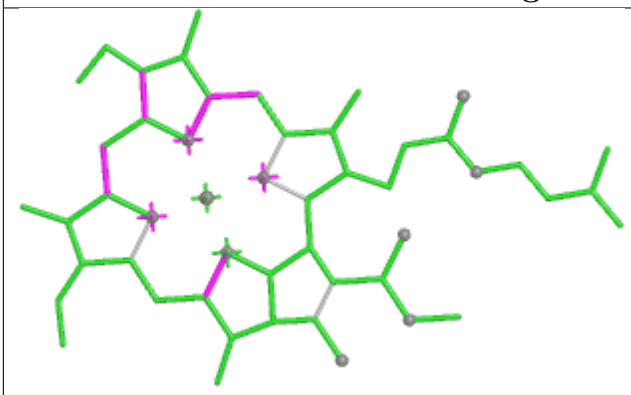


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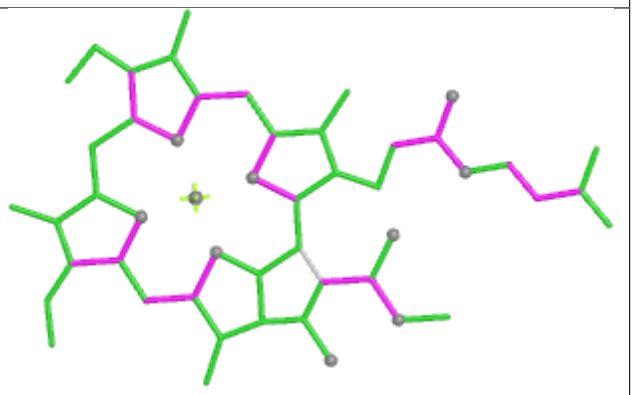


Rings

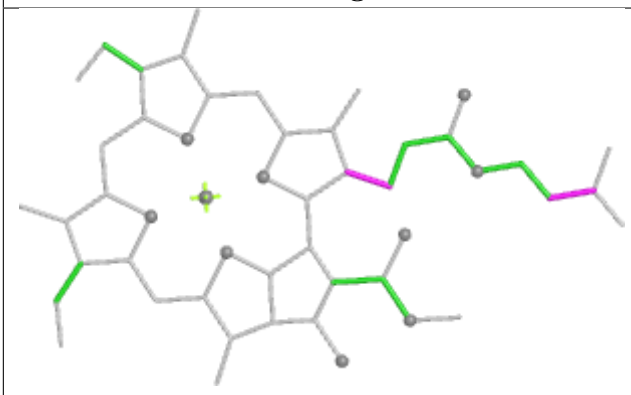
Ligand CLA m 207



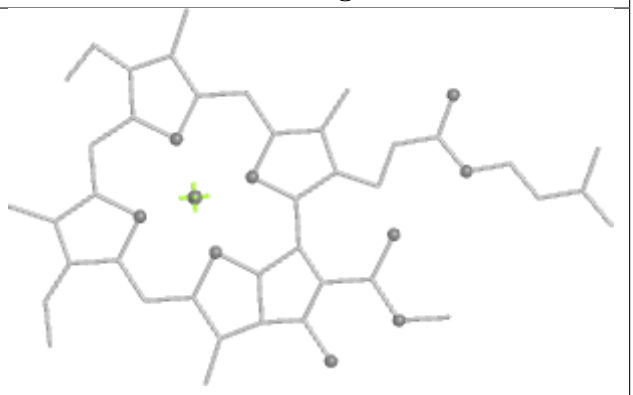
Bond lengths



Bond angles

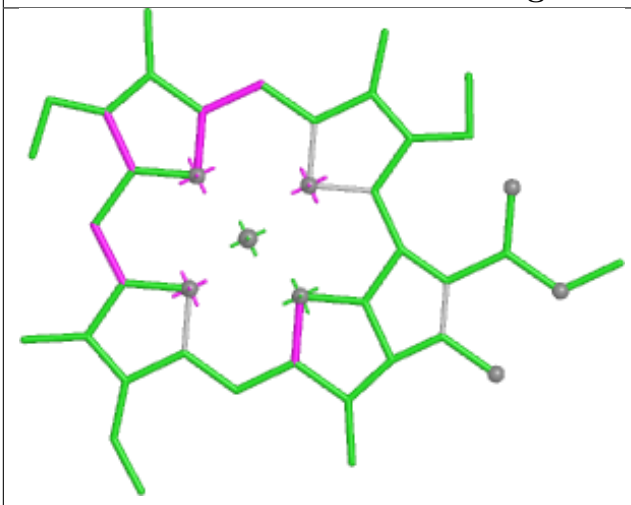


Torsions

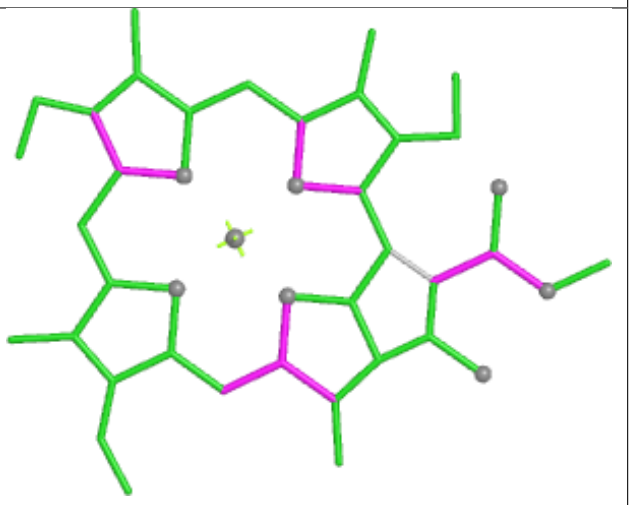


Rings

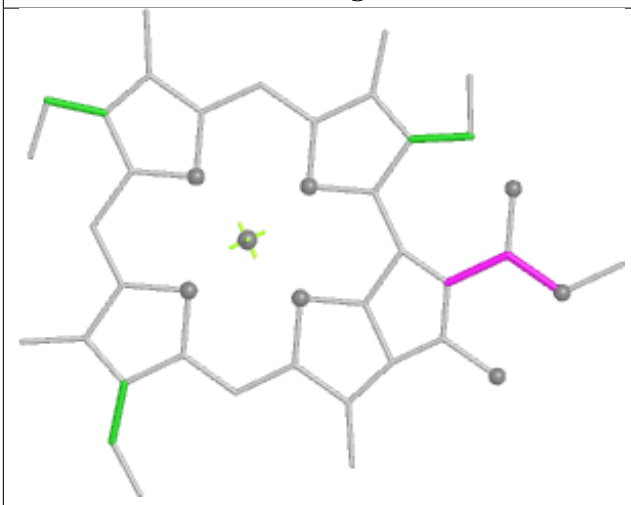
Ligand CLA d 314



Bond lengths



Bond angles

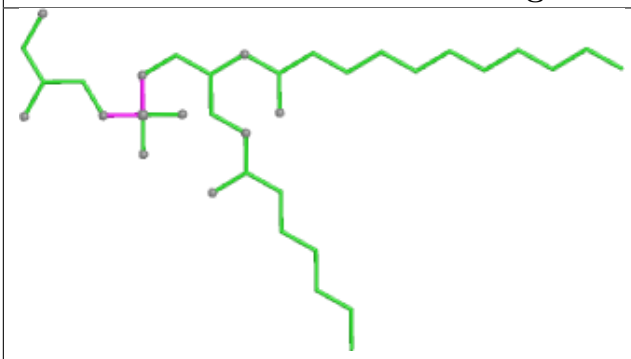


Torsions

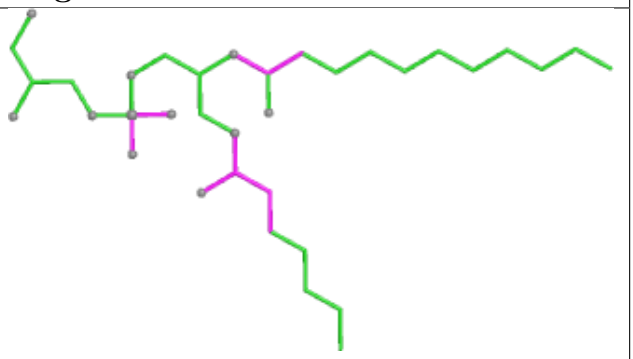


Rings

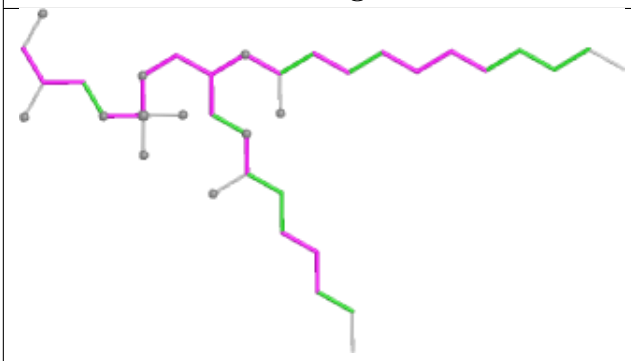
Ligand LHG g 201



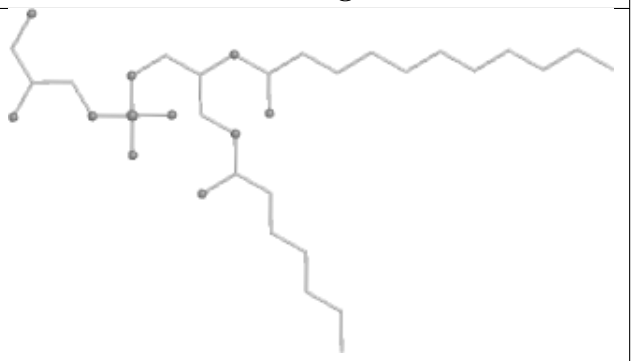
Bond lengths



Bond angles

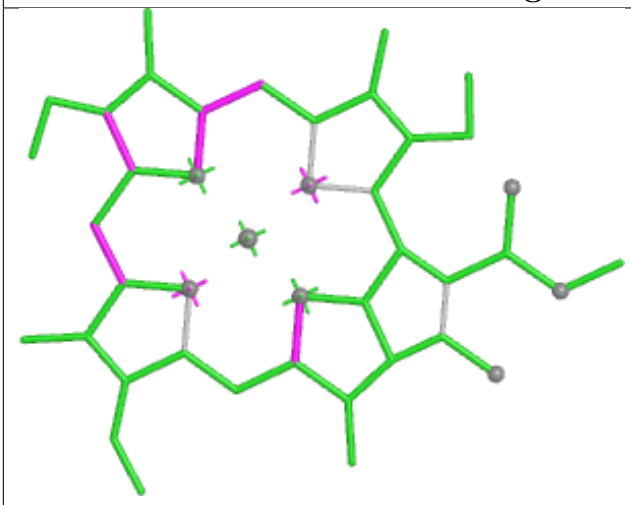


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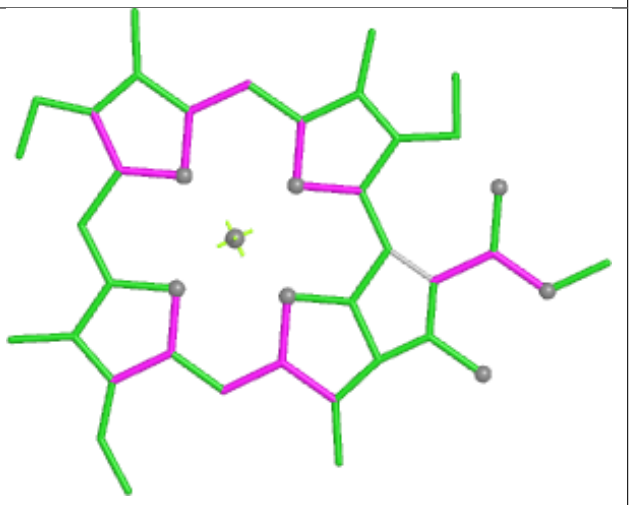


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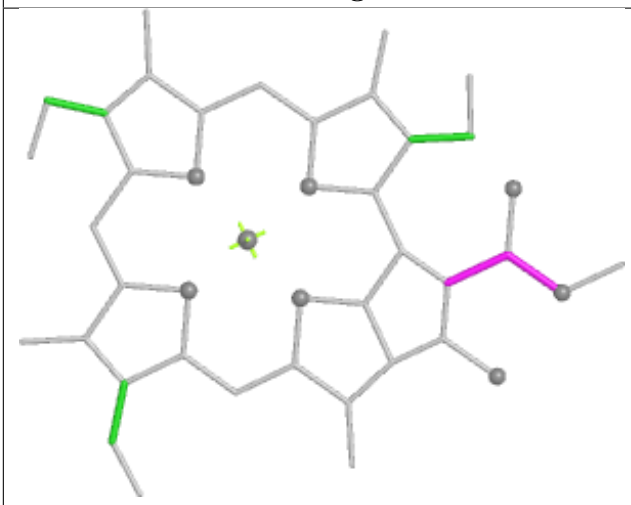
Ligand CLA B 809



Bond lengths



Bond angles

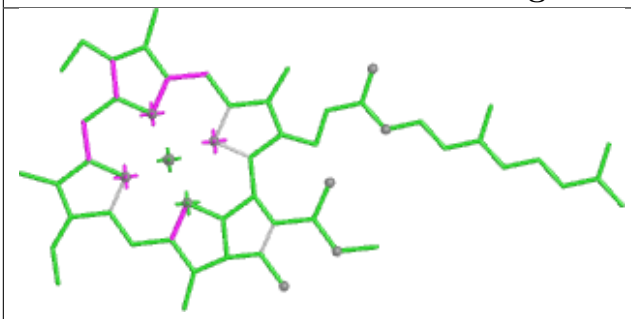


Torsions

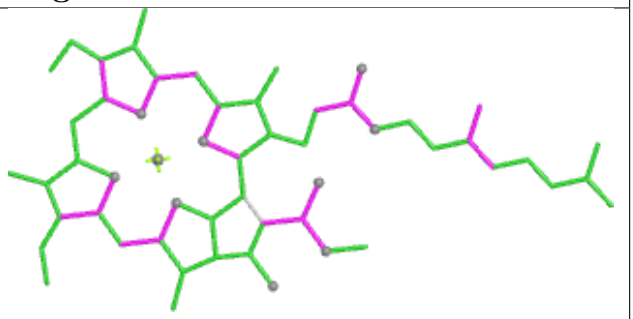


Rings

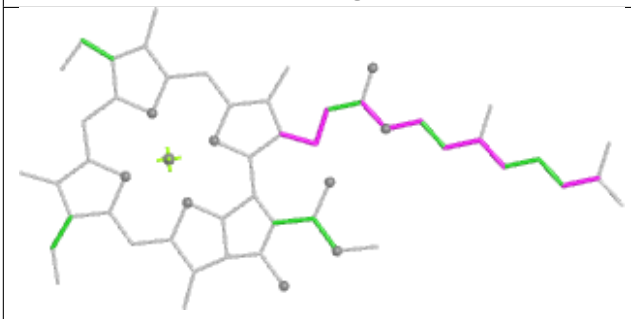
Ligand CLA g 212



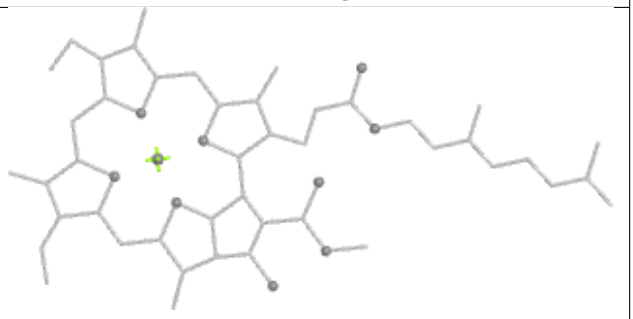
Bond lengths



Bond angles

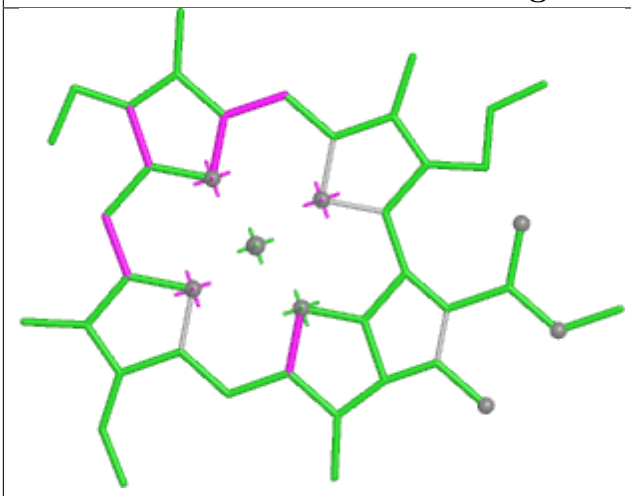


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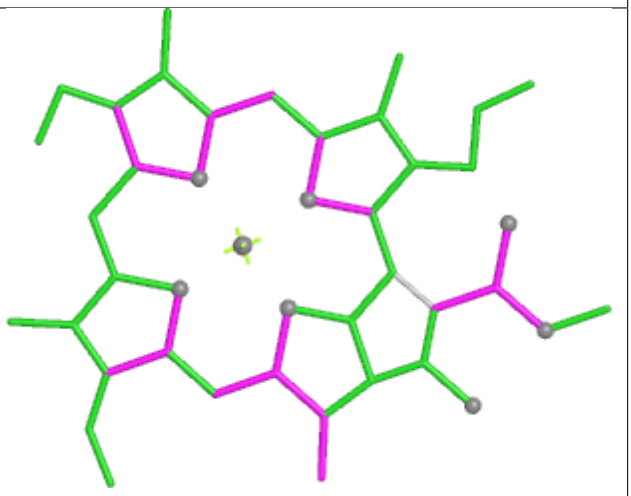


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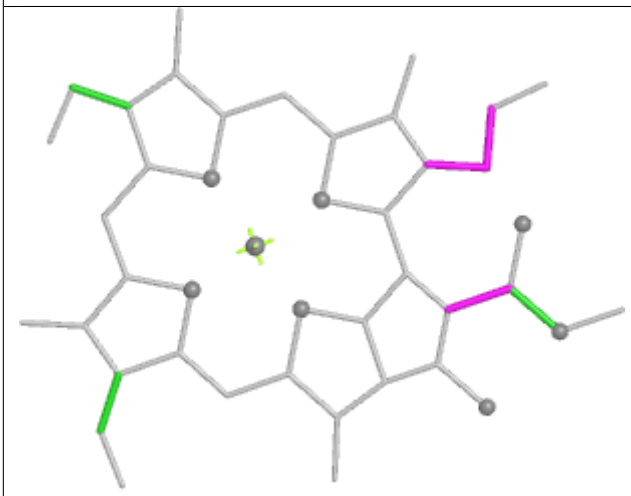
Ligand CLA c 306



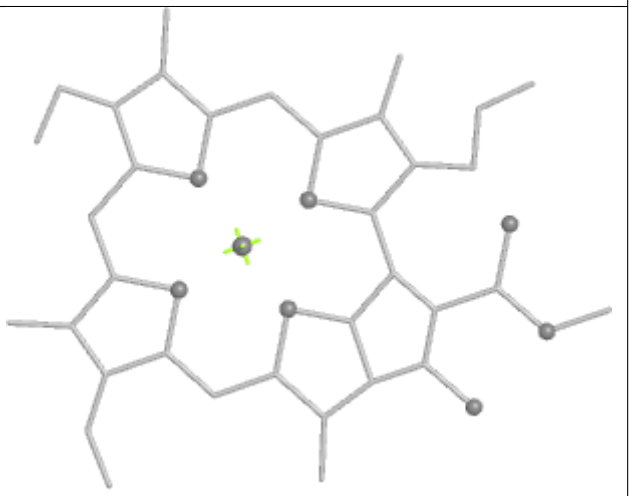
Bond lengths



Bond angles

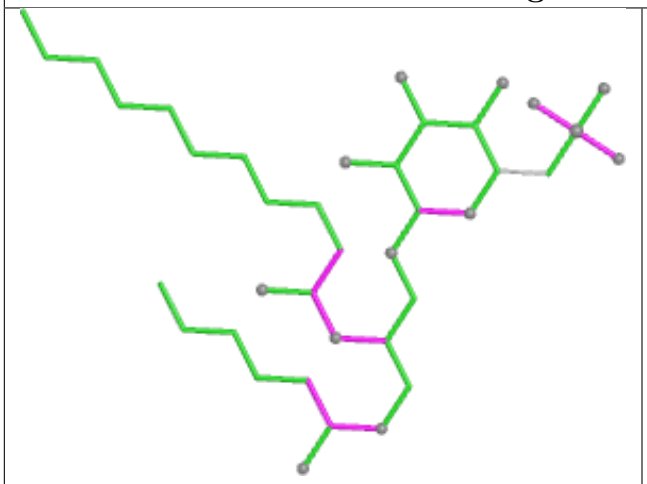


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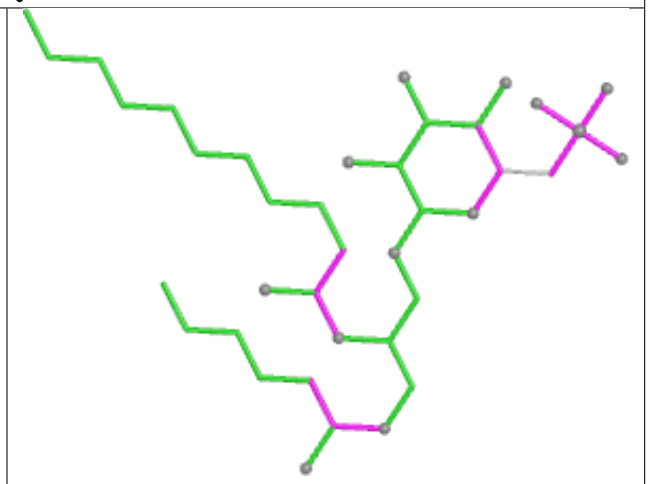


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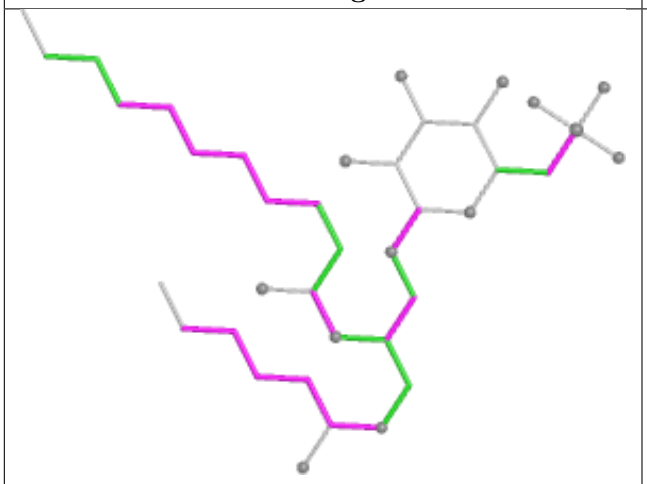
Ligand SQD F 204



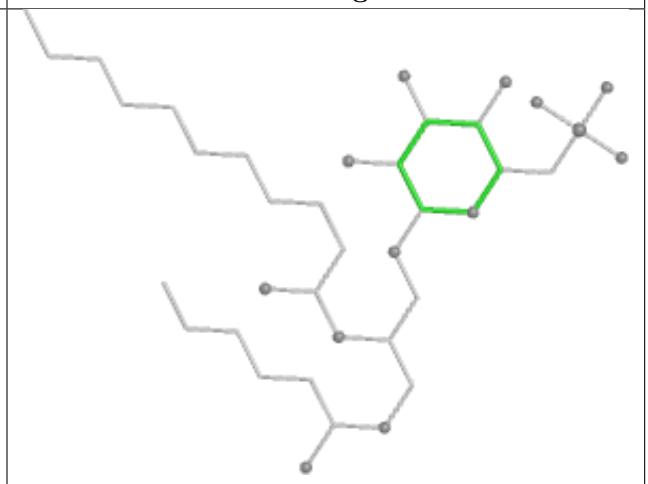
Bond lengths



Bond angles



Torsions

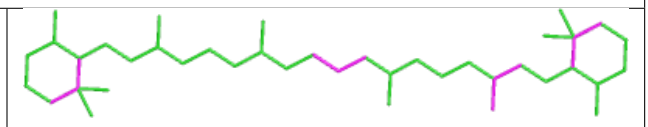


Rings

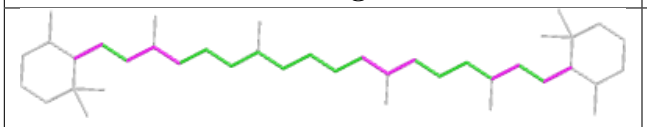
Ligand BCR A 839



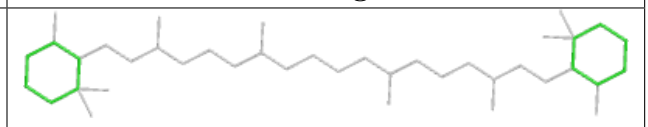
Bond lengths



Bond angles

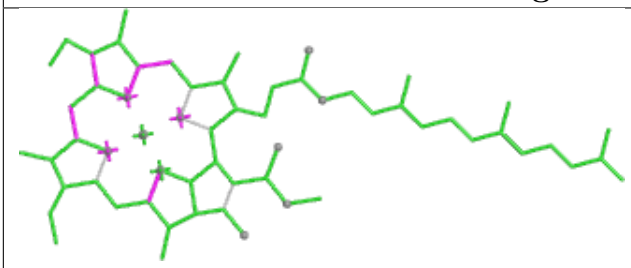


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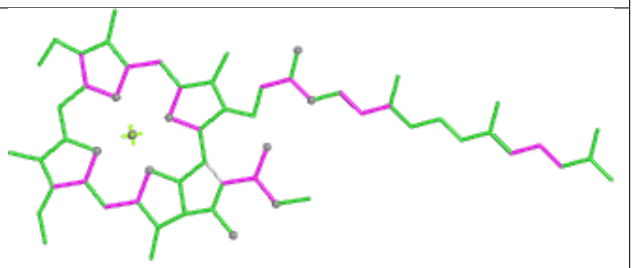


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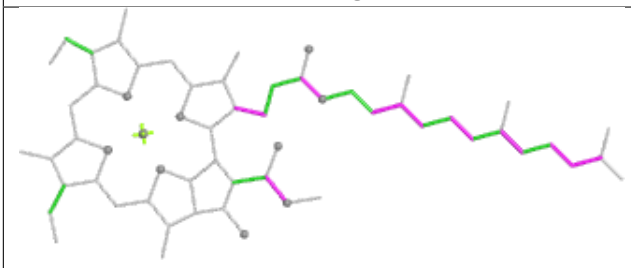
Ligand CLA l 606



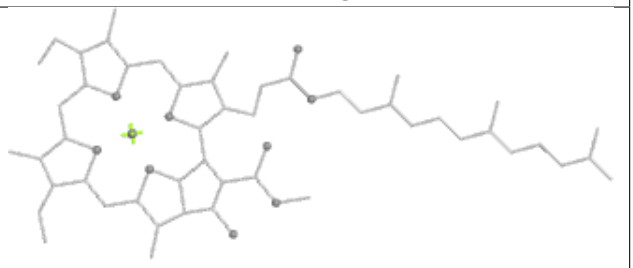
Bond lengths



Bond angles

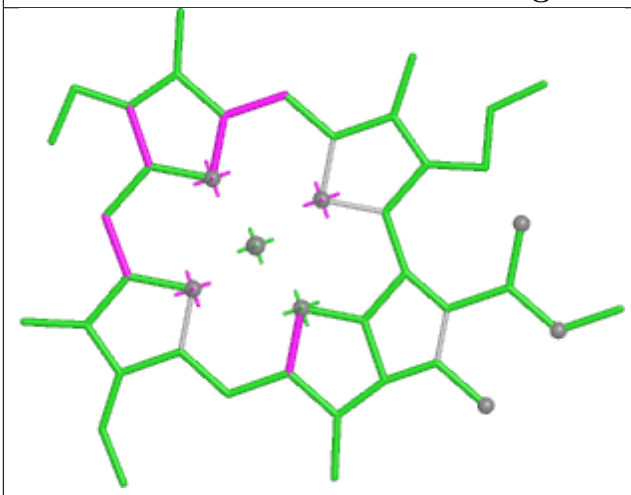


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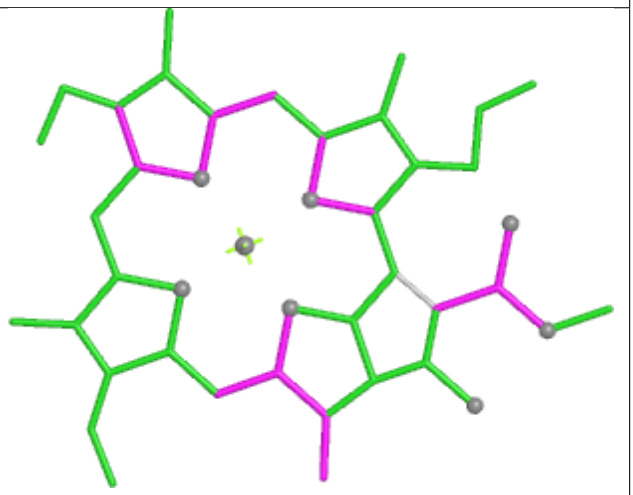


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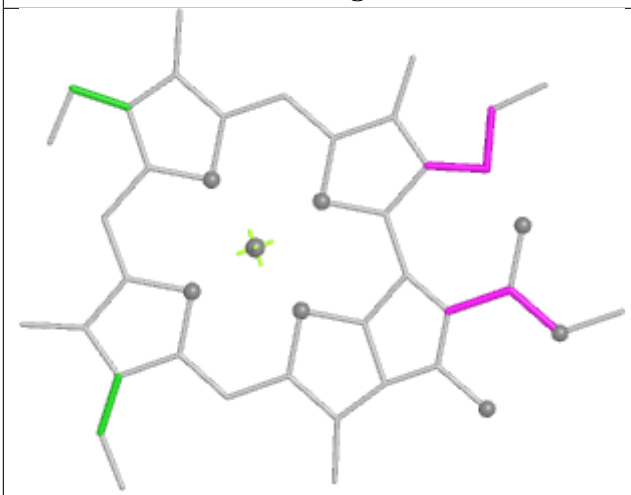
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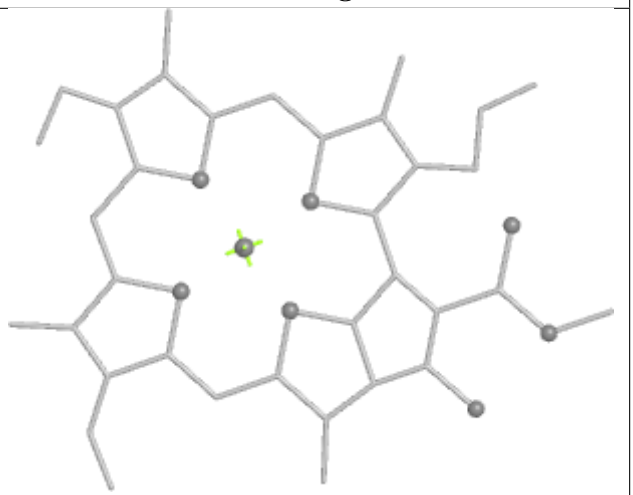
Bond lengths



Bond angles

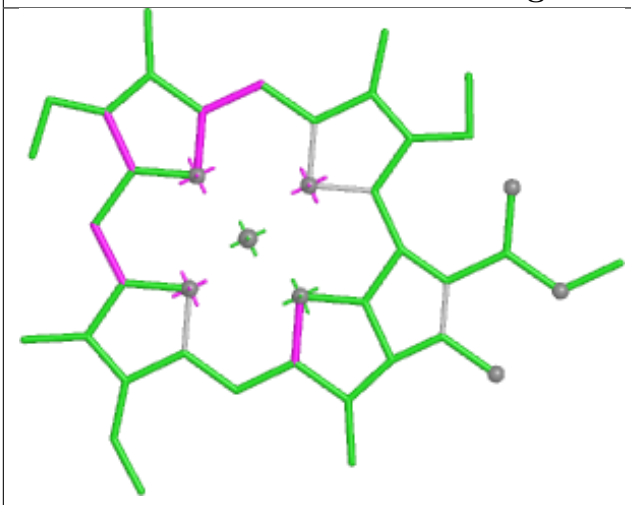


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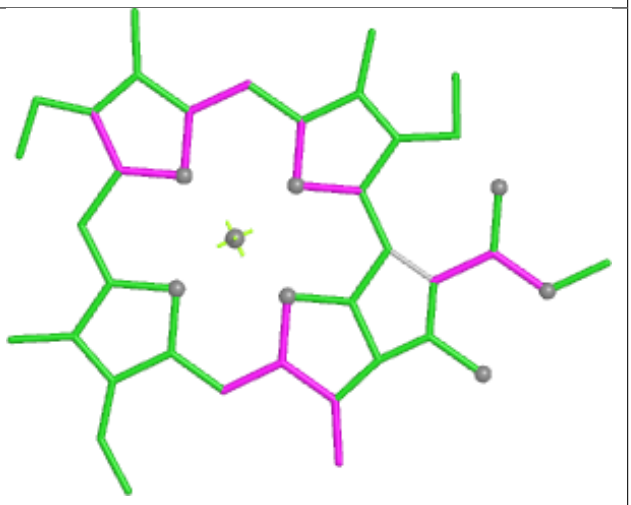


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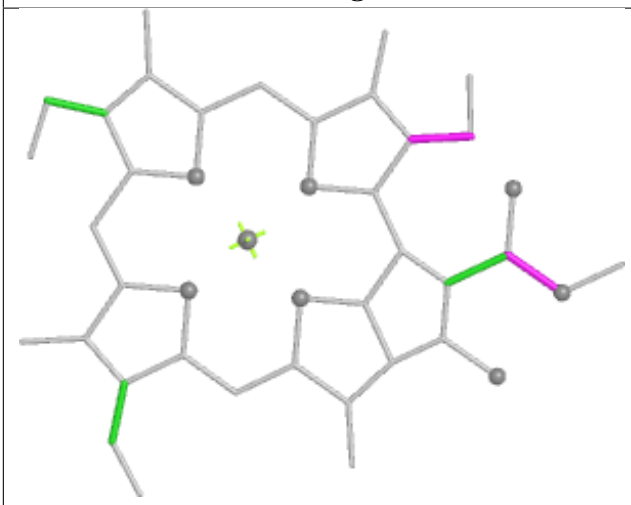
Ligand CLA n 210



Bond lengths



Bond angles

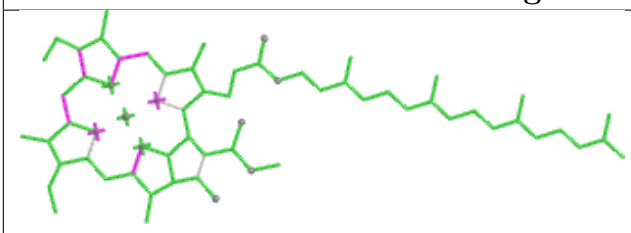


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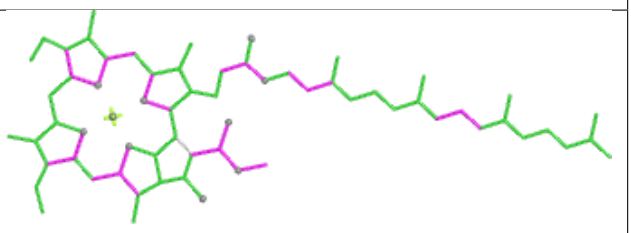


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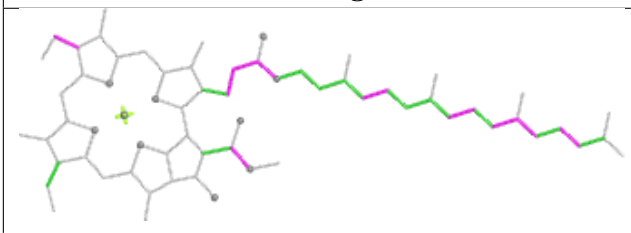
Ligand CLA A 810



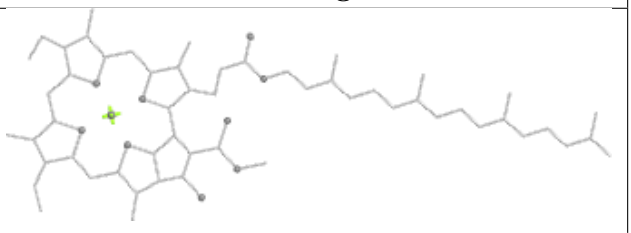
Bond lengths



Bond angles

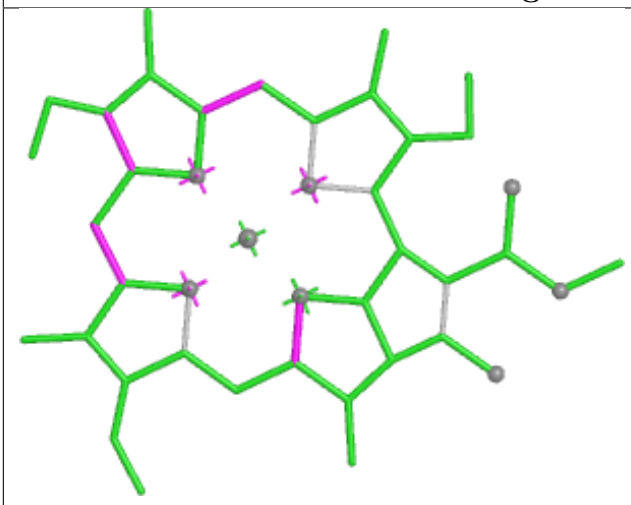


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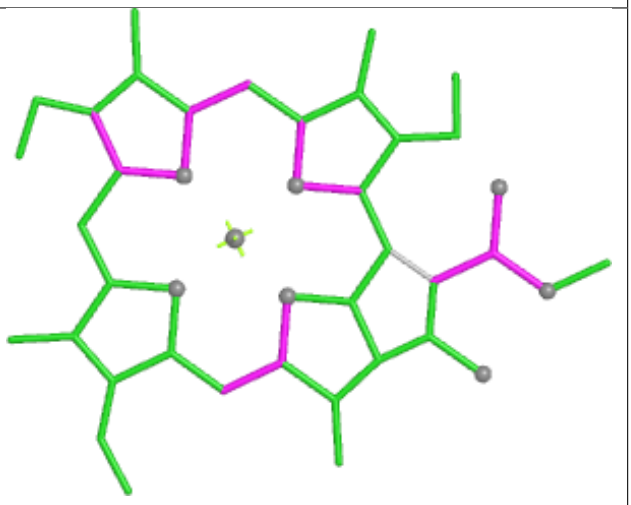


Rings

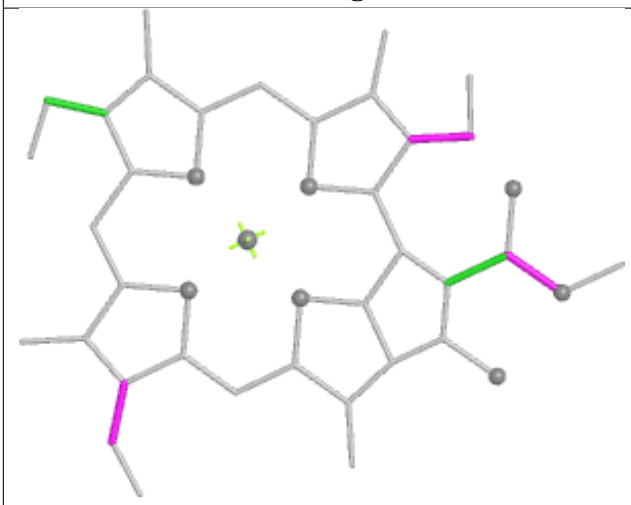
Ligand CLA m 211



Bond lengths



Bond angles

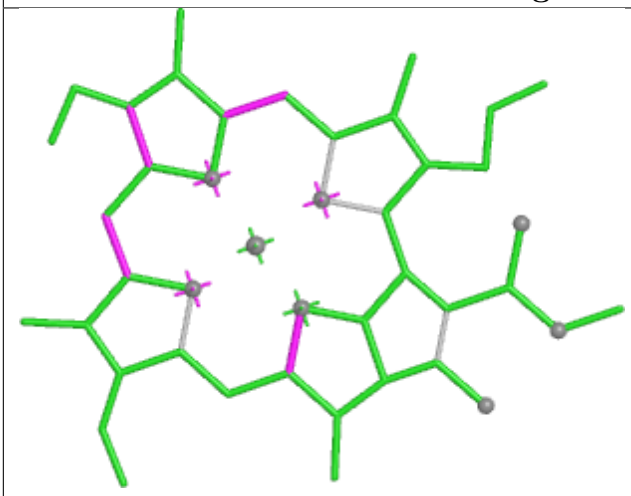


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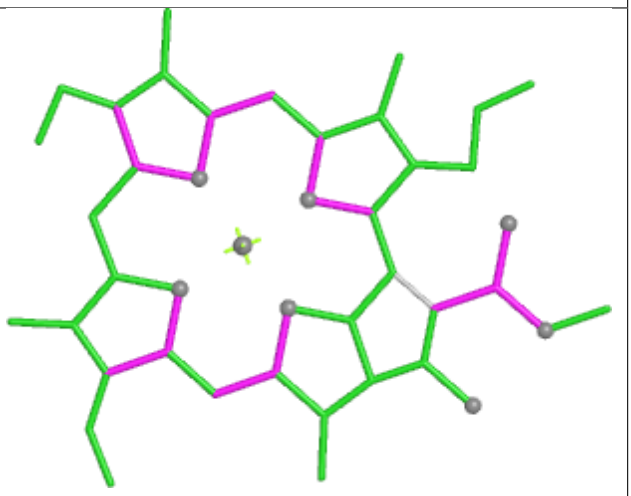


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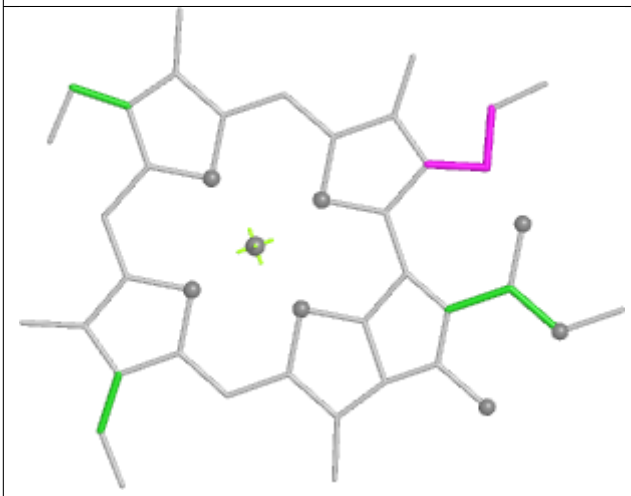
Ligand CLA l 608



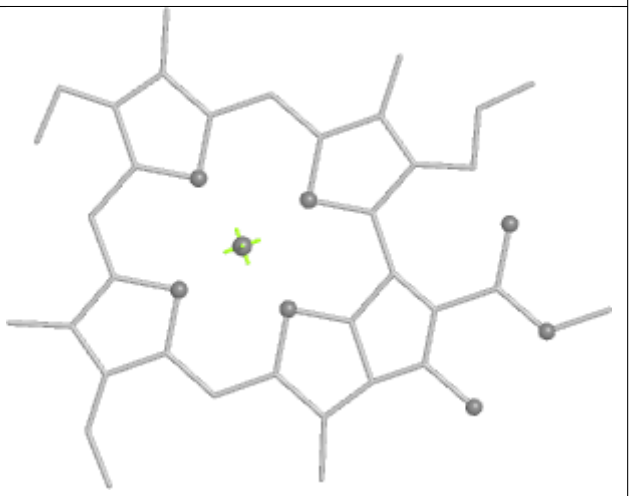
Bond lengths



Bond angles

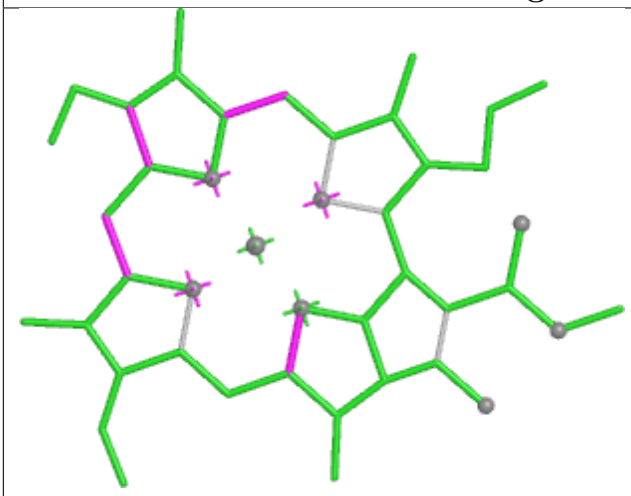


Torsions

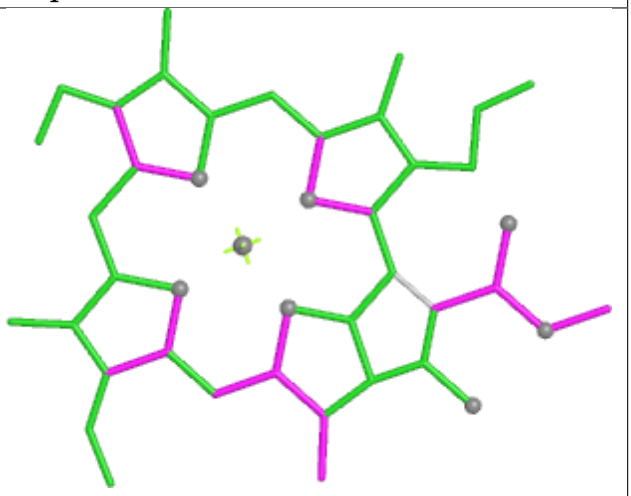


Rings

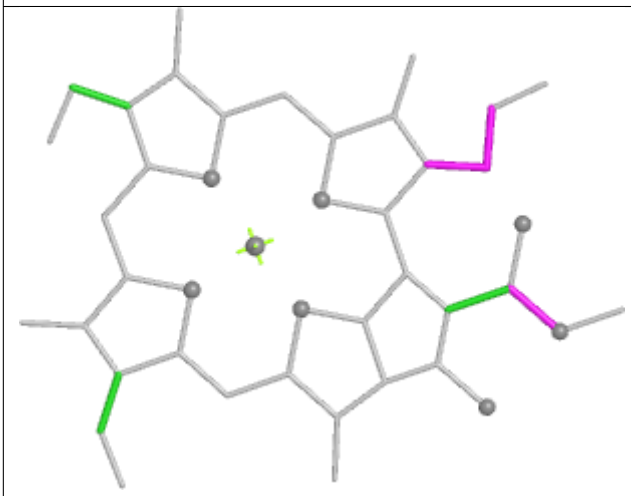
Ligand CLA p 609



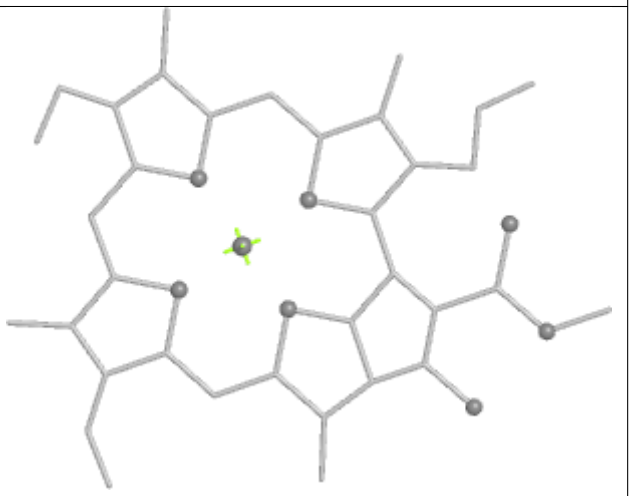
Bond lengths



Bond angles

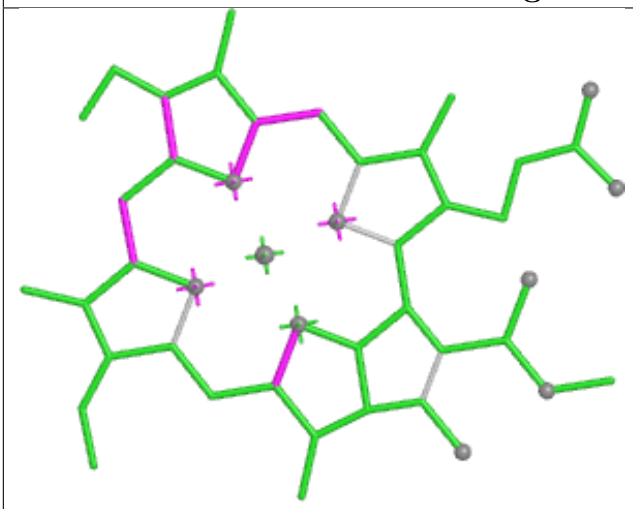


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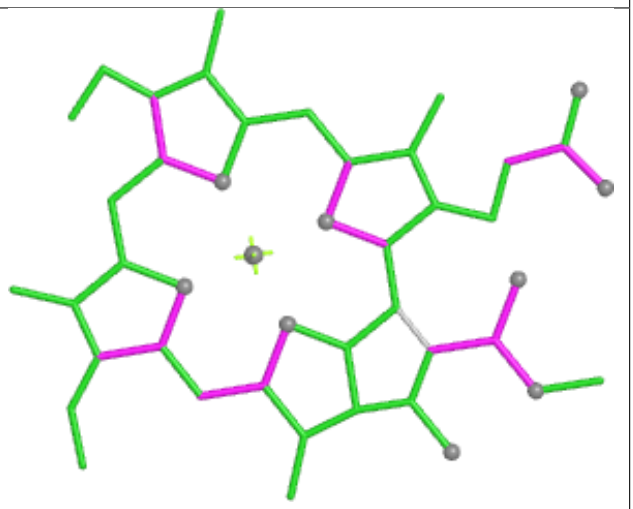


Rings

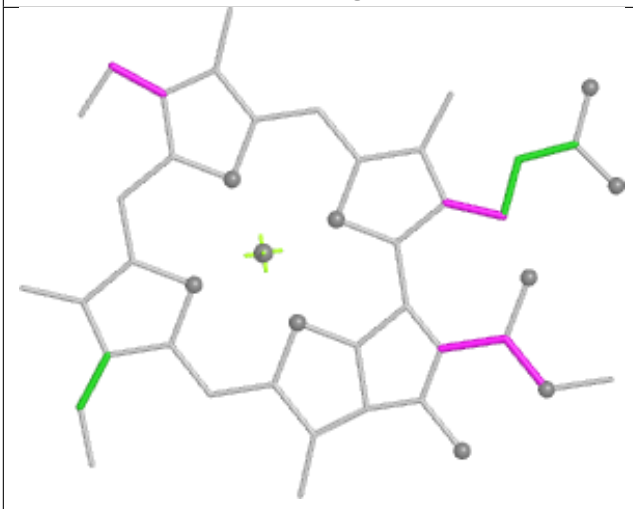
Ligand CLA A 806



Bond lengths



Bond angles

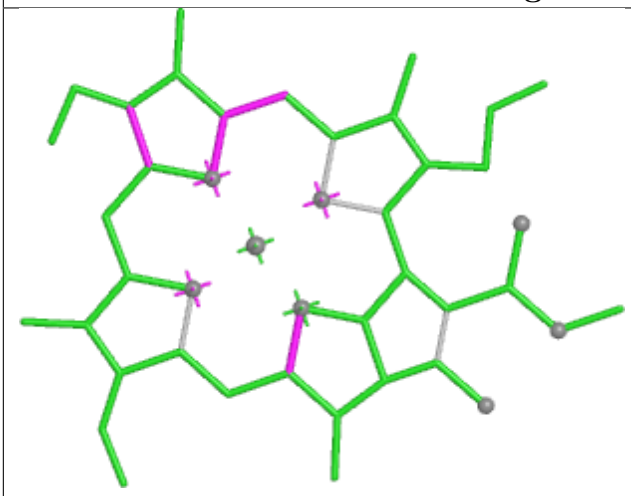


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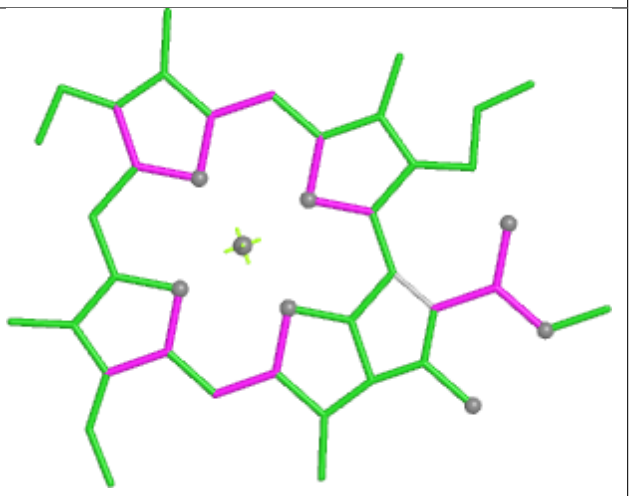


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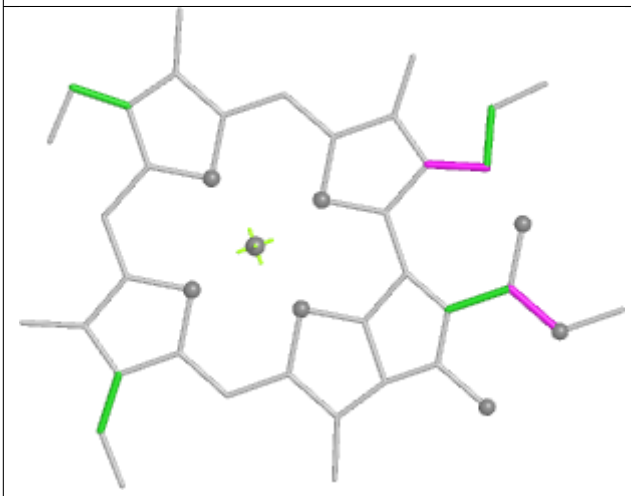
Ligand CLA B 826



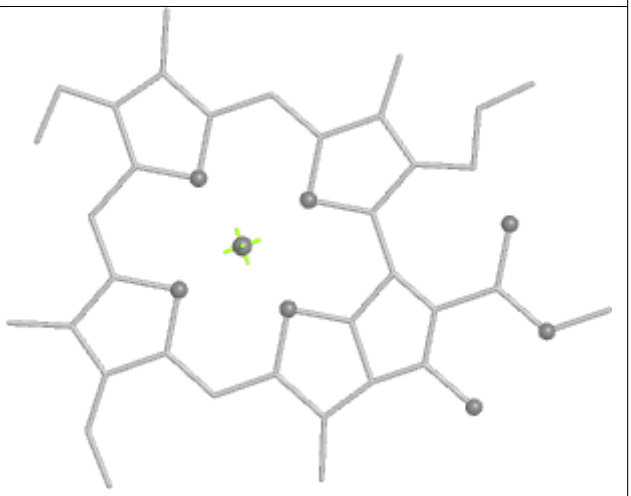
Bond lengths



Bond angles

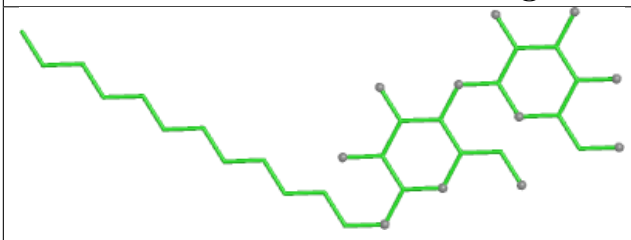


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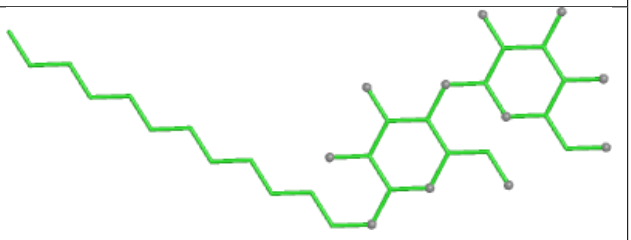


Rings

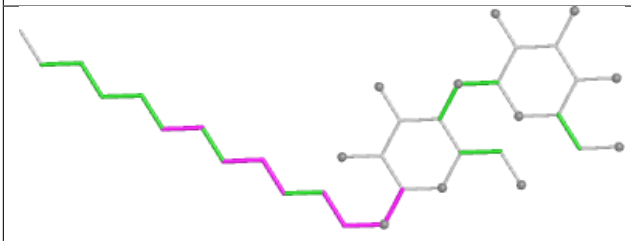
Ligand LMT A 803



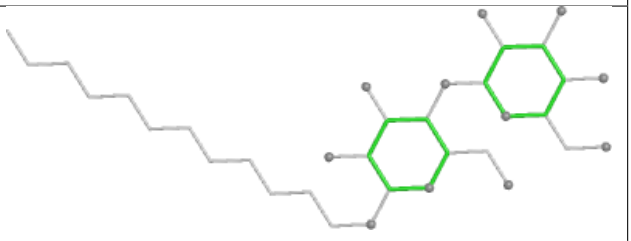
Bond lengths



Bond angles

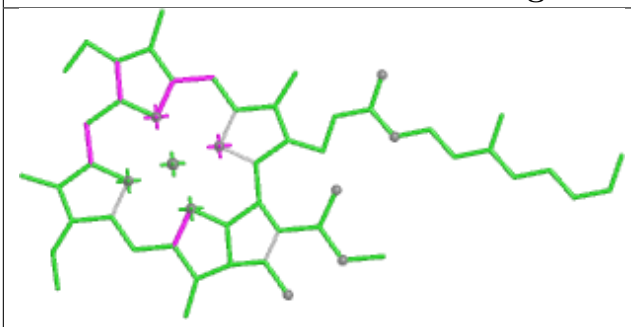


Torsions

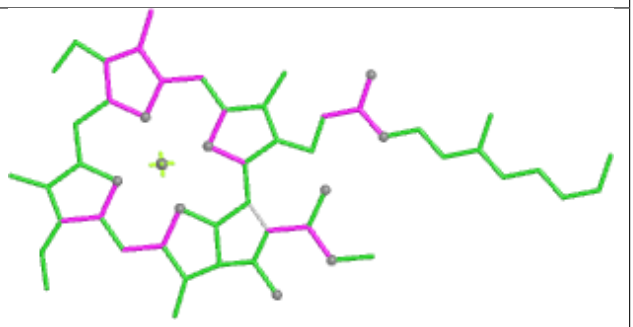


Rings

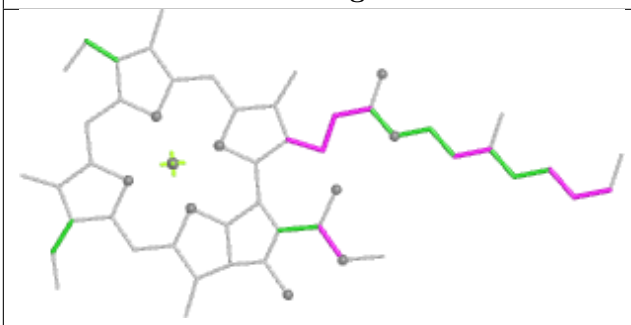
Ligand CLA h 209



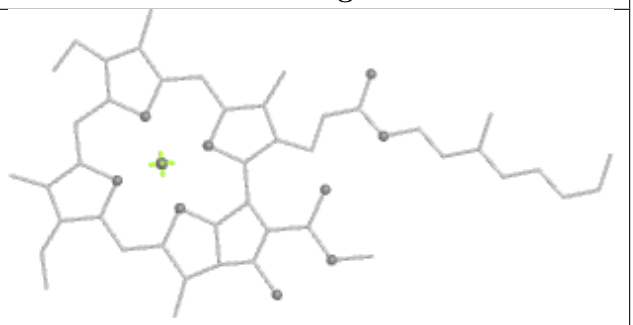
Bond lengths



Bond angles

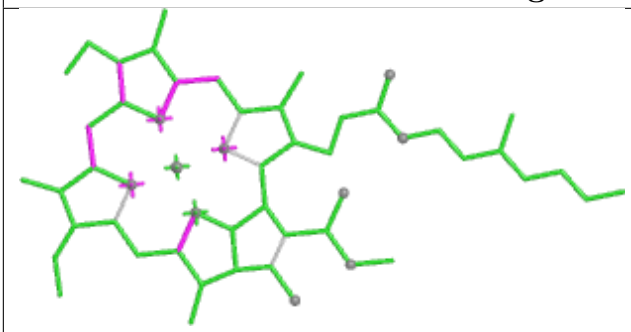


Torsions

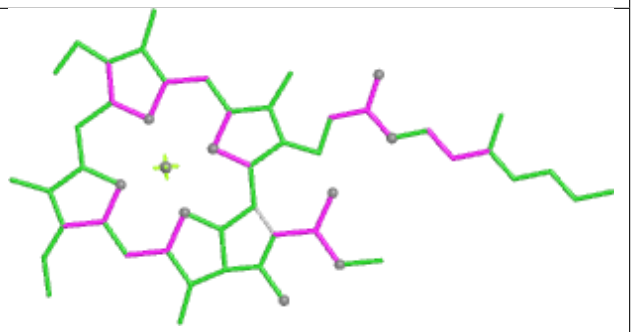


Rings

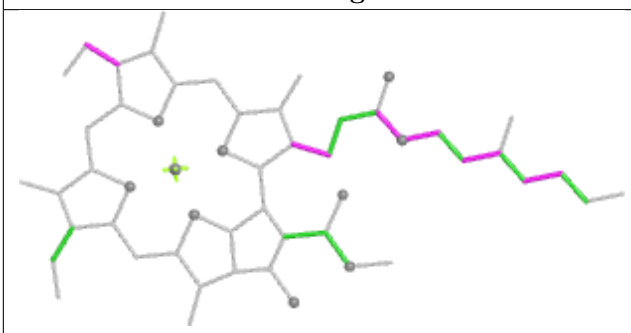
Ligand CLA k 203



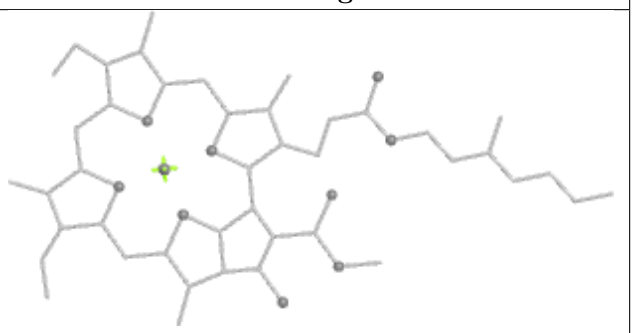
Bond lengths



Bond angles

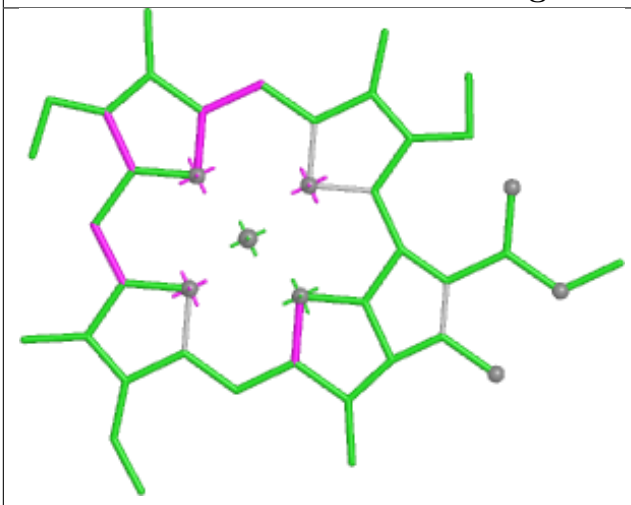


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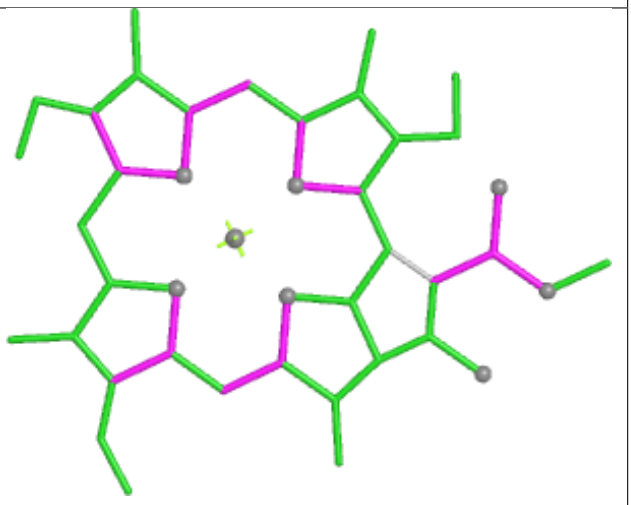


Rings

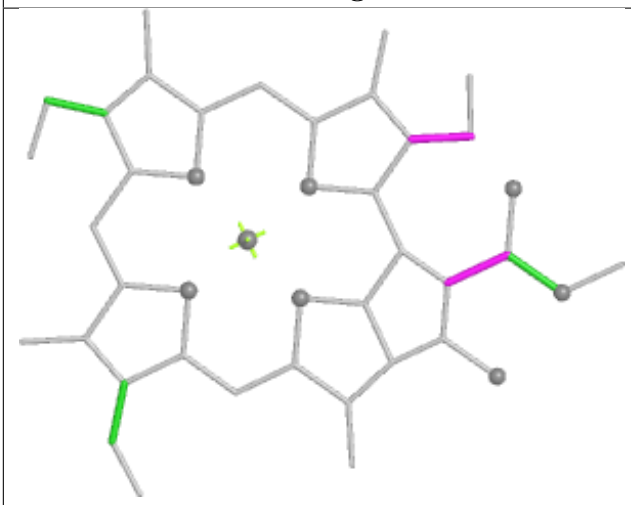
Ligand CLA e 208



Bond lengths



Bond angles

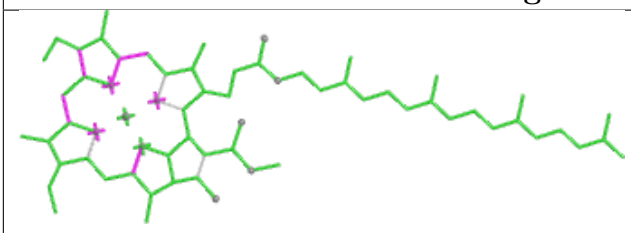


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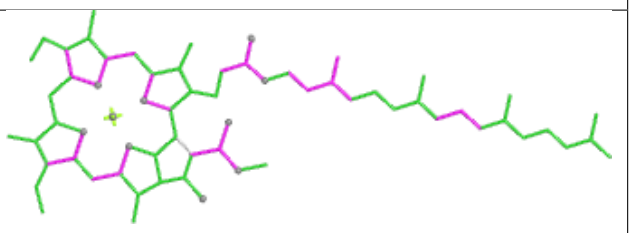


Rings

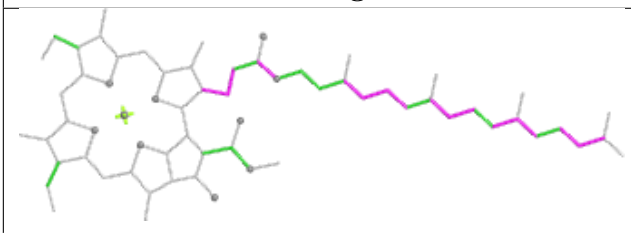
Ligand CLA A 846



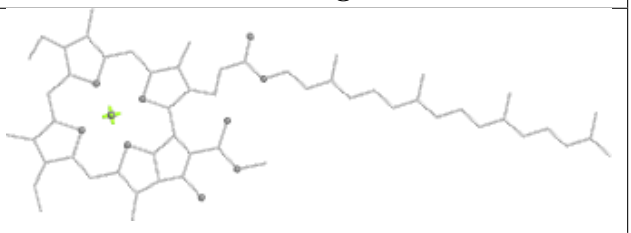
Bond lengths



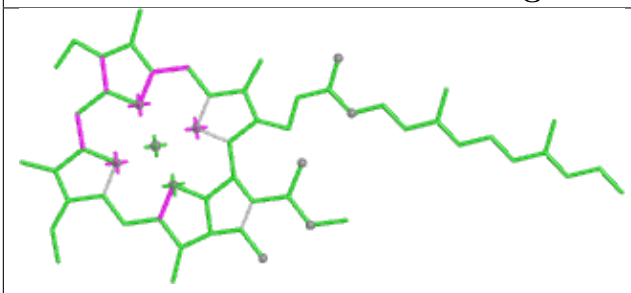
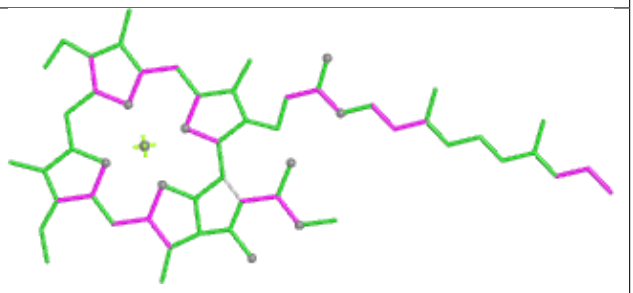
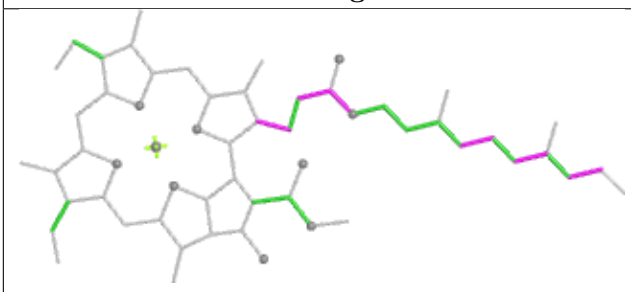
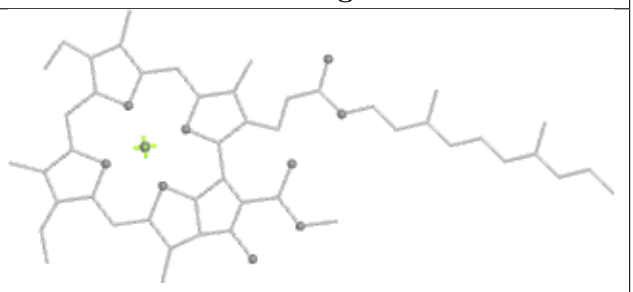
Bond angles



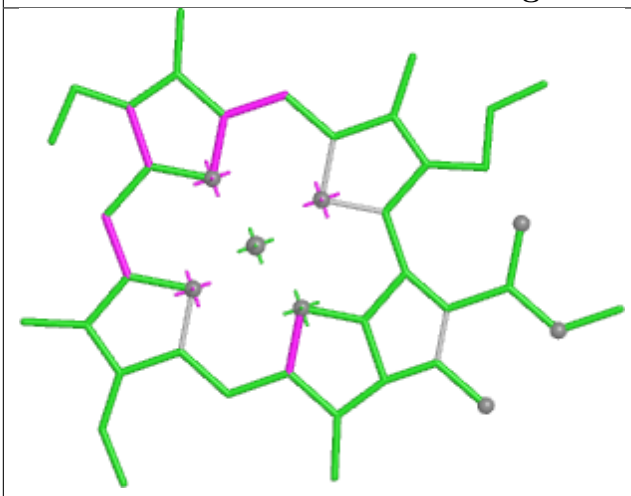
Torsions



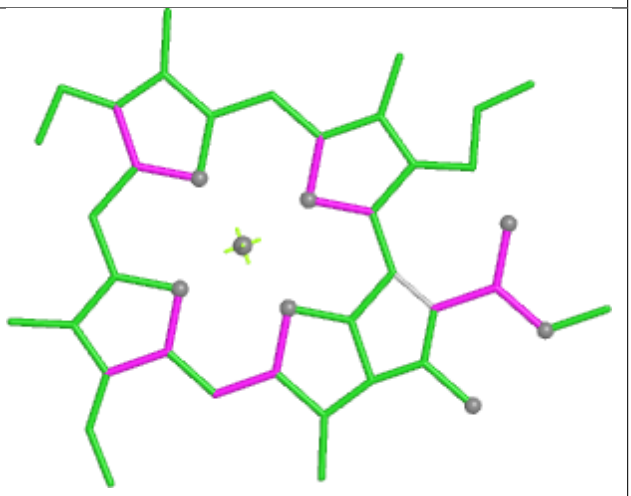
Rings

Ligand CLA A 841	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

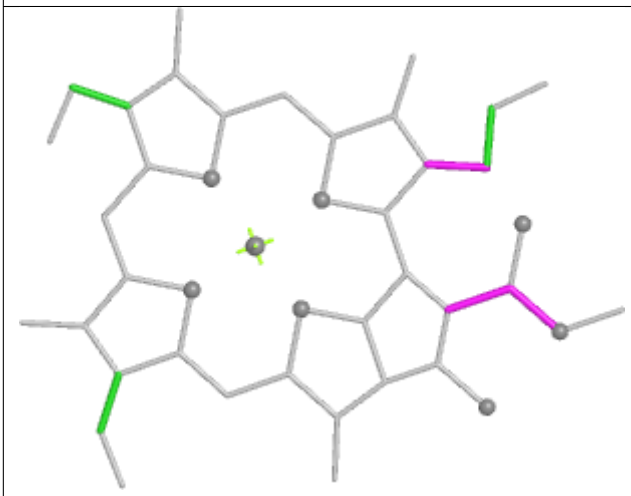
Ligand CLA m 205



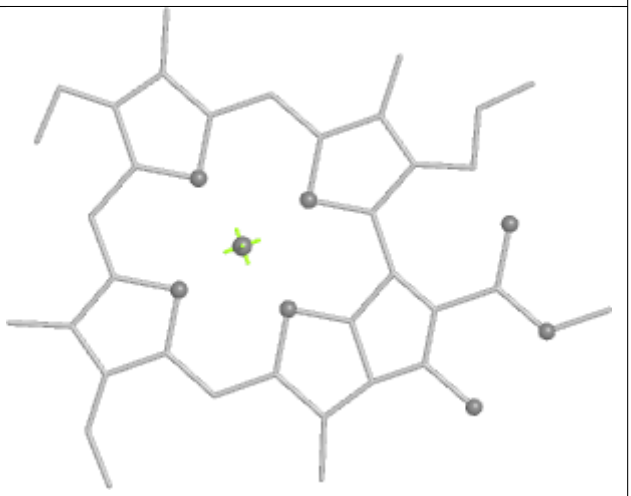
Bond lengths



Bond angles

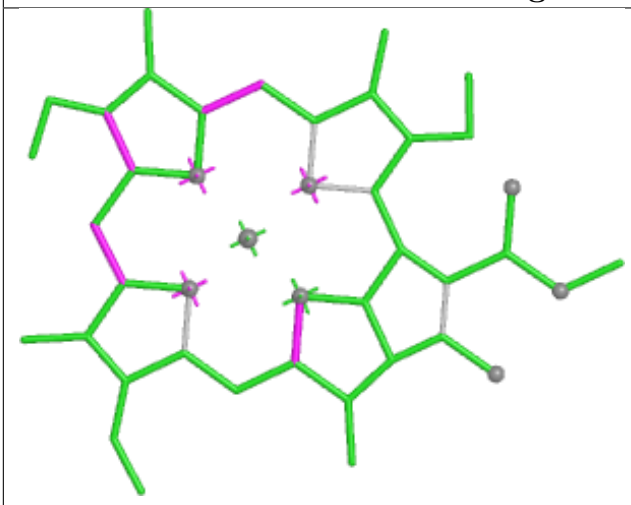


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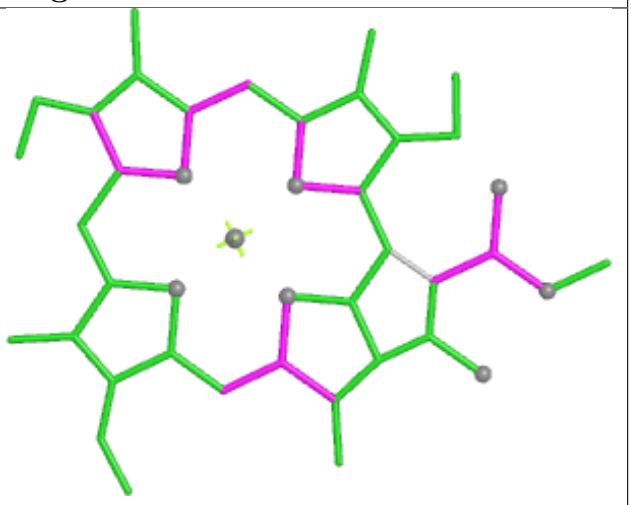


Rings

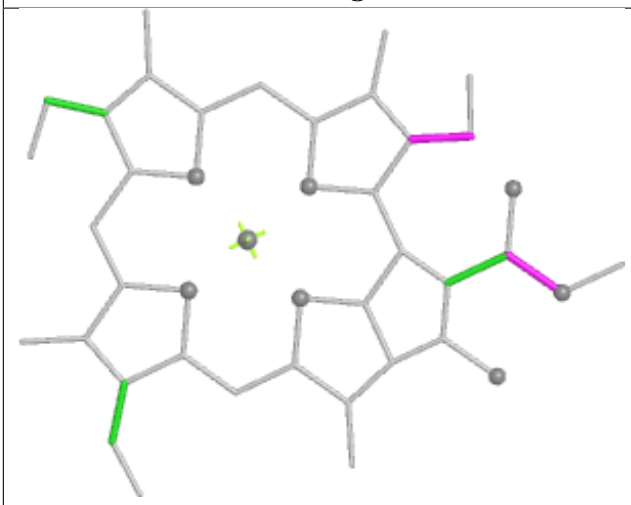
Ligand CLA g 213



Bond lengths



Bond angles

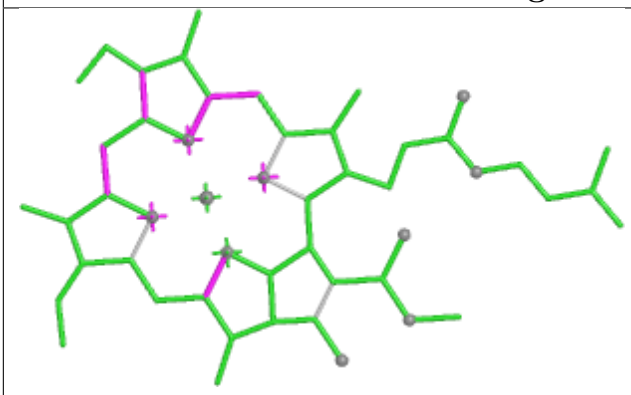


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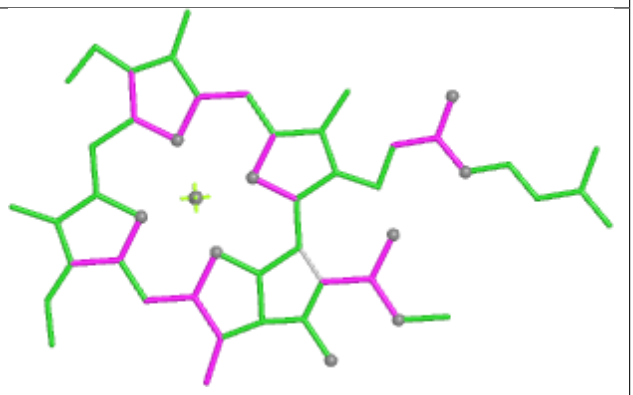


Rings

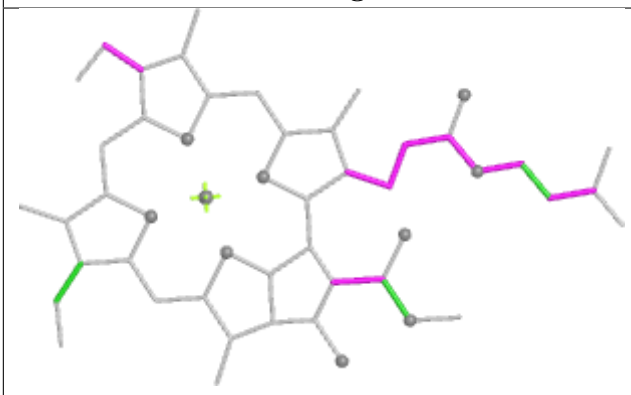
Ligand CLA J 103



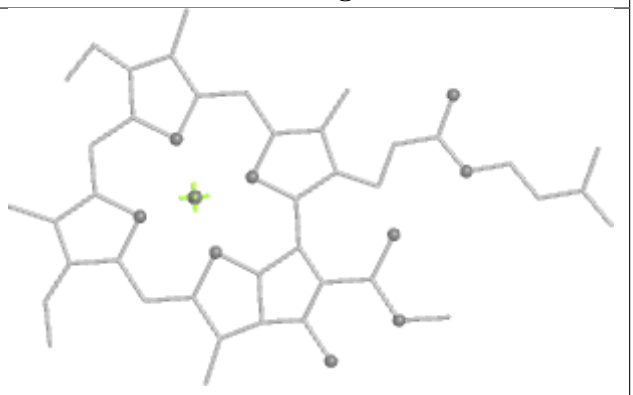
Bond lengths



Bond angles

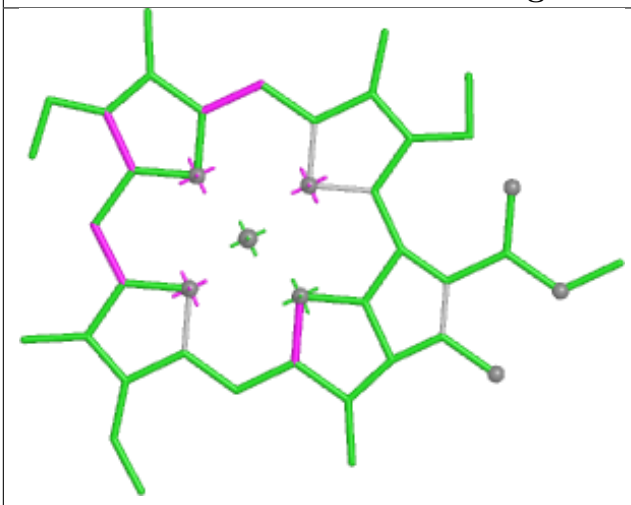


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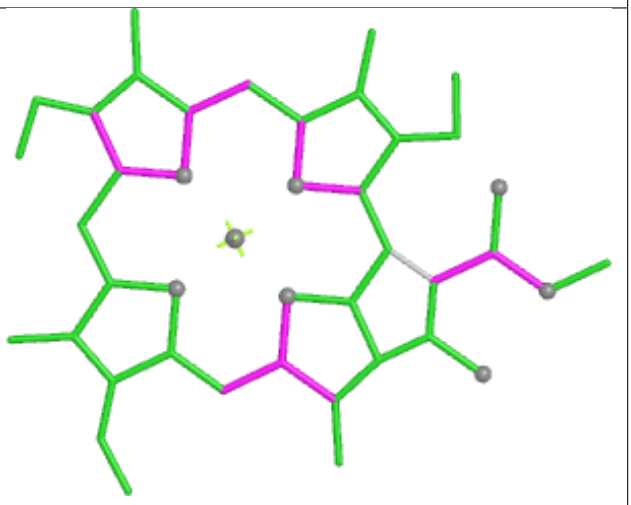


Rings

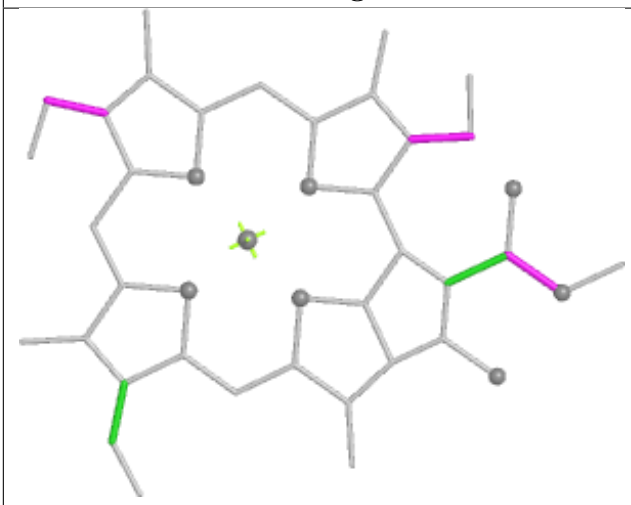
Ligand CLA n 205



Bond lengths



Bond angles

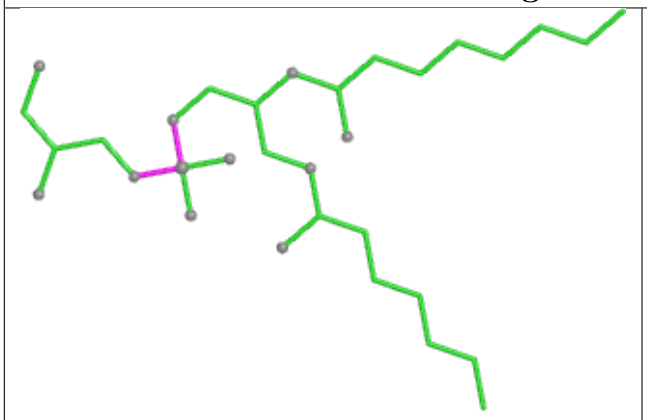


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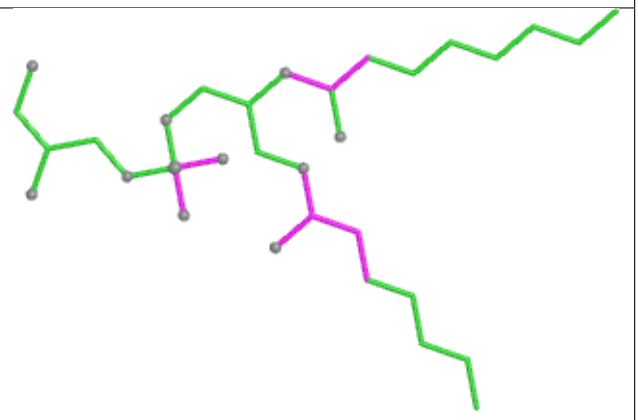


Rings

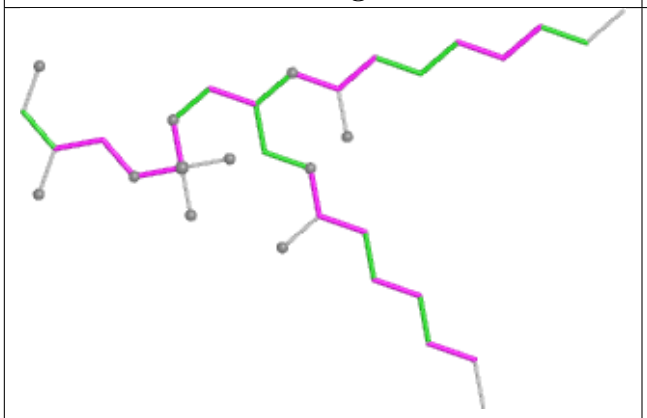
Ligand LHG m 201



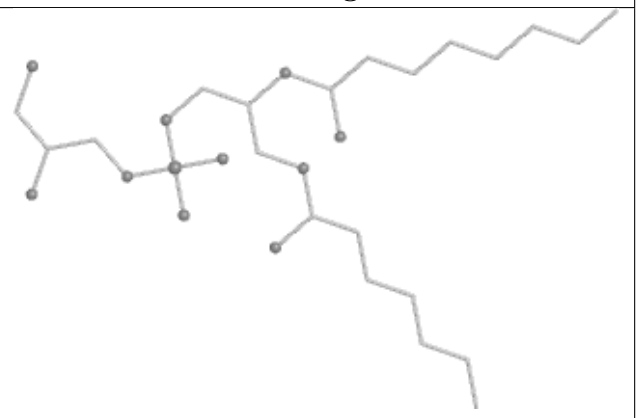
Bond lengths



Bond angles

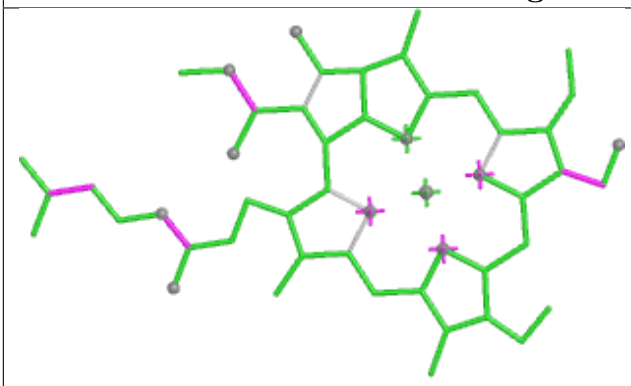


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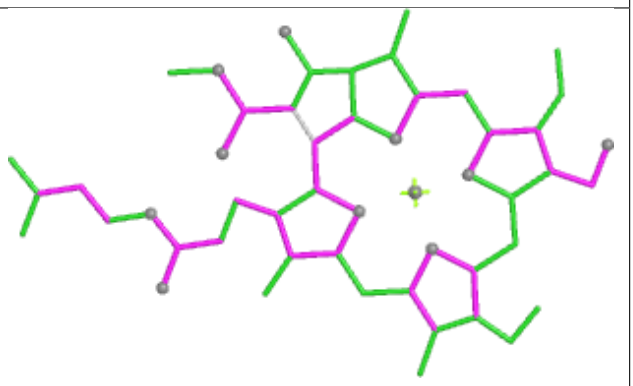


Rings

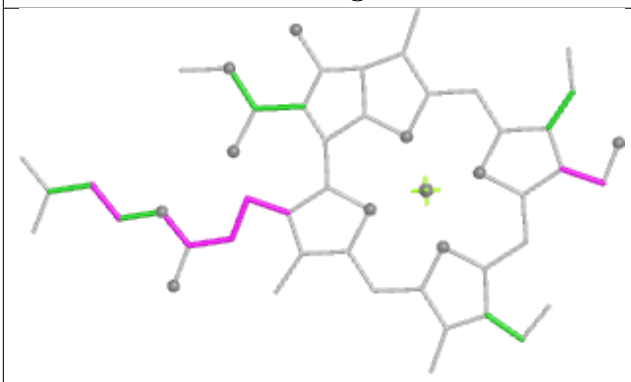
Ligand CHL d 307



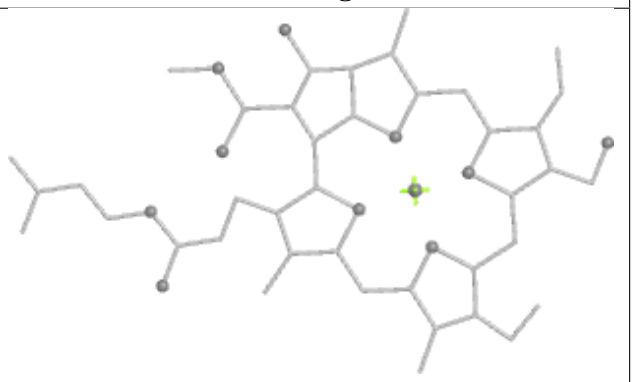
Bond lengths



Bond angles

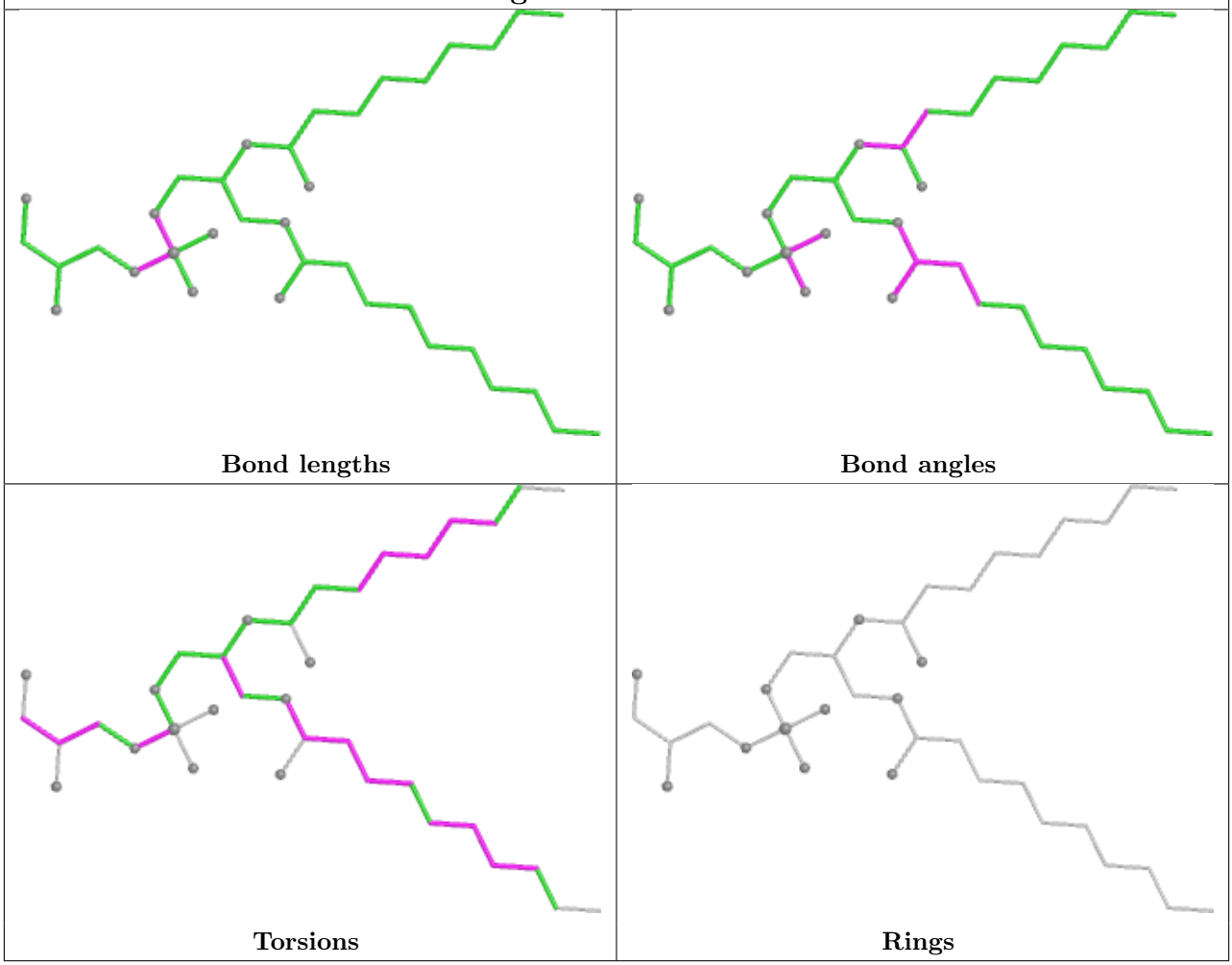


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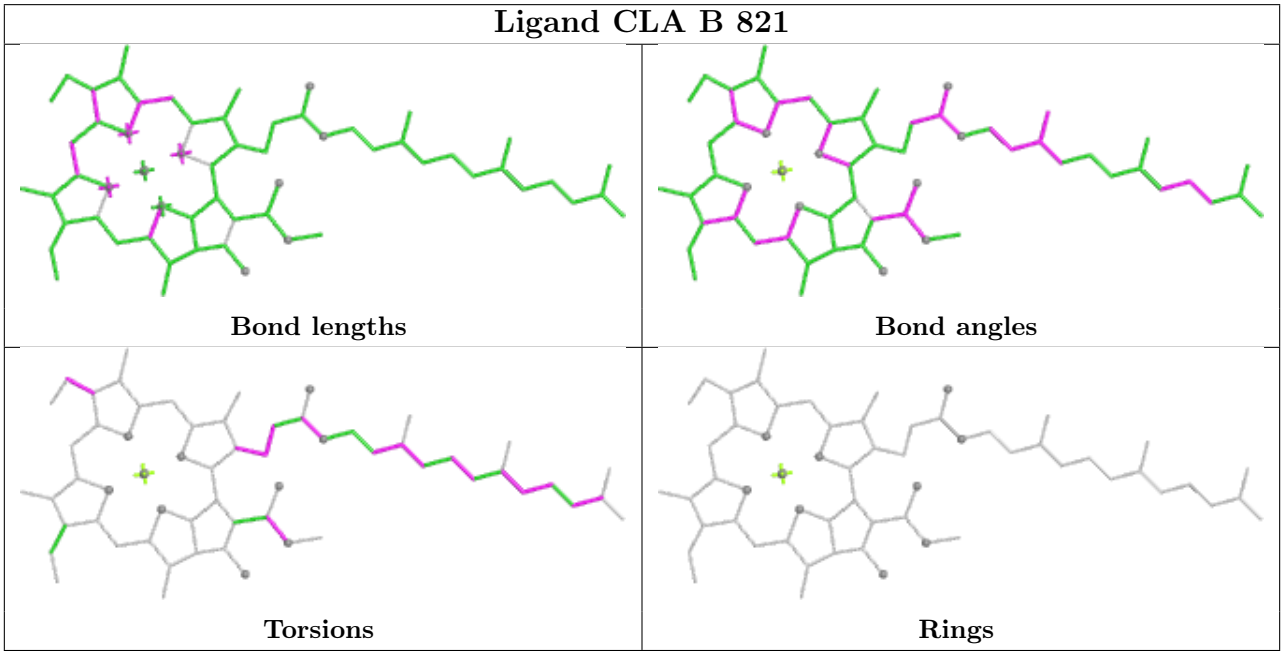


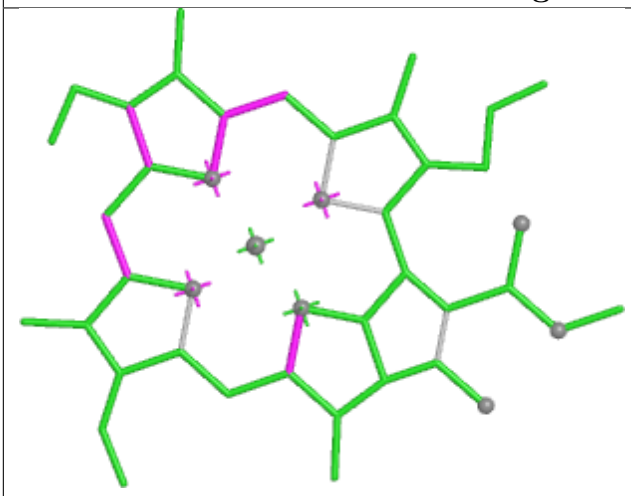
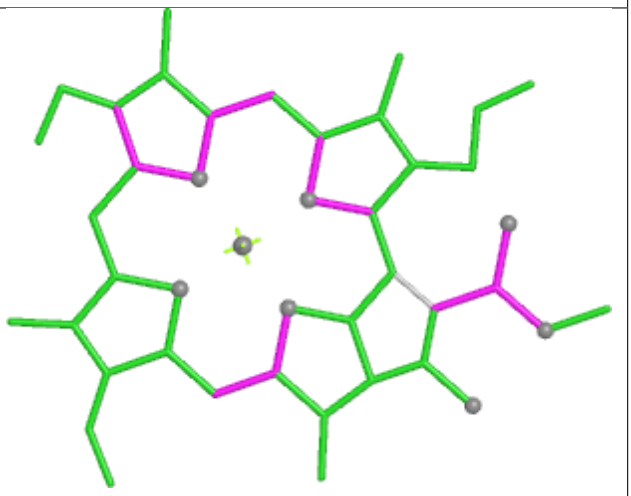
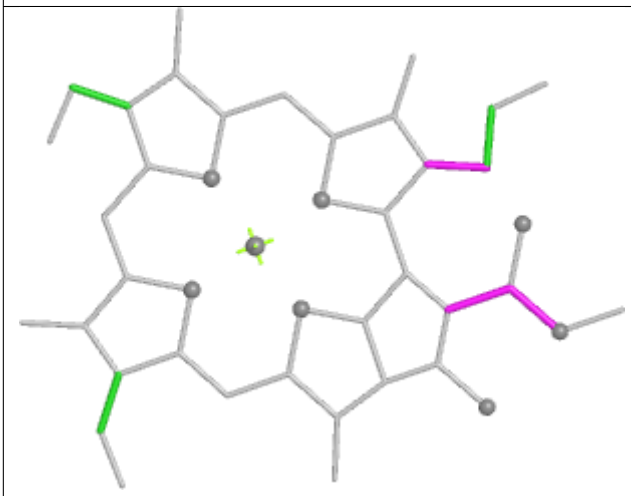
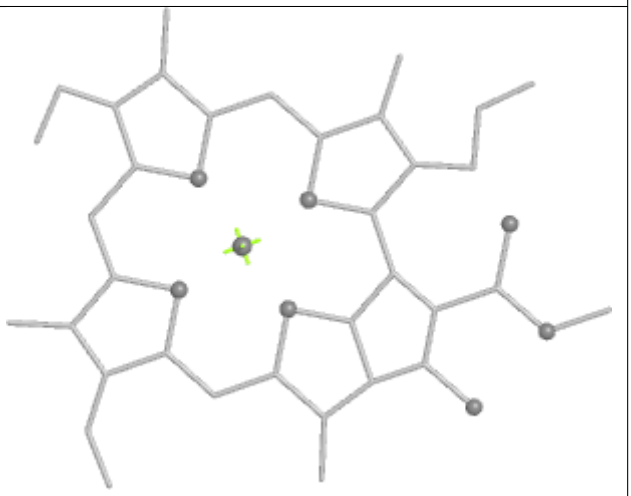
Rings

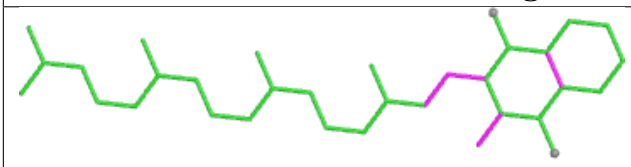
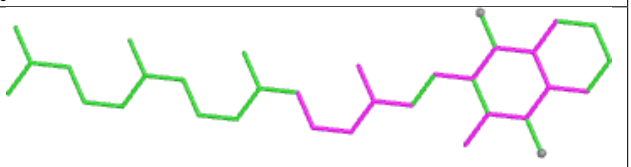
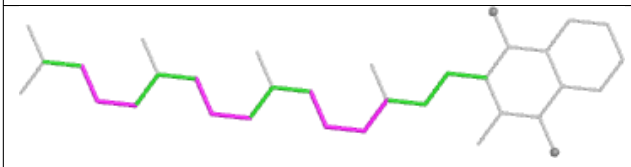
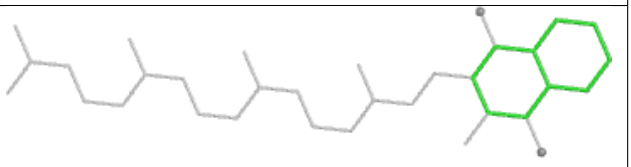
Ligand LHG i 201



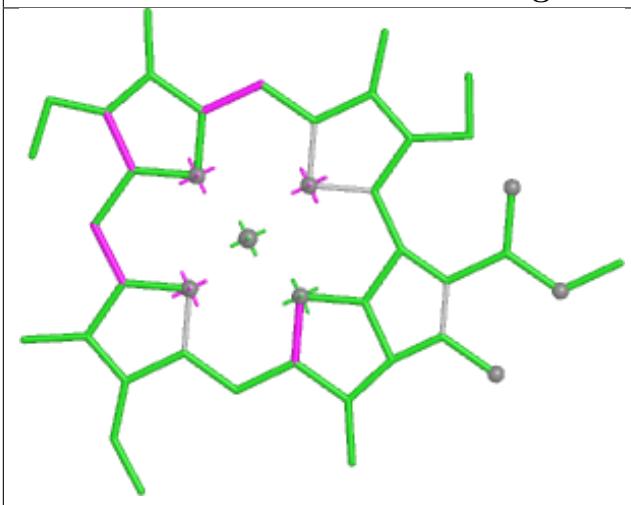
Ligand CLA B 821



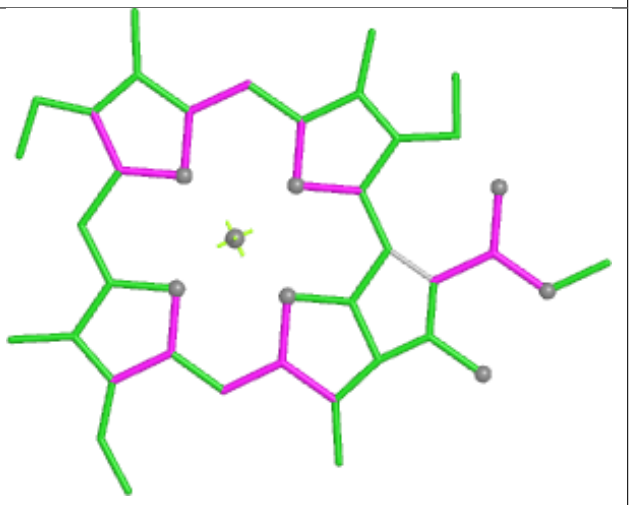
Ligand CLA i 209	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

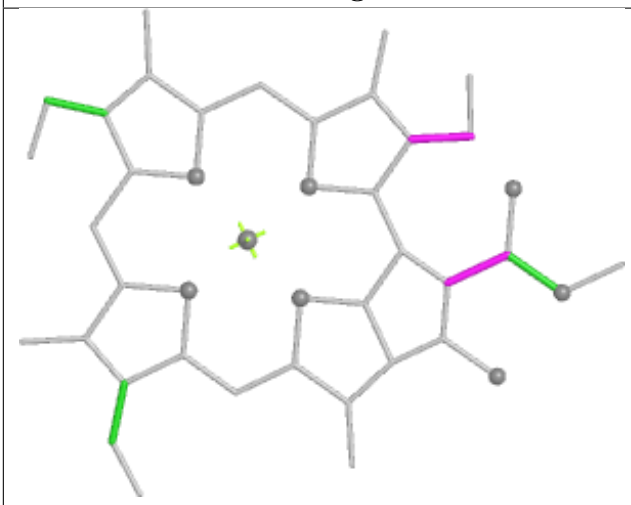
Ligand CLA i 212



Bond lengths



Bond angles

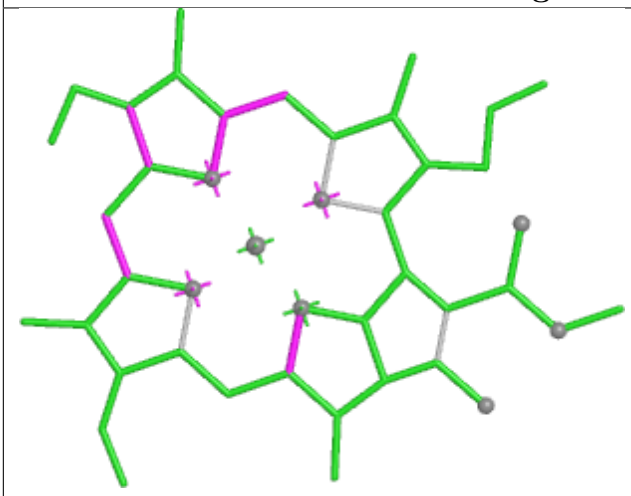


Torsions

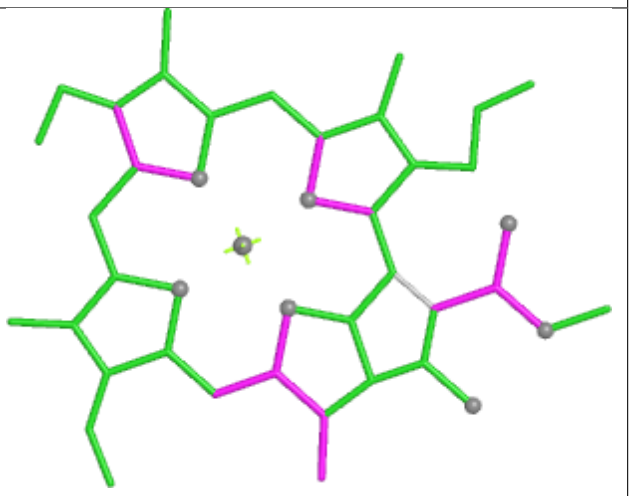


Rings

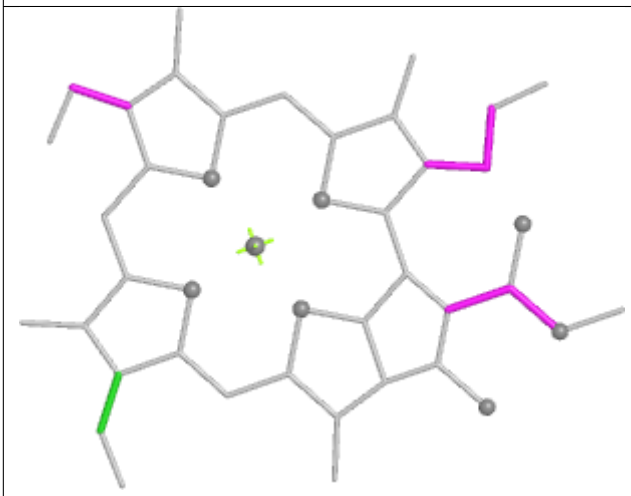
Ligand CLA i 204



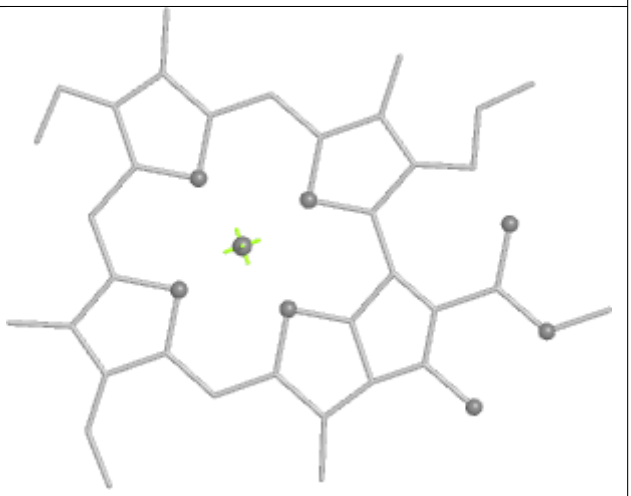
Bond lengths



Bond angles

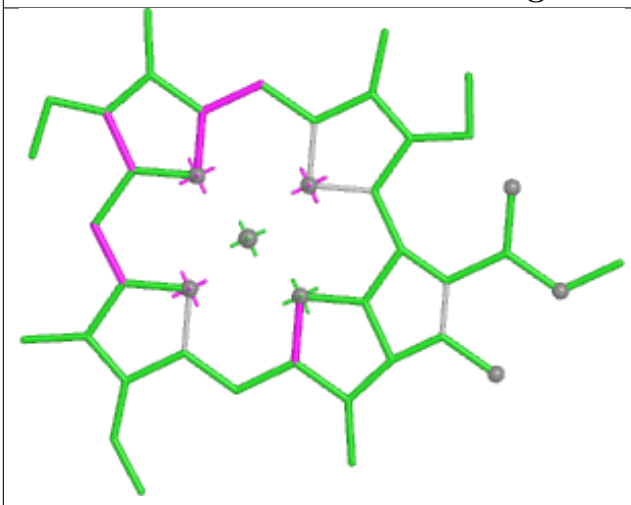


Torsions

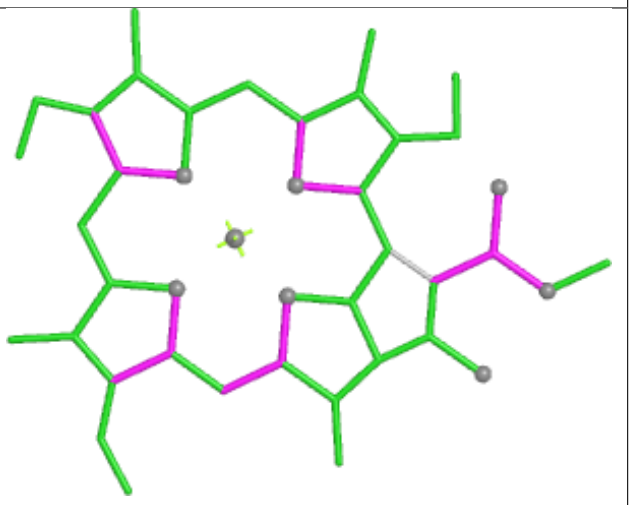


Rings

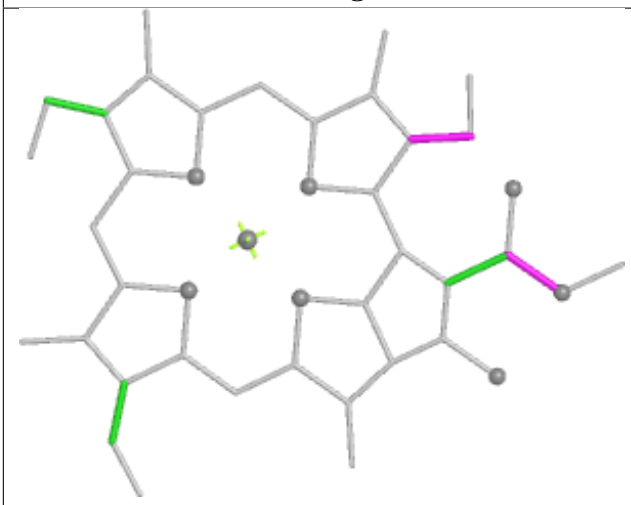
Ligand CLA n 211



Bond lengths



Bond angles

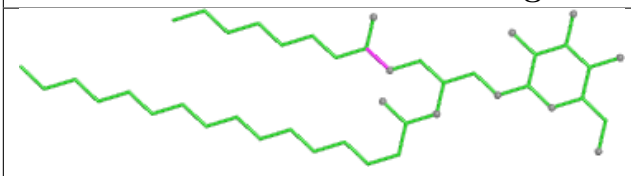


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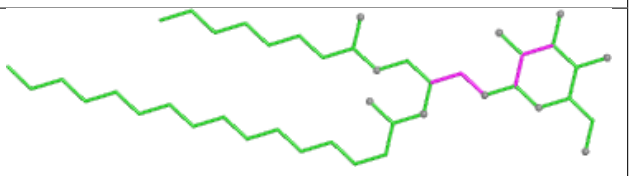


Rings

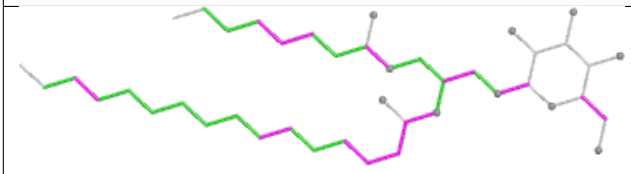
Ligand LMG a 202



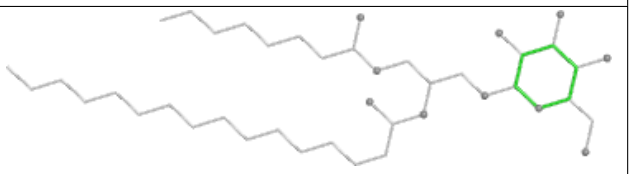
Bond lengths



Bond angles

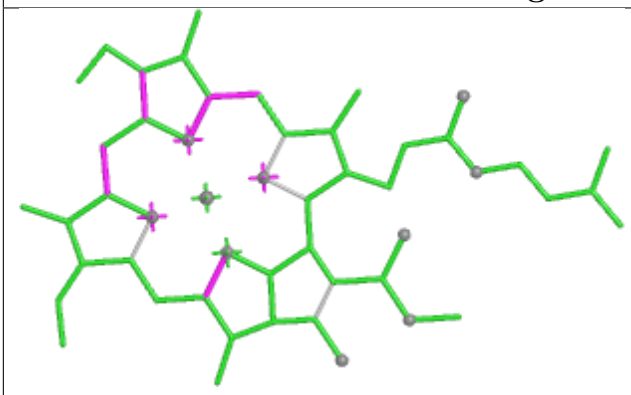


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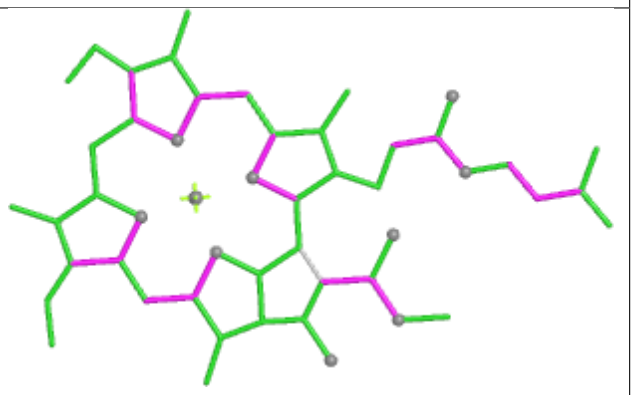


Rings

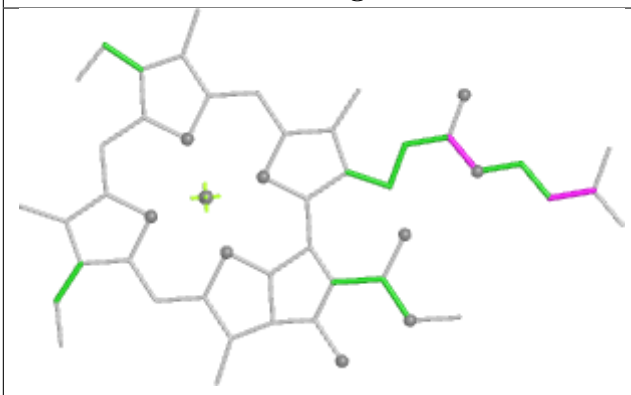
Ligand CLA k 207



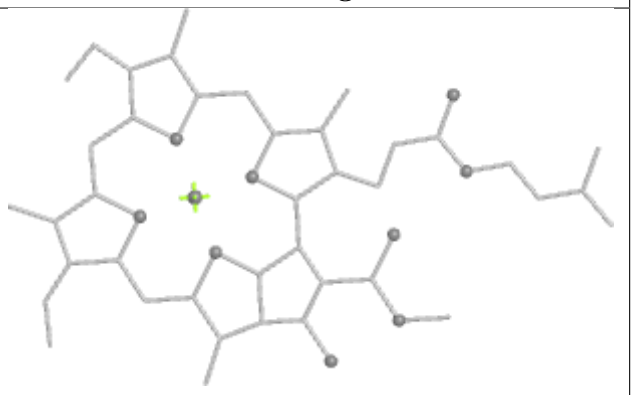
Bond lengths



Bond angles

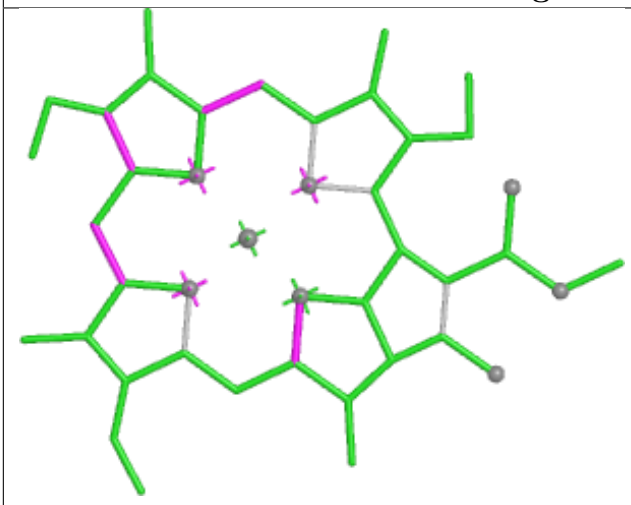


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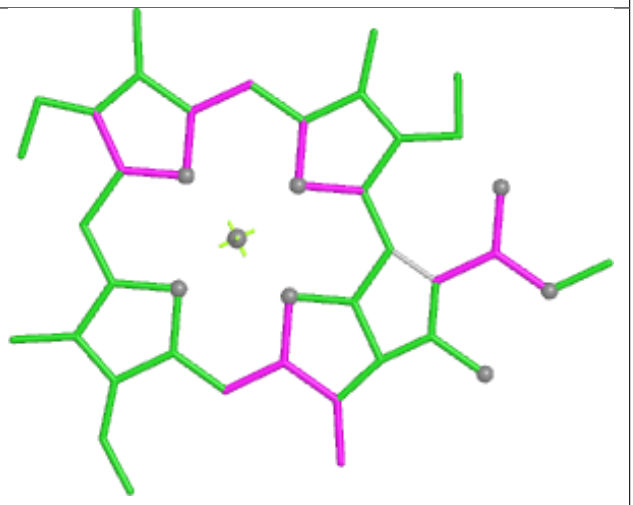


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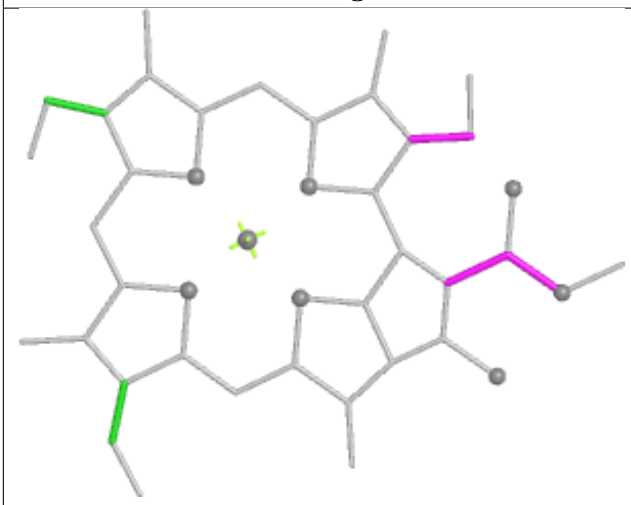
Ligand CLA l 611



Bond lengths



Bond angles

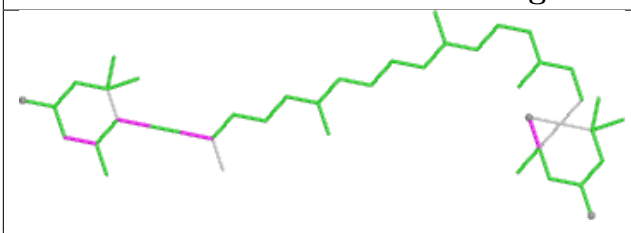


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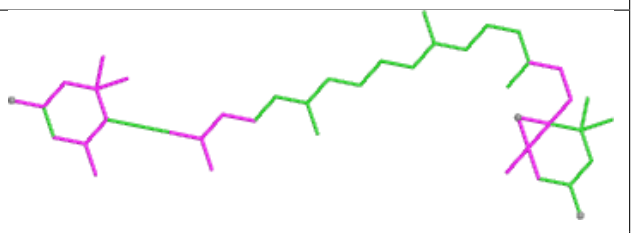


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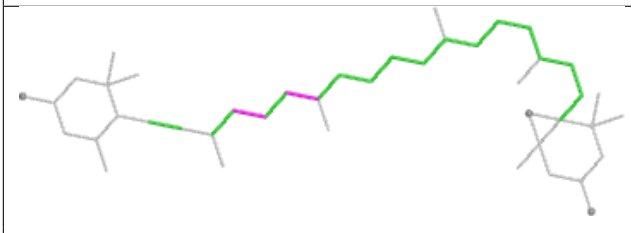
Ligand DD6 k 216



Bond lengths



Bond angles

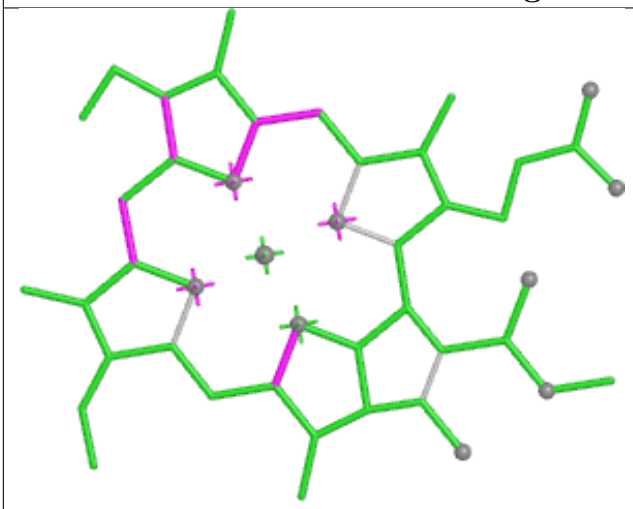


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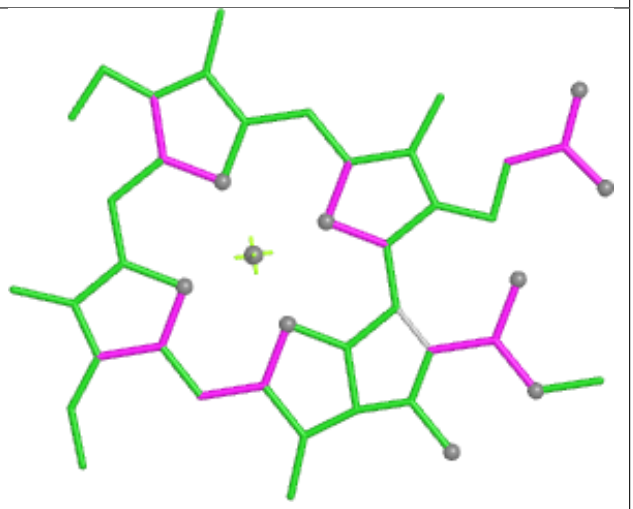


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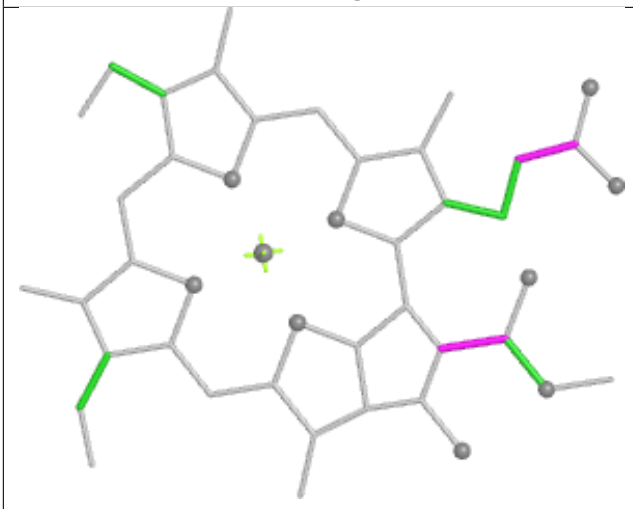
Ligand CLA A 851



Bond lengths



Bond angles

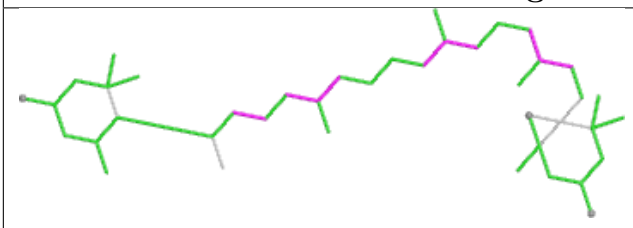


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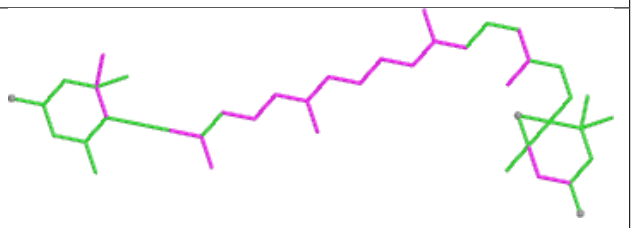


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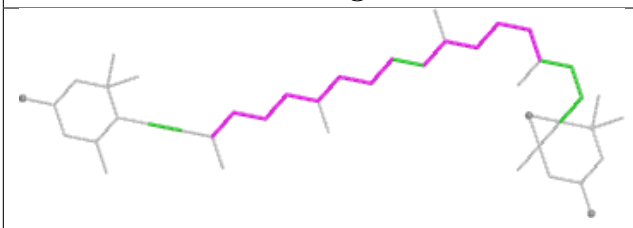
Ligand DD6 F 203



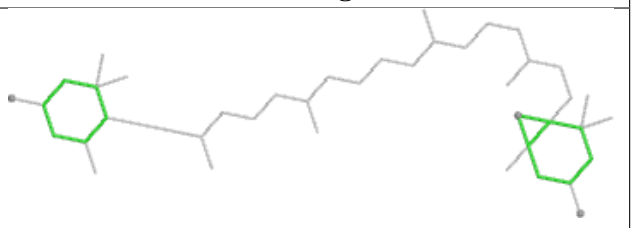
Bond lengths



Bond angles

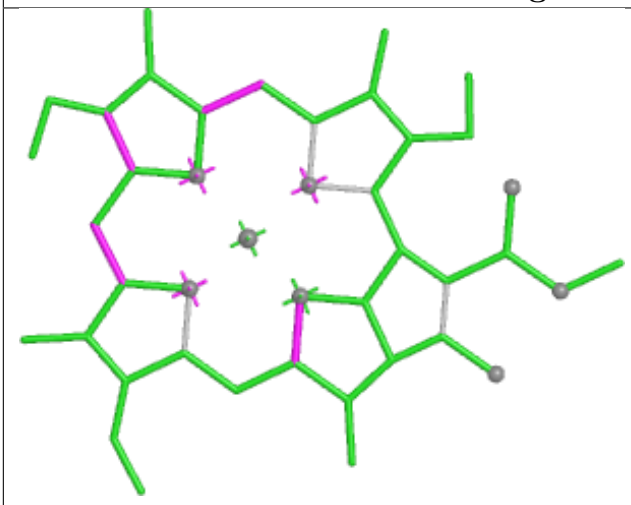


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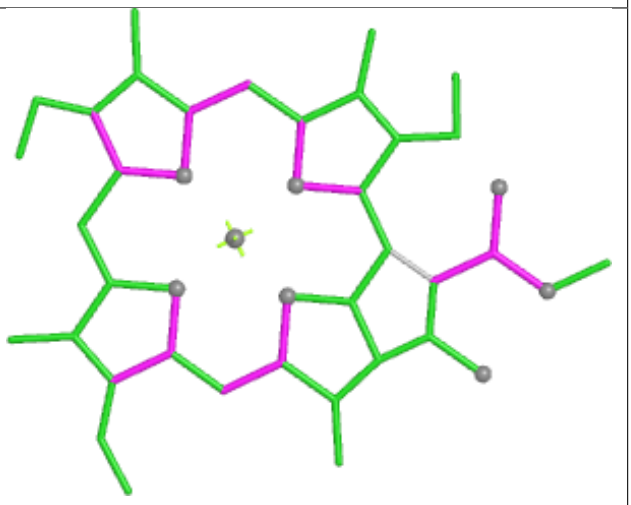


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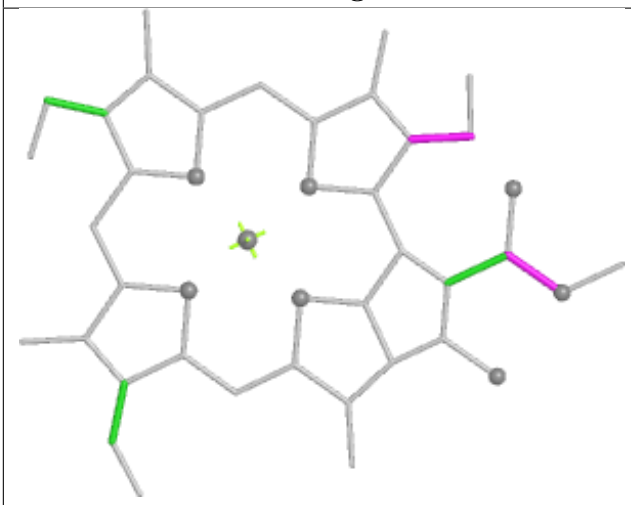
Ligand CLA e 214



Bond lengths



Bond angles

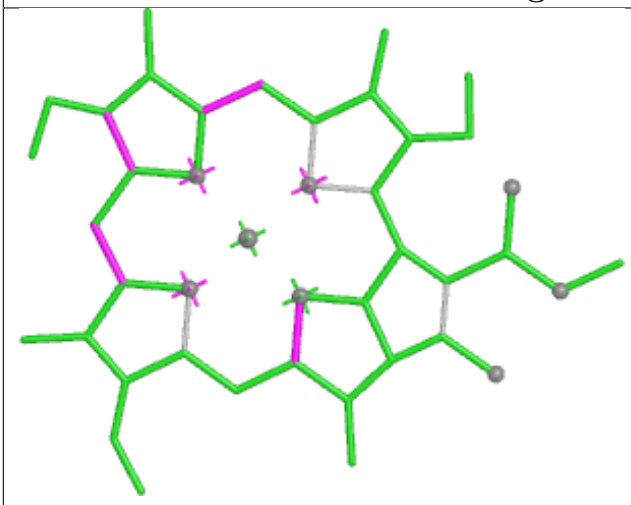


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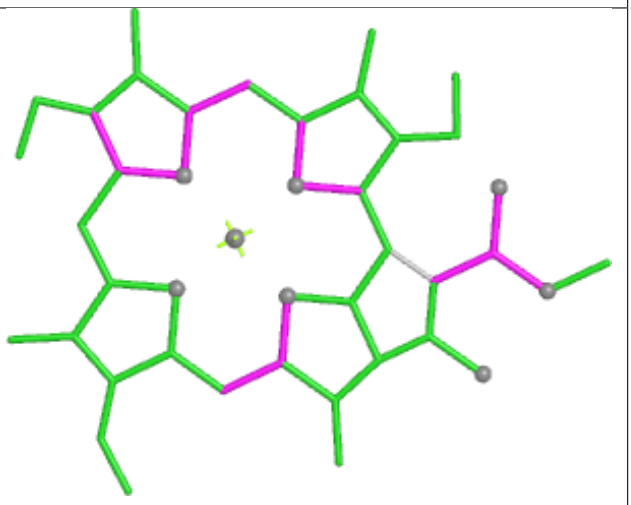


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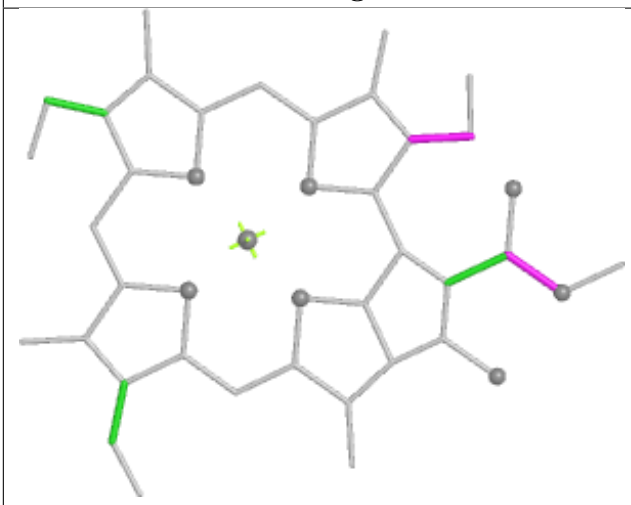
Ligand CLA k 212



Bond lengths



Bond angles

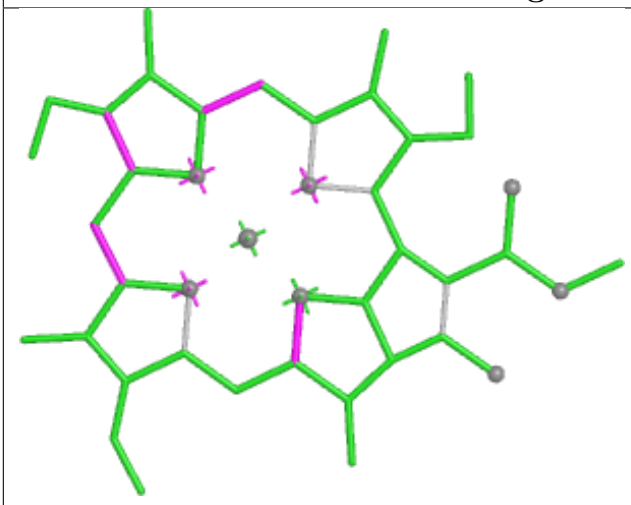


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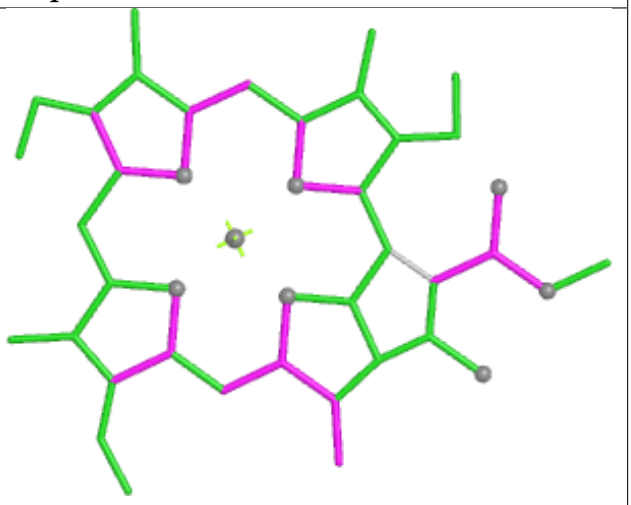


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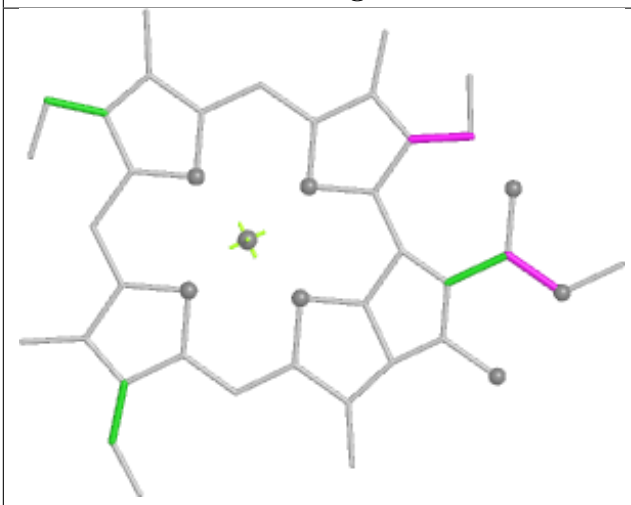
Ligand CLA p 601



Bond lengths



Bond angles

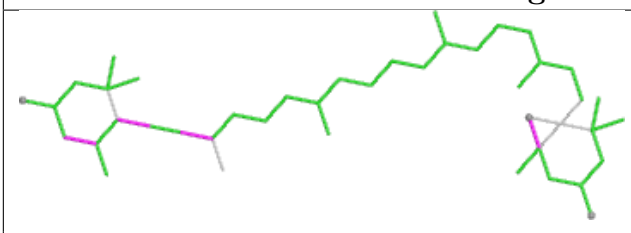


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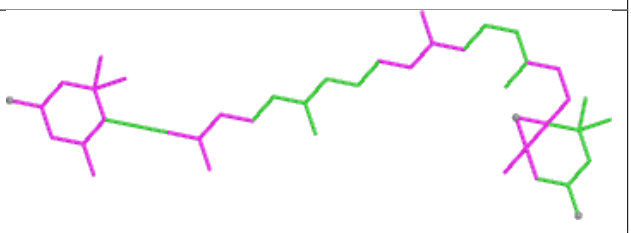


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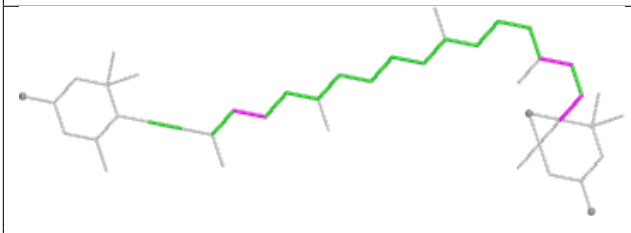
Ligand DD6 d 319



Bond lengths



Bond angles

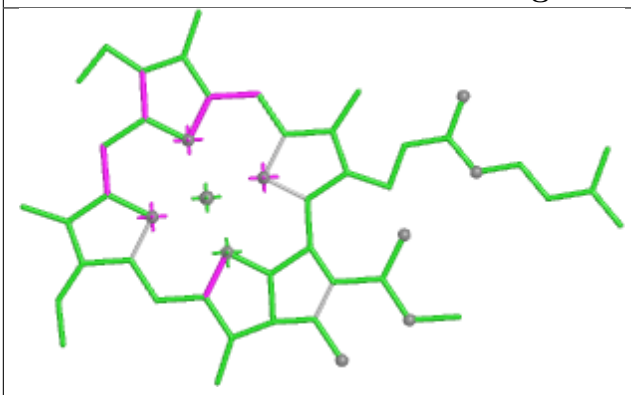


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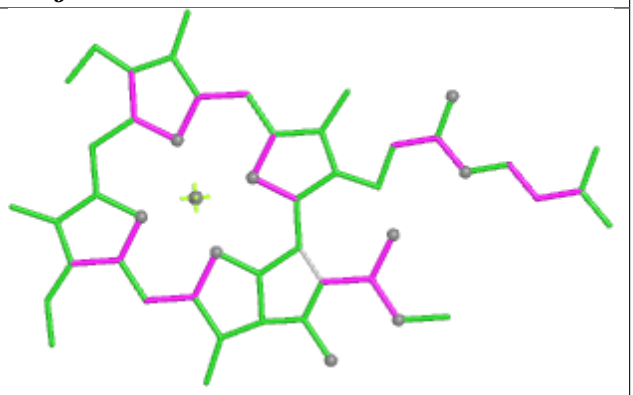


Rings

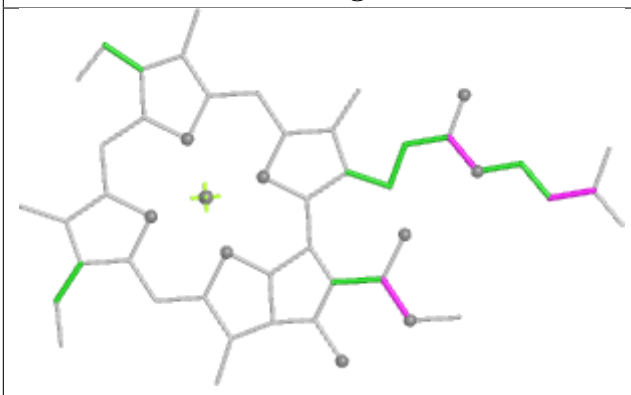
Ligand CLA j 208



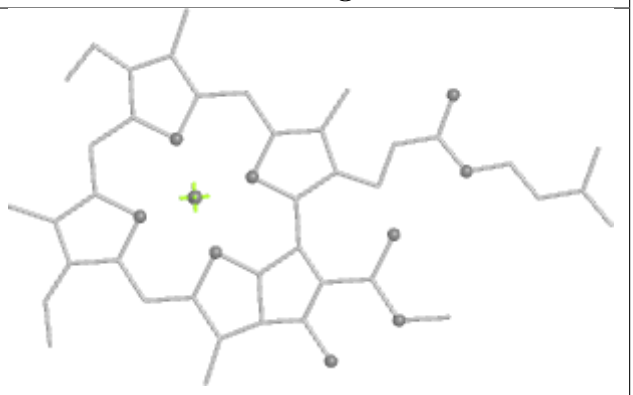
Bond lengths



Bond angles

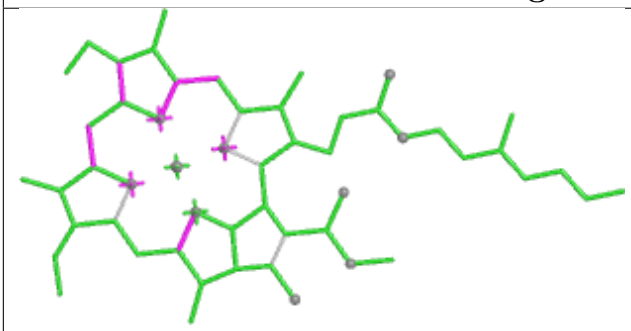


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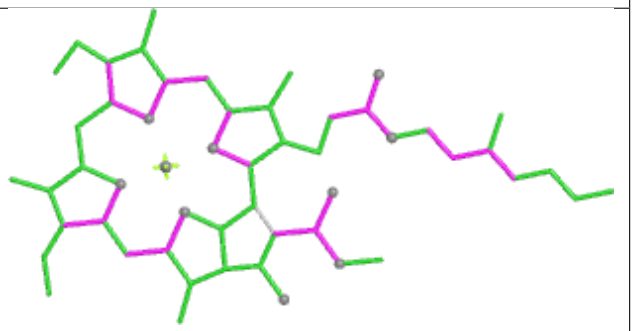


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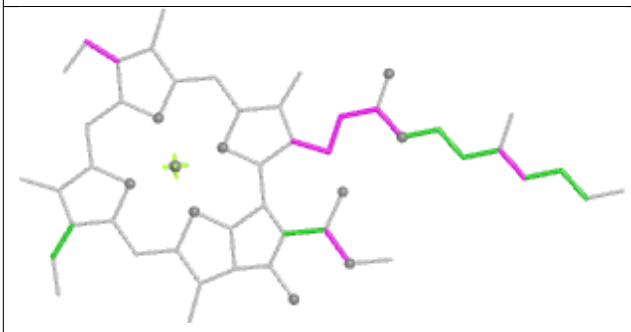
Ligand CLA a 207



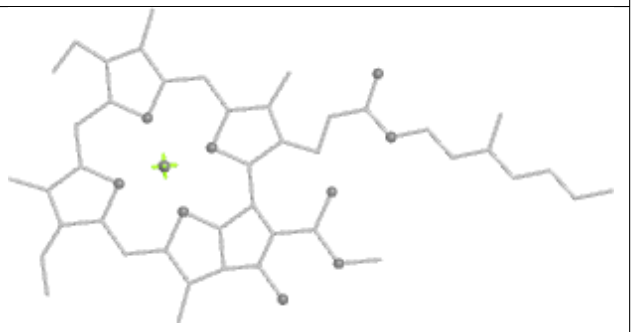
Bond lengths



Bond angles

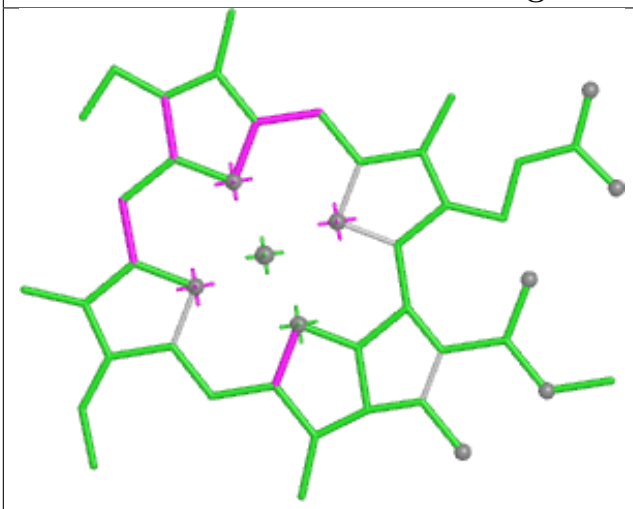


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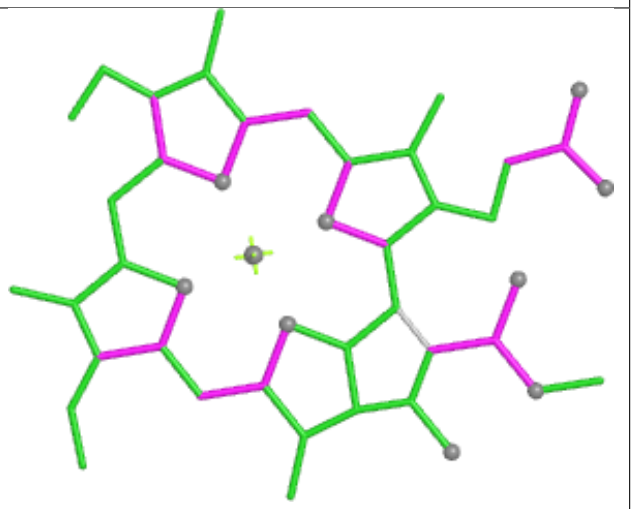


Rings

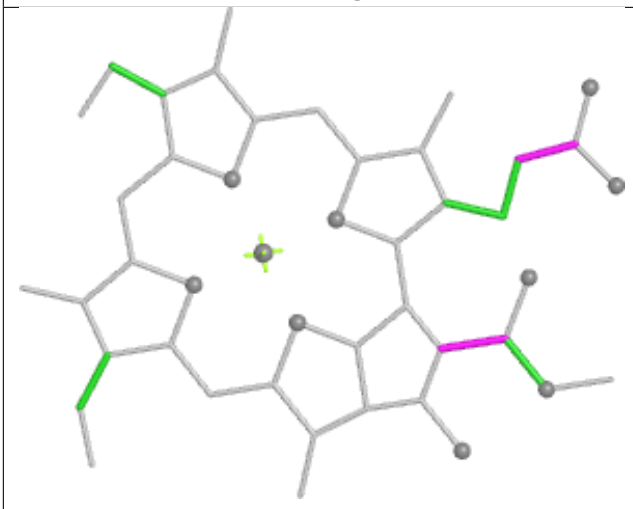
Ligand CLA b 209



Bond lengths



Bond angles

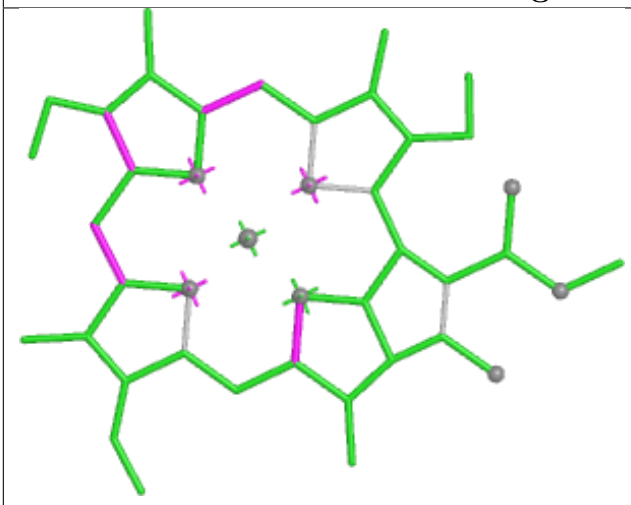


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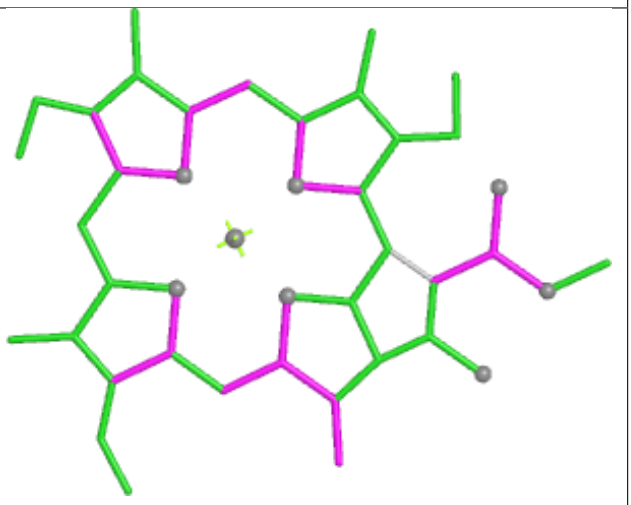


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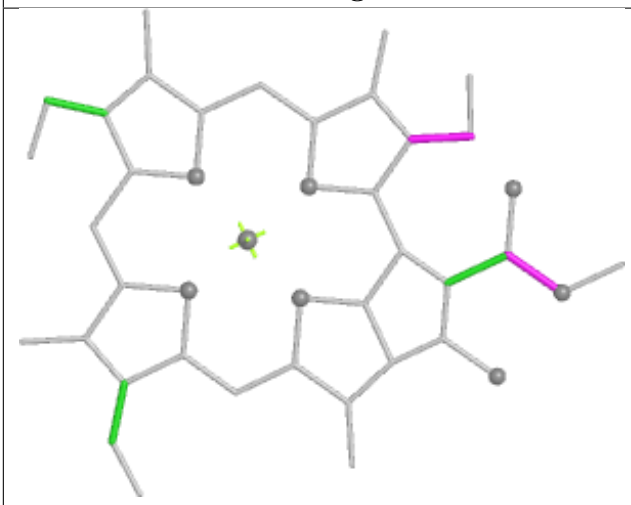
Ligand CLA f 606



Bond lengths



Bond angles

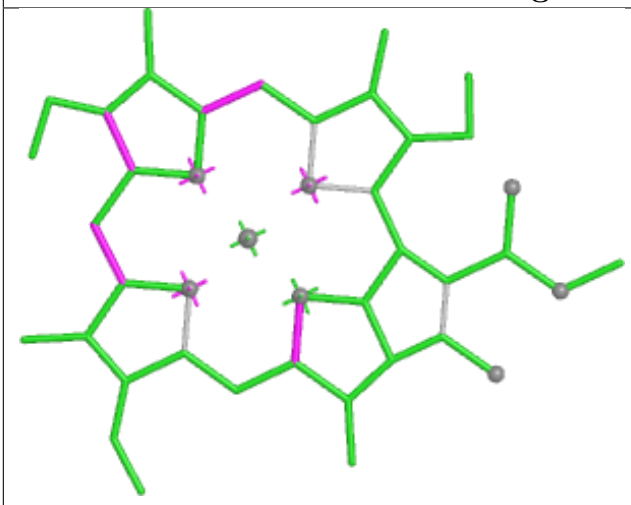


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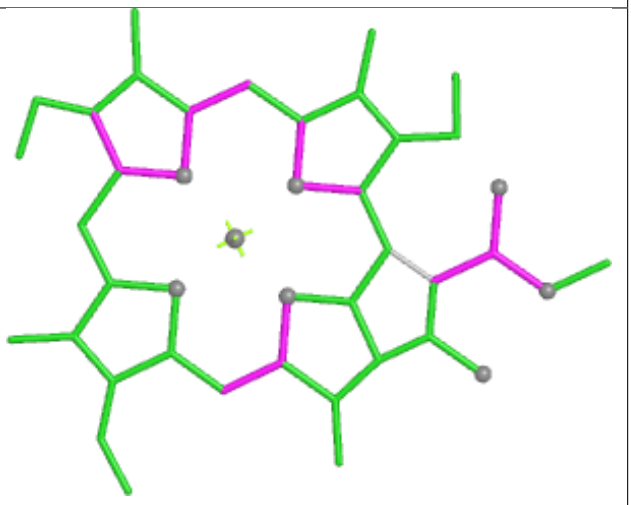


Rings

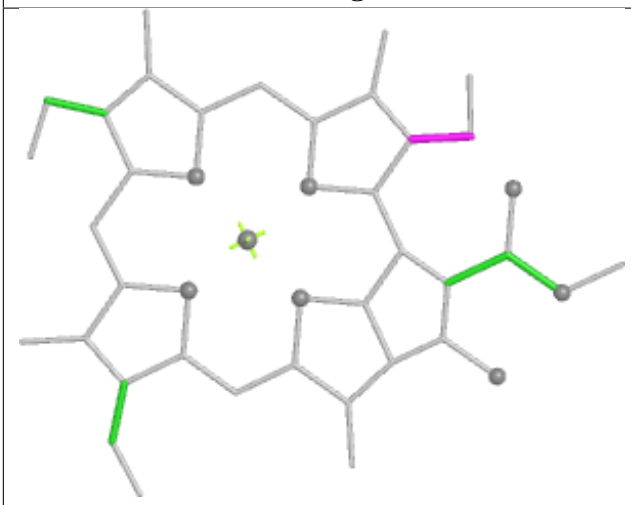
Ligand CLA f 608



Bond lengths



Bond angles

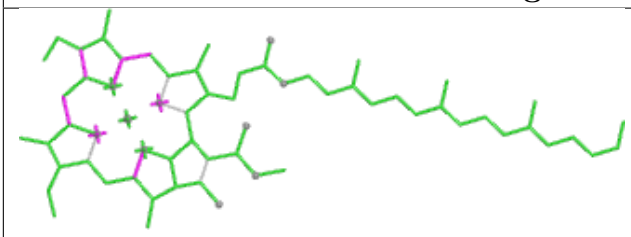


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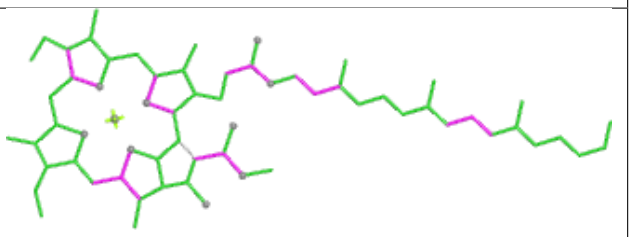


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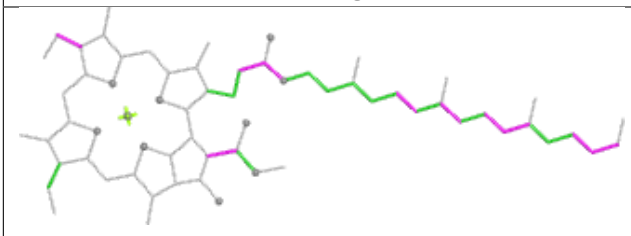
Ligand CLA A 823



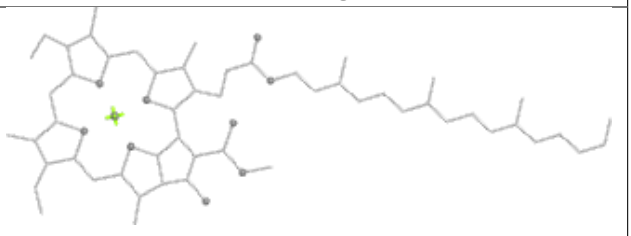
Bond lengths



Bond angles

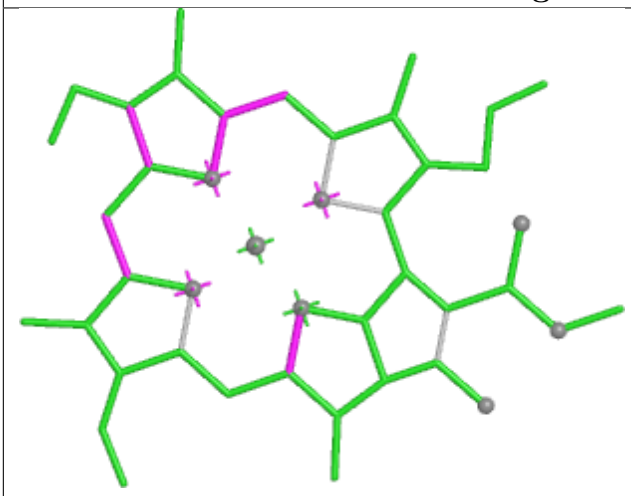


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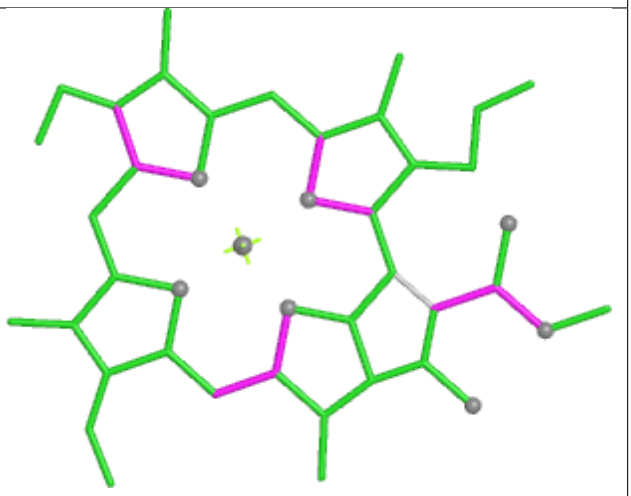


Rings

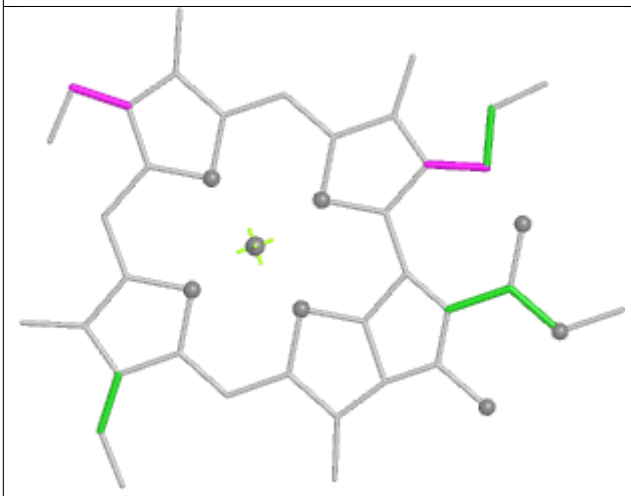
Ligand CLA i 207



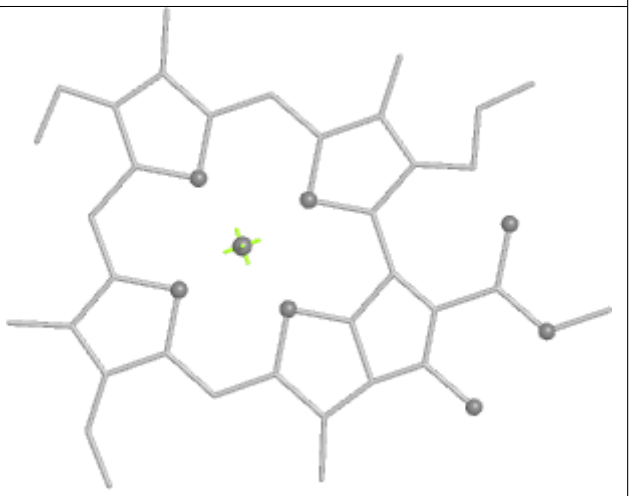
Bond lengths



Bond angles

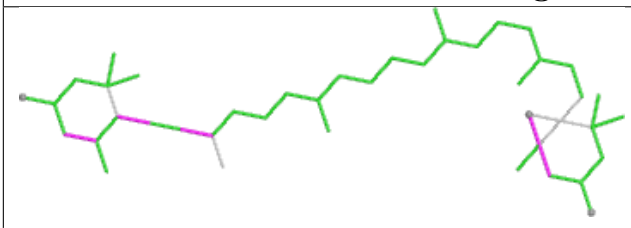


Torsions

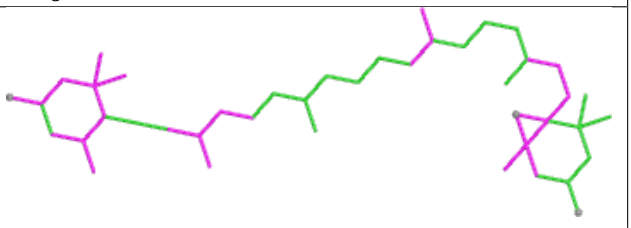


Rings

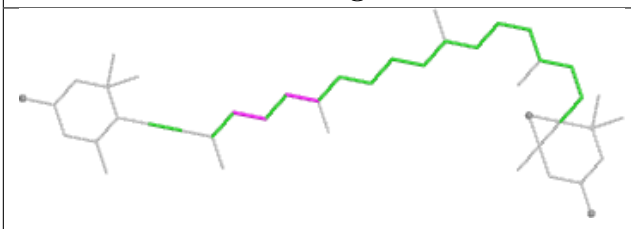
Ligand DD6 j 217



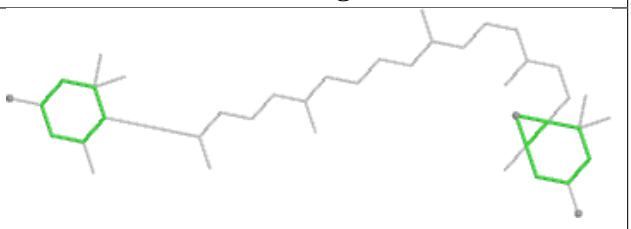
Bond lengths



Bond angles

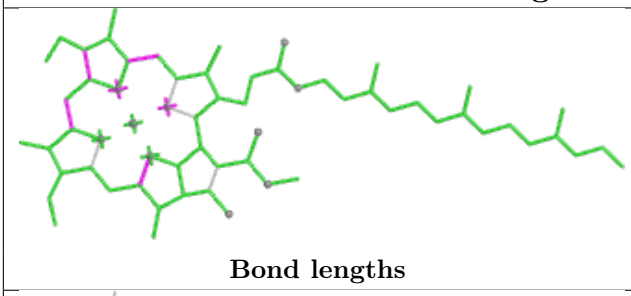


Torsions

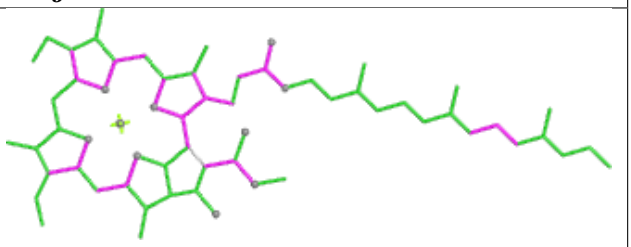


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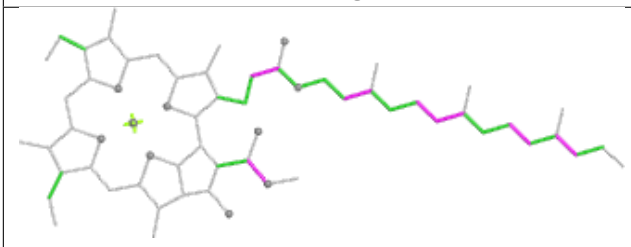
Ligand CLA j 212



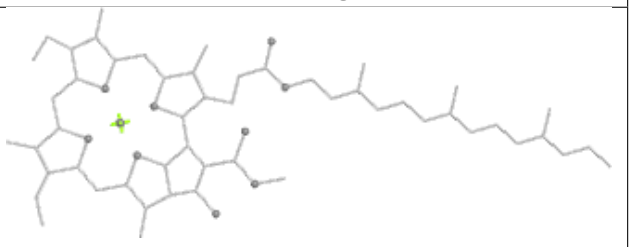
Bond lengths



Bond angles

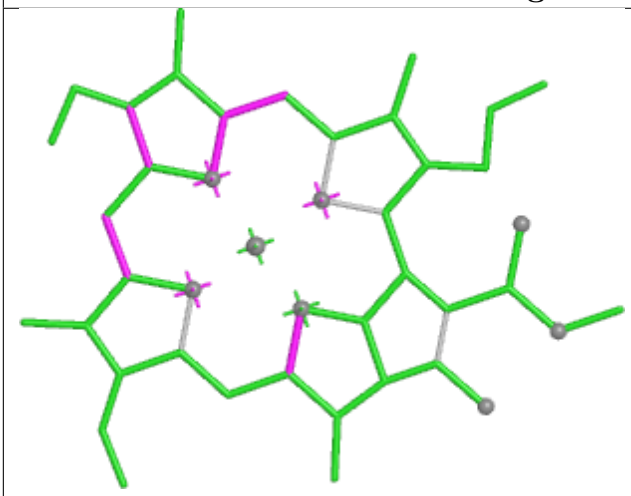


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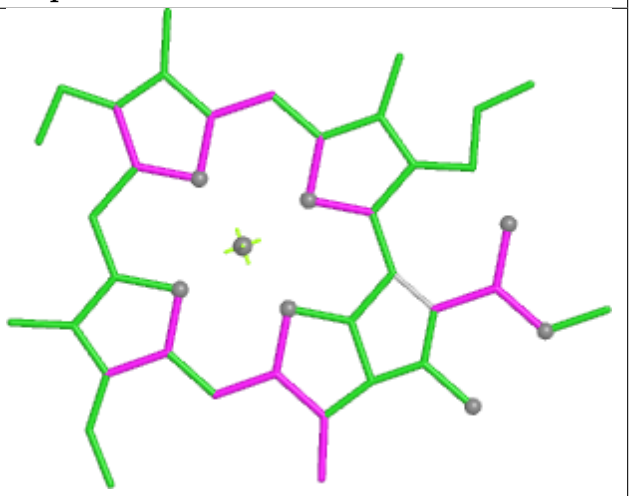


Rings

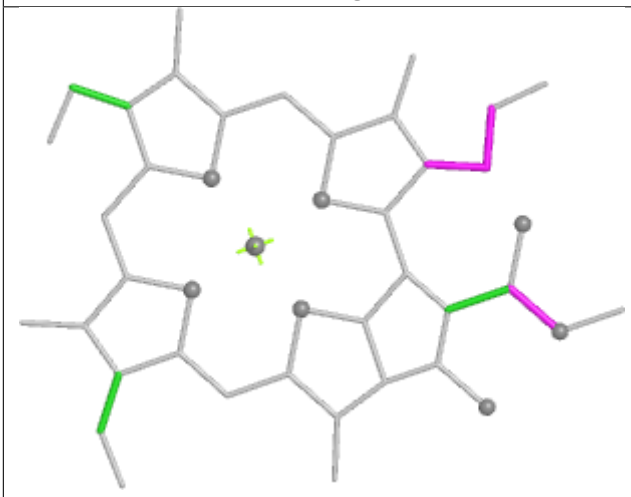
Ligand CLA p 604



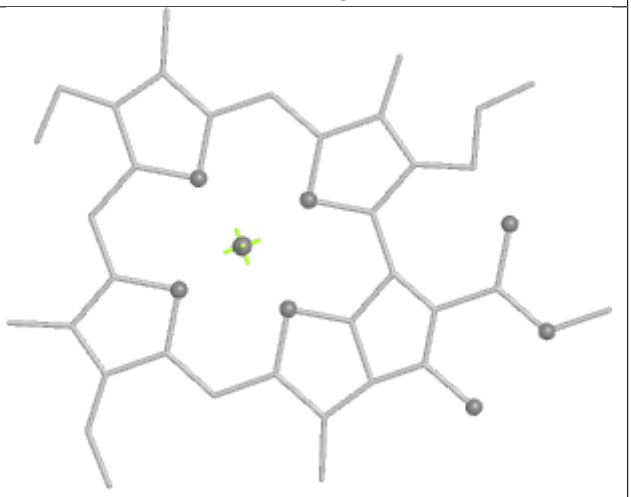
Bond lengths



Bond angles

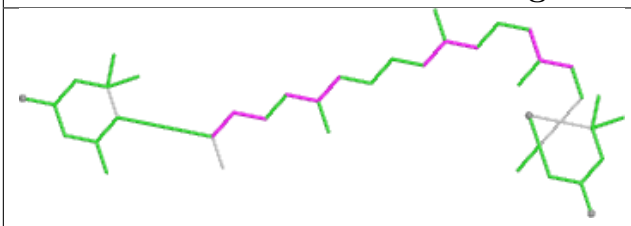


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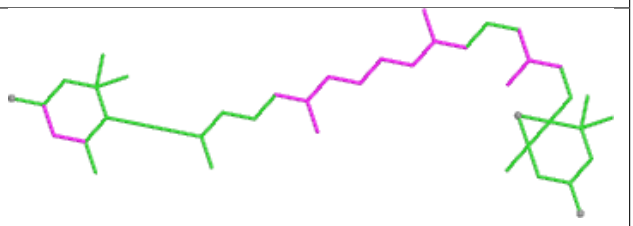


Rings

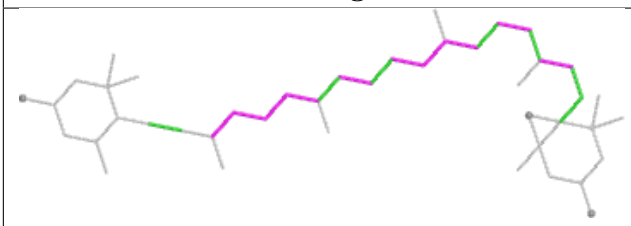
Ligand DD6 J 105



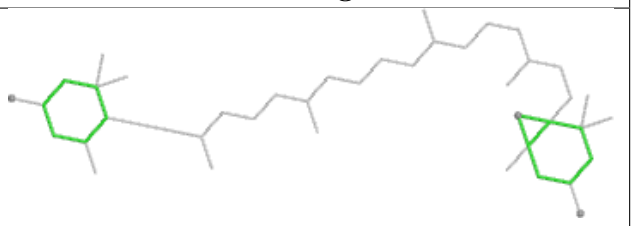
Bond lengths



Bond angles

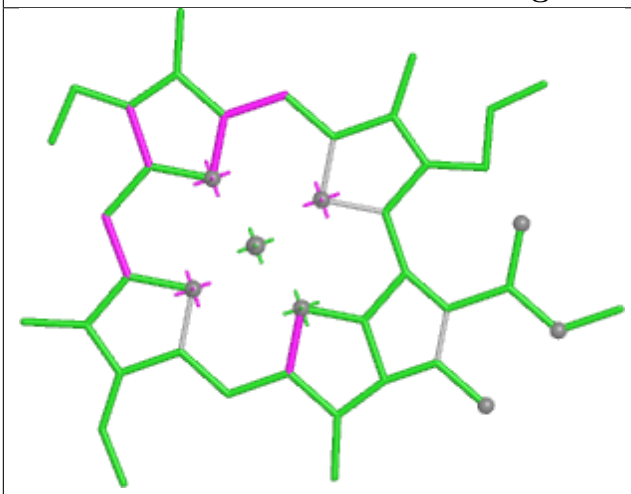


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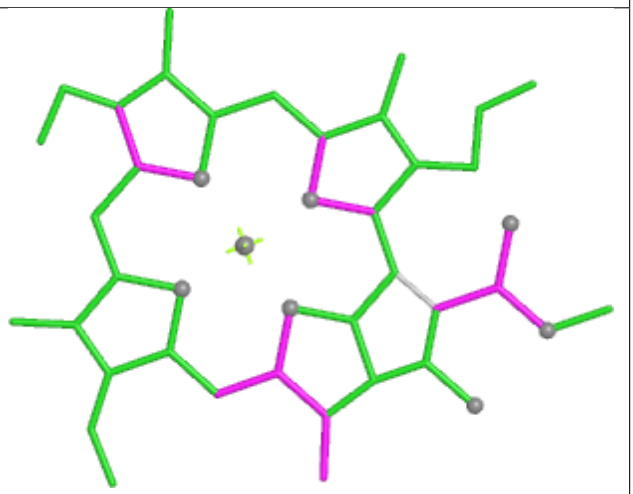


Rings

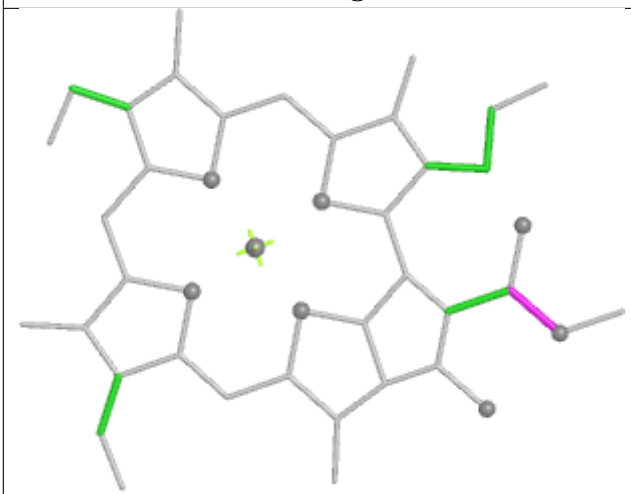
Ligand CLA f 603



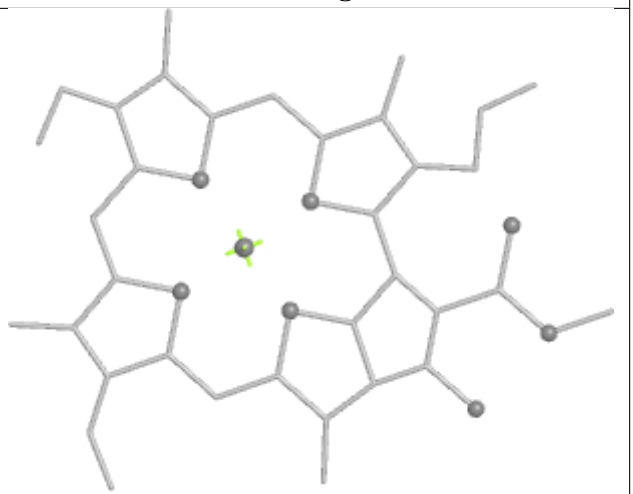
Bond lengths



Bond angles

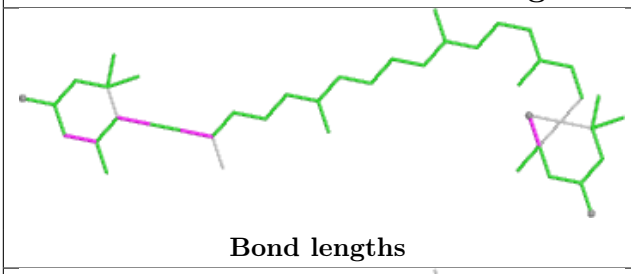


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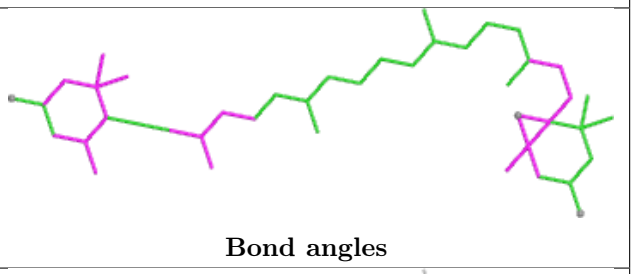


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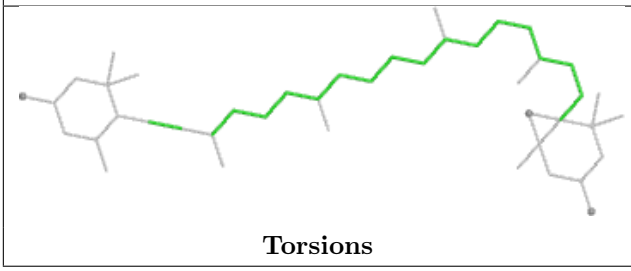
Ligand DD6 h 217



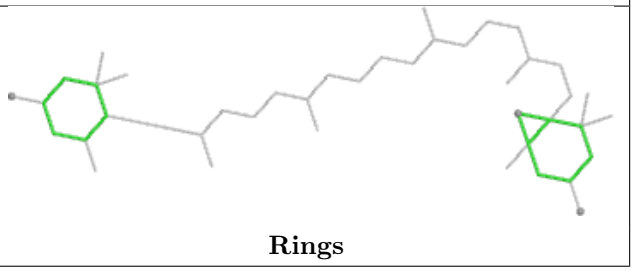
Bond lengths



Bond angles

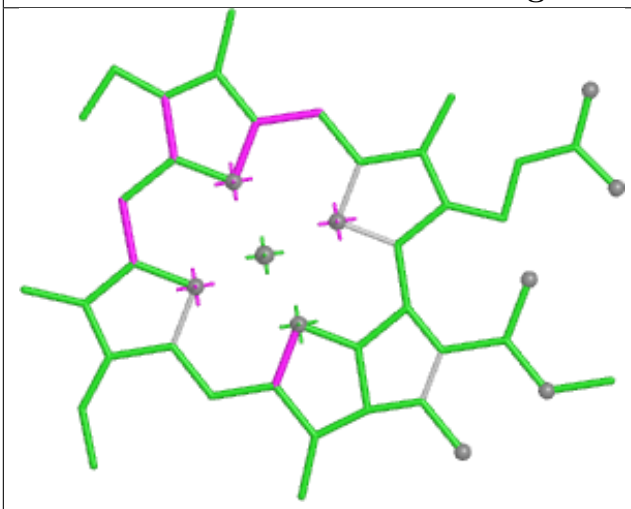


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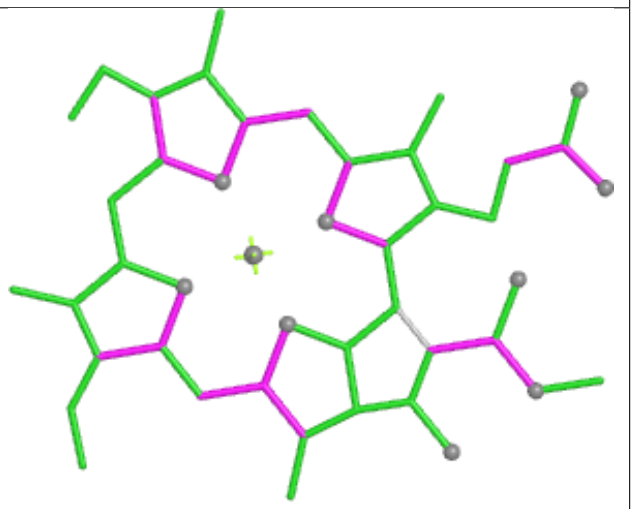


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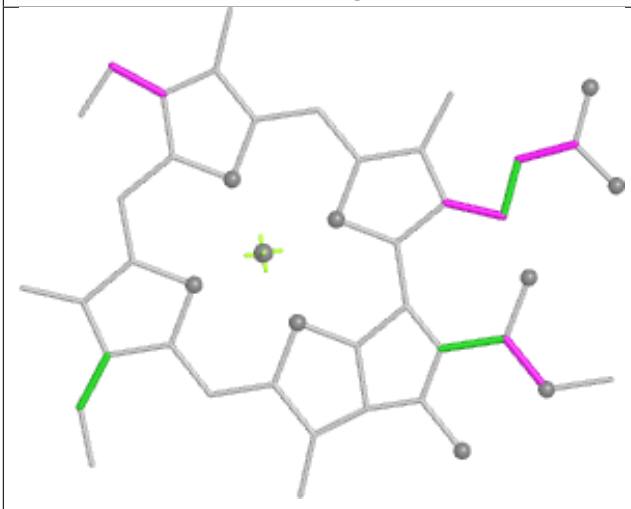
Ligand CLA b 207



Bond lengths



Bond angles

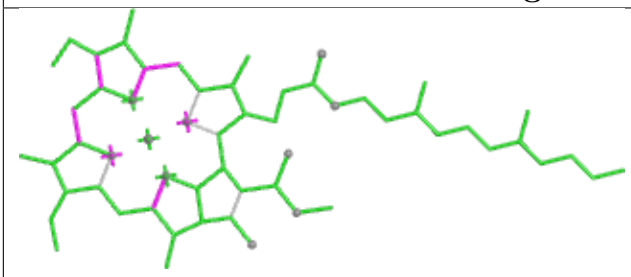


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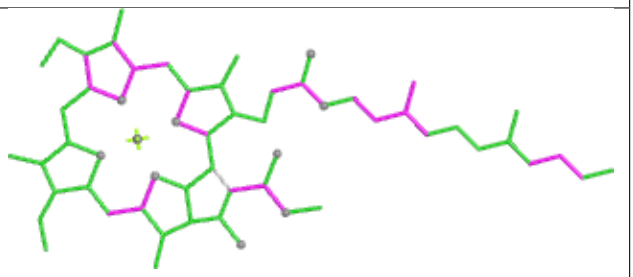


Rings

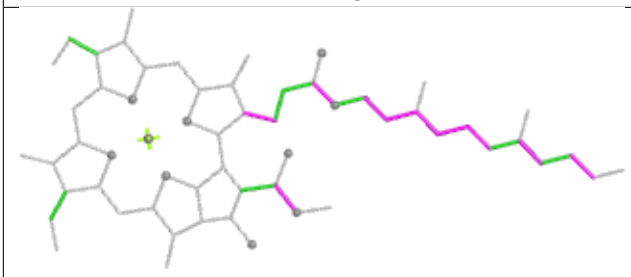
Ligand CLA A 829



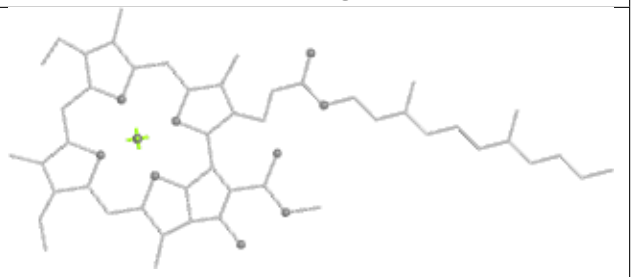
Bond lengths



Bond angles

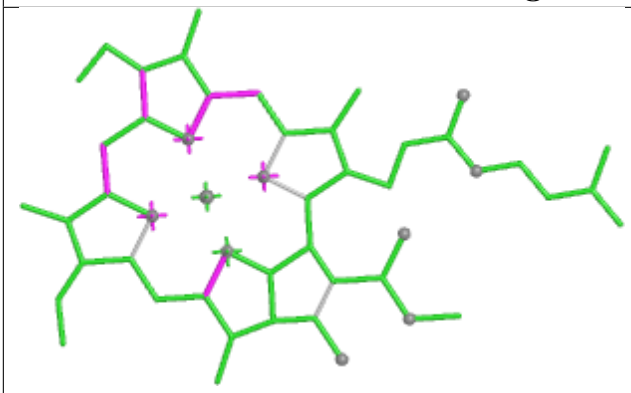


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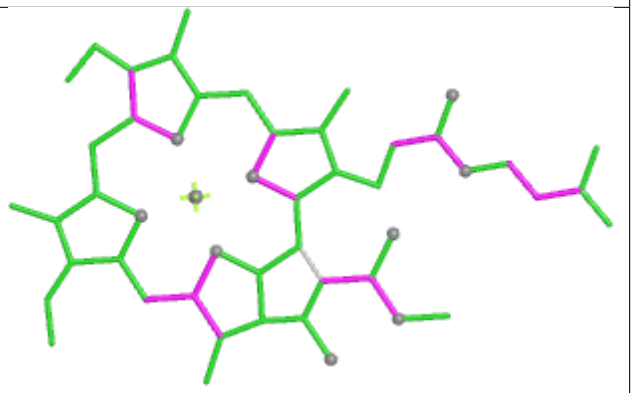


Rings

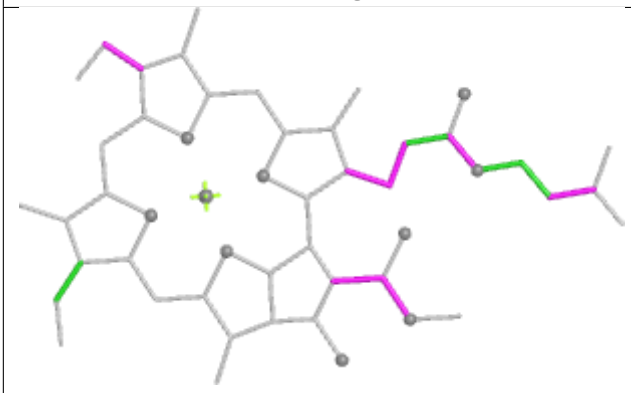
Ligand CLA B 837



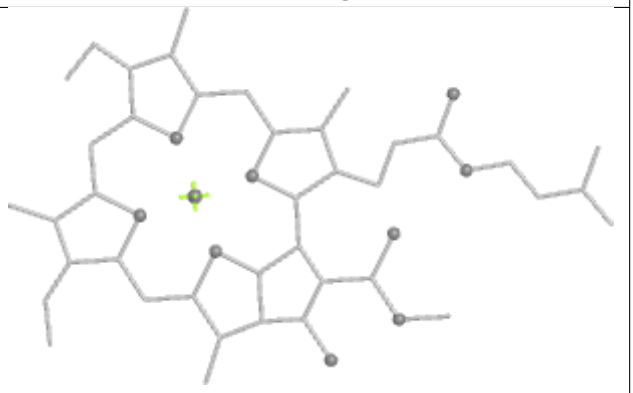
Bond lengths



Bond angles

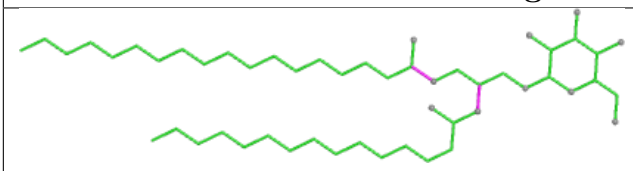


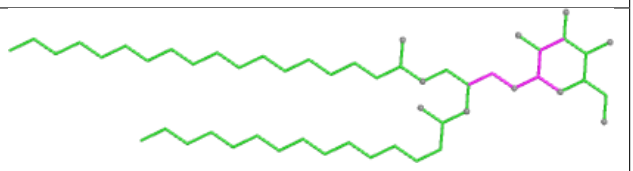
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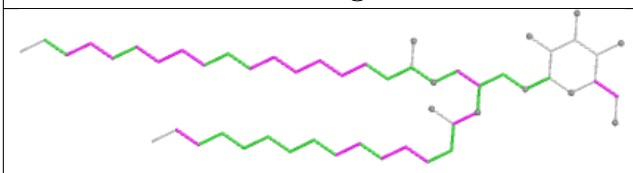


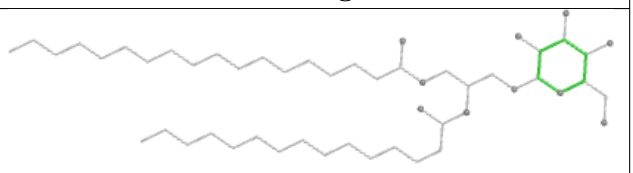
Rings

Ligand LMG e 202

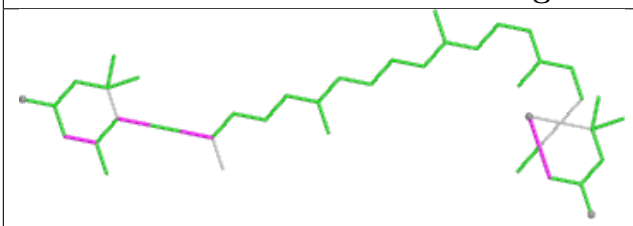

Bond lengths

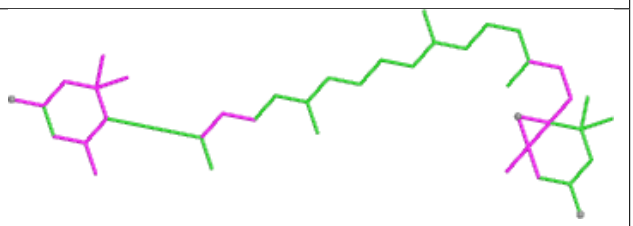

Bond angles

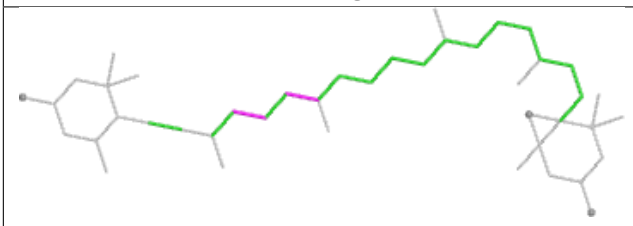

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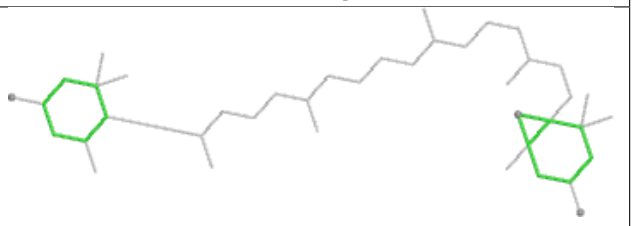

Rings

Ligand DD6 i 215

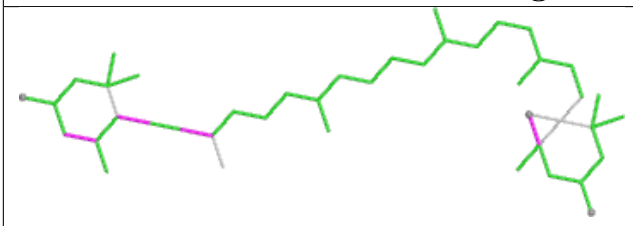

Bond lengths

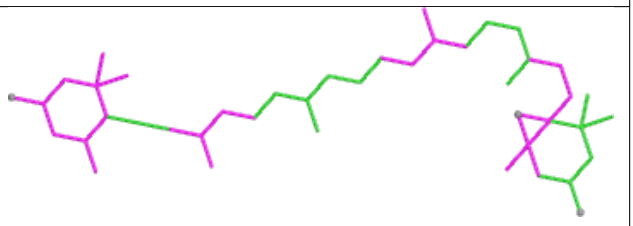

Bond angles

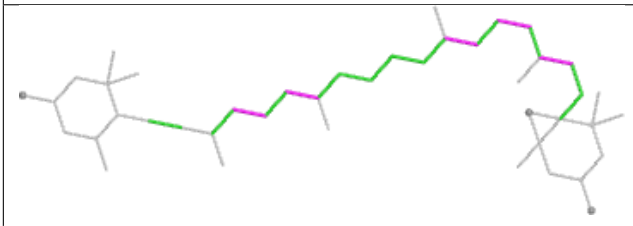

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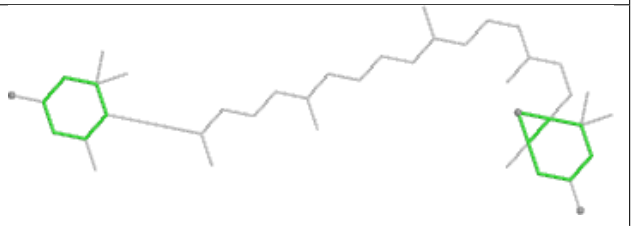

Rings

Ligand DD6 c 318

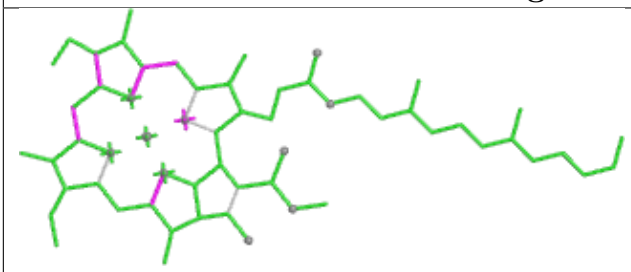

Bond lengths


Bond angles

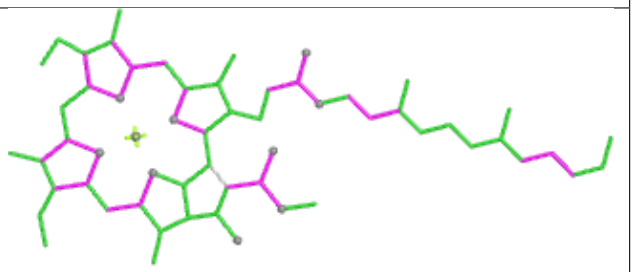

Torsions


Rings

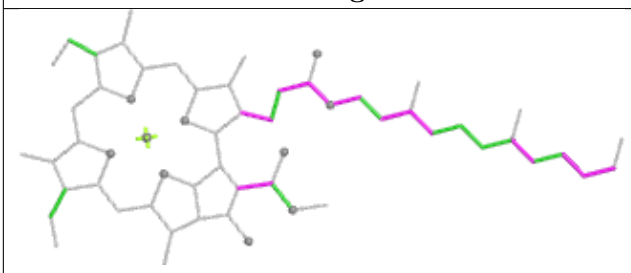
Ligand CLA n 201



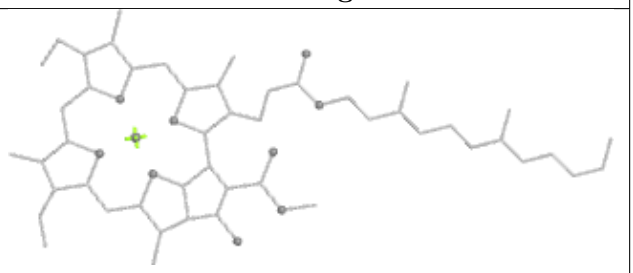
Bond lengths



Bond angles

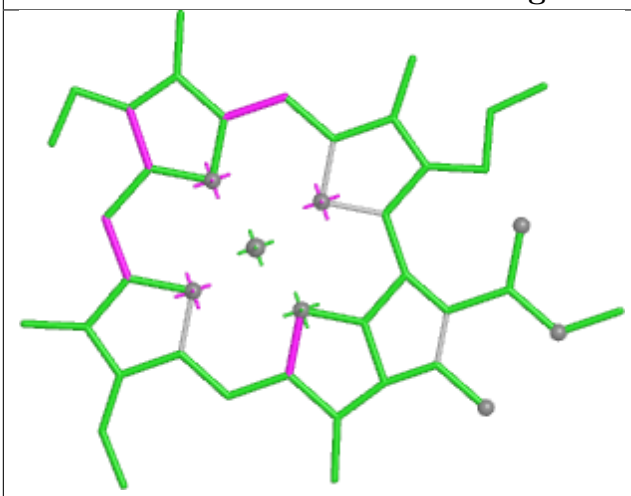


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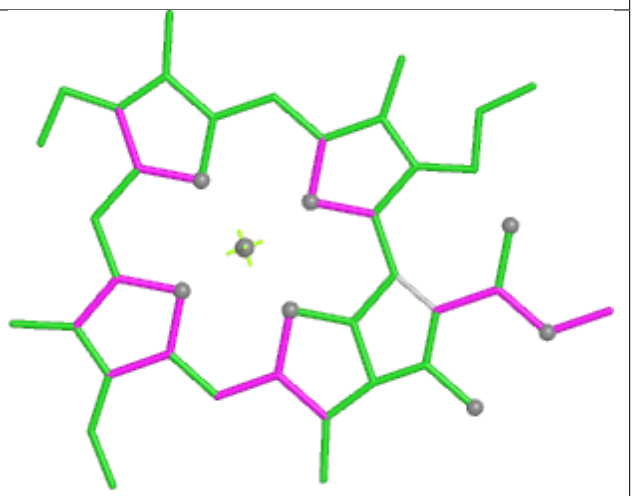


Rings

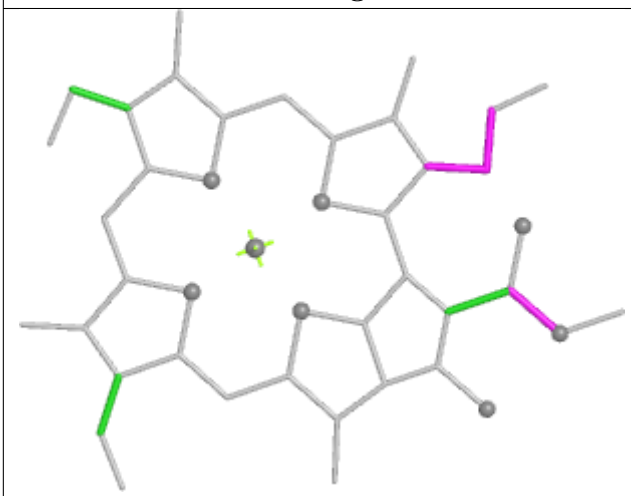
Ligand CLA o 610



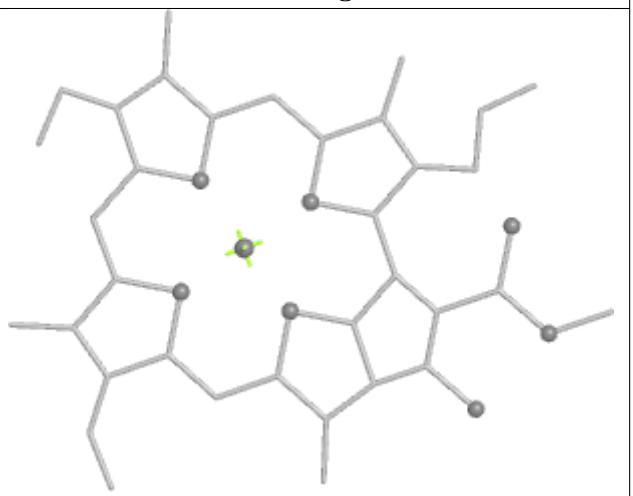
Bond lengths



Bond angles

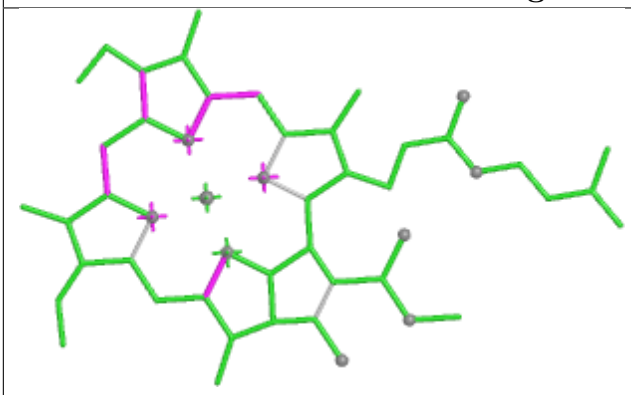


Torsions

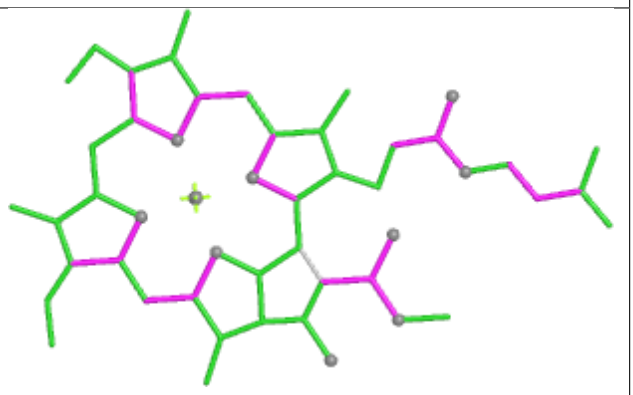


Rings

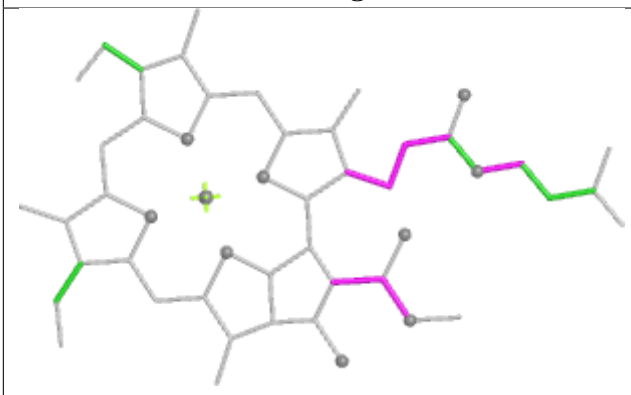
Ligand CLA h 203



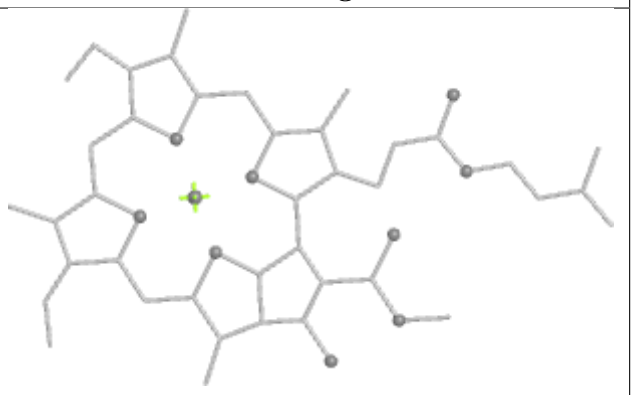
Bond lengths



Bond angles

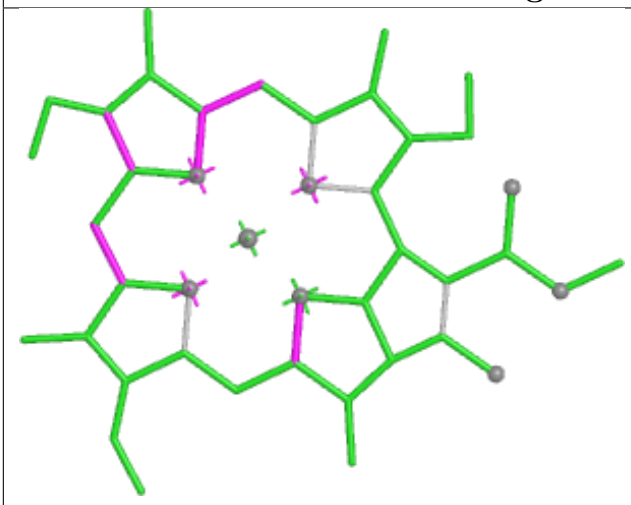


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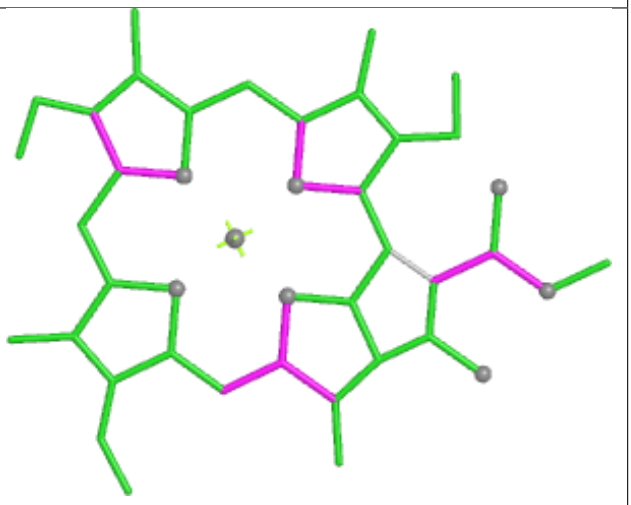


Rings

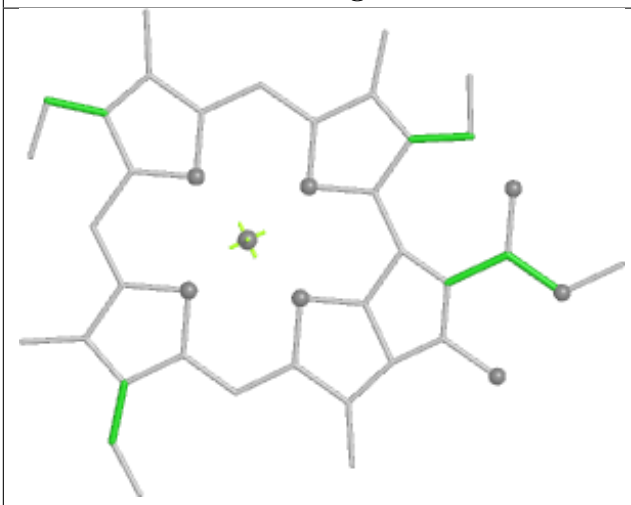
Ligand CLA F 201



Bond lengths



Bond angles

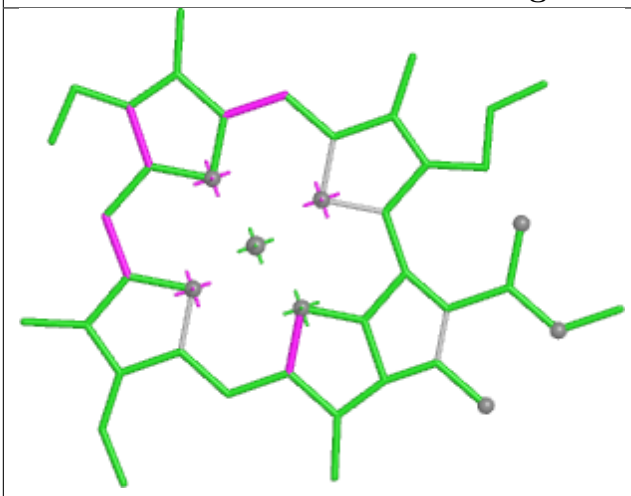


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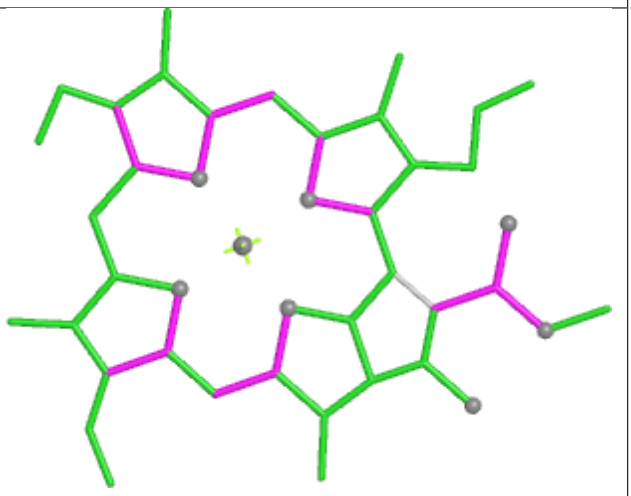


Rings

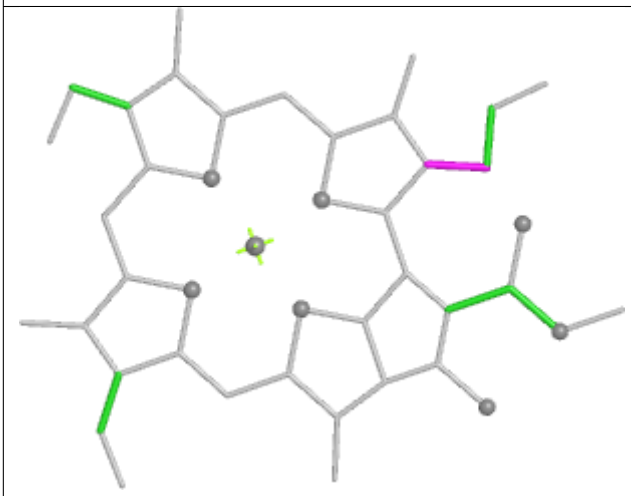
Ligand CLA c 311



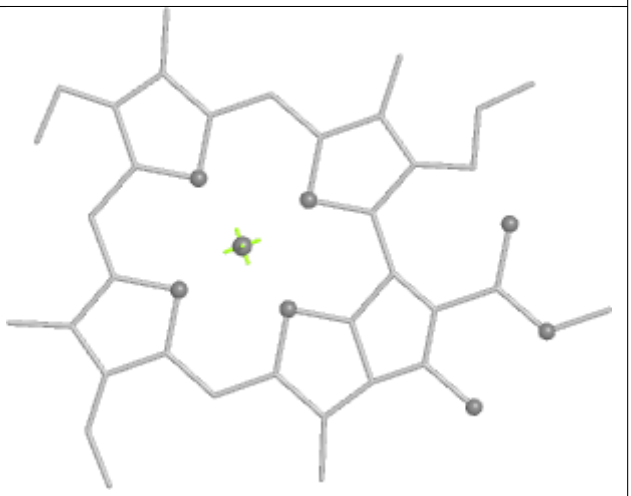
Bond lengths



Bond angles

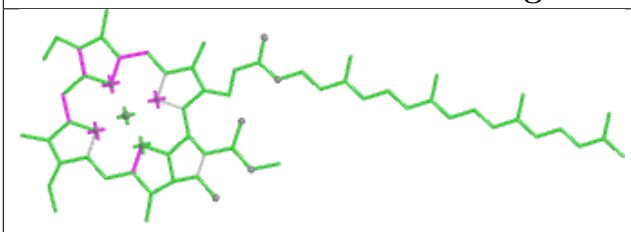


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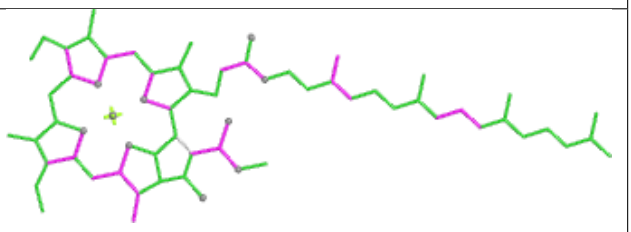


Rings

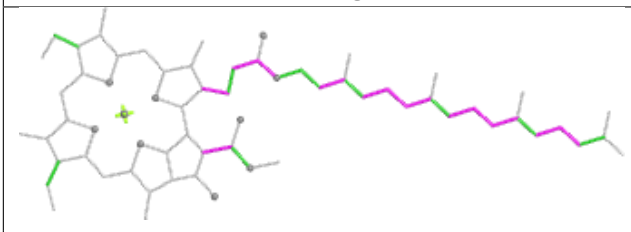
Ligand CLA B 848



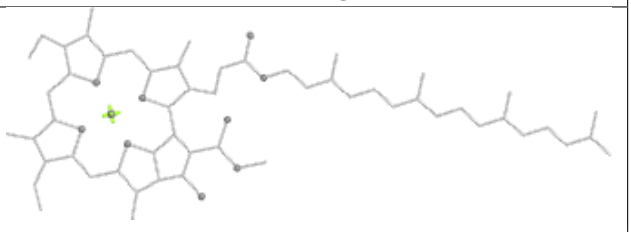
Bond lengths



Bond angles

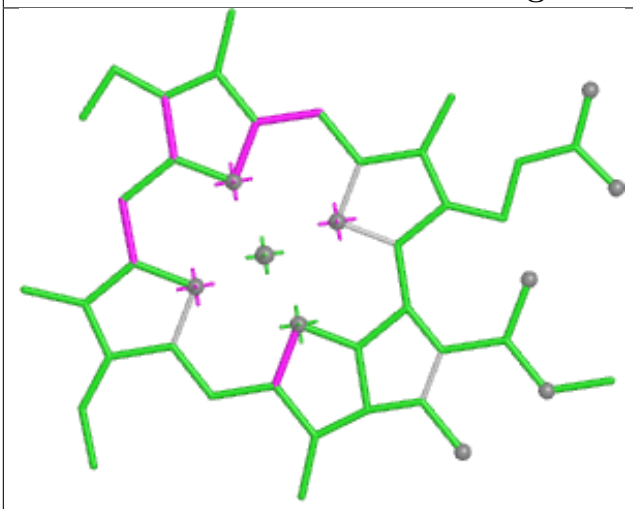


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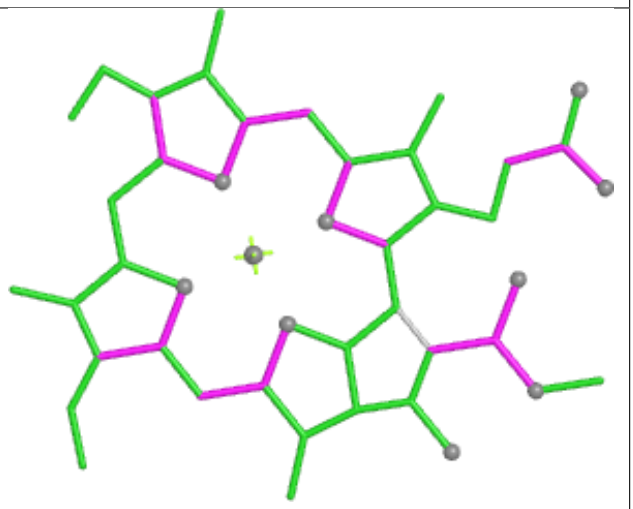


Rings

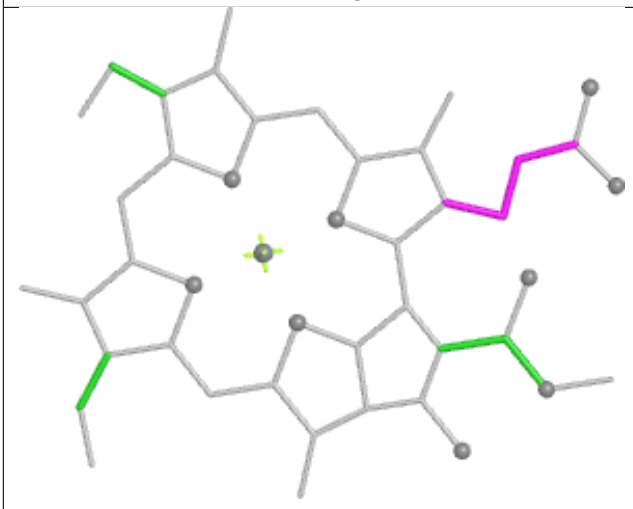
Ligand CLA d 313



Bond lengths



Bond angles

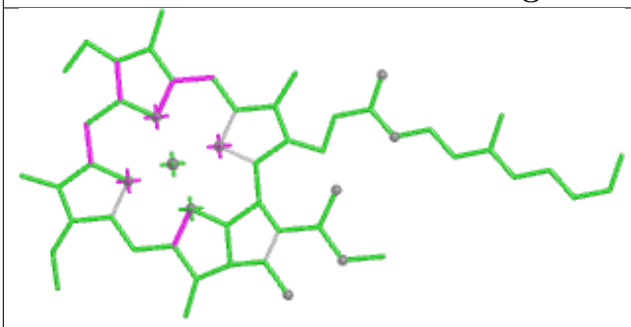


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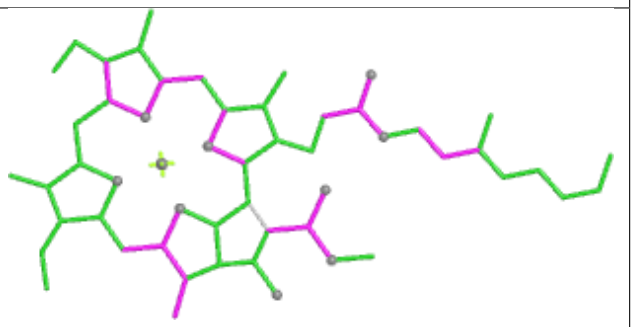


Rings

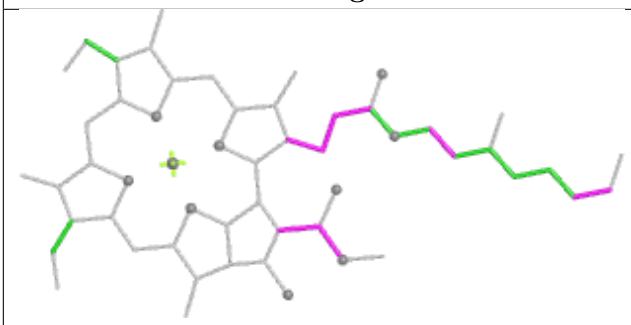
Ligand CLA m 204



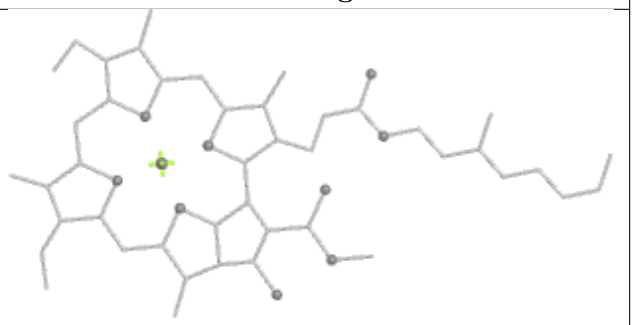
Bond lengths



Bond angles

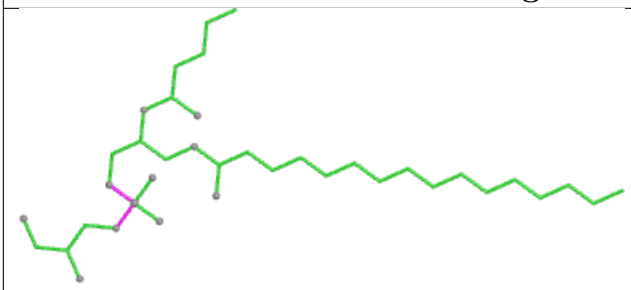


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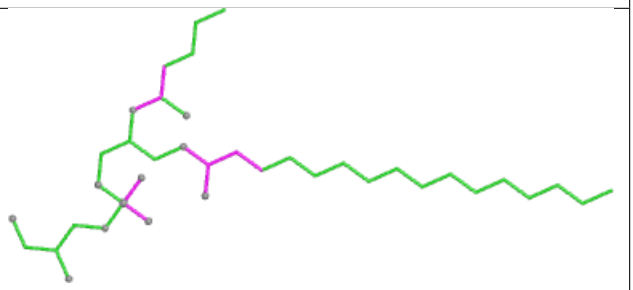


Rings

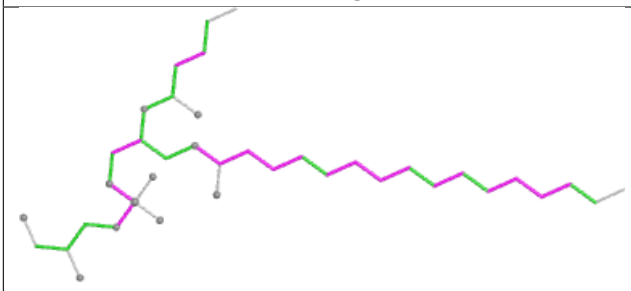
Ligand LHG A 805



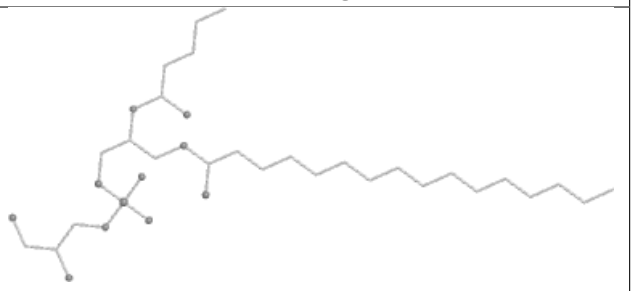
Bond lengths



Bond angles

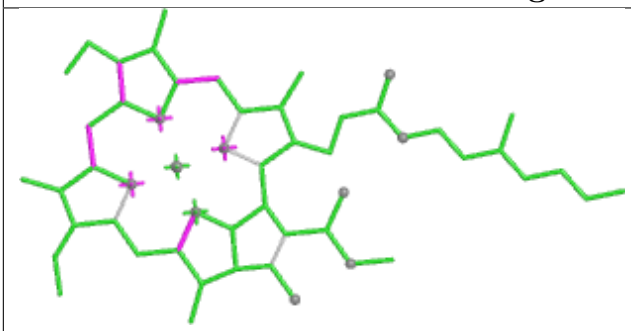


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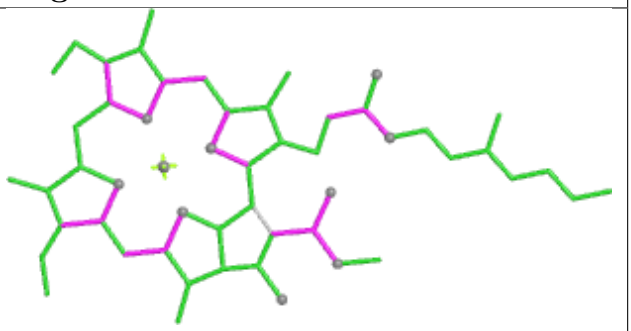


Rings

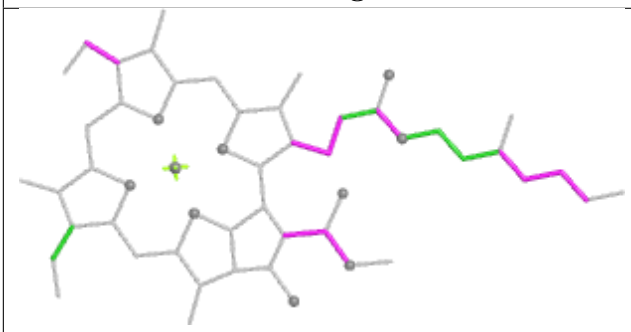
Ligand CLA g 204



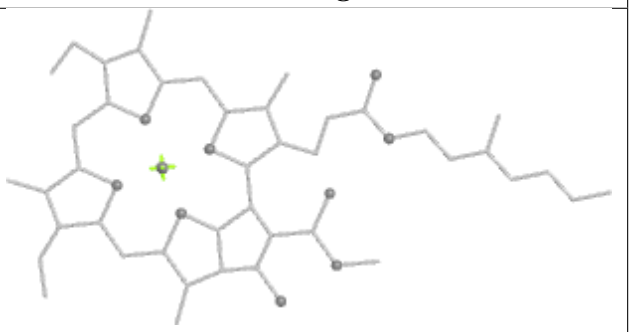
Bond lengths



Bond angles

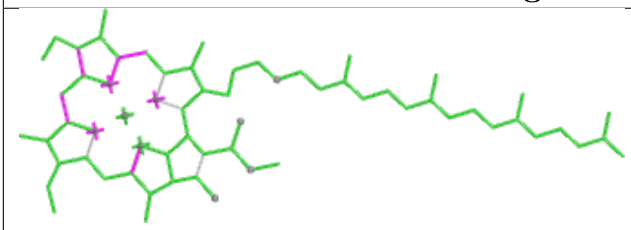


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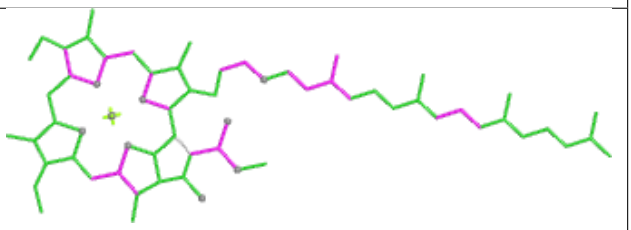


Rings

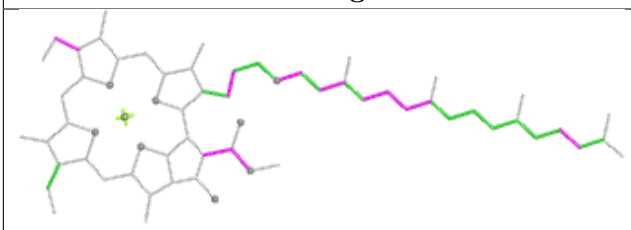
Ligand CLA A 821



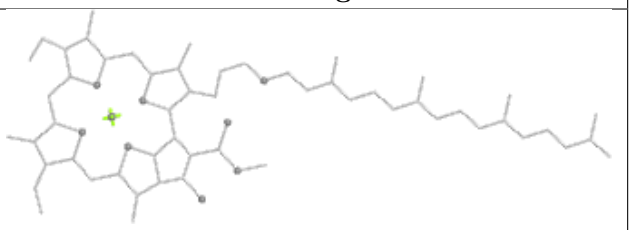
Bond lengths



Bond angles

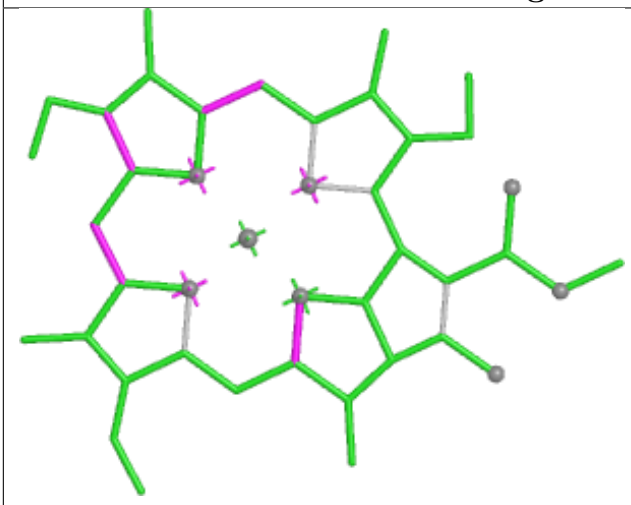


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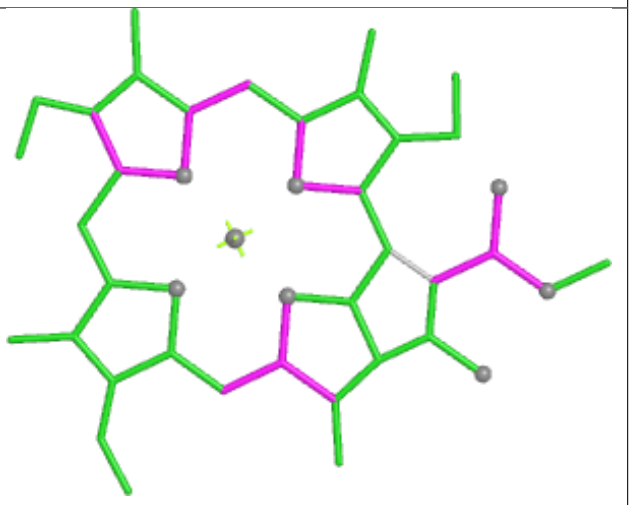


Rings

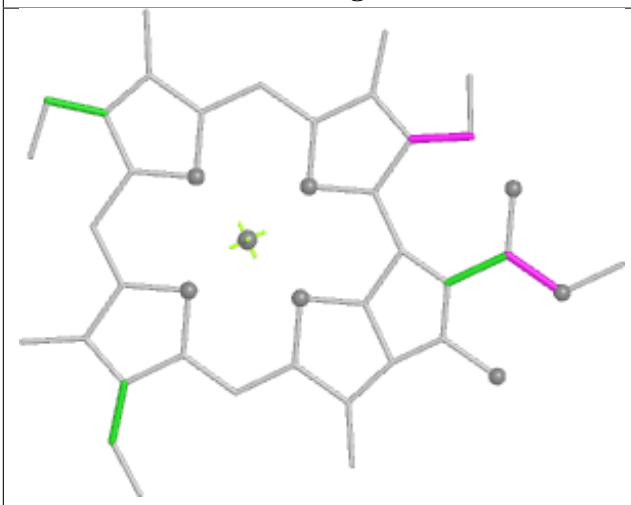
Ligand CLA d 316



Bond lengths



Bond angles

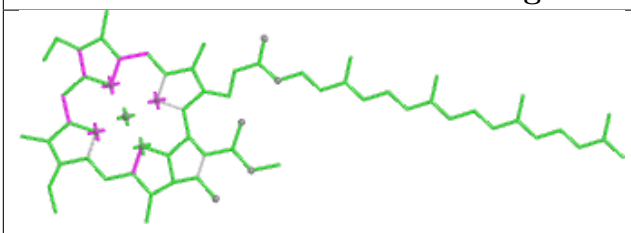


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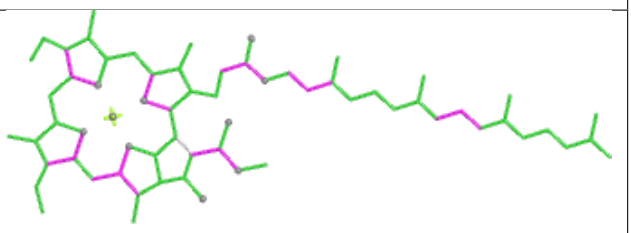


Rings

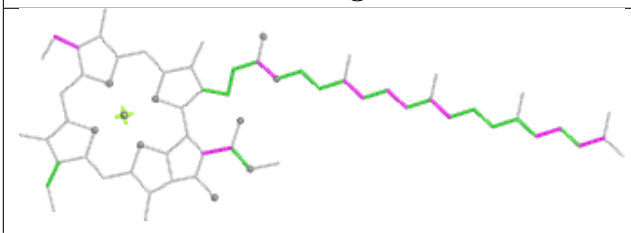
Ligand CLA A 826



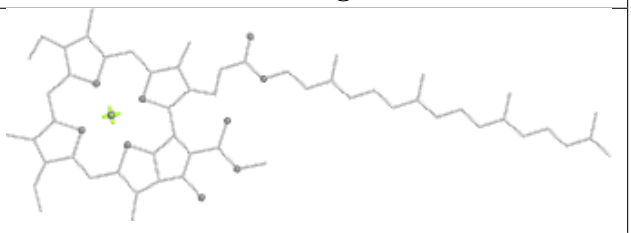
Bond lengths



Bond angles

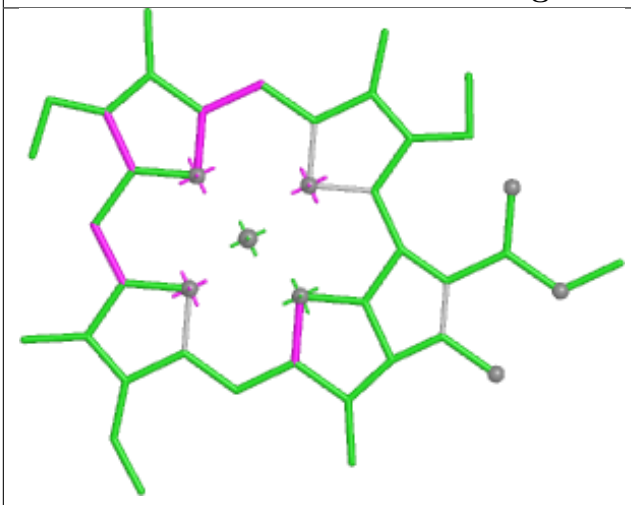


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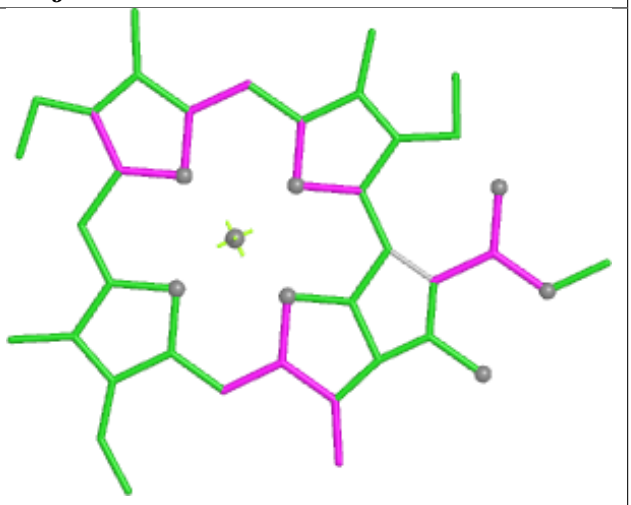


Rings

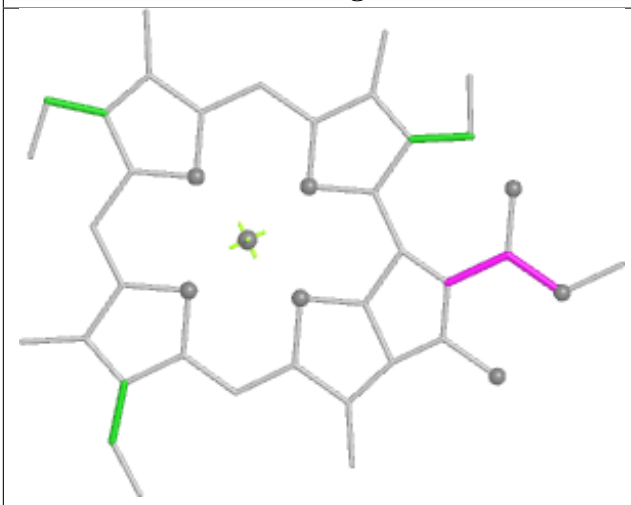
Ligand CLA j 205



Bond lengths



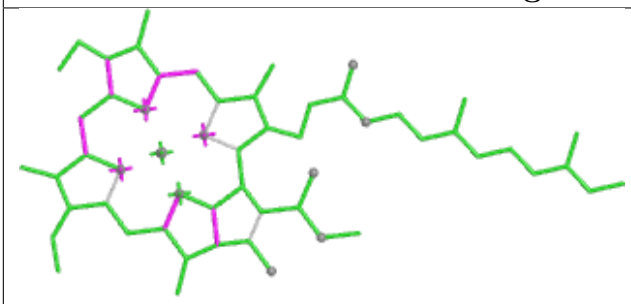
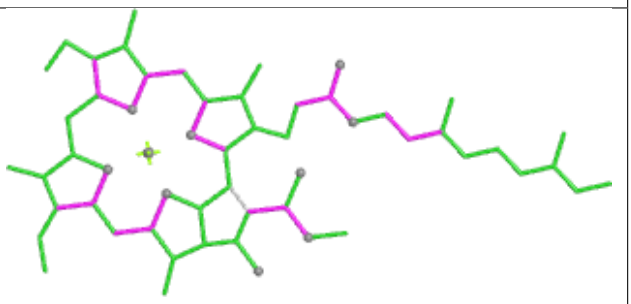
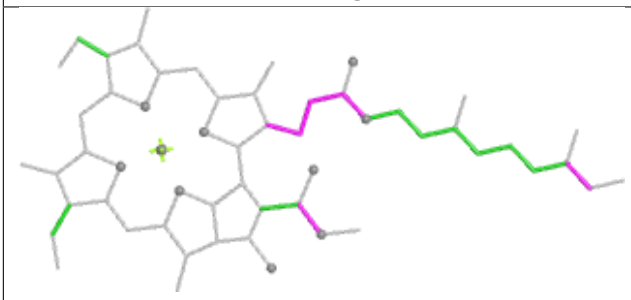
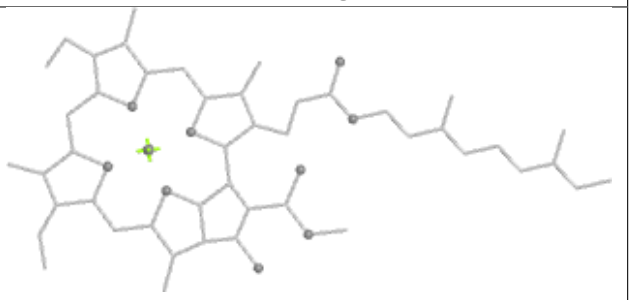
Bond angles

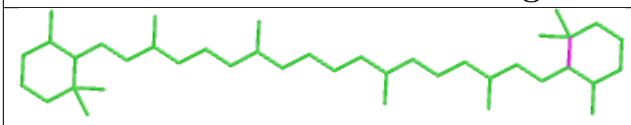
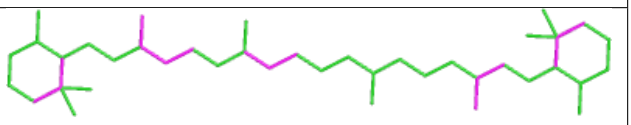
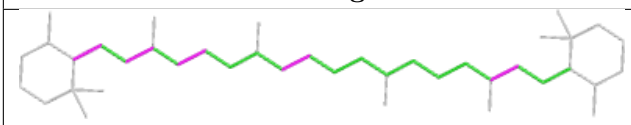
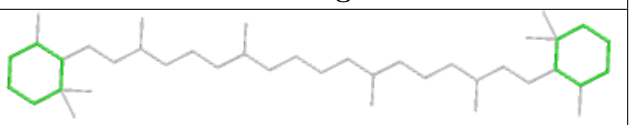


Torsions

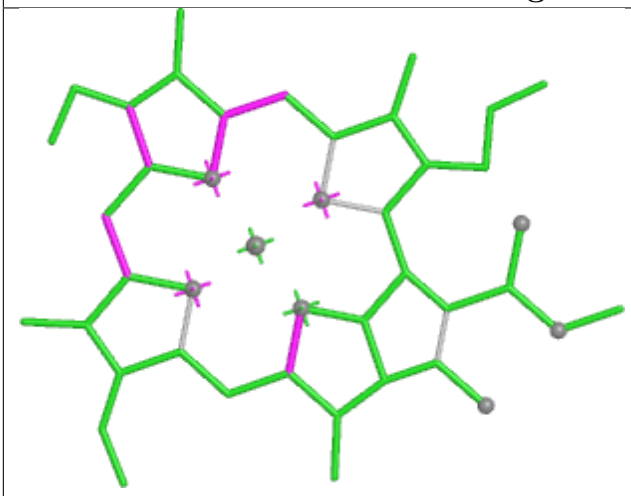


Rings

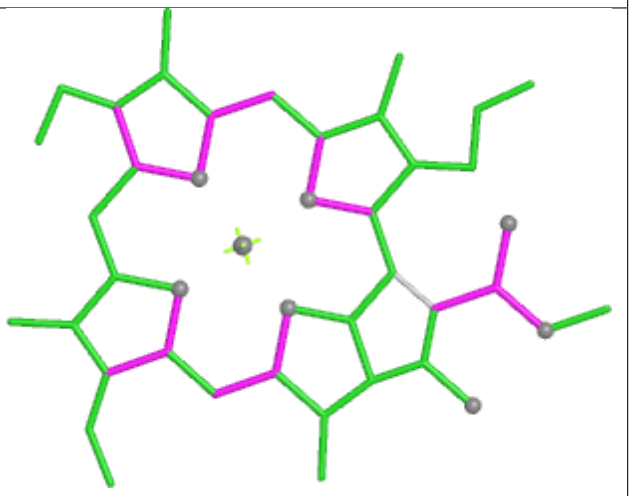
Ligand CLA A 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

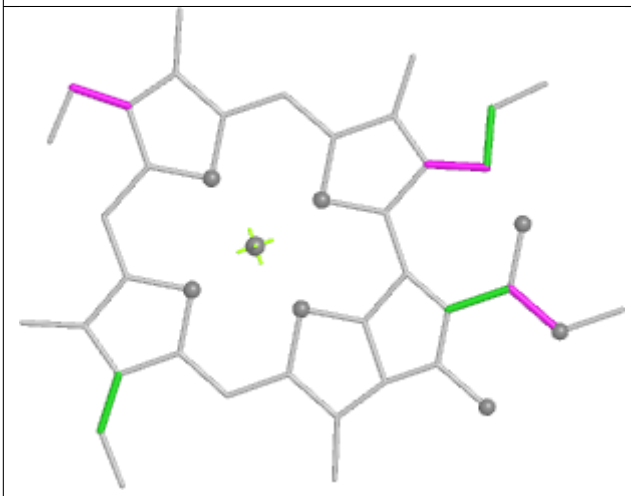
Ligand CLA h 213



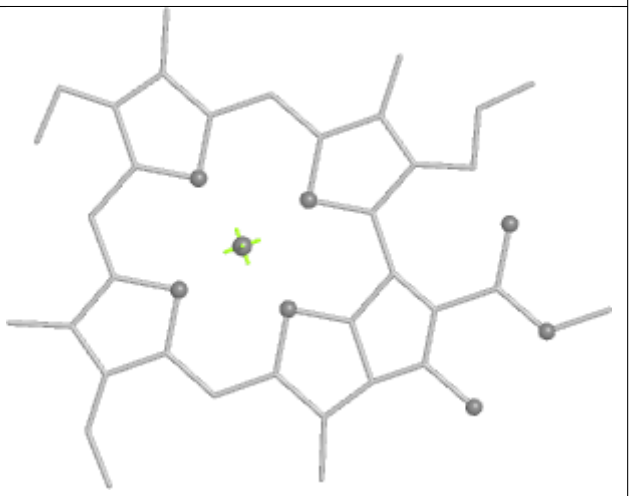
Bond lengths



Bond angles

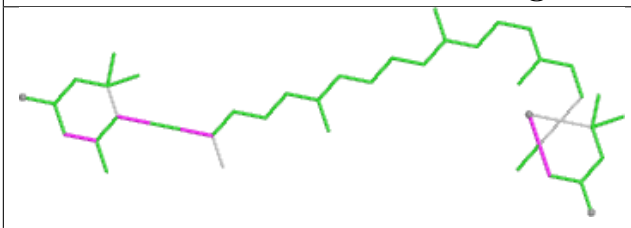


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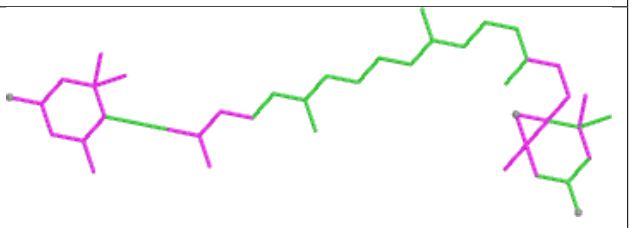


Rings

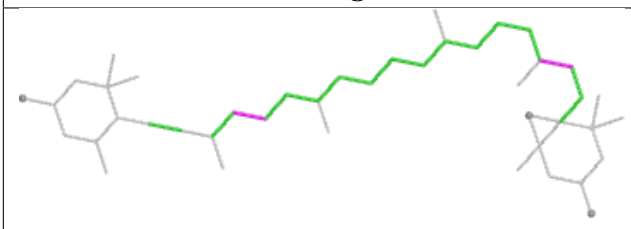
Ligand DD6 d 318



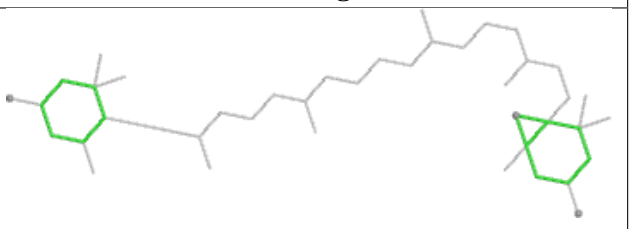
Bond lengths



Bond angles

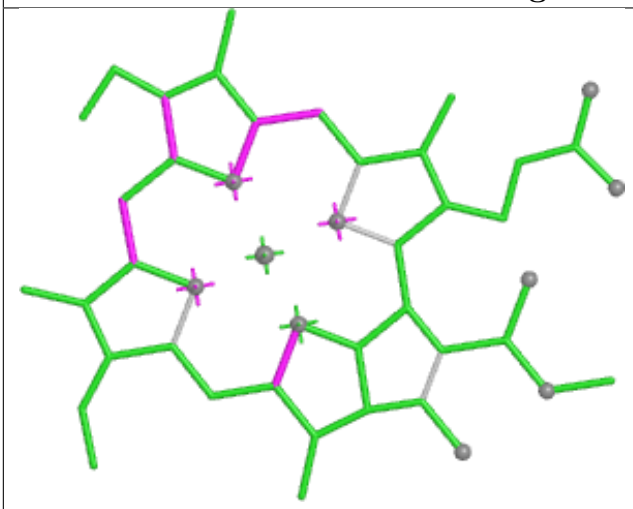


Torsions

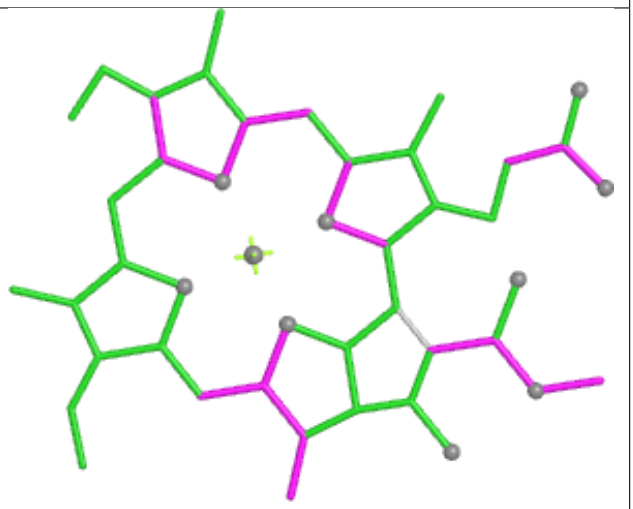


Rings

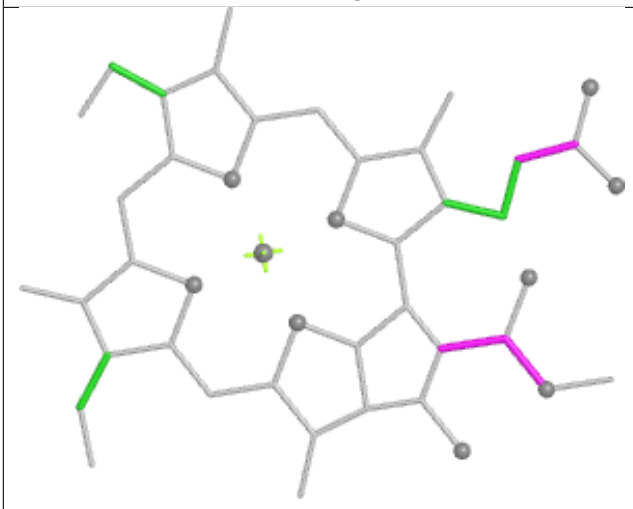
Ligand CLA e 206



Bond lengths



Bond angles

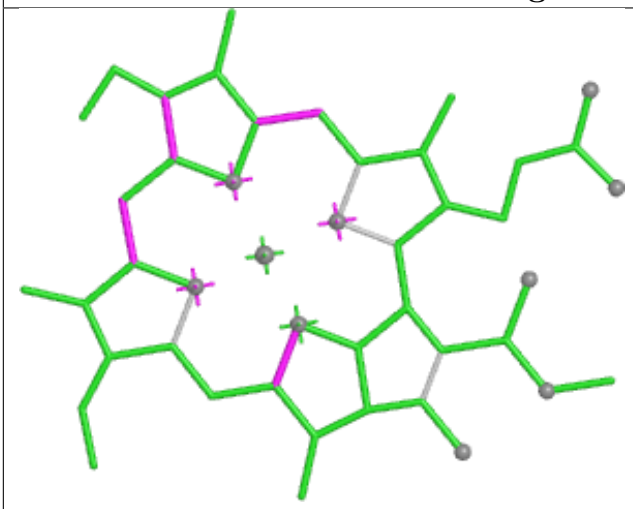


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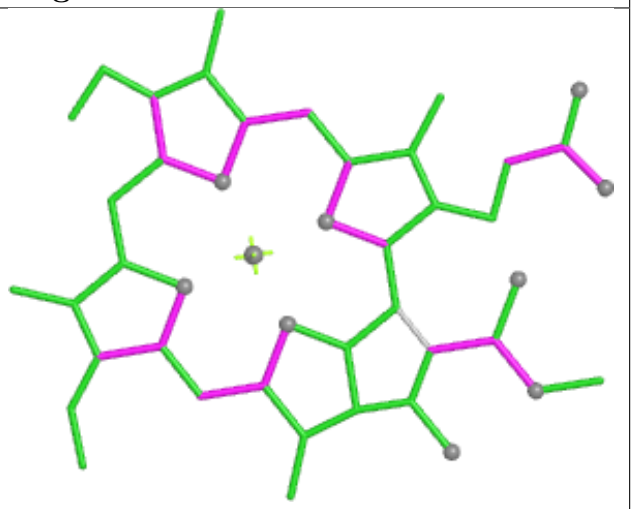


Rings

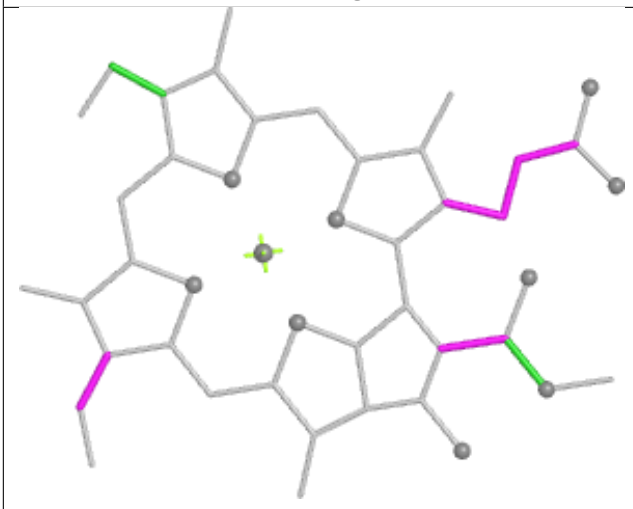
Ligand CLA g 207



Bond lengths



Bond angles

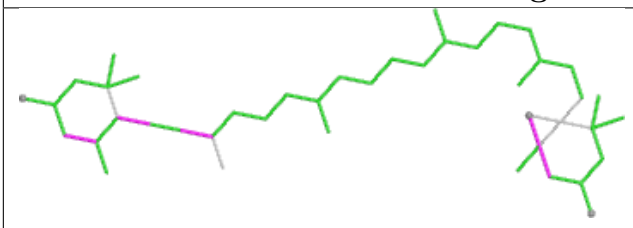


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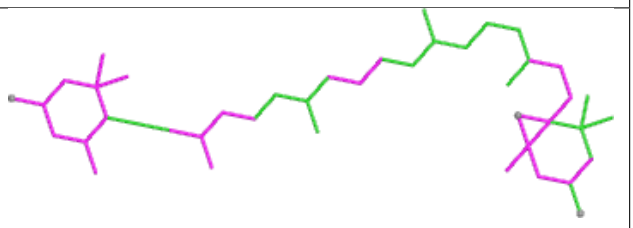


Rings

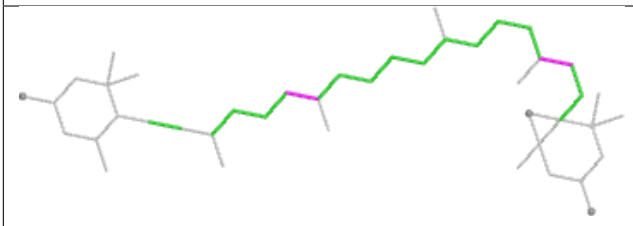
Ligand DD6 c 316



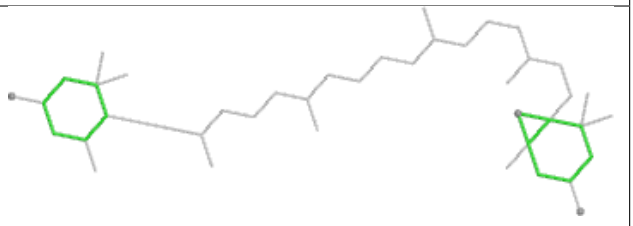
Bond lengths



Bond angles

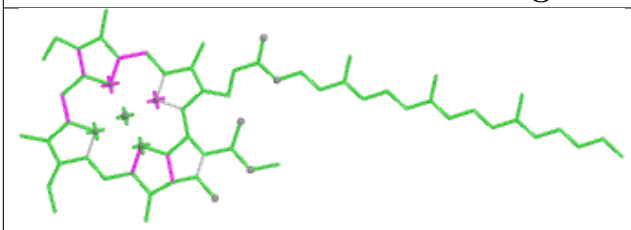


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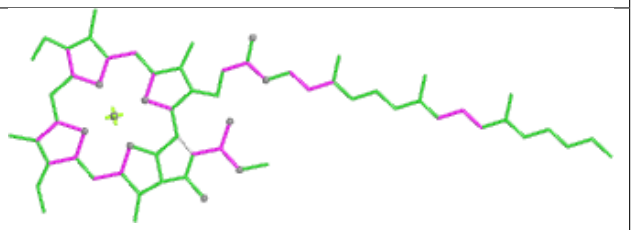


Rings

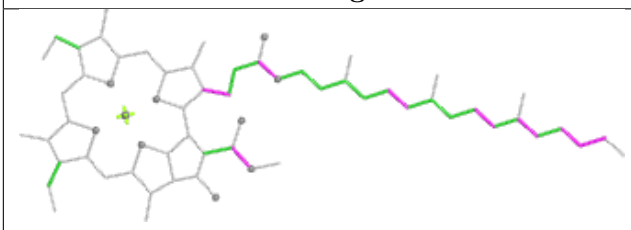
Ligand CLA i 203



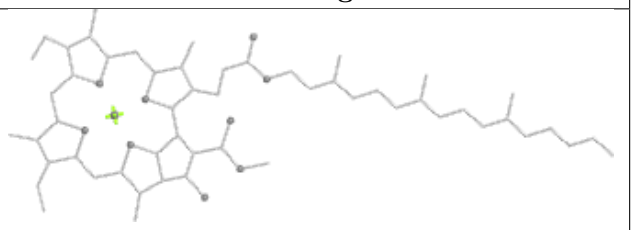
Bond lengths



Bond angles

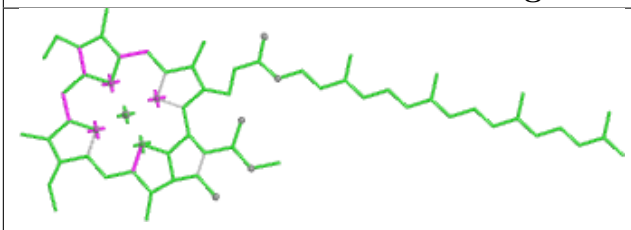


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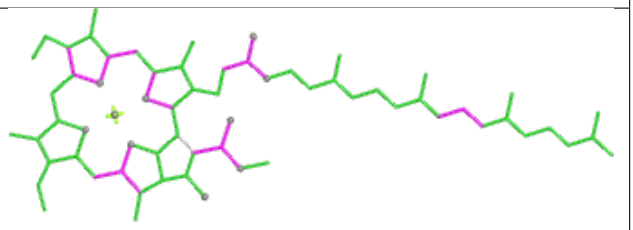


Rings

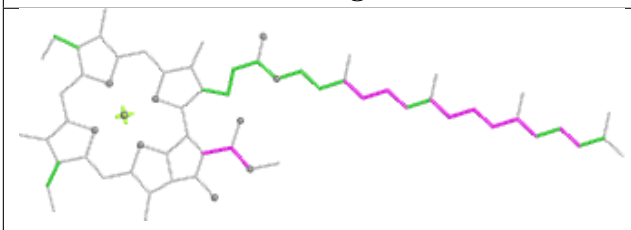
Ligand CLA B 807



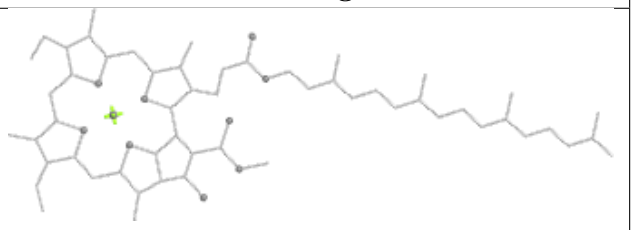
Bond lengths



Bond angles

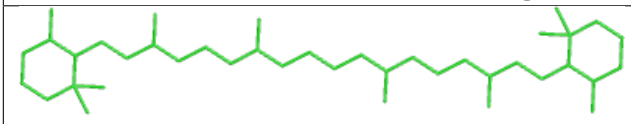


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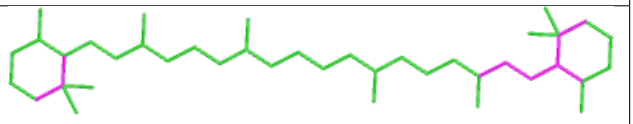


Rings

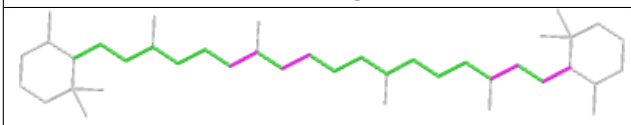
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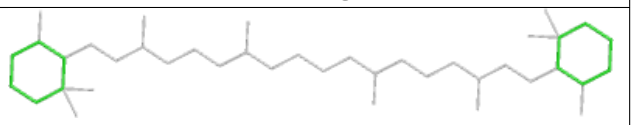
Bond lengths



Bond angles

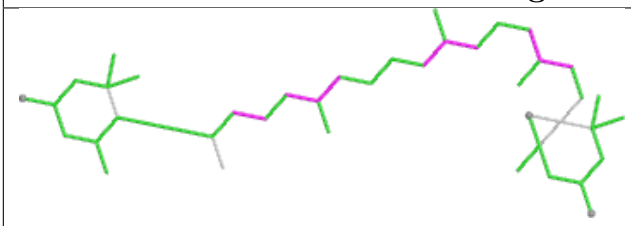


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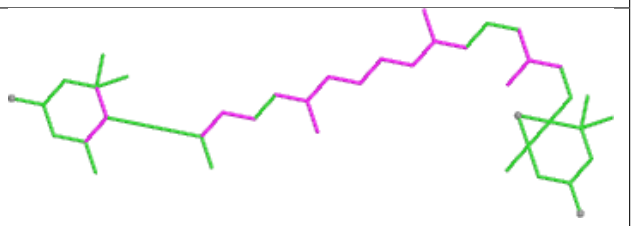


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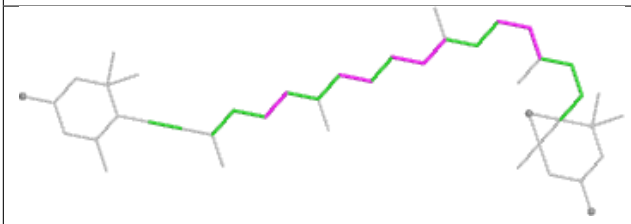
Ligand DD6 n 214



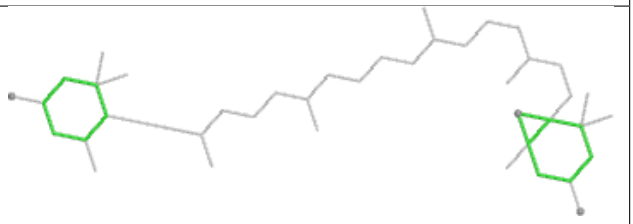
Bond lengths



Bond angles

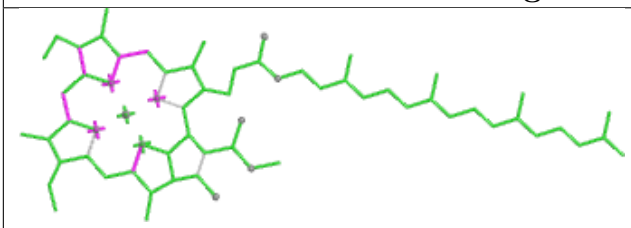


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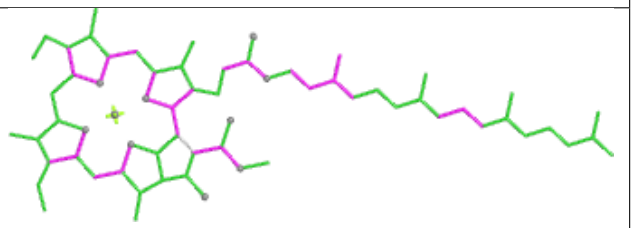


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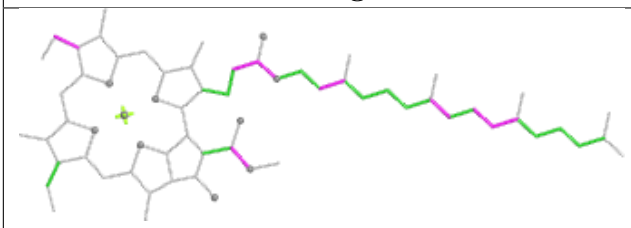
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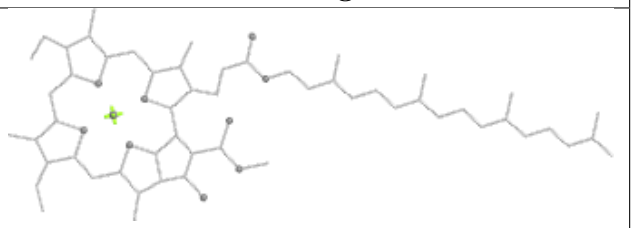
Bond lengths



Bond angles

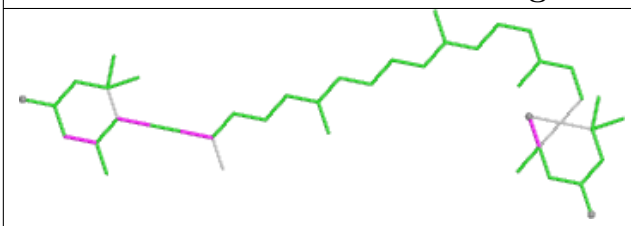


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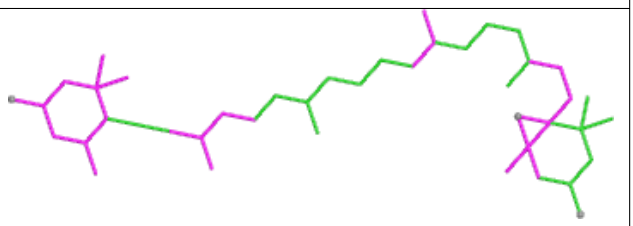


Rings

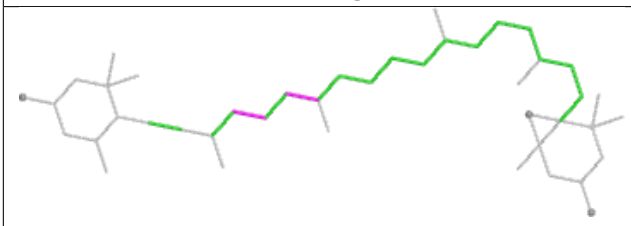
Ligand DD6 o 612



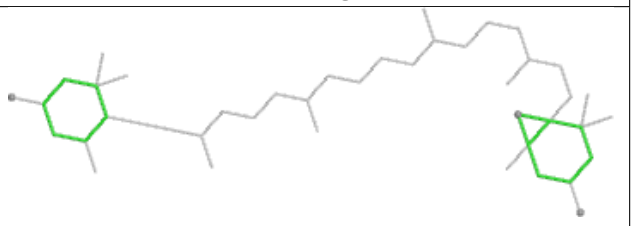
Bond lengths



Bond angles

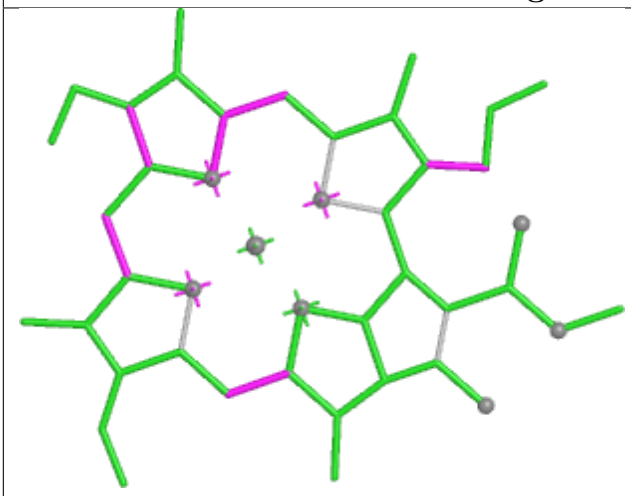


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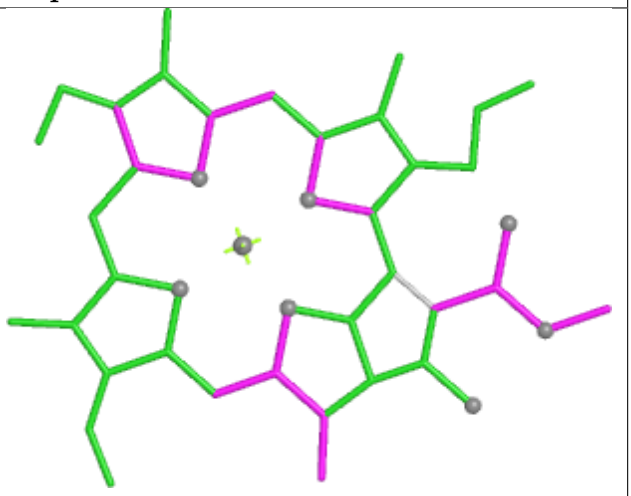


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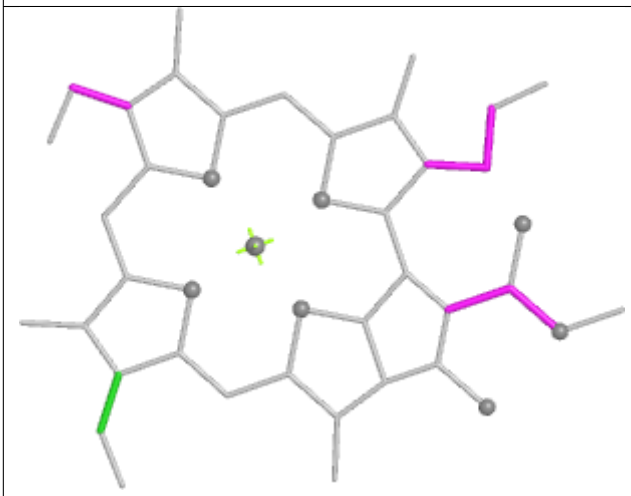
Ligand CLA p 602



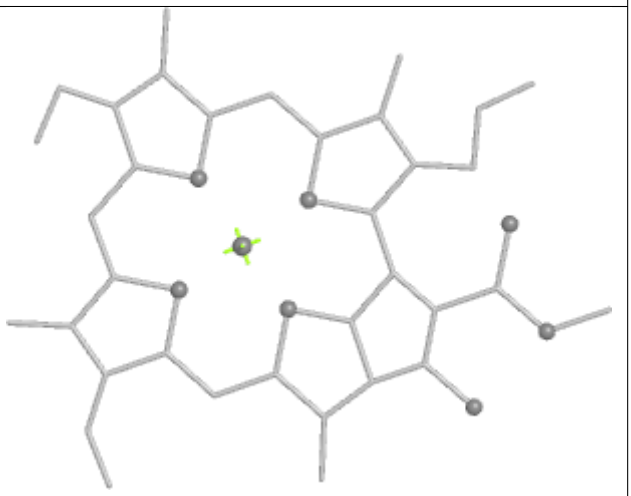
Bond lengths



Bond angles

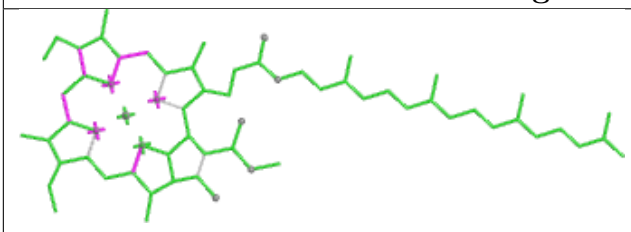


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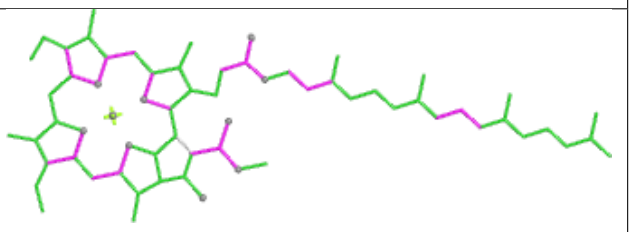


Rings

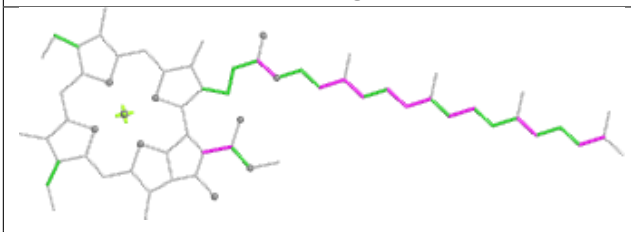
Ligand CLA i 206



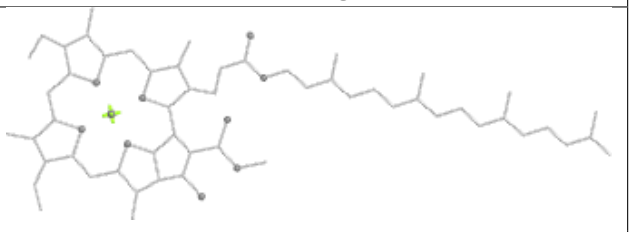
Bond lengths



Bond angles

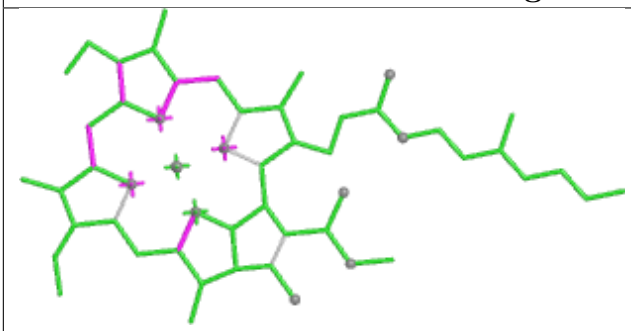


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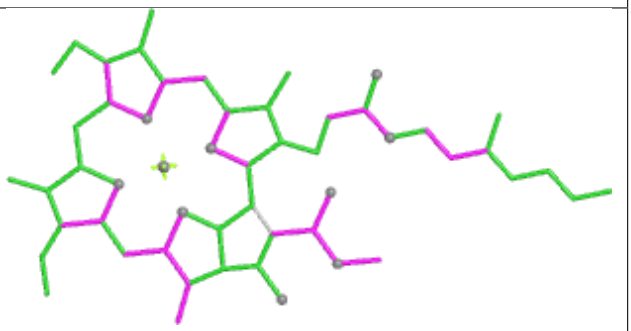


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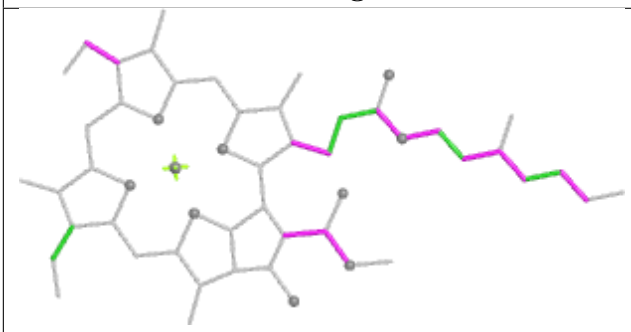
Ligand CLA B 842



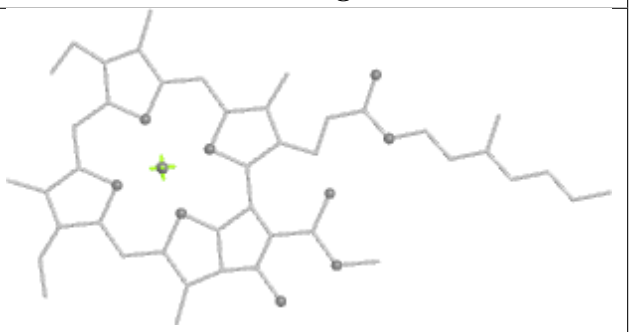
Bond lengths



Bond angles

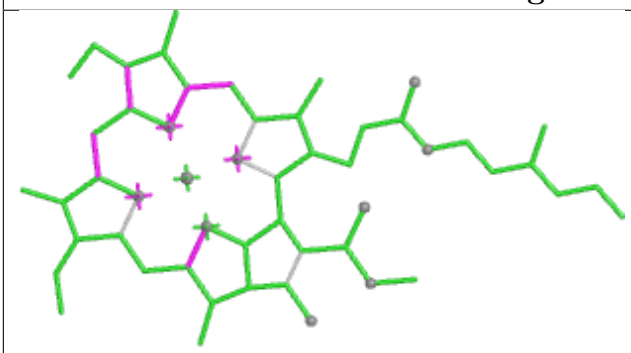


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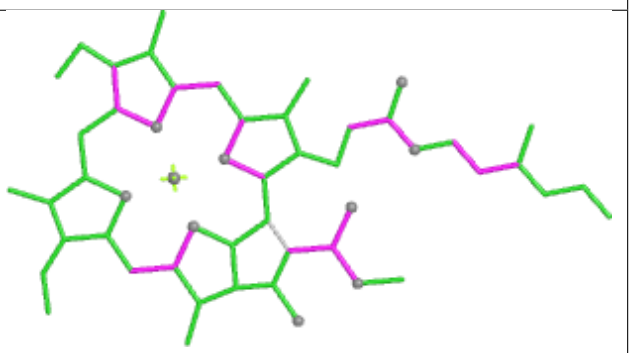


Rings

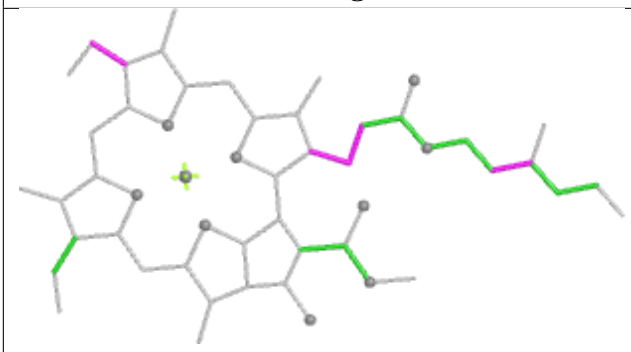
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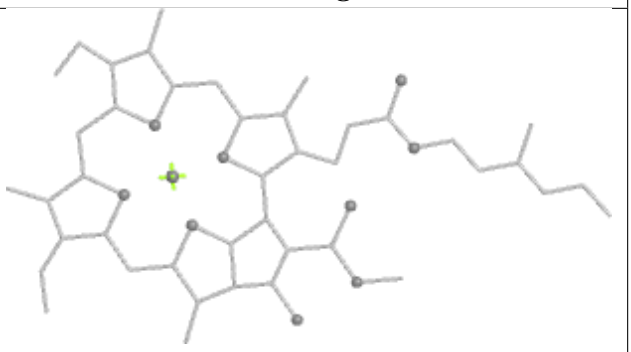
Bond lengths



Bond angles

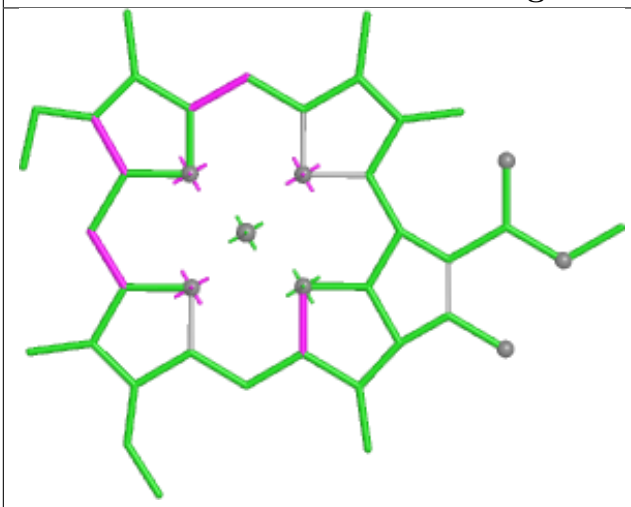


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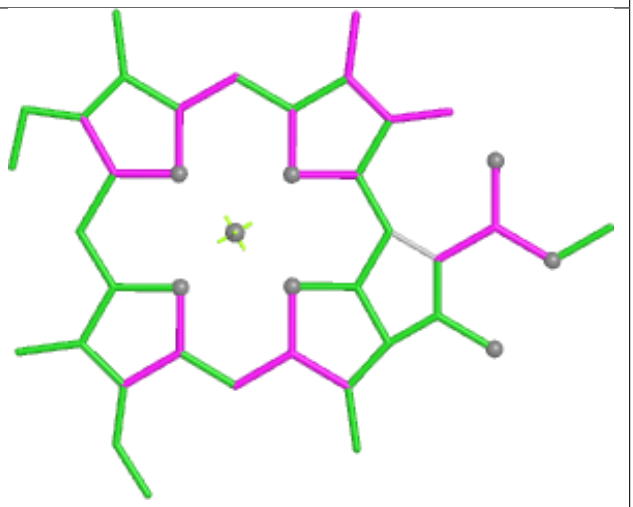


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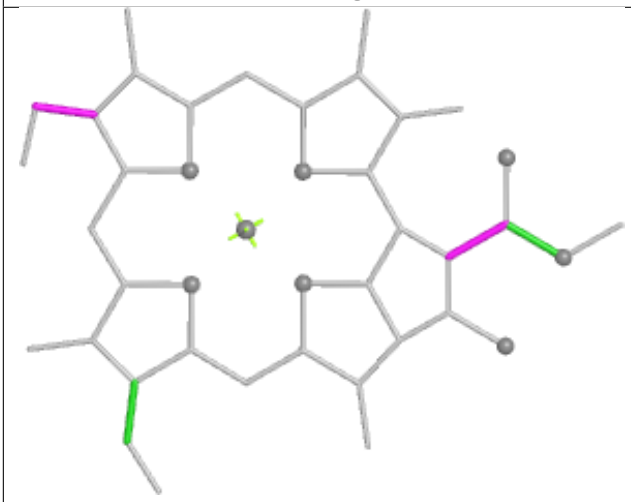
Ligand CLA n 209



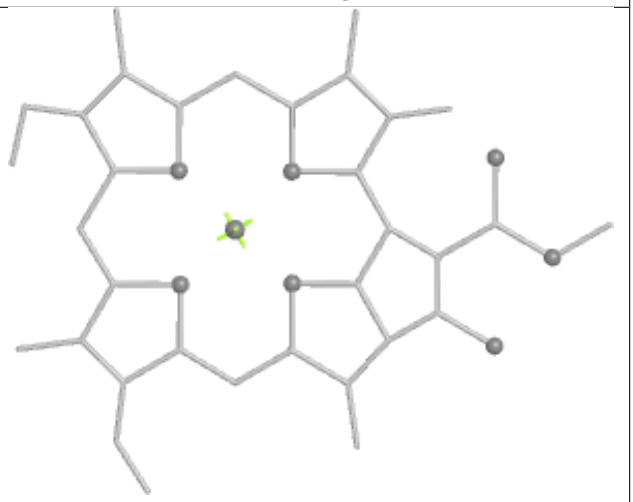
Bond lengths



Bond angles

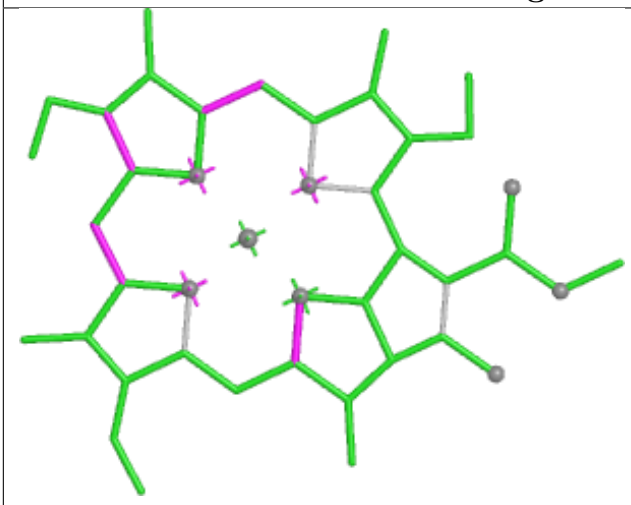


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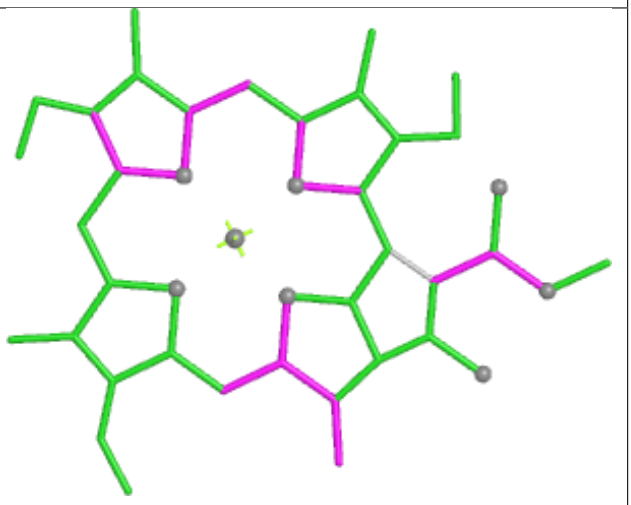


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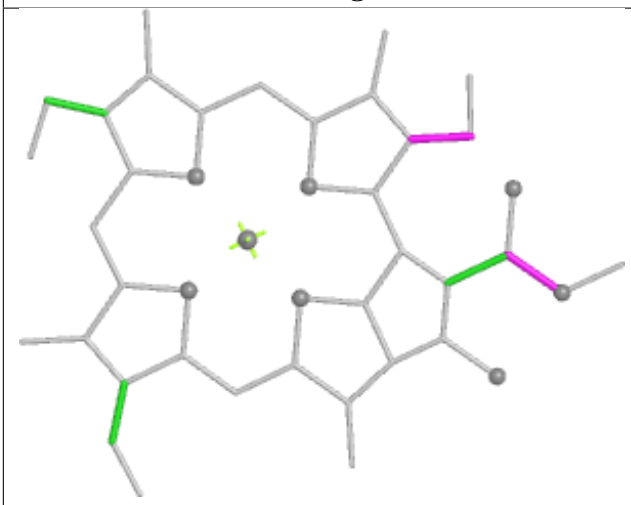
Ligand CLA b 203



Bond lengths



Bond angles

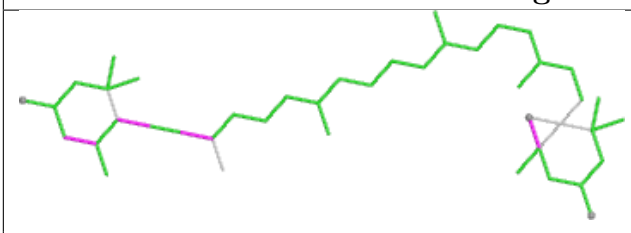


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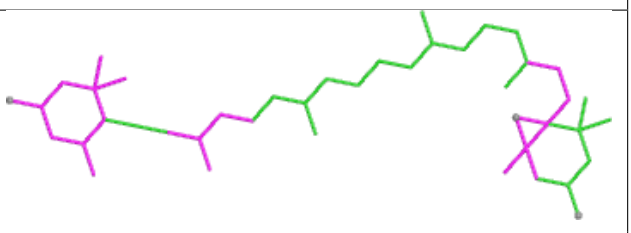


Rings

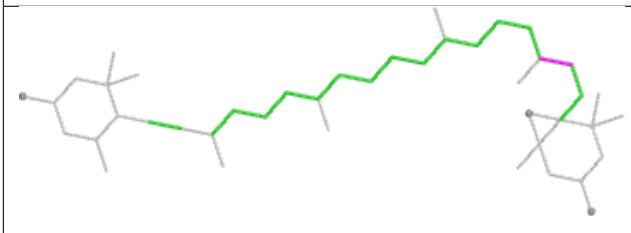
Ligand DD6 l 613



Bond lengths



Bond angles

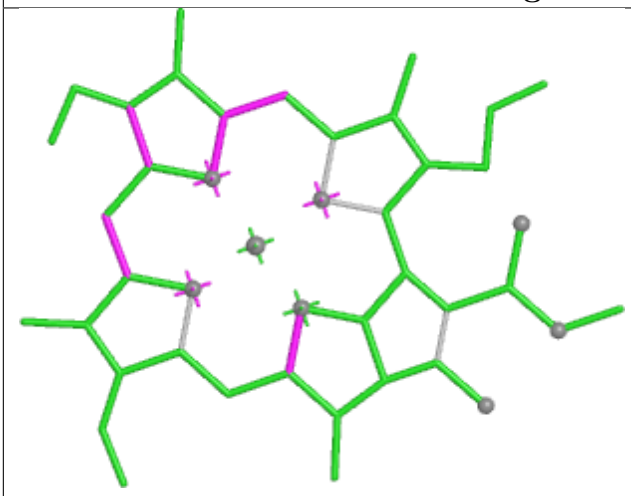


Torsions

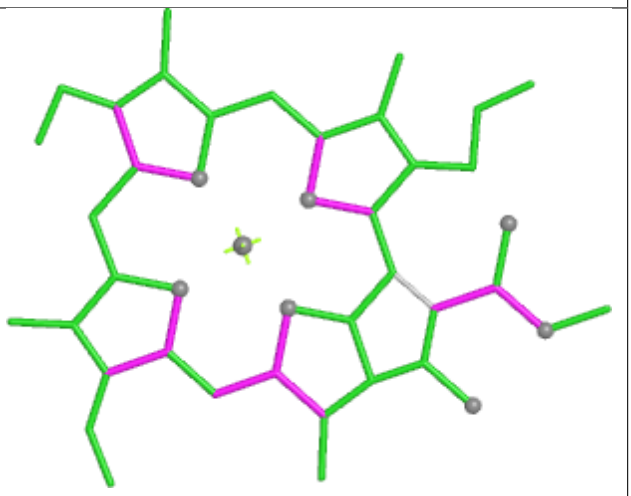


Rings

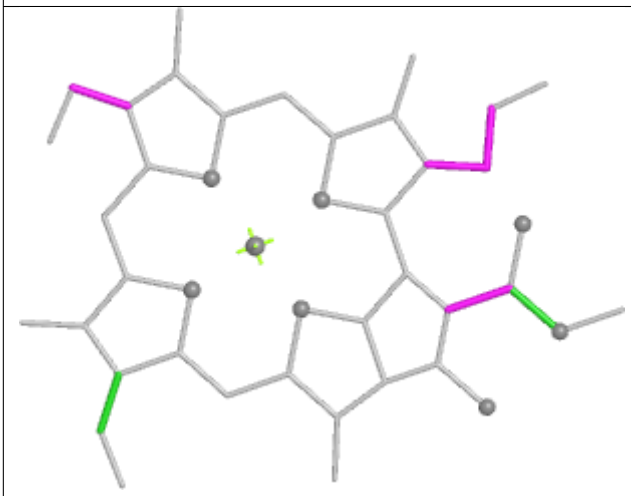
Ligand CLA A 816



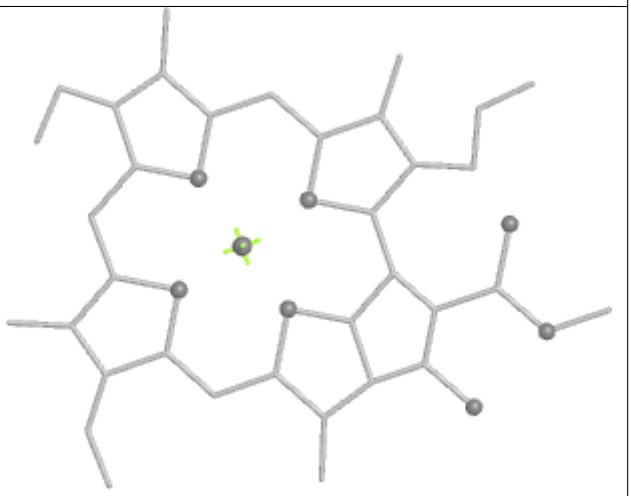
Bond lengths



Bond angles

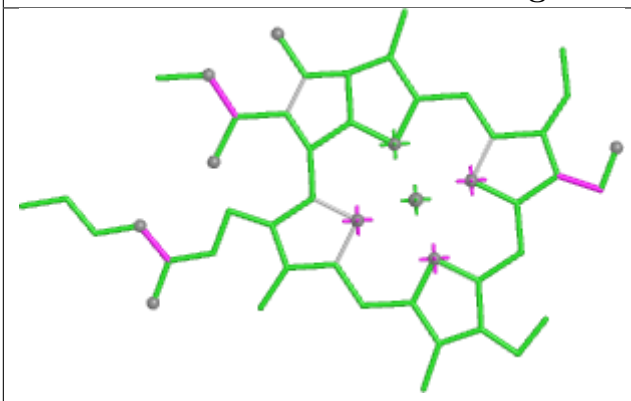


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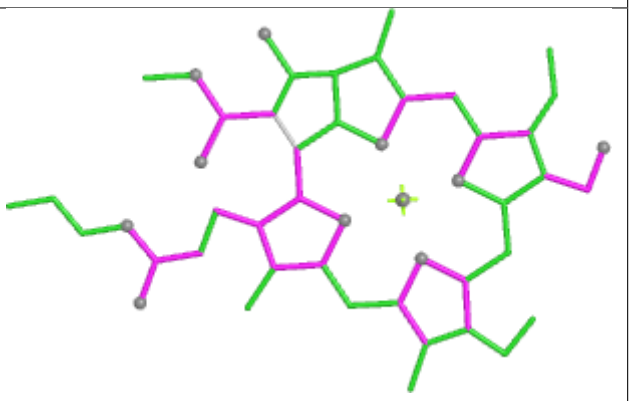


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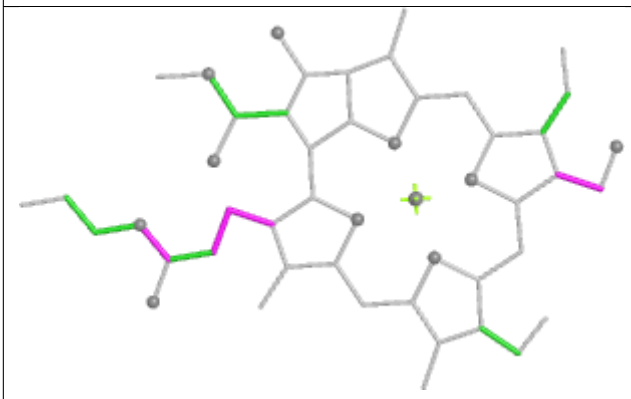
Ligand CHL c 307



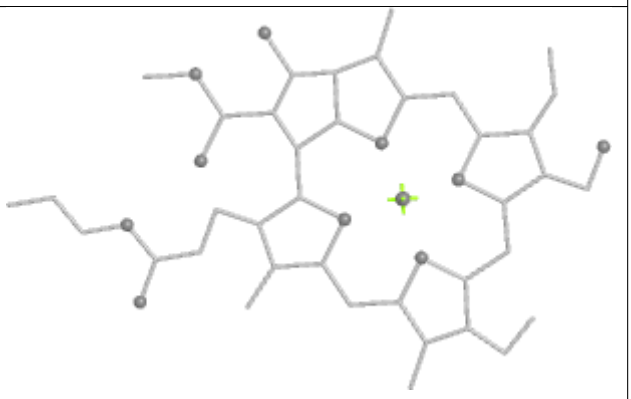
Bond lengths



Bond angles

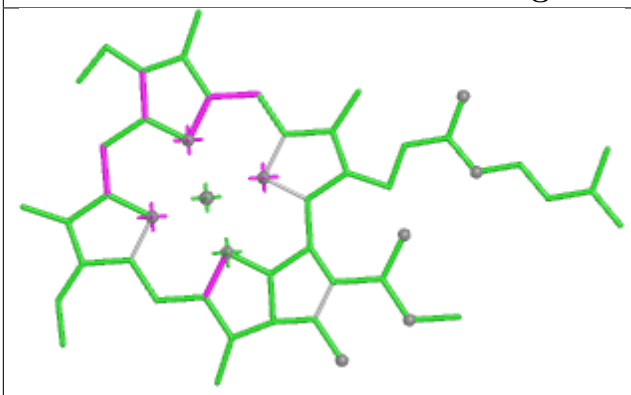


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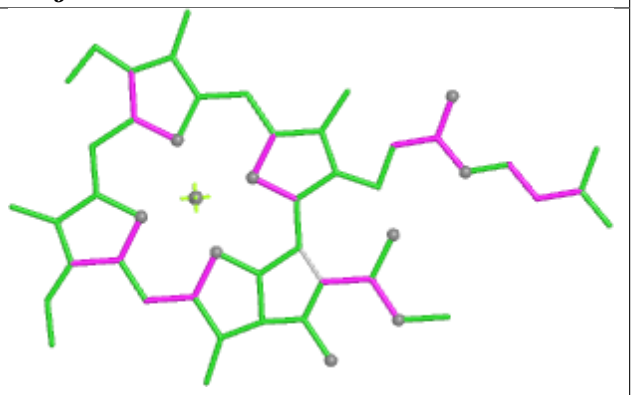


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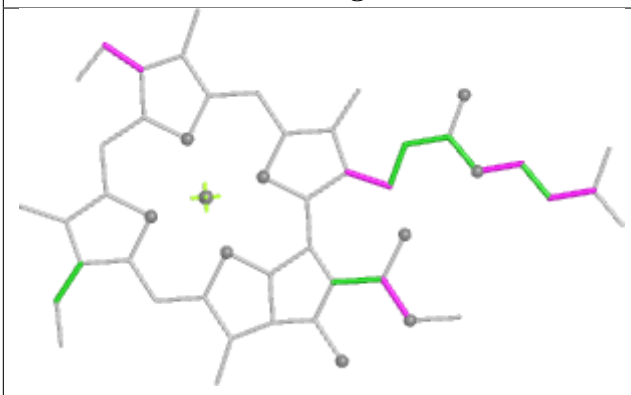
Ligand CLA j 210



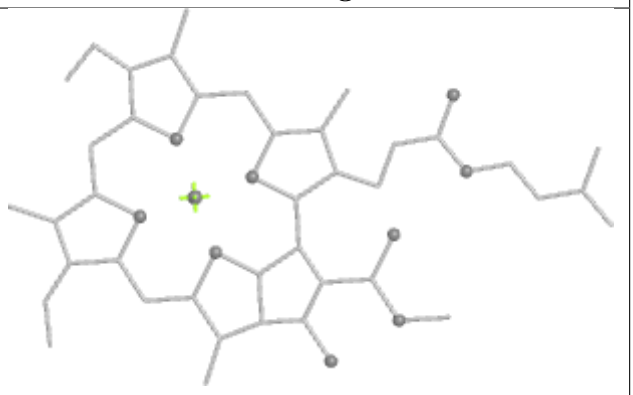
Bond lengths



Bond angles

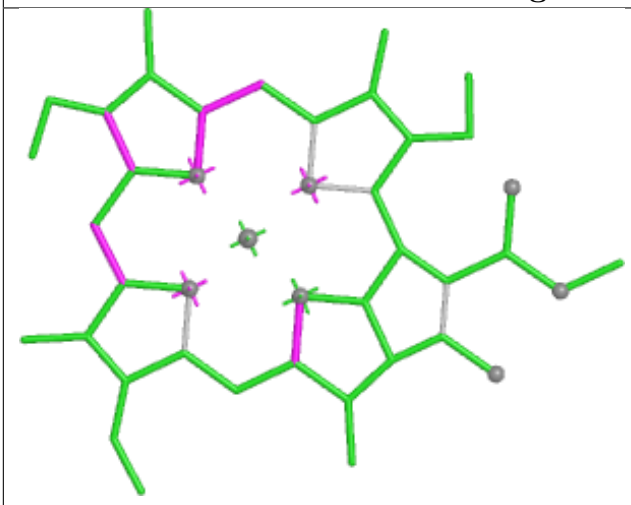


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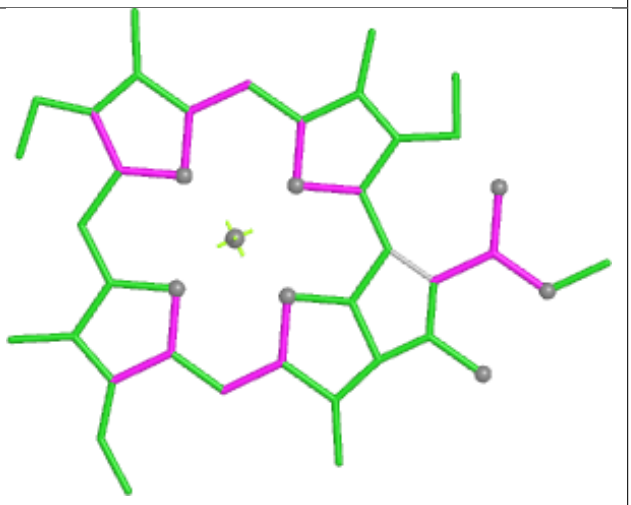


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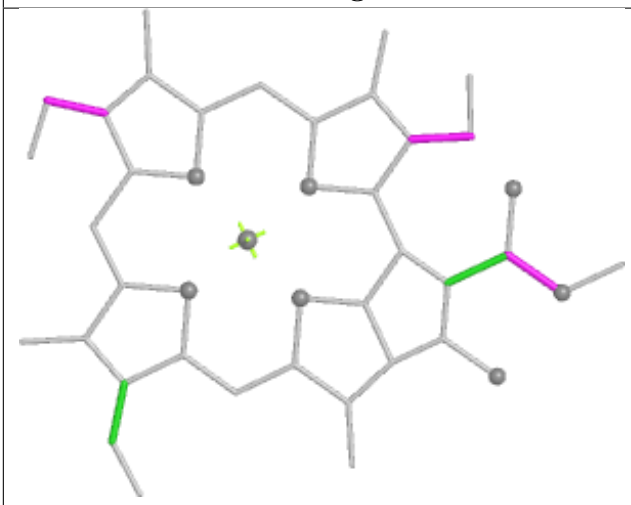
Ligand CLA c 314



Bond lengths



Bond angles

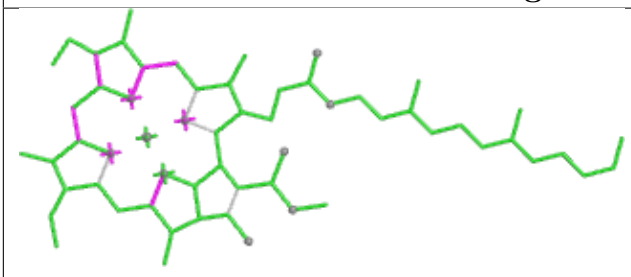


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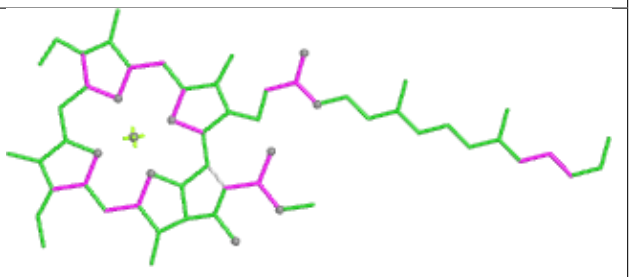


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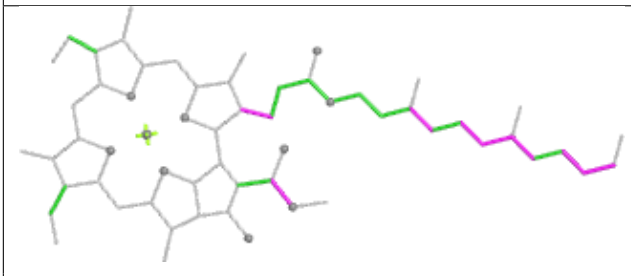
Ligand CLA B 814



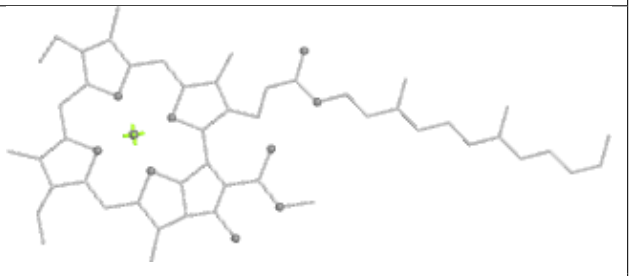
Bond lengths



Bond angles

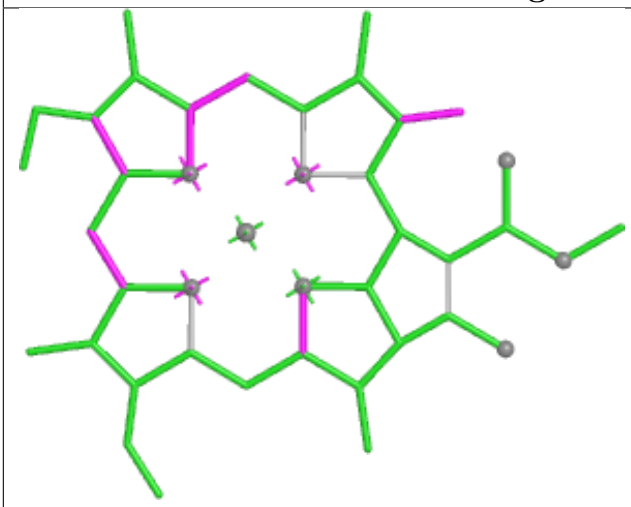


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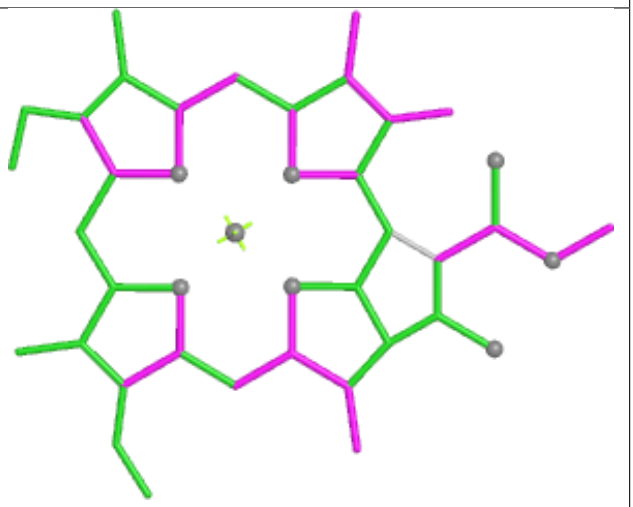


Rings

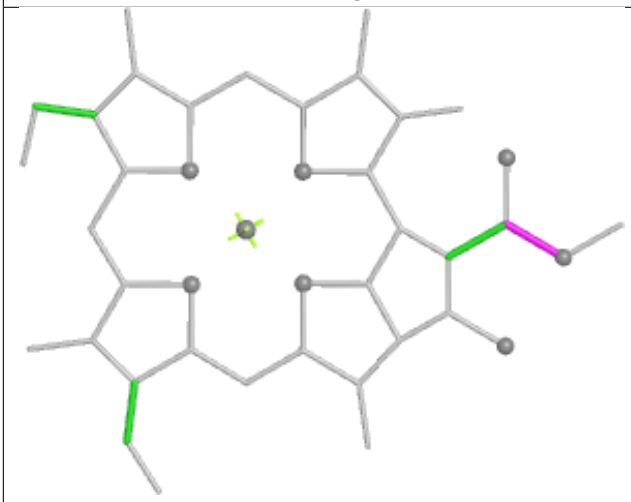
Ligand CLA o 601



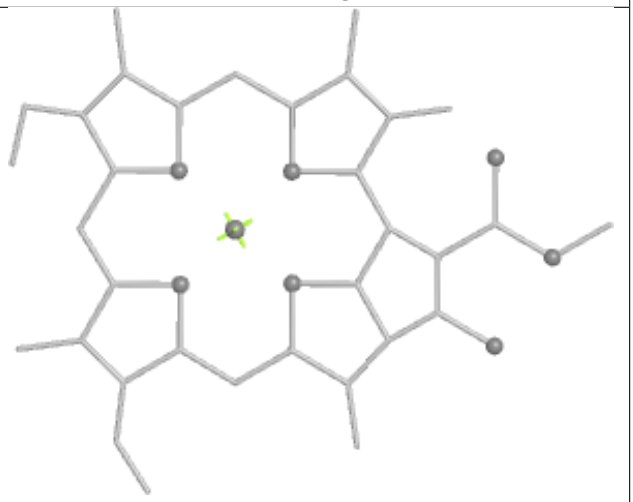
Bond lengths



Bond angles

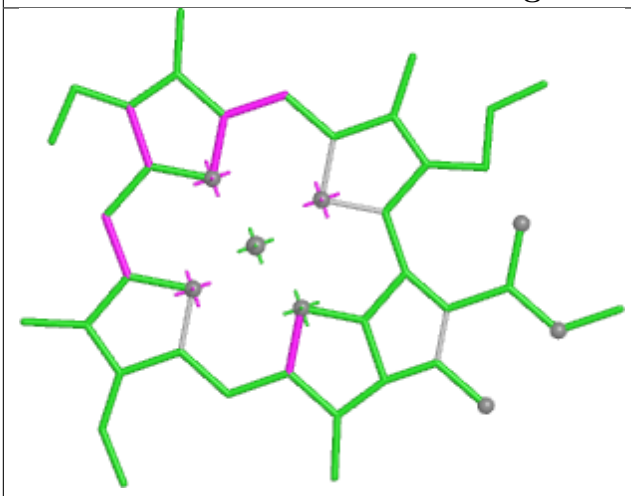


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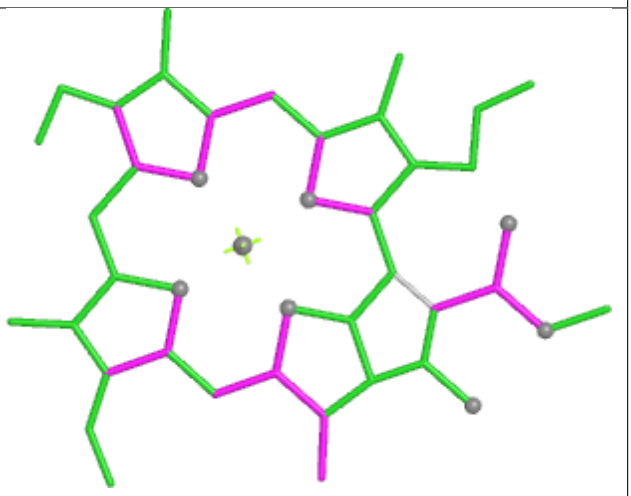


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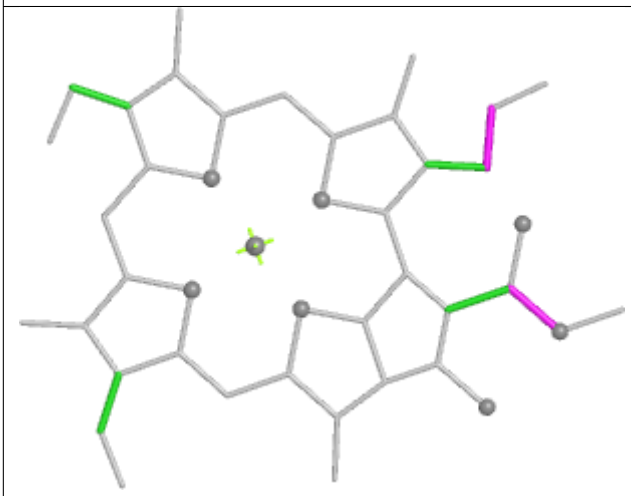
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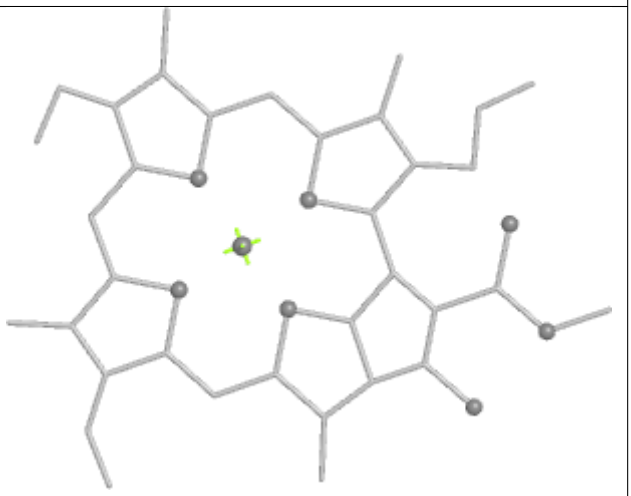
Bond lengths



Bond angles

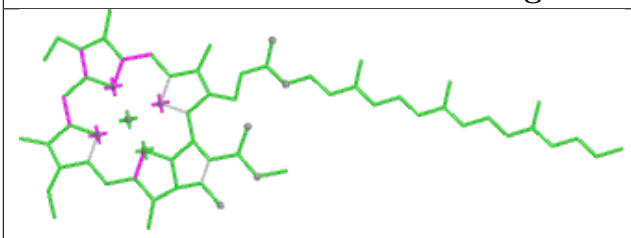


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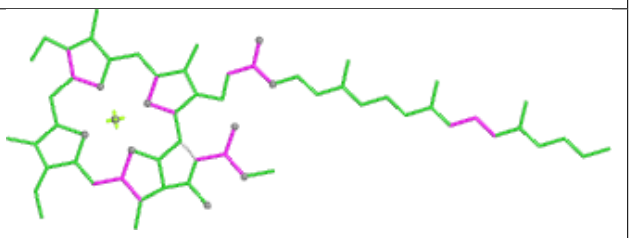


Rings

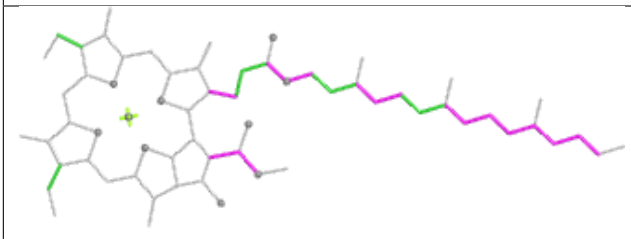
Ligand CLA B 811



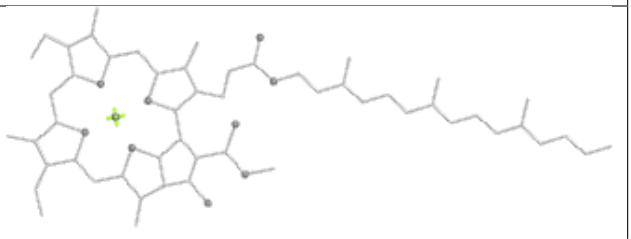
Bond lengths



Bond angles

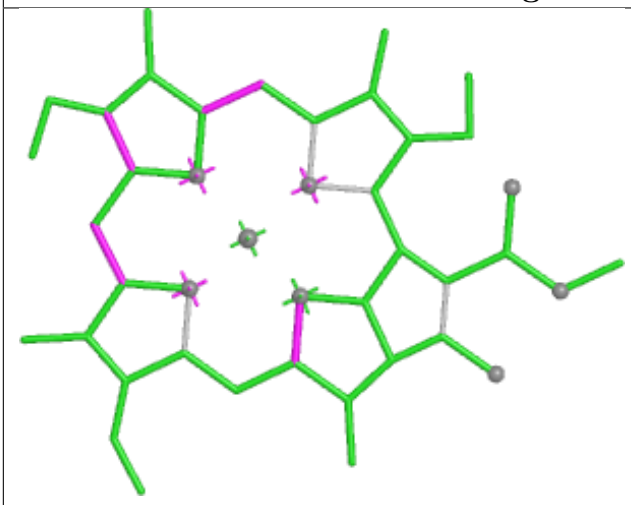


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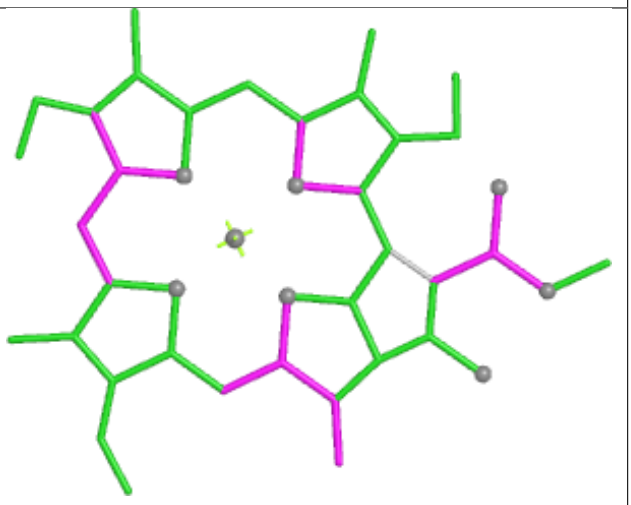


Rings

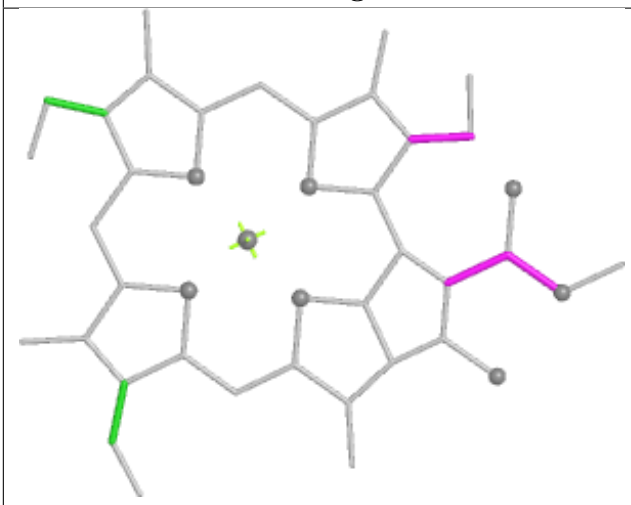
Ligand CLA m 202



Bond lengths



Bond angles

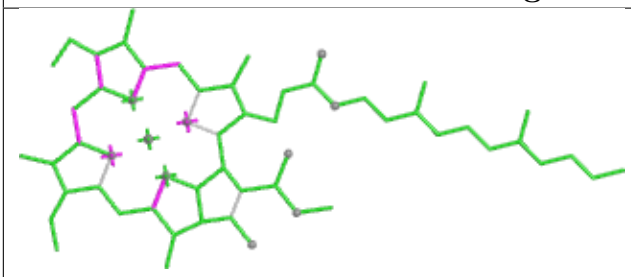


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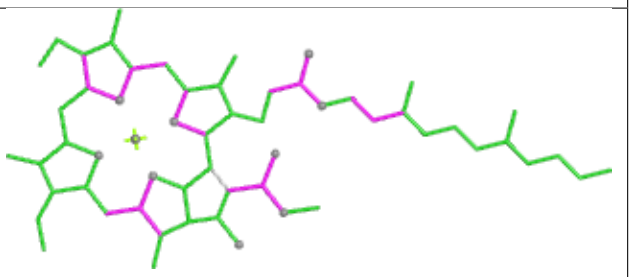


Rings

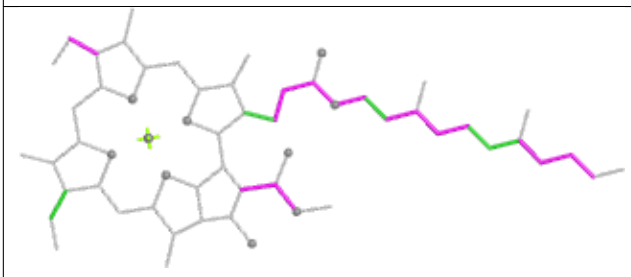
Ligand CLA A 815



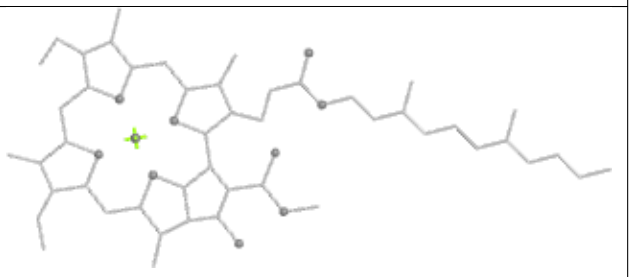
Bond lengths



Bond angles

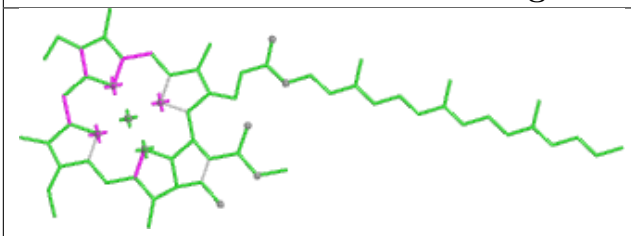


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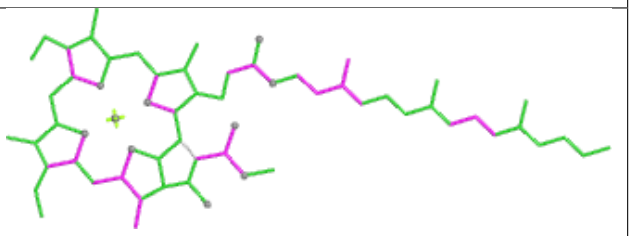


Rings

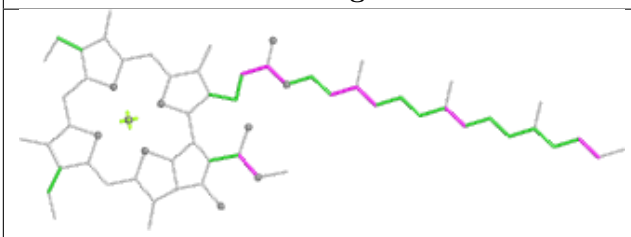
Ligand CLA a 213



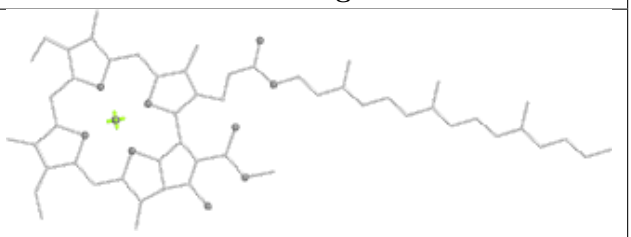
Bond lengths



Bond angles

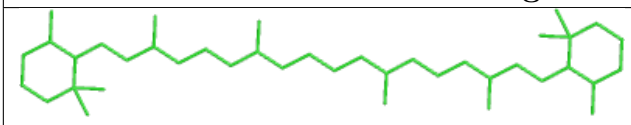


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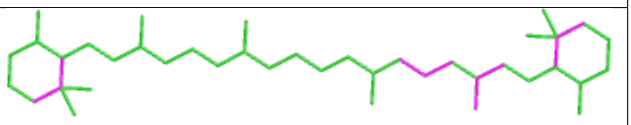


Rings

Ligand BCR B 829



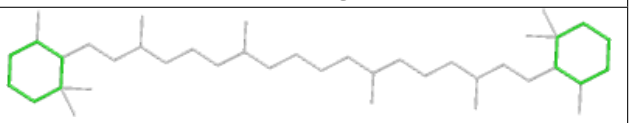
Bond lengths



Bond angles

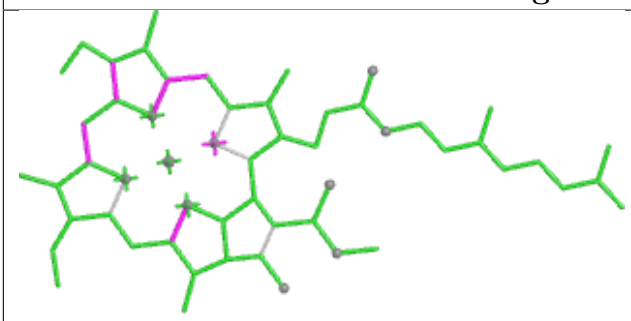


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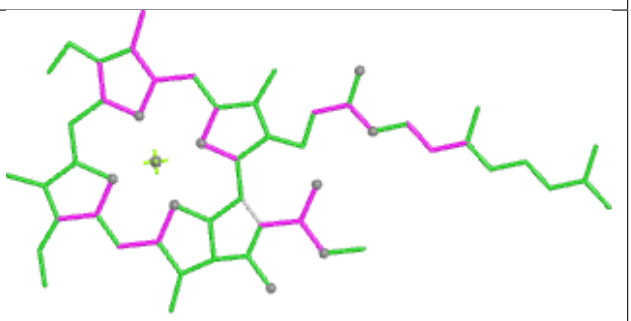


Rings

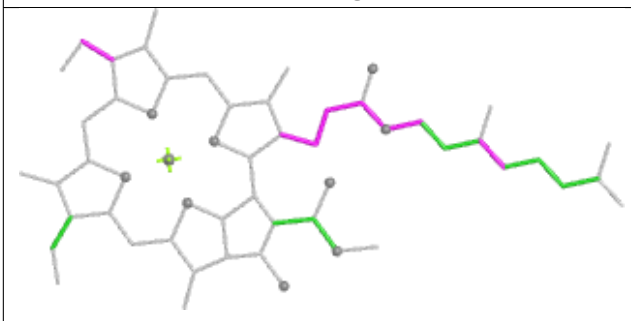
Ligand CLA i 208



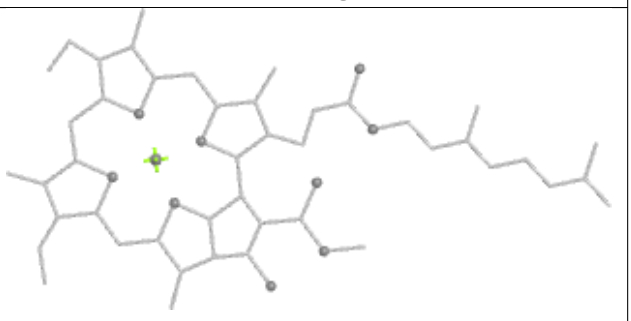
Bond lengths



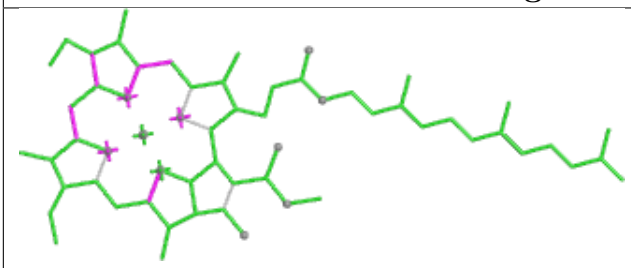
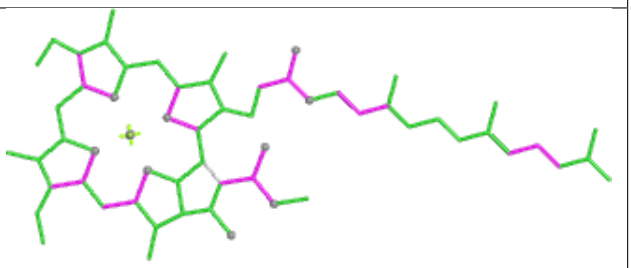
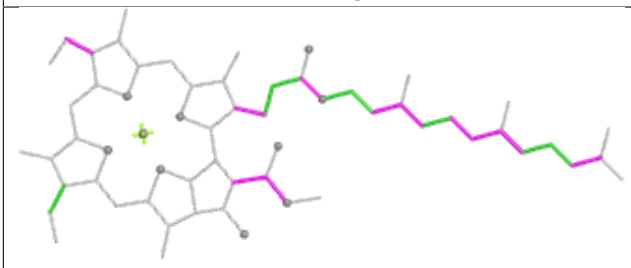
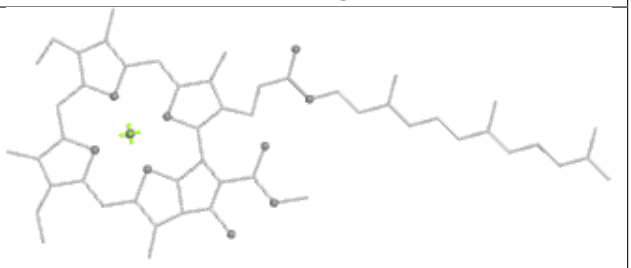
Bond angles

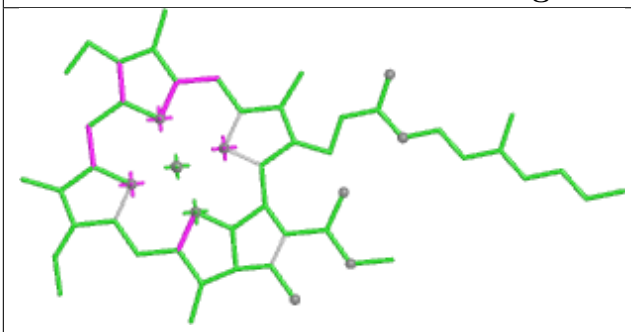
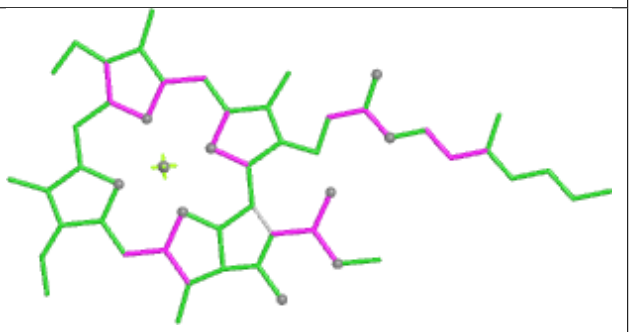
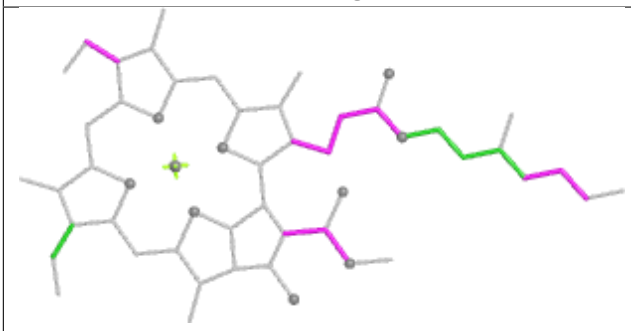
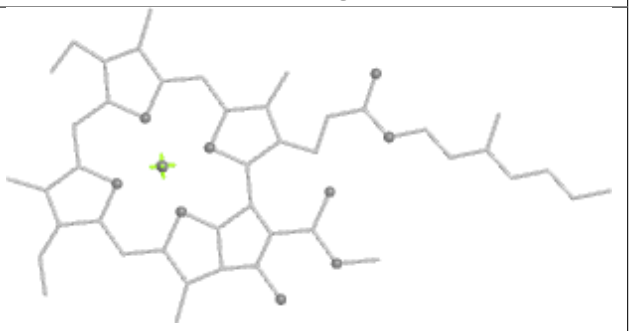


Torsions

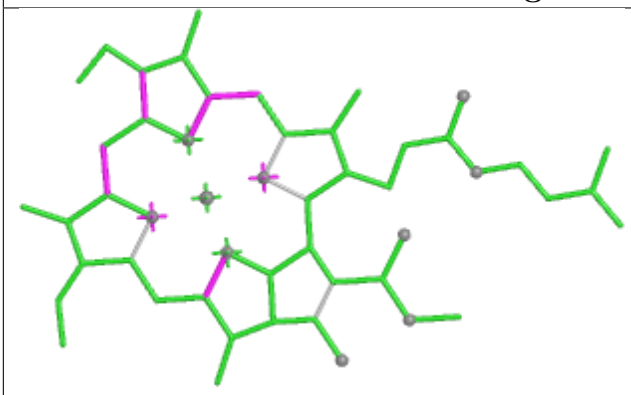


Rings

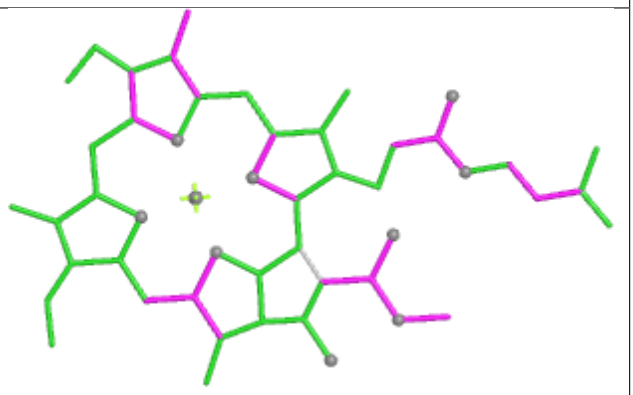
Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA i 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

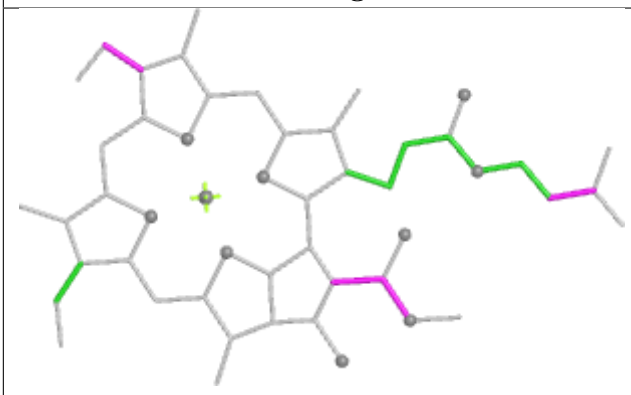
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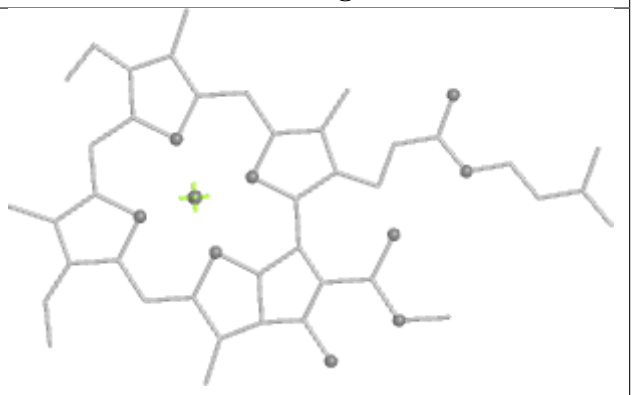
Bond lengths



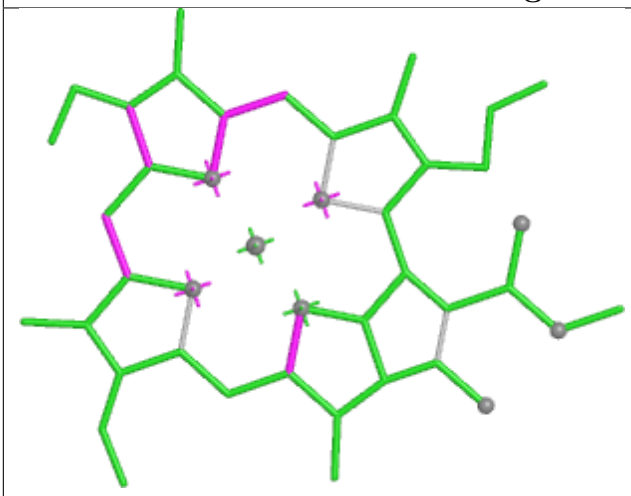
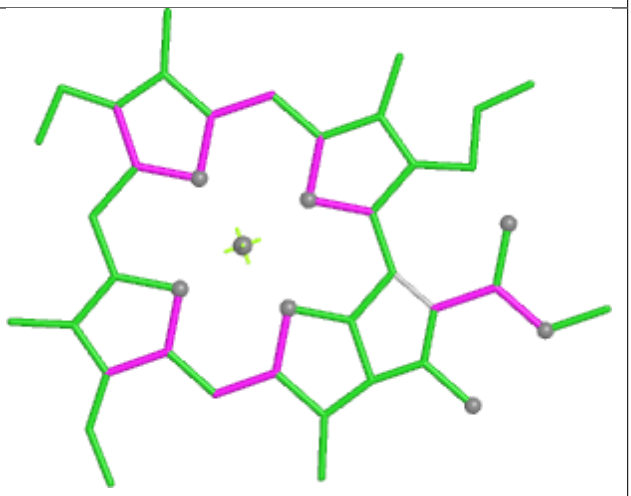
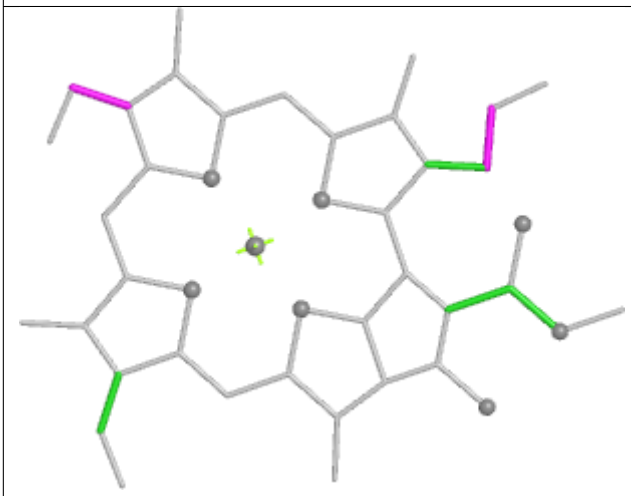
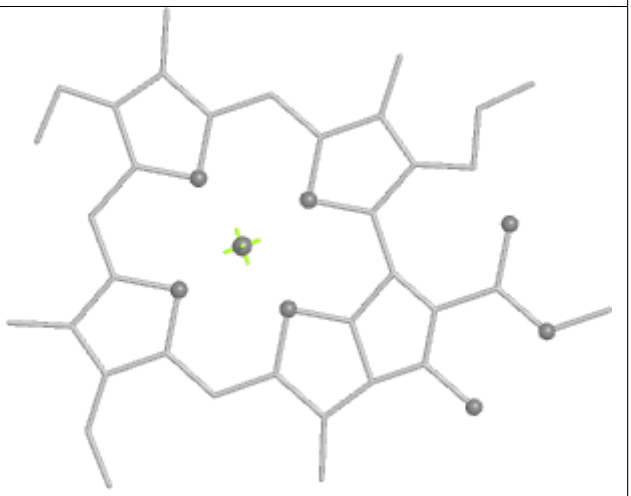
Bond angles



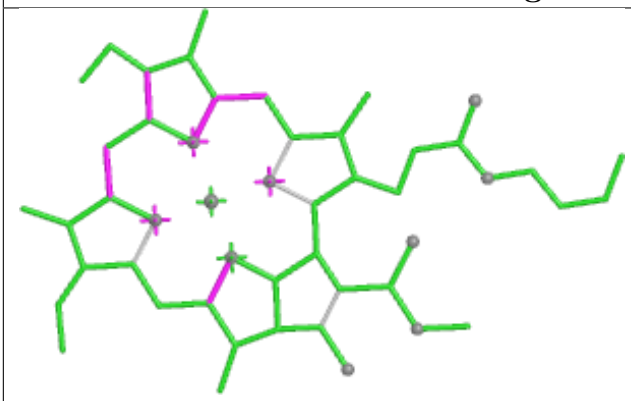
Torsions



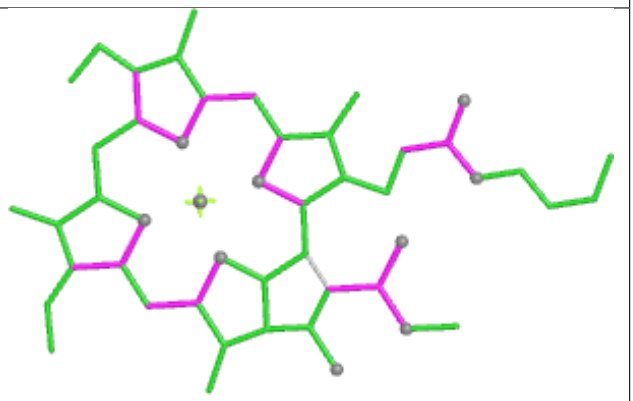
Rings

Ligand CLA B 808	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

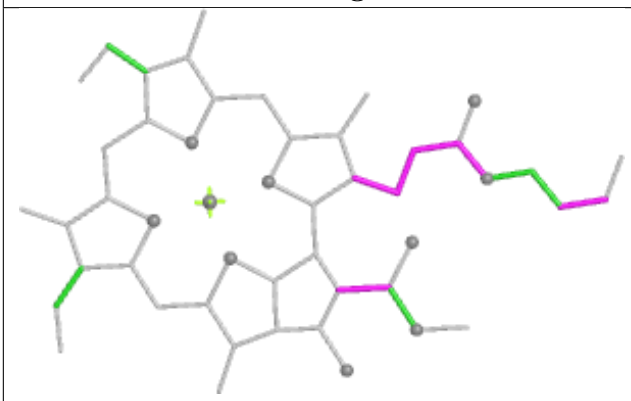
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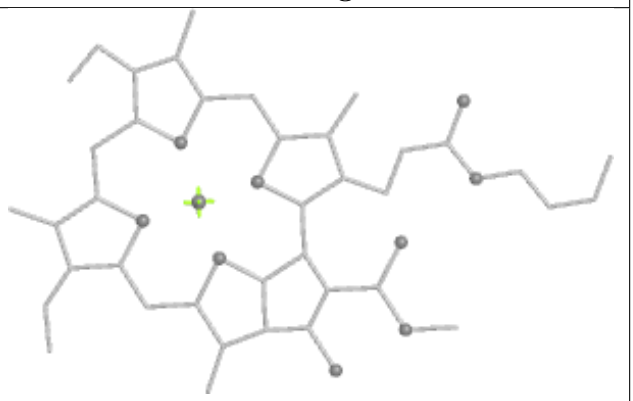
Bond lengths



Bond angles

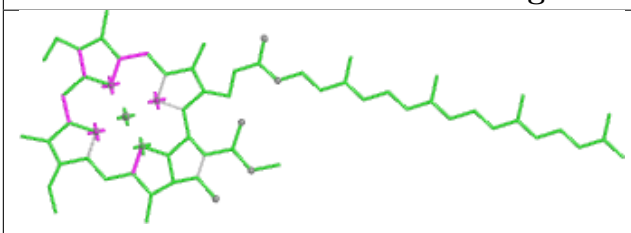


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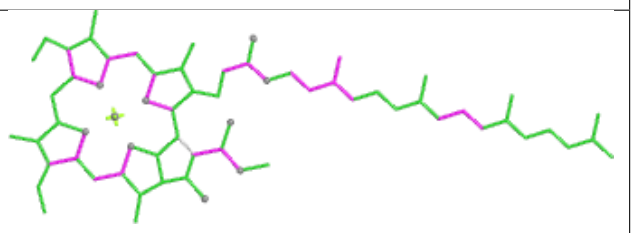


Rings

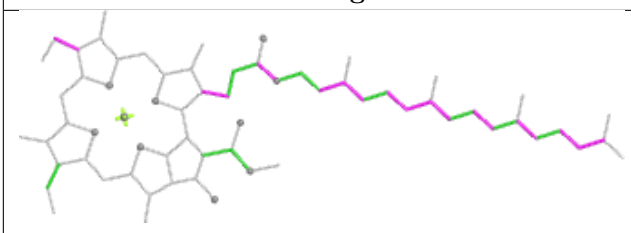
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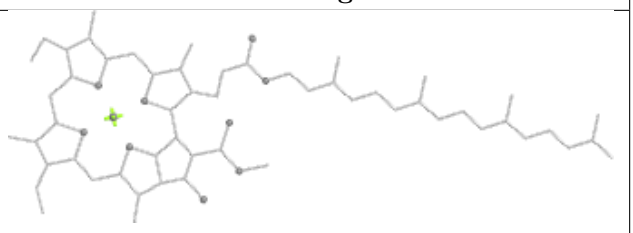
Bond lengths



Bond angles

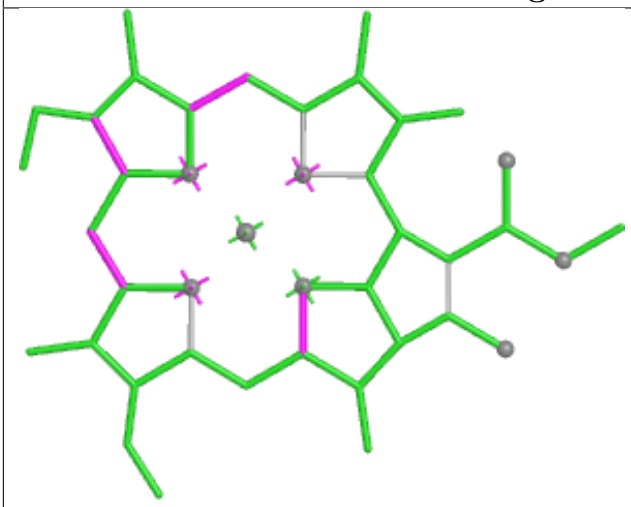


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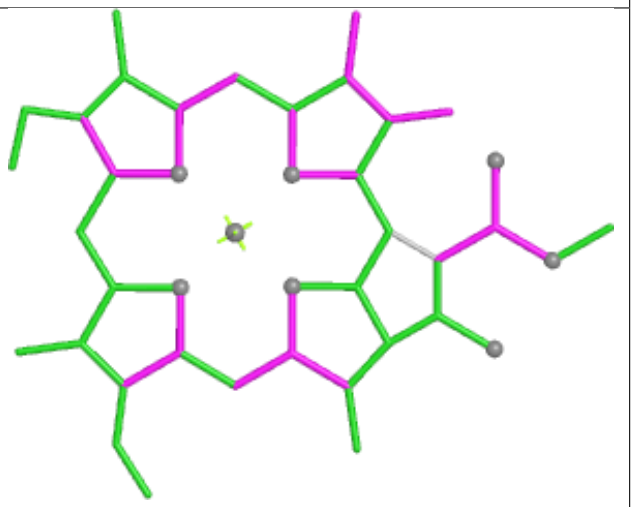


Rings

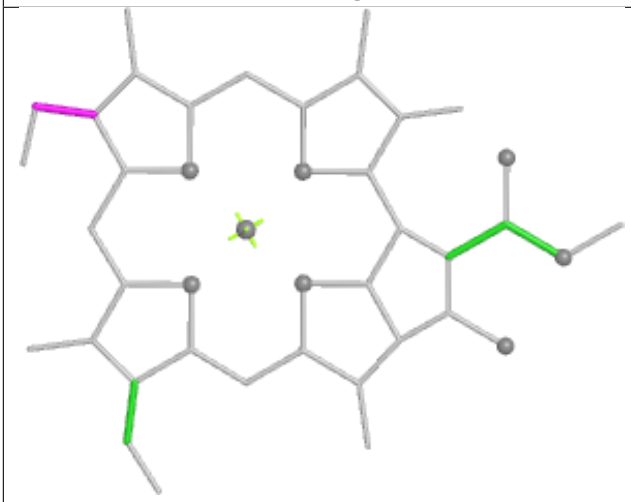
Ligand CLA o 607



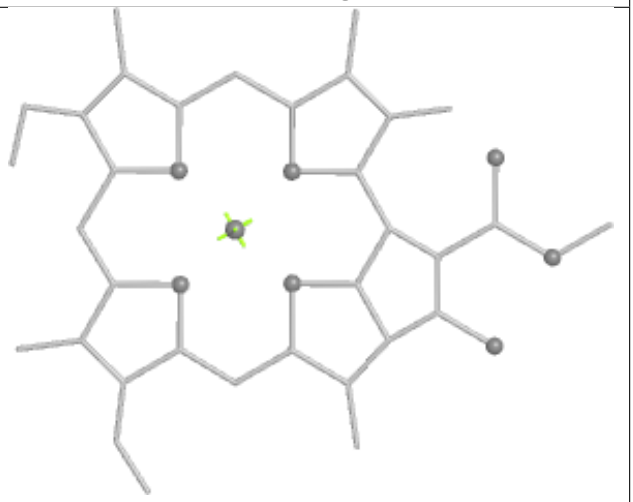
Bond lengths



Bond angles

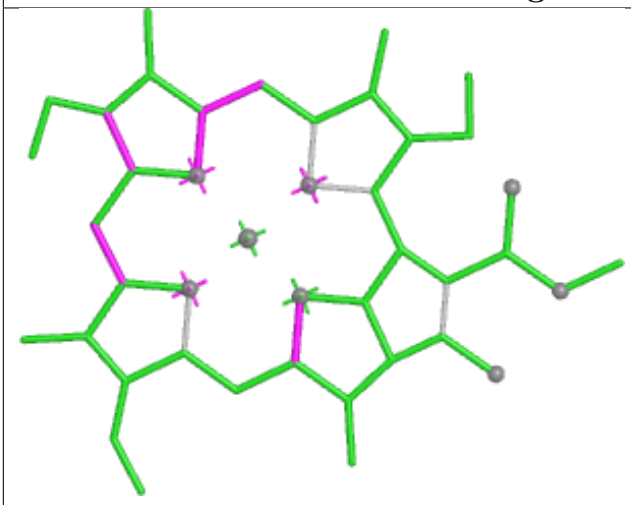


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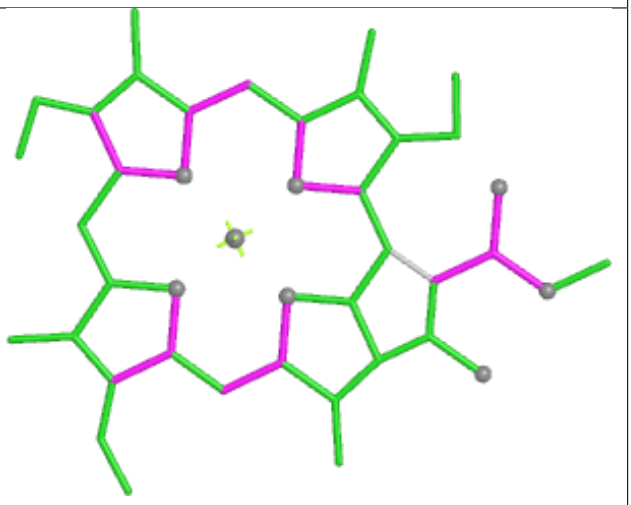


Rings

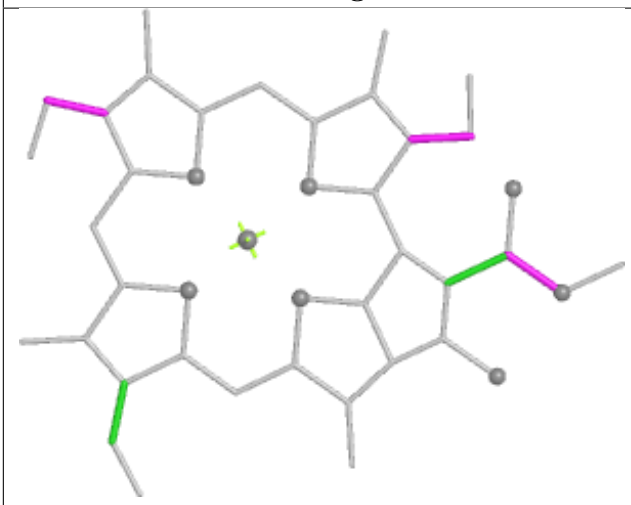
Ligand CLA h 214



Bond lengths



Bond angles

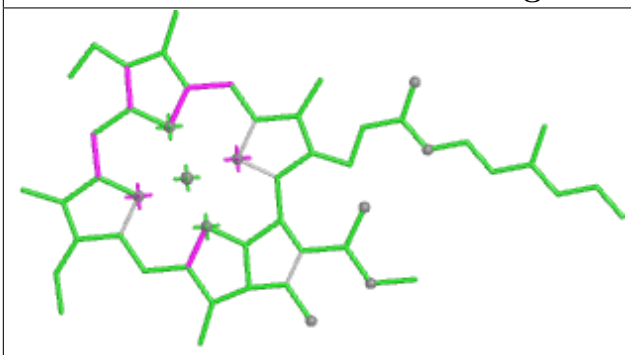


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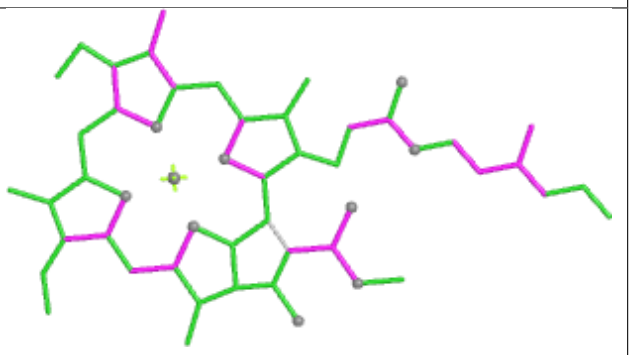


Rings

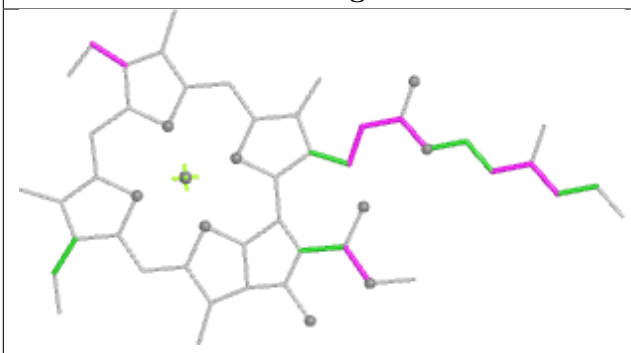
Ligand CLA A 843



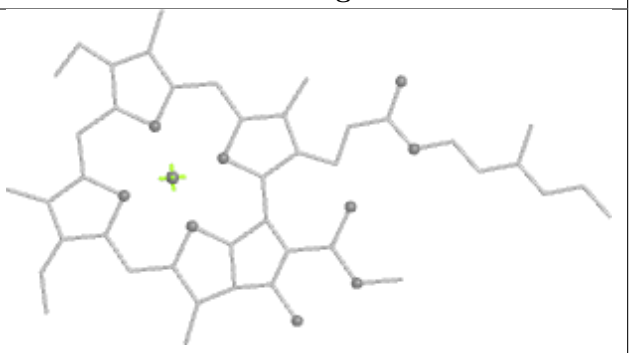
Bond lengths



Bond angles

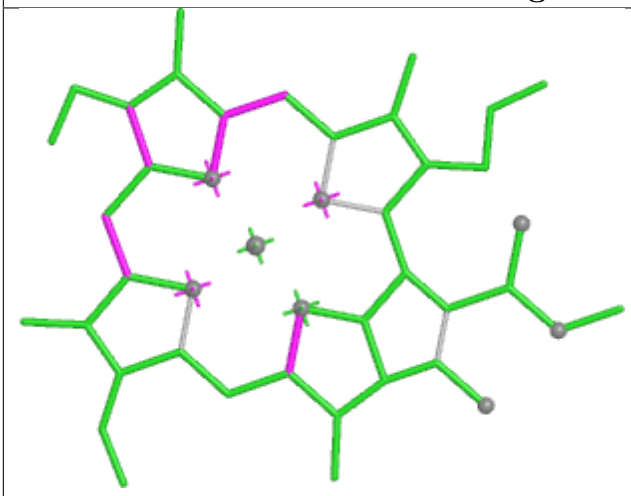


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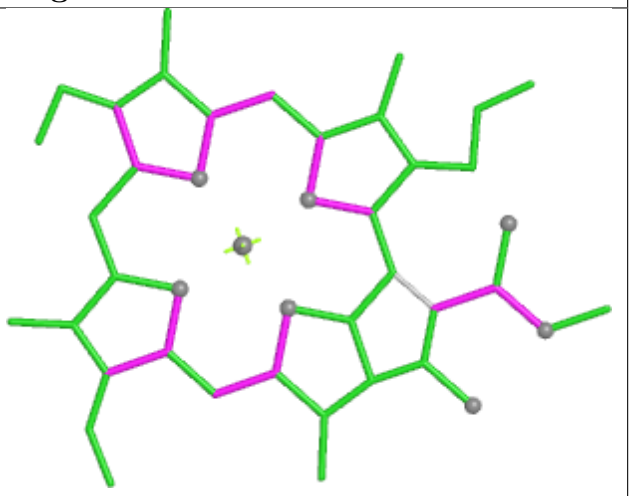


Rings

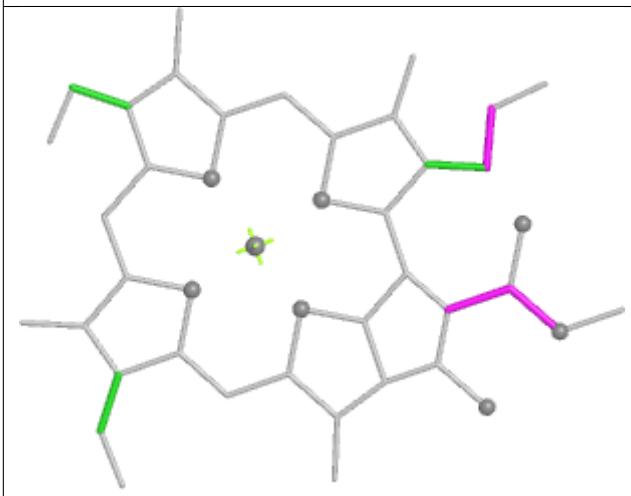
Ligand CLA g 206



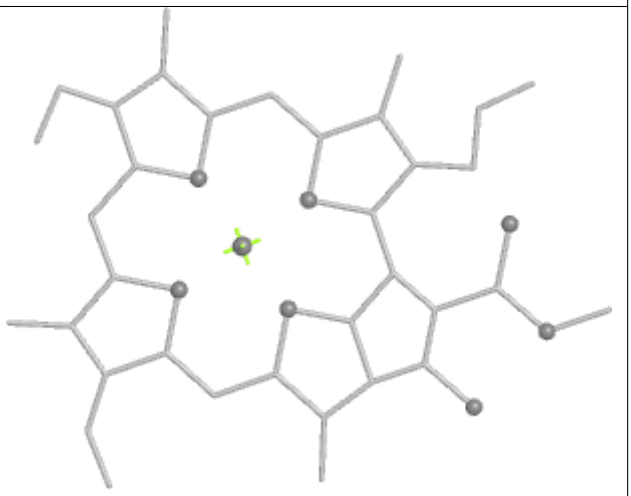
Bond lengths



Bond angles

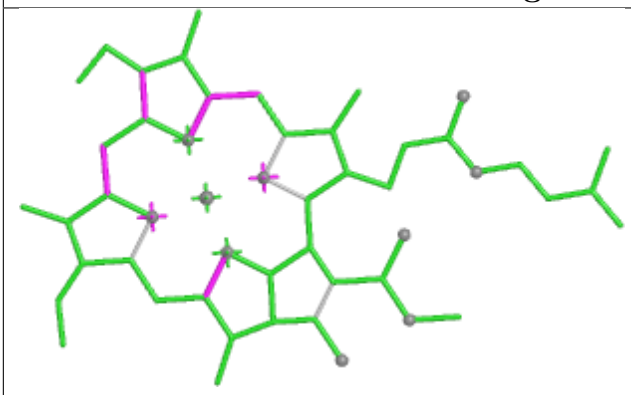


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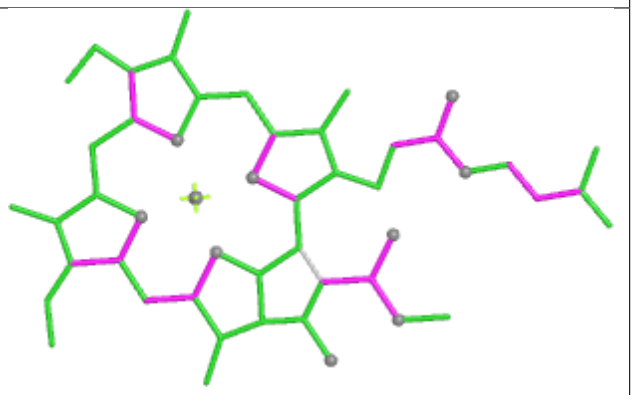


Rings

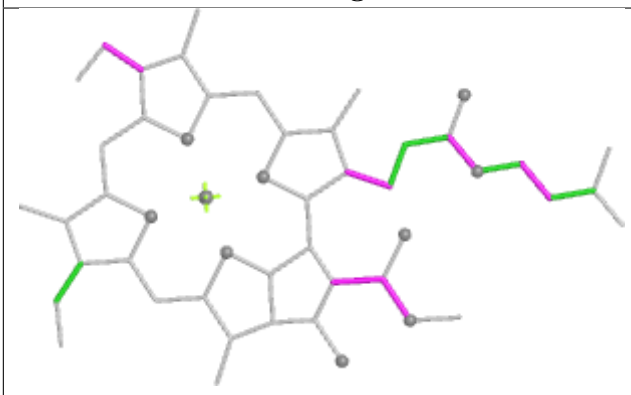
Ligand CLA A 849



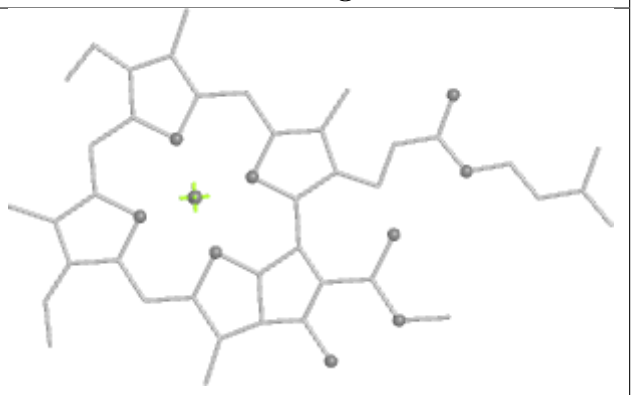
Bond lengths



Bond angles

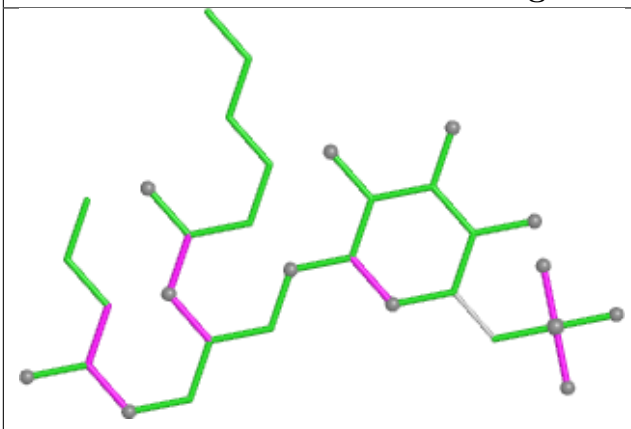


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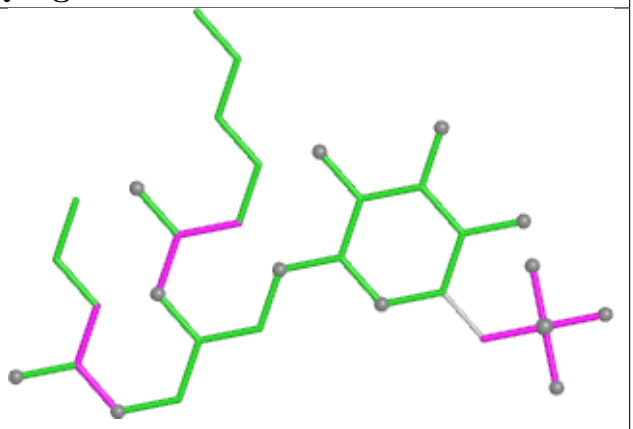


Rings

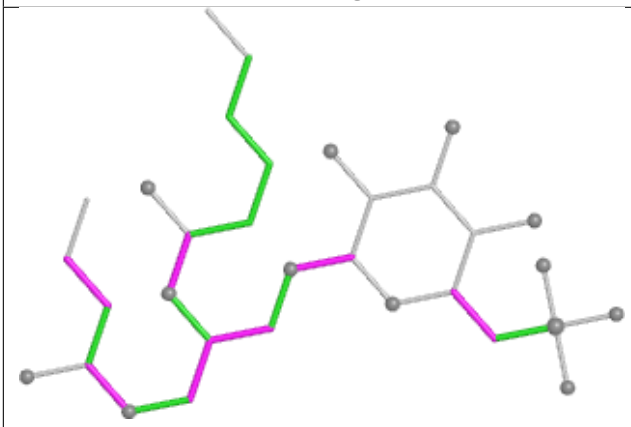
Ligand SQD g 202



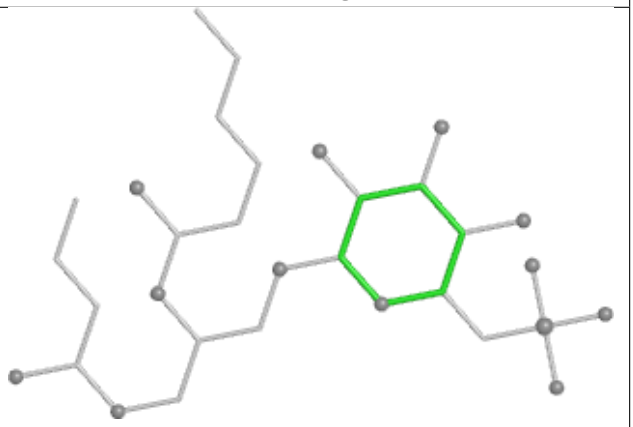
Bond lengths



Bond angles

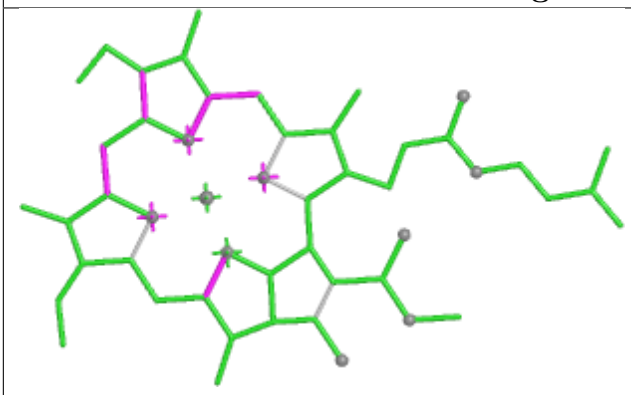


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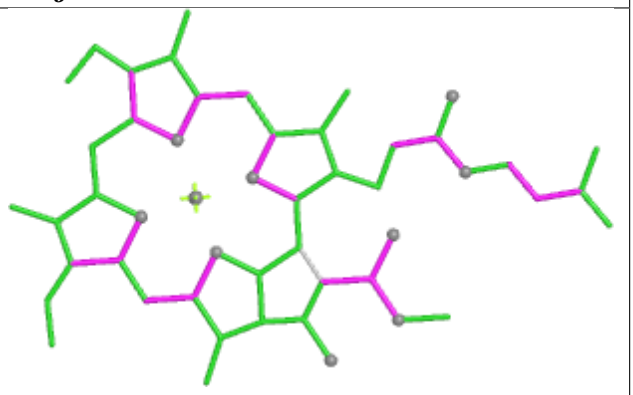


Rings

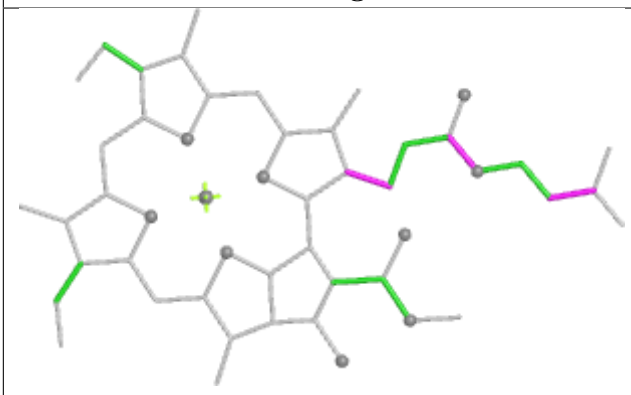
Ligand CLA j 215



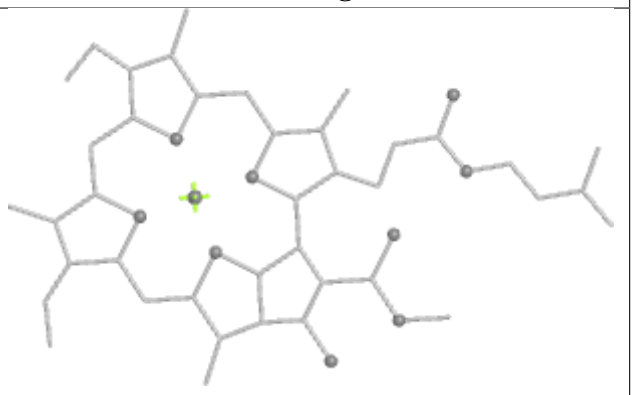
Bond lengths



Bond angles

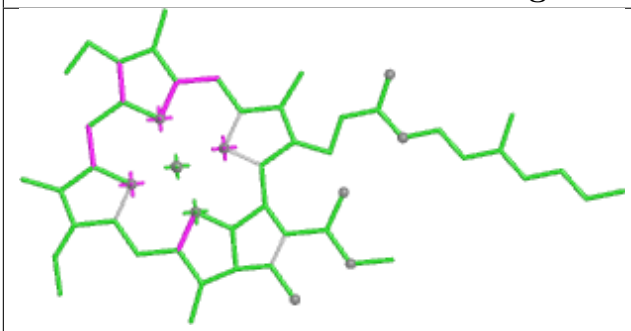


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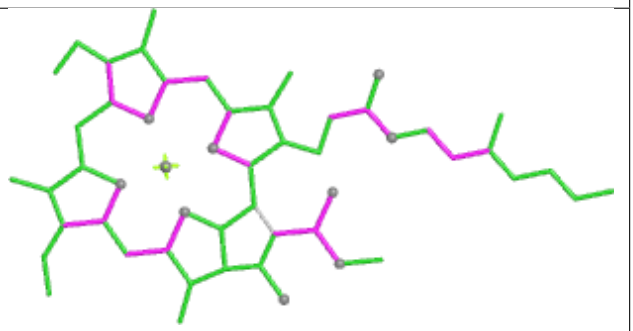


Rings

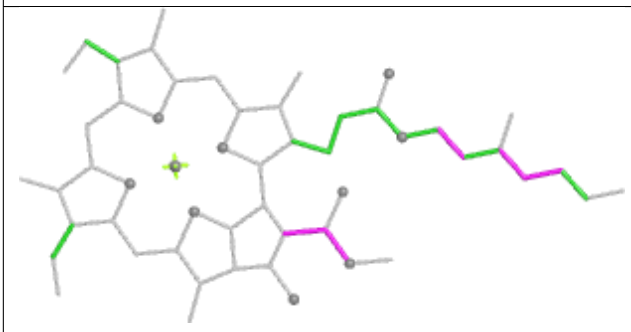
Ligand CLA e 201



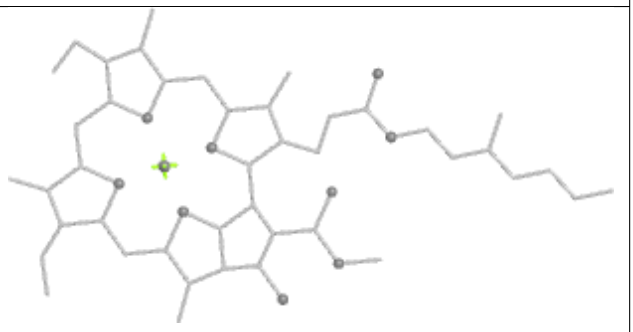
Bond lengths



Bond angles

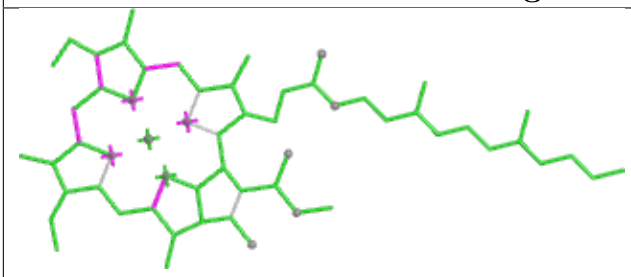


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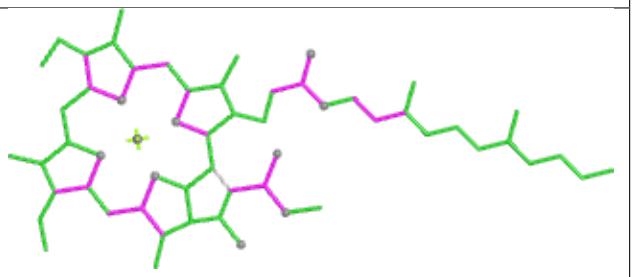


Rings

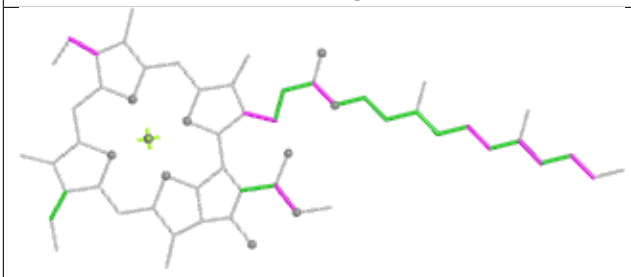
Ligand CLA A 813



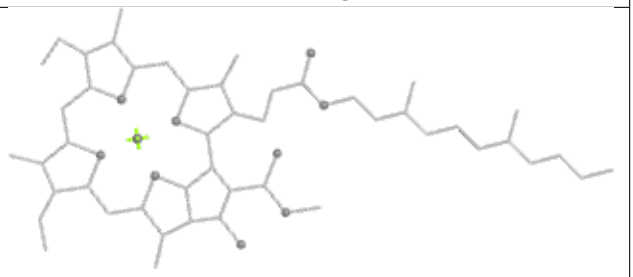
Bond lengths



Bond angles

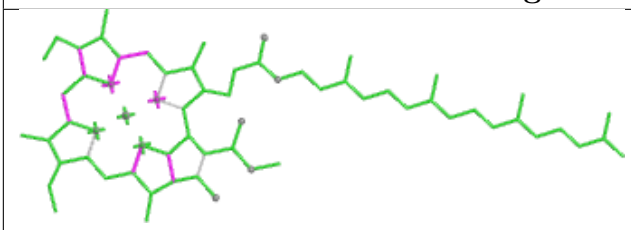


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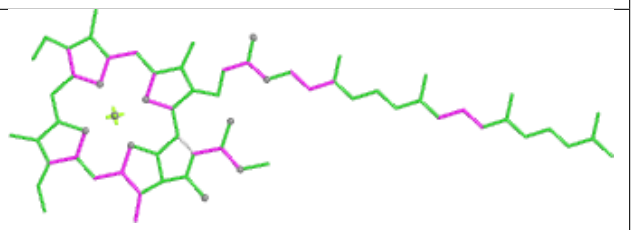


Rings

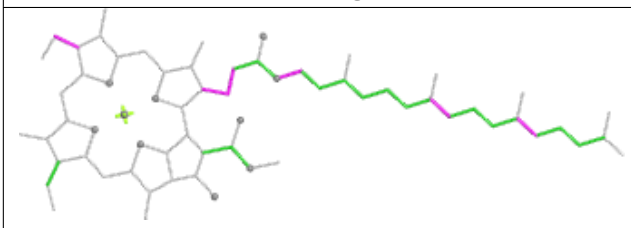
Ligand CLA A 807



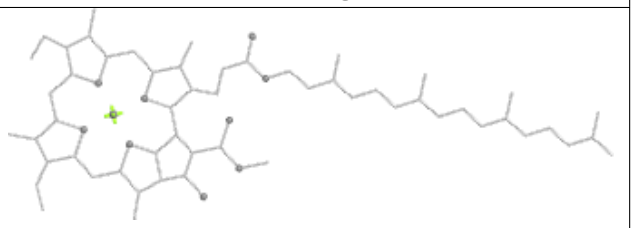
Bond lengths



Bond angles

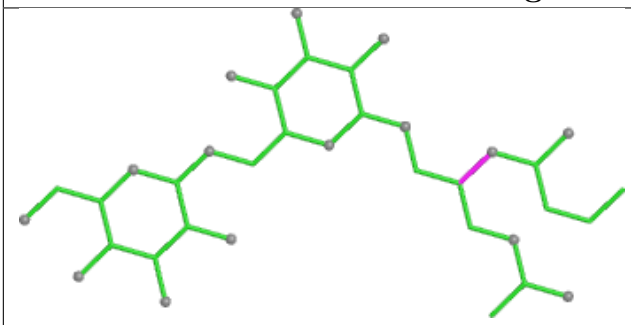


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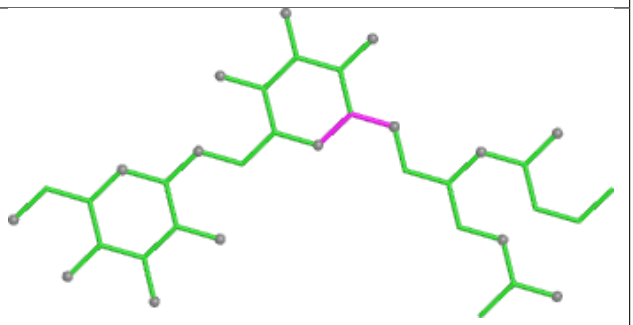


Rings

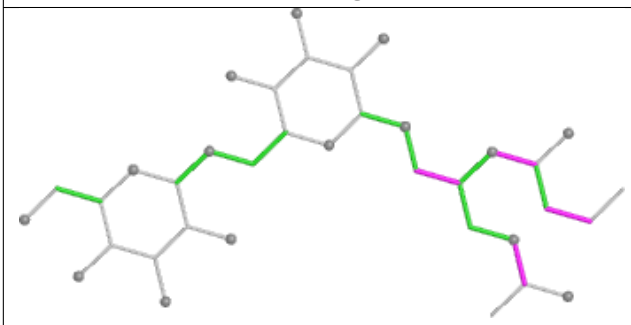
Ligand DGD e 203



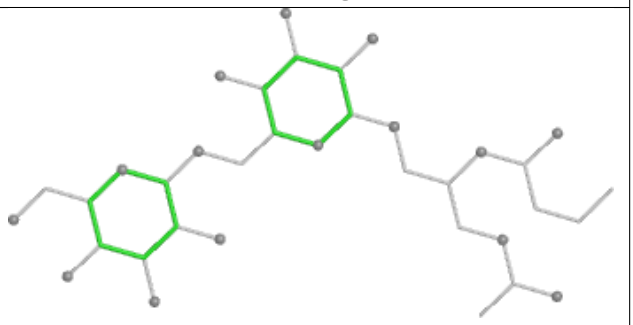
Bond lengths



Bond angles

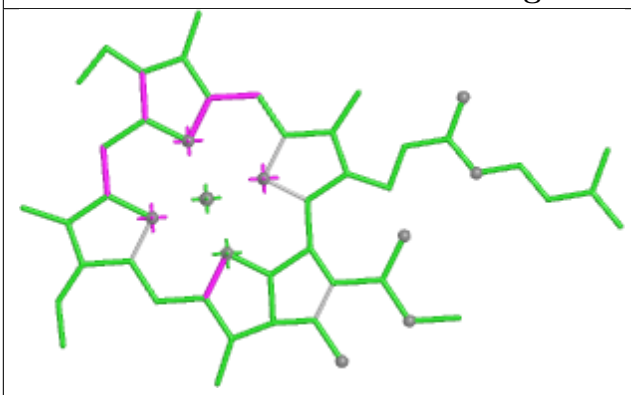


Torsions

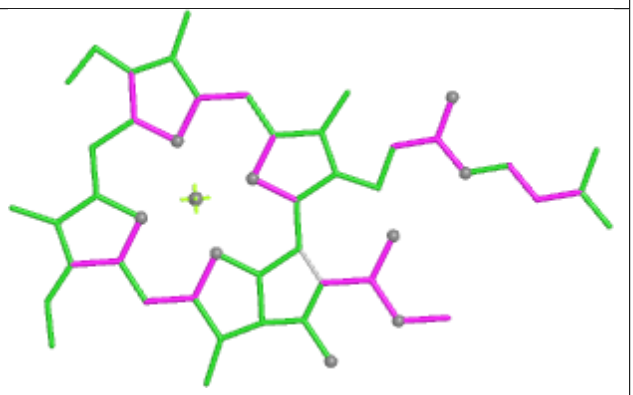


Rings

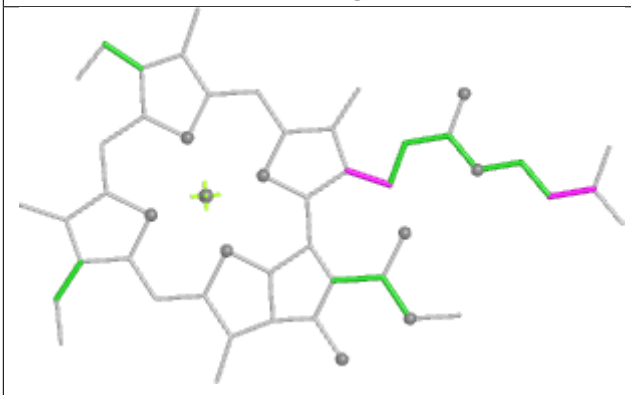
Ligand CLA A 811



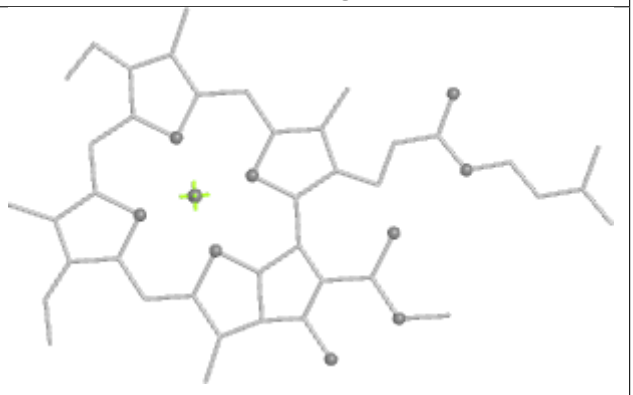
Bond lengths



Bond angles

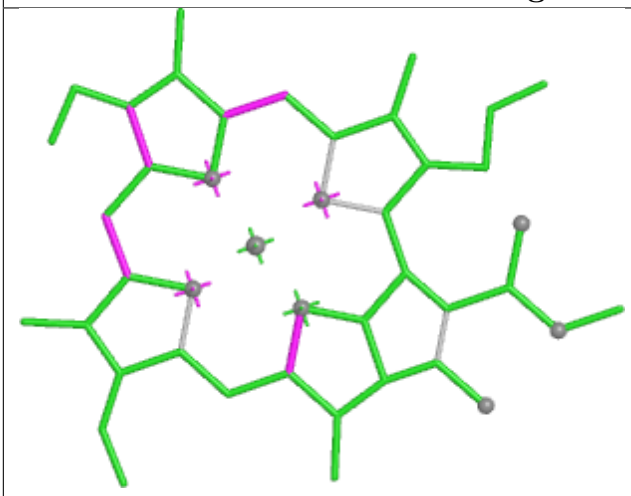


Torsions

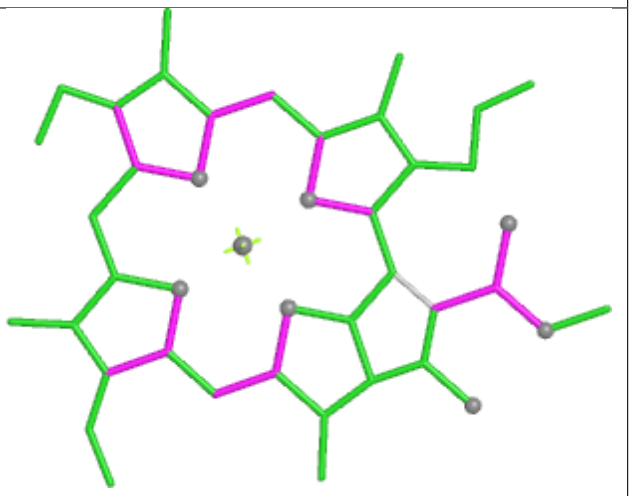


Rings

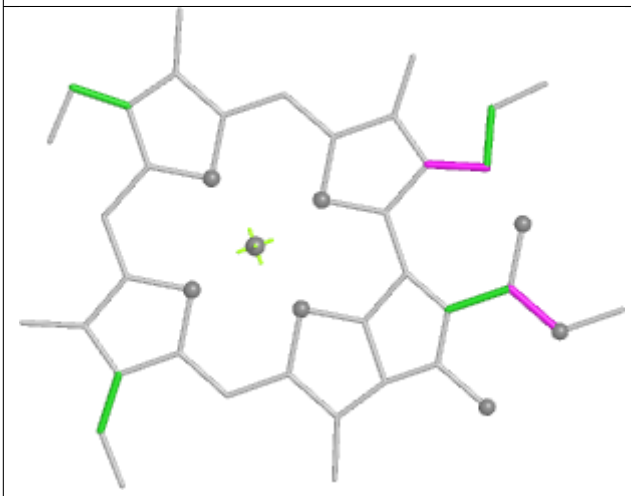
Ligand CLA k 202



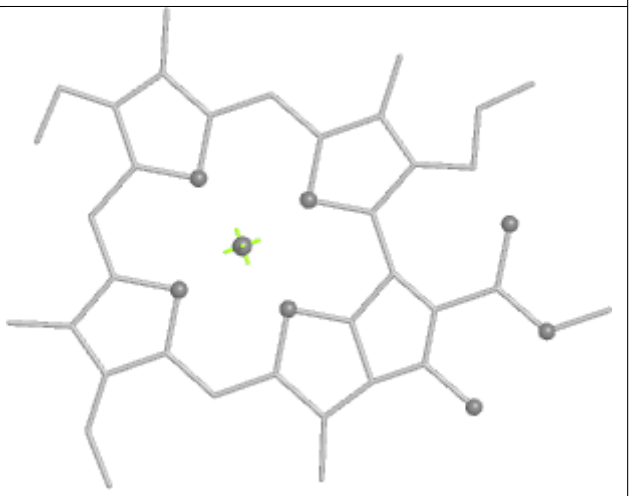
Bond lengths



Bond angles

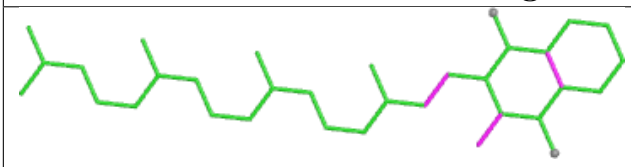


Torsions

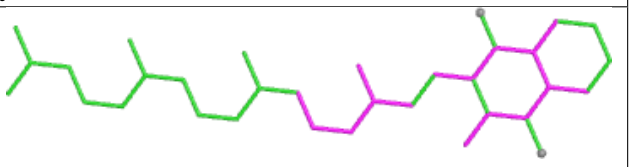


Rings

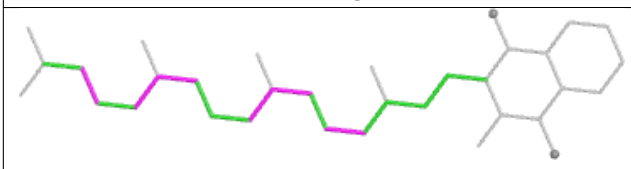
Ligand PQN A 834



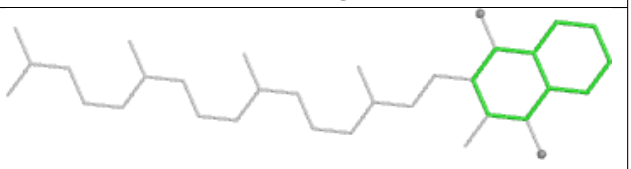
Bond lengths



Bond angles

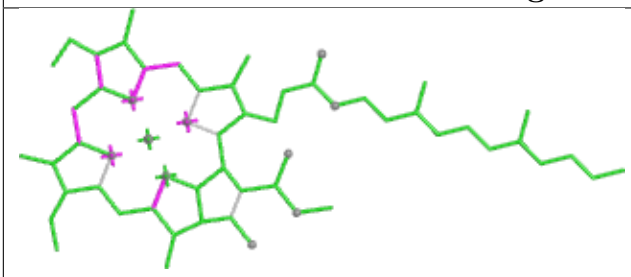


Torsions

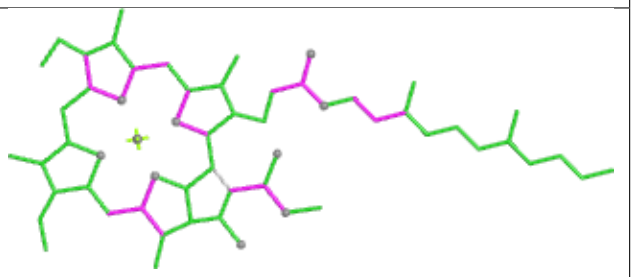


Rings

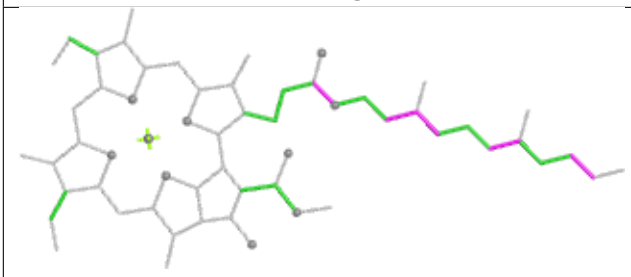
Ligand CLA h 211



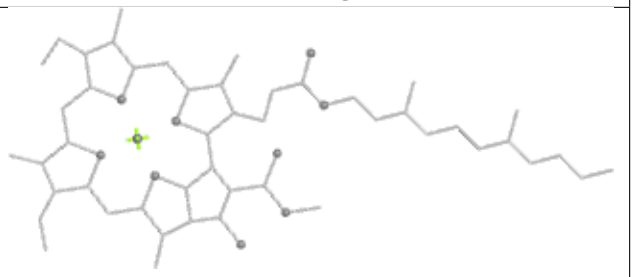
Bond lengths



Bond angles

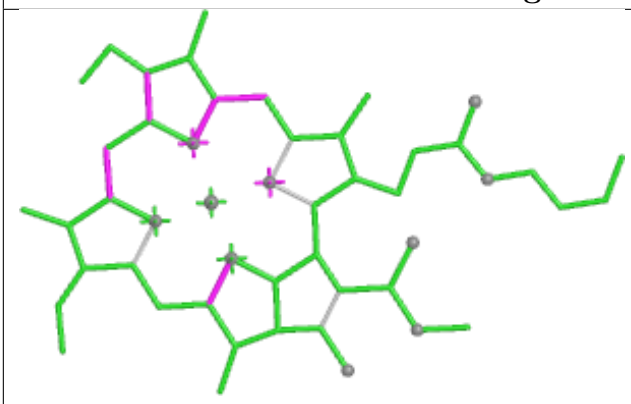


Torsions

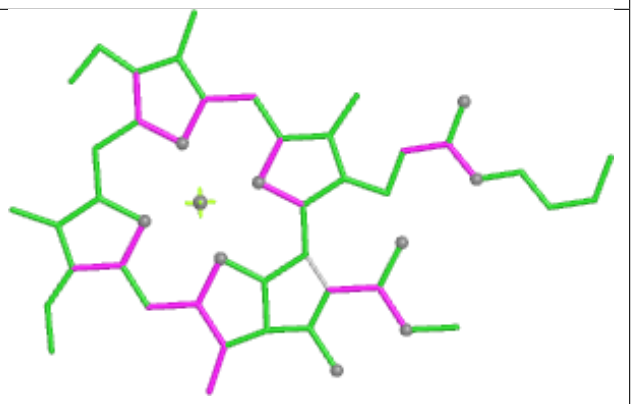


Rings

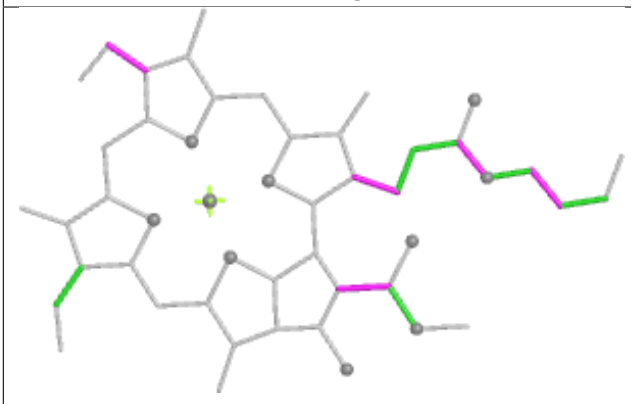
Ligand CLA A 842



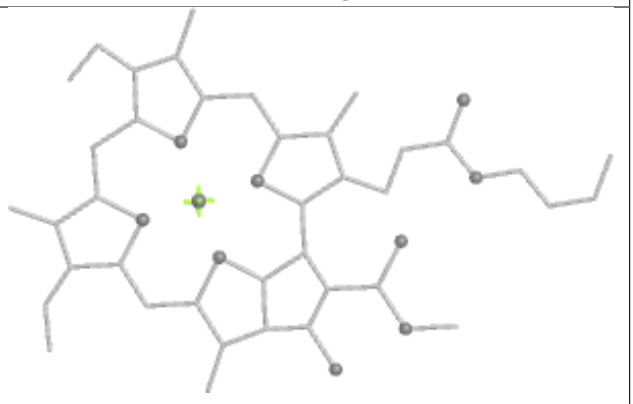
Bond lengths



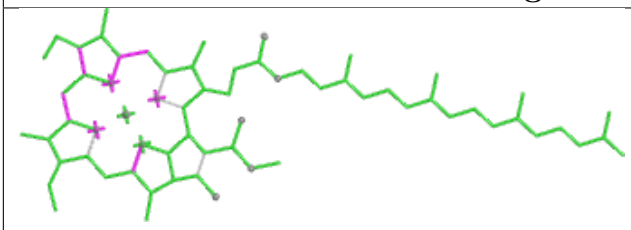
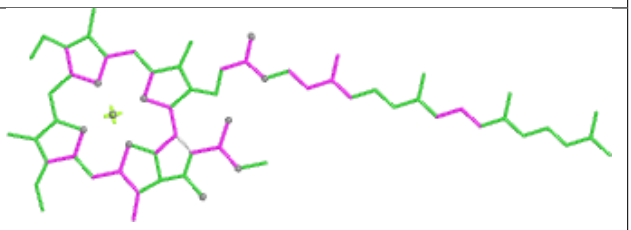
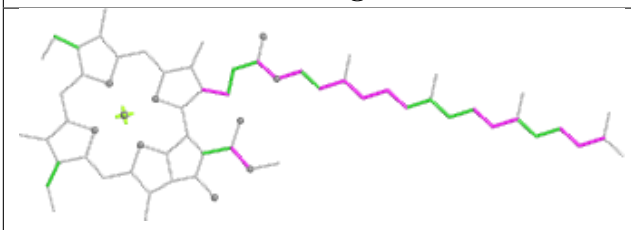
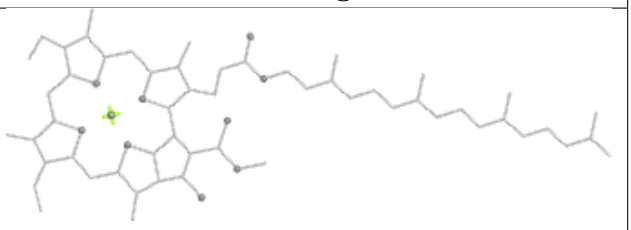
Bond angles

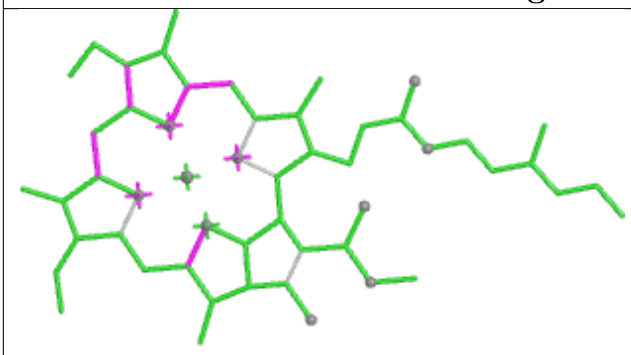
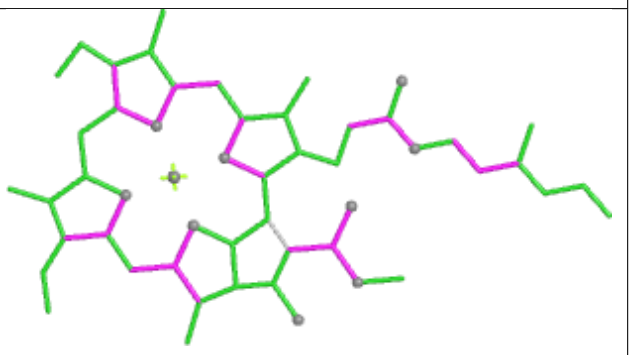
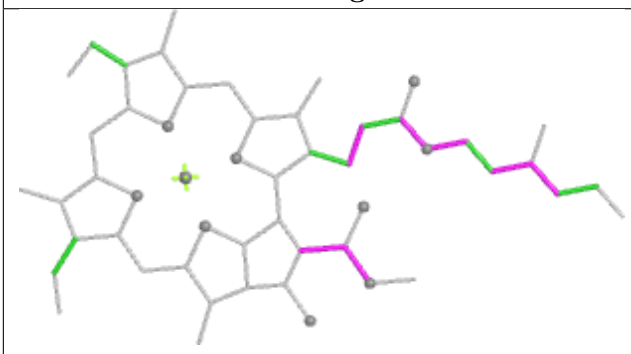
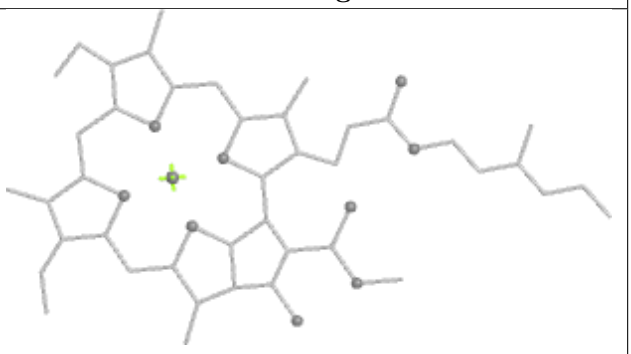


Torsions

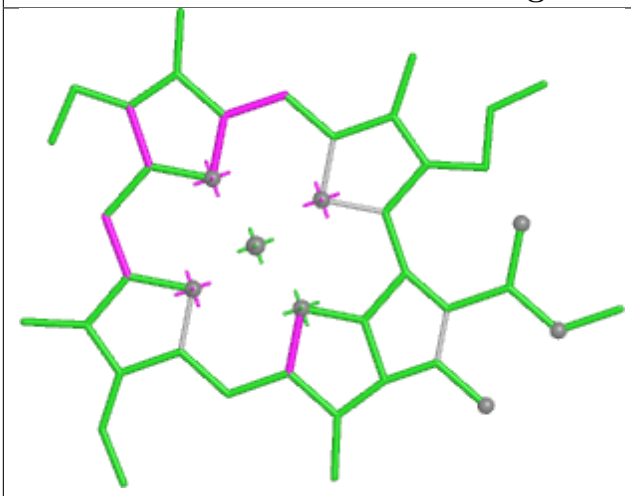


Rings

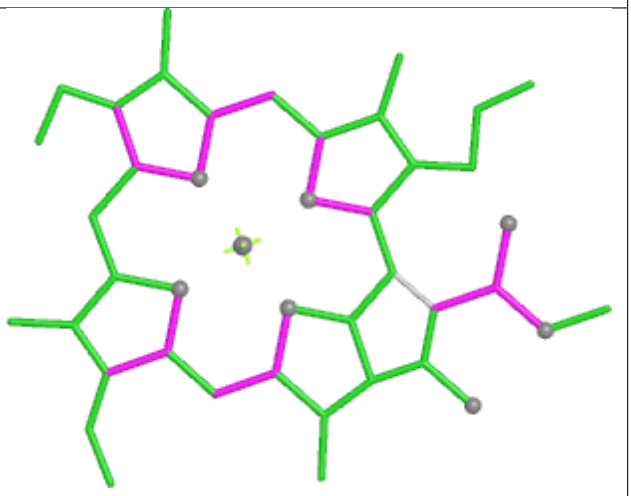
Ligand CLA B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

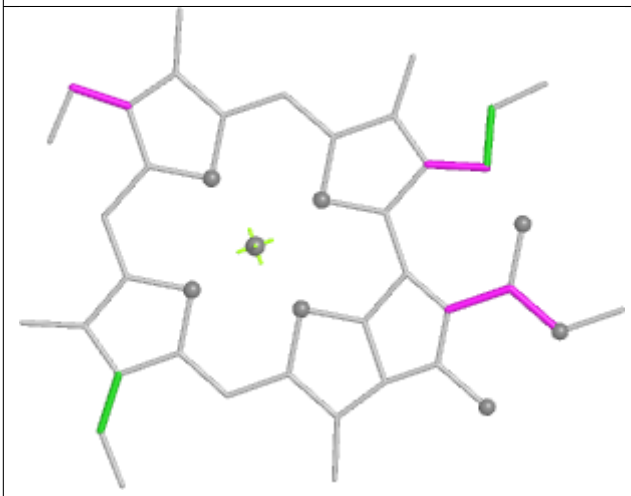
Ligand CLA h 210



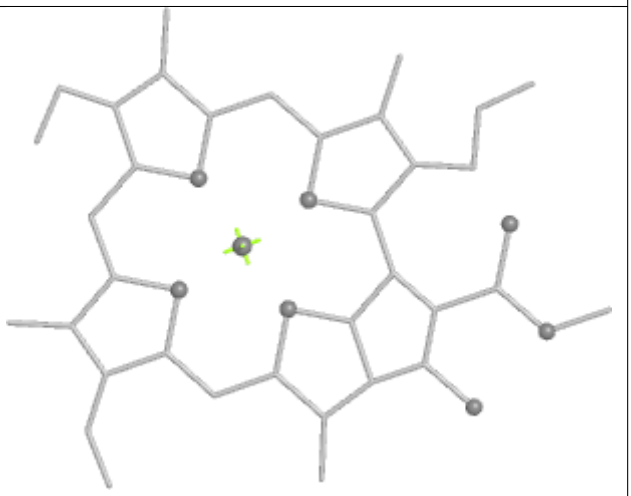
Bond lengths



Bond angles

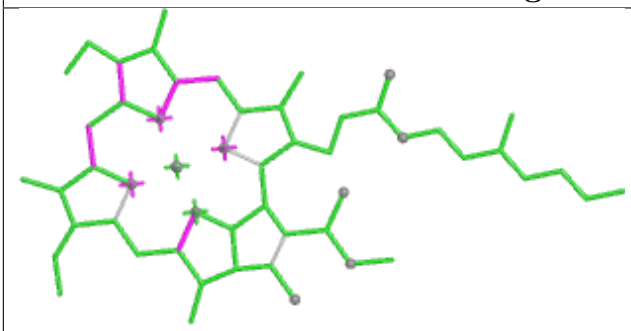


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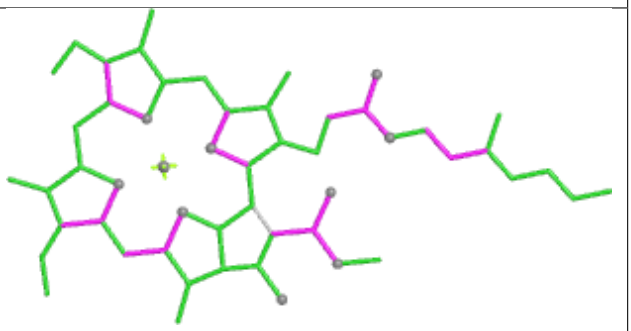


Rings

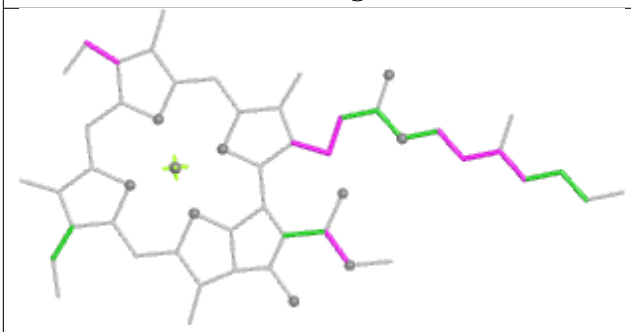
Ligand CLA B 836



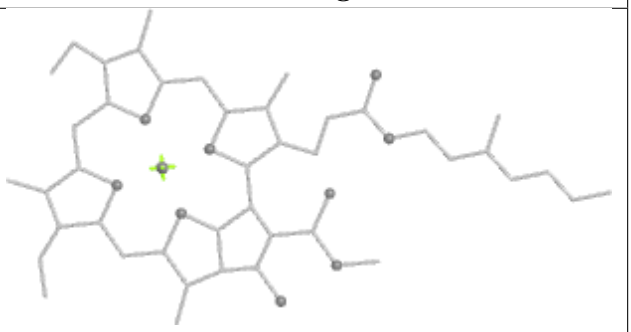
Bond lengths



Bond angles

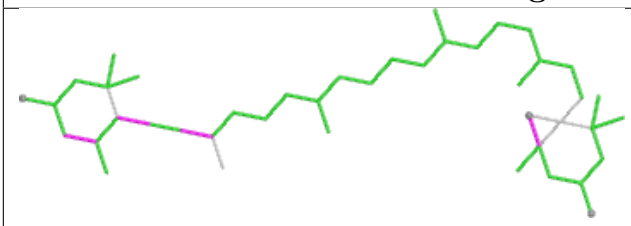


Torsions

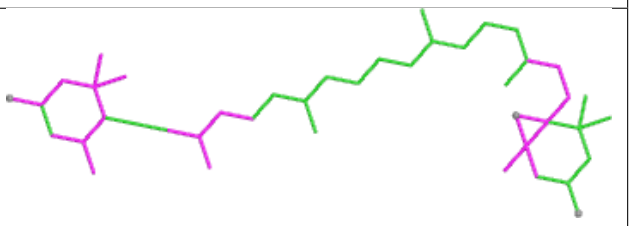


Rings

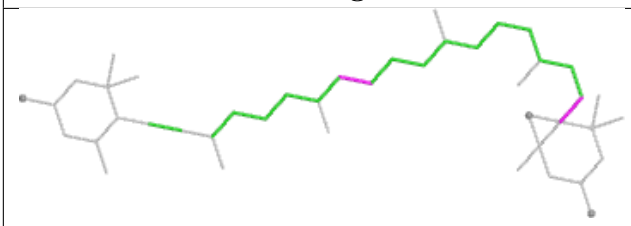
Ligand DD6 J 104



Bond lengths



Bond angles

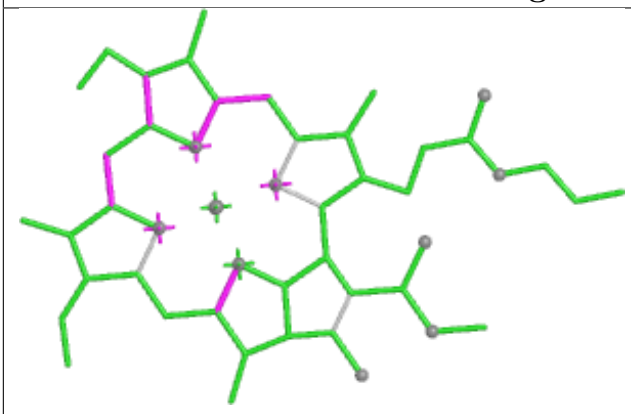


Torsions

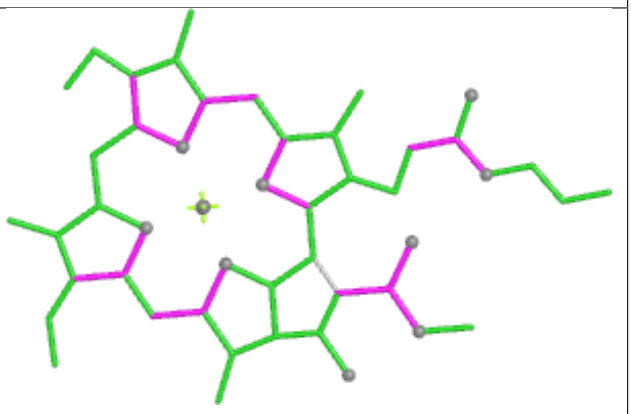


Rings

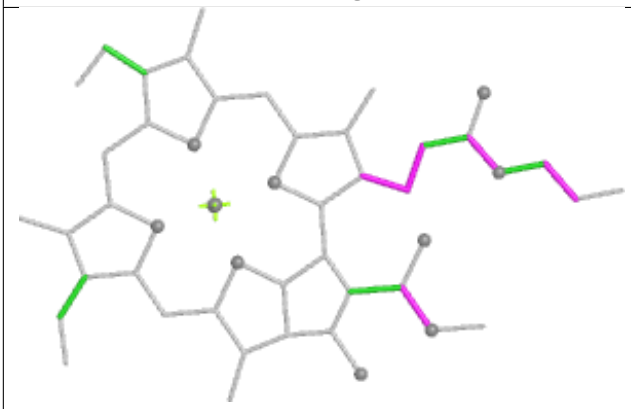
Ligand CLA e 211



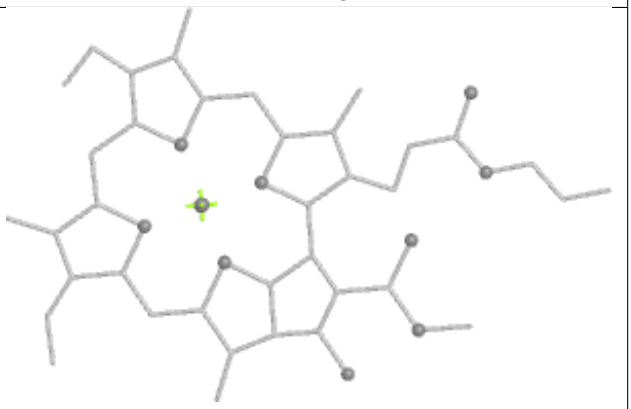
Bond lengths



Bond angles

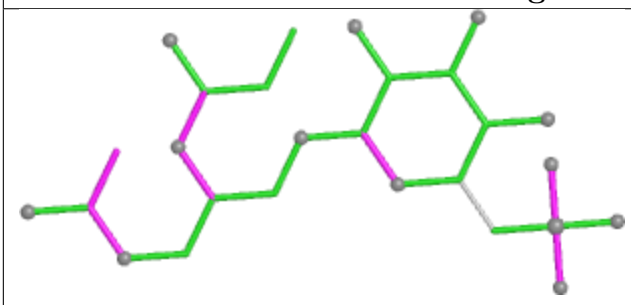


Torsions

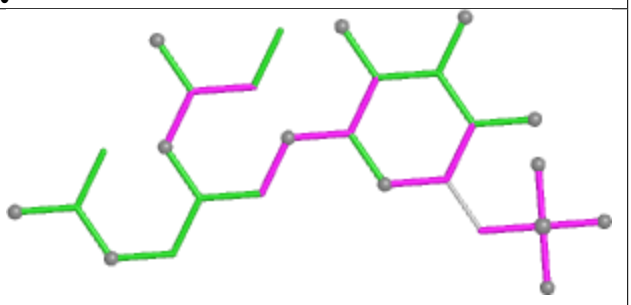


Rings

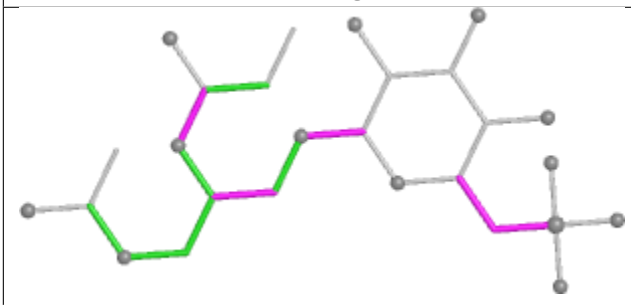
Ligand SQD J 102



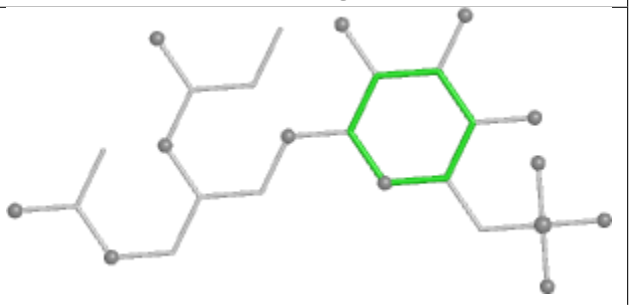
Bond lengths



Bond angles

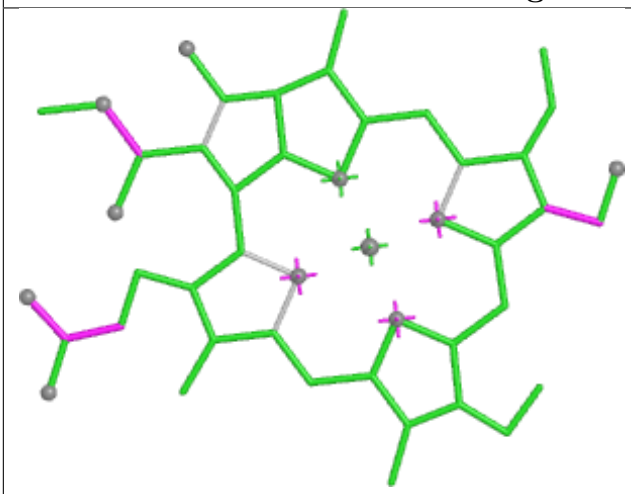


Torsions

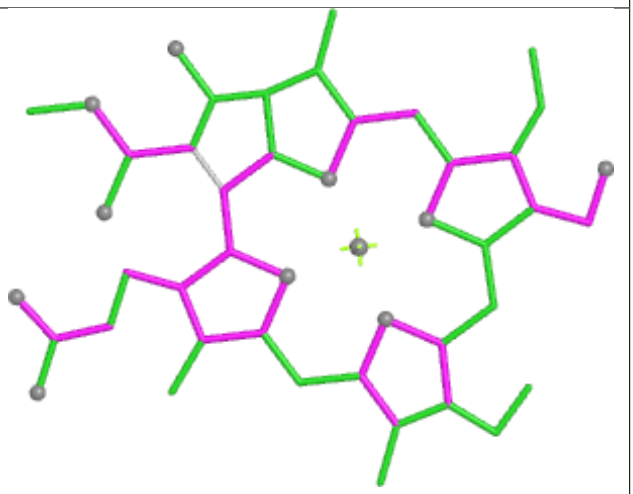


Rings

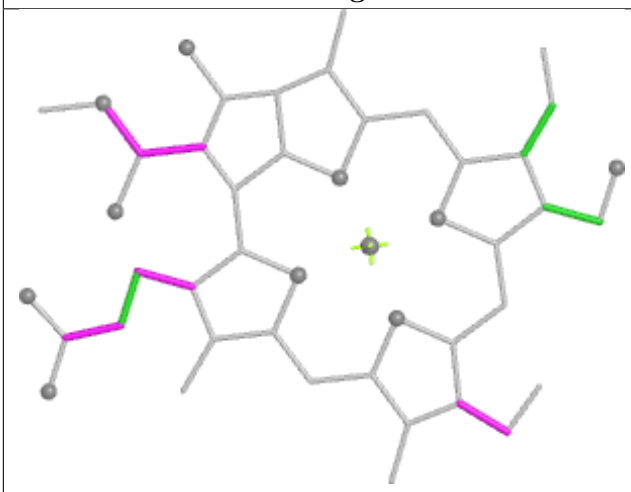
Ligand CHL d 310



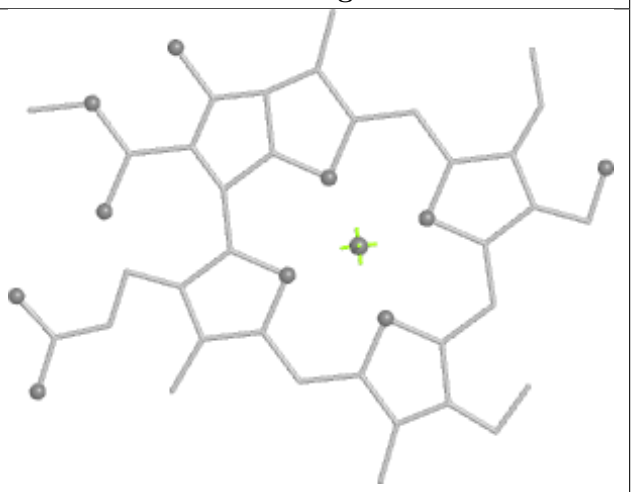
Bond lengths



Bond angles

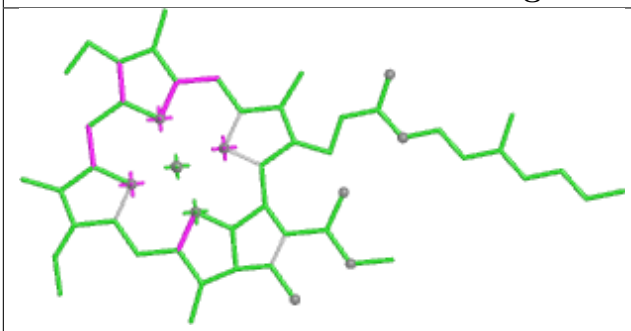


Torsions

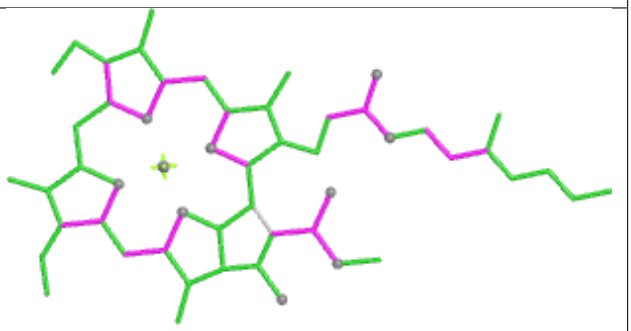


Rings

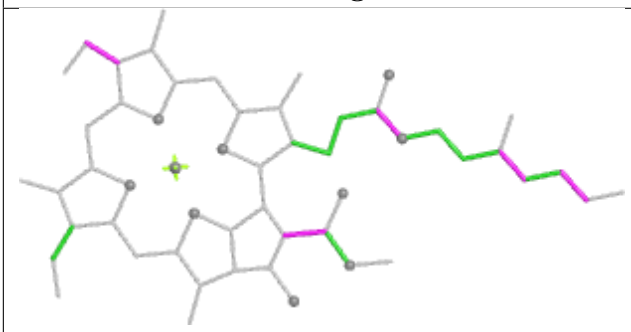
Ligand CLA A 822



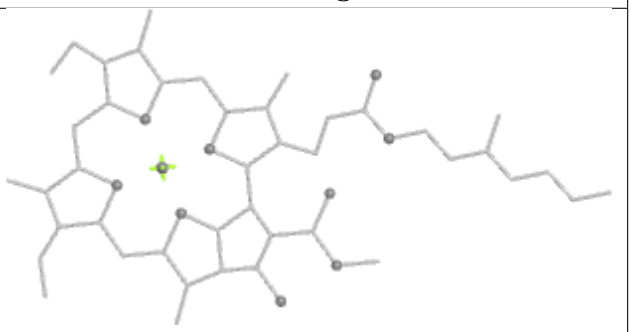
Bond lengths



Bond angles

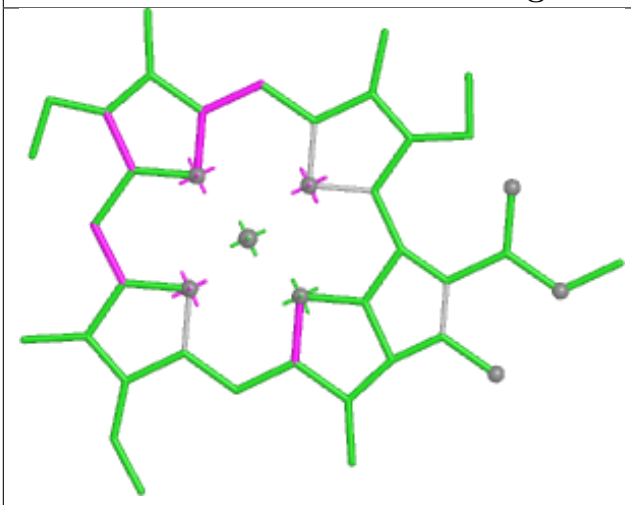


Torsions

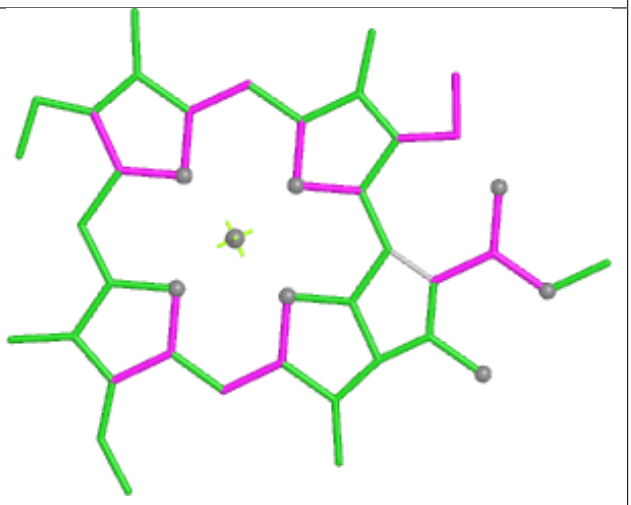


Rings

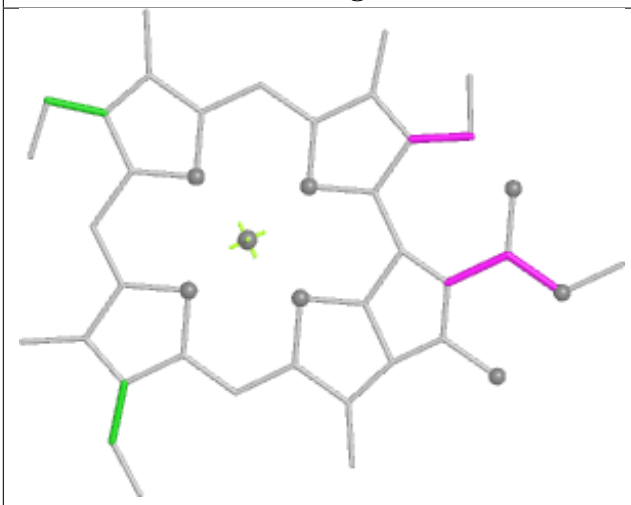
Ligand CLA b 213



Bond lengths



Bond angles

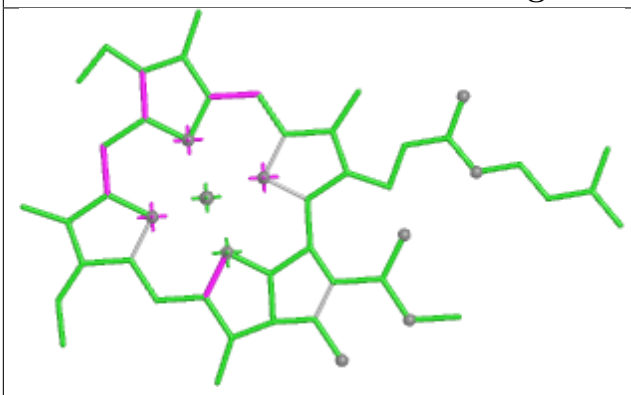


Torsions

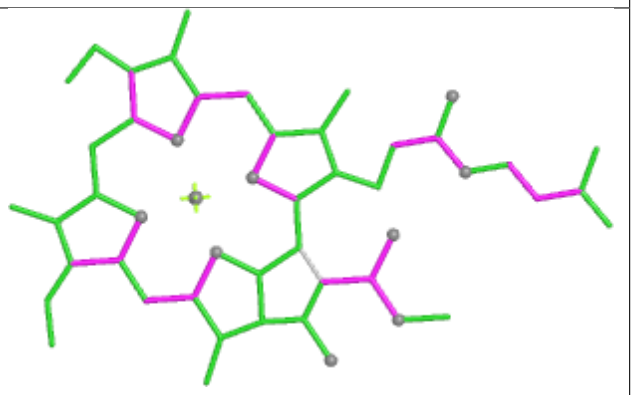


Rings

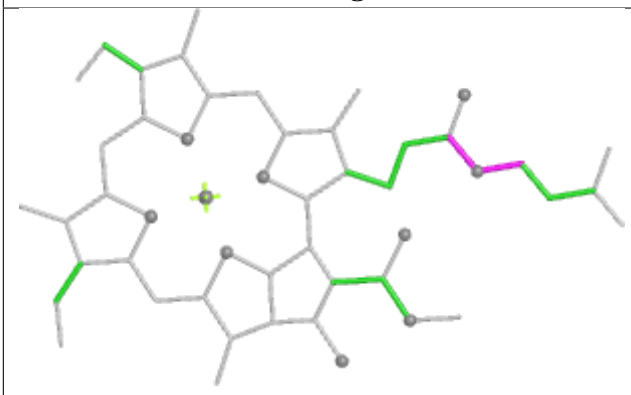
Ligand CLA k 214



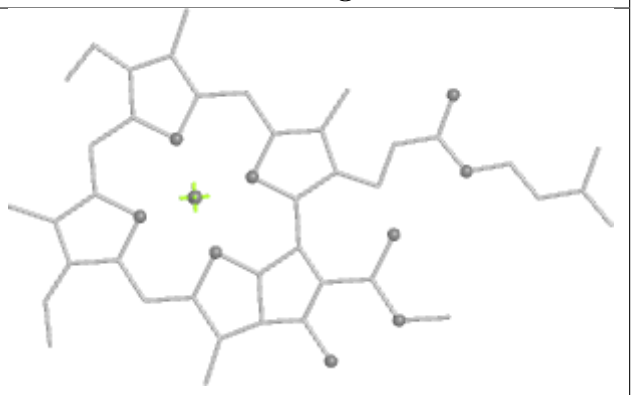
Bond lengths



Bond angles

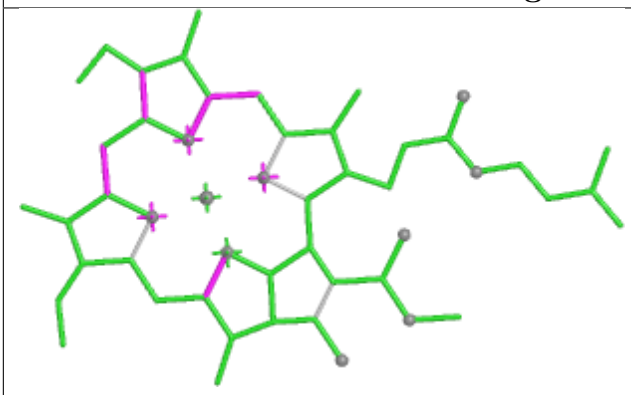


Torsions

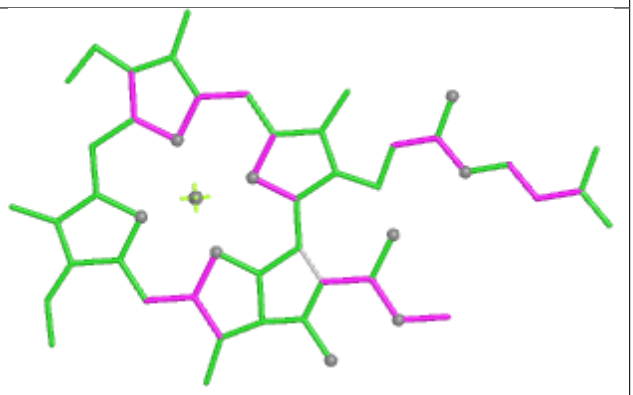


Rings

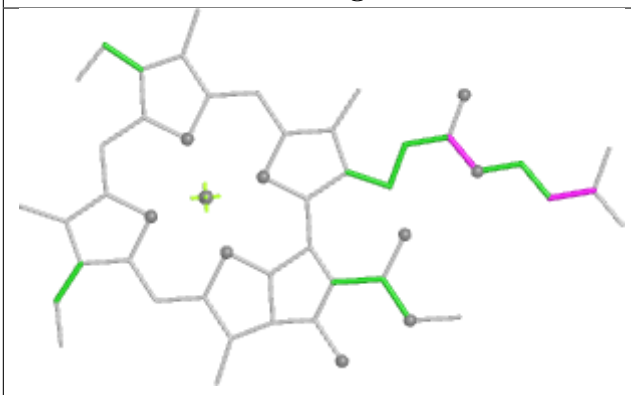
Ligand CLA B 847



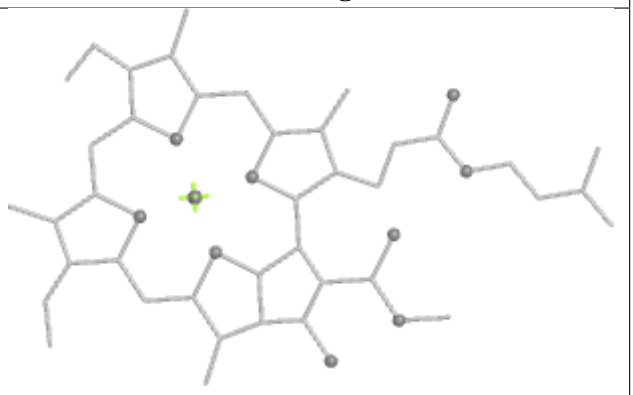
Bond lengths



Bond angles

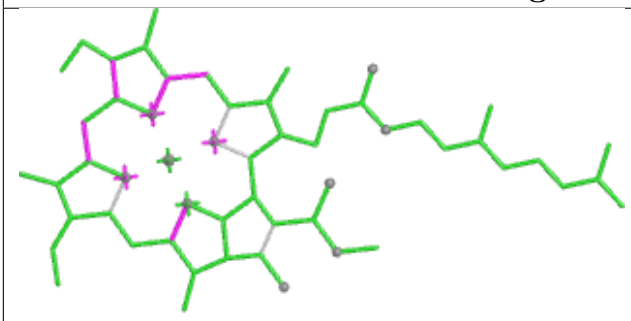


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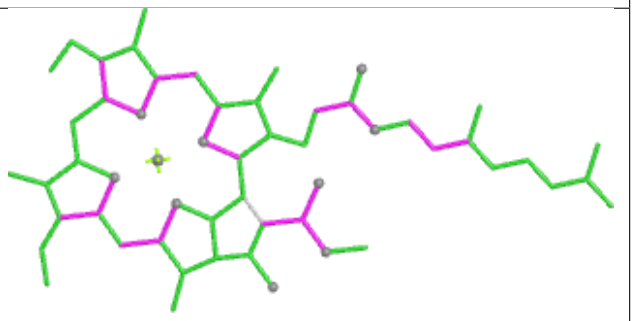


Rings

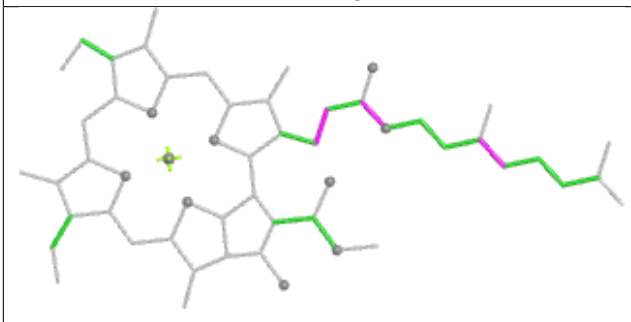
Ligand CLA e 216



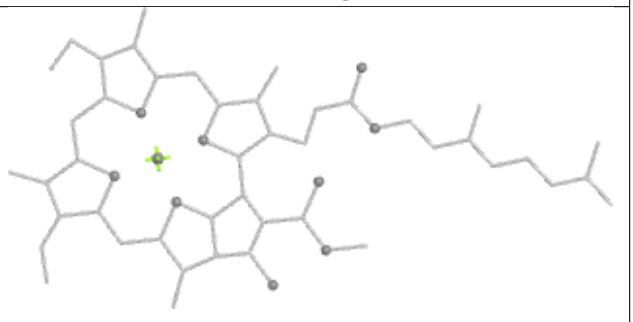
Bond lengths



Bond angles

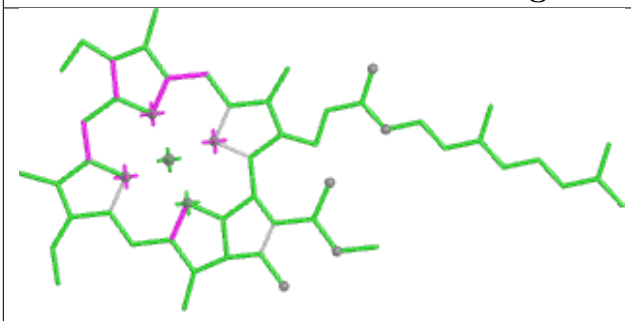


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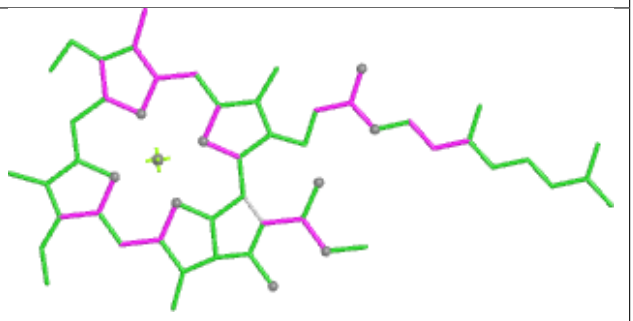


Rings

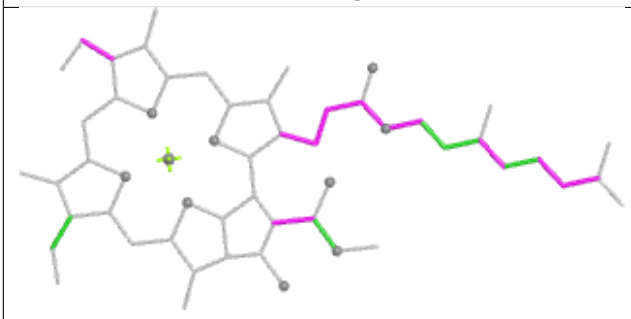
Ligand CLA c 310



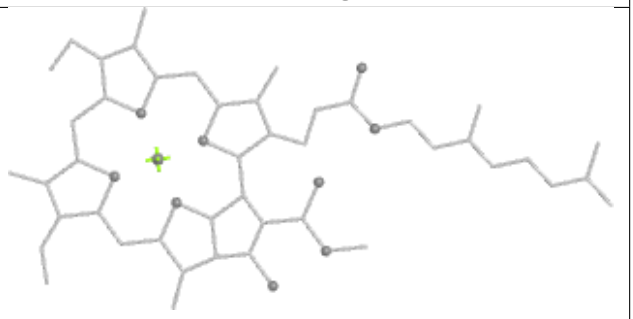
Bond lengths



Bond angles

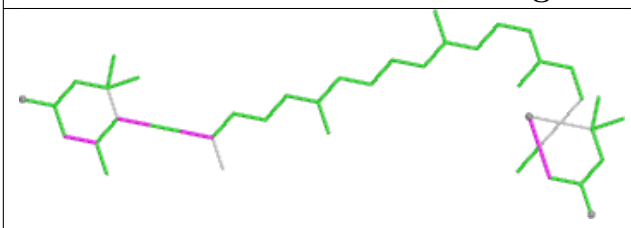


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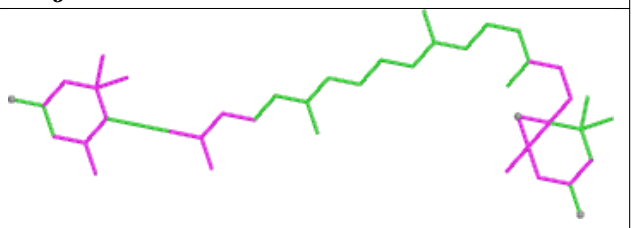


Rings

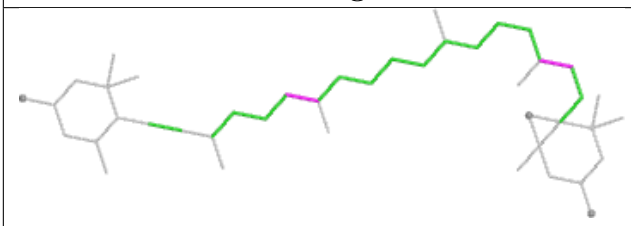
Ligand DD6 j 216



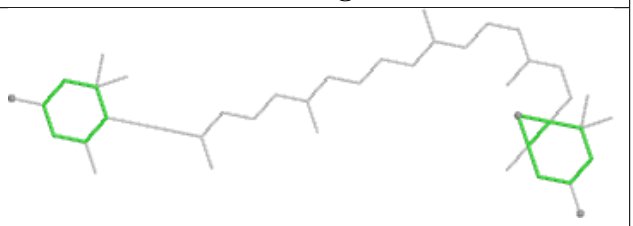
Bond lengths



Bond angles

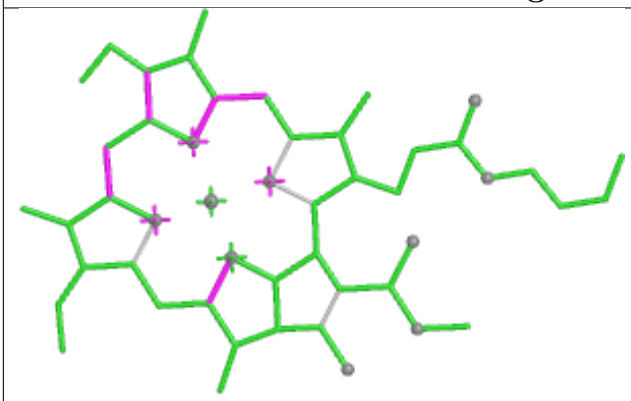


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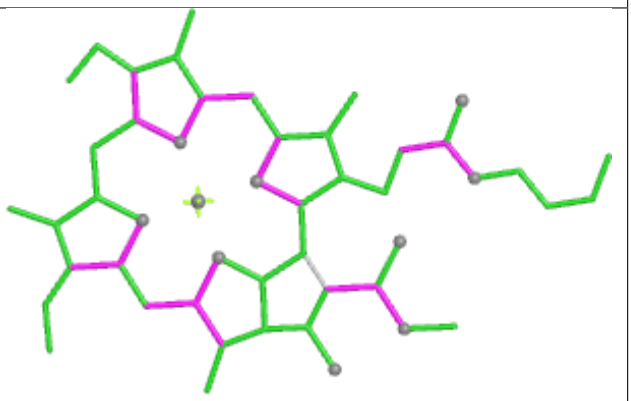


Rings

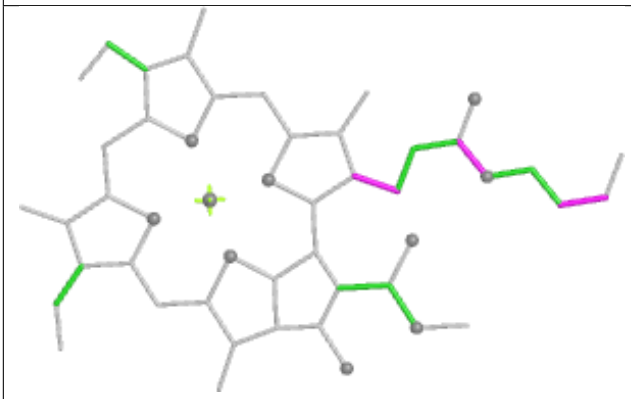
Ligand CLA d 311



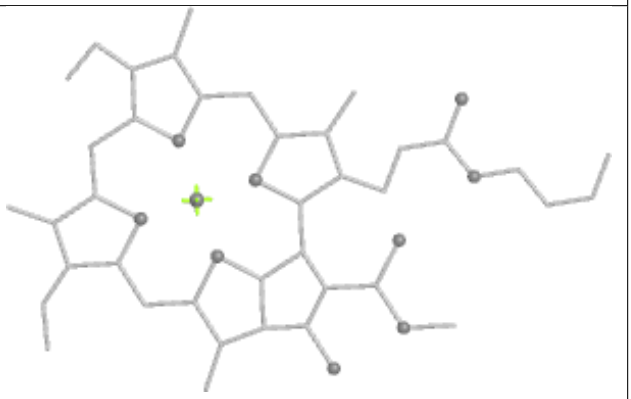
Bond lengths



Bond angles

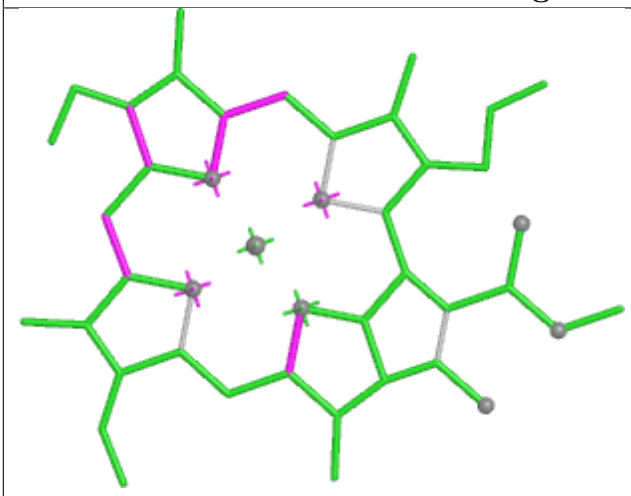


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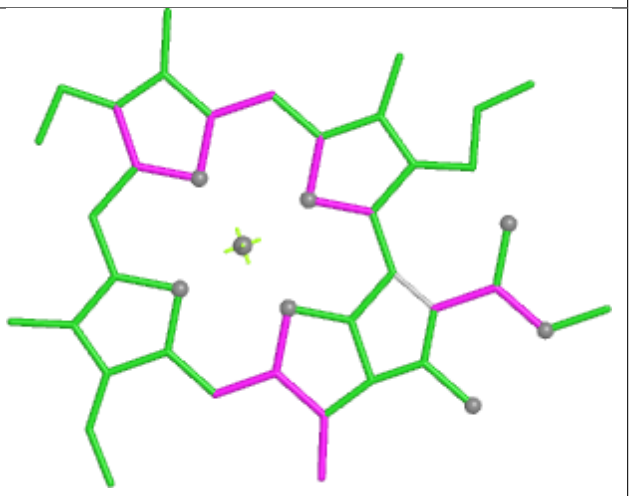


Rings

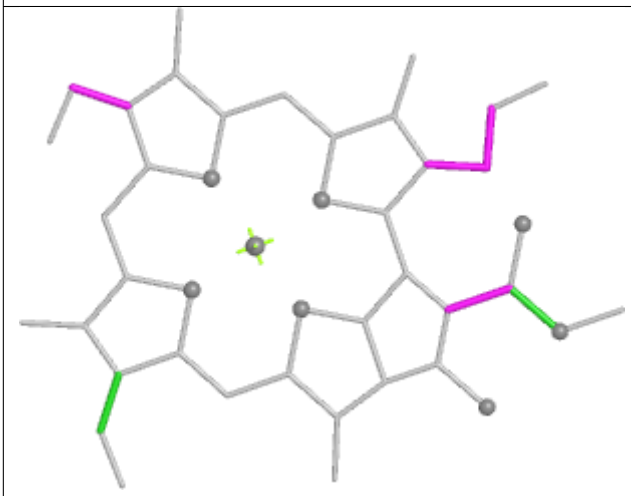
Ligand CLA l 605



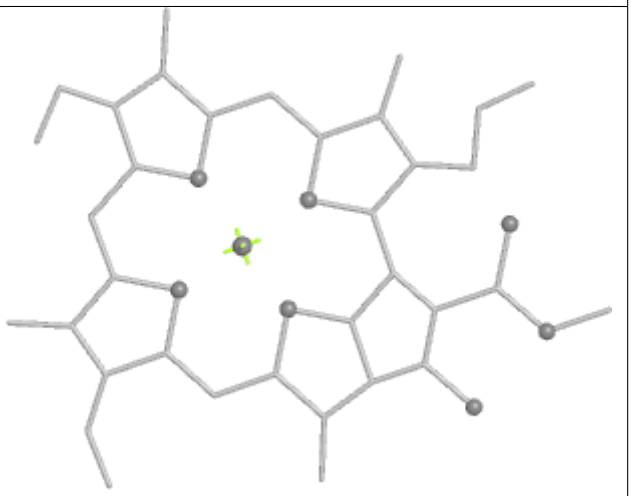
Bond lengths



Bond angles

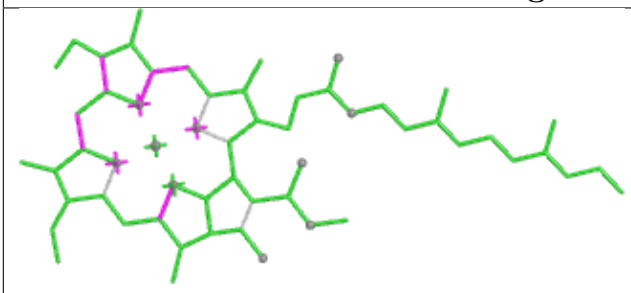


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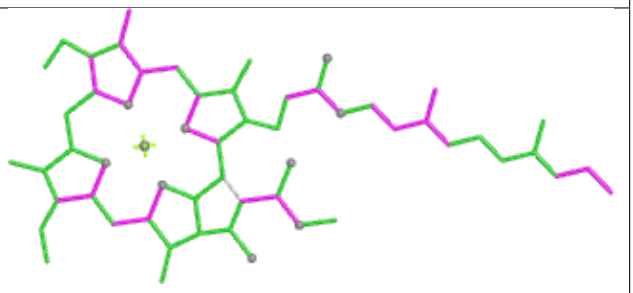


Rings

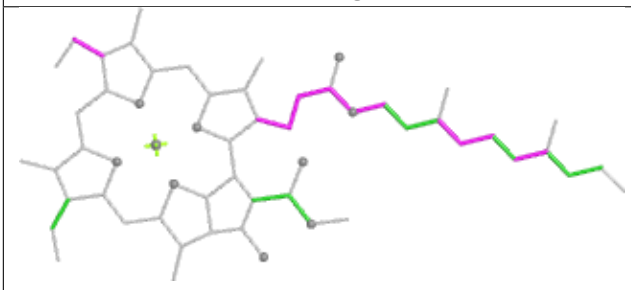
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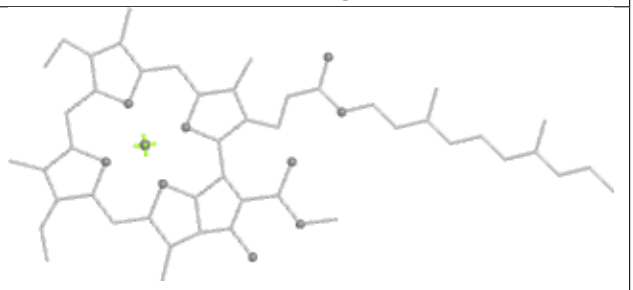
Bond lengths



Bond angles

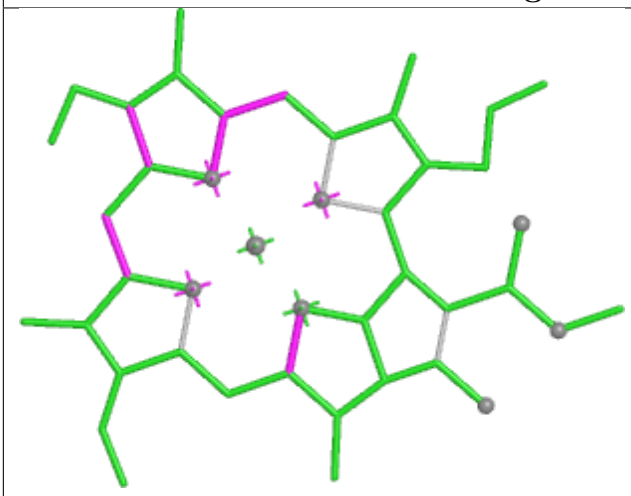


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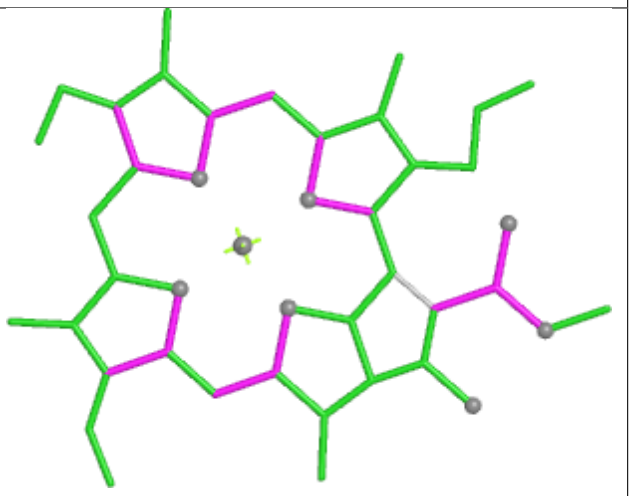


Rings

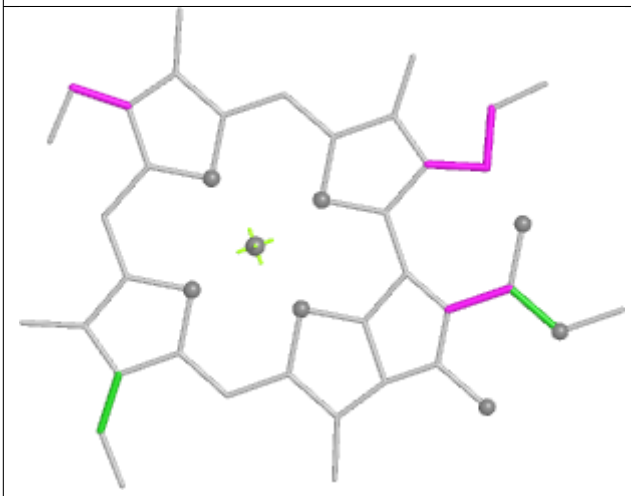
Ligand CLA B 825



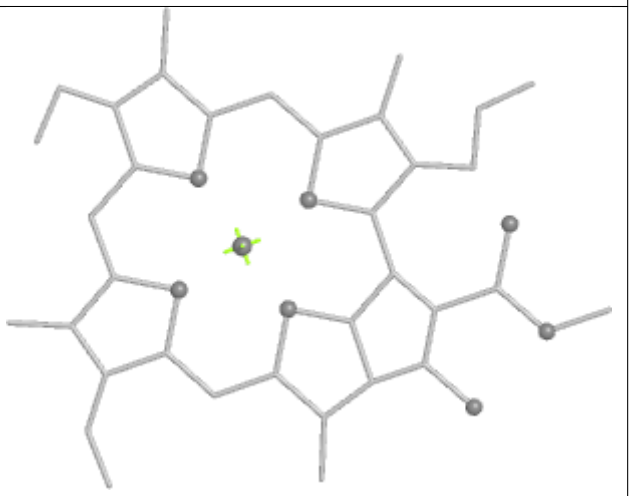
Bond lengths



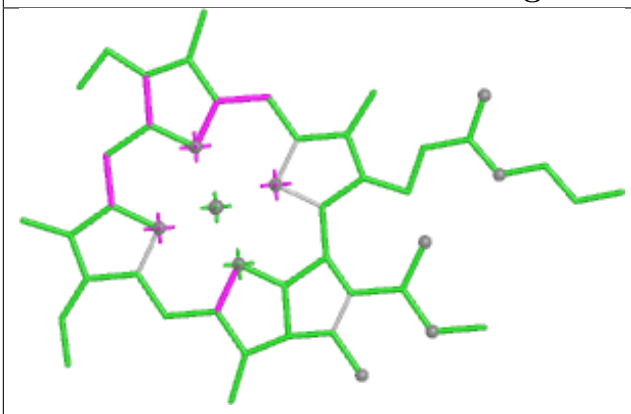
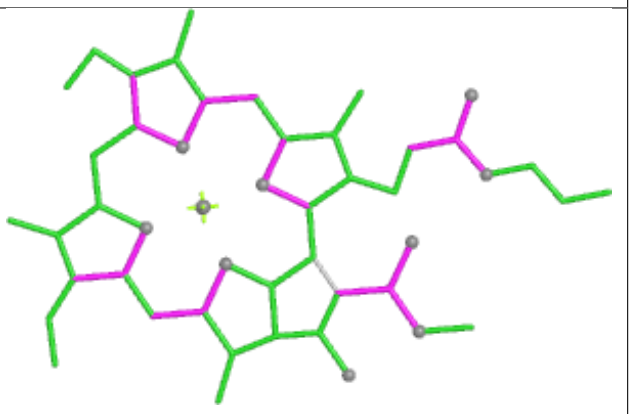
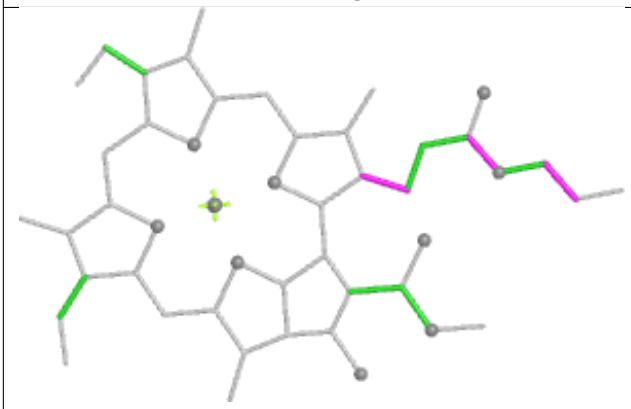
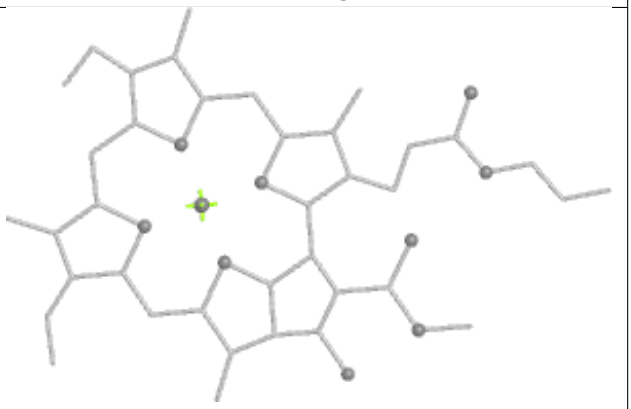
Bond angles

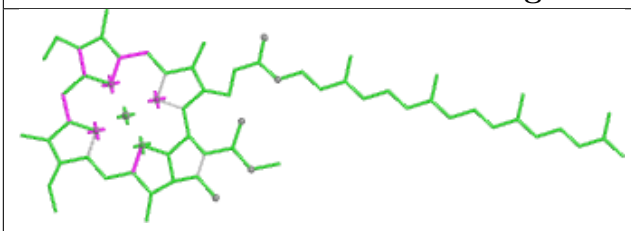
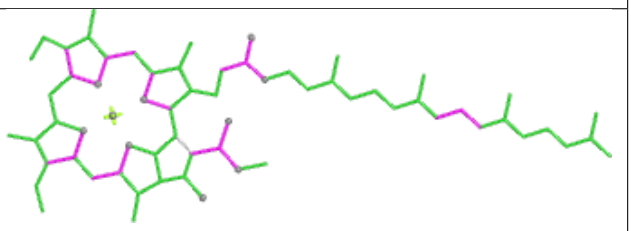
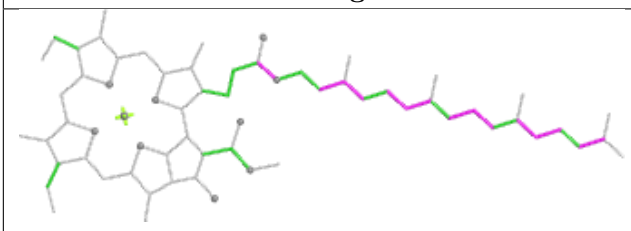
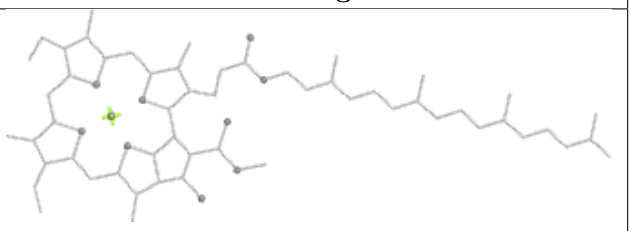


Torsions

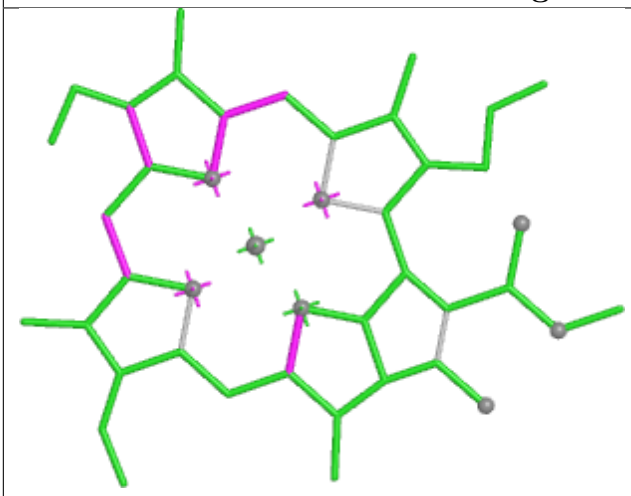


Rings

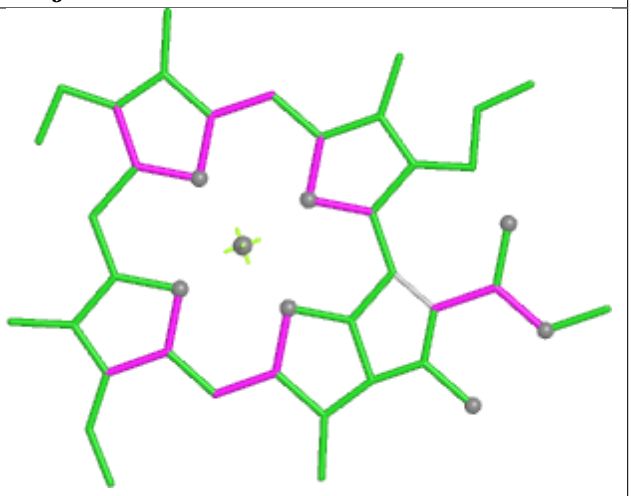
Ligand CLA A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

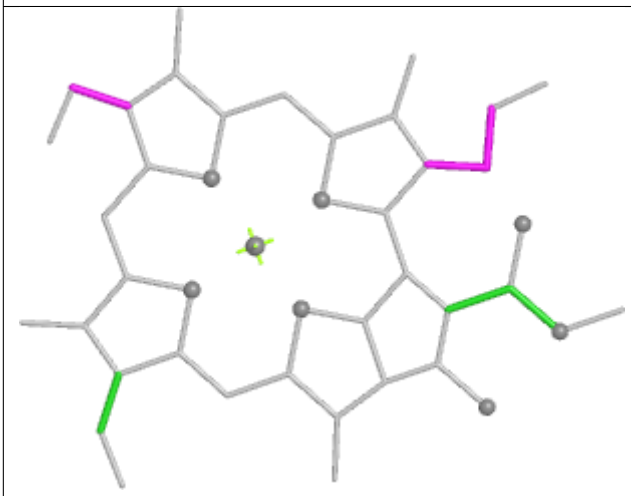
Ligand CLA j 214



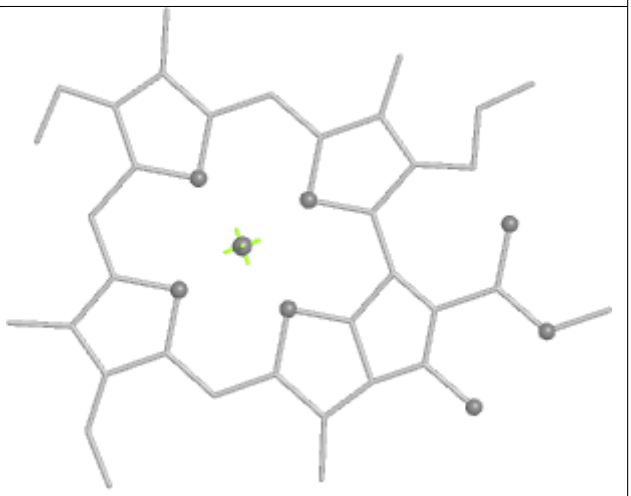
Bond lengths



Bond angles

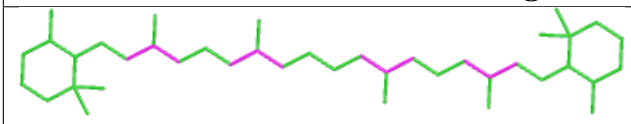


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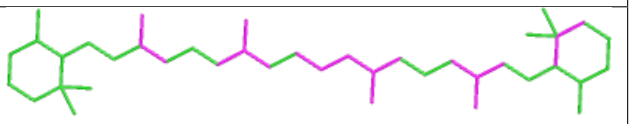


Rings

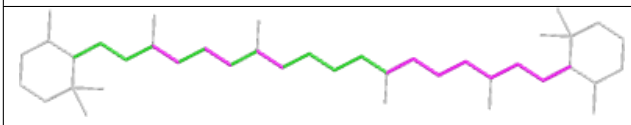
Ligand BCR B 832



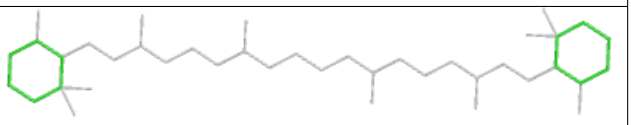
Bond lengths



Bond angles

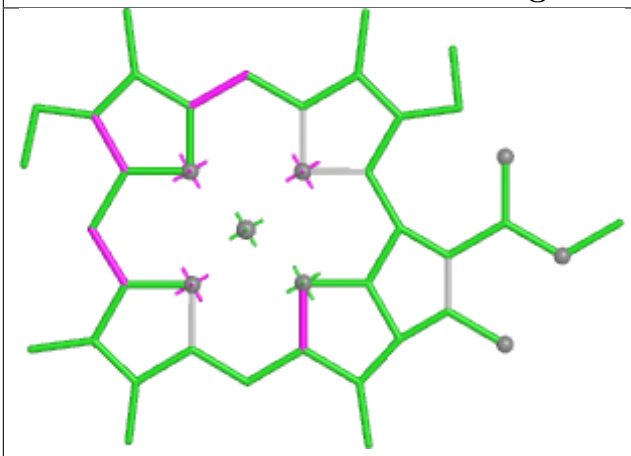


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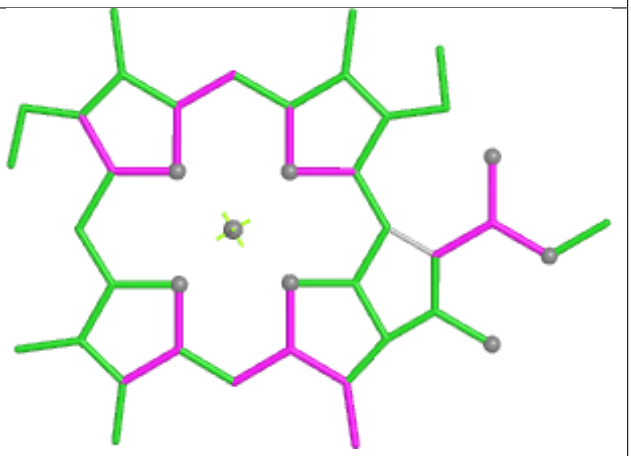


Rings

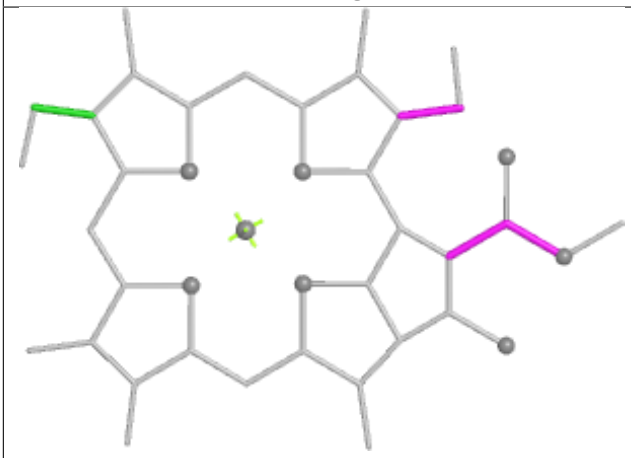
Ligand CLA e 204



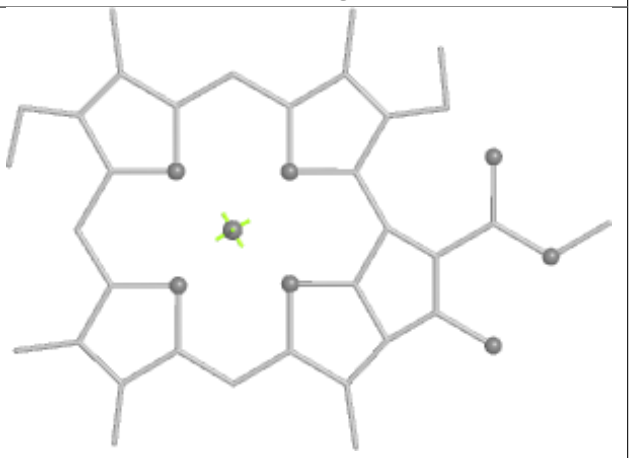
Bond lengths



Bond angles

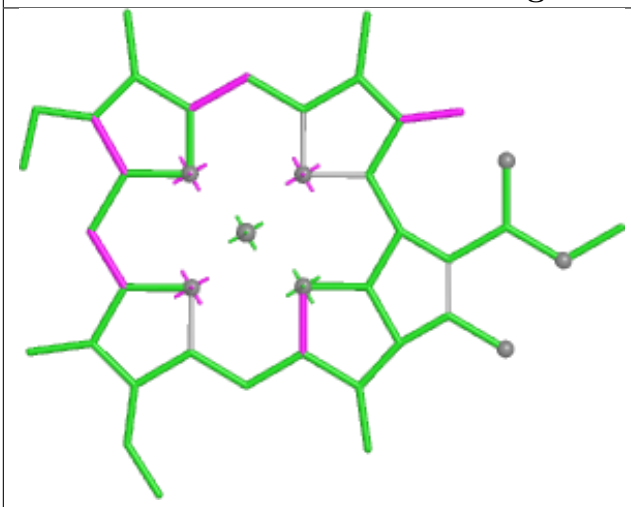


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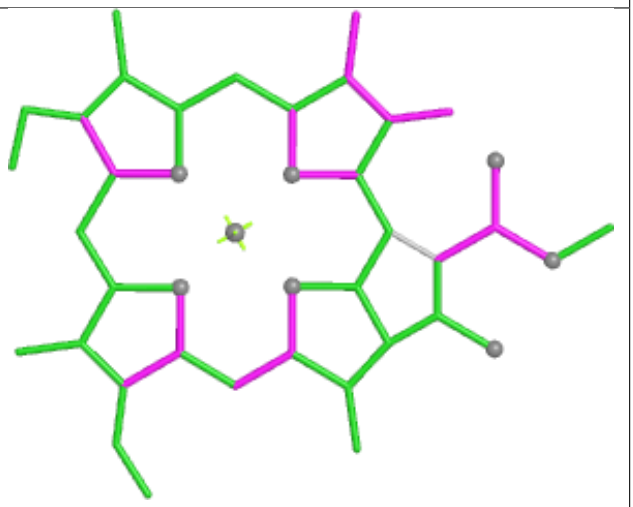


Rings

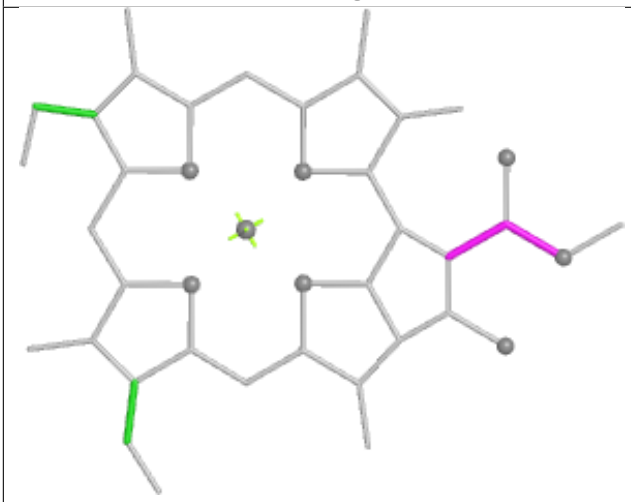
Ligand CLA d 301



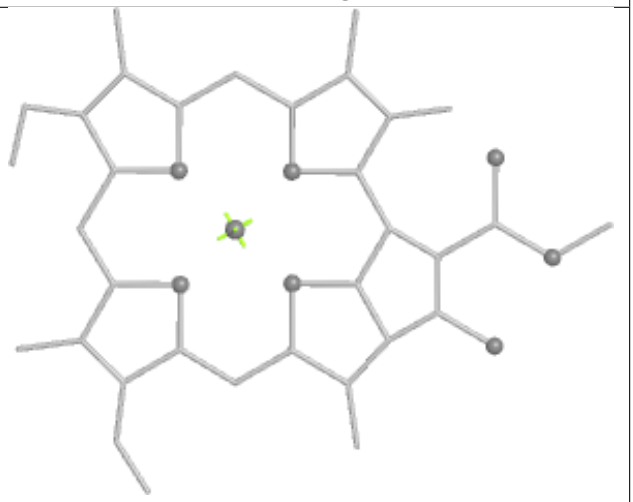
Bond lengths



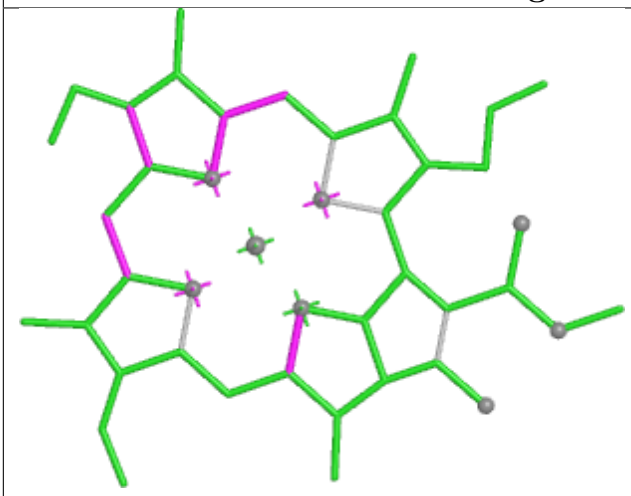
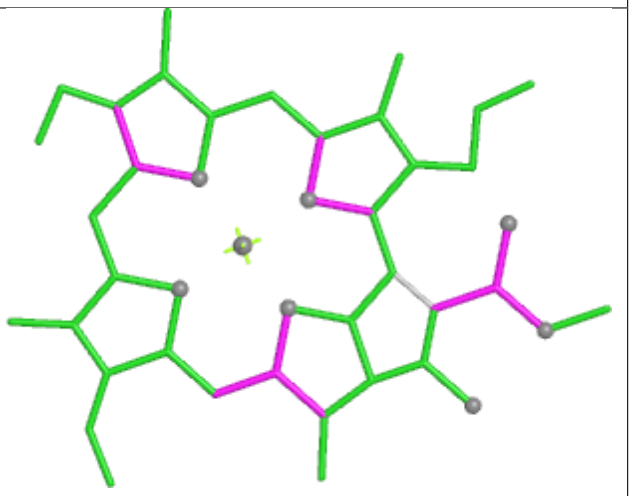
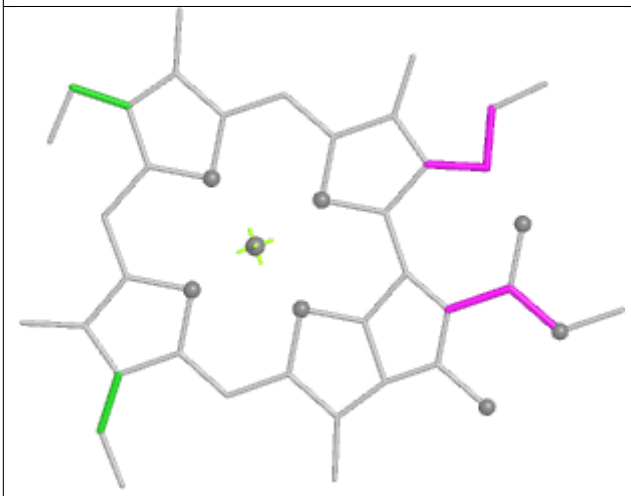
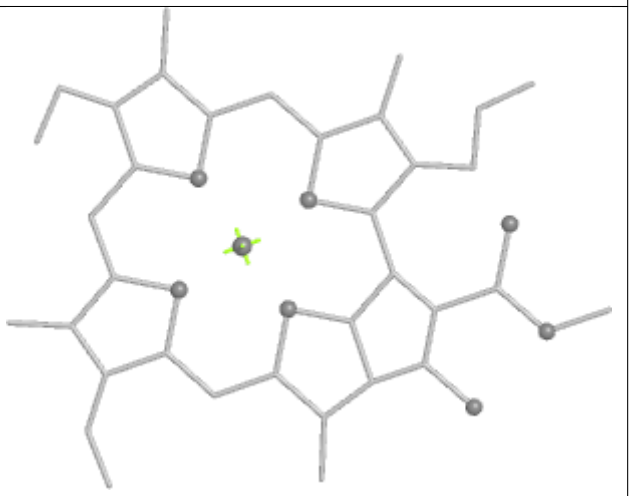
Bond angles

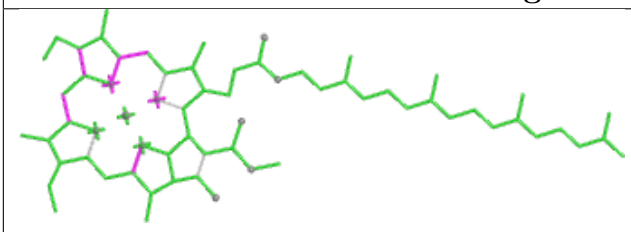
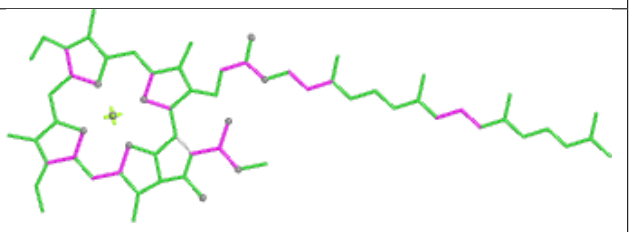
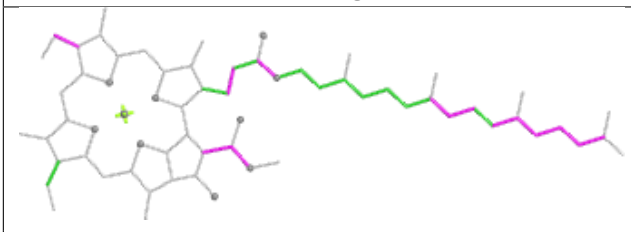
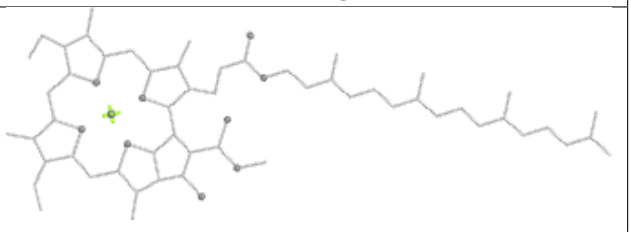


Torsions

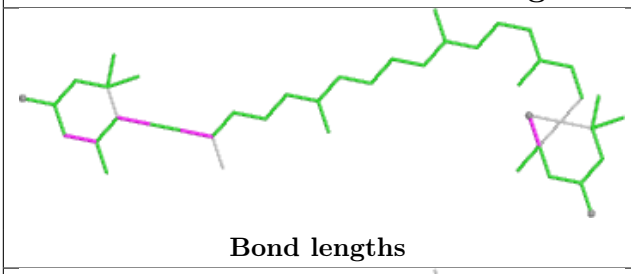


Rings

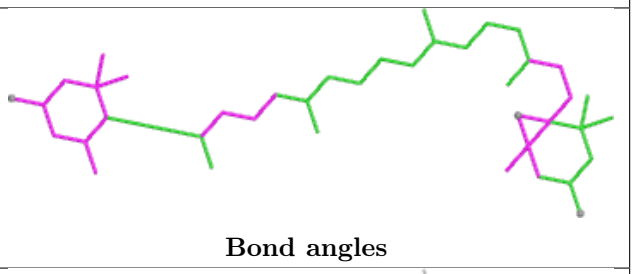
Ligand CLA a 211	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

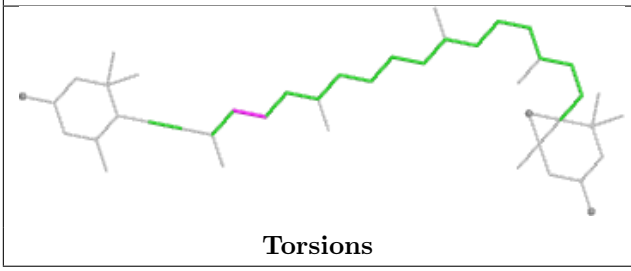
Ligand DD6 b 215



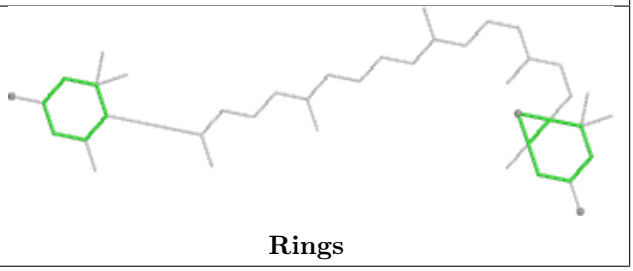
Bond lengths



Bond angles

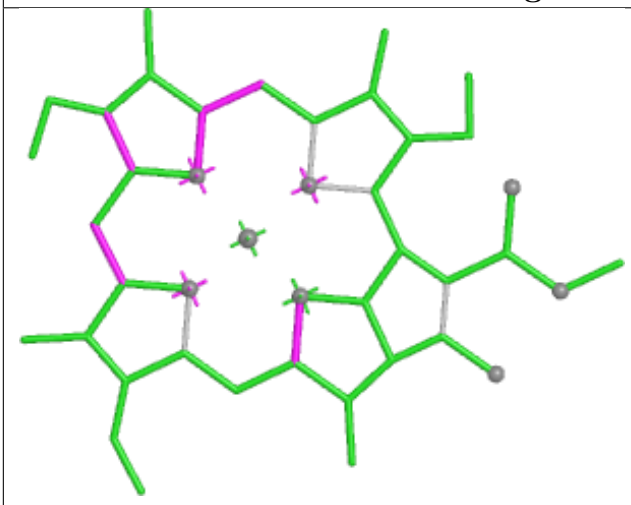


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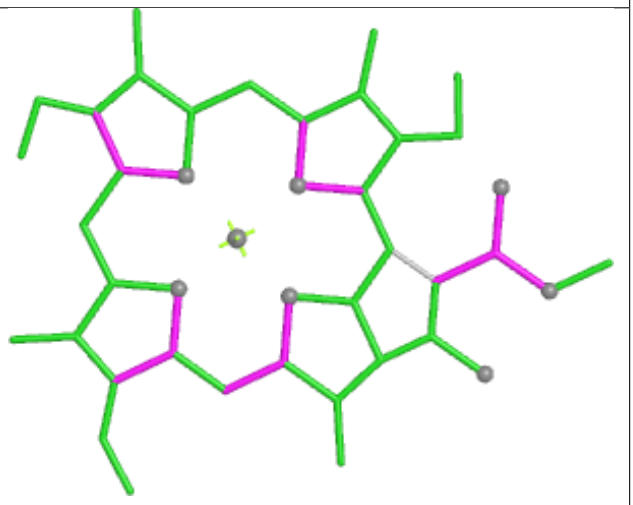


Rings

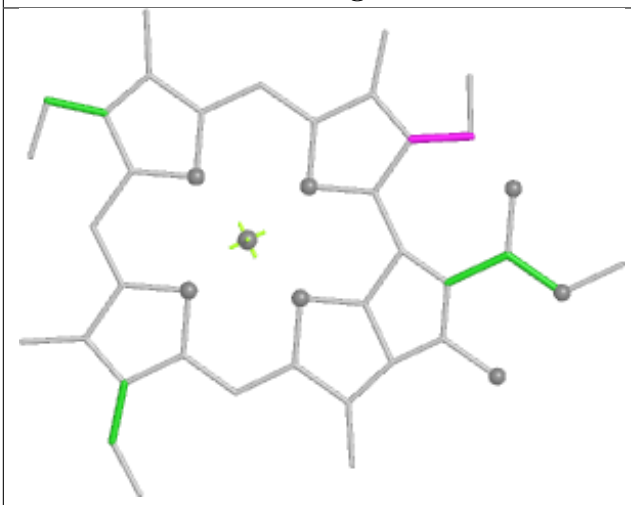
Ligand CLA B 806



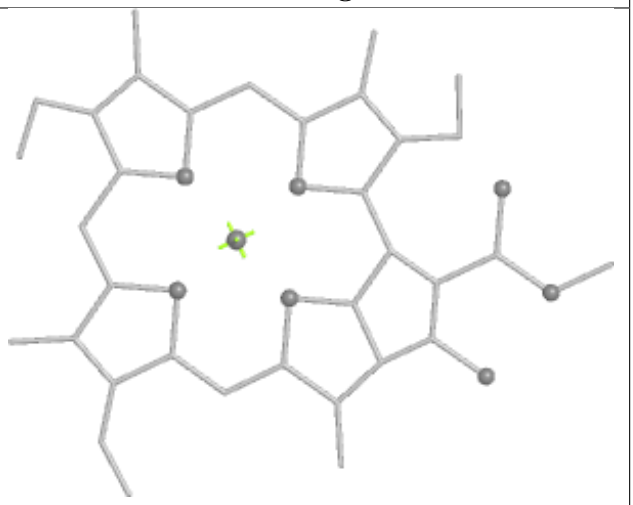
Bond lengths



Bond angles

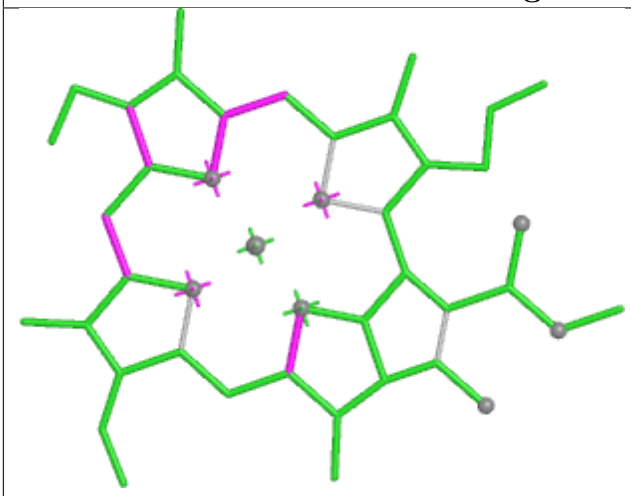


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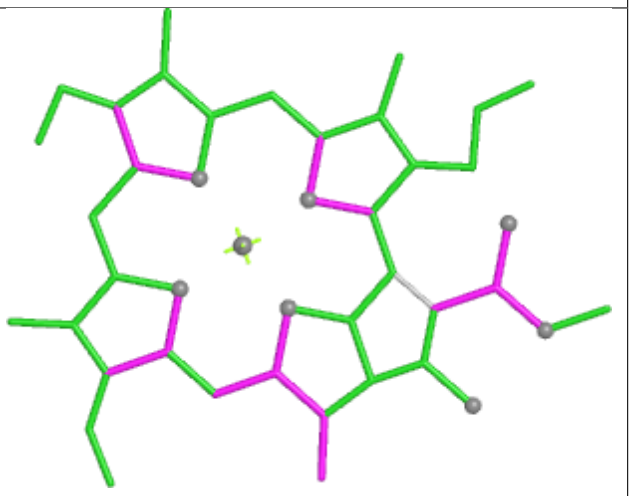


Rings

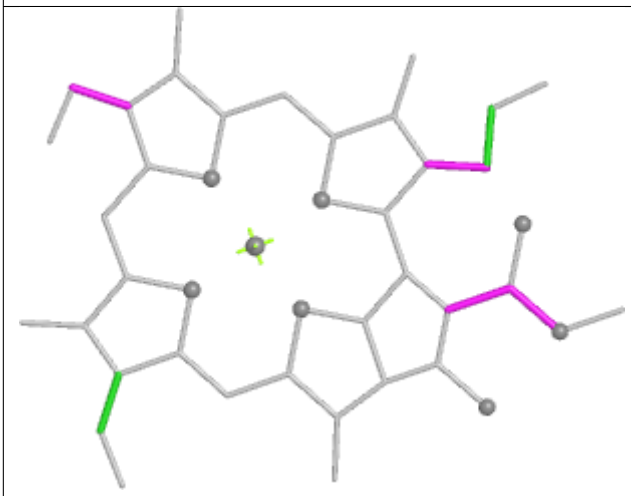
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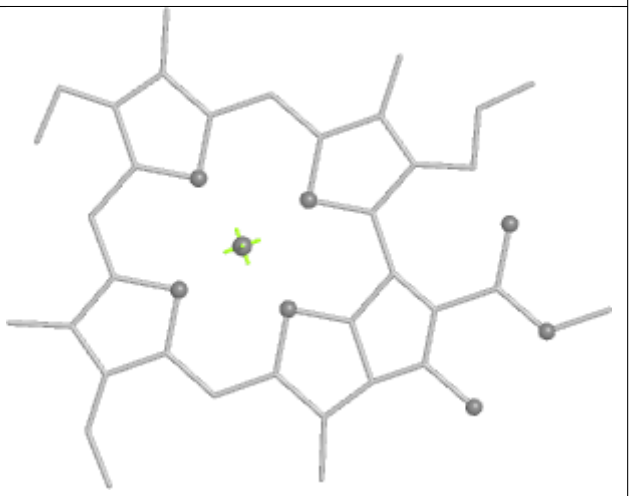
Bond lengths



Bond angles

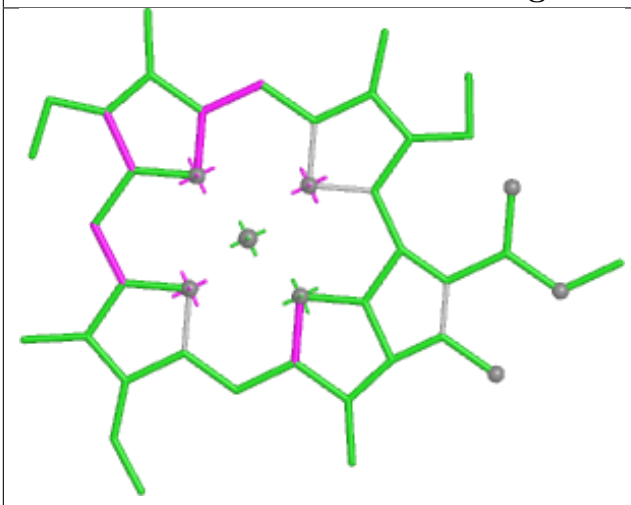


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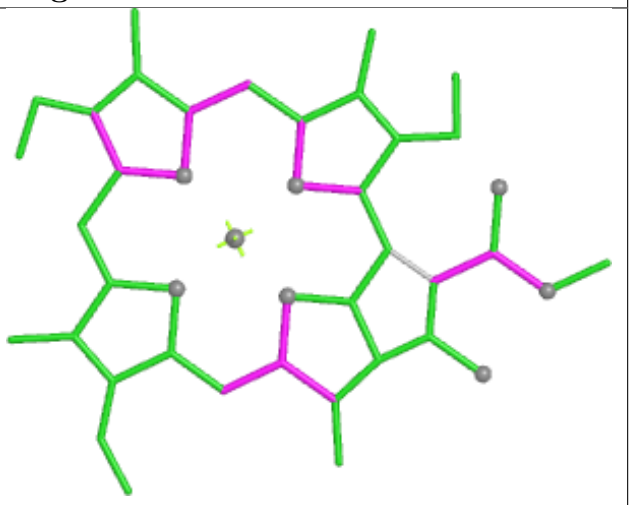


Rings

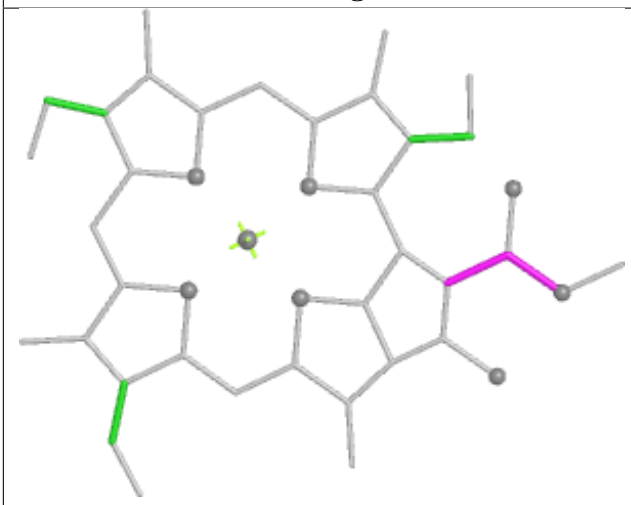
Ligand CLA g 211



Bond lengths



Bond angles

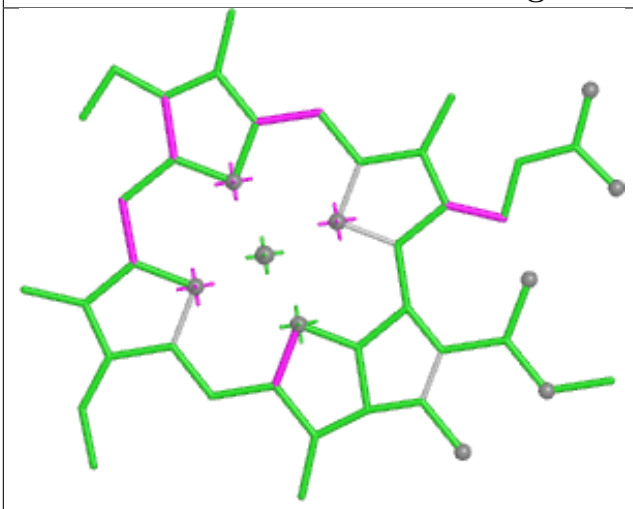


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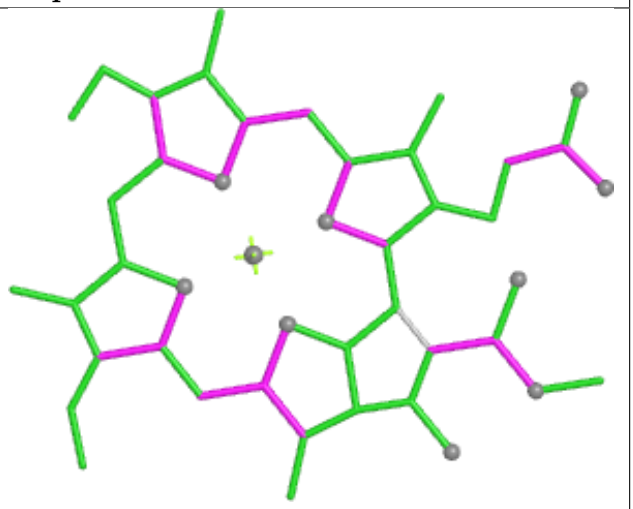


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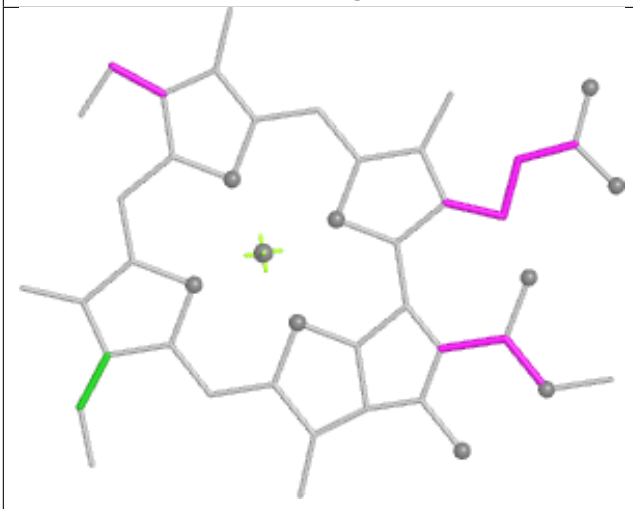
Ligand CLA p 607



Bond lengths



Bond angles

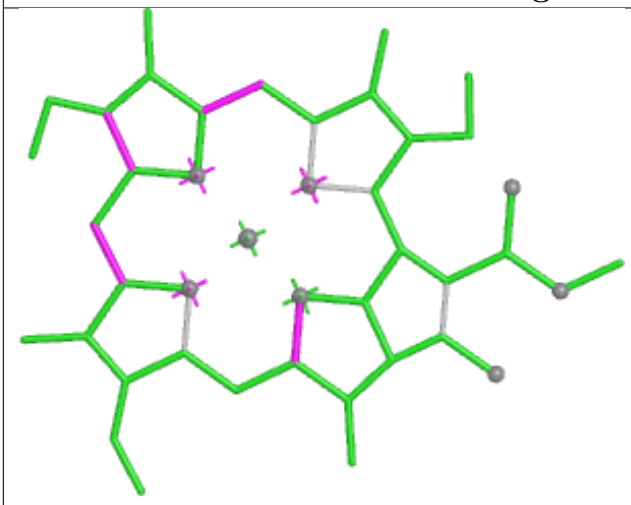


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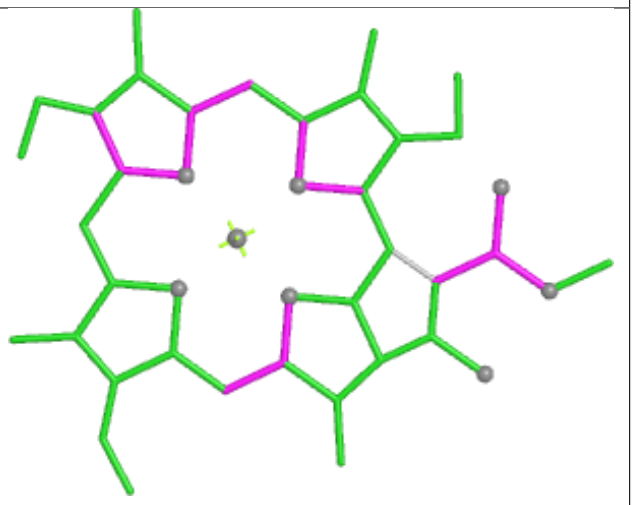


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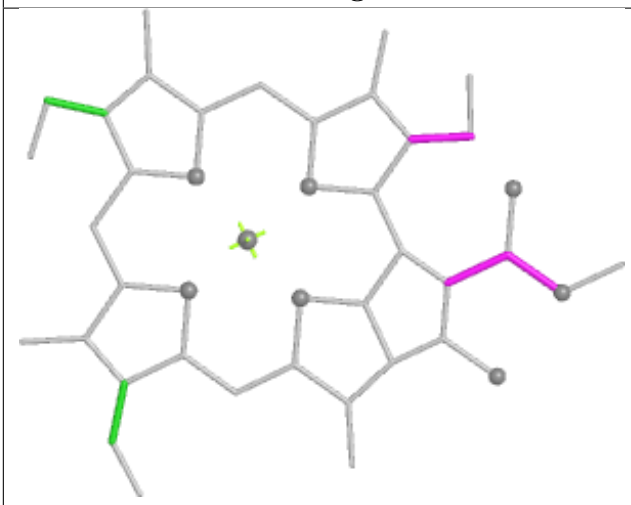
Ligand CLA l 601



Bond lengths



Bond angles

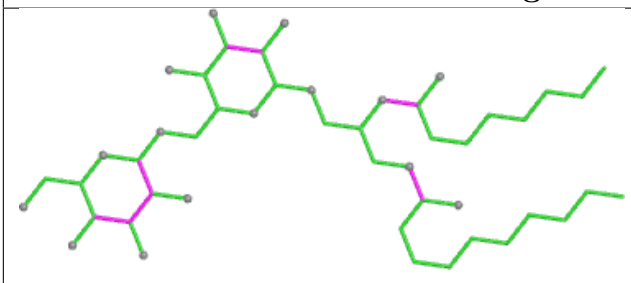


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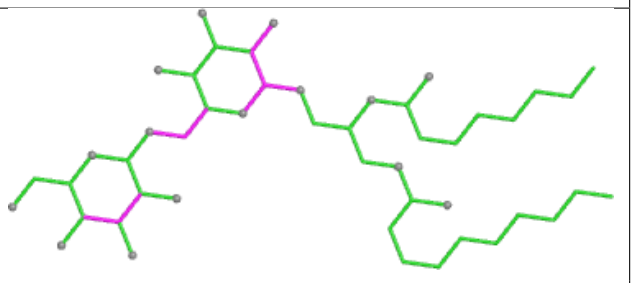


Rings

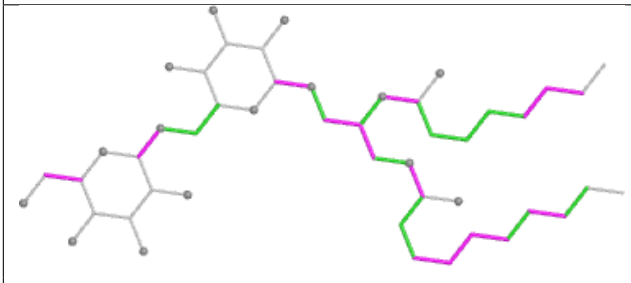
Ligand DGD b 202



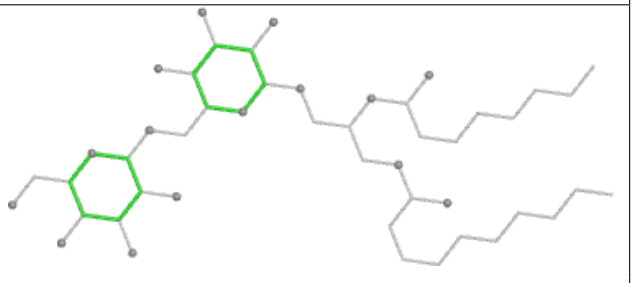
Bond lengths



Bond angles

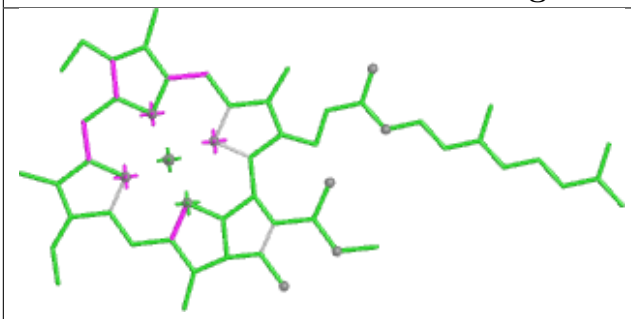


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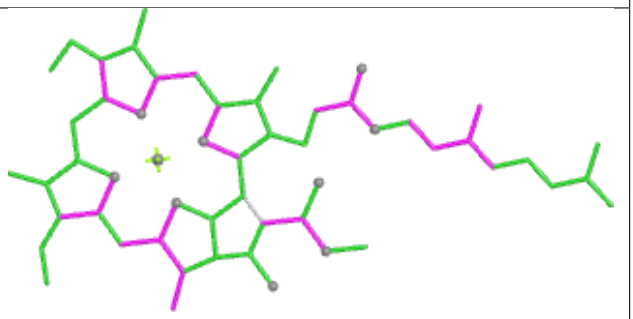


Rings

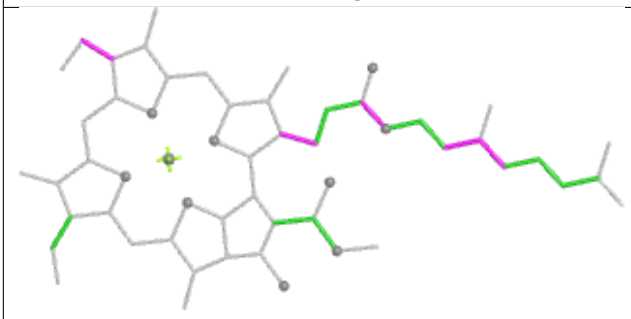
Ligand CLA e 213



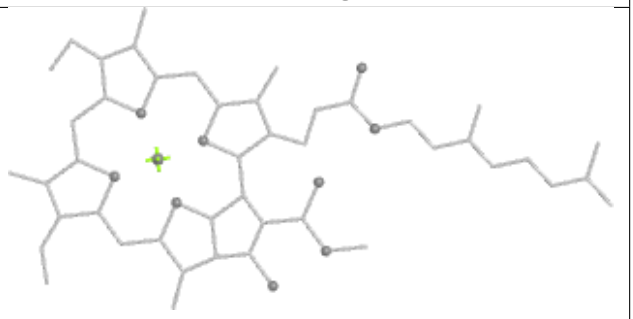
Bond lengths



Bond angles

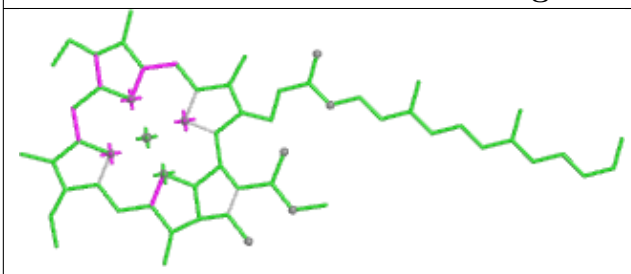


Torsions

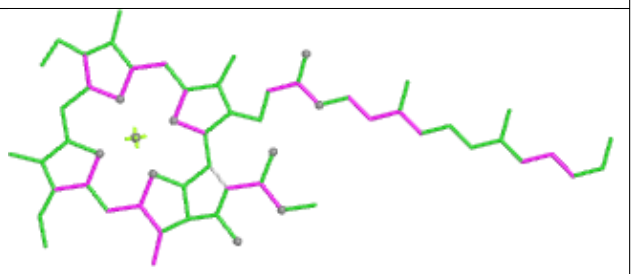


Rings

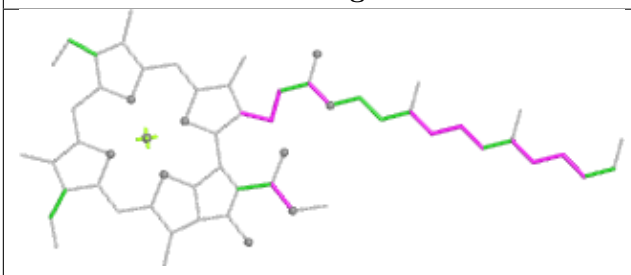
Ligand CLA f 610



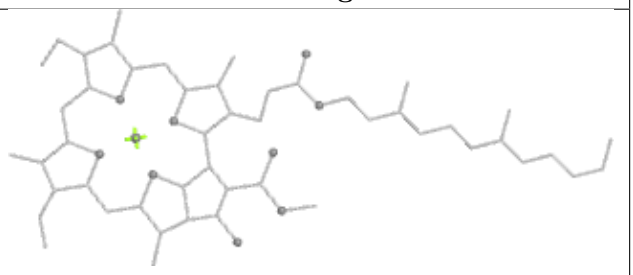
Bond lengths



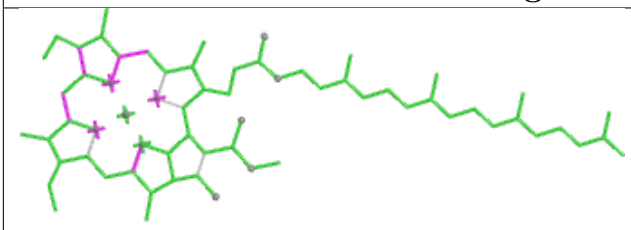
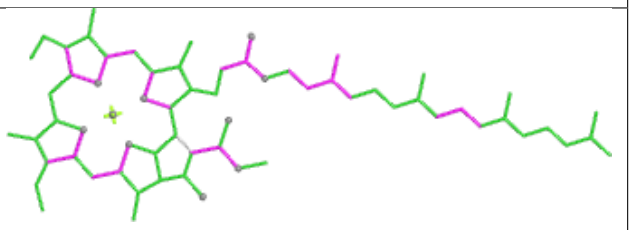
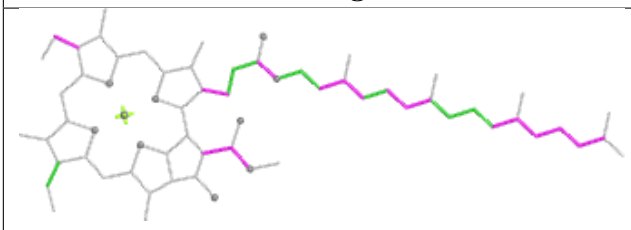
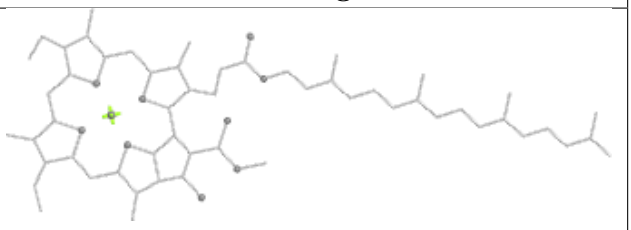
Bond angles

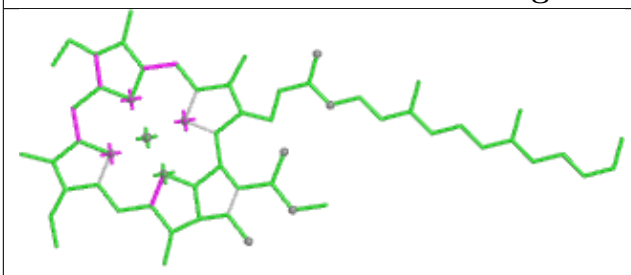
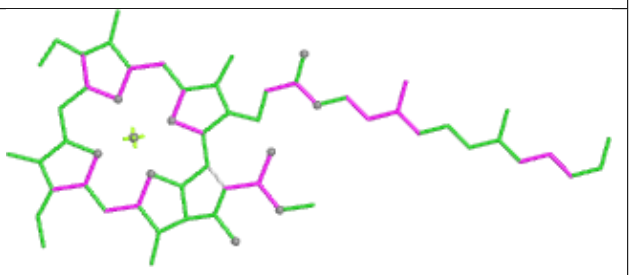
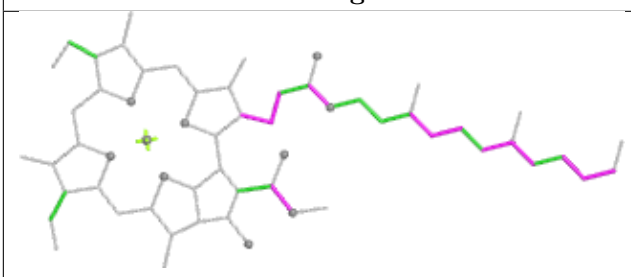
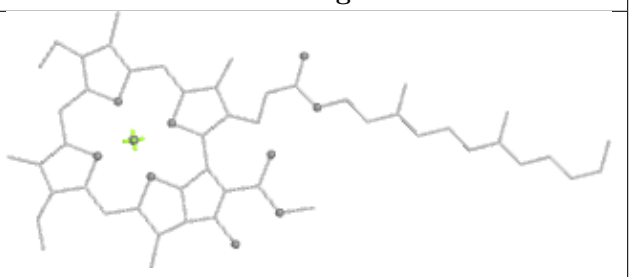


Torsions

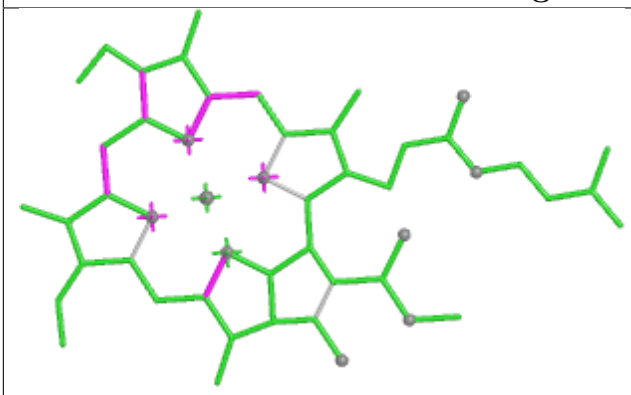


Rings

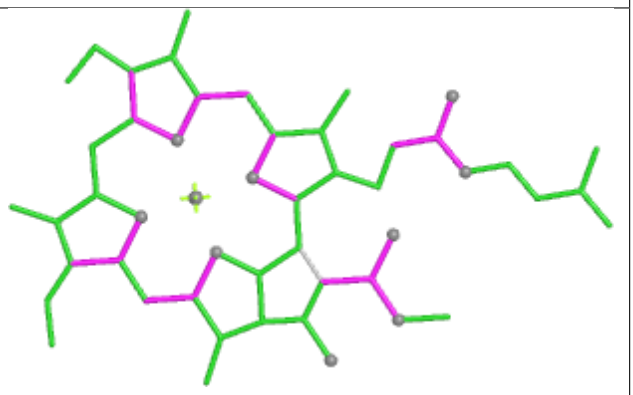
Ligand CLA B 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

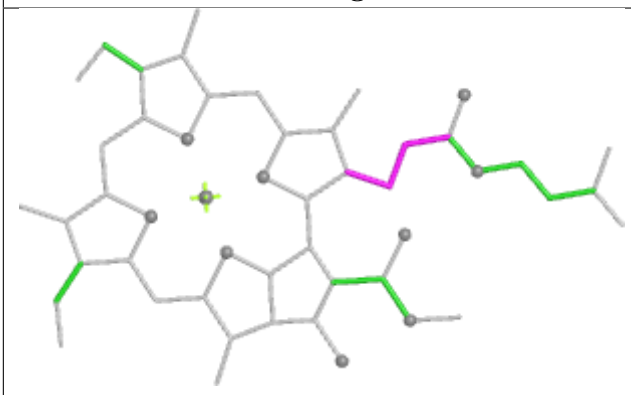
Ligand CLA i 213



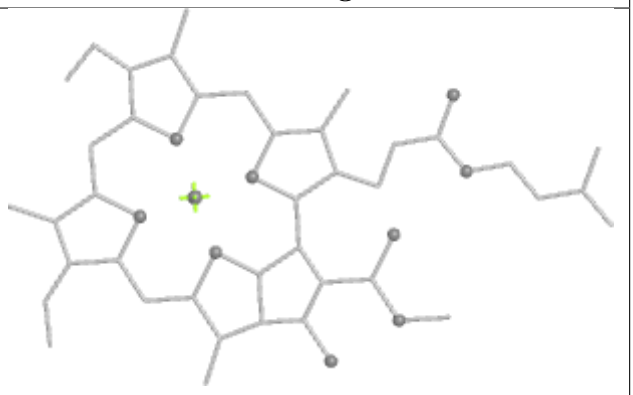
Bond lengths



Bond angles

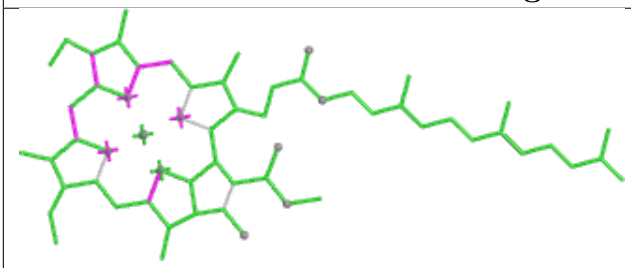


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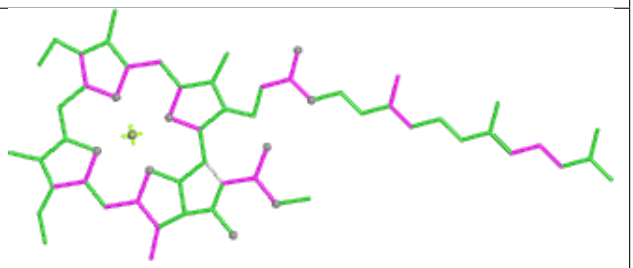


Rings

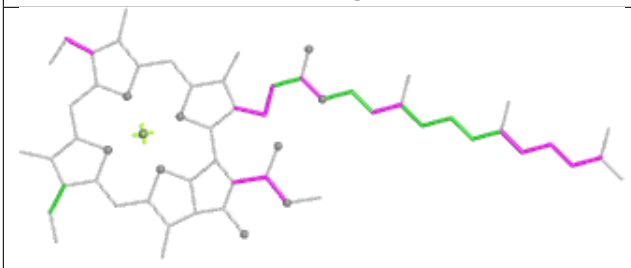
Ligand CLA A 844



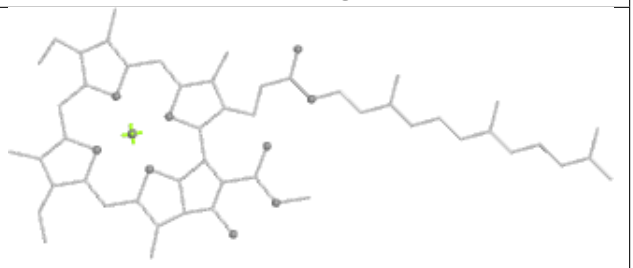
Bond lengths



Bond angles

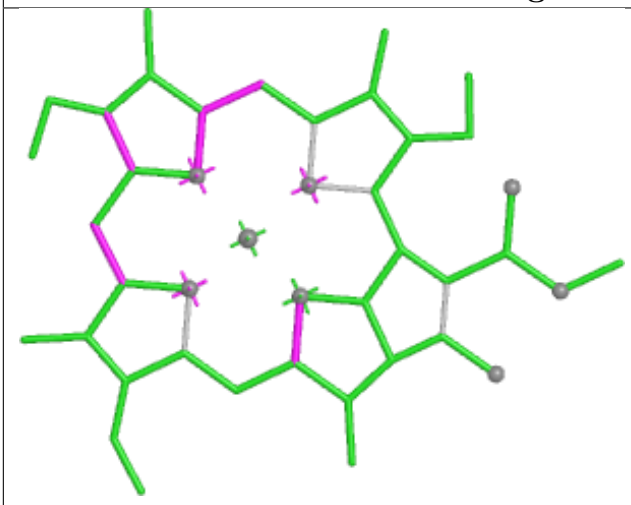


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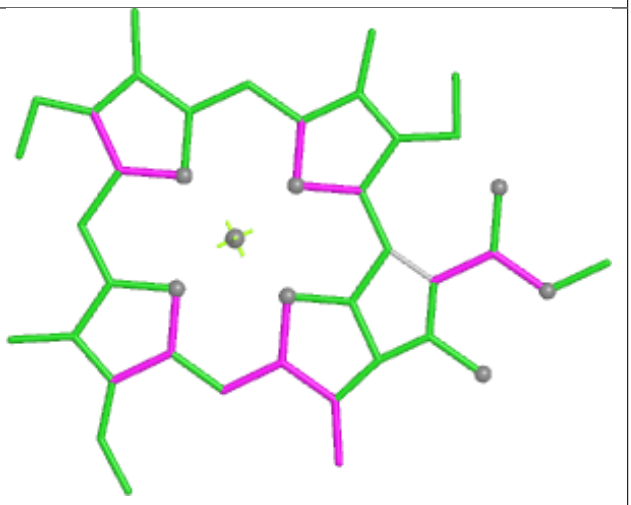


Rings

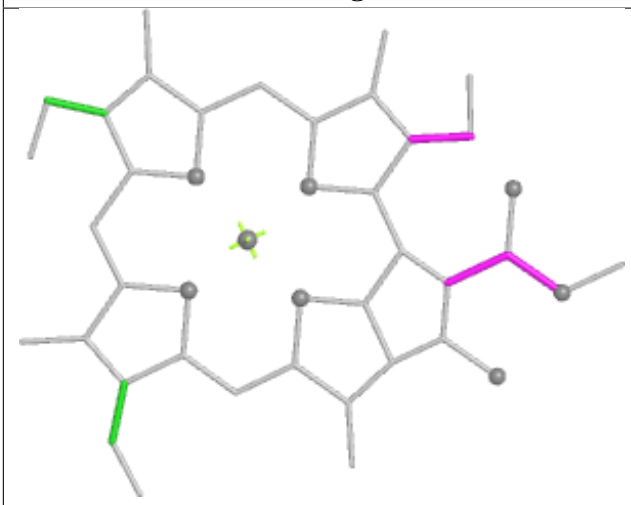
Ligand CLA k 204



Bond lengths



Bond angles

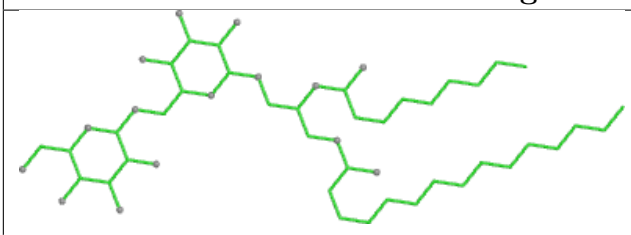


Torsions

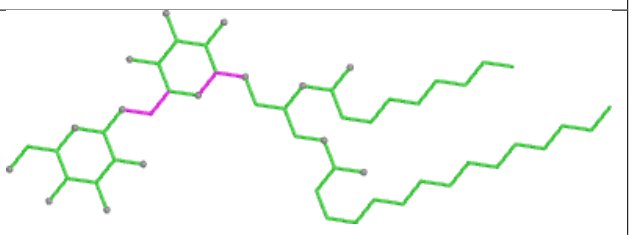


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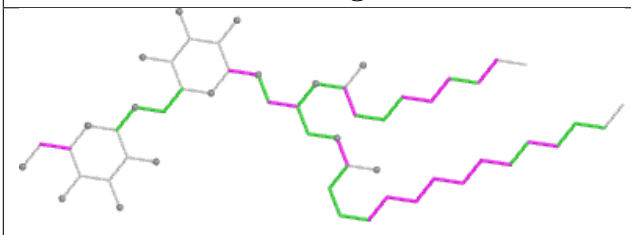
Ligand DGD B 849



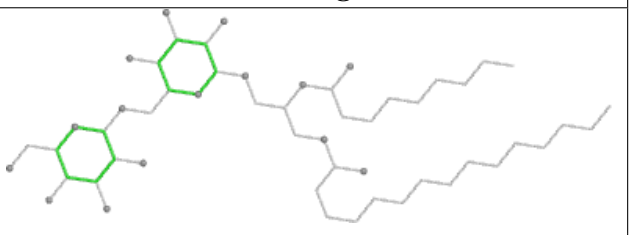
Bond lengths



Bond angles

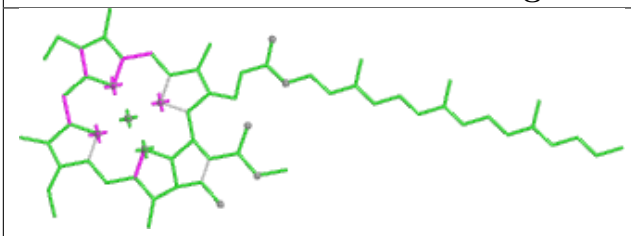


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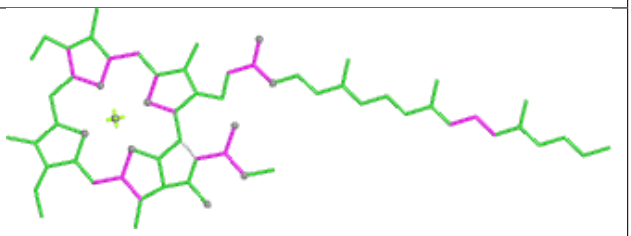


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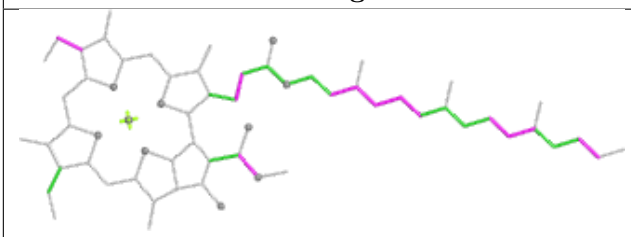
Ligand CLA A 840



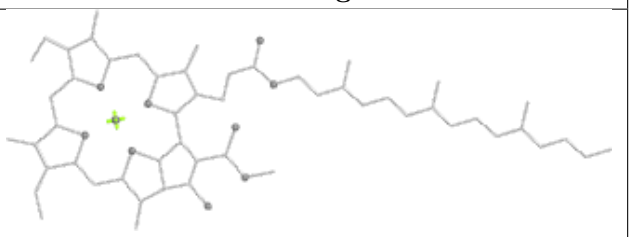
Bond lengths



Bond angles

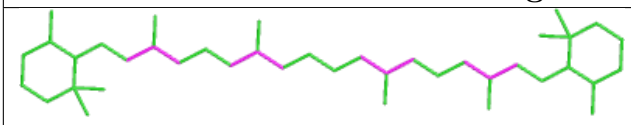


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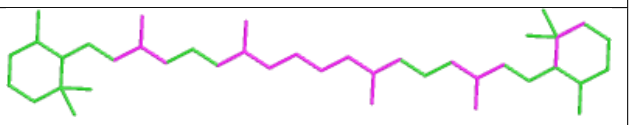


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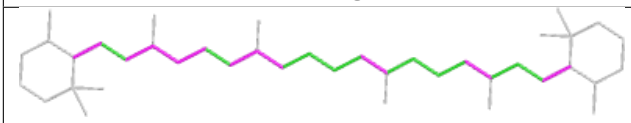
Ligand BCR J 101



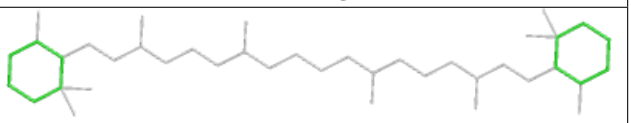
Bond lengths



Bond angles

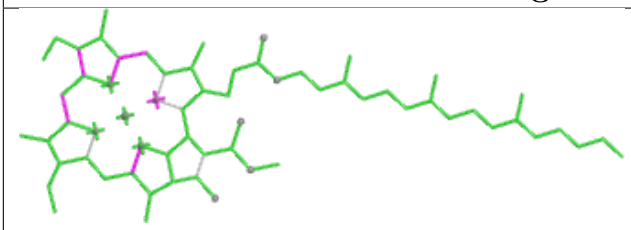


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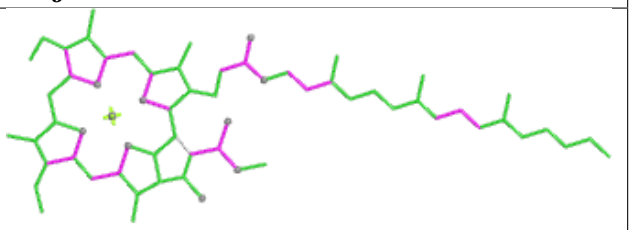


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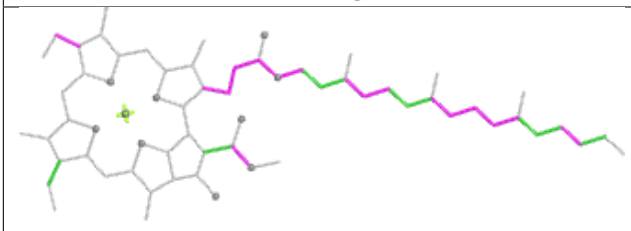
Ligand CLA j 209



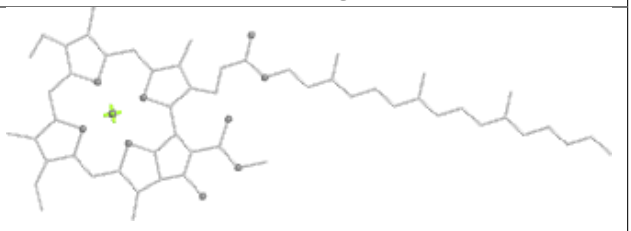
Bond lengths



Bond angles

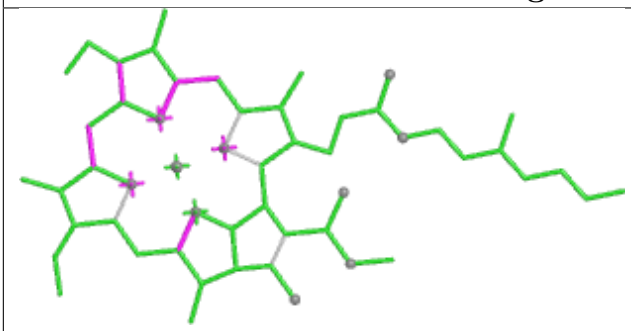


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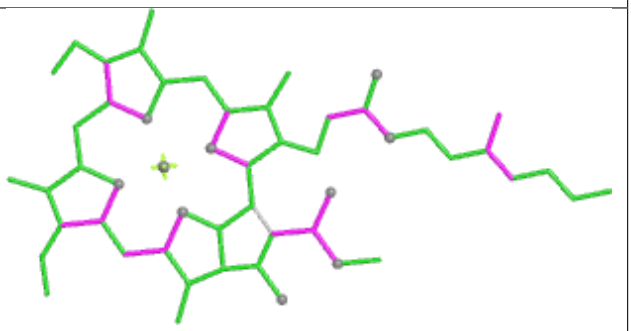


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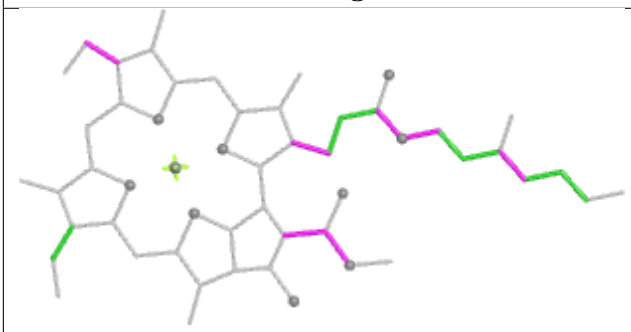
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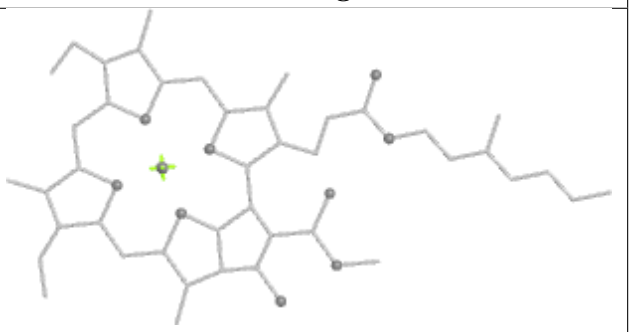
Bond lengths



Bond angles

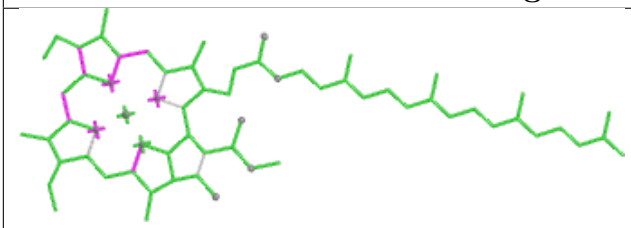


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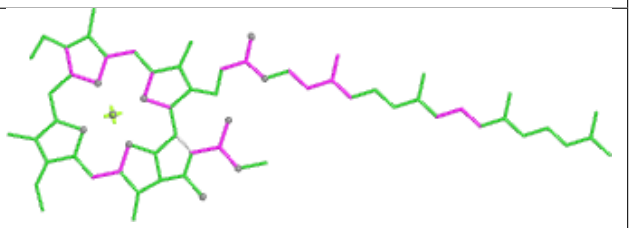


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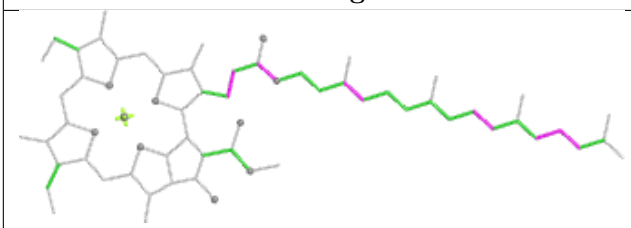
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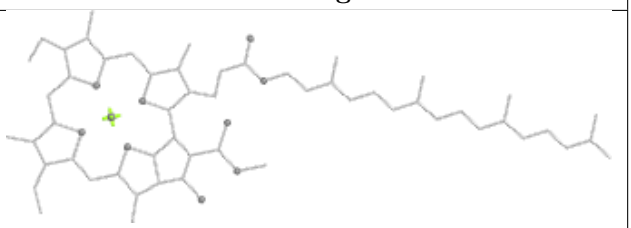
Bond lengths



Bond angles

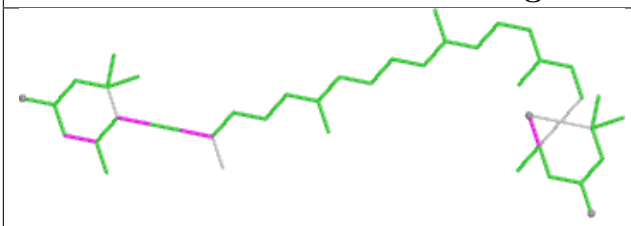


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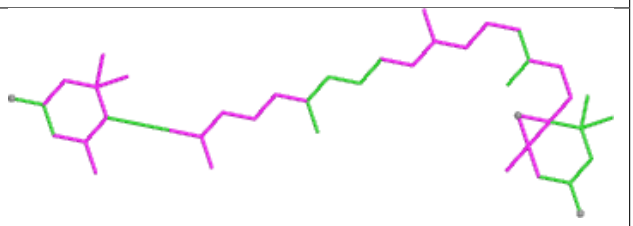


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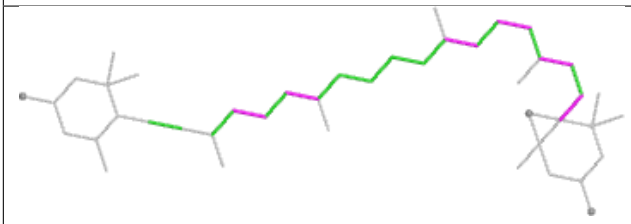
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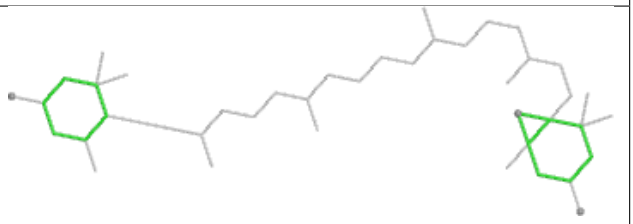
Bond lengths



Bond angles

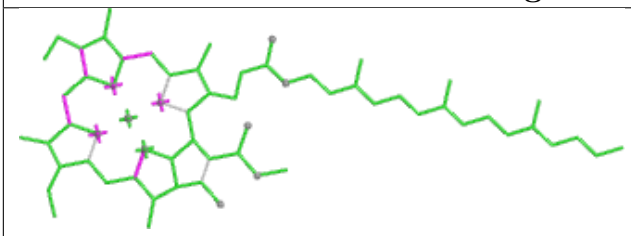


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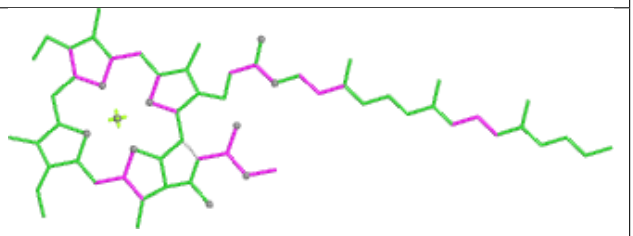


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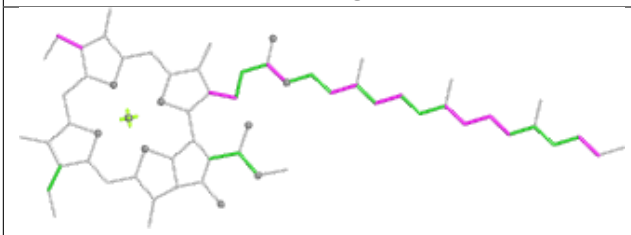
Ligand CLA B 843



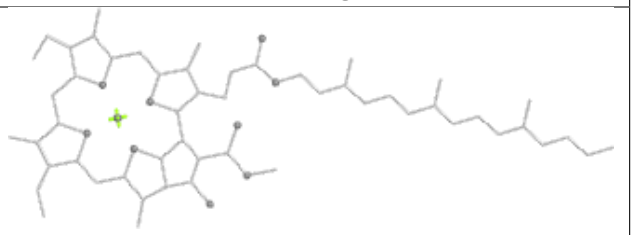
Bond lengths



Bond angles

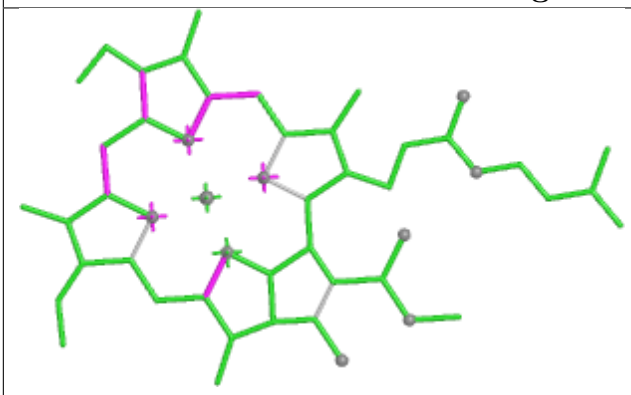


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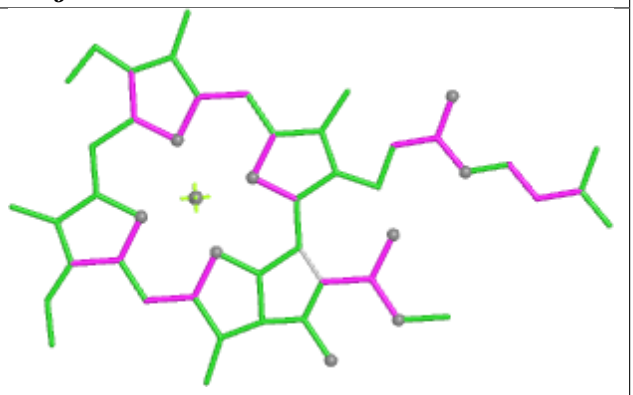


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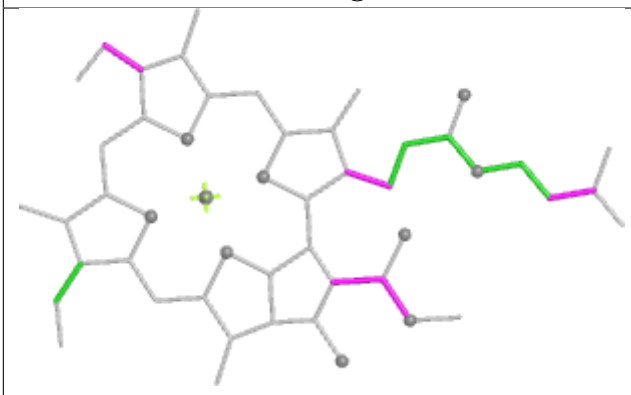
Ligand CLA j 203



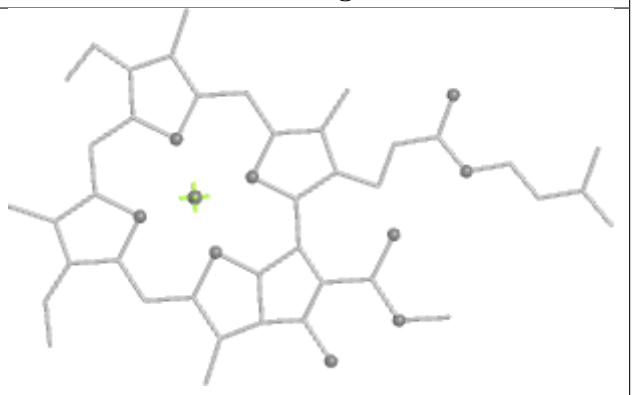
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Bond angles

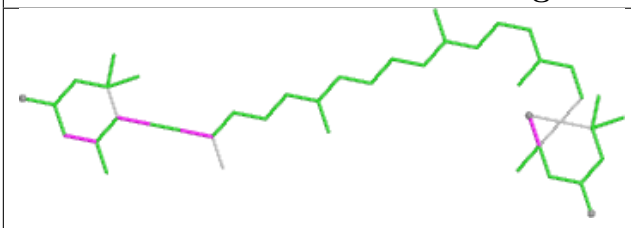


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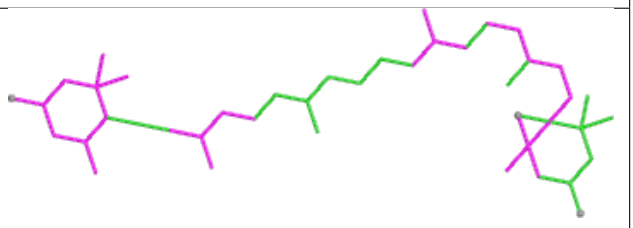


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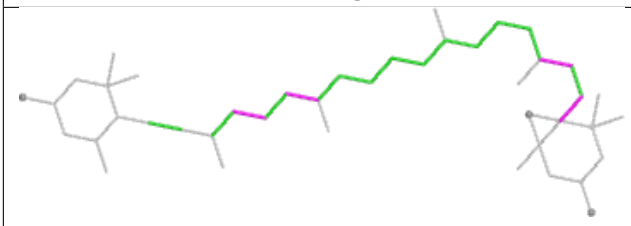
Ligand DD6 f 614



Bond lengths



Bond angles

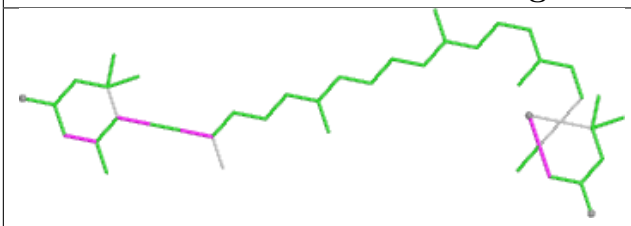


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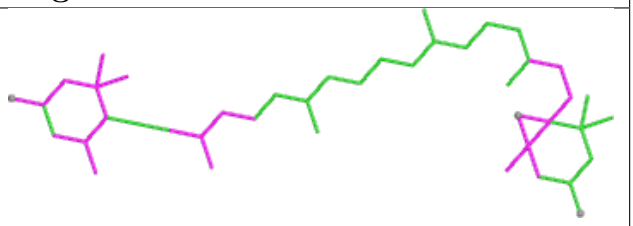


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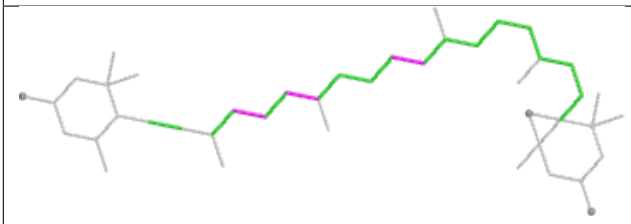
Ligand DD6 g 217



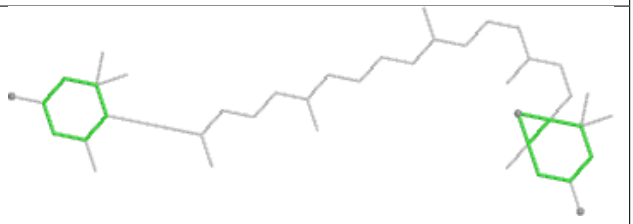
Bond lengths



Bond angles

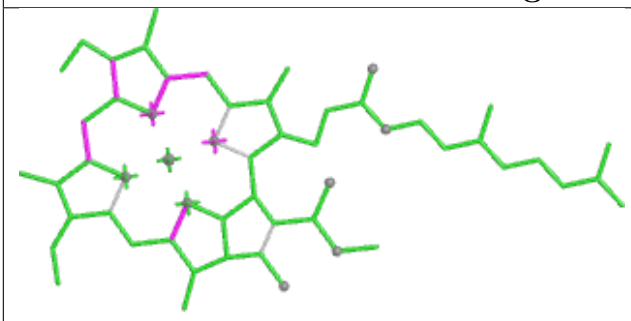


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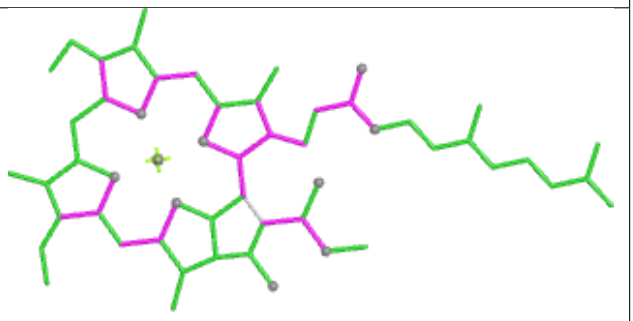


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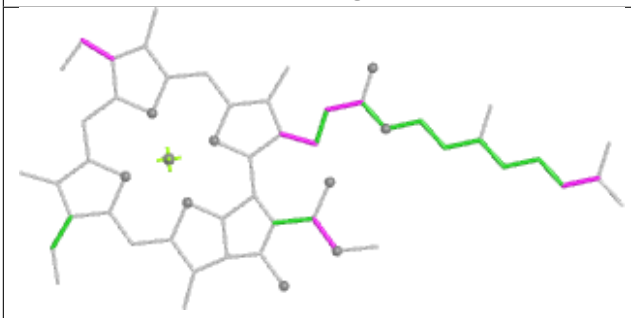
Ligand CLA A 850



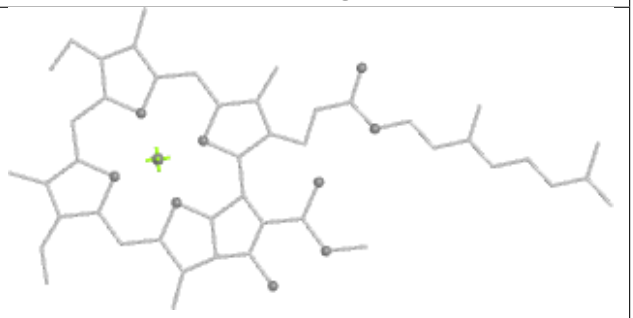
Bond lengths



Bond angles

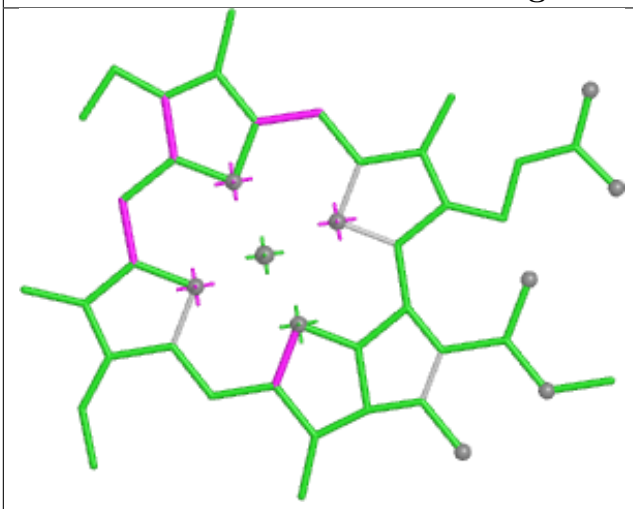


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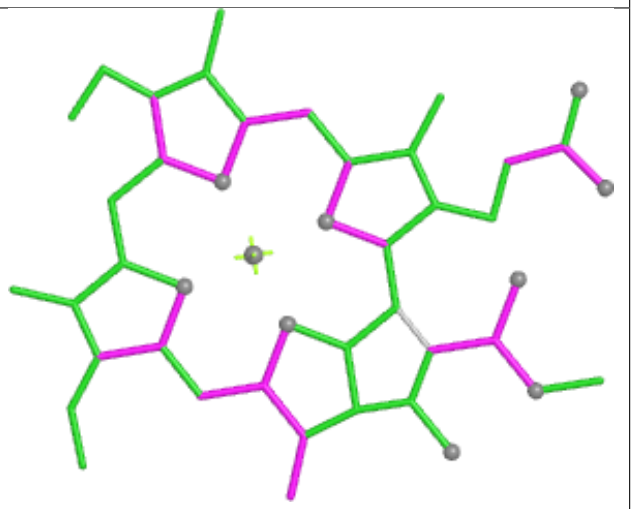


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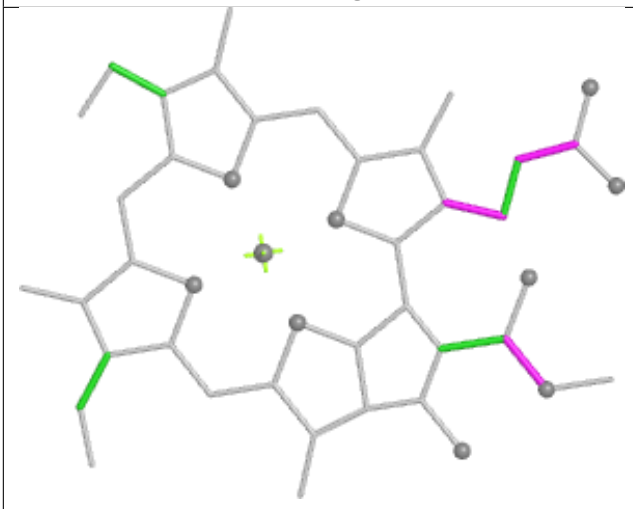
Ligand CLA o 606



Bond lengths



Bond angles

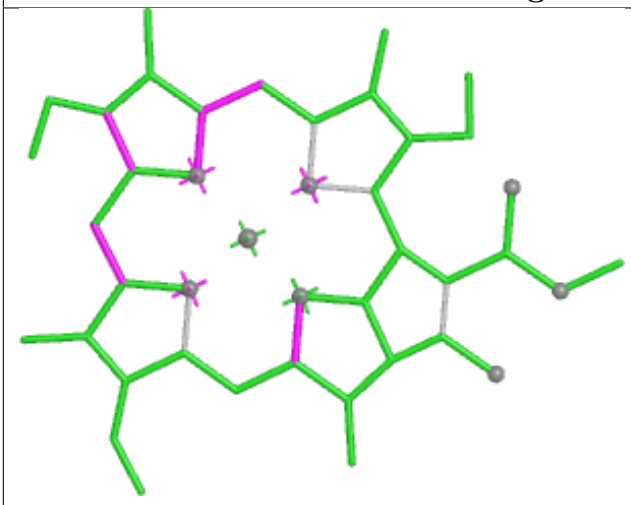


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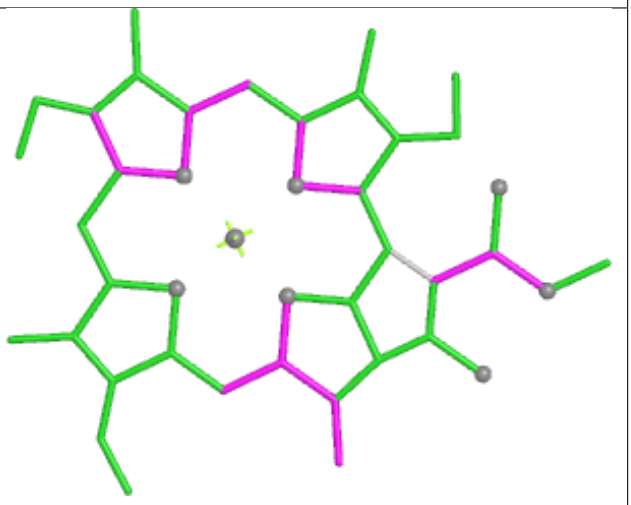


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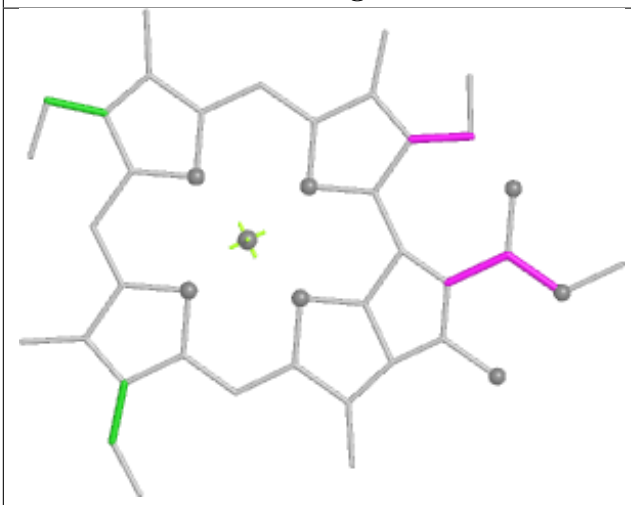
Ligand CLA d 305



Bond lengths



Bond angles

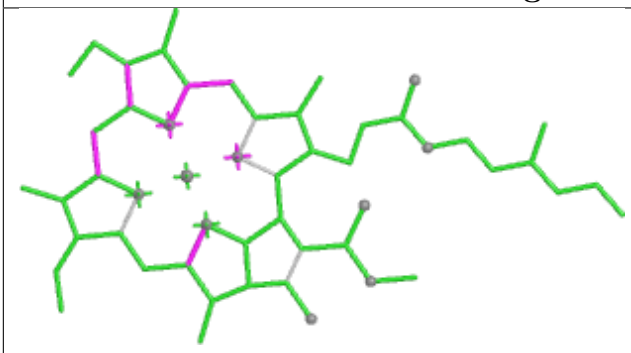


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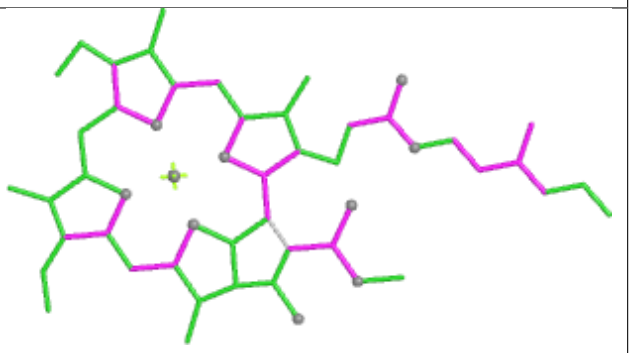


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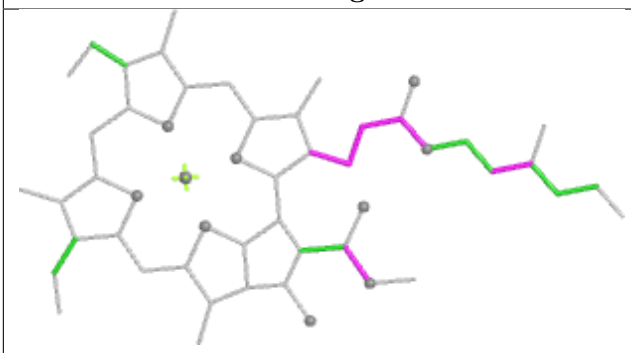
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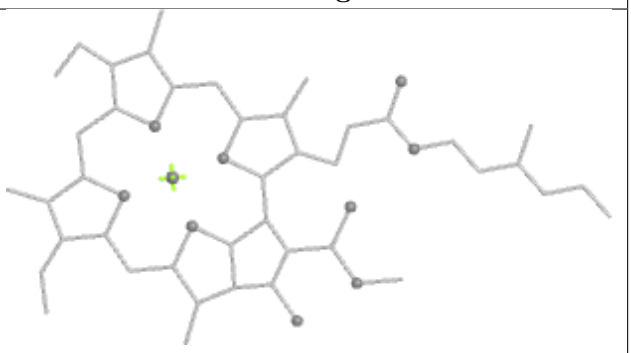
Bond lengths



Bond angles

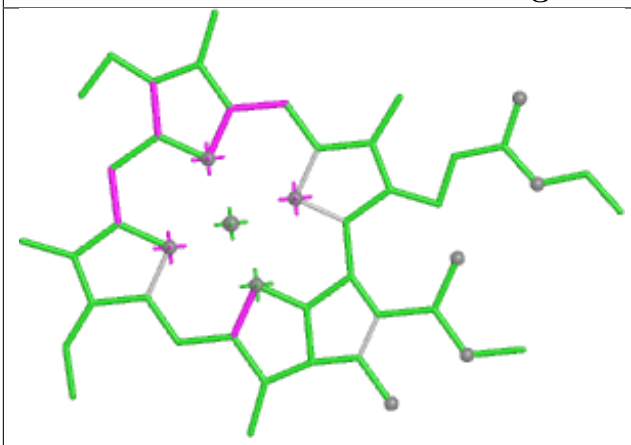


Torsions

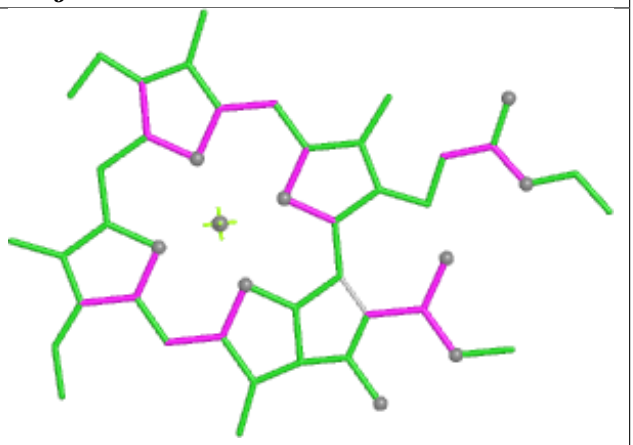


Rings

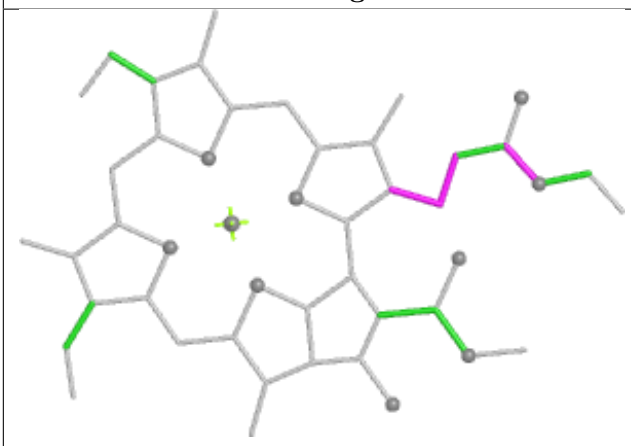
Ligand CLA j 207



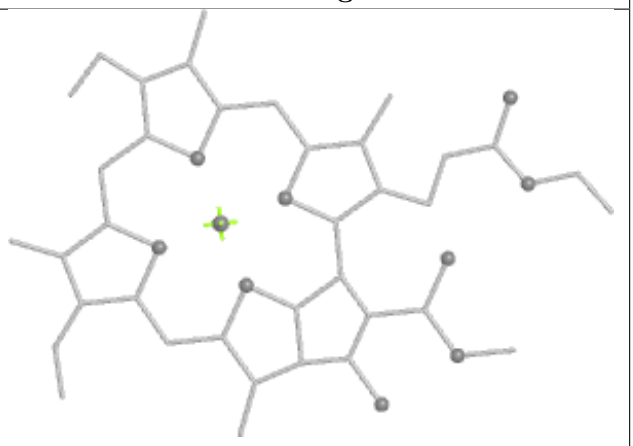
Bond lengths



Bond angles

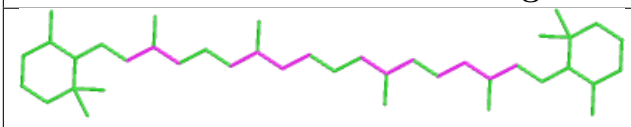


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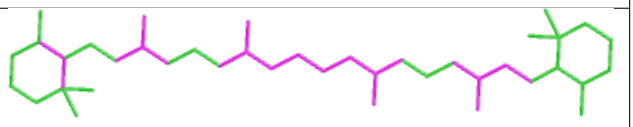


Rings

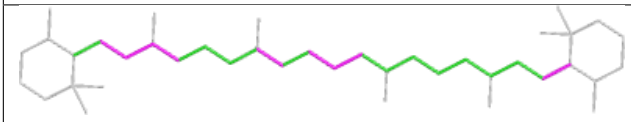
Ligand BCR A 837



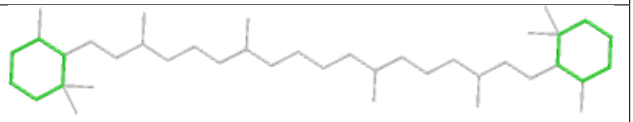
Bond lengths



Bond angles

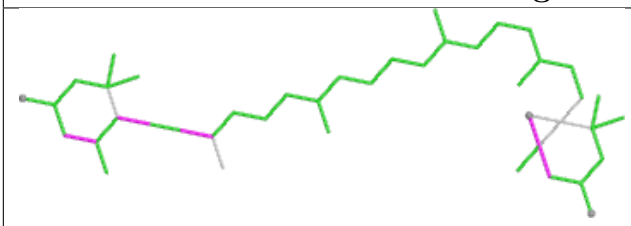


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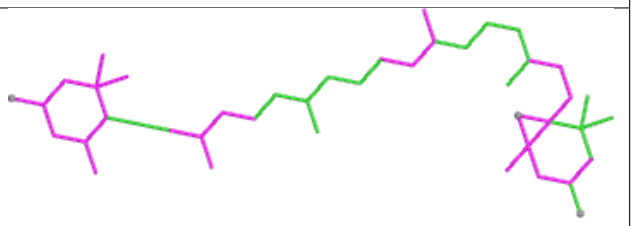


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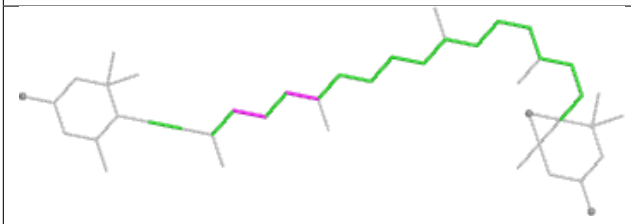
Ligand DD6 l 614



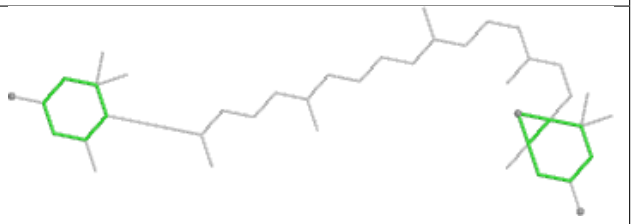
Bond lengths



Bond angles

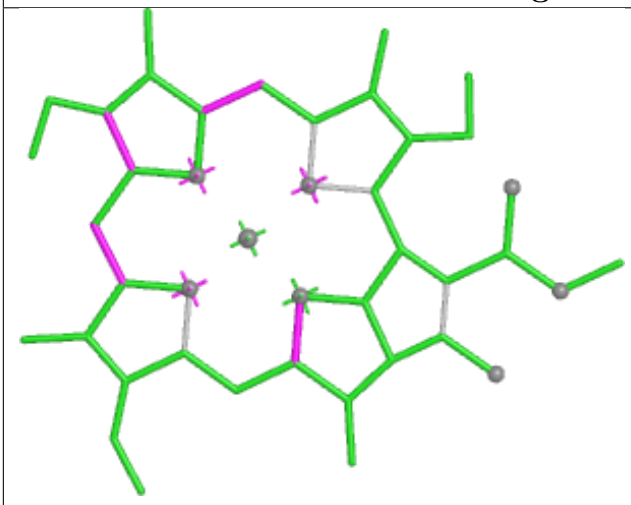


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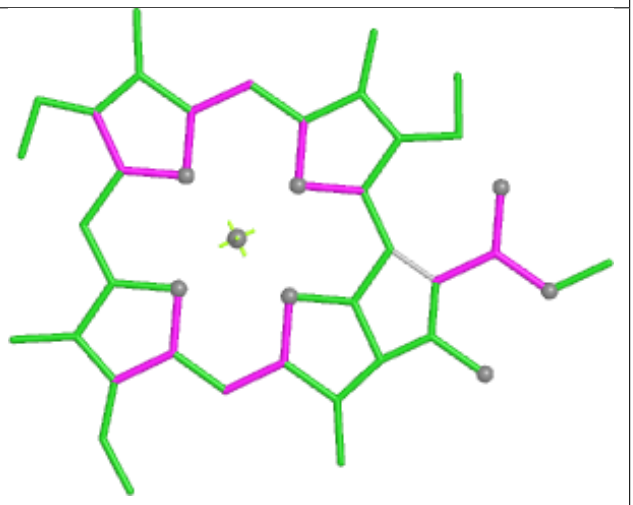


Rings

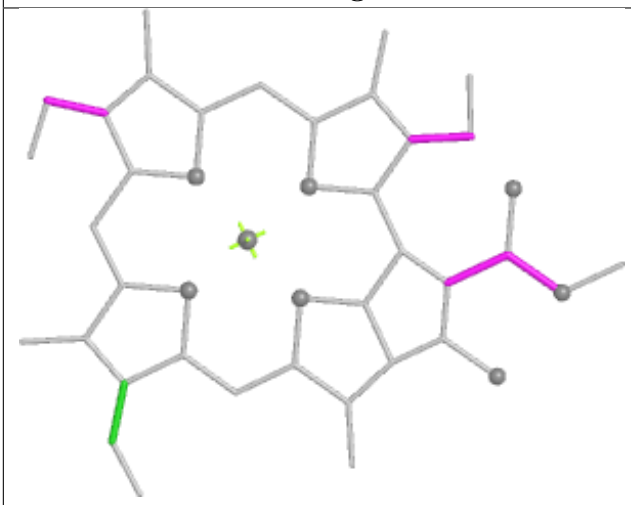
Ligand CLA f 601



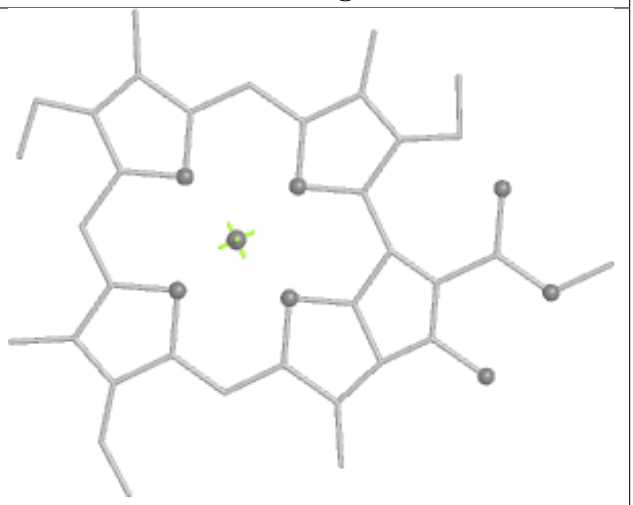
Bond lengths



Bond angles

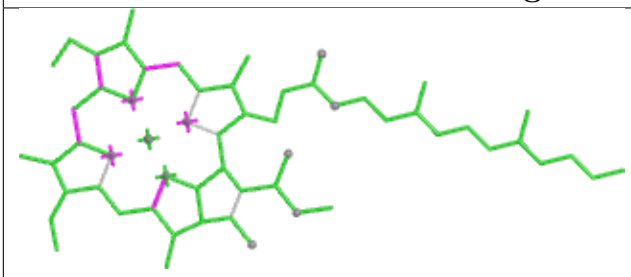


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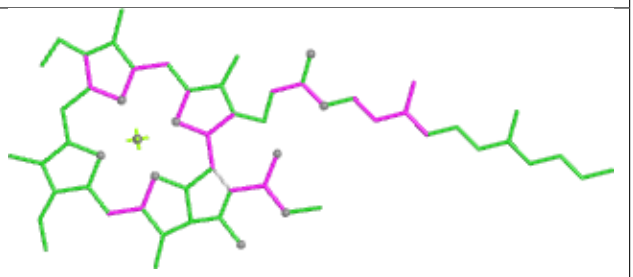


Rings

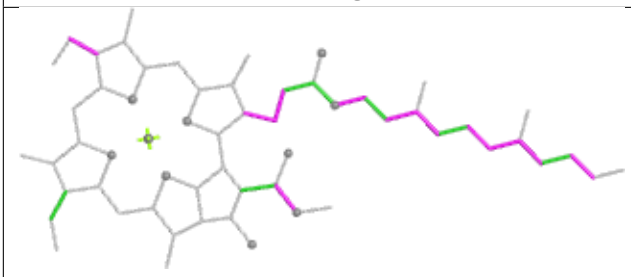
Ligand CLA A 824



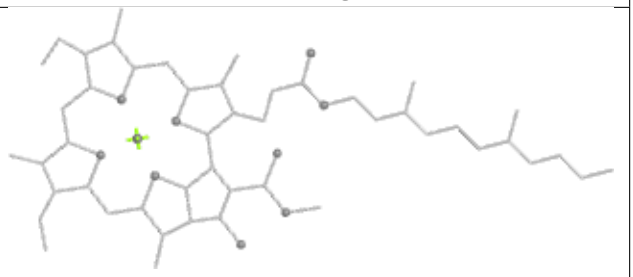
Bond lengths



Bond angles

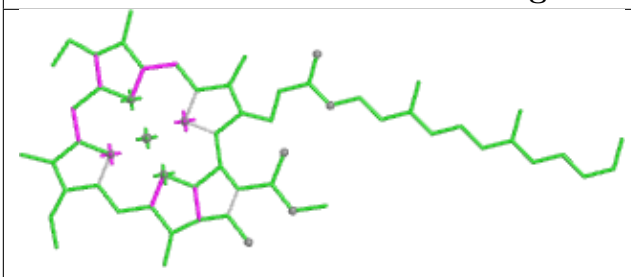


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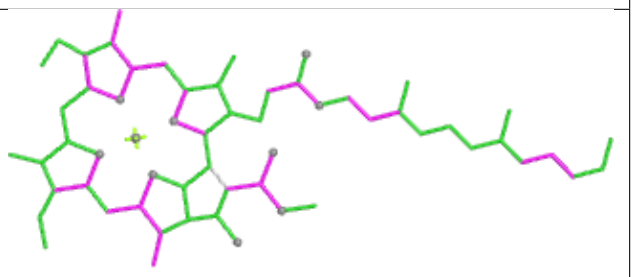


Rings

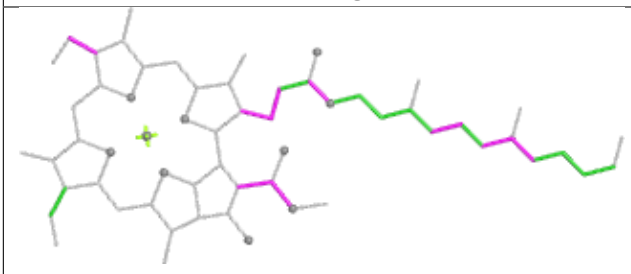
Ligand CLA c 303



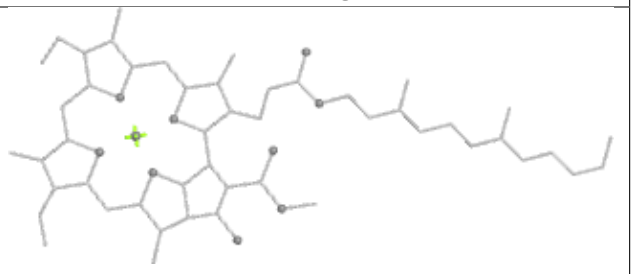
Bond lengths



Bond angles

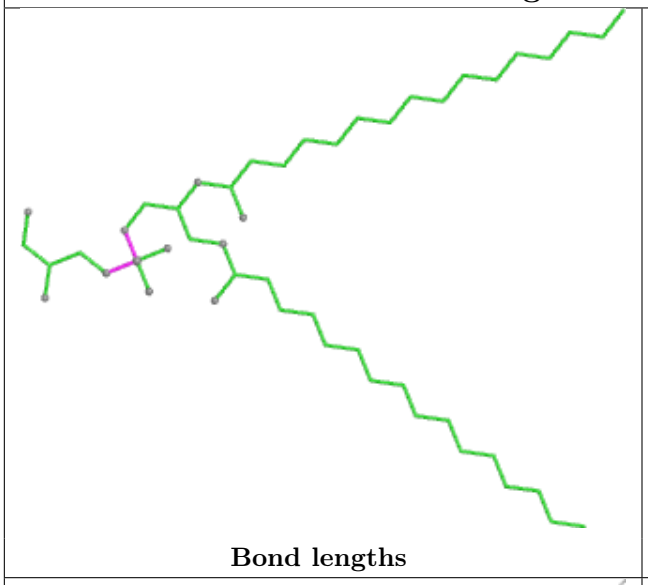


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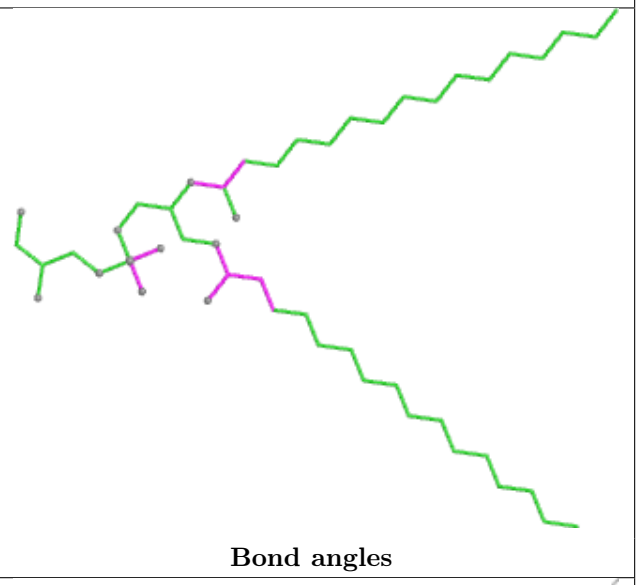


Rings

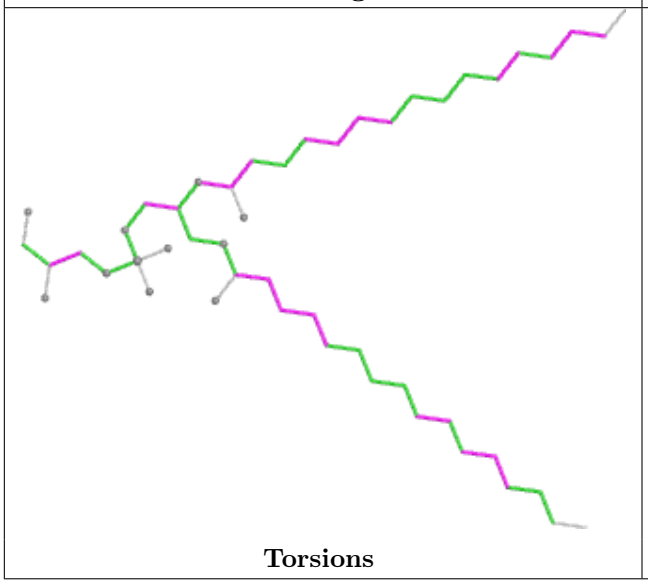
Ligand LHG A 835



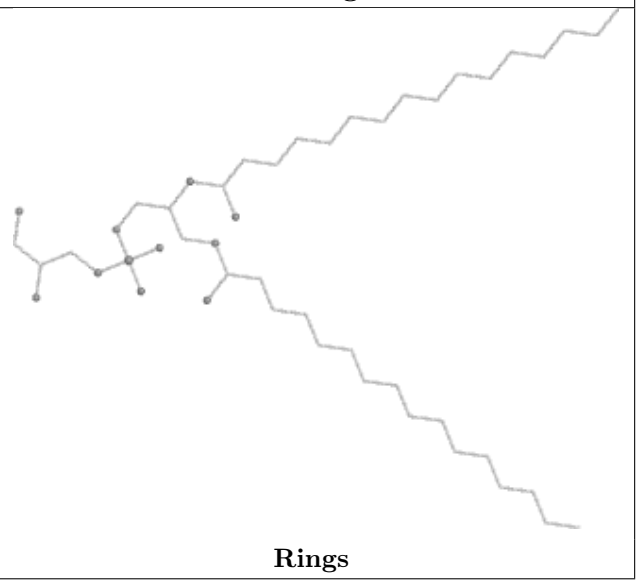
Bond lengths



Bond angles

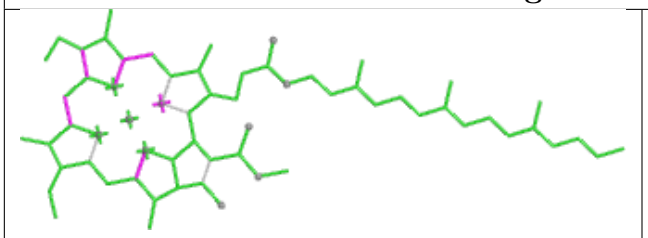


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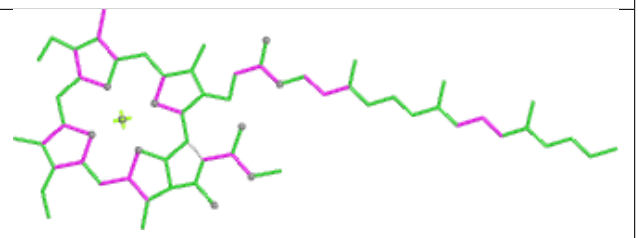


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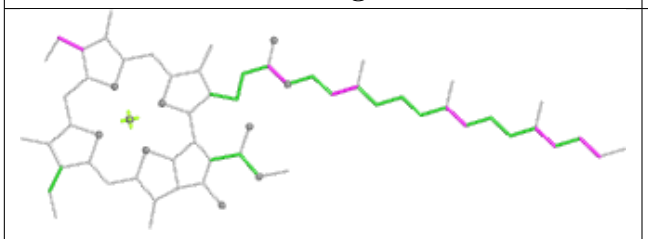
Ligand CLA A 802



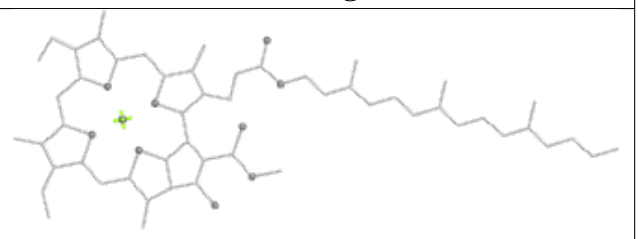
Bond lengths



Bond angles

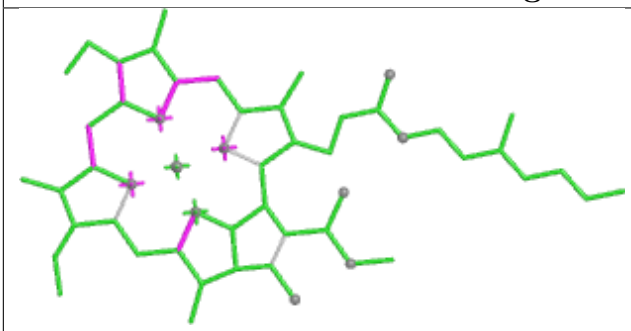


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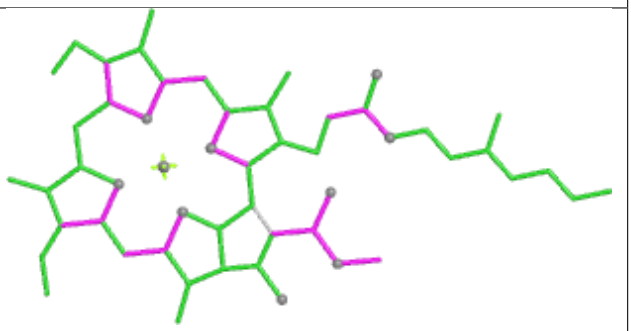


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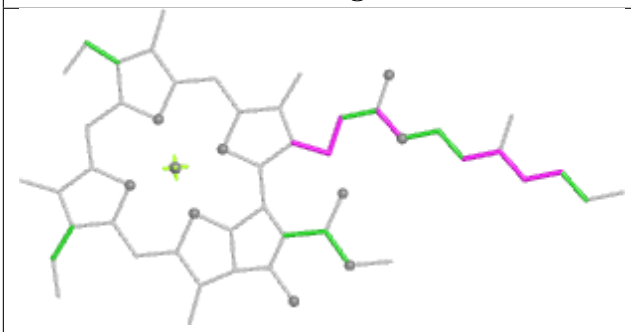
Ligand CLA A 857



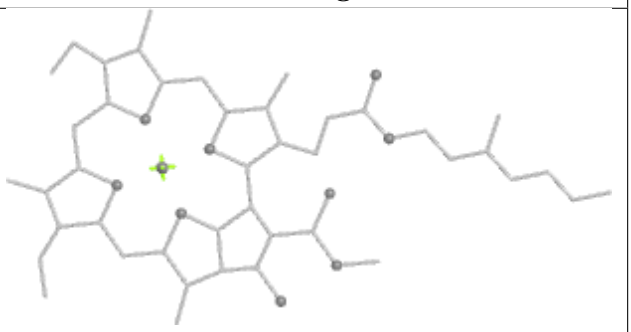
Bond lengths



Bond angles

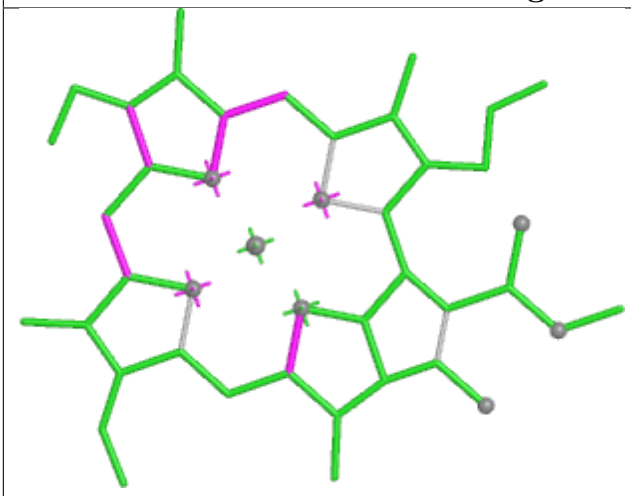


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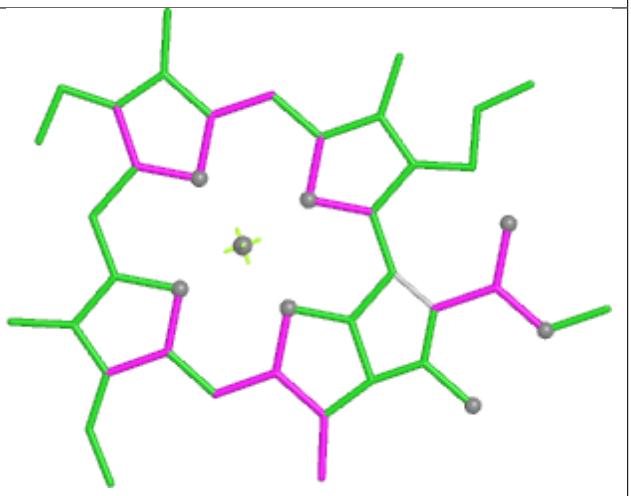


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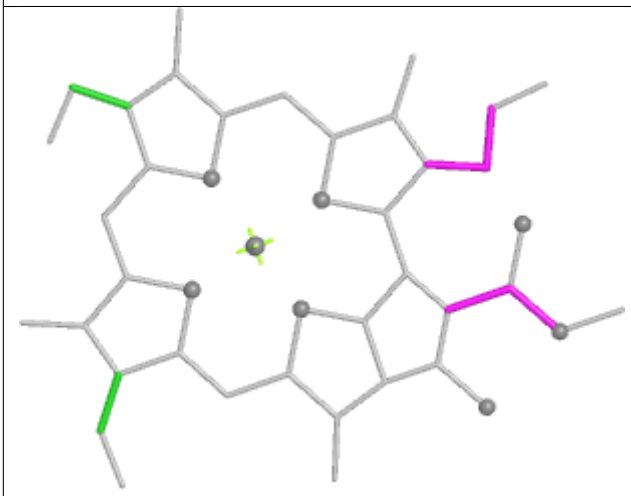
Ligand CLA h 205



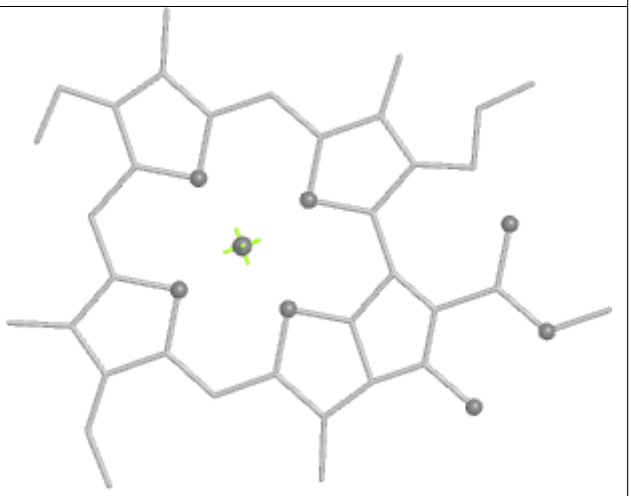
Bond lengths



Bond angles

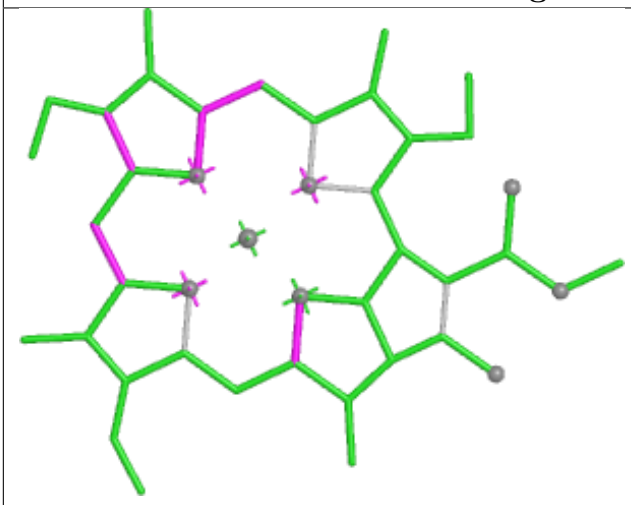


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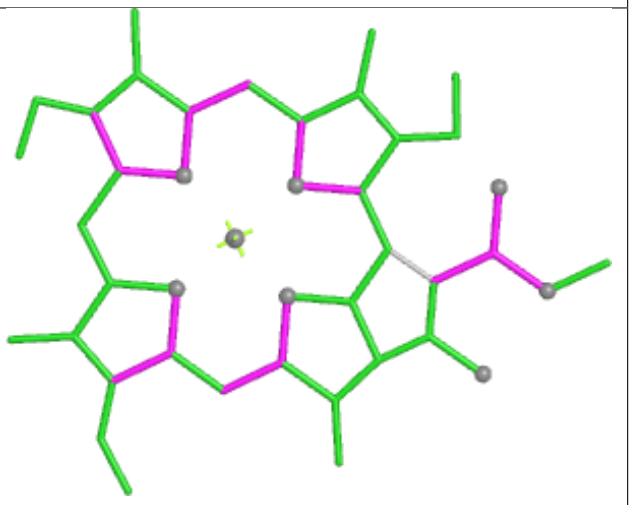


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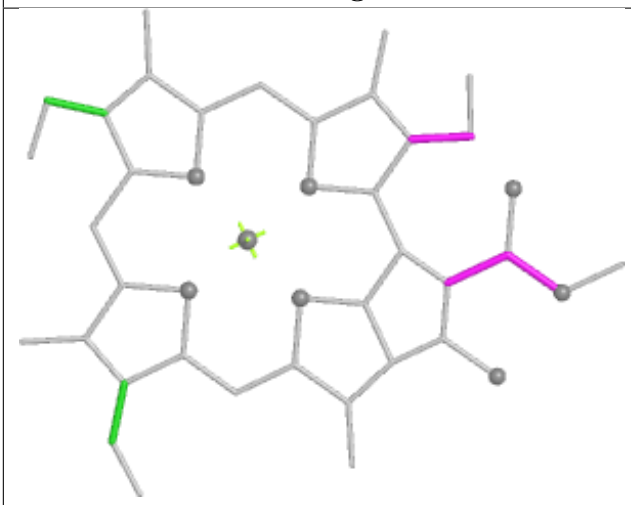
Ligand CLA c 302



Bond lengths



Bond angles

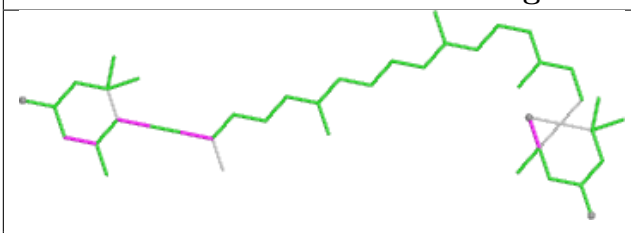


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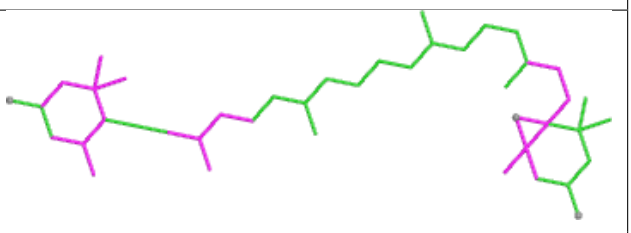


Rings

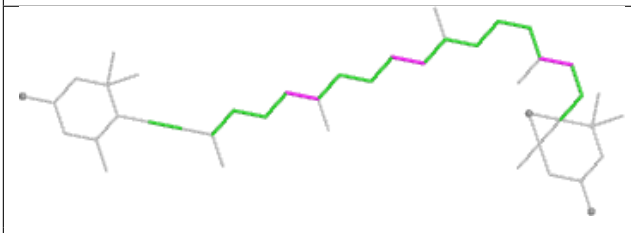
Ligand DD6 m 212



Bond lengths



Bond angles

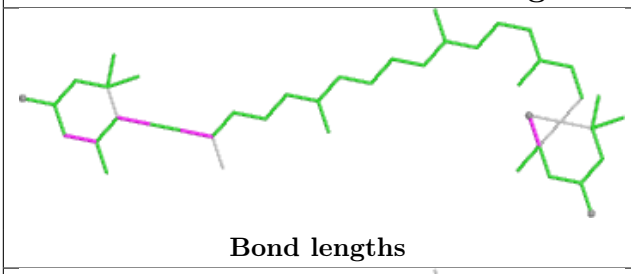


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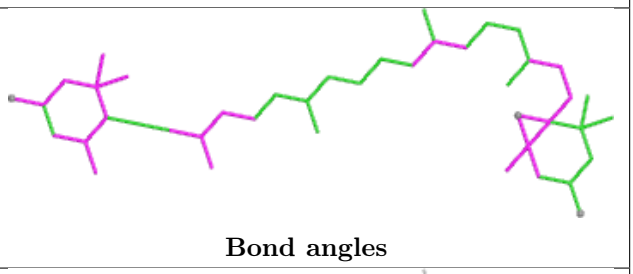


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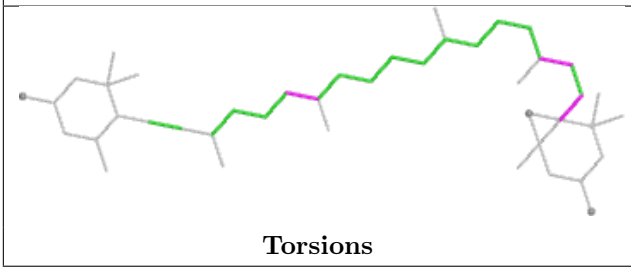
Ligand DD6 b 214



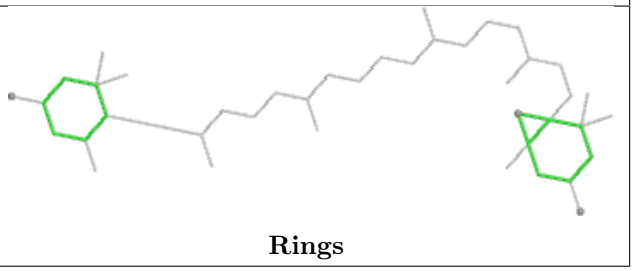
Bond lengths



Bond angles

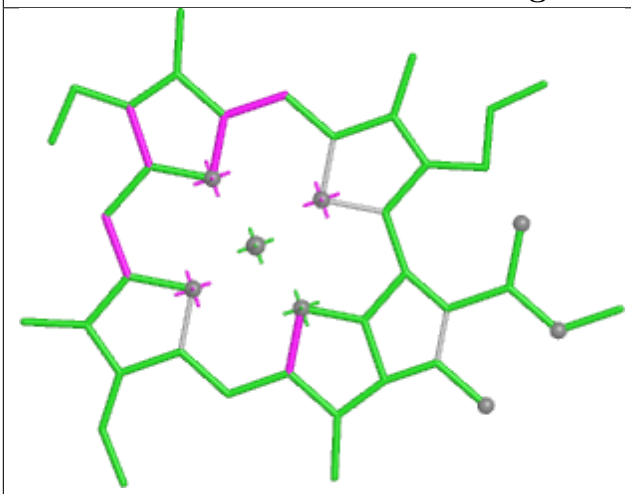


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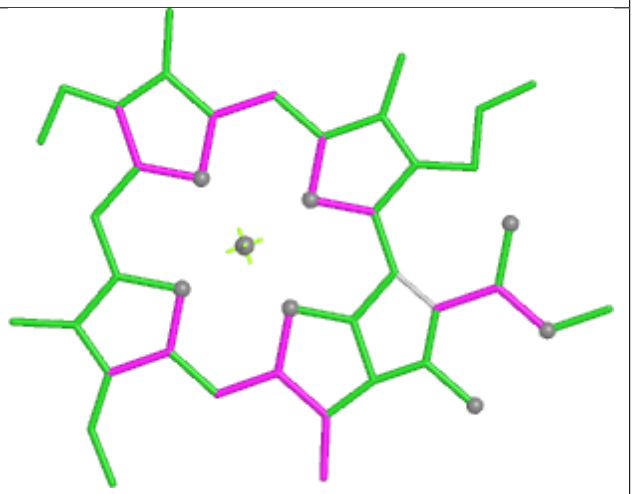


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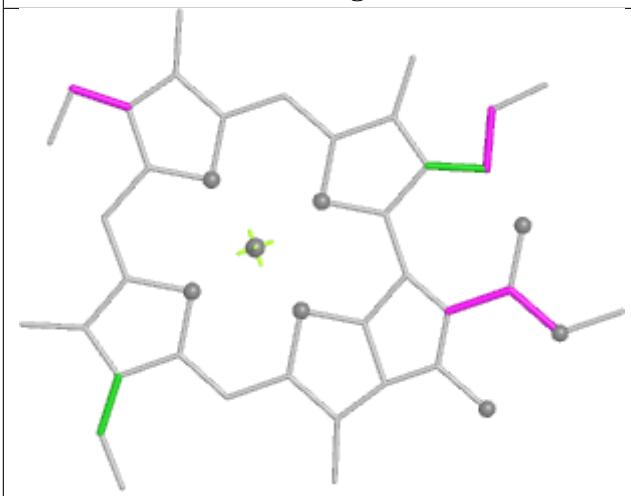
Ligand CLA e 210



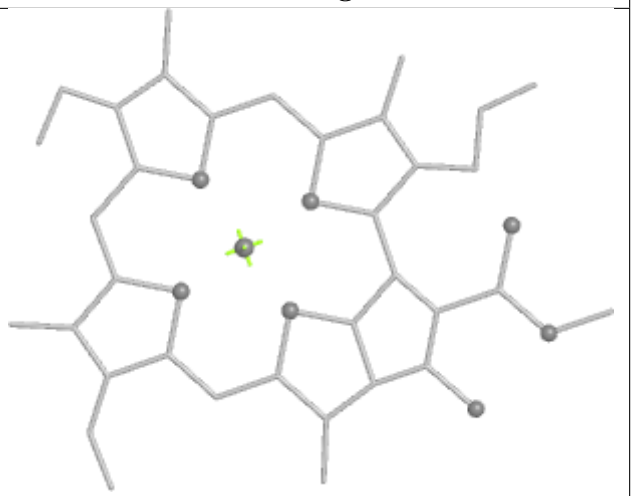
Bond lengths



Bond angles

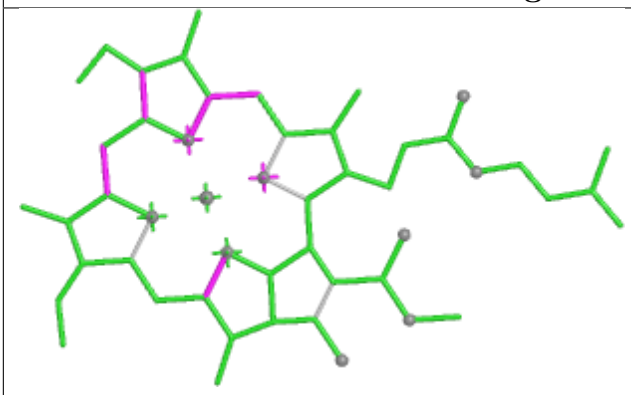


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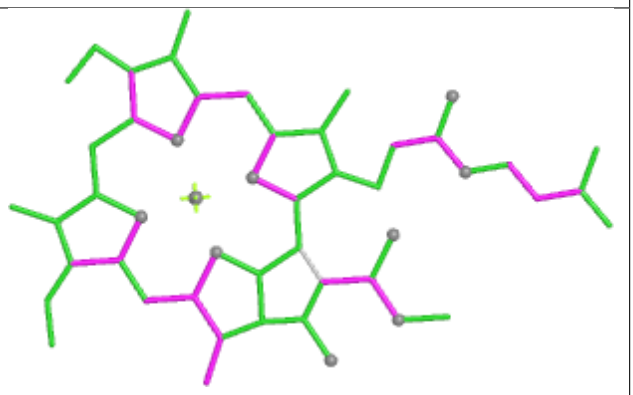


Rings

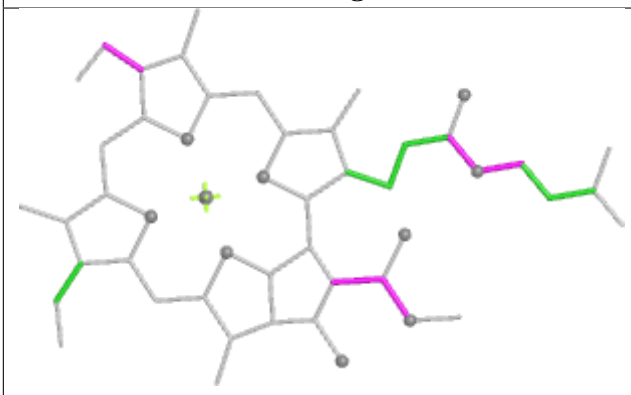
Ligand CLA B 817



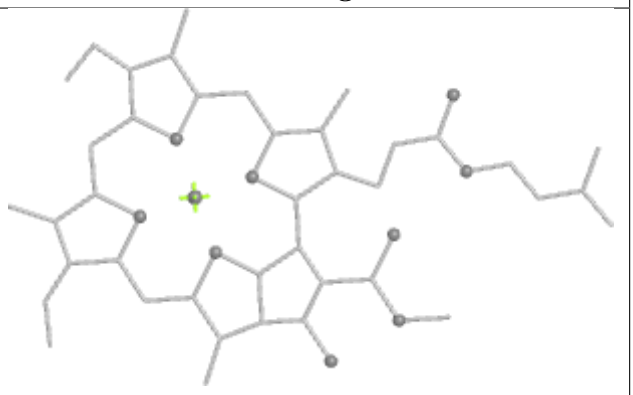
Bond lengths



Bond angles

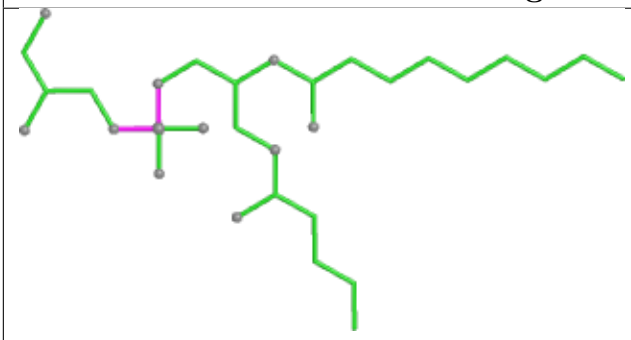


Torsions

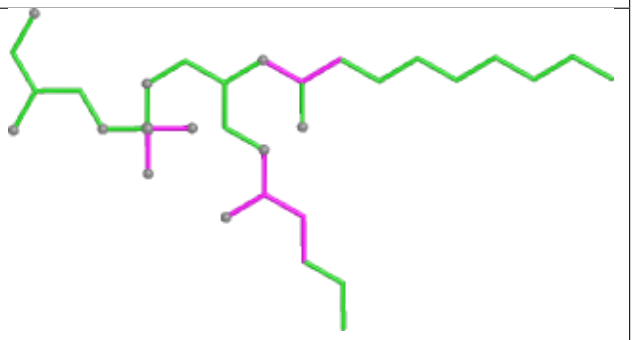


Rings

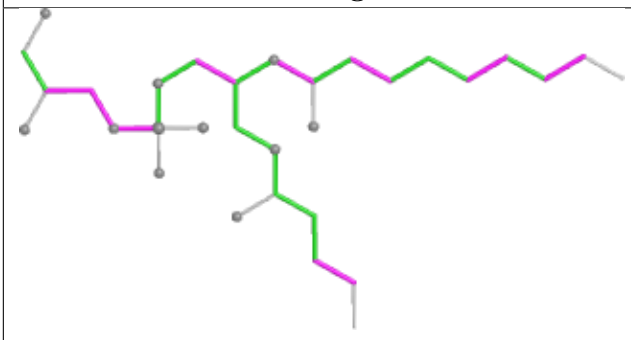
Ligand LHG h 202



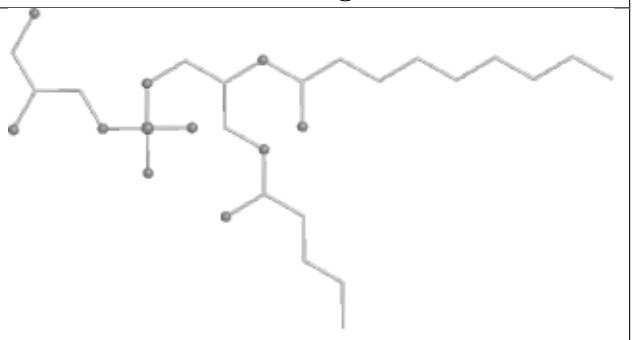
Bond lengths



Bond angles

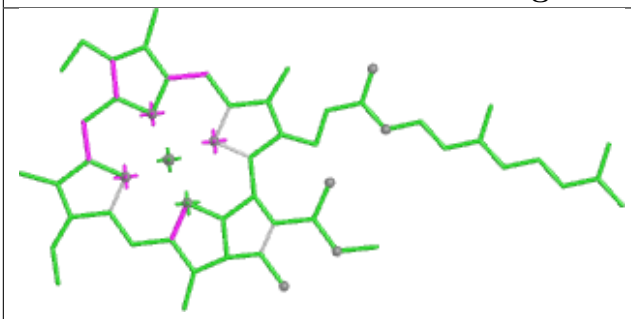


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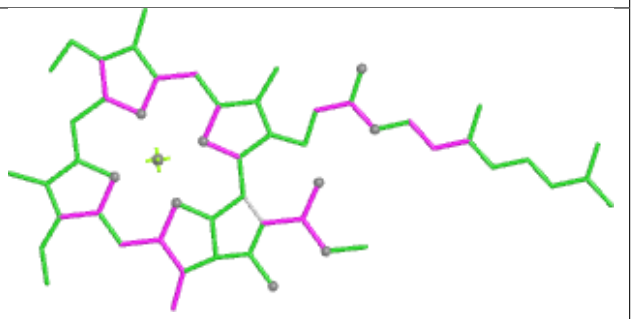


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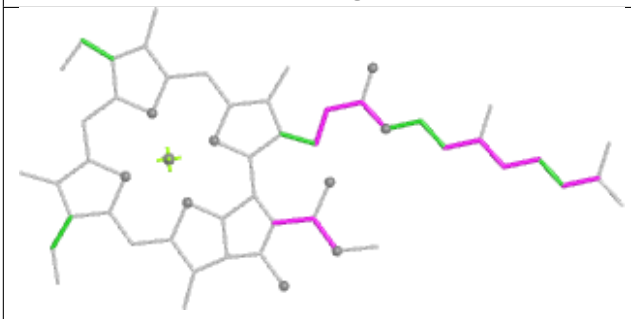
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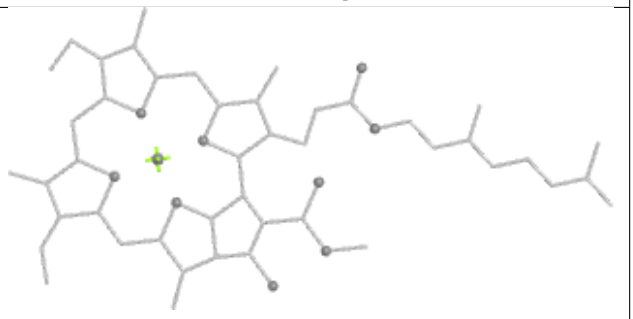
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Bond angles

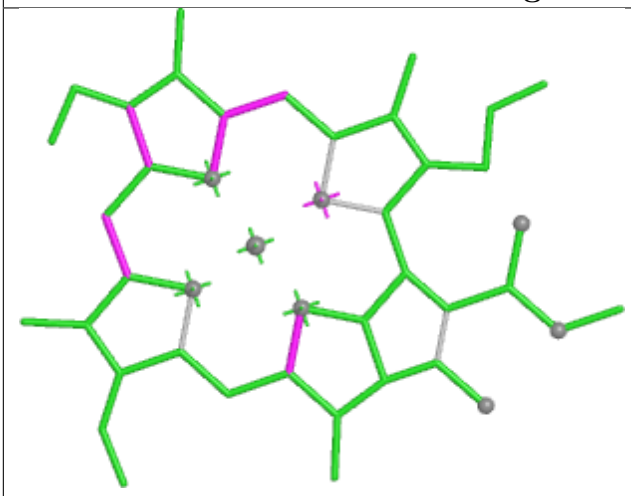


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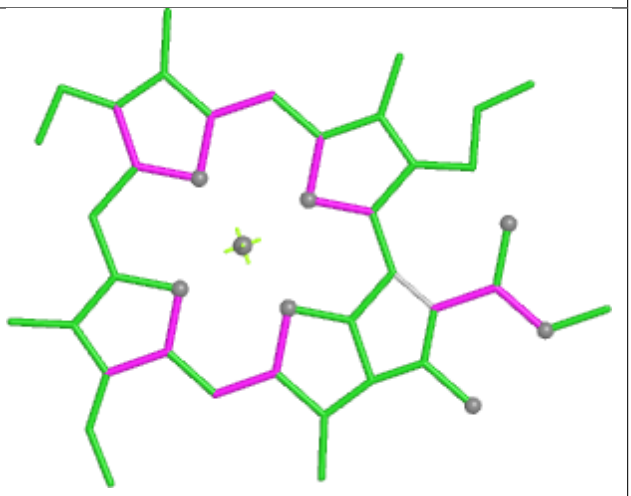


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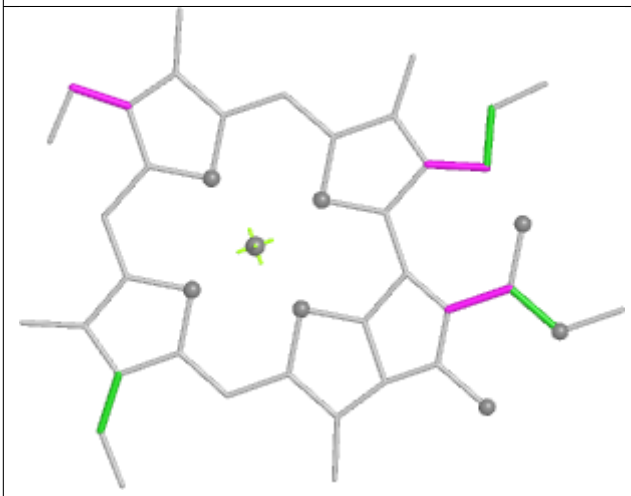
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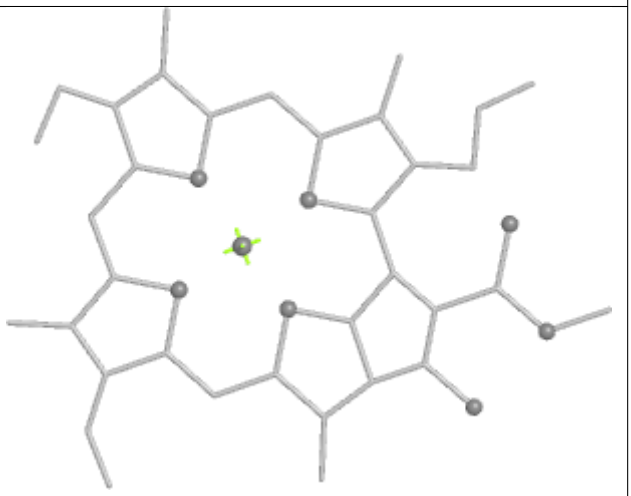
Bond lengths



Bond angles

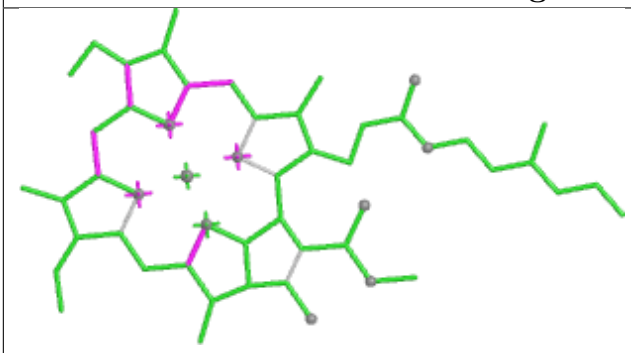


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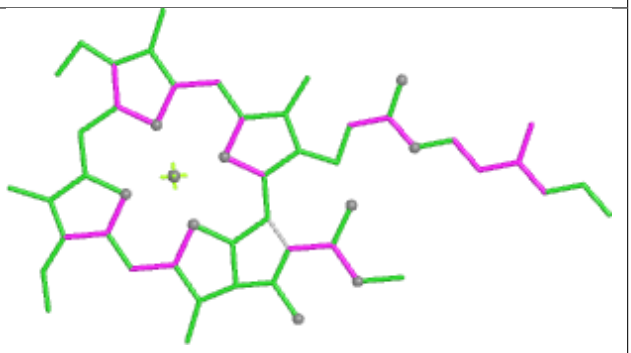


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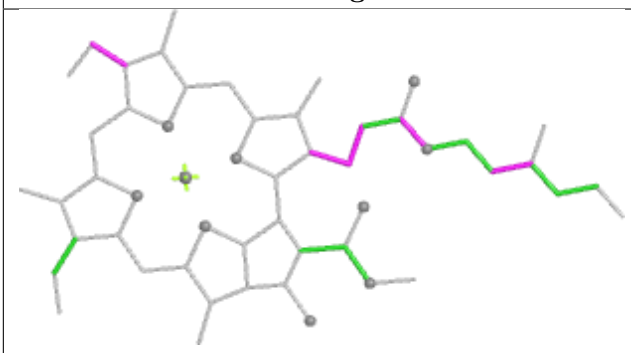
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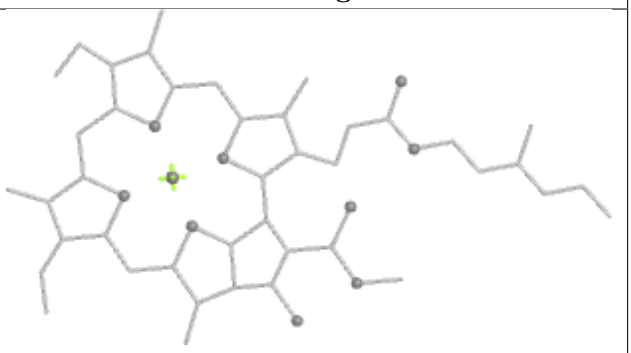
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Bond angles

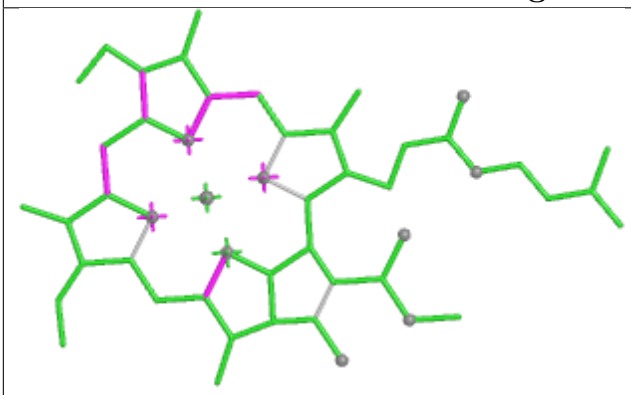


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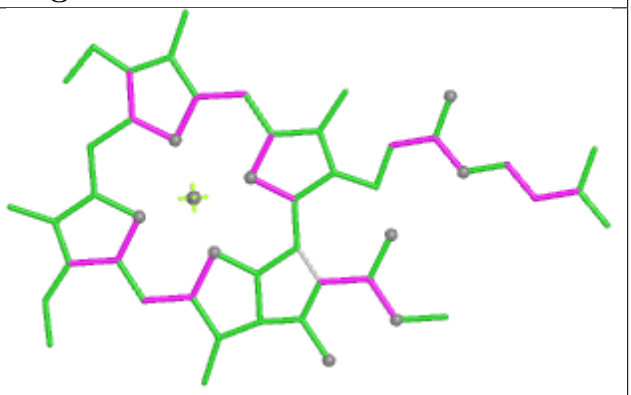


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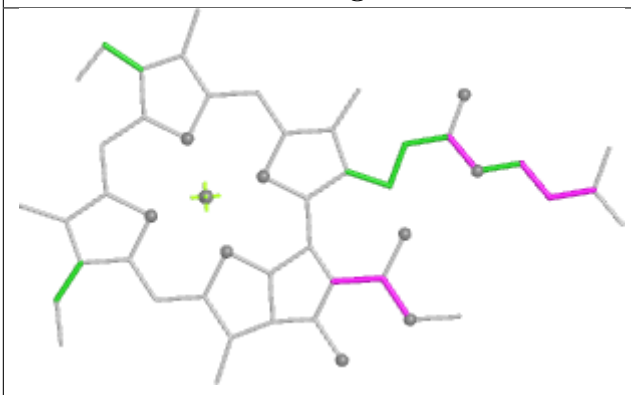
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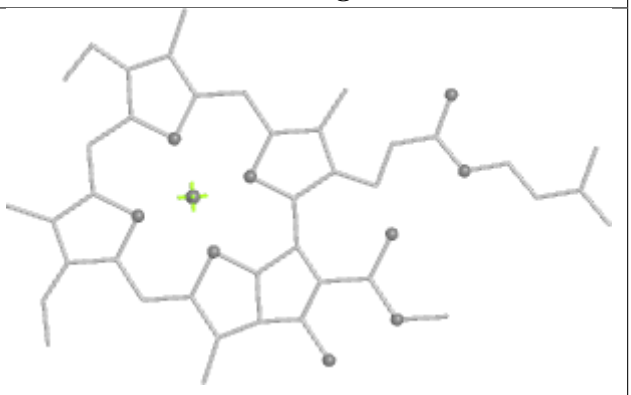
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Bond angles

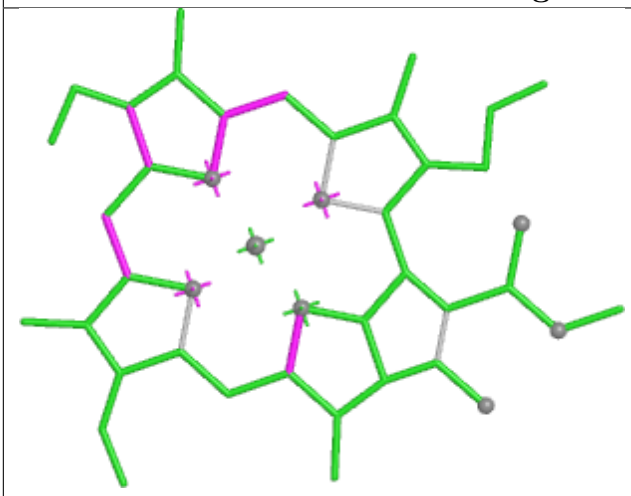


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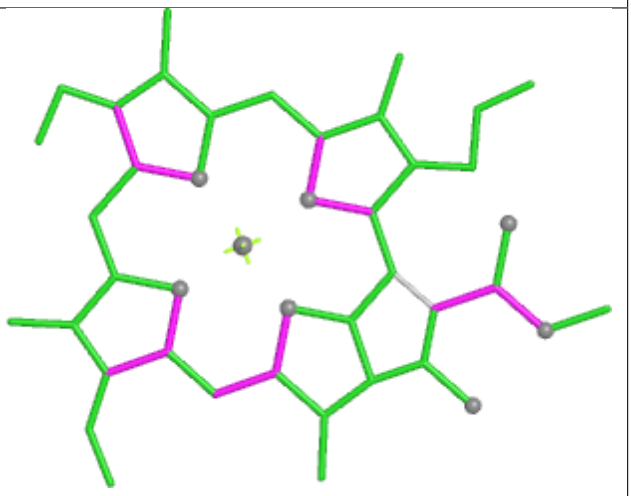


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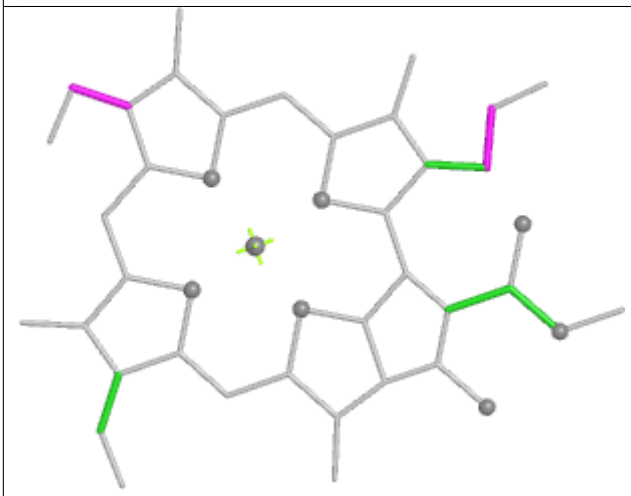
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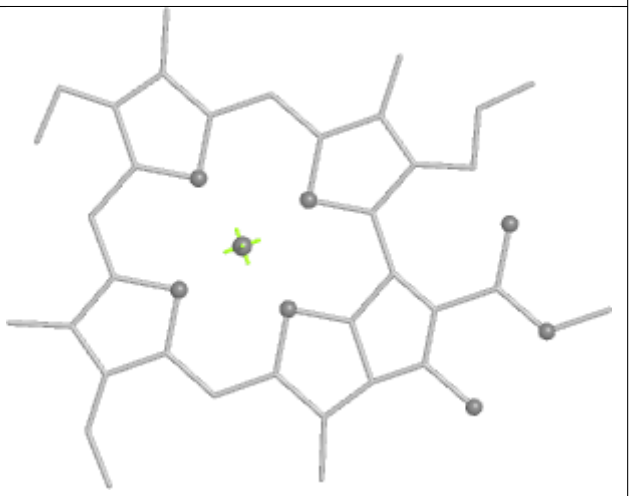
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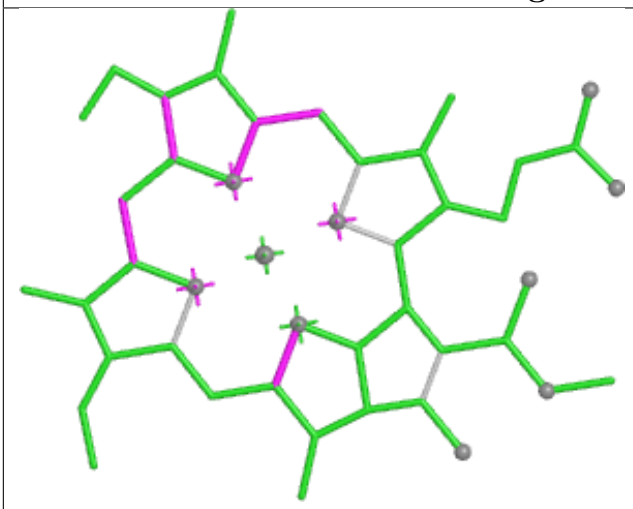


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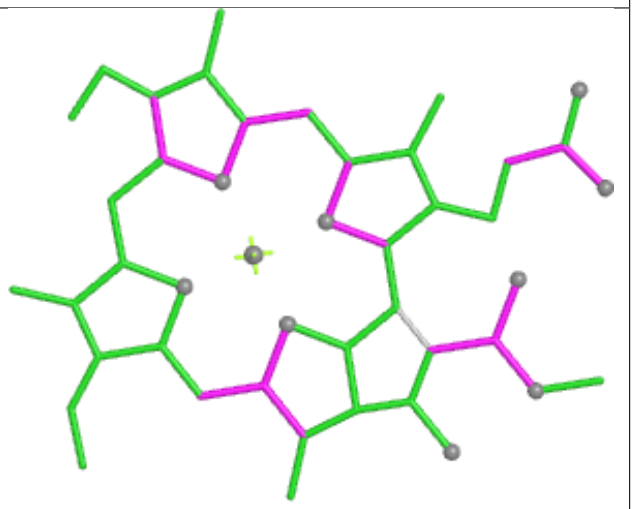


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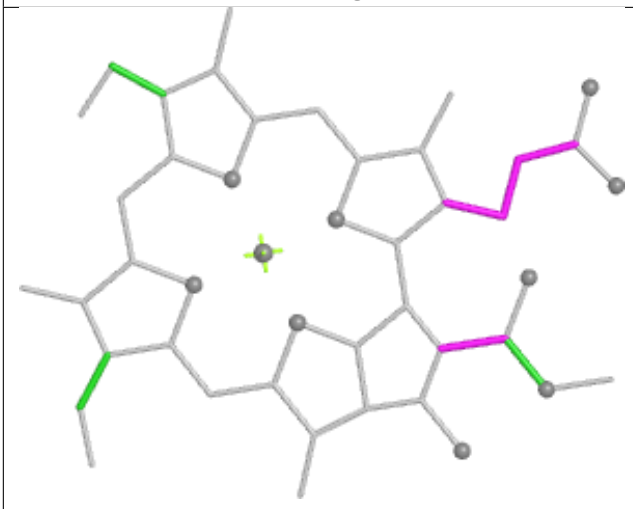
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Bond lengths



Bond angles

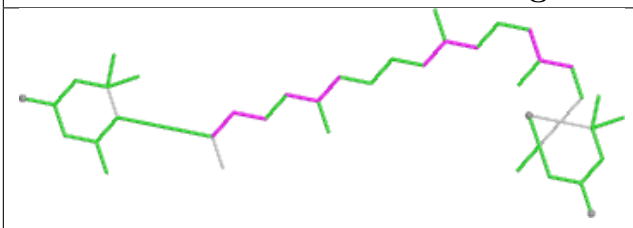


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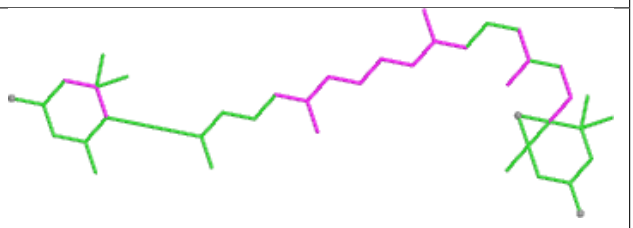


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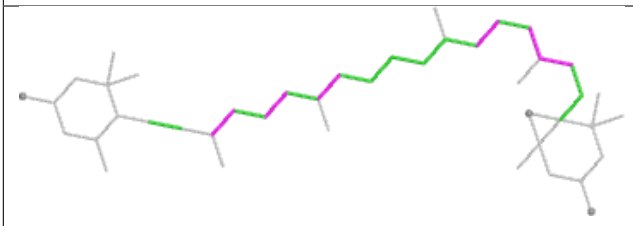
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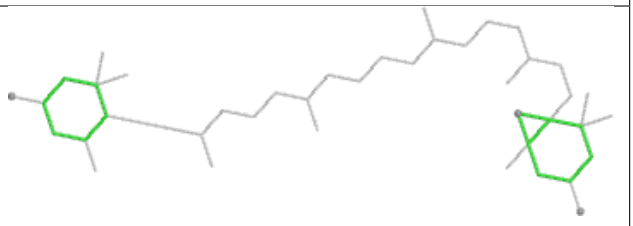
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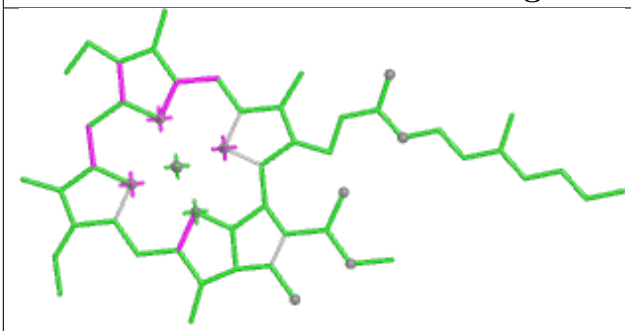


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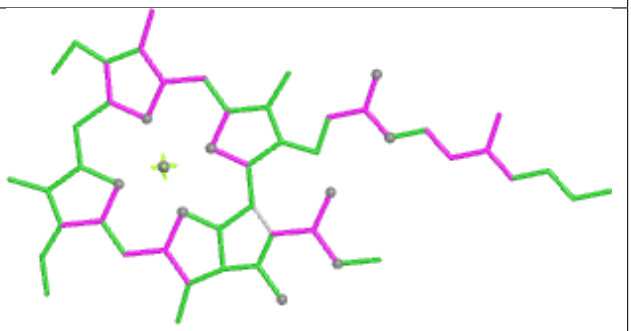


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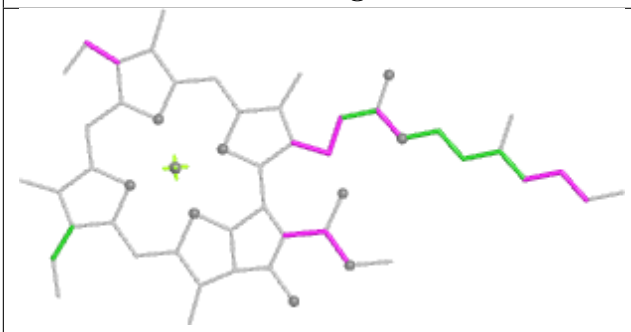
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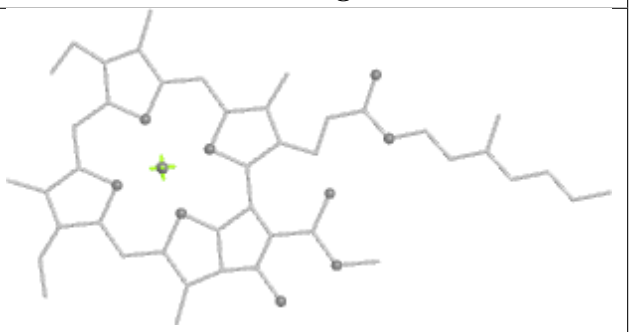
Bond lengths



Bond angles

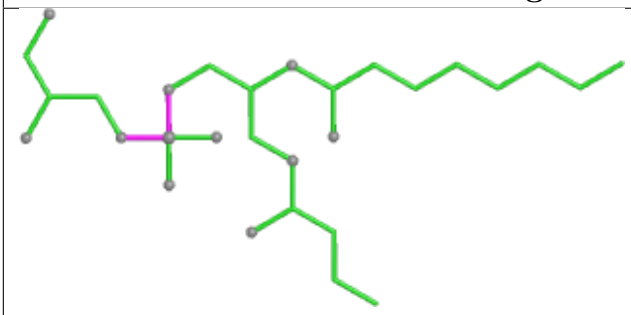


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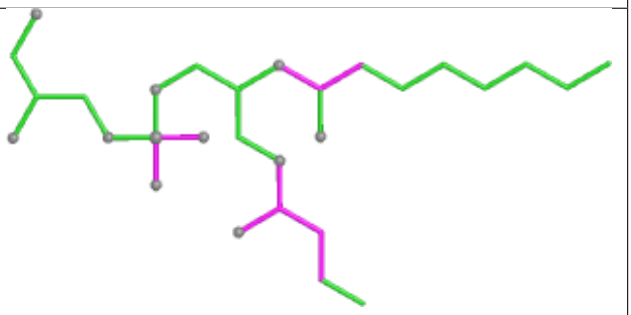


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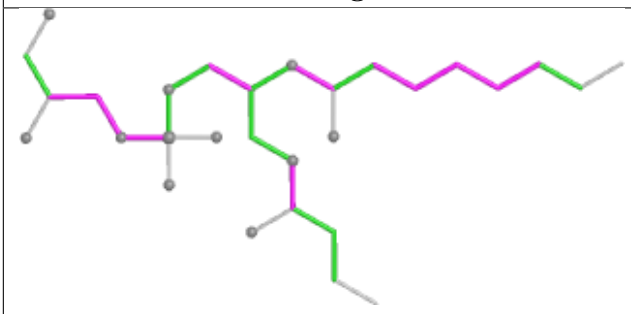
Ligand LHG d 302



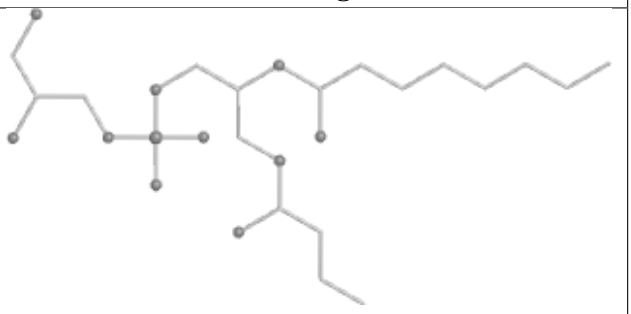
Bond lengths



Bond angles

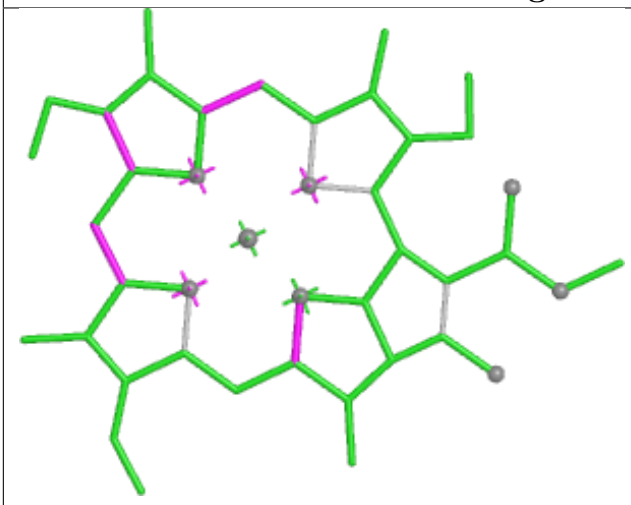


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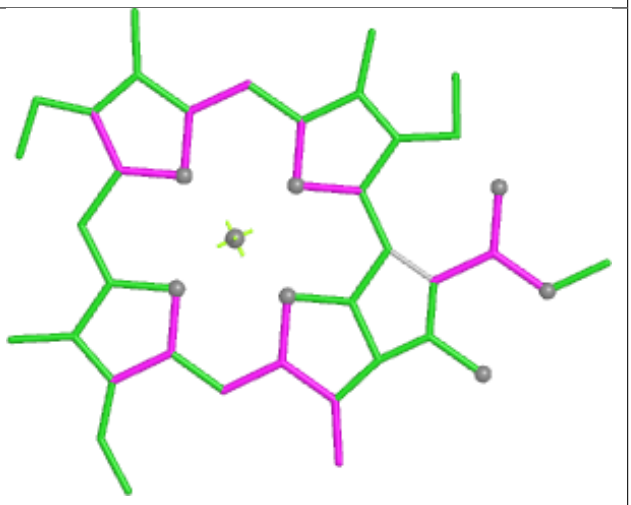


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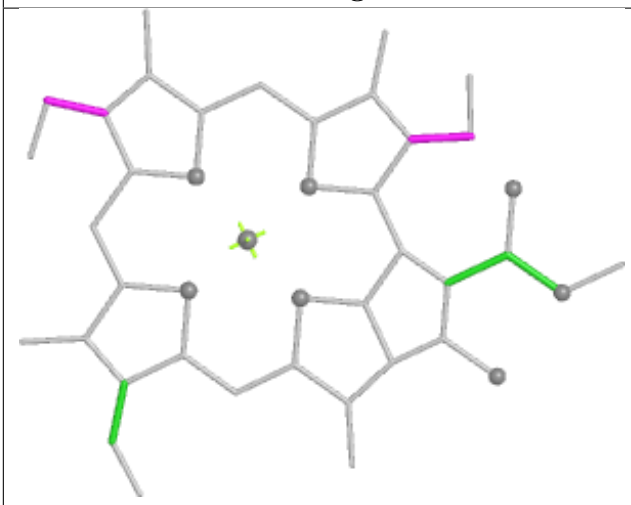
Ligand CLA o 604



Bond lengths



Bond angles

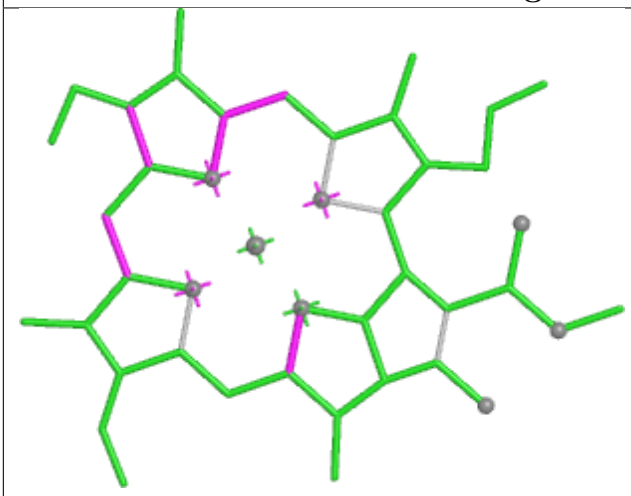


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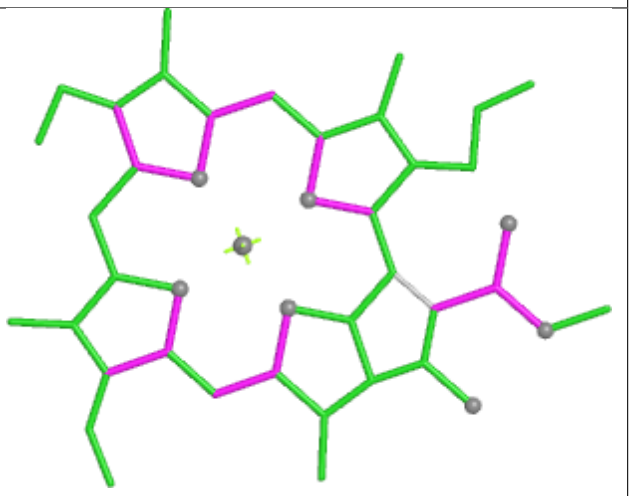


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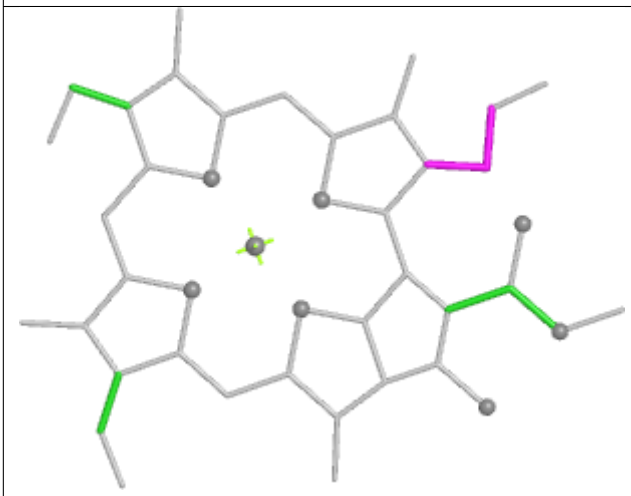
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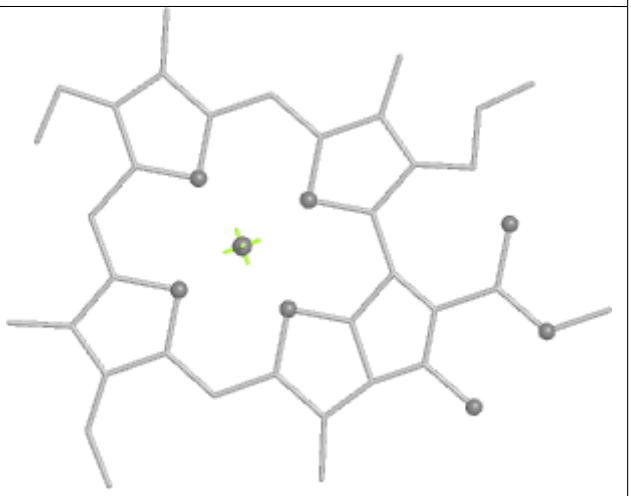
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Bond angles

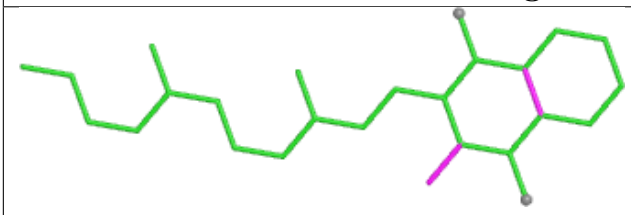


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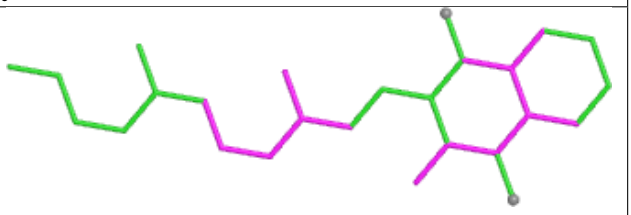


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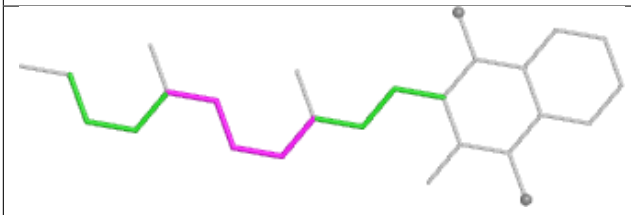
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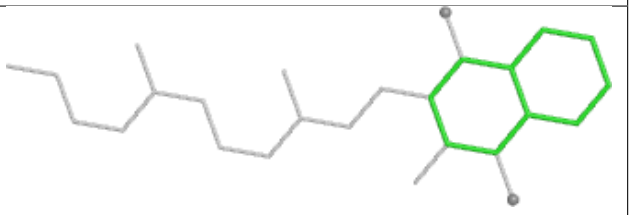
Bond lengths



Bond angles

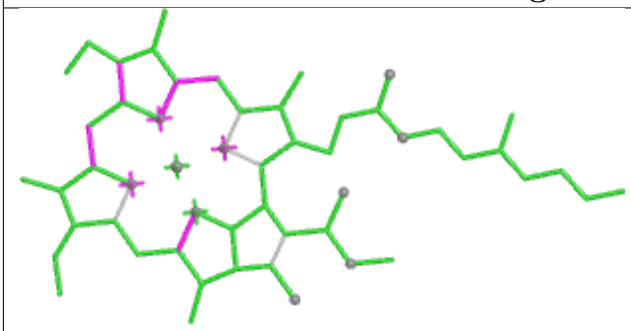


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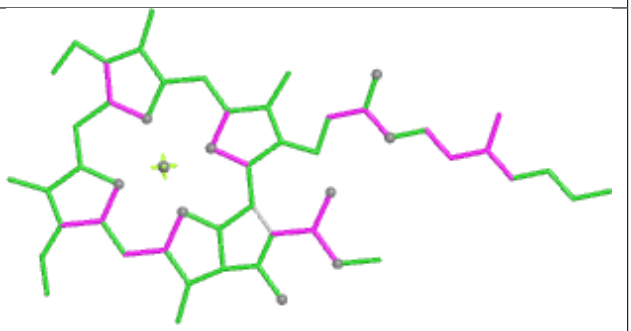


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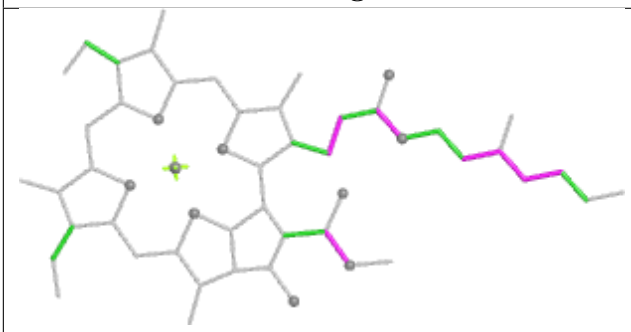
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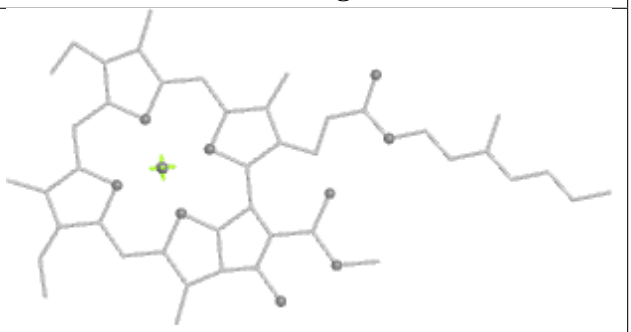
Bond lengths



Bond angles



Torsions

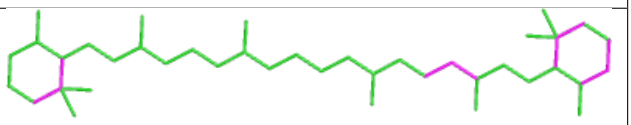


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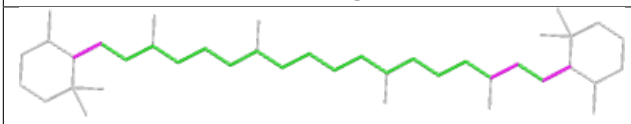
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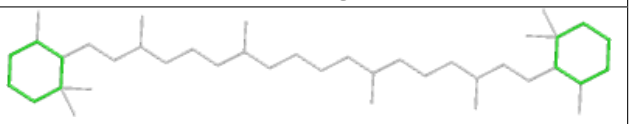
Bond lengths



Bond angles

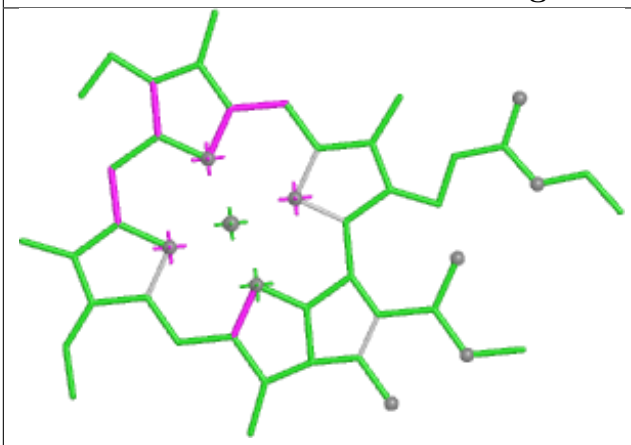


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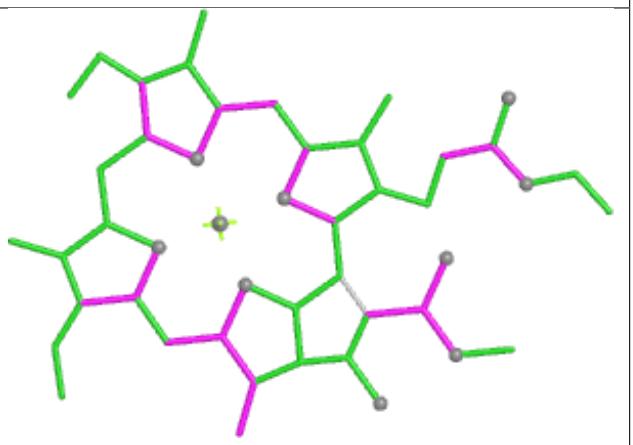


Rings

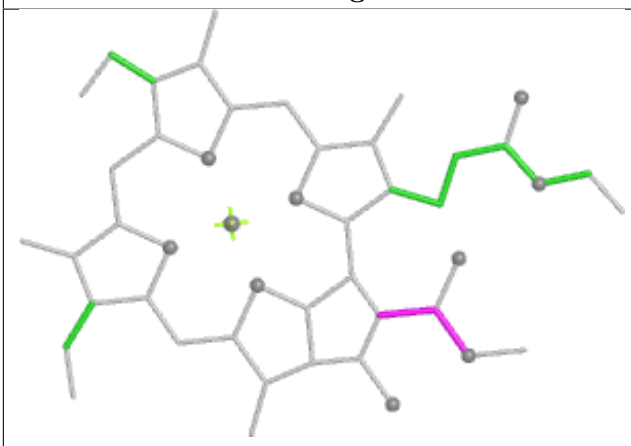
Ligand CLA c 315



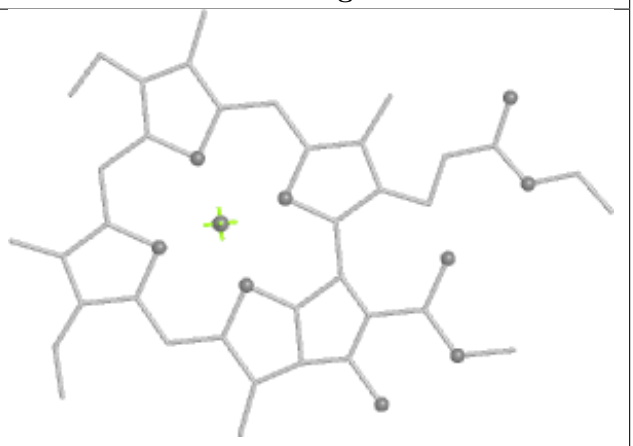
Bond lengths



Bond angles

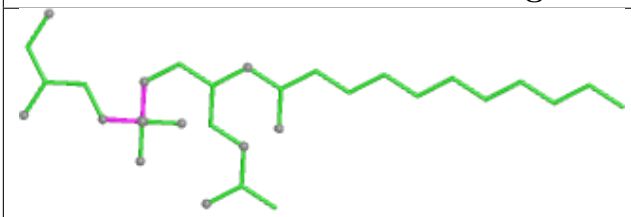


Torsions

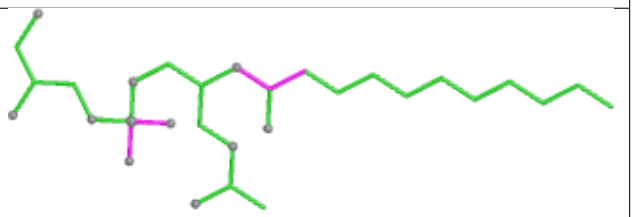


Rings

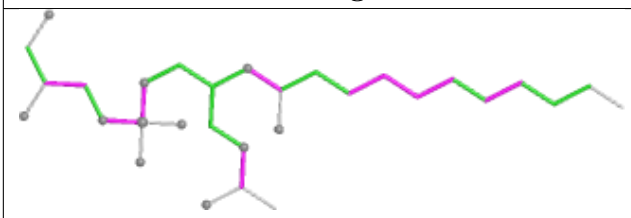
Ligand LHG h 201



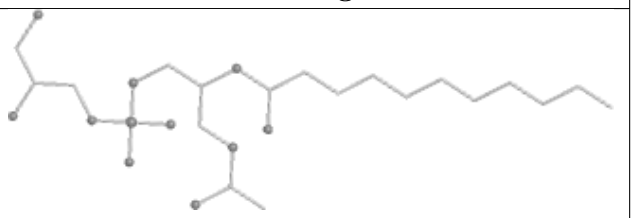
Bond lengths



Bond angles

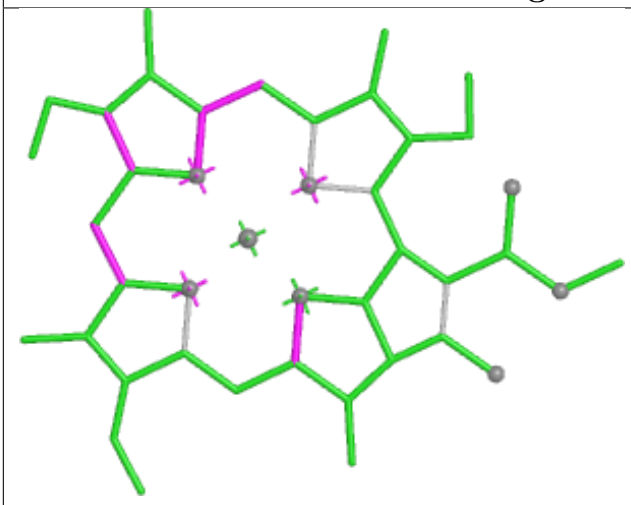


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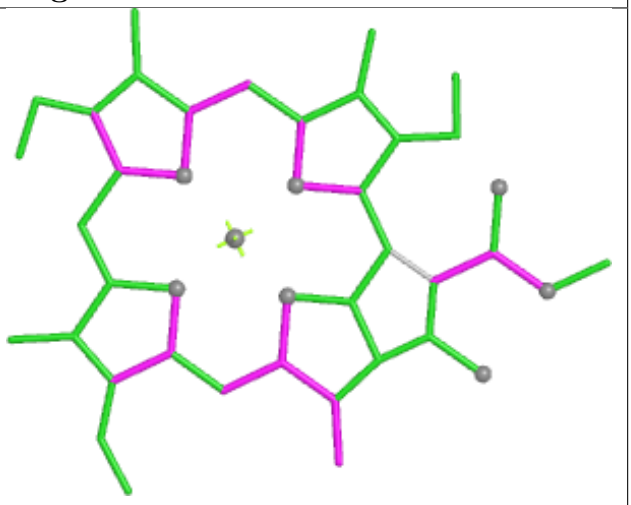


Rings

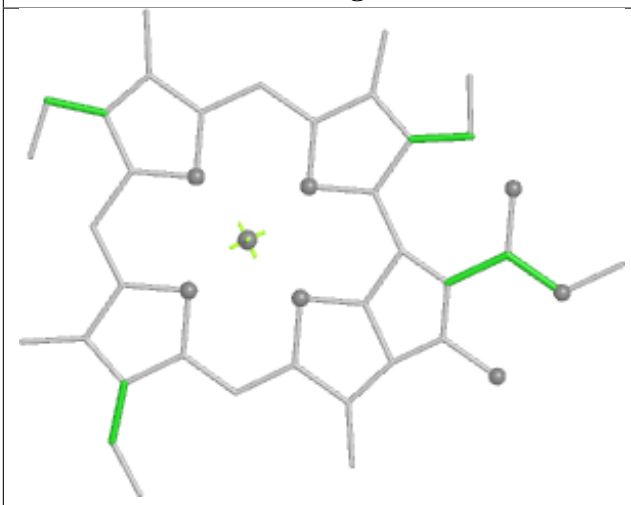
Ligand CLA g 214



Bond lengths



Bond angles

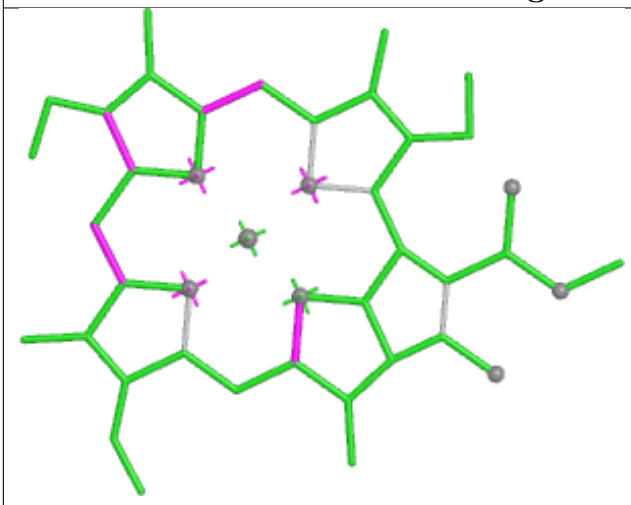


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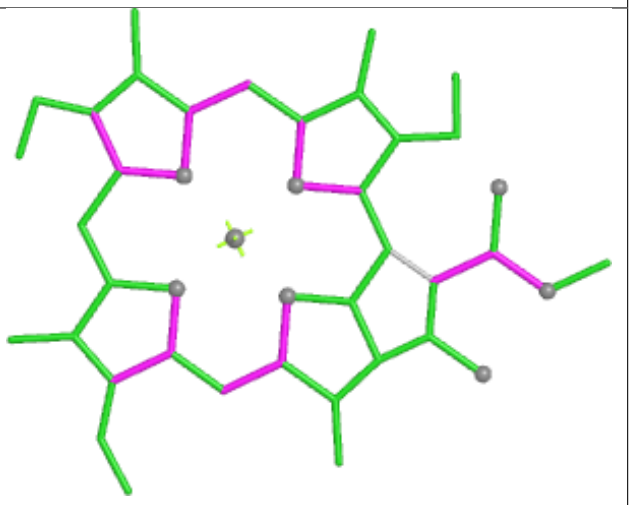


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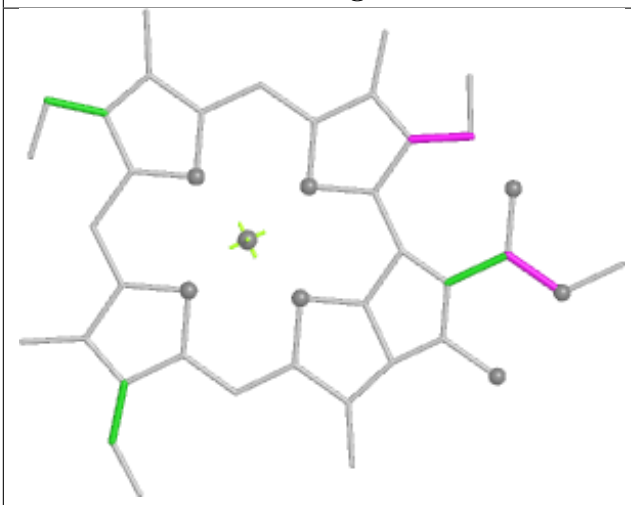
Ligand CLA n 206



Bond lengths



Bond angles

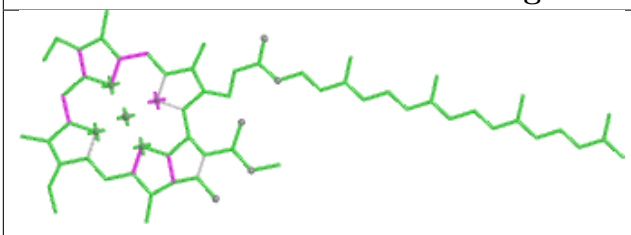


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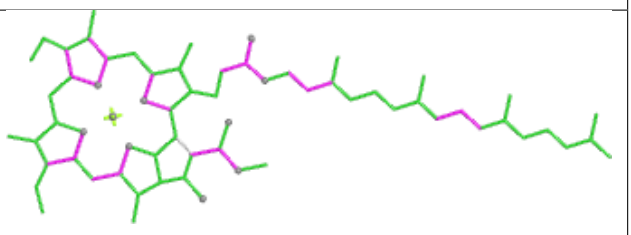


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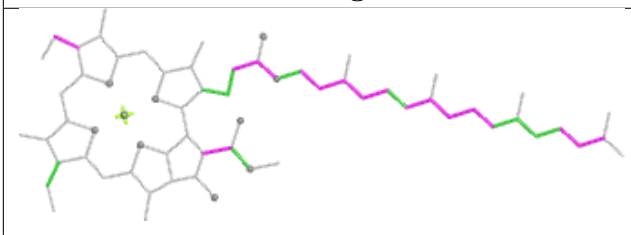
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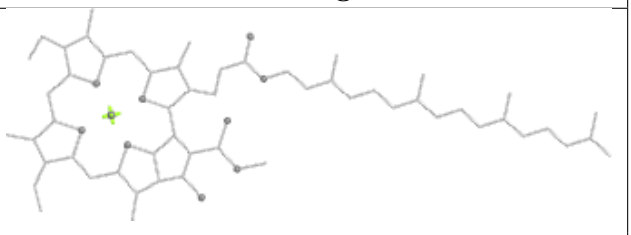
Bond lengths



Bond angles



Torsions

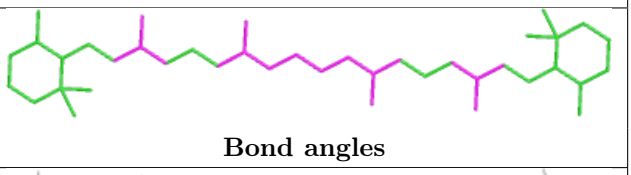


Rings

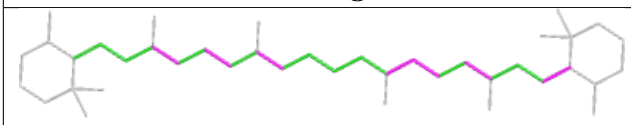
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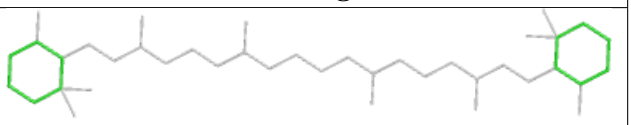
Bond lengths



Bond angles

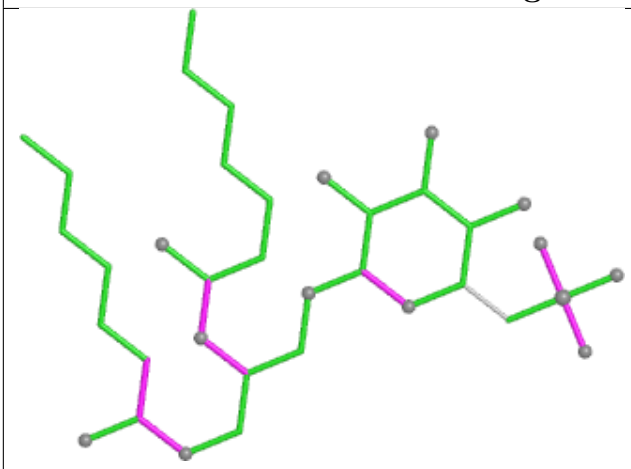


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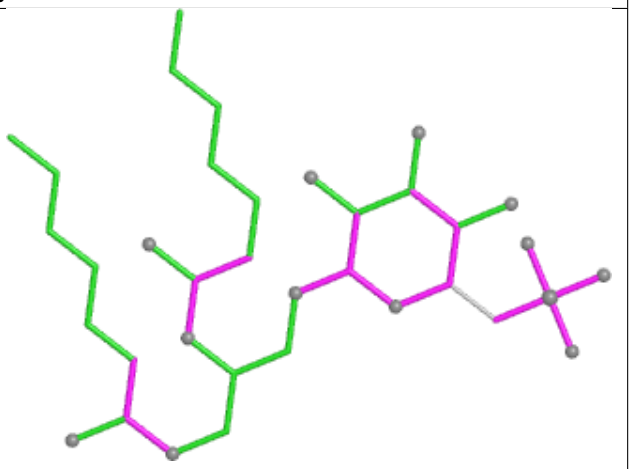


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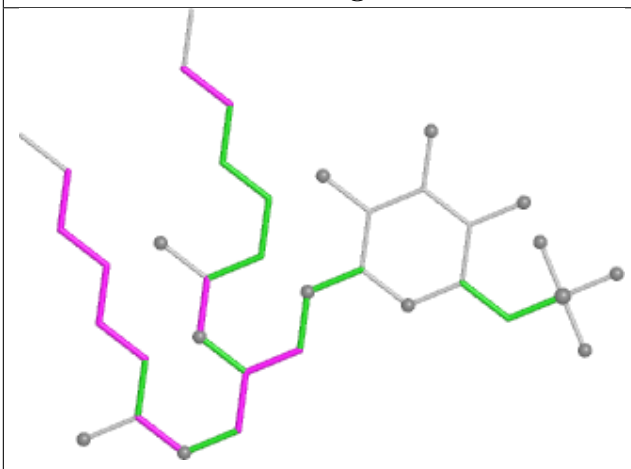
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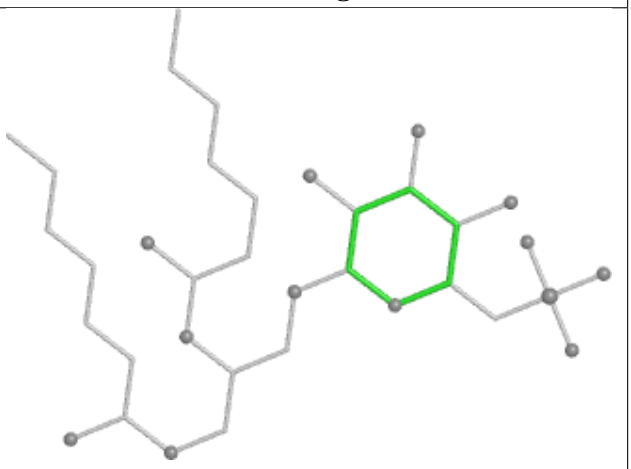
Bond lengths



Bond angles

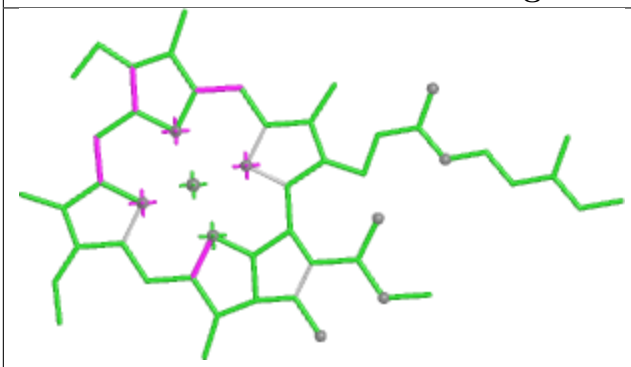


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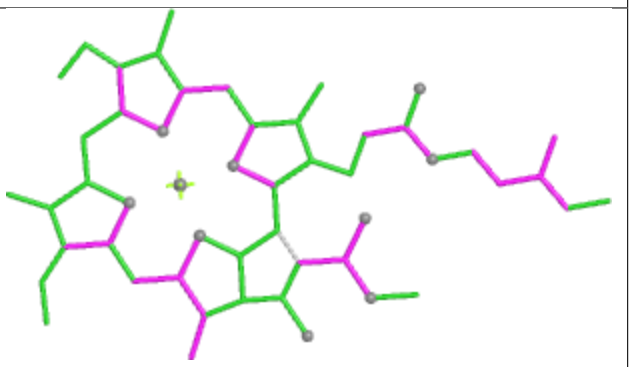


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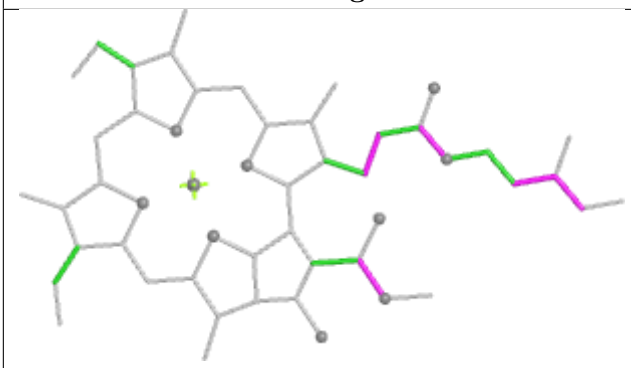
Ligand CLA A 848



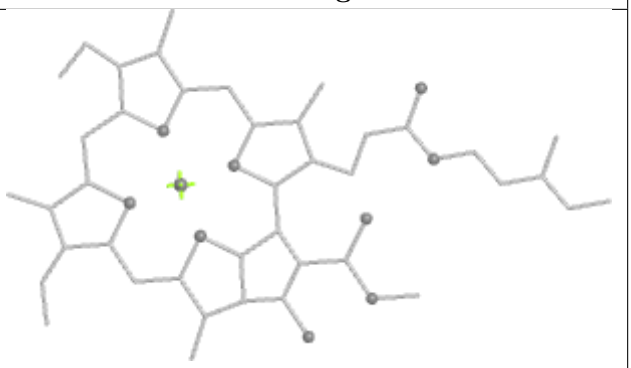
Bond lengths



Bond angles

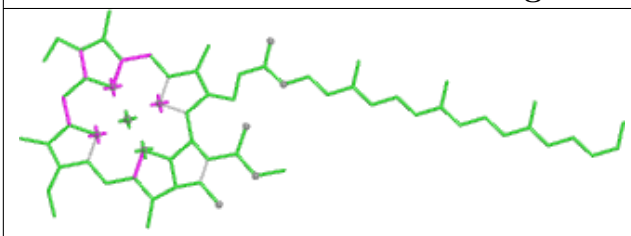


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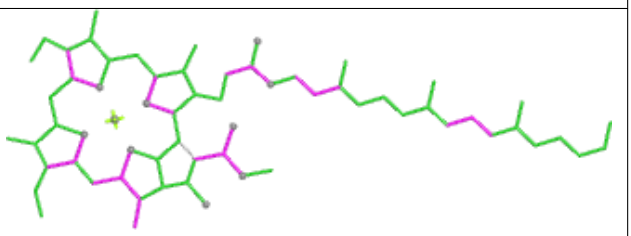


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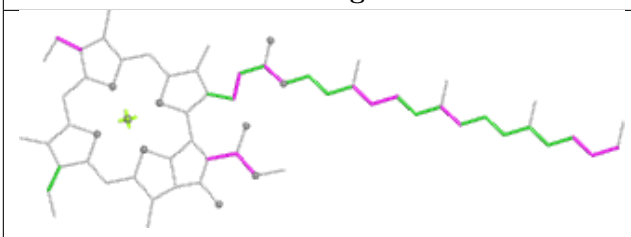
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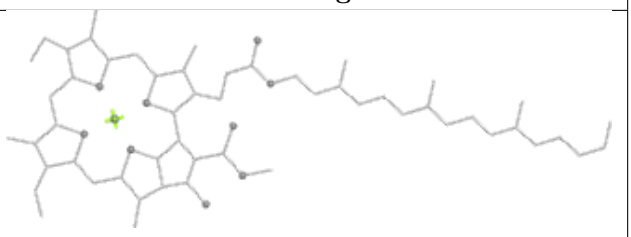
Bond lengths



Bond angles

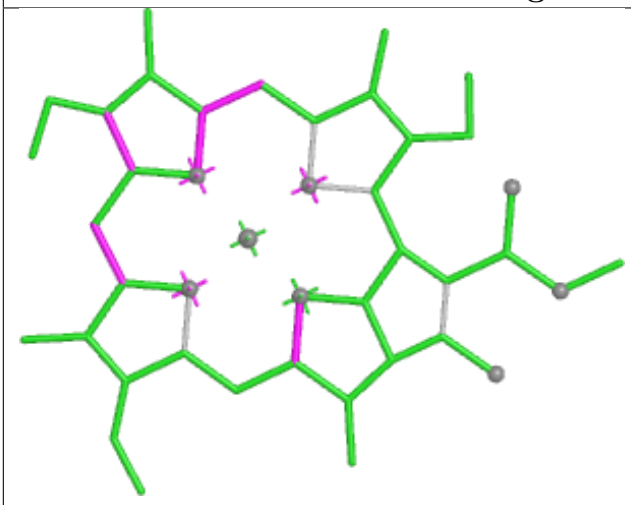


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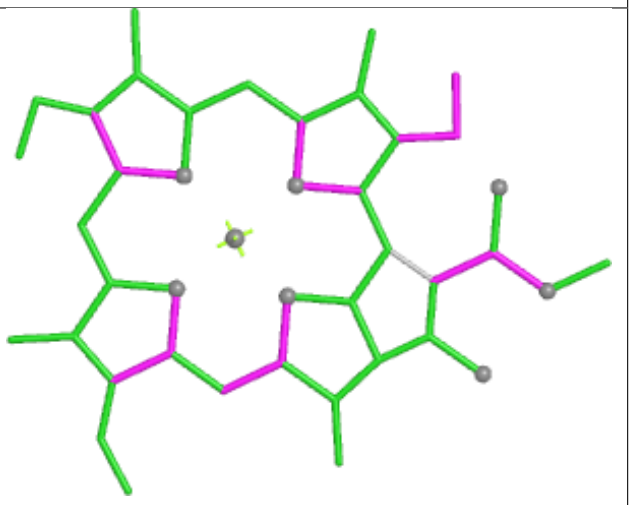


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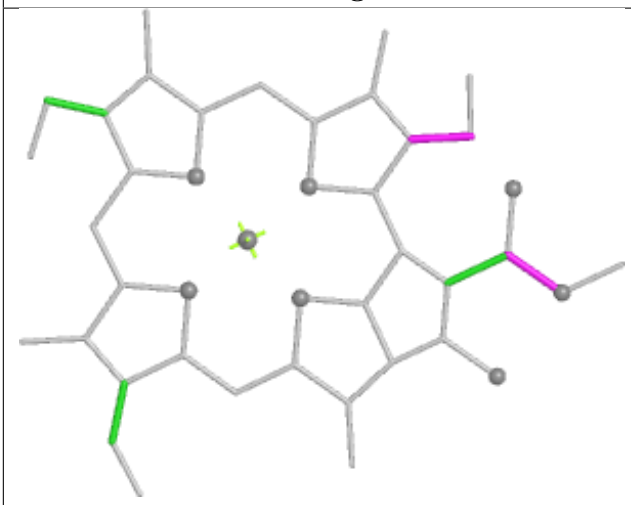
Ligand CLA d 315



Bond lengths



Bond angles

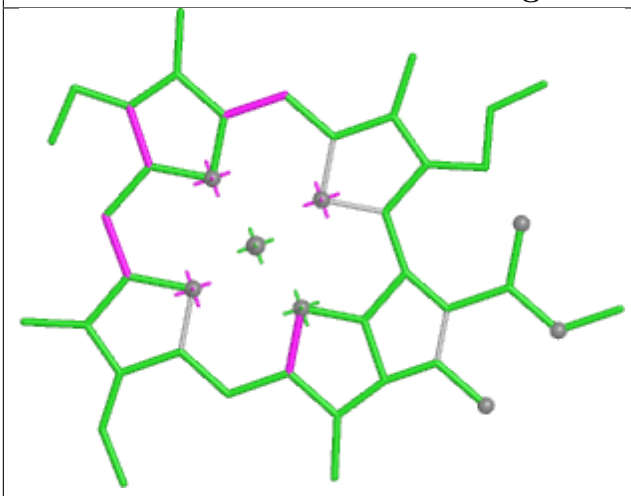


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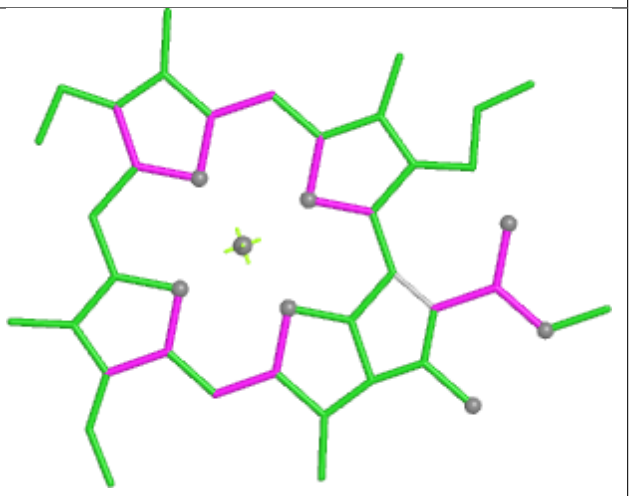


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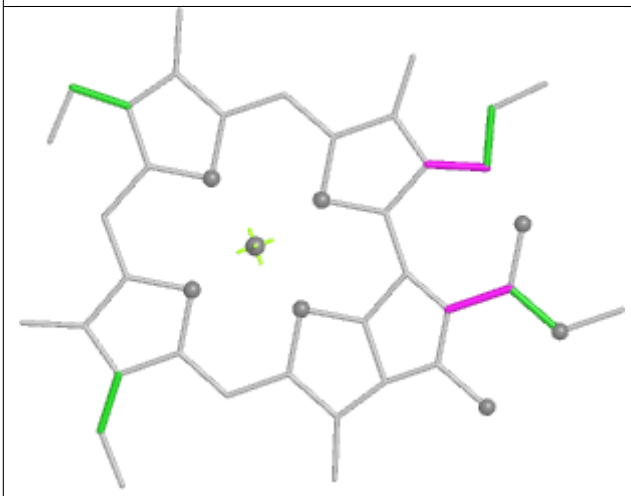
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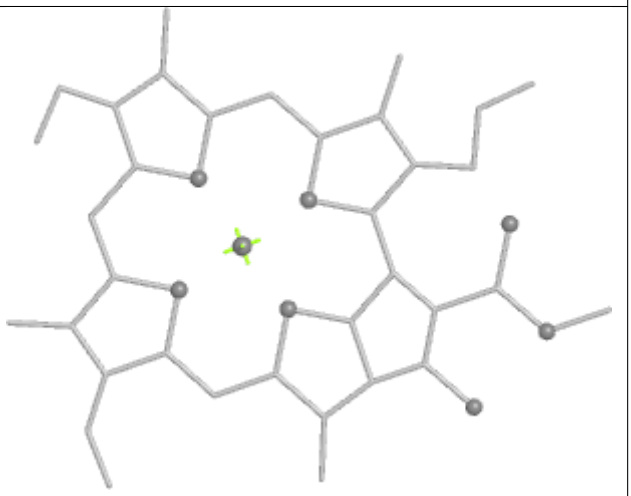
Bond lengths



Bond angles

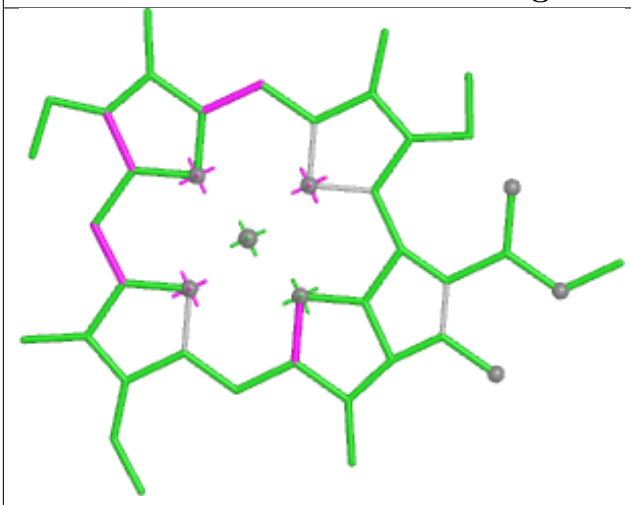


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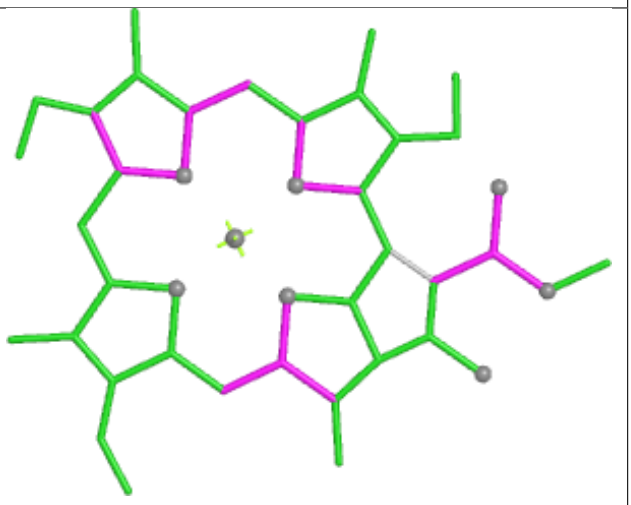


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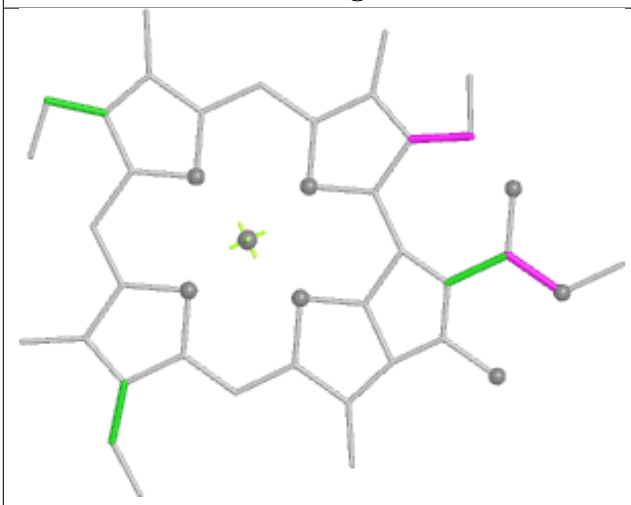
Ligand CLA f 609



Bond lengths



Bond angles

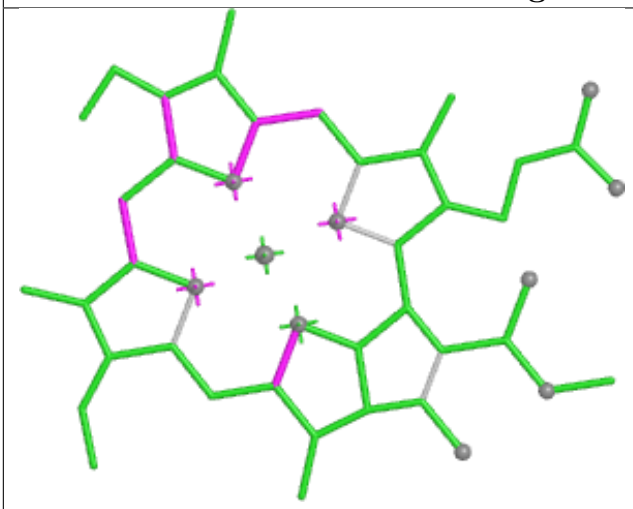


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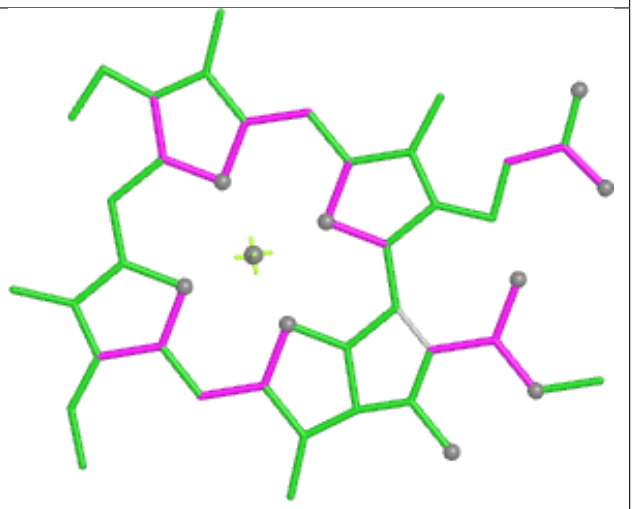


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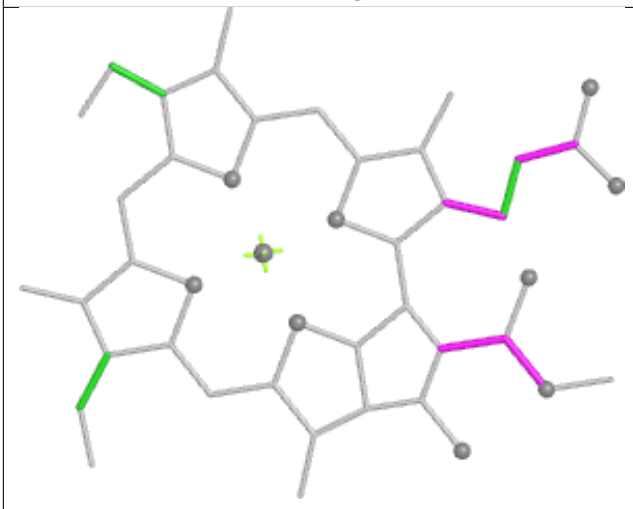
Ligand CLA a 206



Bond lengths



Bond angles

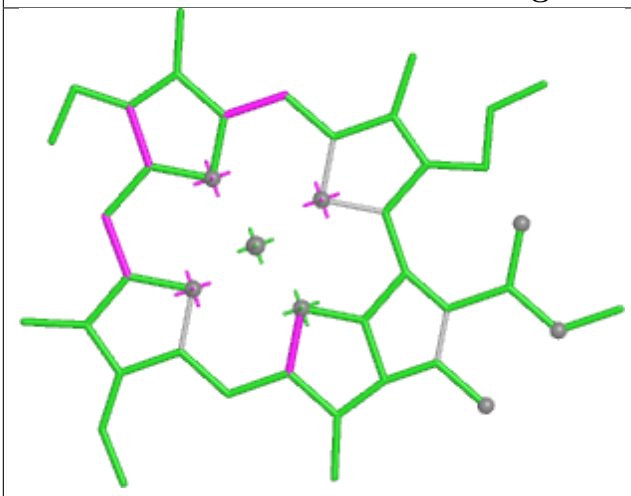


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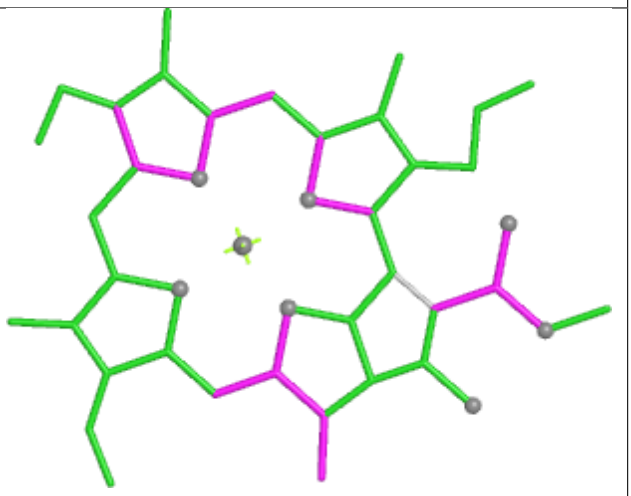


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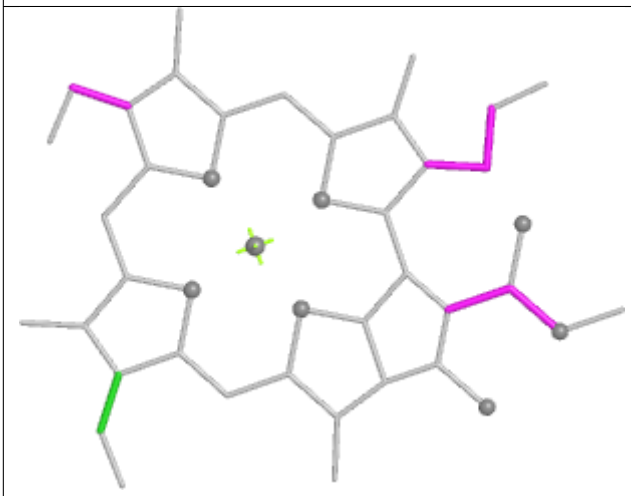
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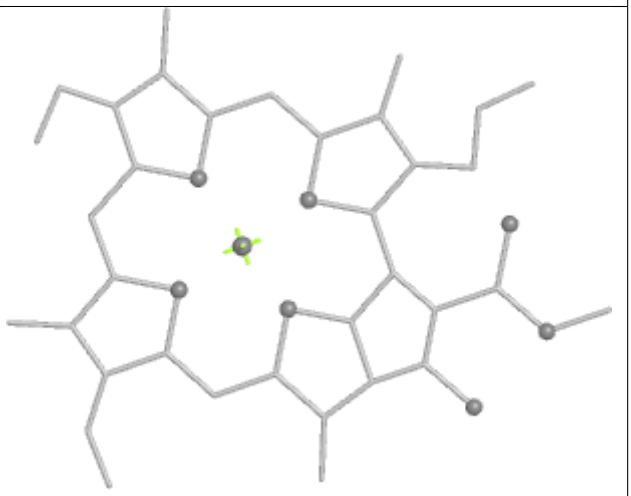
Bond lengths



Bond angles

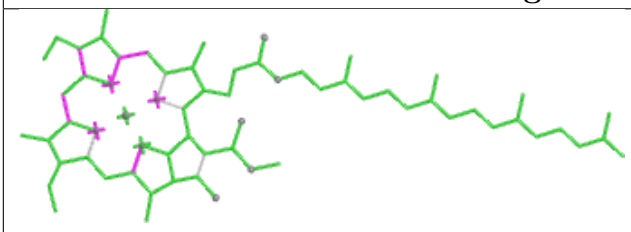


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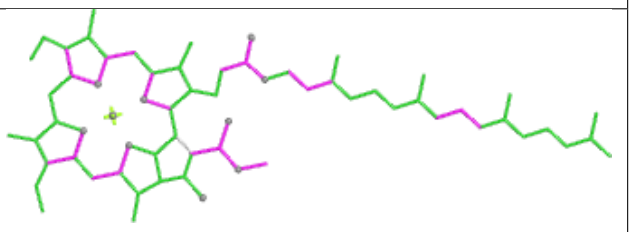


Rings

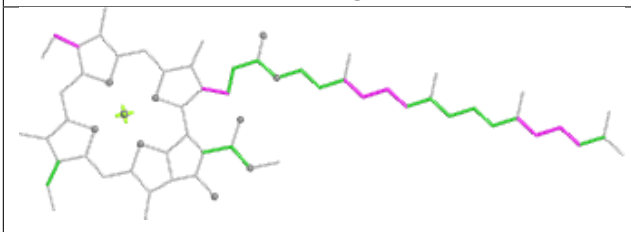
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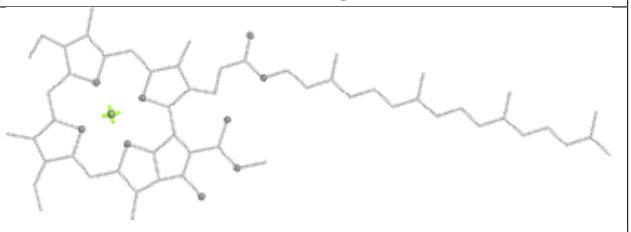
Bond lengths



Bond angles

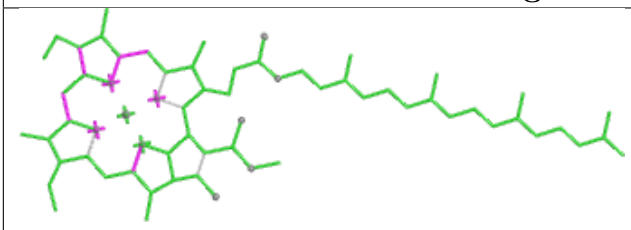


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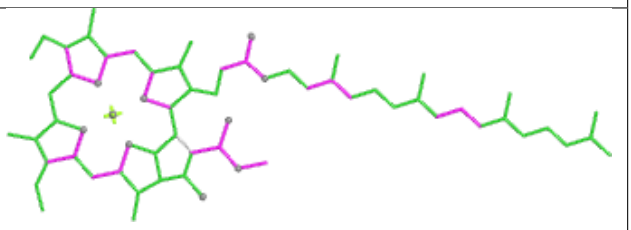


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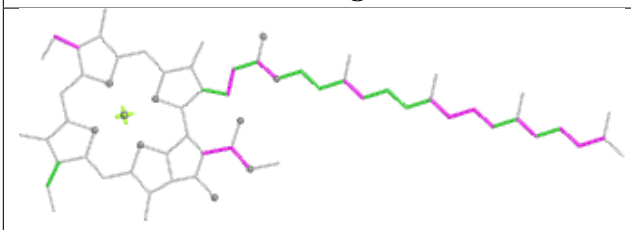
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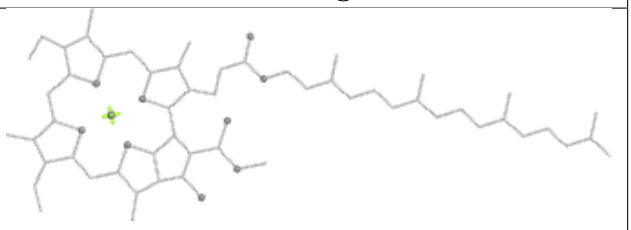
Bond lengths



Bond angles

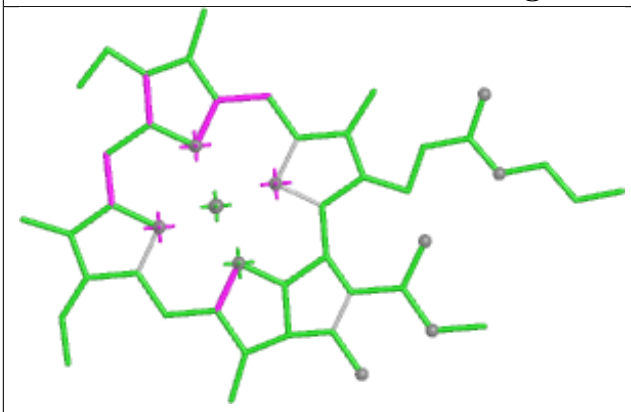


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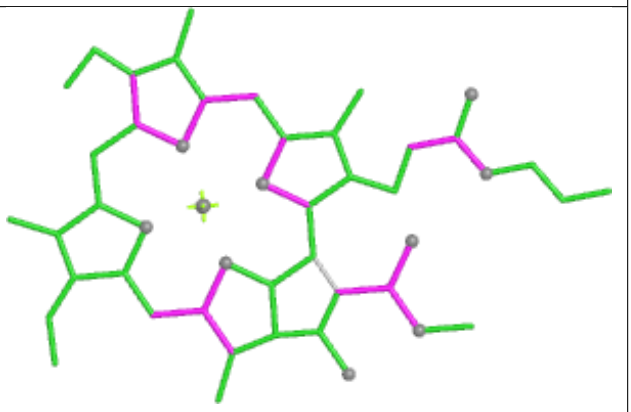


Rings

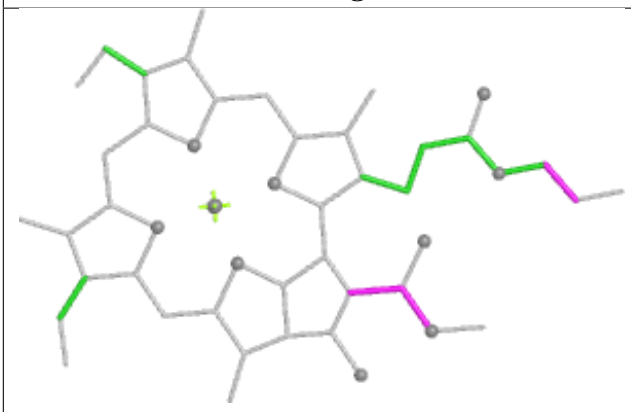
Ligand CLA A 831



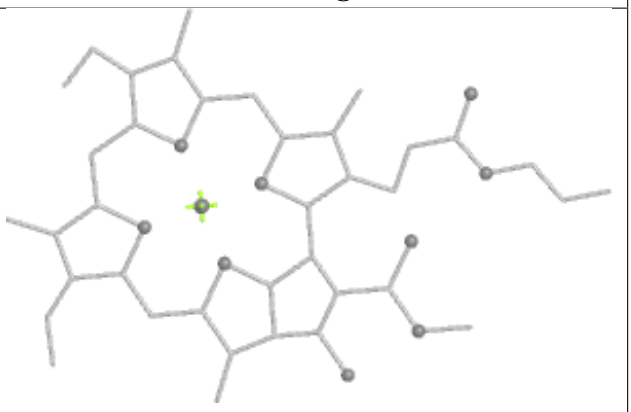
Bond lengths



Bond angles

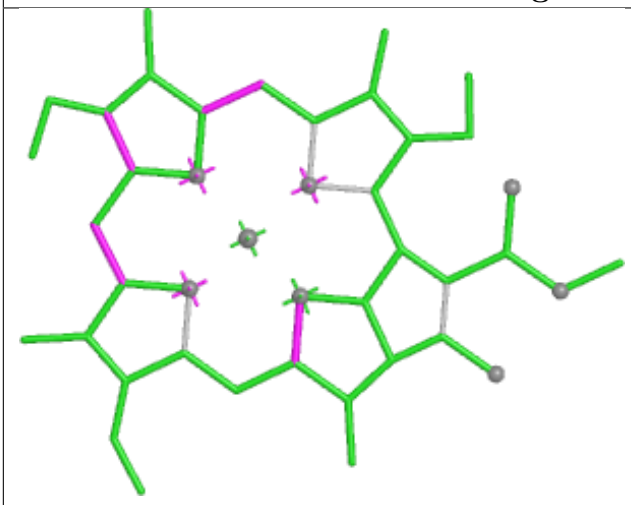


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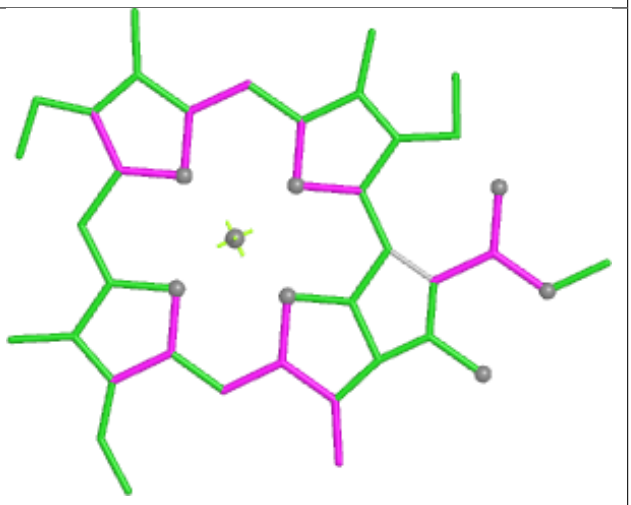


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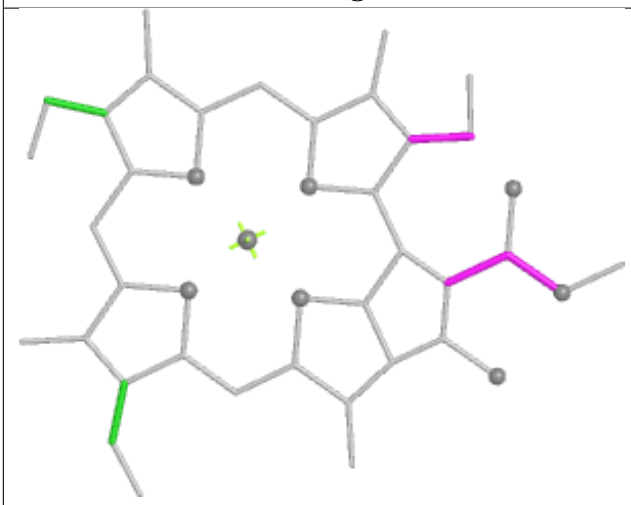
Ligand CLA f 611



Bond lengths



Bond angles

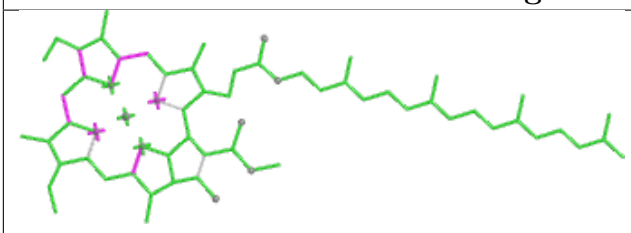


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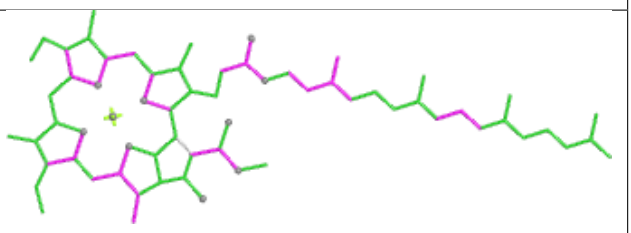


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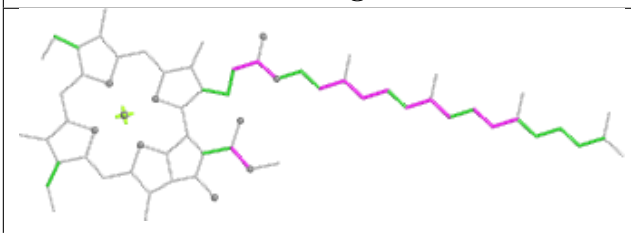
Ligand CLA B 805



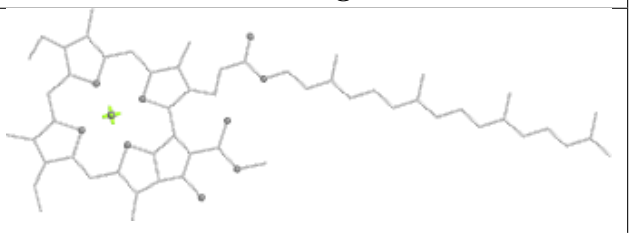
Bond lengths



Bond angles

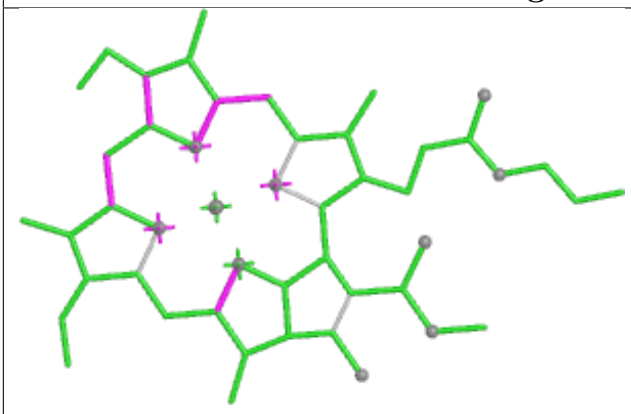


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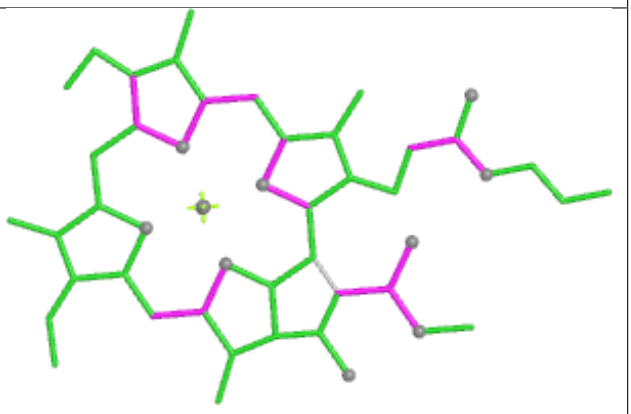


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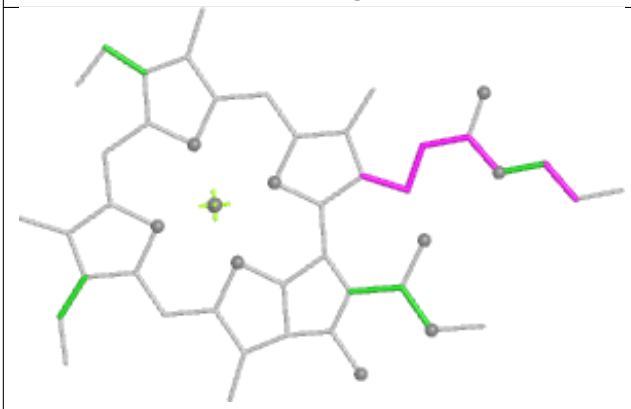
Ligand CLA h 207



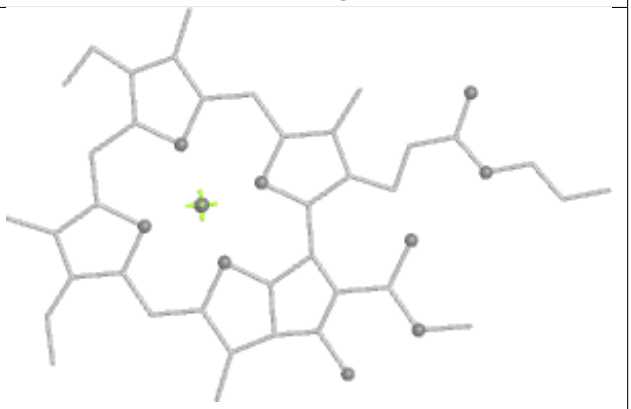
Bond lengths



Bond angles

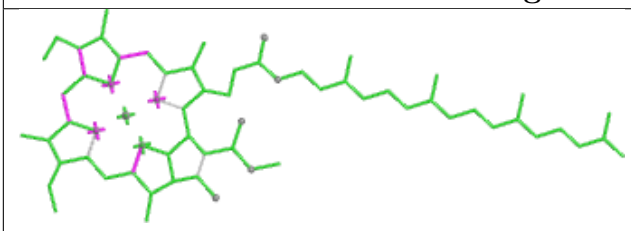


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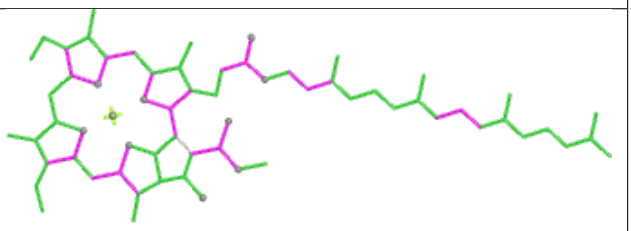


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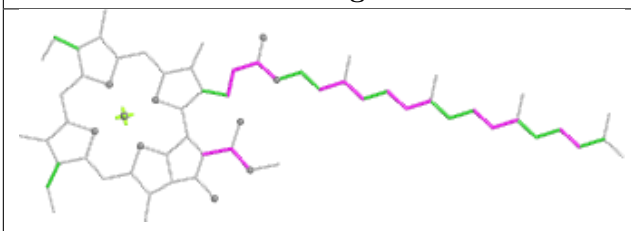
Ligand CLA A 833



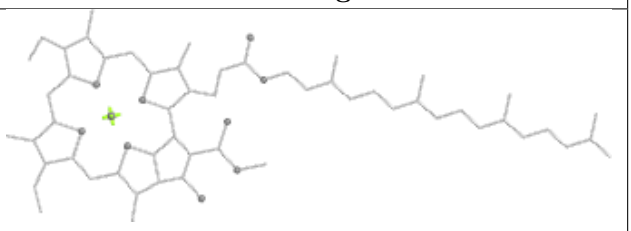
Bond lengths



Bond angles

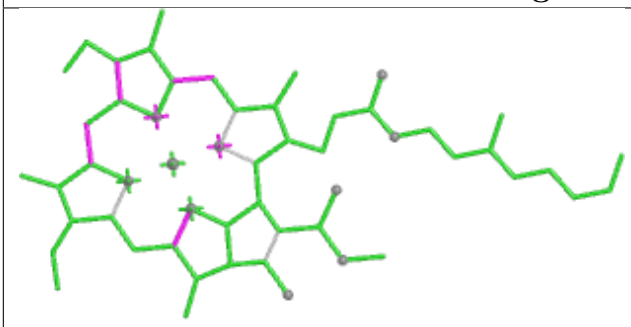


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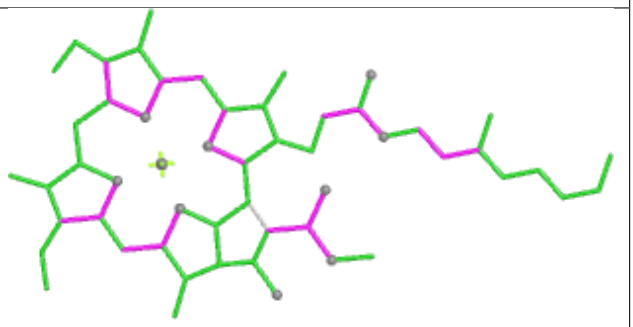


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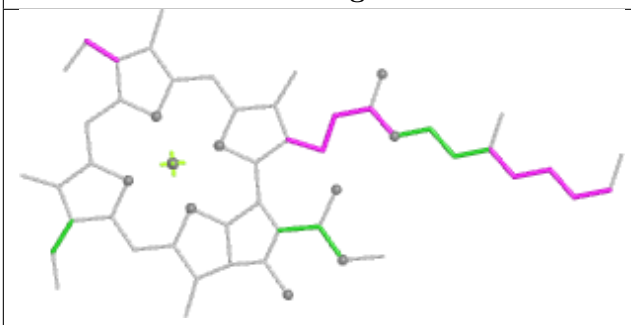
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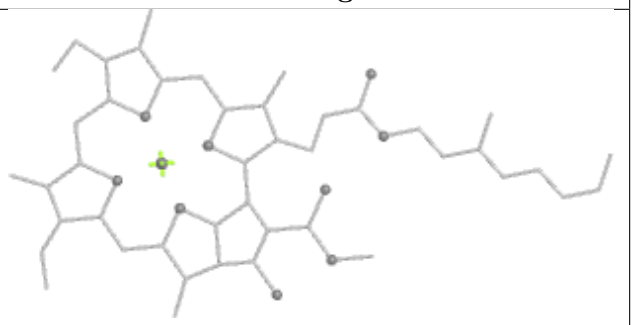
Bond lengths



Bond angles

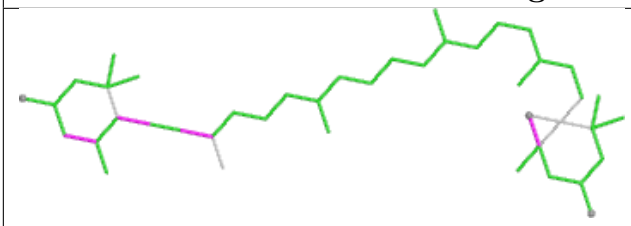


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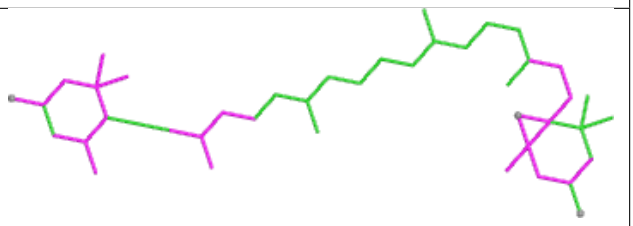


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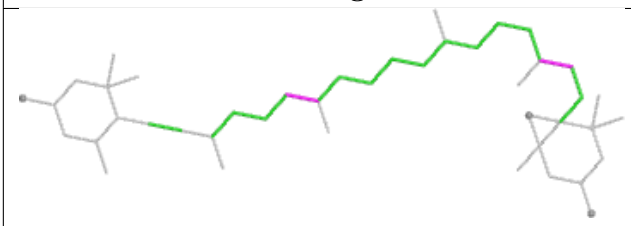
Ligand DD6 h 216



Bond lengths



Bond angles

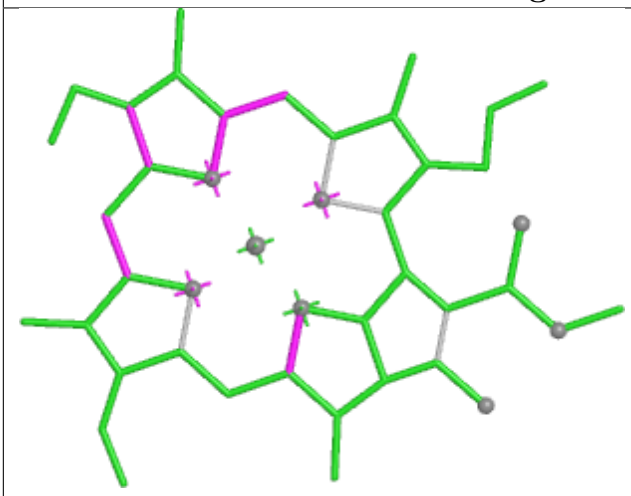


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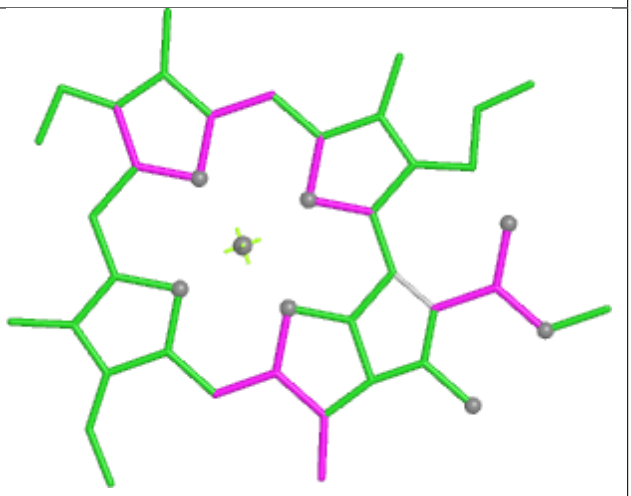


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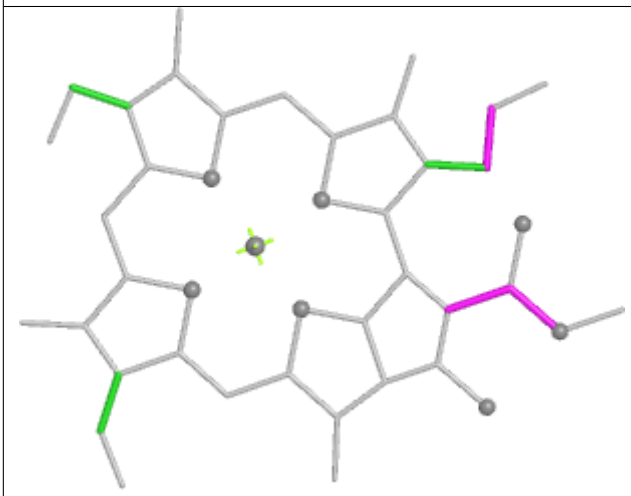
Ligand CLA c 312



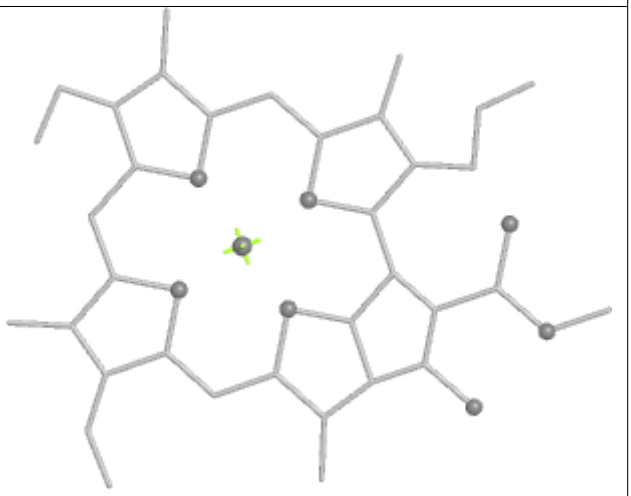
Bond lengths



Bond angles

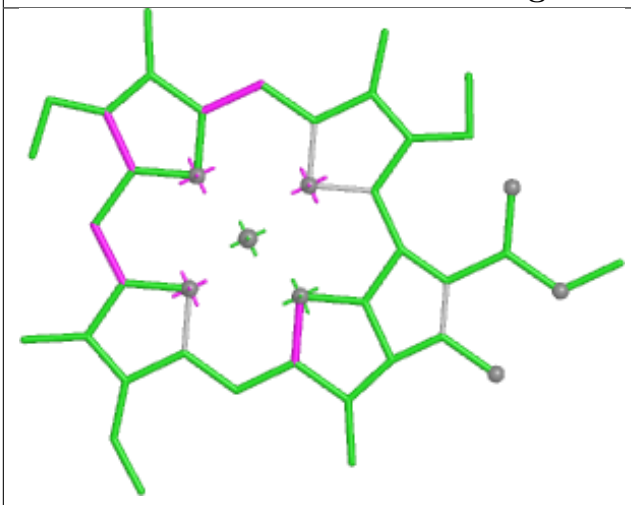


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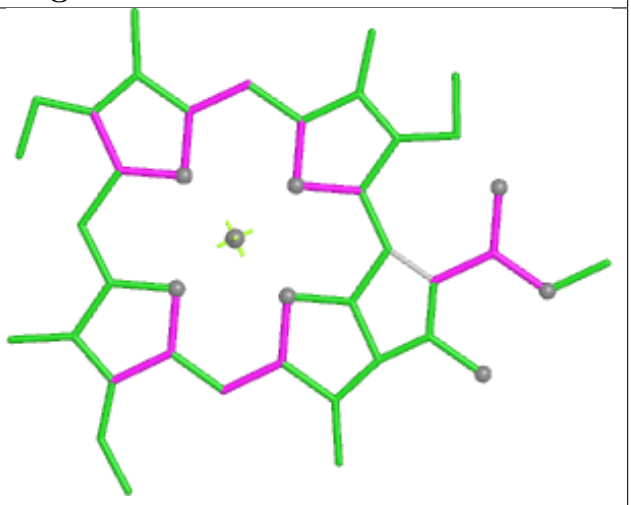


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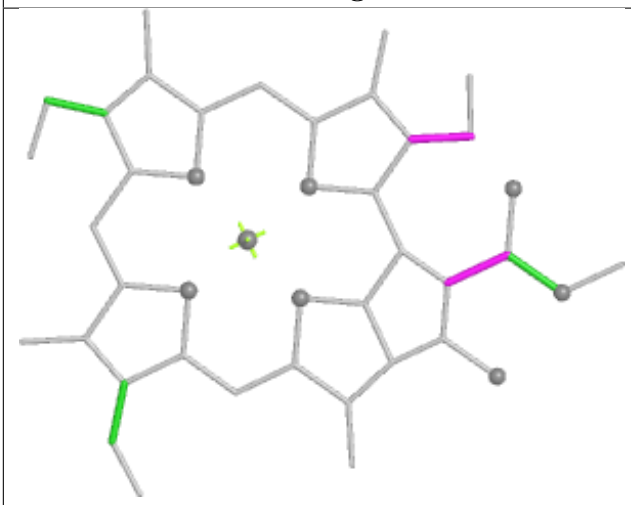
Ligand CLA g 210



Bond lengths



Bond angles

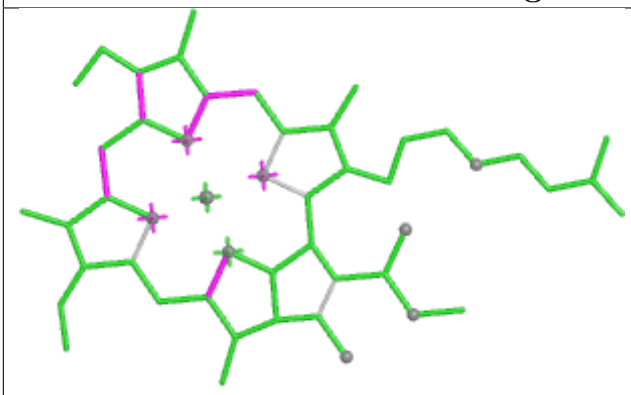


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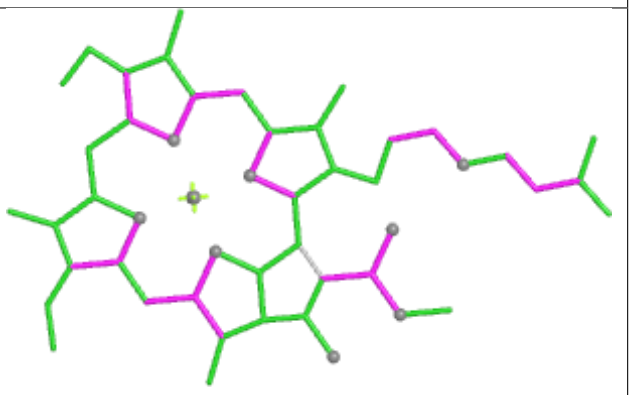


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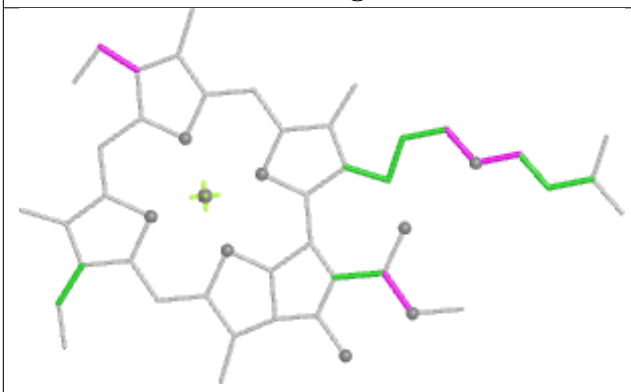
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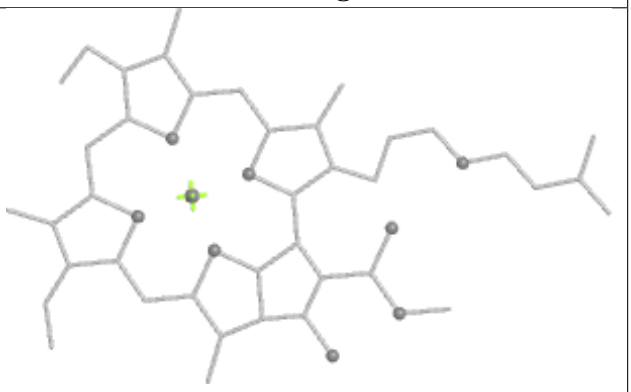
Bond lengths



Bond angles

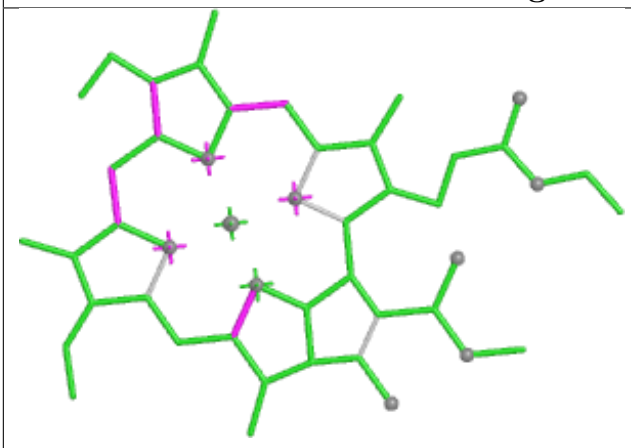


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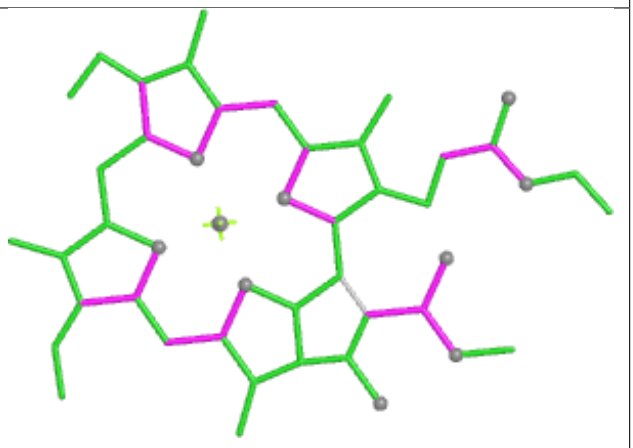


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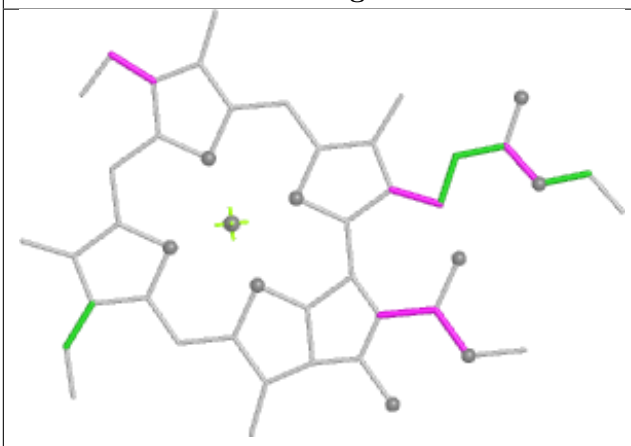
Ligand CLA o 602



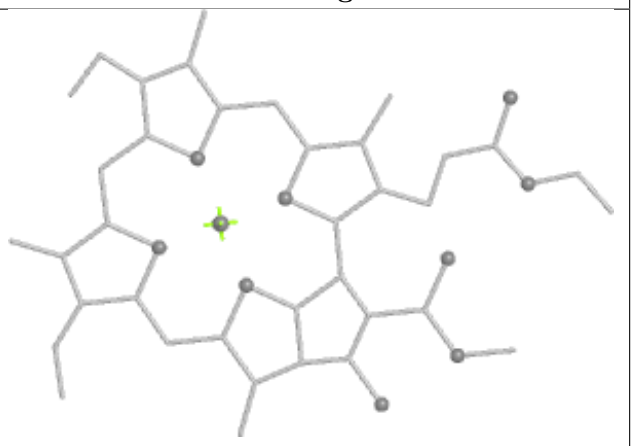
Bond lengths



Bond angles



Torsions



Rings

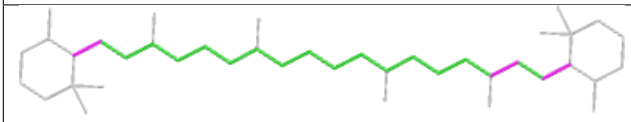
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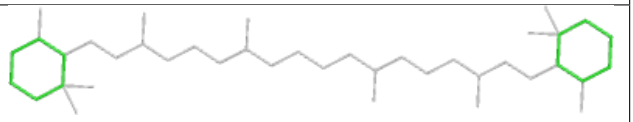
Bond lengths



Bond angles

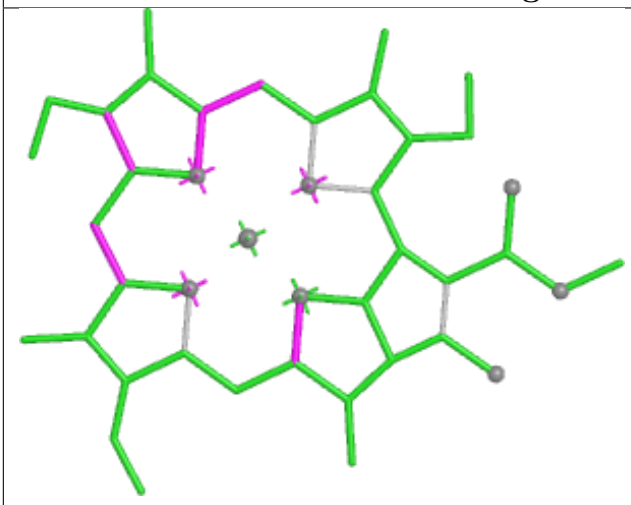


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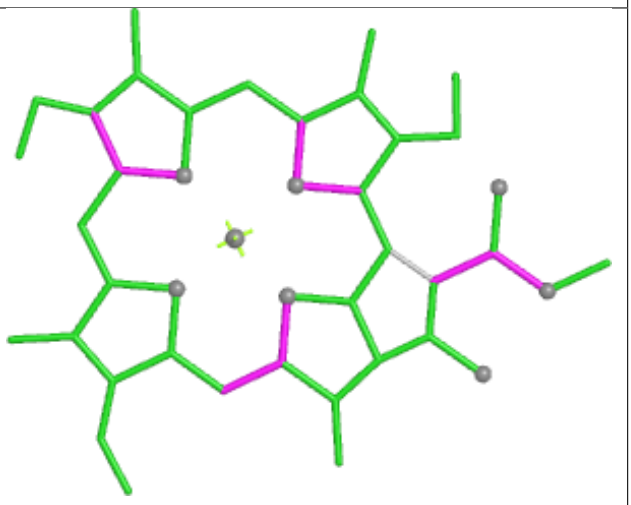


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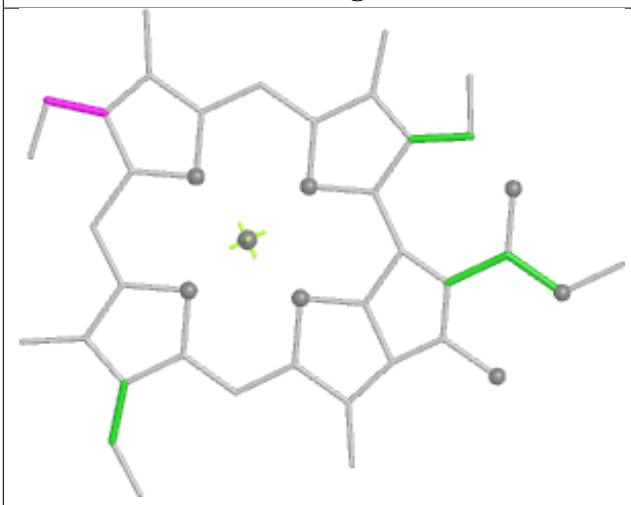
Ligand CLA m 206



Bond lengths



Bond angles

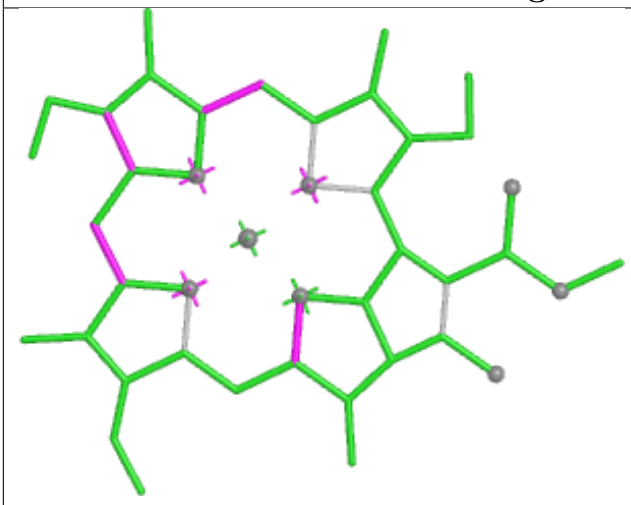


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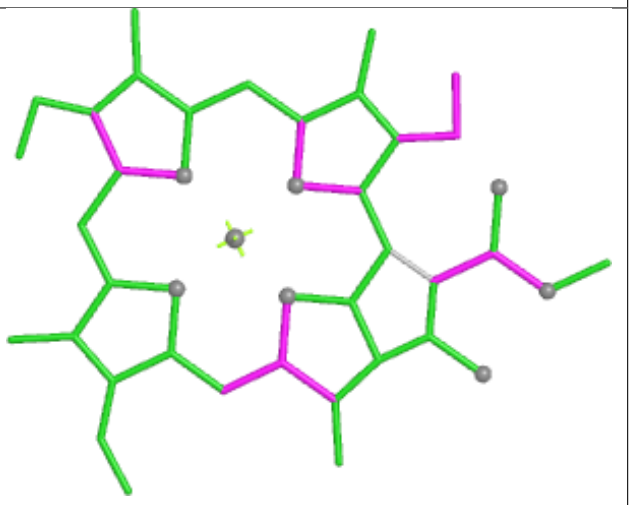


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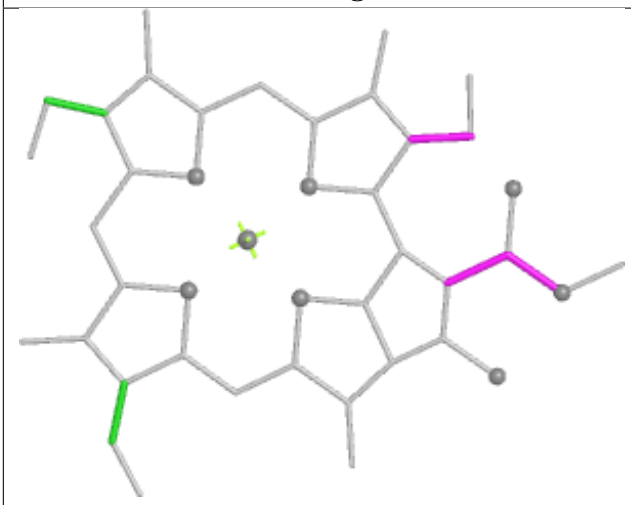
Ligand CLA o 609



Bond lengths



Bond angles

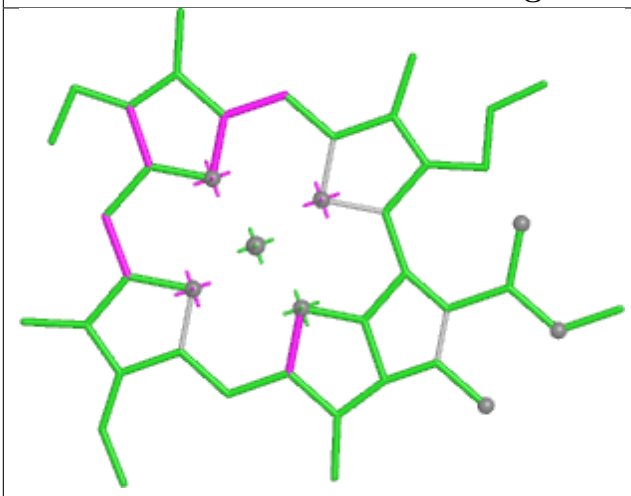


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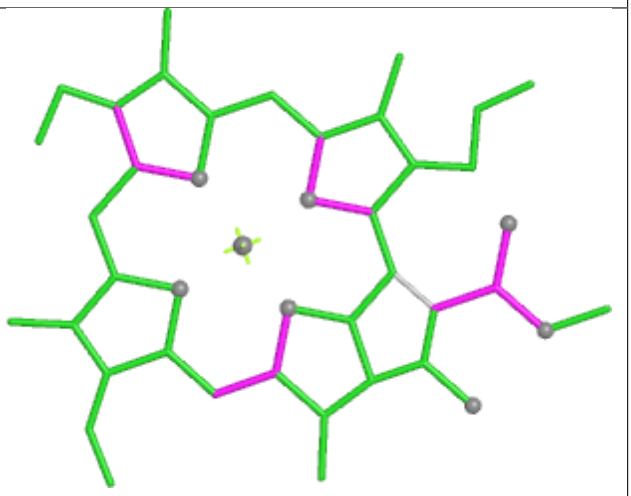


Rings

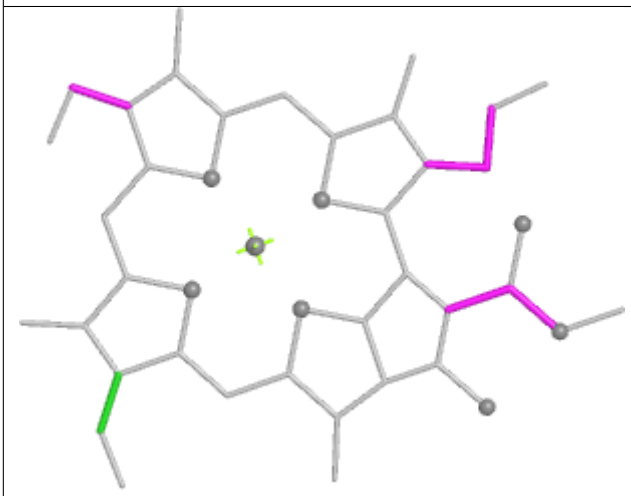
Ligand CLA B 820



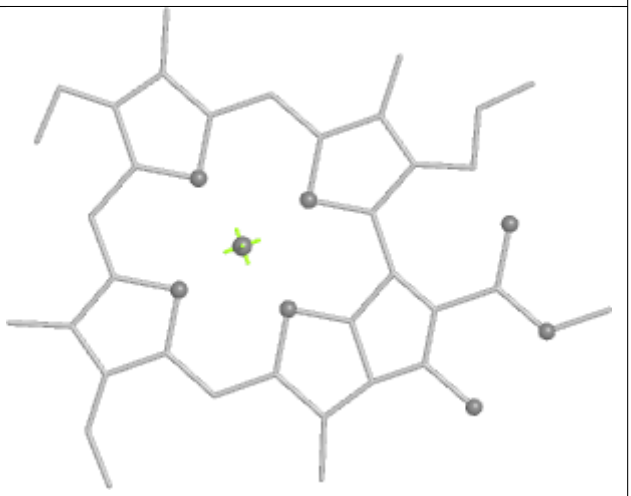
Bond lengths



Bond angles

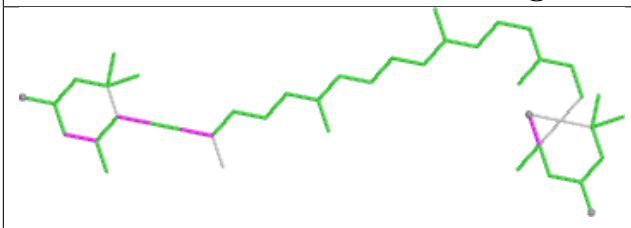


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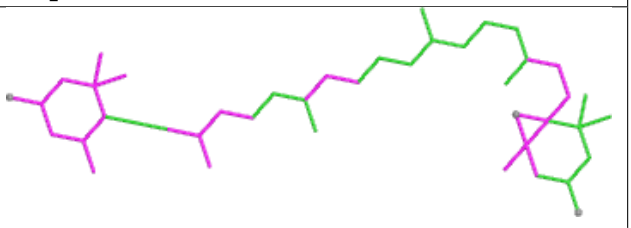


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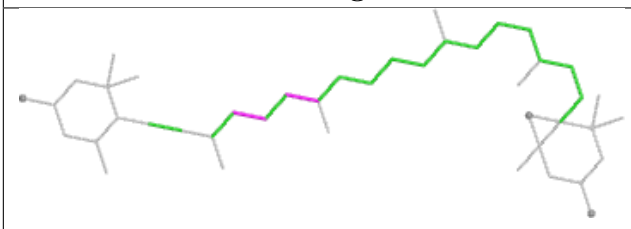
Ligand DD6 p 610



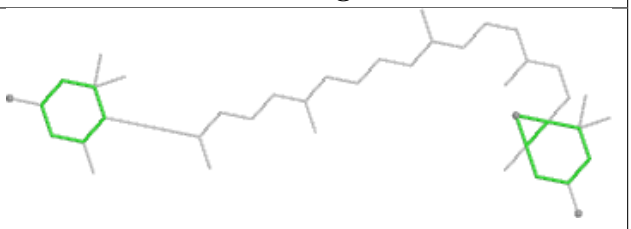
Bond lengths



Bond angles

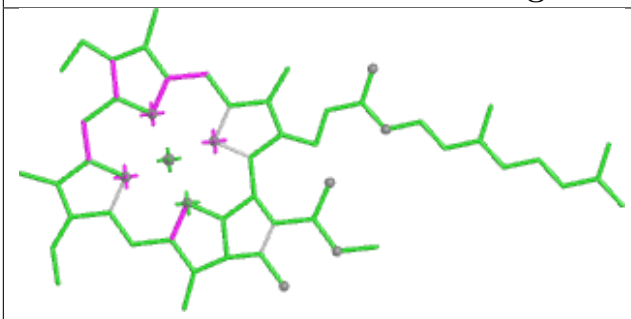


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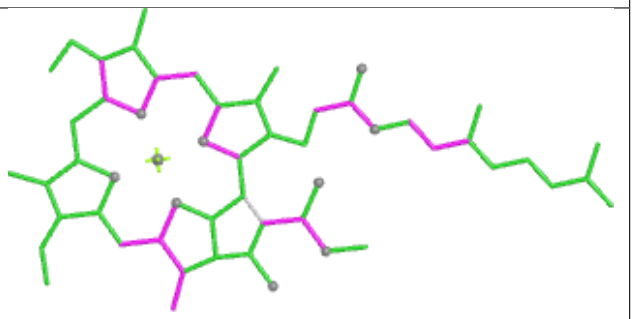


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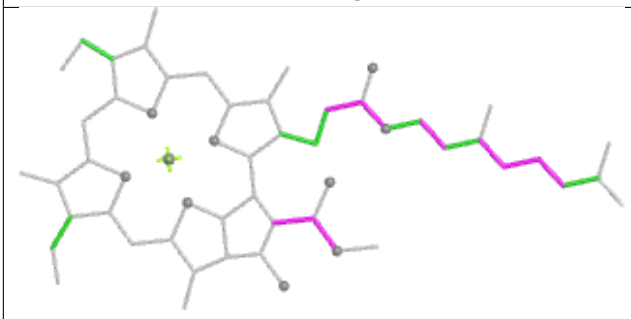
Ligand CLA n 202



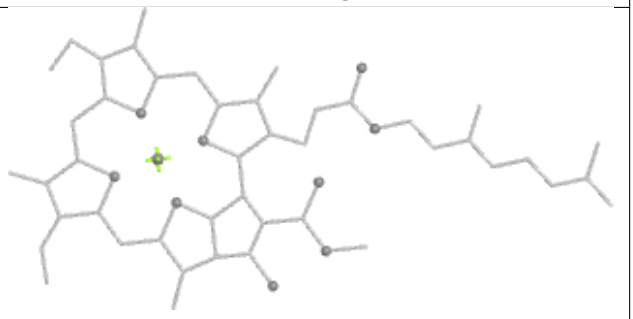
Bond lengths



Bond angles

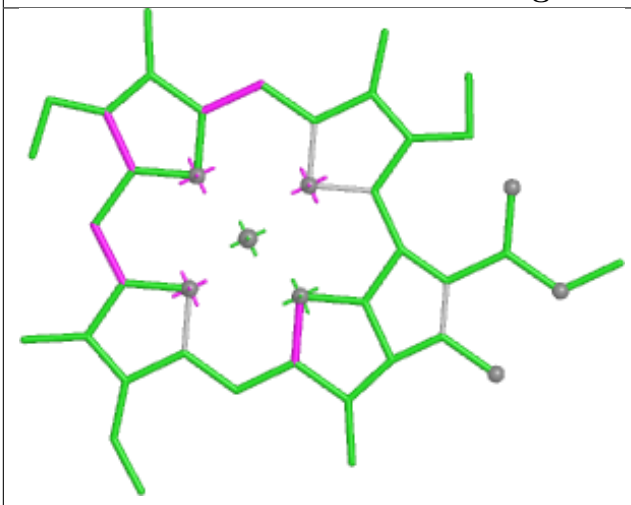


Torsions

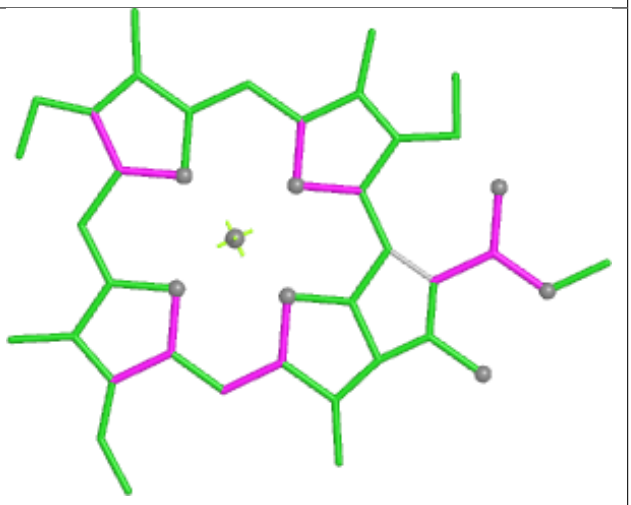


Rings

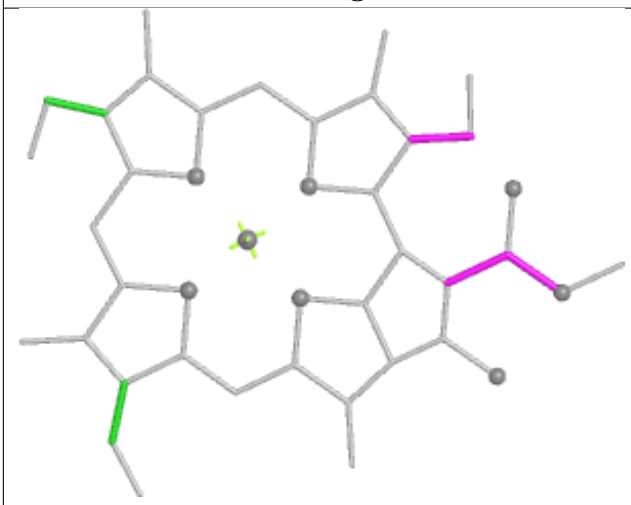
Ligand CLA l 612



Bond lengths



Bond angles

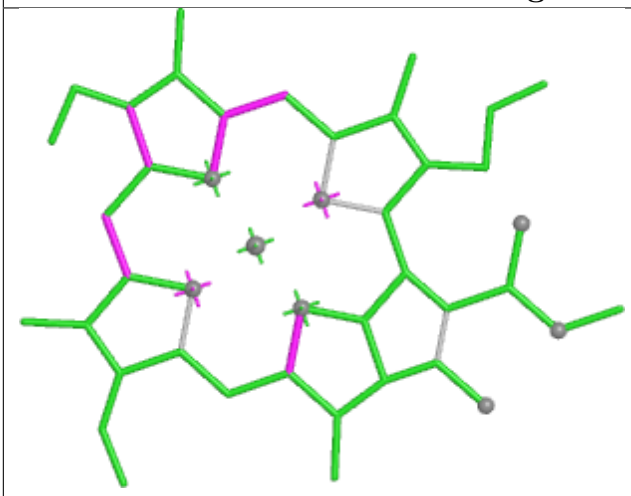


Torsions

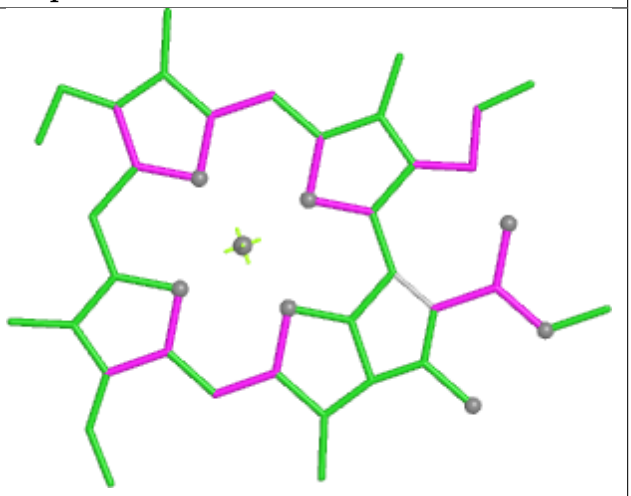


Rings

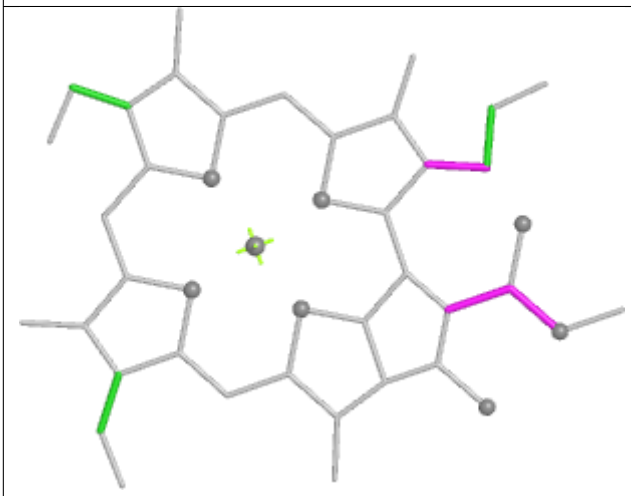
Ligand CLA p 608



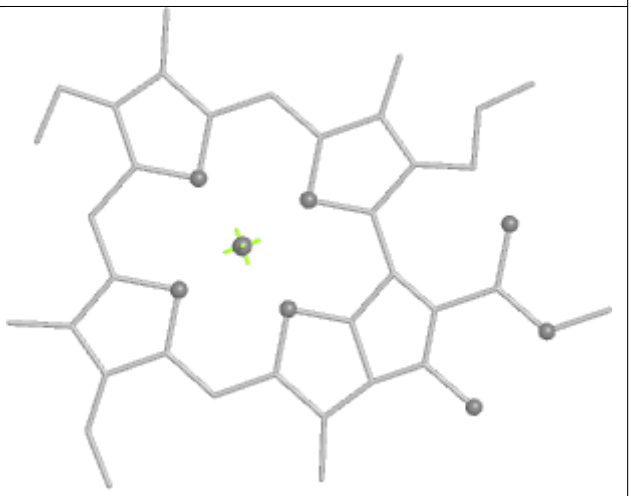
Bond lengths



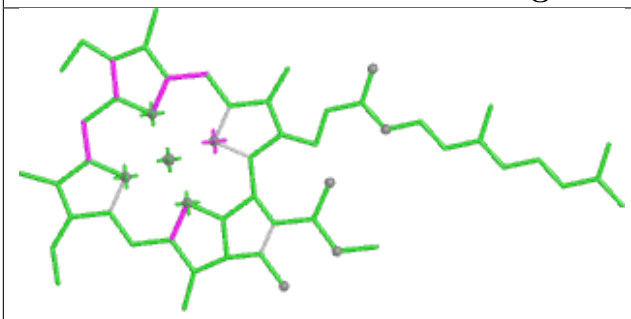
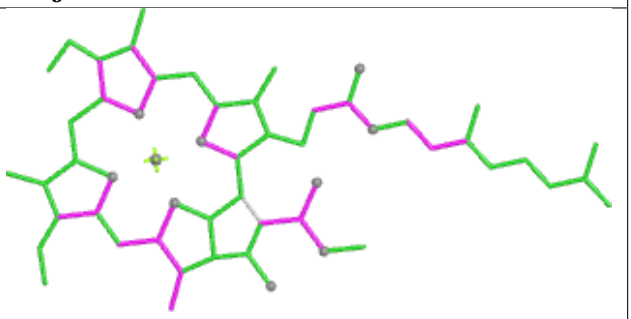
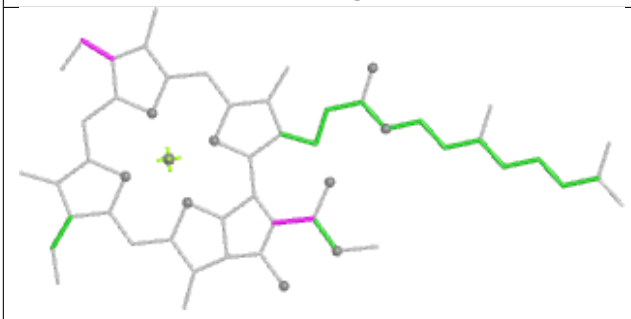
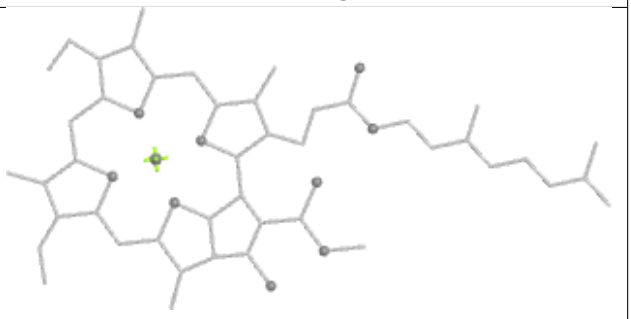
Bond angles

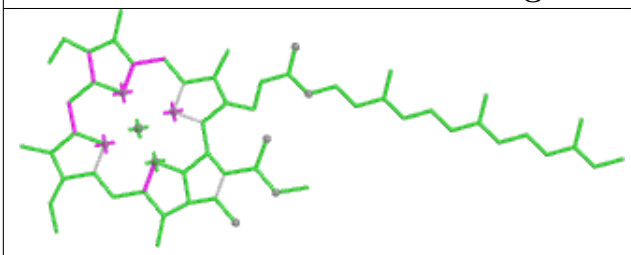
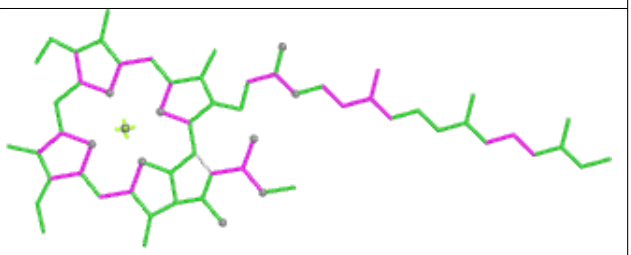
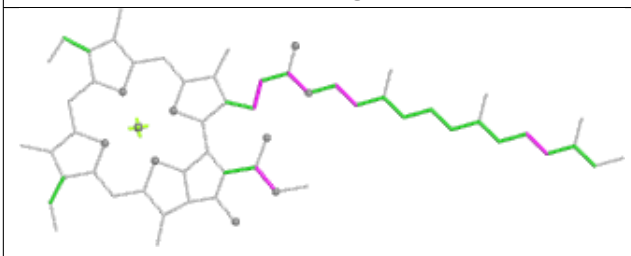
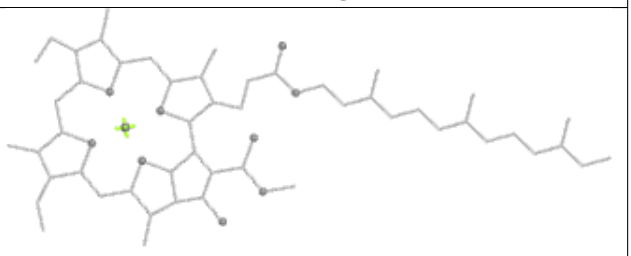


Torsions

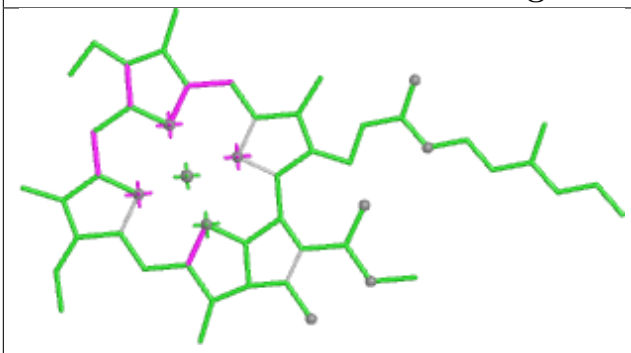


Rings

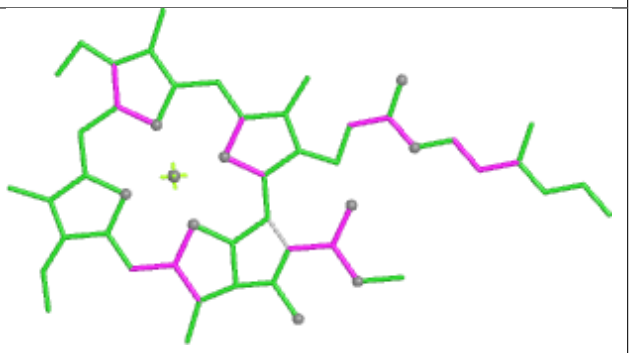
Ligand CLA j 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

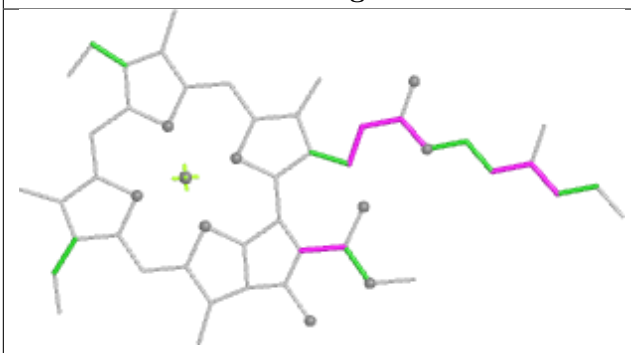
Ligand CLA b 212



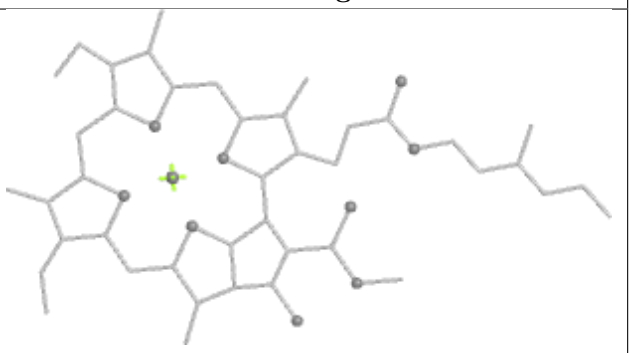
Bond lengths



Bond angles

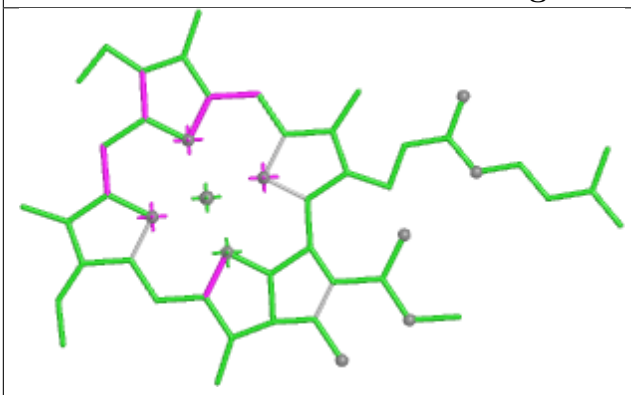


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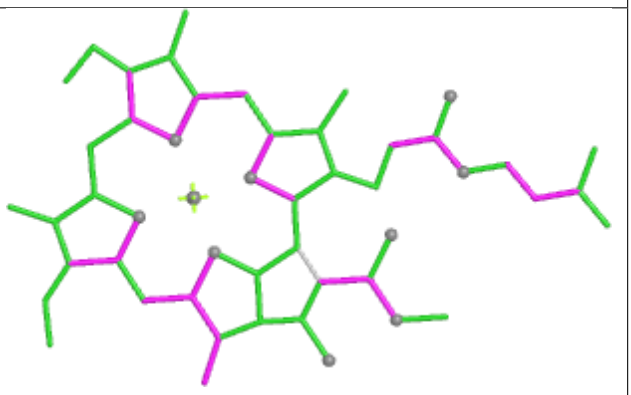


Rings

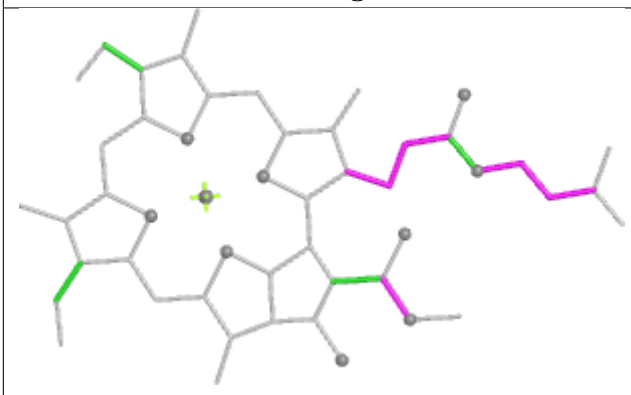
Ligand CLA c 308



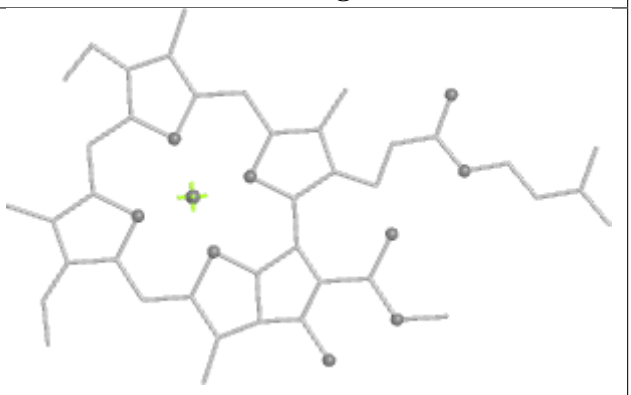
Bond lengths



Bond angles

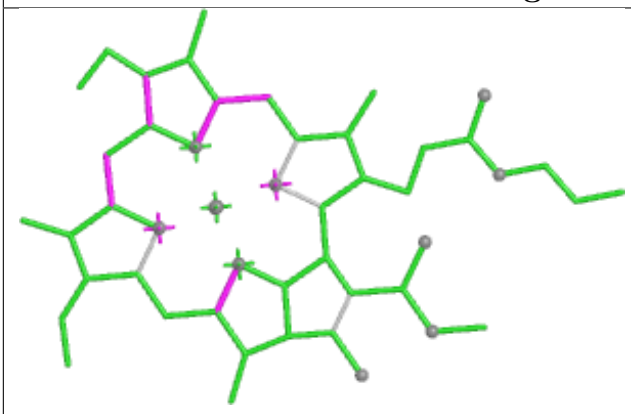


Torsions

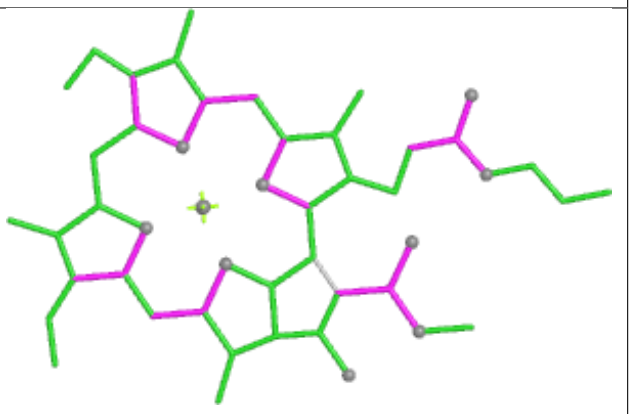


Rings

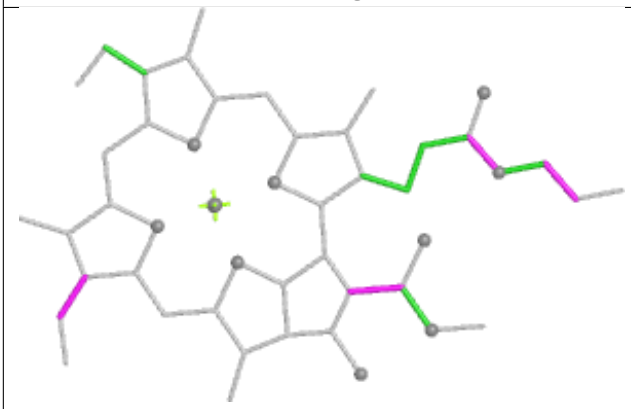
Ligand CLA A 852



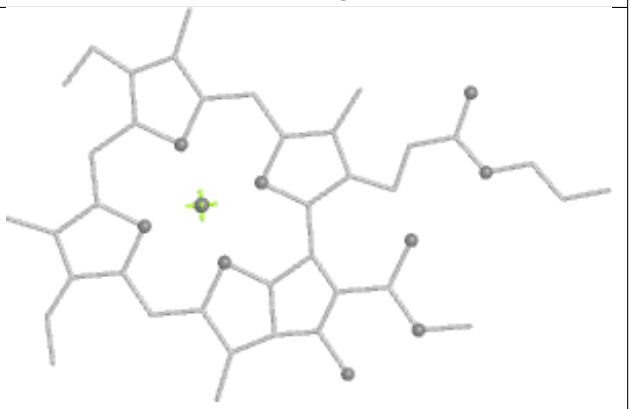
Bond lengths



Bond angles

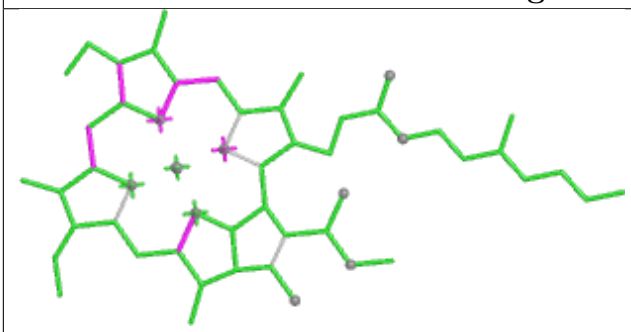


Torsions

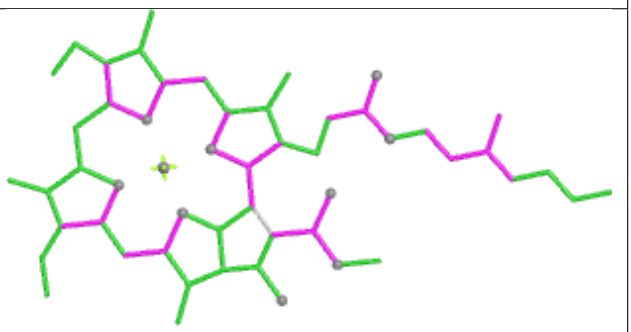


Rings

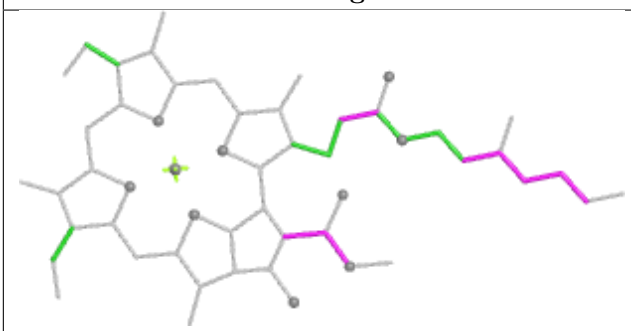
Ligand CLA h 212



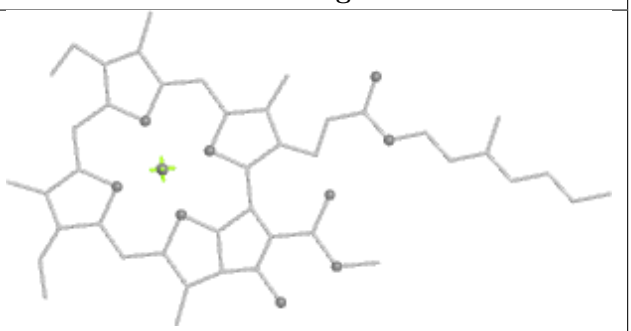
Bond lengths



Bond angles

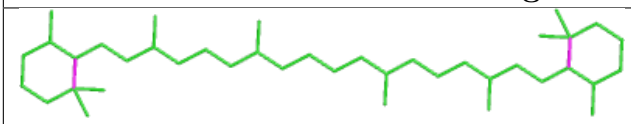


Torsions

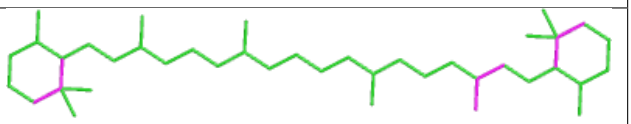


Rings

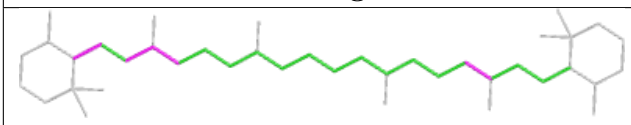
Ligand BCR B 830



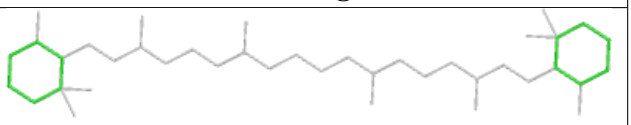
Bond lengths



Bond angles

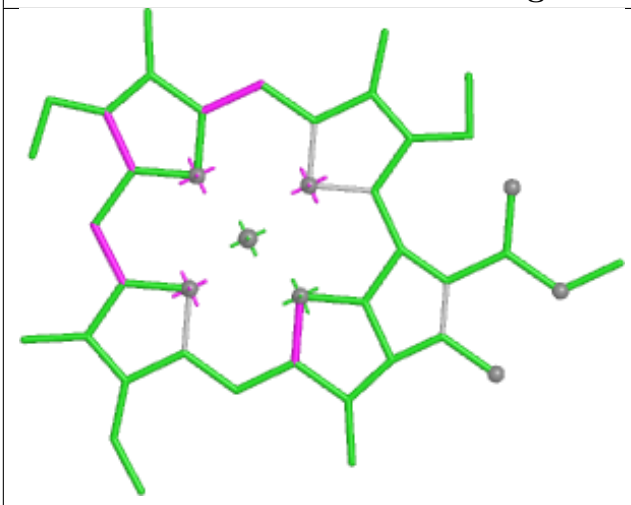


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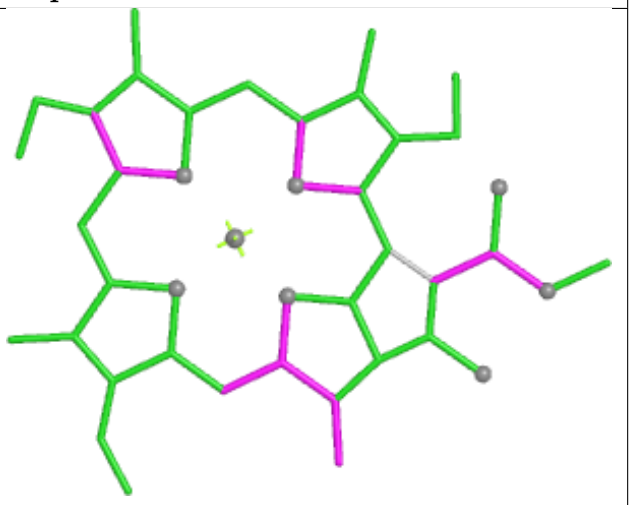


Rings

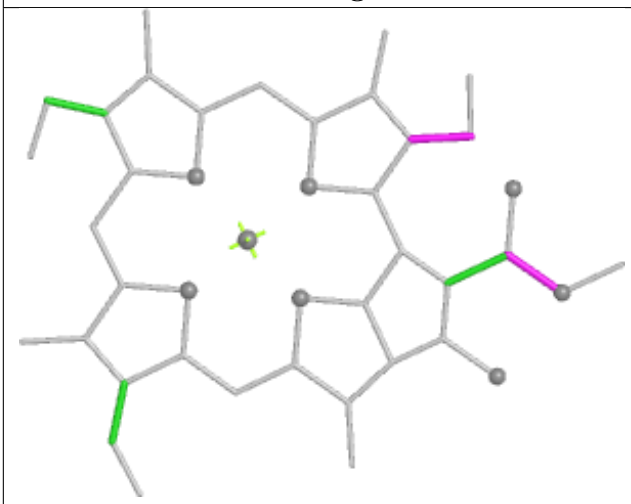
Ligand CLA p 603



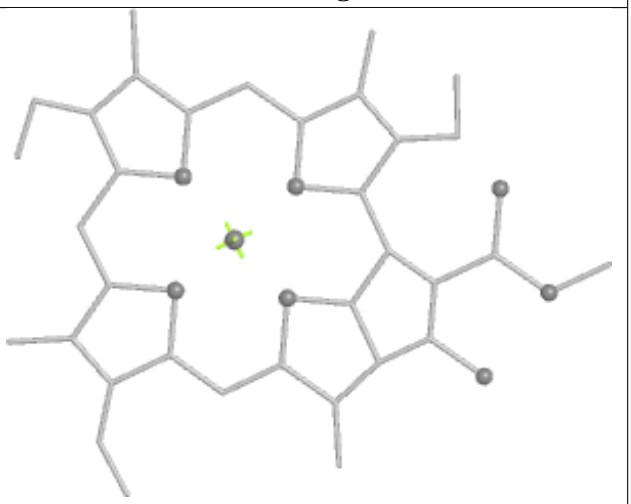
Bond lengths



Bond angles

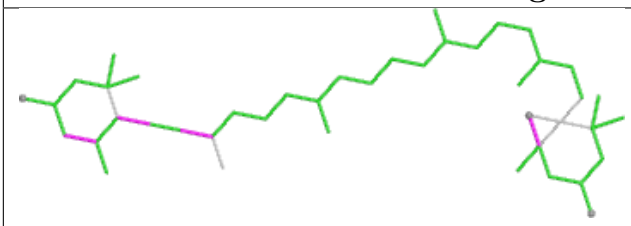


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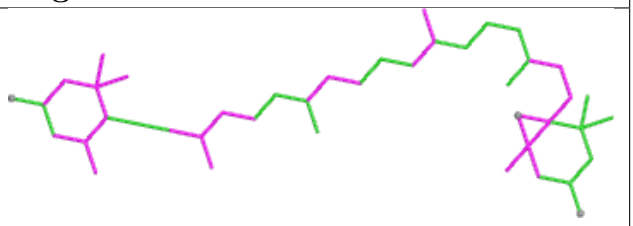


Rings

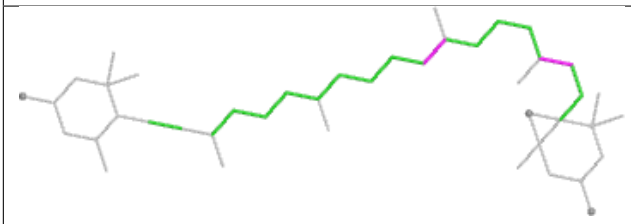
Ligand DD6 g 216



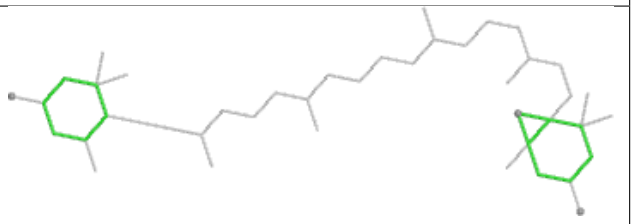
Bond lengths



Bond angles

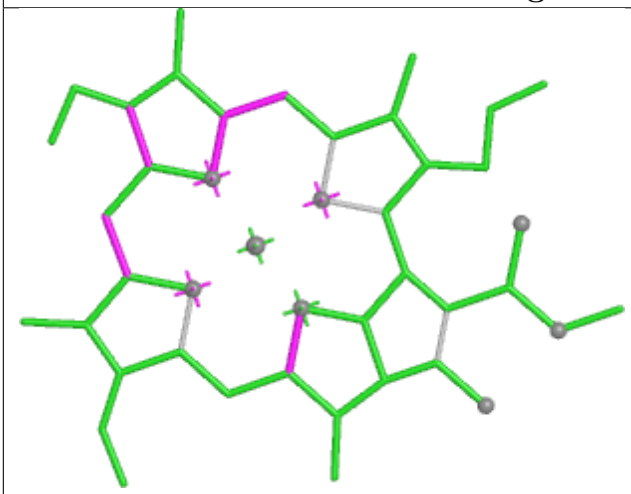


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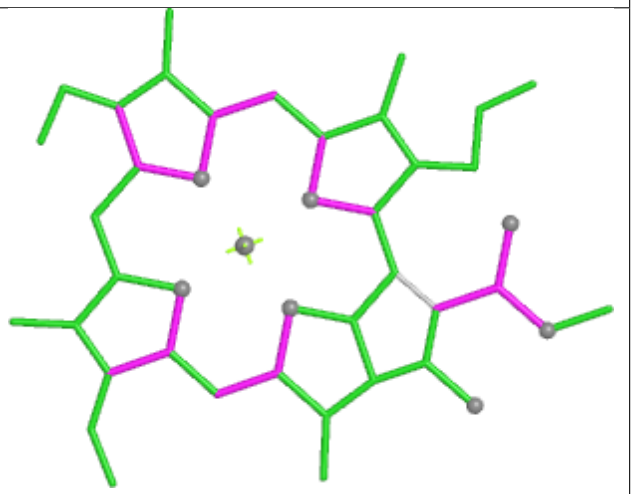


Rings

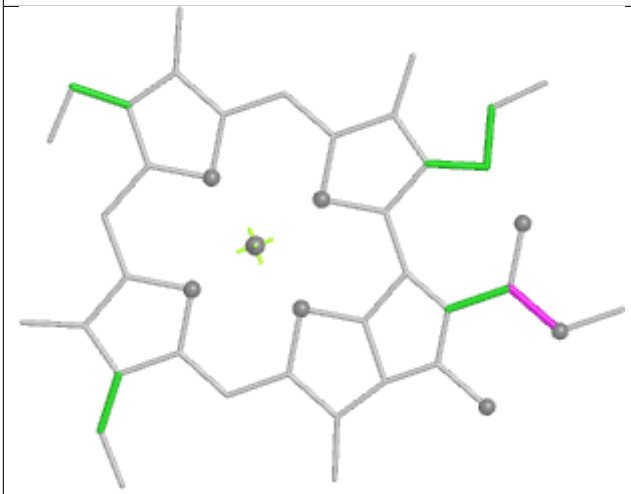
Ligand CLA h 215



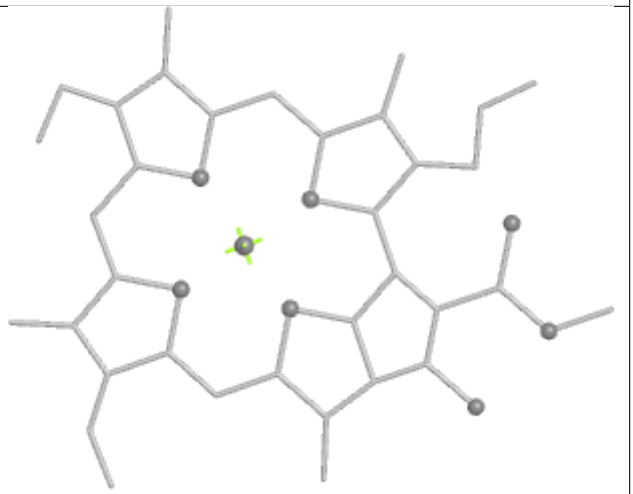
Bond lengths



Bond angles

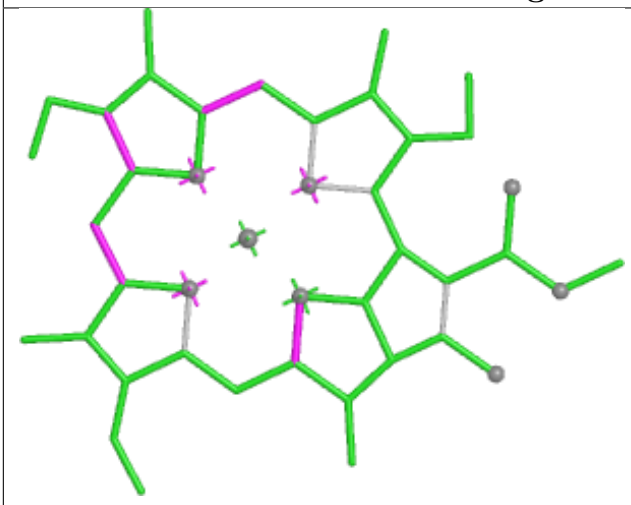


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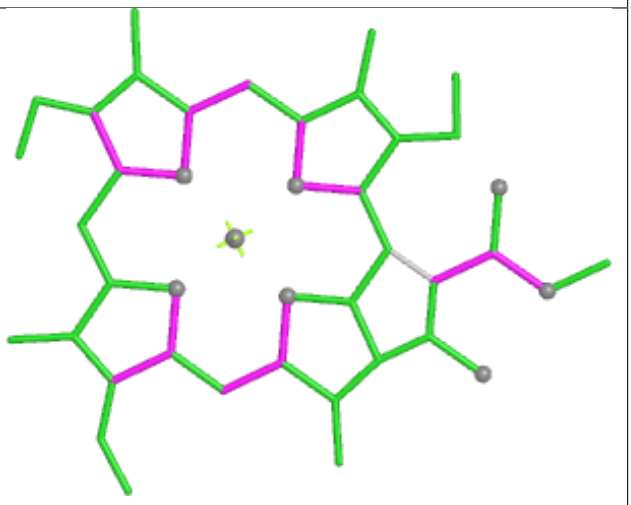


Rings

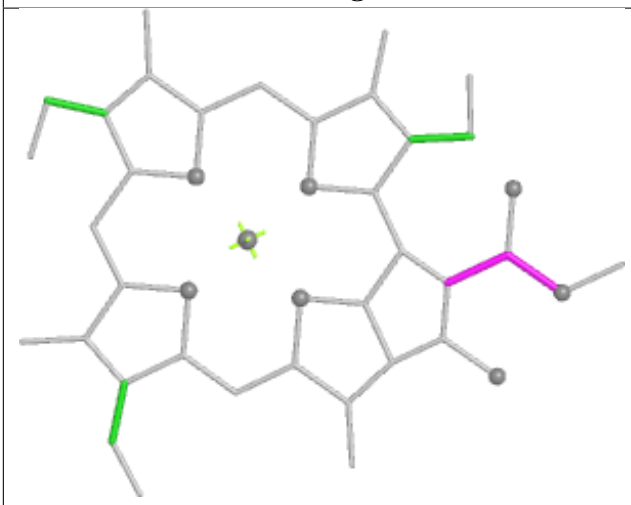
Ligand CLA b 211



Bond lengths



Bond angles

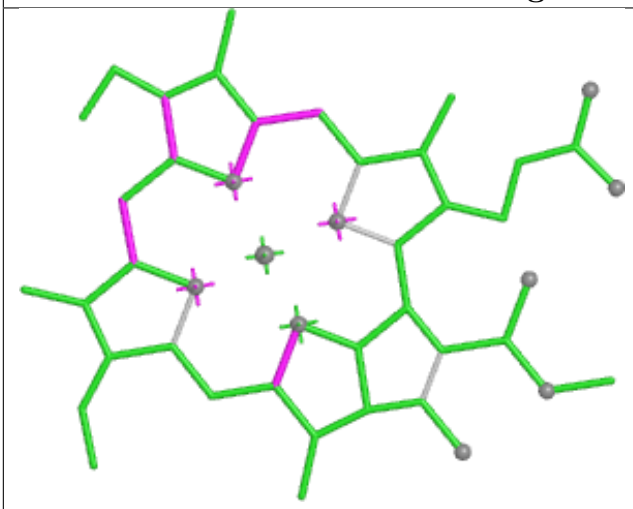


Torsions

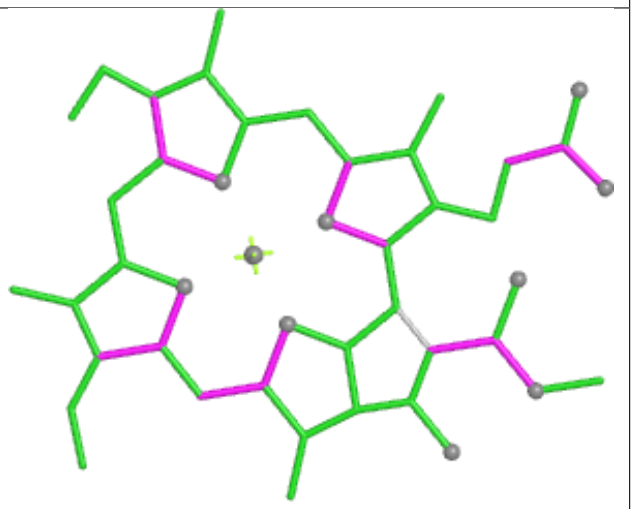


Rings

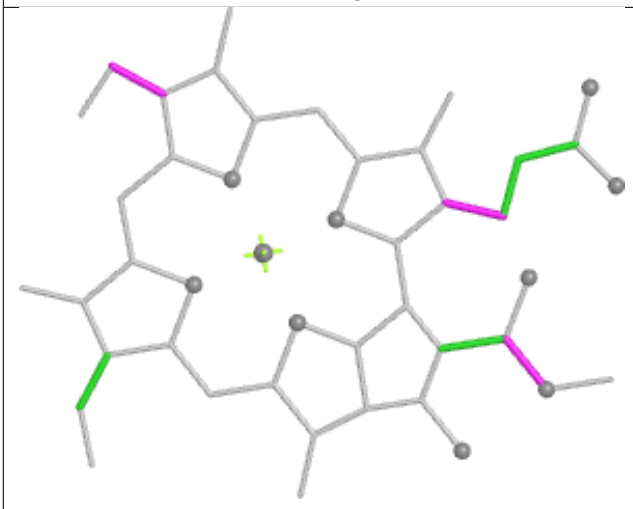
Ligand CLA b 206



Bond lengths



Bond angles

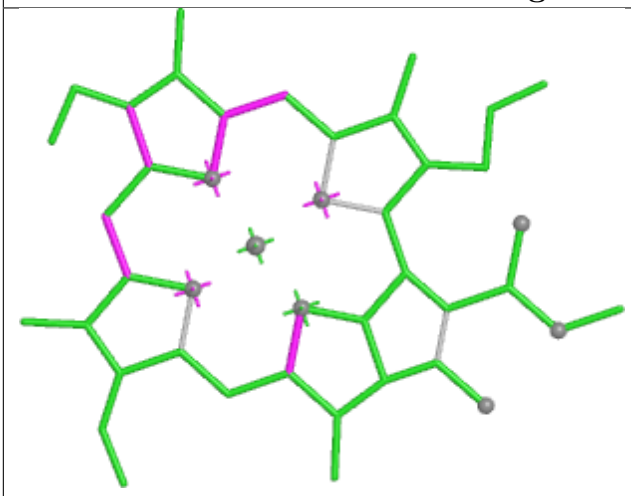


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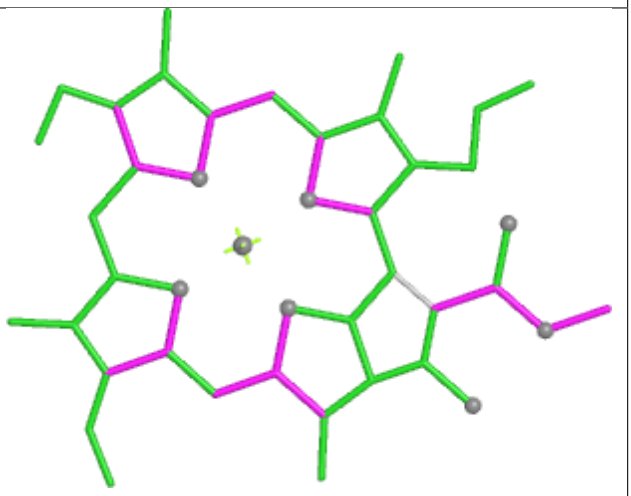


Rings

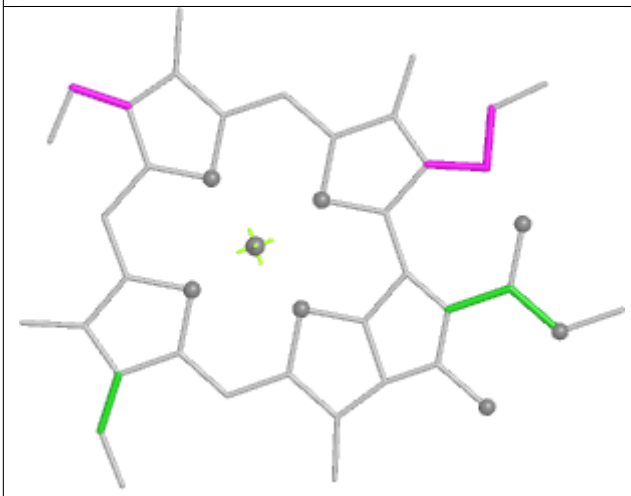
Ligand CLA o 605



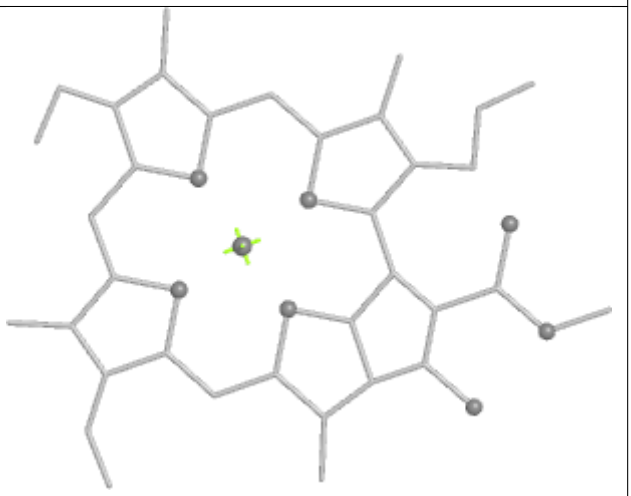
Bond lengths



Bond angles

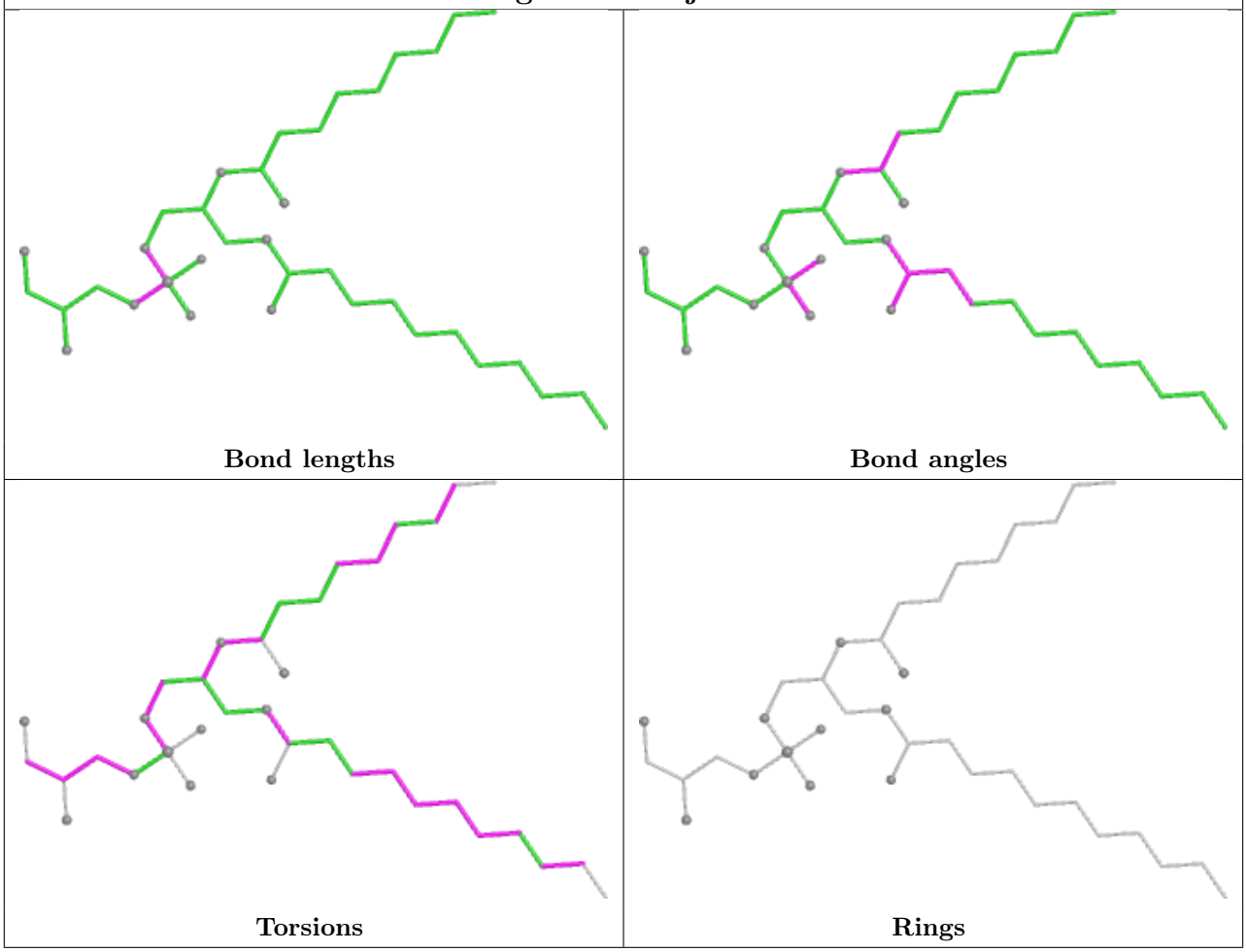


Torsions

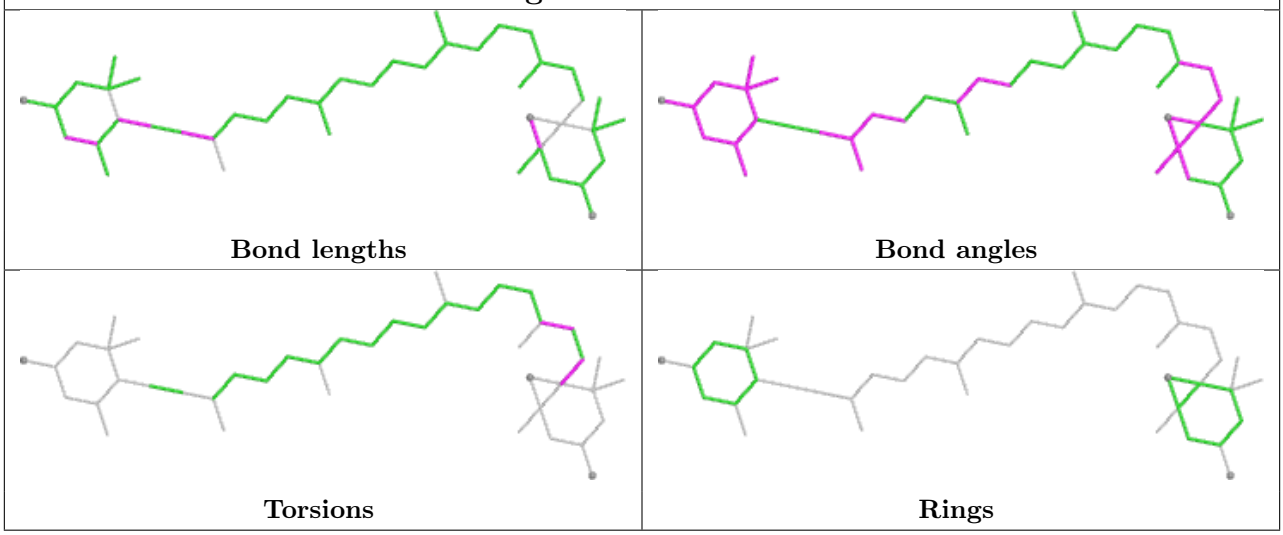


Rings

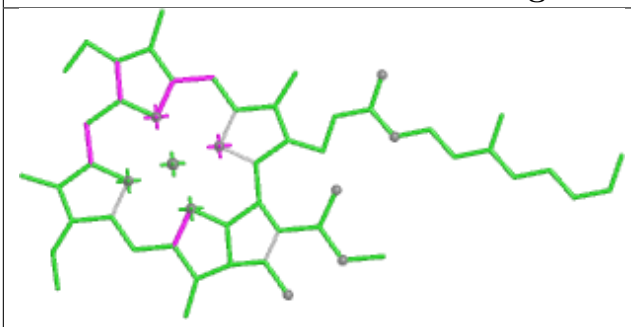
Ligand LHG j 202



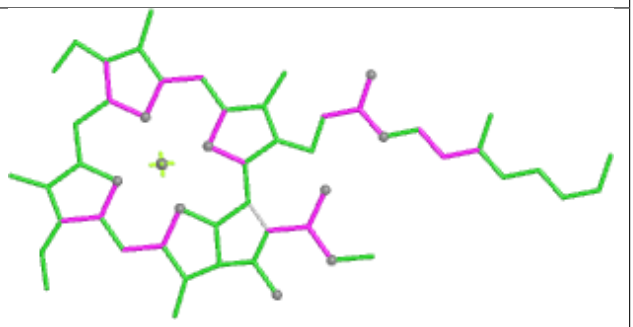
Ligand DD6 A 854



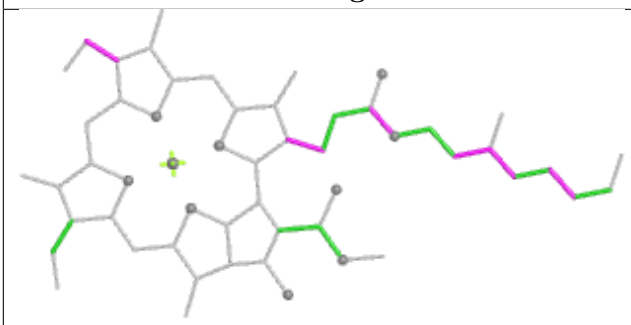
Ligand CLA a 209



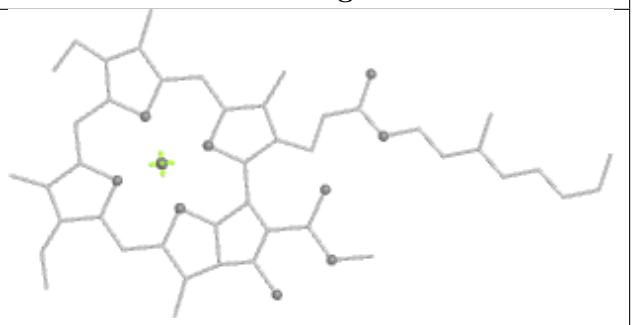
Bond lengths



Bond angles

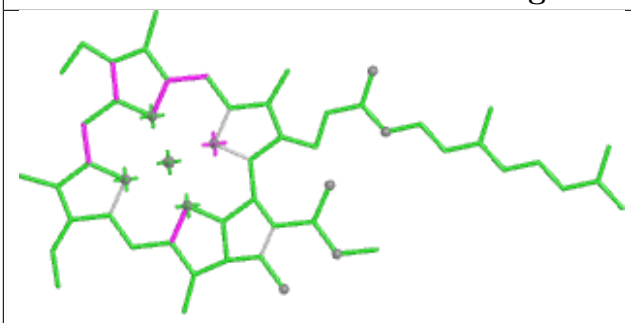


Torsions

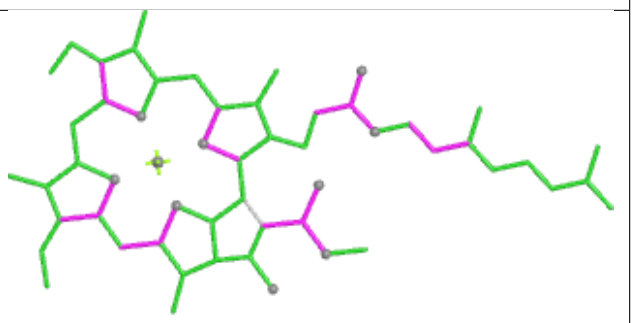


Rings

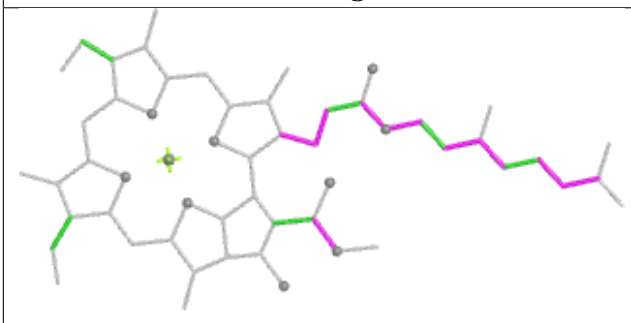
Ligand CLA a 212



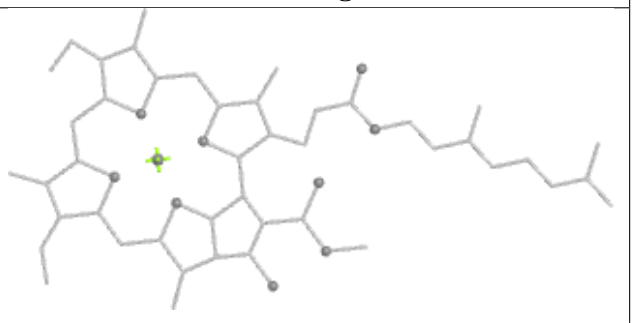
Bond lengths



Bond angles

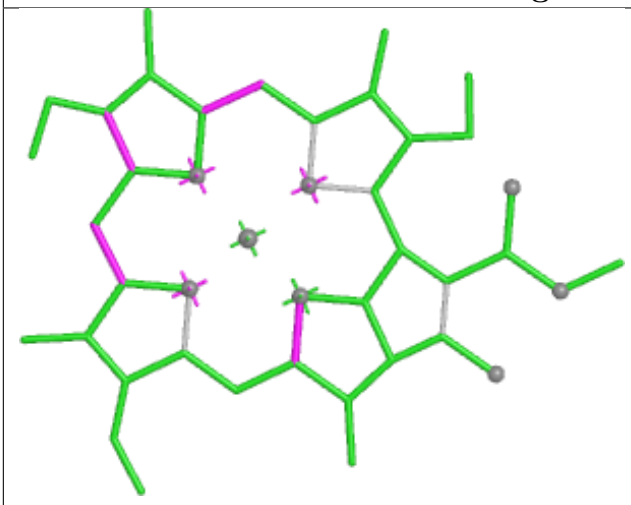


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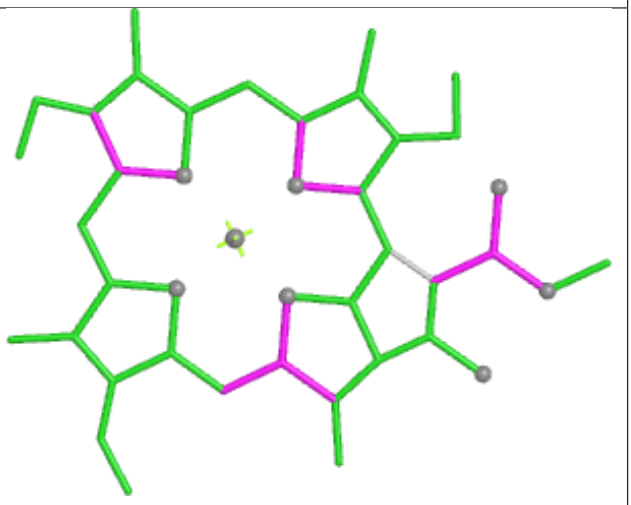


Rings

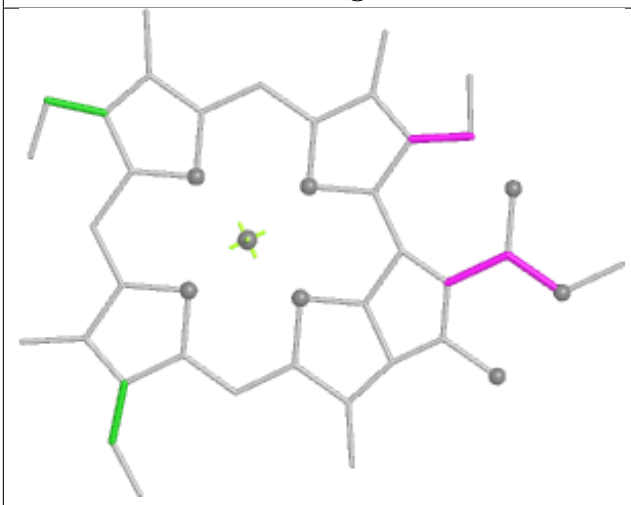
Ligand CLA f 604



Bond lengths



Bond angles



Torsions

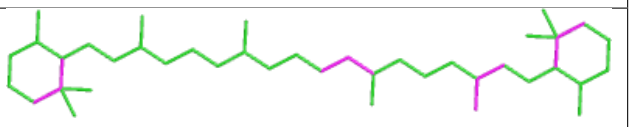


Rings

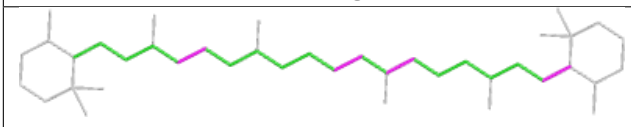
Ligand BCR A 836



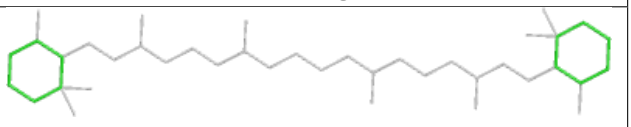
Bond lengths



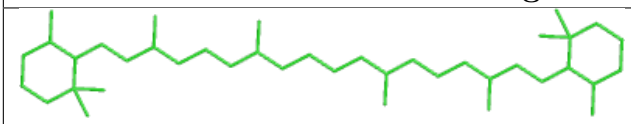
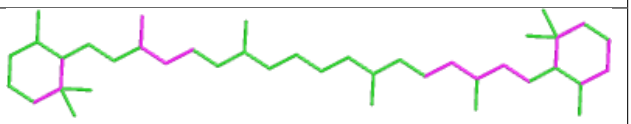
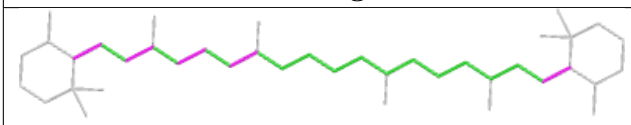
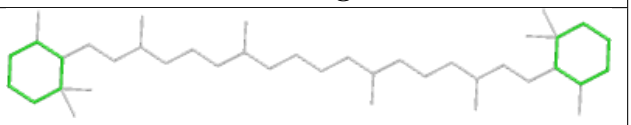
Bond angles

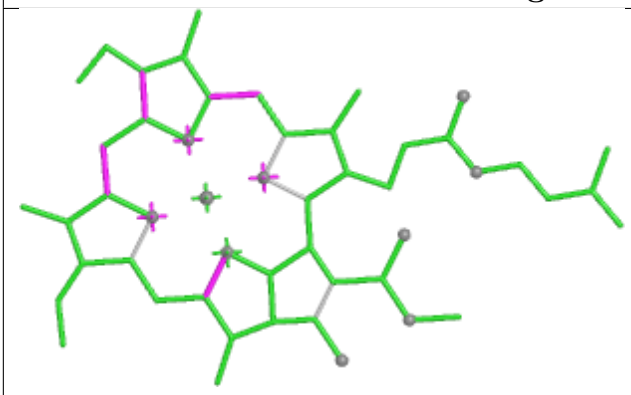
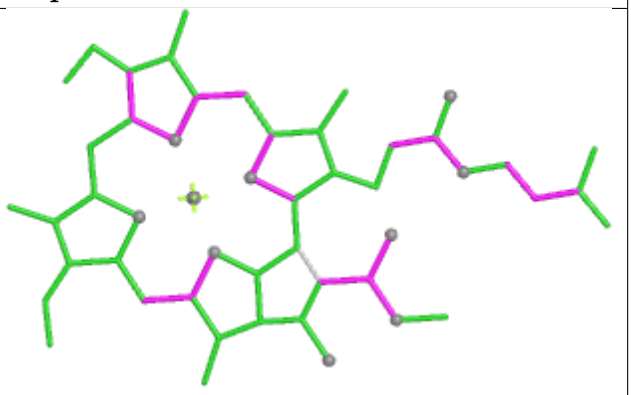
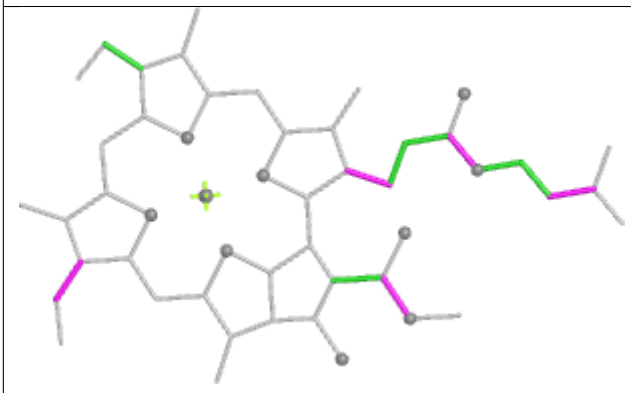
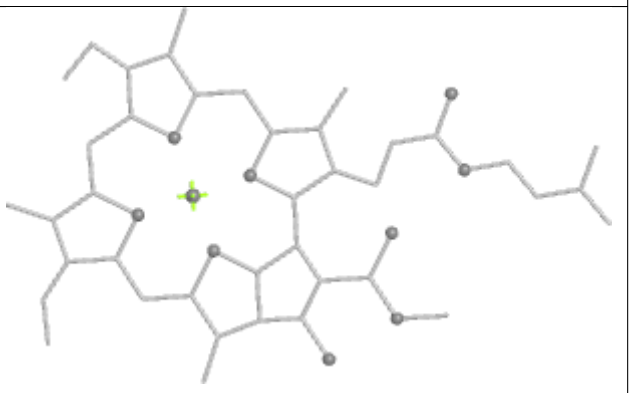


Torsions

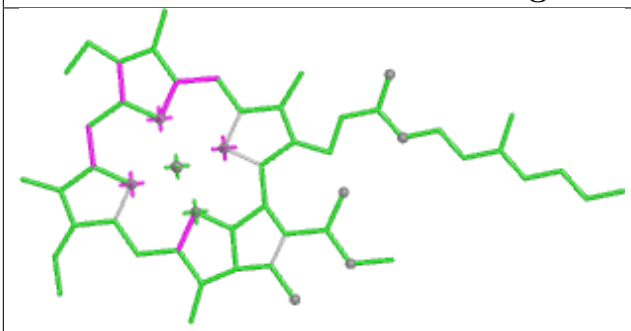


Rings

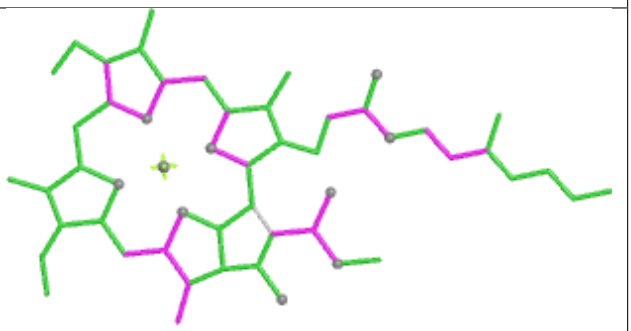
Ligand BCR B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

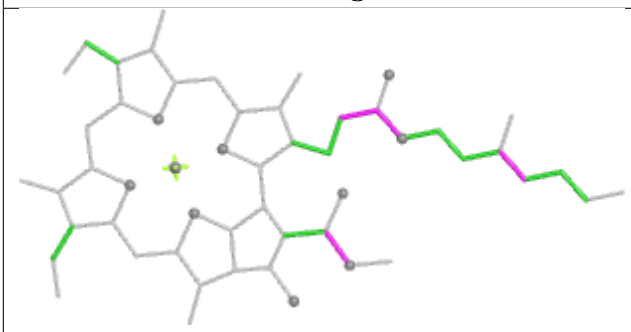
Ligand CLA c 304



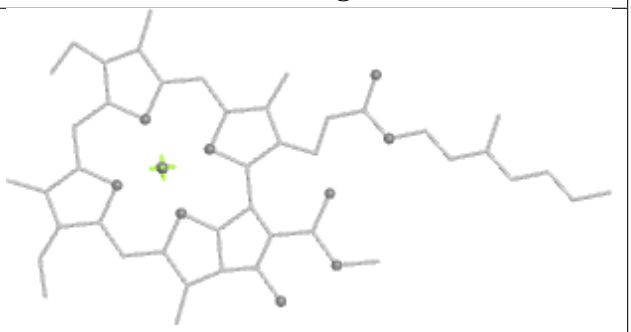
Bond lengths



Bond angles

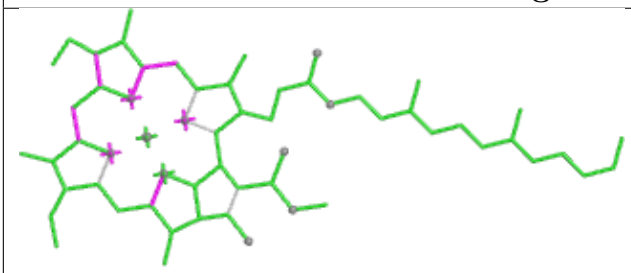


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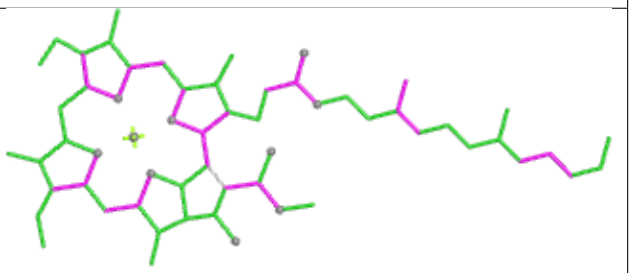


Rings

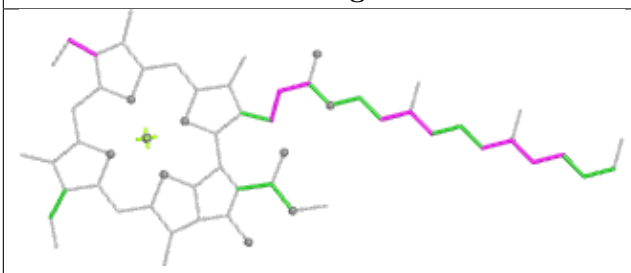
Ligand CLA i 211



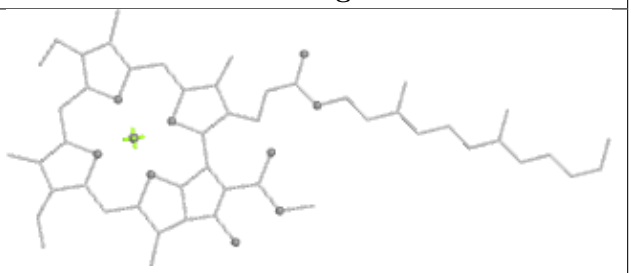
Bond lengths



Bond angles

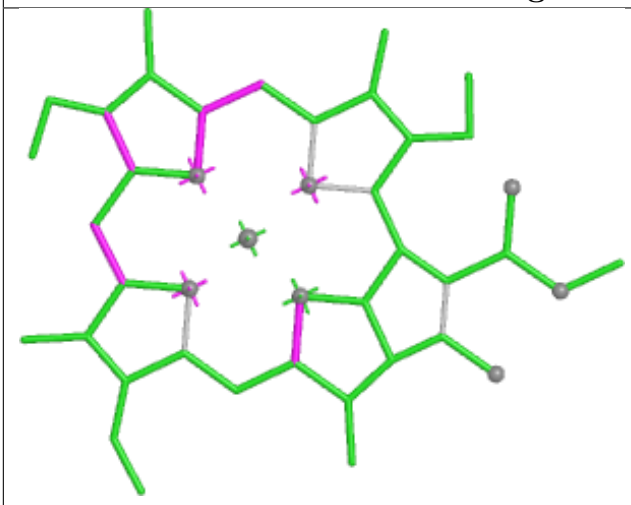


Torsions

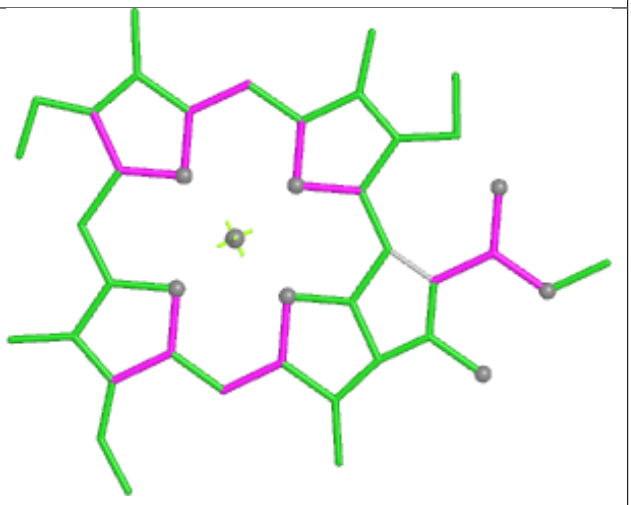


Rings

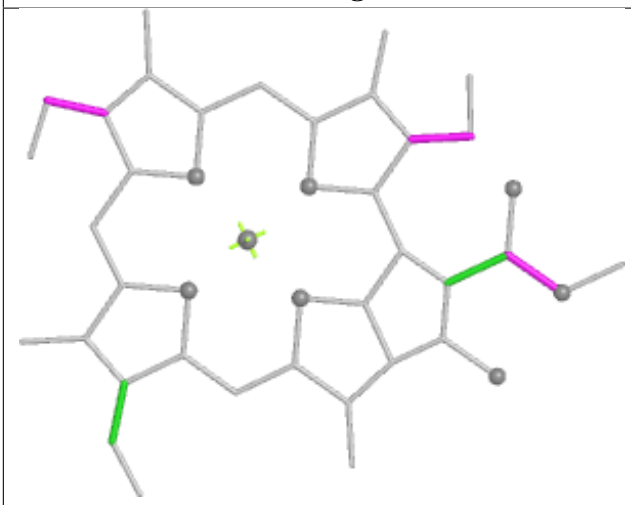
Ligand CLA k 213



Bond lengths



Bond angles

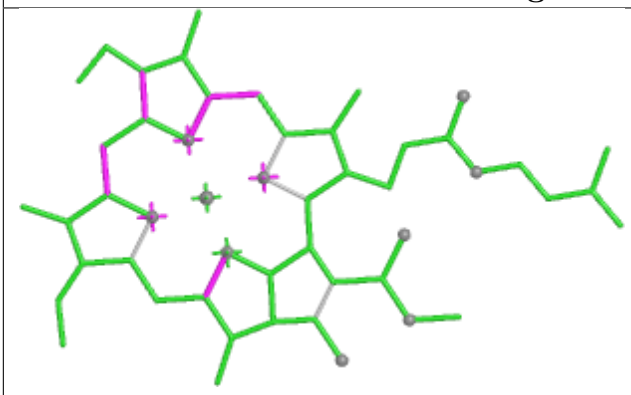


Torsions

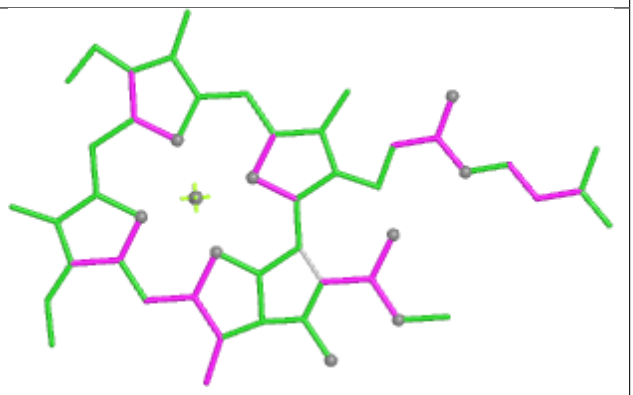


Rings

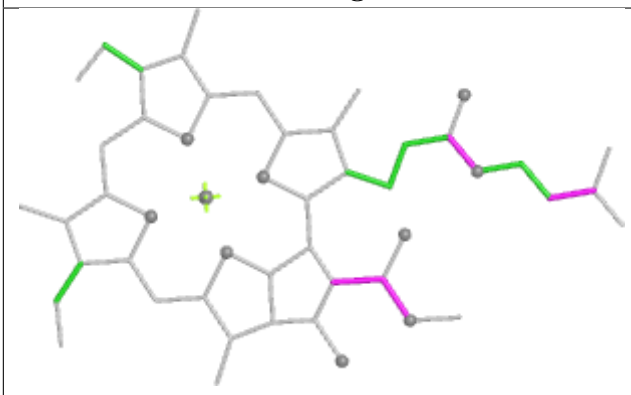
Ligand CLA d 303



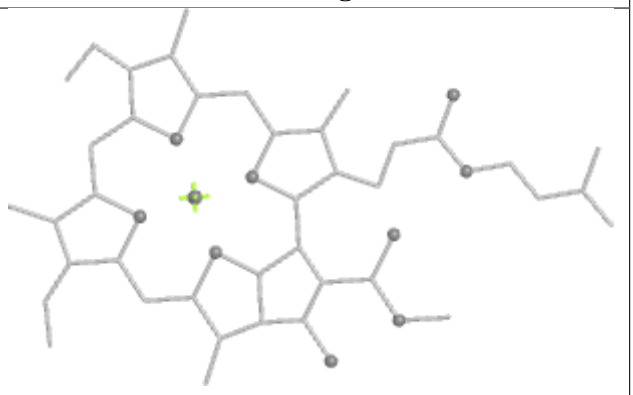
Bond lengths



Bond angles

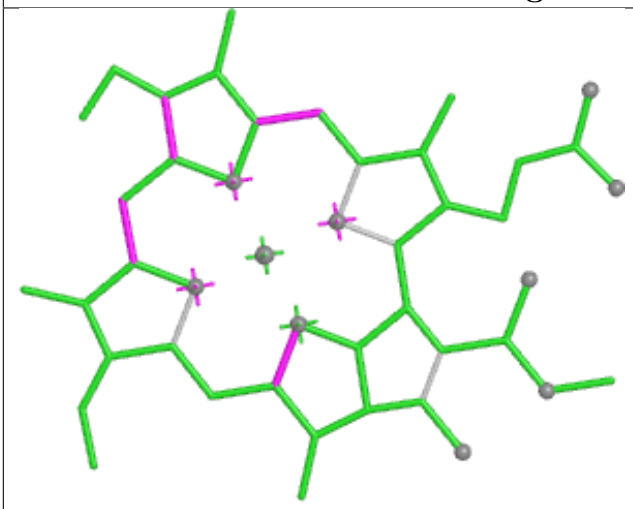


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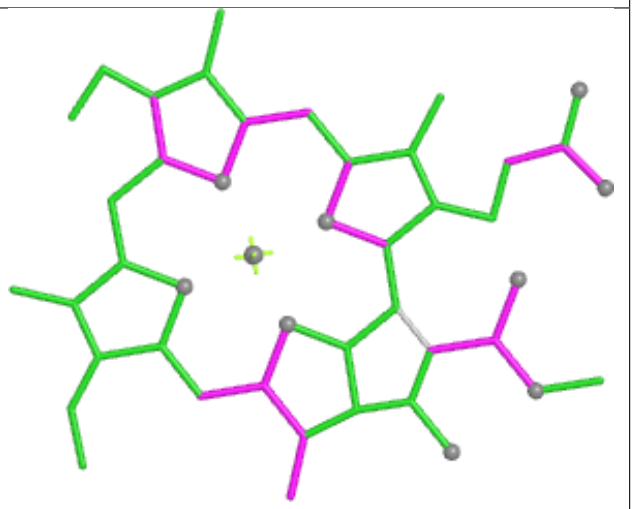


Rings

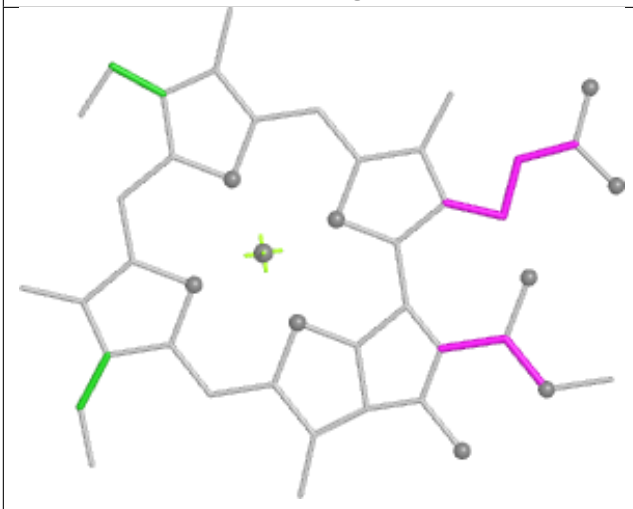
Ligand CLA F 202



Bond lengths



Bond angles

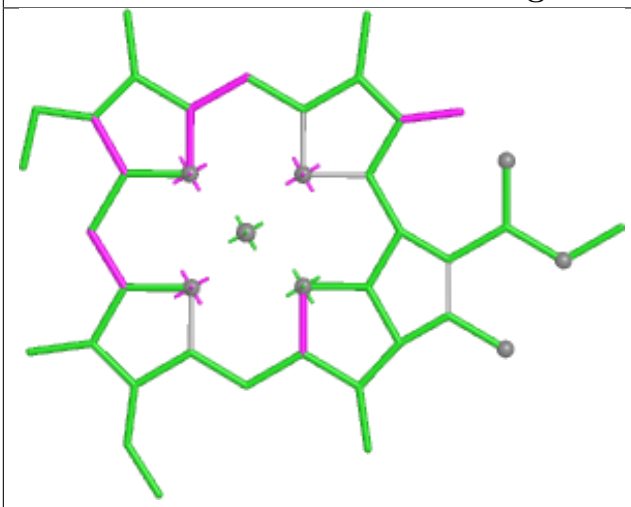


Torsions

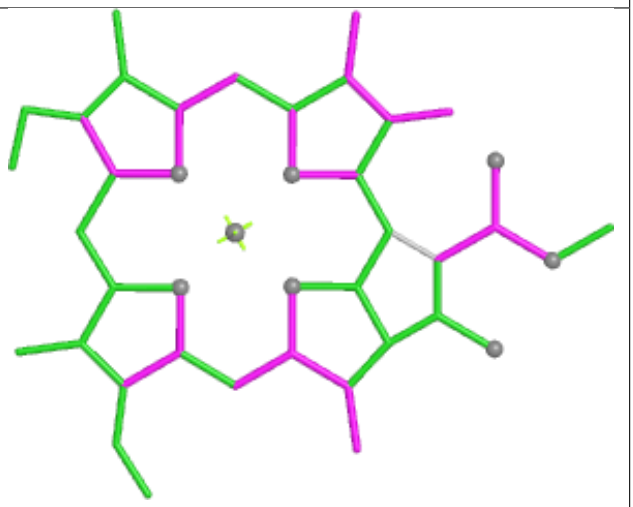


Rings

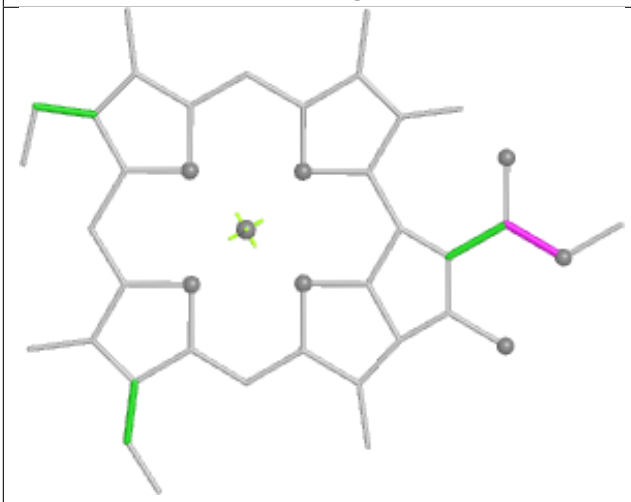
Ligand CLA n 207



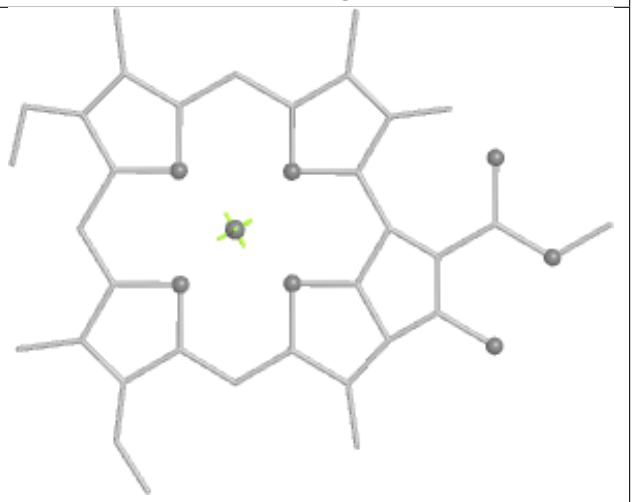
Bond lengths



Bond angles

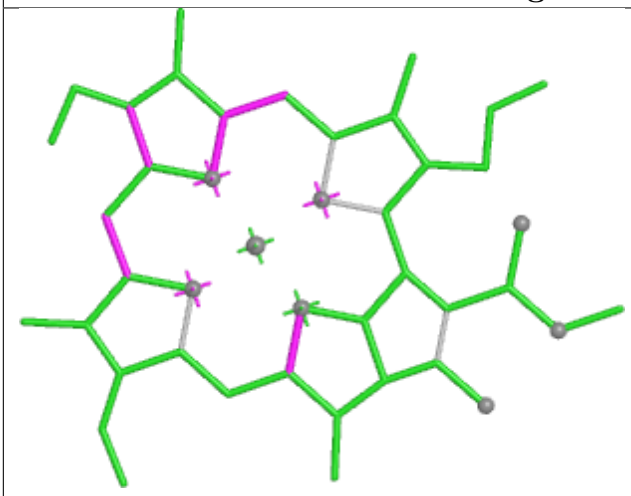


Torsions

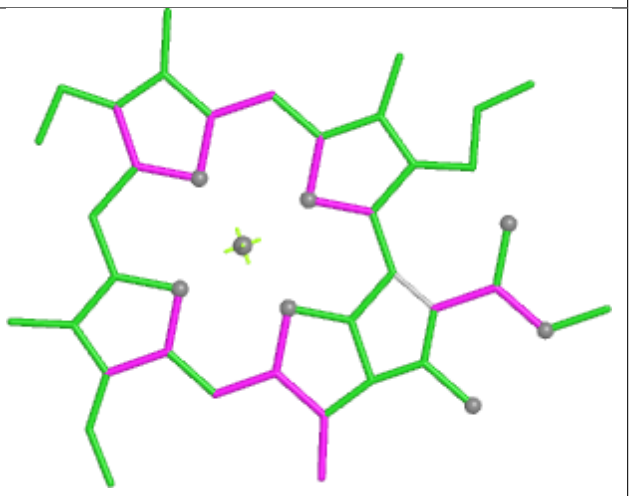


Rings

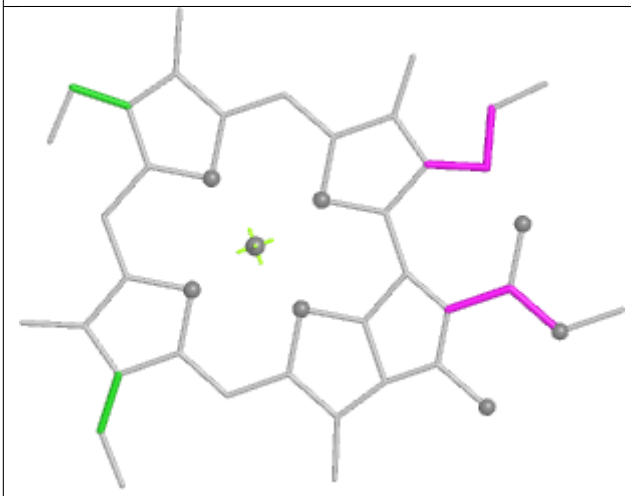
Ligand CLA b 205



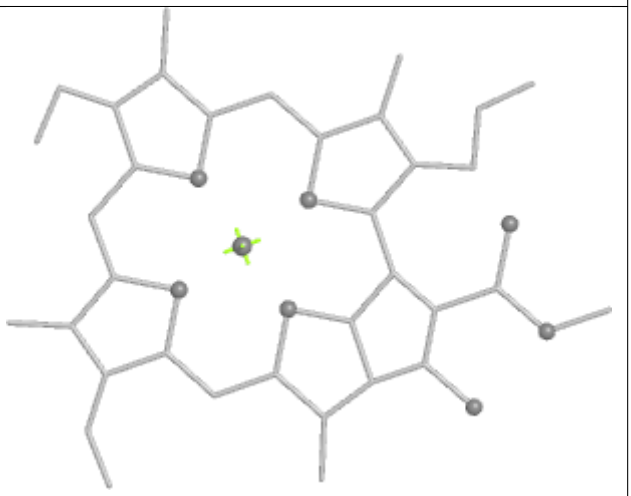
Bond lengths



Bond angles

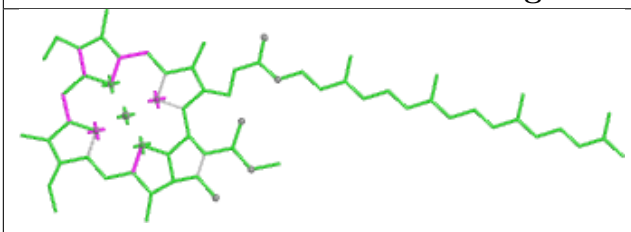


Torsions

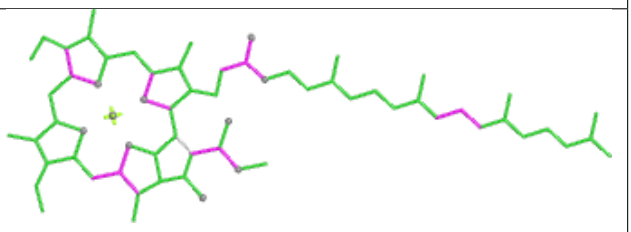


Rings

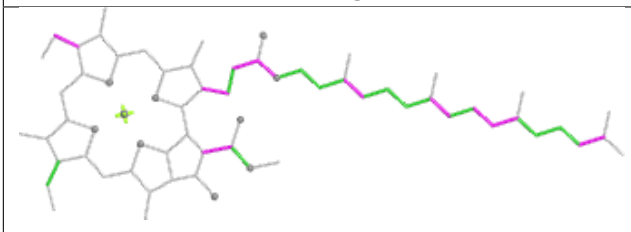
Ligand CLA B 804



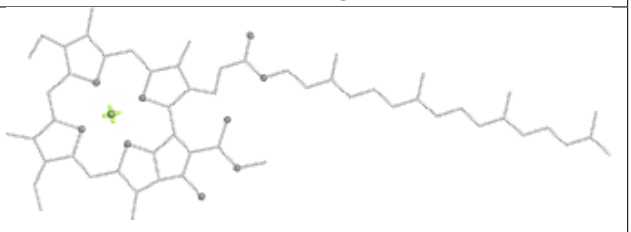
Bond lengths



Bond angles

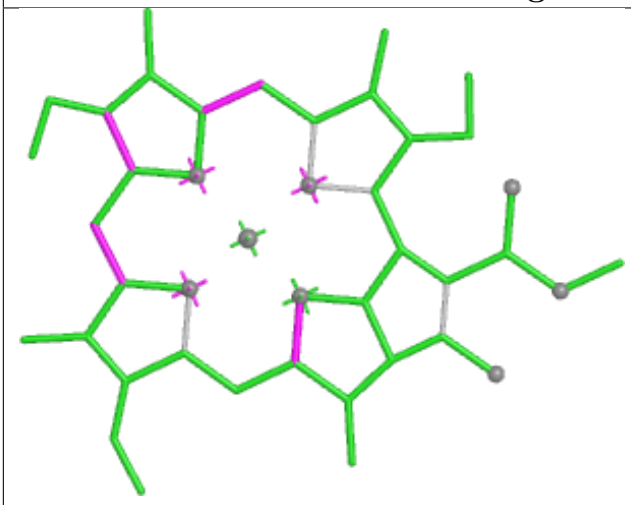


Torsions

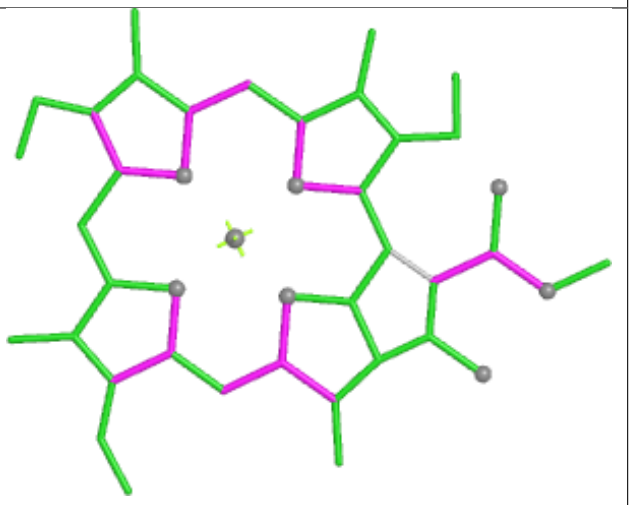


Rings

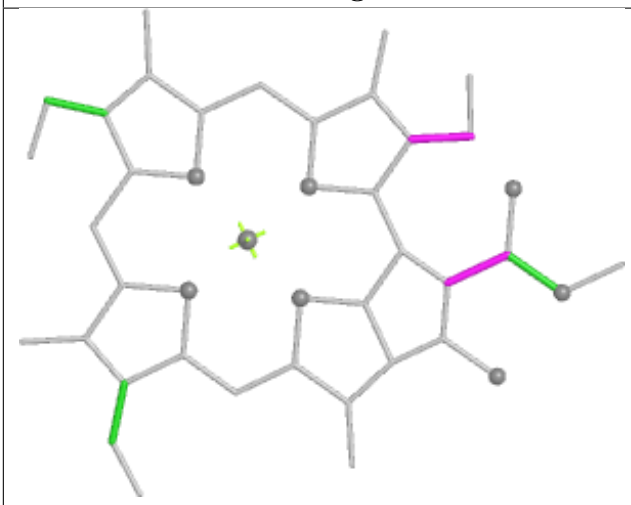
Ligand CLA k 209



Bond lengths



Bond angles

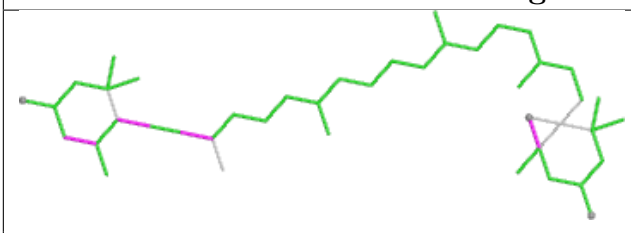


Torsions

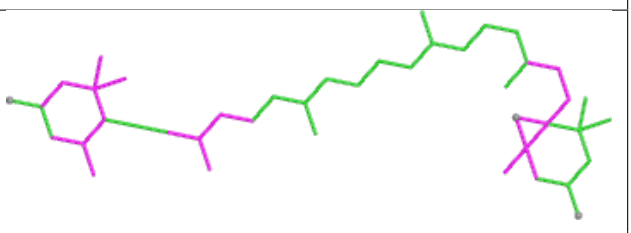


Rings

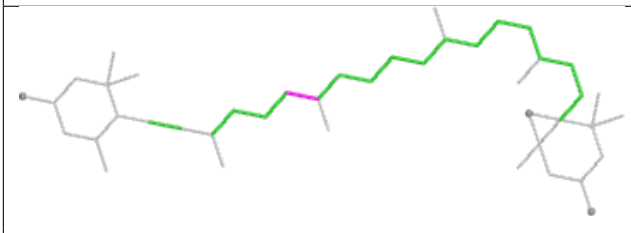
Ligand DD6 k 215



Bond lengths



Bond angles

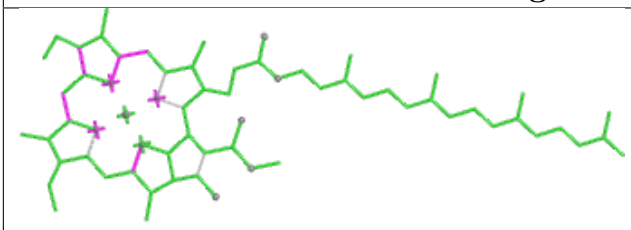


Torsions

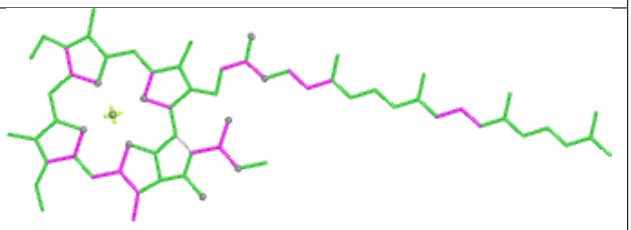


Rings

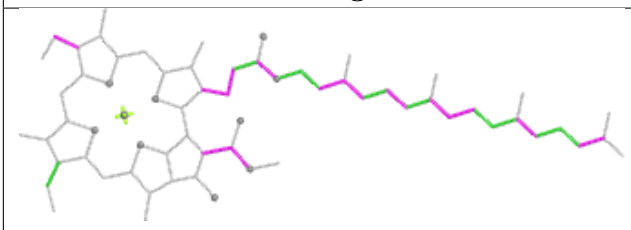
Ligand CLA e 205



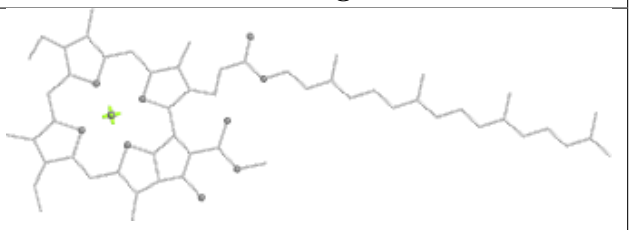
Bond lengths



Bond angles

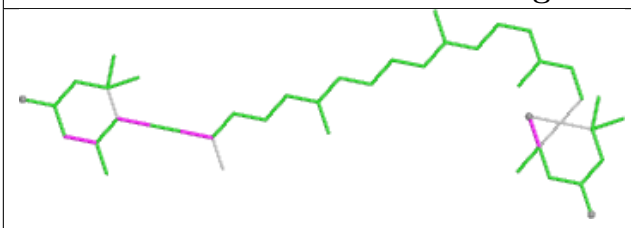


Torsions

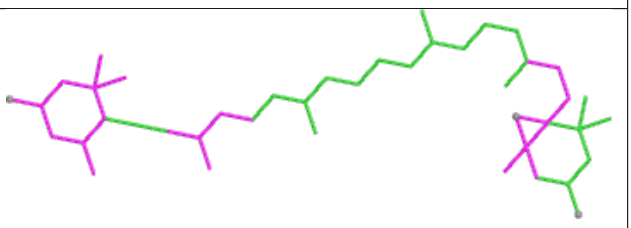


Rings

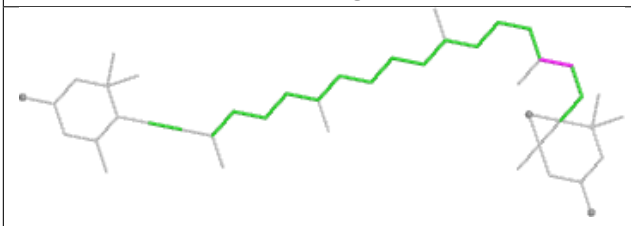
Ligand DD6 i 216



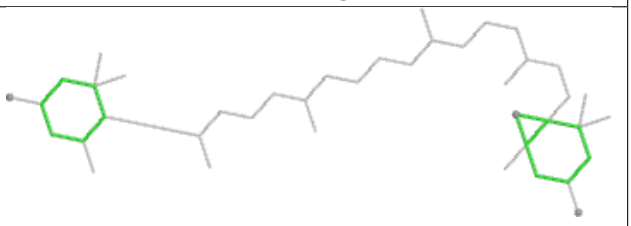
Bond lengths



Bond angles

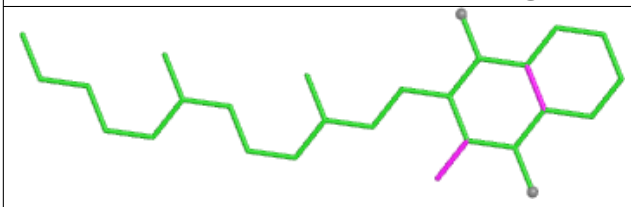


Torsions

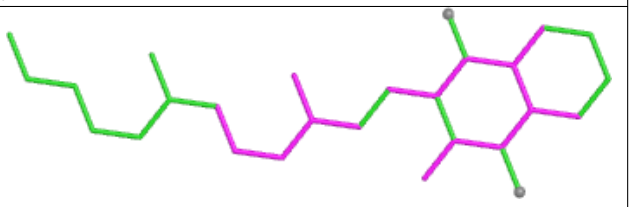


Rings

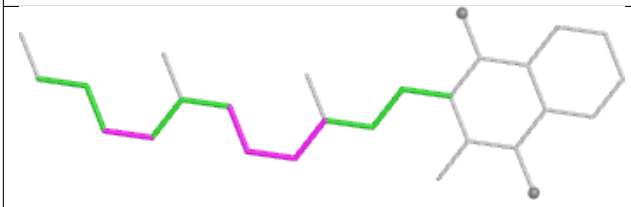
Ligand PQN B 835



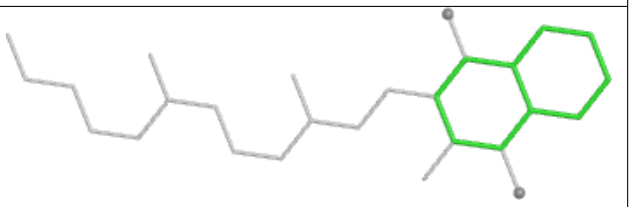
Bond lengths



Bond angles

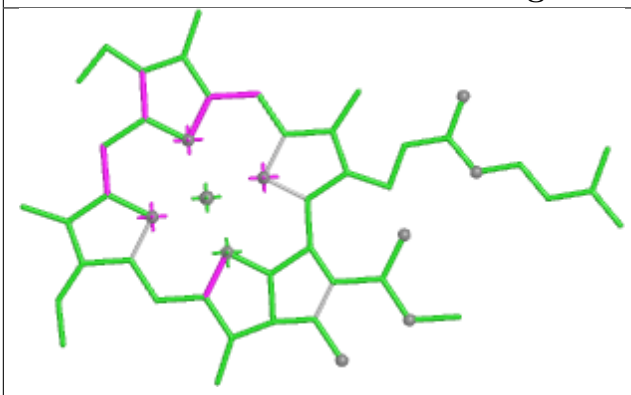


Torsions

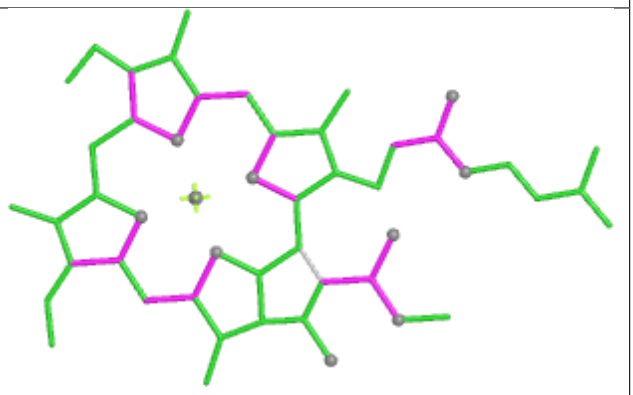


Rings

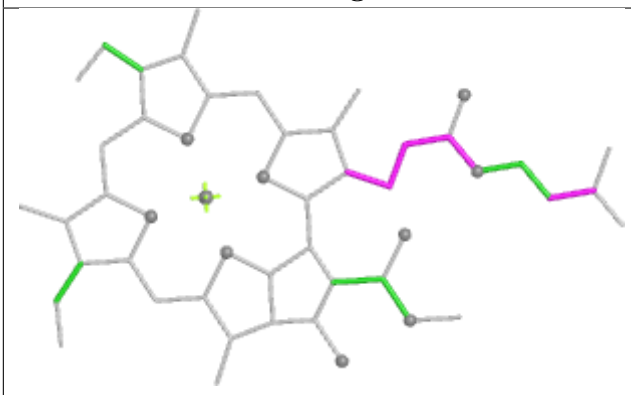
Ligand CLA h 208



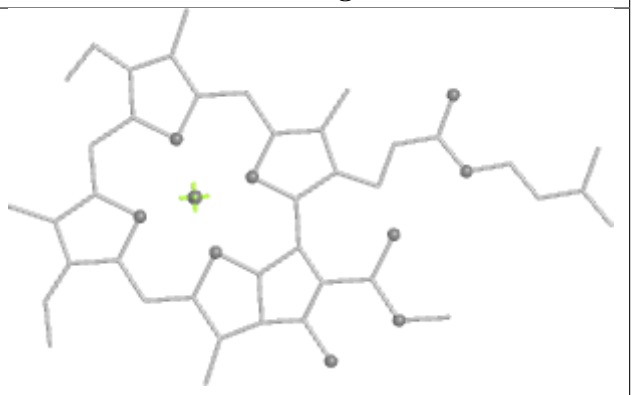
Bond lengths



Bond angles

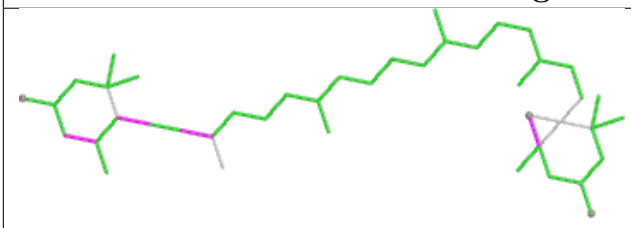


Torsions

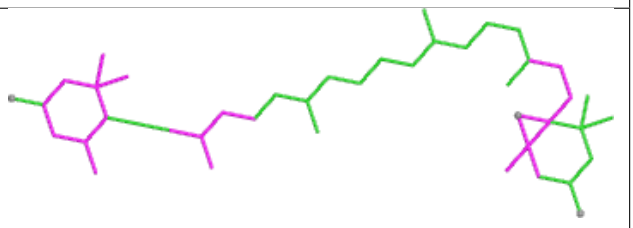


Rings

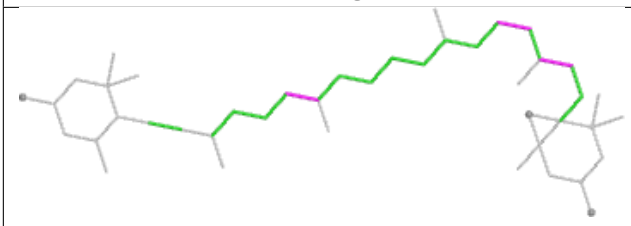
Ligand DD6 f 613



Bond lengths



Bond angles

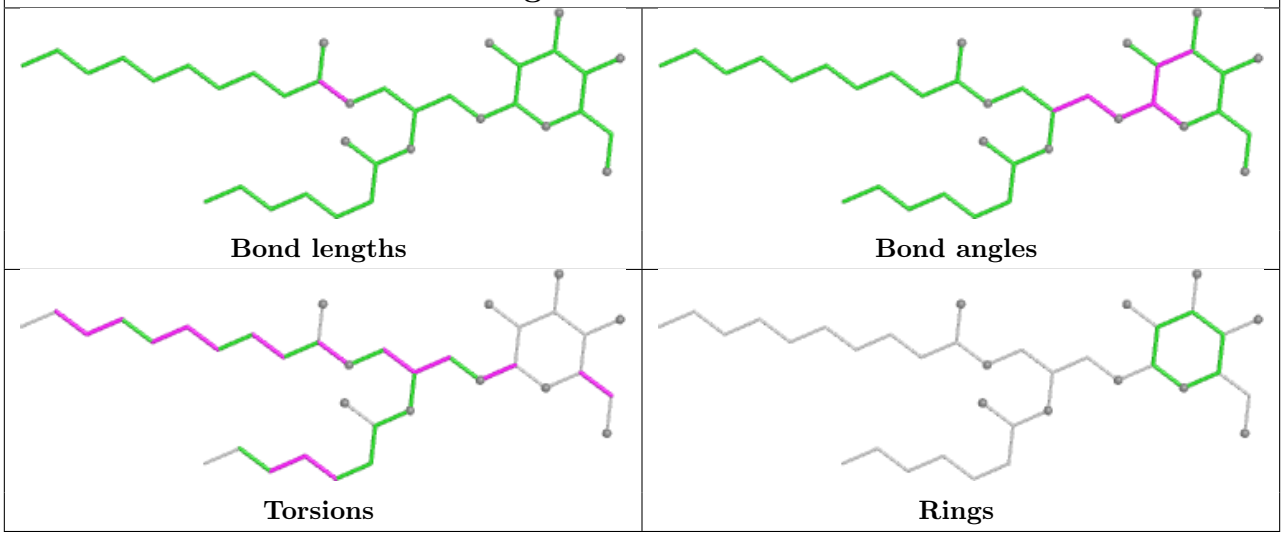


Torsions



Rings

Ligand LMG k 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

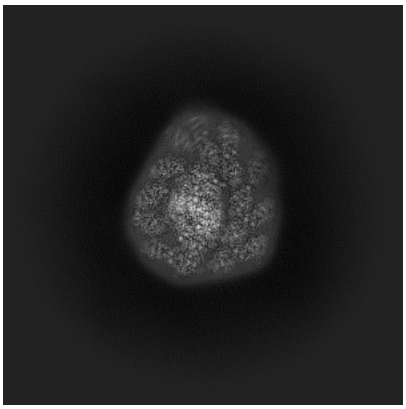
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64823. These allow visual inspection of the internal detail of the map and identification of artifacts.

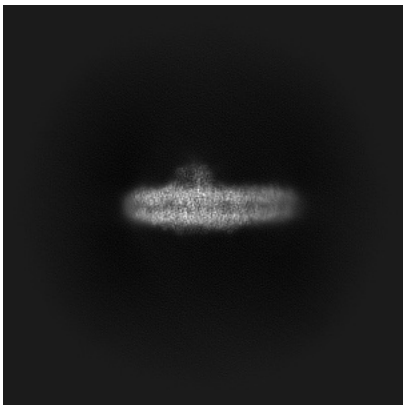
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

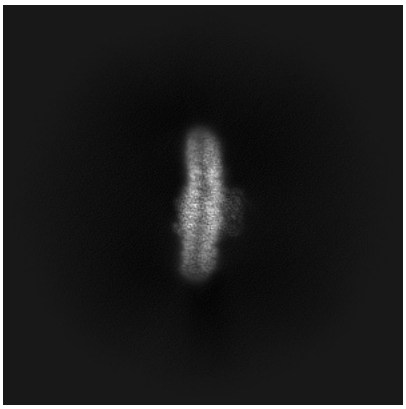
6.1.1 Primary map



X

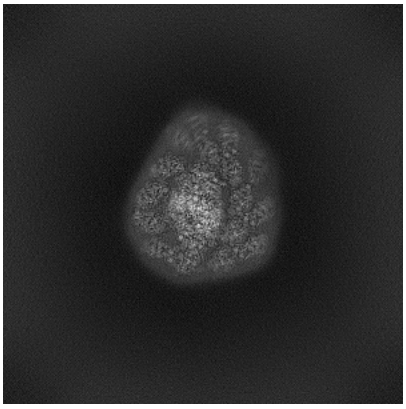


Y

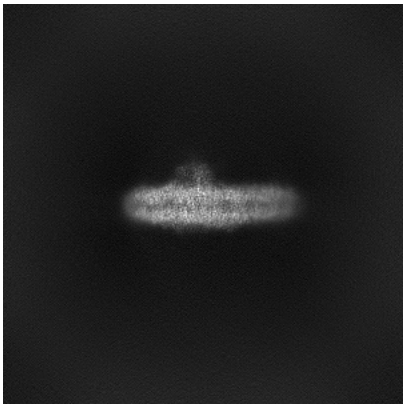


Z

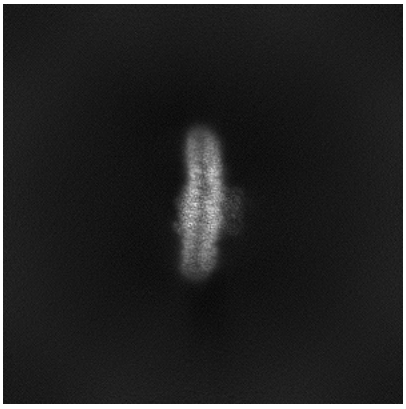
6.1.2 Raw map



X



Y

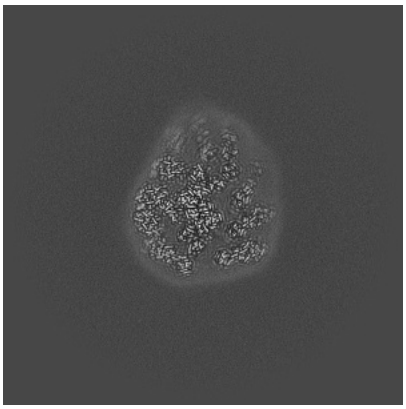


Z

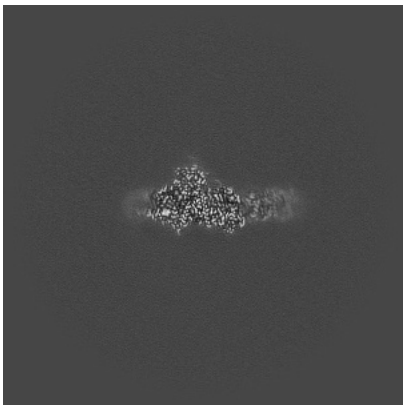
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

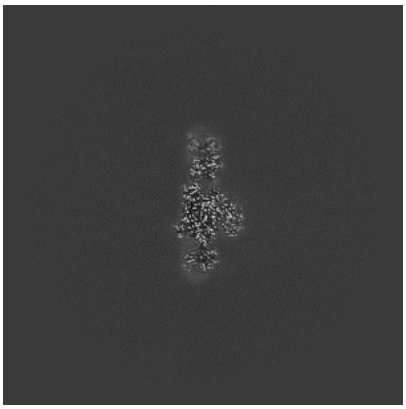
6.2.1 Primary map



X Index: 256

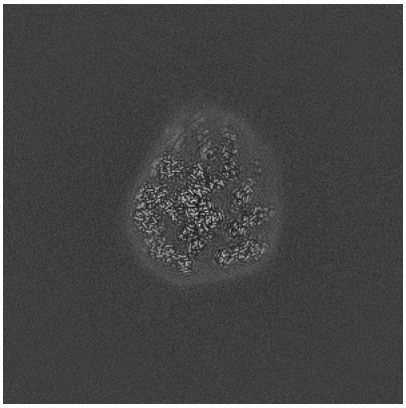


Y Index: 256

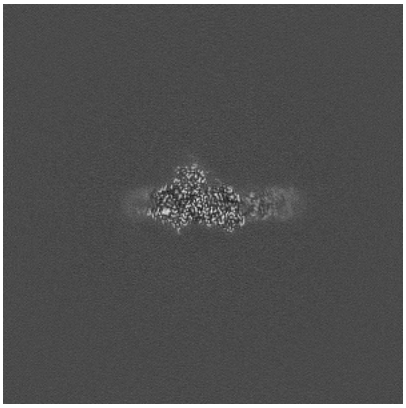


Z Index: 256

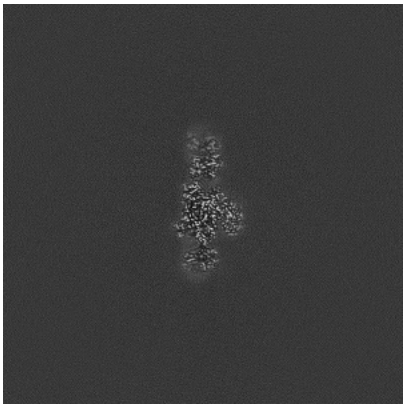
6.2.2 Raw map



X Index: 256



Y Index: 256

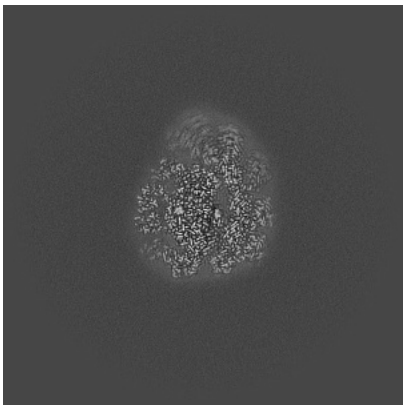


Z Index: 256

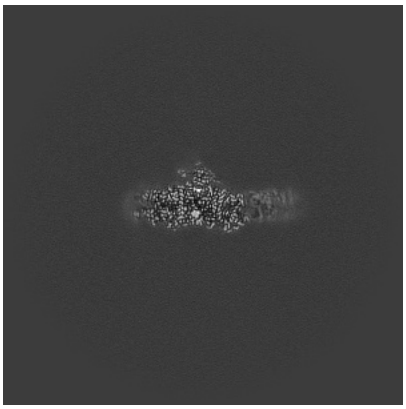
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

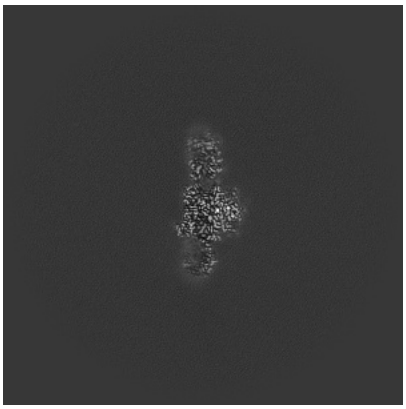
6.3.1 Primary map



X Index: 267

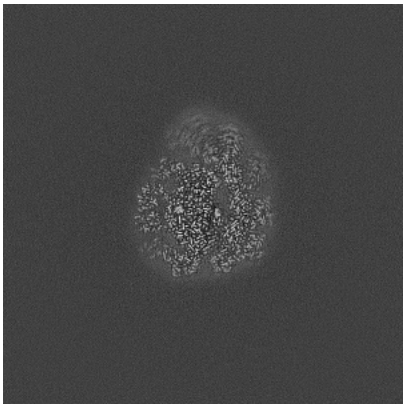


Y Index: 249

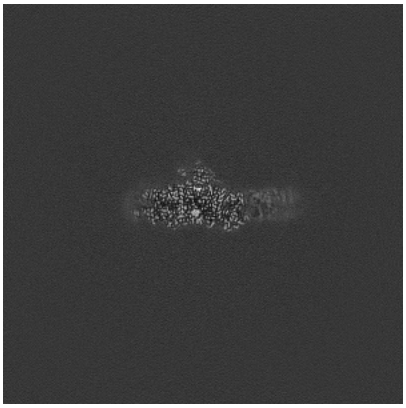


Z Index: 250

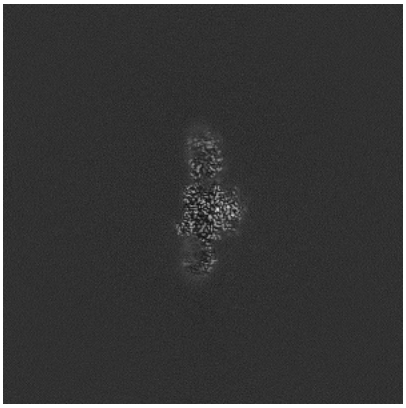
6.3.2 Raw map



X Index: 267



Y Index: 249

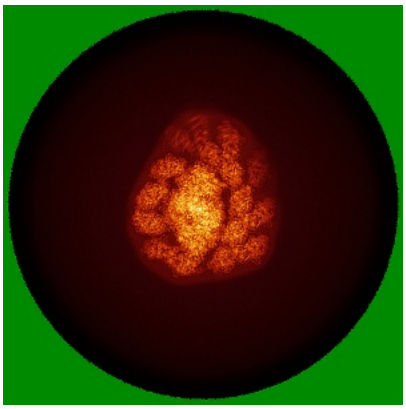


Z Index: 250

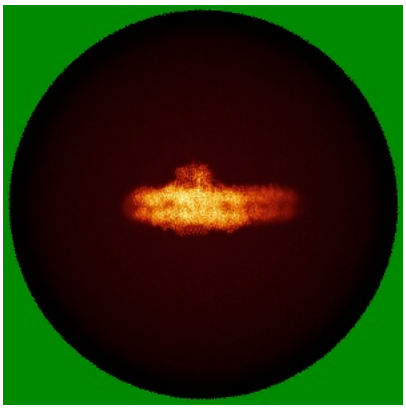
The images above show the largest variance slices of the map in three orthogonal directions.

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

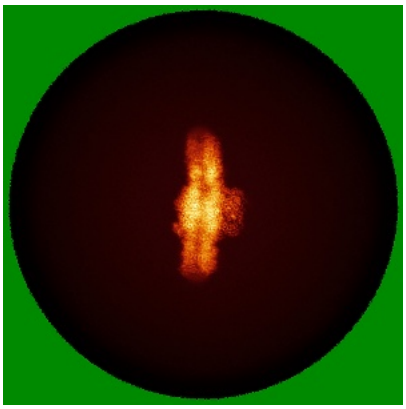
6.4.1 Primary map



X

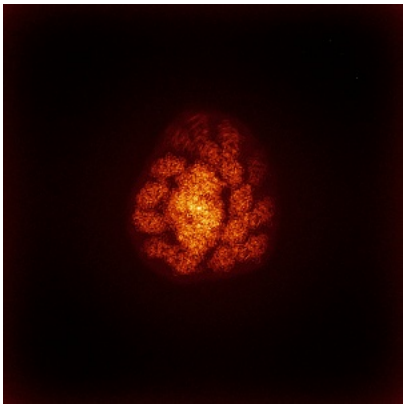


Y

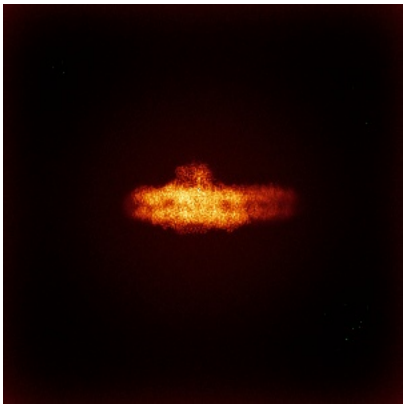


Z

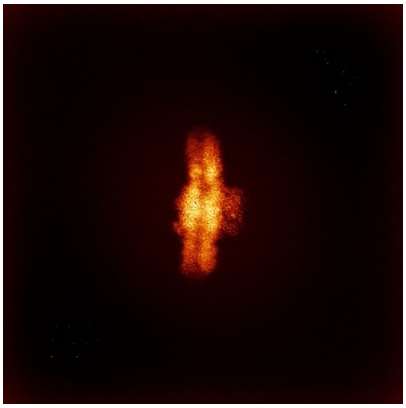
6.4.2 Raw map



X



Y

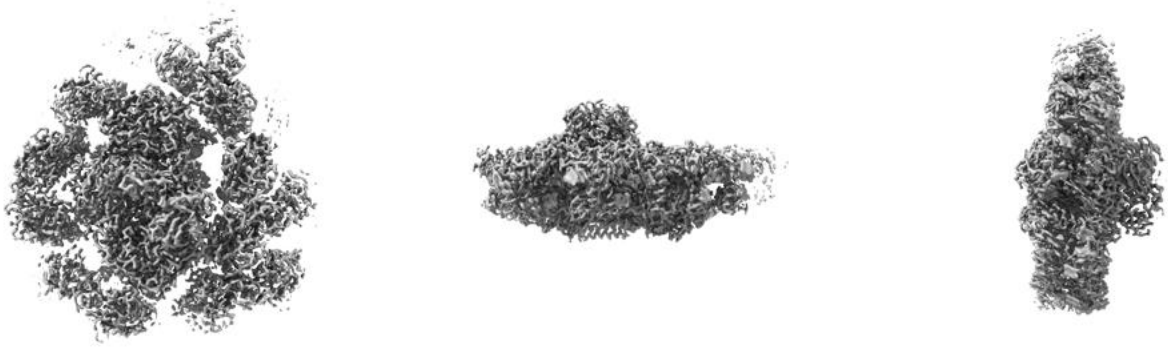


Z

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

6.5 Orthogonal surface views (i)

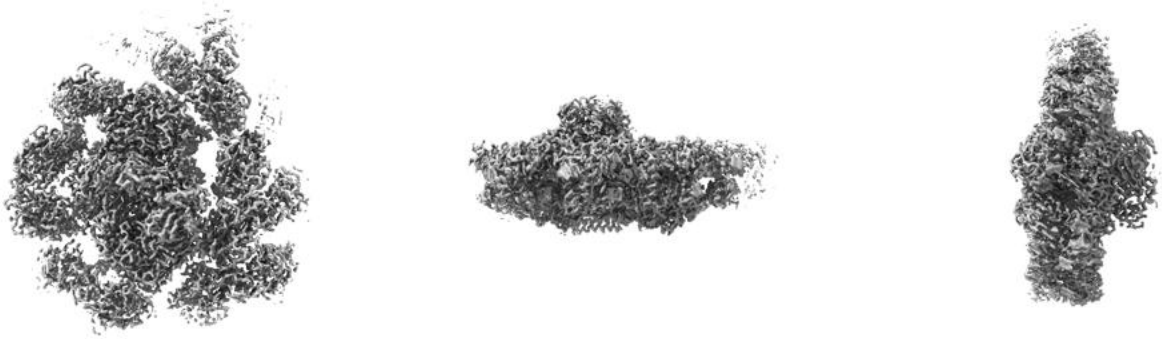
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

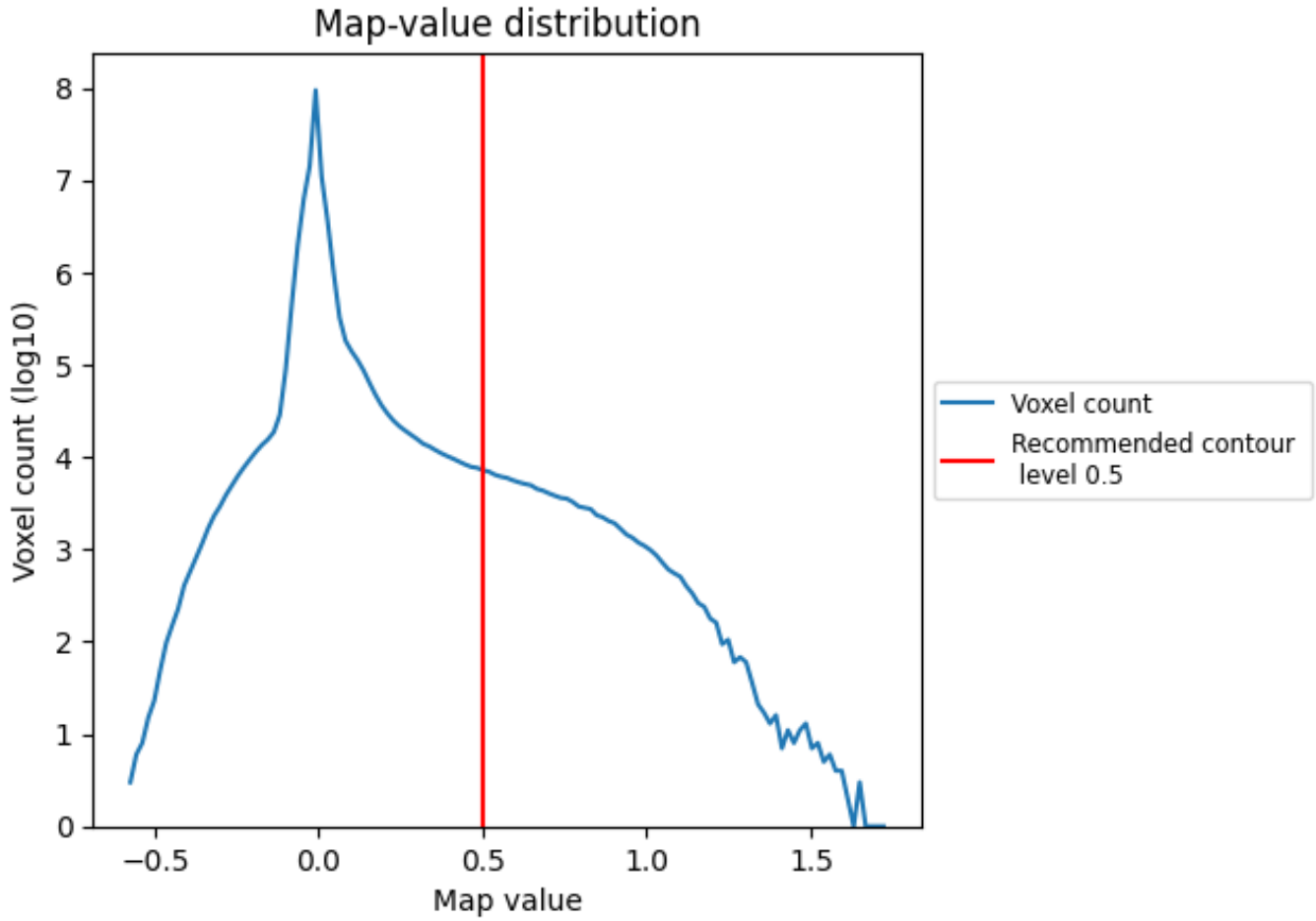
6.6 Mask visualisation (i)

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

7 Map analysis

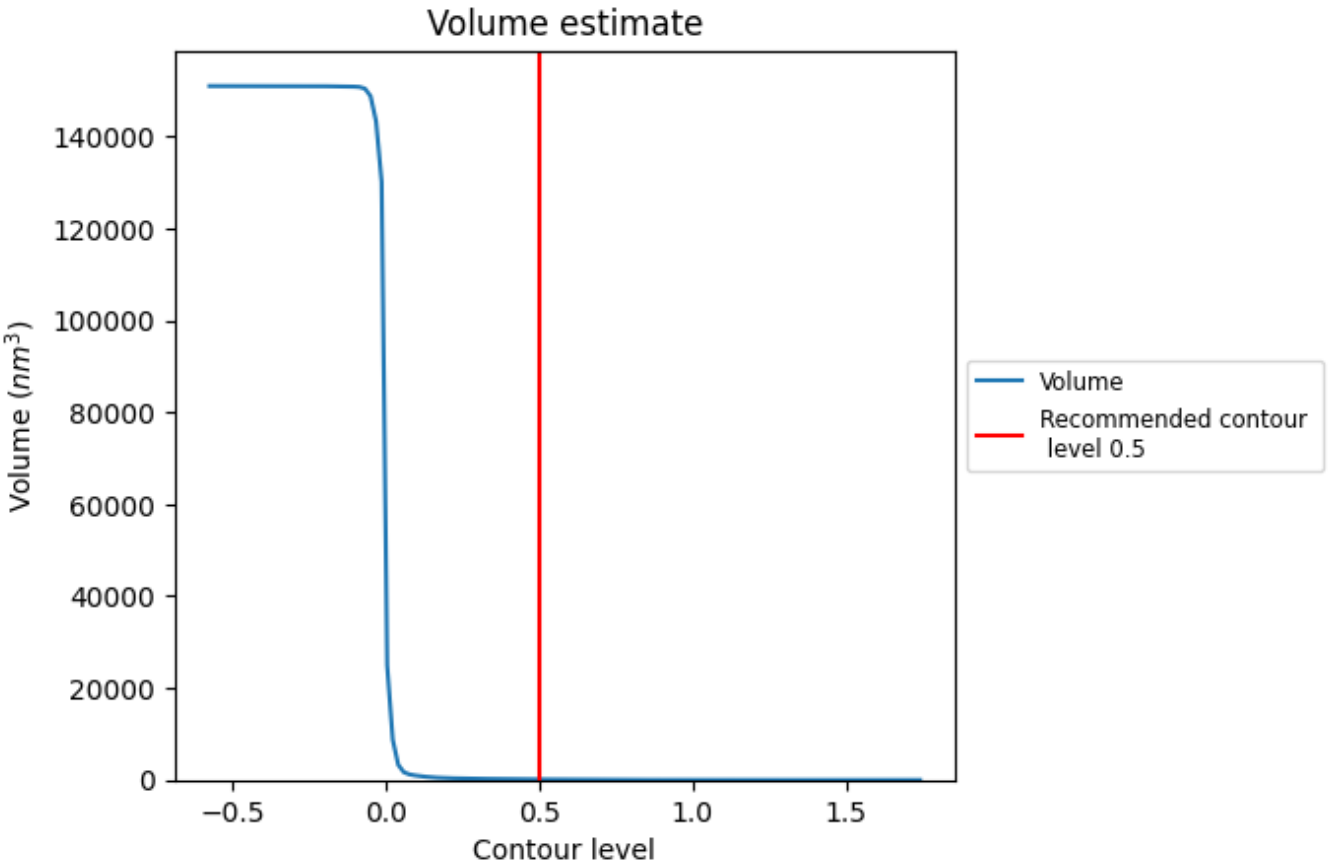
This section contains the results of statistical analysis of the map.

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.

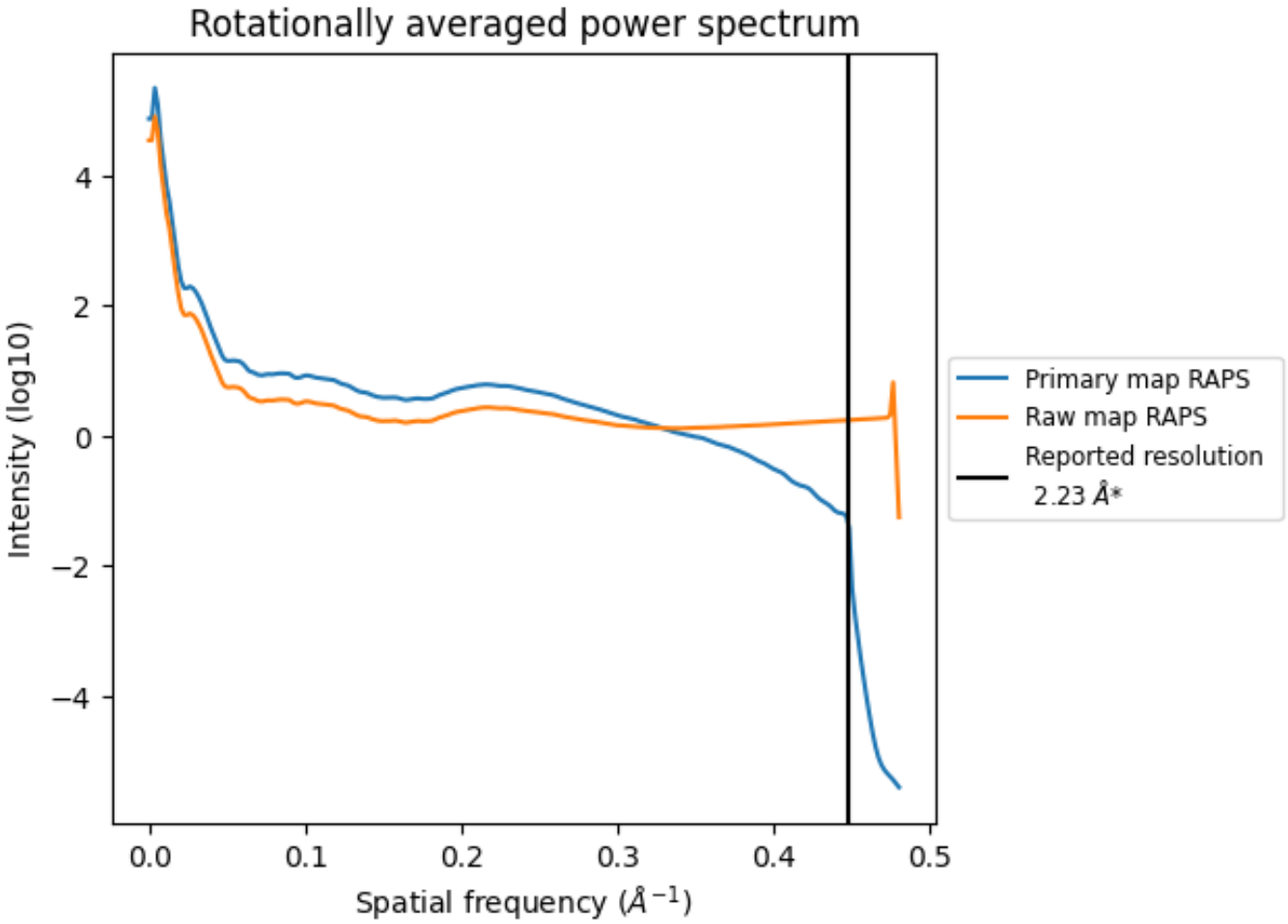
7.2 Volume estimate



The volume at the recommended contour level is 125 nm^3; this corresponds to an approximate mass of 113 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)

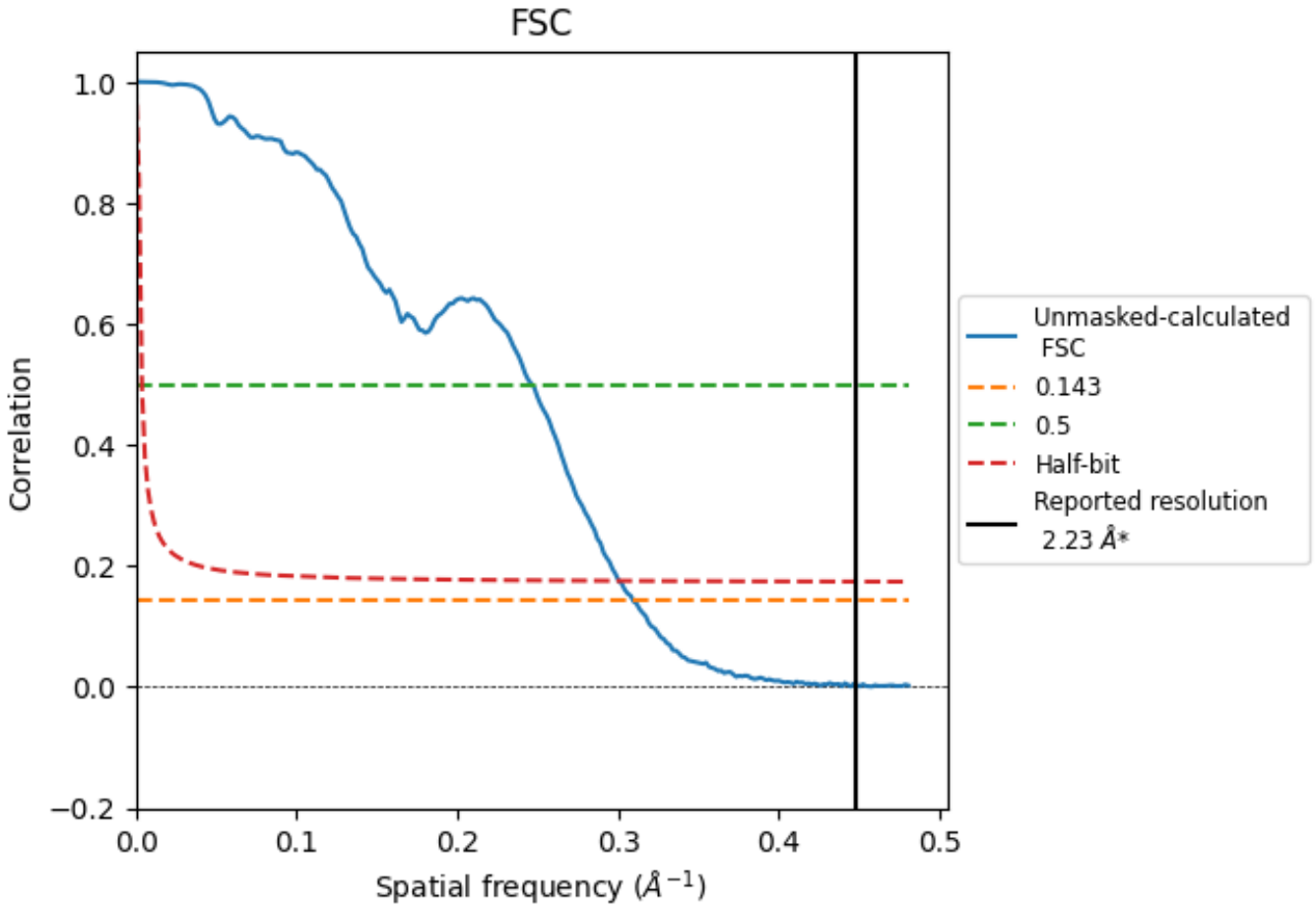


*Reported resolution corresponds to spatial frequency of 0.448 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.448 Å^{-1}

8.2 Resolution estimates (i)

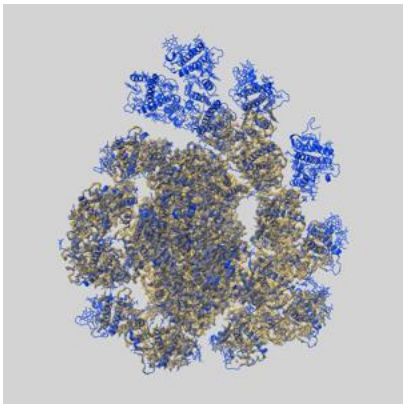
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	4.06	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.23 by more than 10 %

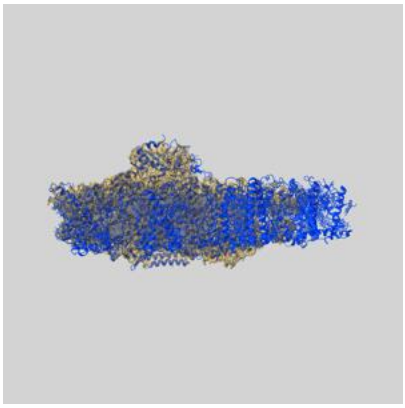
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64823 and PDB model 9V7T. Per-residue inclusion information can be found in section 3 on page 31.

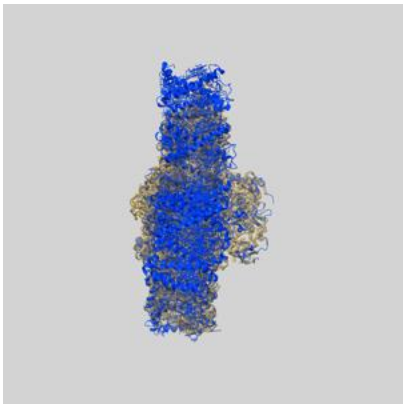
9.1 Map-model overlay



X



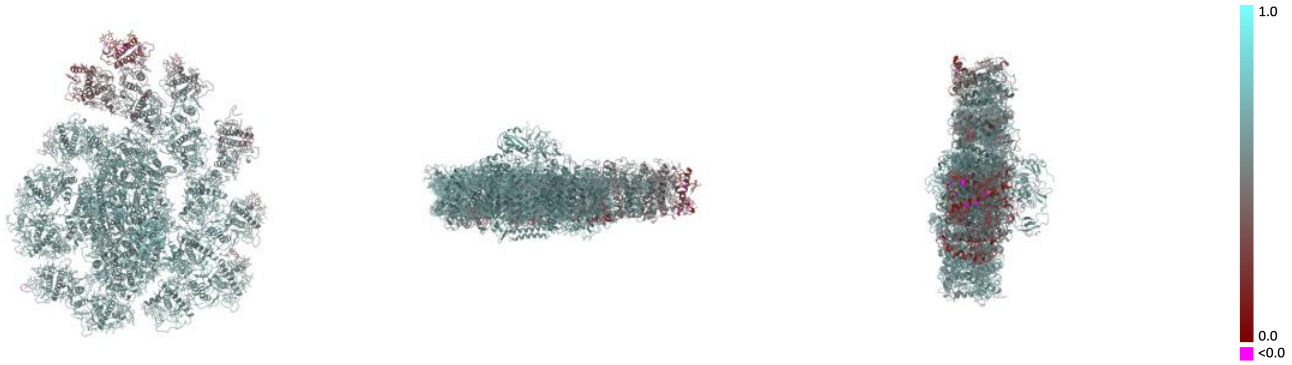
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

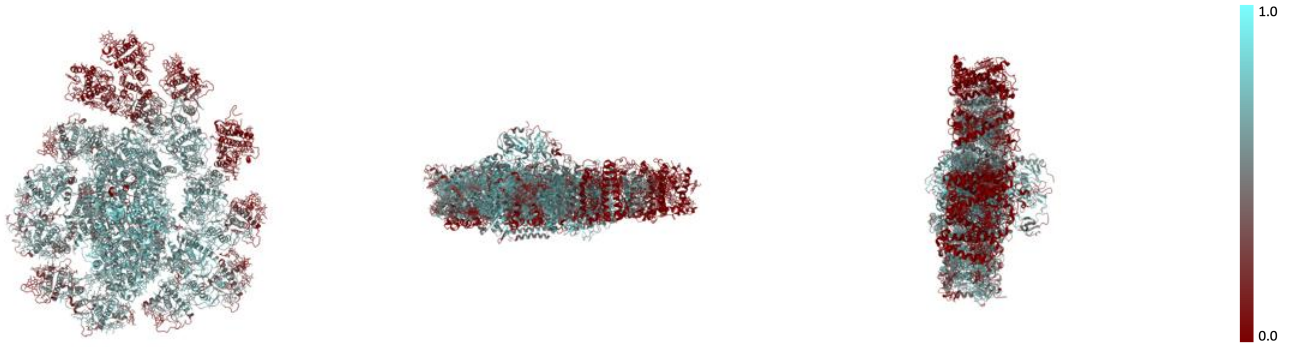
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

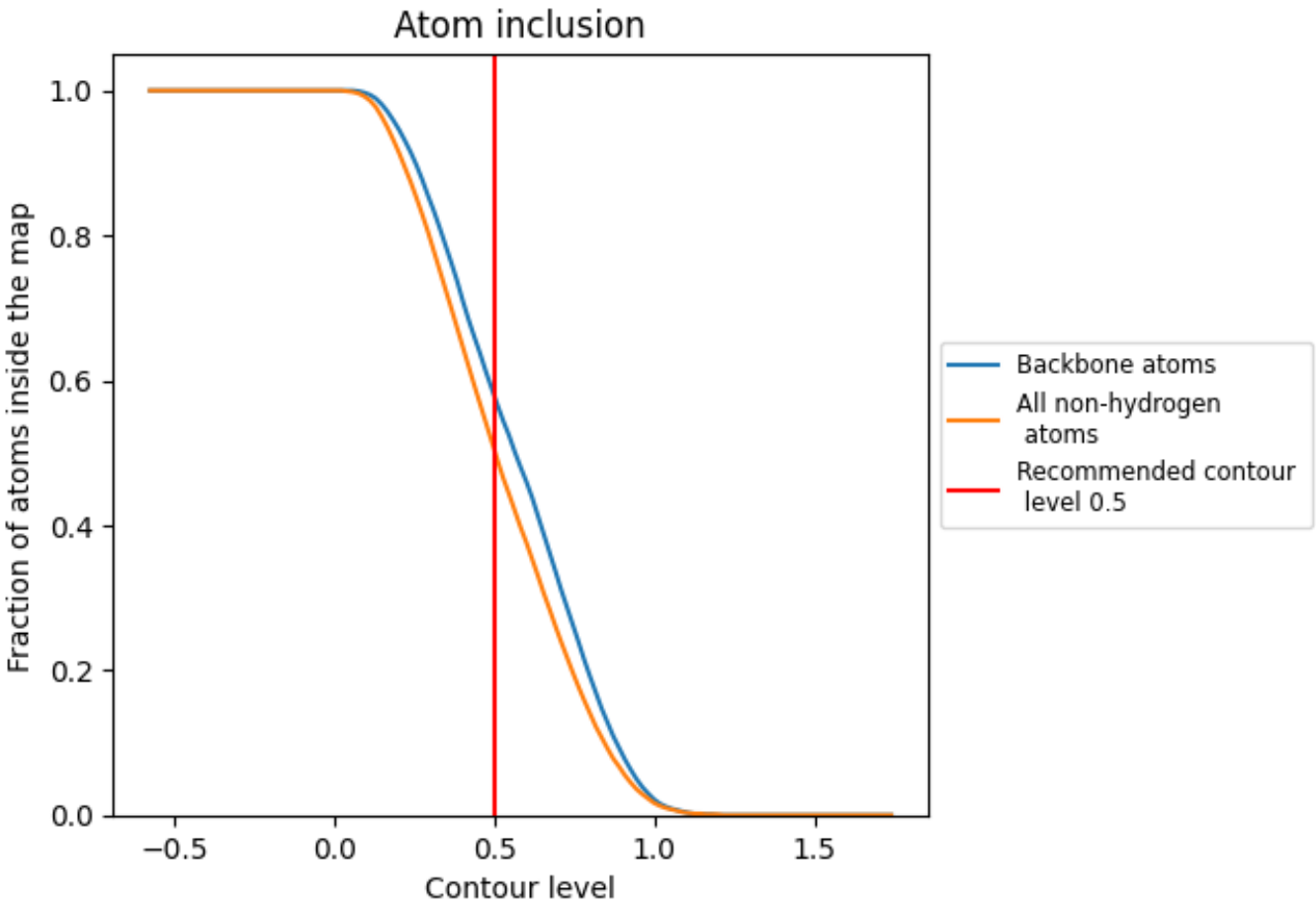
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 58% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5050	0.6030
A	0.7400	0.6620
B	0.7250	0.6600
C	0.7380	0.6460
D	0.4850	0.6250
E	0.5280	0.6170
F	0.5600	0.6410
J	0.5890	0.6490
M	0.5350	0.6370
a	0.5050	0.6250
b	0.3480	0.5970
c	0.5130	0.6240
d	0.5520	0.6300
e	0.4470	0.6190
f	0.0030	0.3560
g	0.2530	0.5450
h	0.5780	0.6320
i	0.6060	0.6350
j	0.6640	0.6490
k	0.4950	0.6240
l	0.3890	0.5840
m	0.2650	0.5670
n	0.0050	0.4830
o	0.1340	0.5040
p	0.0000	0.2870

