Full wwPDB EM Validation Report

Mar 20, 2026 – 05:38 PM UTC

PDB ID	:	8Z9D / pdb_00008z9d
EMDB ID	:	EMD-39860
Title	:	cryo-EM structure of PSII-LHCII megacomplex from spinach
Authors	:	Shan, J.Y.; Liu, Z.F.
Deposited on	:	2024-04-23
Resolution	:	3.22 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:

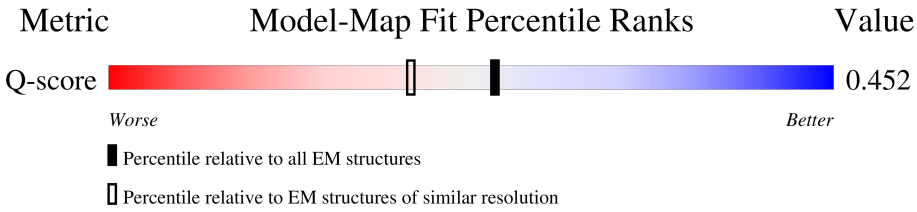
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.22 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	14612 (2.72 - 3.72)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	PL9	A	410	-	X	-	-
35	PL9	AA	410	-	X	-	-
35	PL9	D	407	-	X	-	-
35	PL9	DD	406	-	X	-	-
35	PL9	Dd	404	-	X	-	-
35	PL9	d	404	-	X	-	-

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 339330 atoms, of which 168031 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 II protein D1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	0
			5145	1710	2526	431	465	13		
1	a	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		
1	AA	335	Total	C	H	N	O	S	0	0
			5146	1710	2527	431	465	13		
1	Aa	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		

- Molecule 2 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Oo	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	O	236	Total	C	H	N	O	S	0	0
			3559	1136	1765	292	363	3		
2	o	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	OO	236	Total	C	H	N	O	S	0	0
			3561	1136	1767	292	363	3		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Rr	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	R	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		
3	r	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	RR	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ss	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	S	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		
4	s	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	SS	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Tt	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	T	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	t	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	TT	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		

- Molecule 6 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Uu	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	U	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		
6	u	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	UU	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		

- Molecule 7 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Ww	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	W	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	w	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	WW	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

- Molecule 8 is a protein called Photosystem II reaction center X protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Xx	34	Total	C	H	N	O	0	0
			487	158	250	37	42		
8	X	46	Total	C	H	N	O	0	0
			667	213	341	53	60		
8	x	34	Total	C	H	N	O	0	0
			487	158	250	37	42		
8	XX	48	Total	C	H	N	O	S	0	0
			701	223	359	55	62	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Xx	45	GLY	SER	conflict	UNP A0A9R0JQ89
X	45	GLY	SER	conflict	UNP A0A9R0JQ89
x	45	GLY	SER	conflict	UNP A0A9R0JQ89
XX	45	GLY	SER	conflict	UNP A0A9R0JQ89

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Yy	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	G	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	N	217	Total	C	H	N	O	S	0	0
			3245	1077	1589	269	303	7		
9	Y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	g	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	n	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	GG	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	NN	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	YY	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	Gg	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	Nn	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Zz	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	Z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	ZZ	61	Total	C	H	N	O	0	0
			933	306	479	68	80		

- Molecule 11 is a protein called Chlorophyll a-b binding protein CP24, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	44	186	Total	C	H	N	O	S	0	0
			2847	952	1395	234	262	4		
11	4	186	Total	C	H	N	O	S	0	0
			2847	952	1395	234	262	4		

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Pp	187	Total	C	H	N	O	S	0	0
			2827	912	1394	234	285	2		
12	p	187	Total	C	H	N	O	S	0	0
			2827	912	1394	234	285	2		
12	P	187	Total	C	H	N	O	S	0	0
			2827	912	1394	234	285	2		
12	PP	187	Total	C	H	N	O	S	0	0
			2827	912	1394	234	285	2		

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Qq	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	Q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	QQ	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	11	206	Total	C	H	N	O	S	0	0
			3075	1021	1505	254	288	7		
14	22	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		
14	1	207	Total	C	H	N	O	S	0	0
			3086	1024	1510	255	290	7		
14	2	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	33	207	Total	C	H	N	O	S	0	0
			3189	1061	1575	258	290	5		
15	3	209	Total	C	H	N	O	S	0	0
			3195	1063	1573	260	294	5		

- Molecule 16 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	0	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		
16	00	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		

- Molecule 17 is a protein called Photosystem II reaction center proteins PsbY, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
17	55	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

- Molecule 18 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	C	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	c	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		
18	CC	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	Cc	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		

- Molecule 19 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	D	339	Total	C	H	N	O	S	0	0
			5274	1780	2580	441	461	12		
19	d	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		
19	DD	339	Total	C	H	N	O	S	0	0
			5275	1780	2581	441	461	12		
19	Dd	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		

- Molecule 20 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	e	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		
20	EE	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	Ee	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		

- Molecule 21 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	F	34	Total	C	H	N	O	S	0	0
			558	187	282	45	43	1		
21	f	31	Total	C	H	N	O	S	0	0
			509	169	259	42	38	1		
21	FF	34	Total	C	H	N	O	S	0	0
			558	187	282	45	43	1		
21	Ff	31	Total	C	H	N	O	S	0	0
			509	169	259	42	38	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	H	59	Total	C	H	N	O	S	0	0
			893	288	459	65	78	3		
22	h	59	Total	C	H	N	O	S	0	0
			893	288	459	65	78	3		
22	HH	59	Total	C	H	N	O	S	0	0
			893	288	459	65	78	3		
22	Hh	59	Total	C	H	N	O	S	0	0
			893	288	459	65	78	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	I	35	Total	C	H	N	O	S	0	0
			581	195	295	44	46	1		
23	i	33	Total	C	H	N	O	S	0	0
			542	184	276	39	42	1		
23	II	35	Total	C	H	N	O	S	0	0
			581	195	295	44	46	1		
23	Ii	33	Total	C	H	N	O	S	0	0
			542	184	276	39	42	1		

- Molecule 24 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	37	Total	C	H	N	O	0	0
			552	182	283	41	46		
24	j	34	Total	C	H	N	O	0	0
			505	168	258	38	41		
24	JJ	37	Total	C	H	N	O	0	0
			552	182	283	41	46		

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	Jj	34	Total	C	H	N	O	0	0
			505	168	258	38	41		

- Molecule 25 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	37	Total	C	H	N	O	S	0	0
			617	217	310	43	46	1		
25	k	37	Total	C	H	N	O	S	0	0
			617	217	310	43	46	1		
25	KK	37	Total	C	H	N	O	S	0	0
			617	217	310	43	46	1		
25	Kk	37	Total	C	H	N	O	S	0	0
			616	217	310	43	45	1		

- Molecule 26 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	35	Total	C	H	N	O	0	0
			579	196	284	46	53		
26	l	36	Total	C	H	N	O	0	0
			596	201	292	48	55		
26	LL	35	Total	C	H	N	O	0	0
			579	196	284	46	53		
26	Ll	36	Total	C	H	N	O	0	0
			596	201	292	48	55		

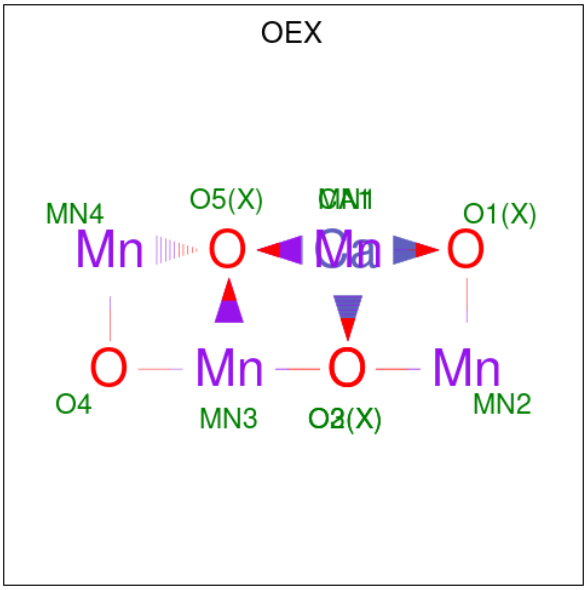
- Molecule 27 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	M	33	Total	C	H	N	O	S	0	0
			543	177	285	37	43	1		
27	m	32	Total	C	H	N	O		0	0
			523	172	273	36	42			
27	MM	33	Total	C	H	N	O	S	0	0
			543	177	285	37	43	1		
27	Mm	32	Total	C	H	N	O		0	0
			523	172	273	36	42			

- Molecule 28 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		
28	BB	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	B	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	Bb	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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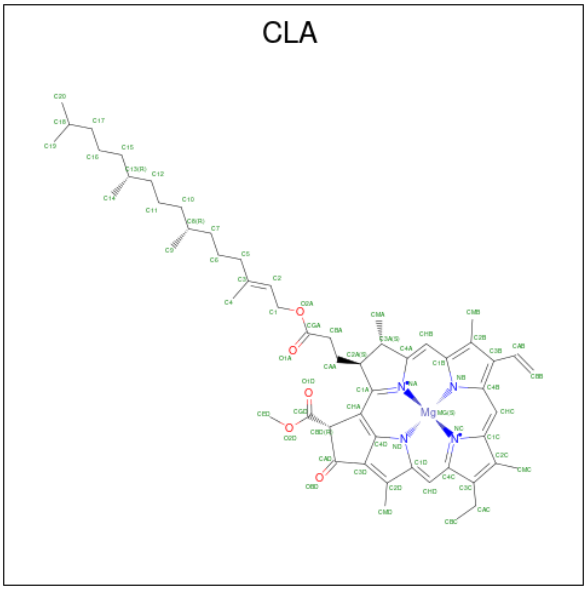
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Mol	Chain	Residues	Atoms	AltConf
30	AA	1	Total Fe 1 1	0
30	Aa	1	Total Fe 1 1	0

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
31	A	2	Total Cl 2 2	0
31	a	2	Total Cl 2 2	0
31	AA	2	Total Cl 2 2	0
31	Aa	2	Total Cl 2 2	0

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C H Mg N O 137 55 72 1 4 5	0
32	A	1	Total C H Mg N O 88 39 39 1 4 5	0
32	A	1	Total C H Mg N O 119 50 59 1 4 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	22	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	33	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	2	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	3	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	G	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	S	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	S	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	X	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	n	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	AA	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	AA	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	DD	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	DD	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	DD	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	SS	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	XX	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	YY	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	YY	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	YY	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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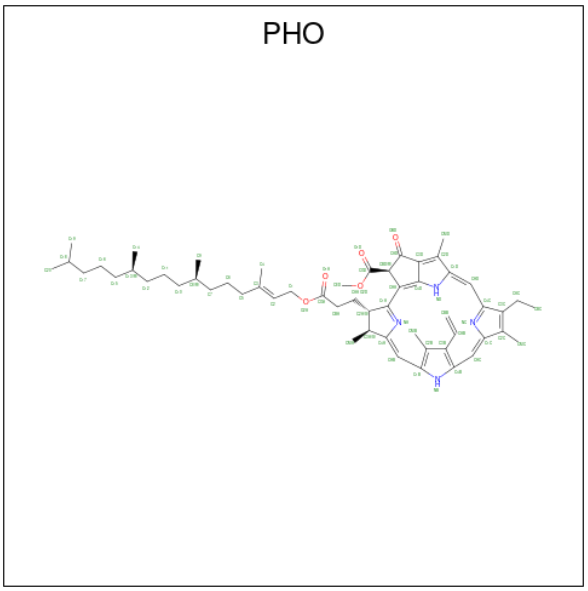
Mol	Chain	Residues	Atoms						AltConf
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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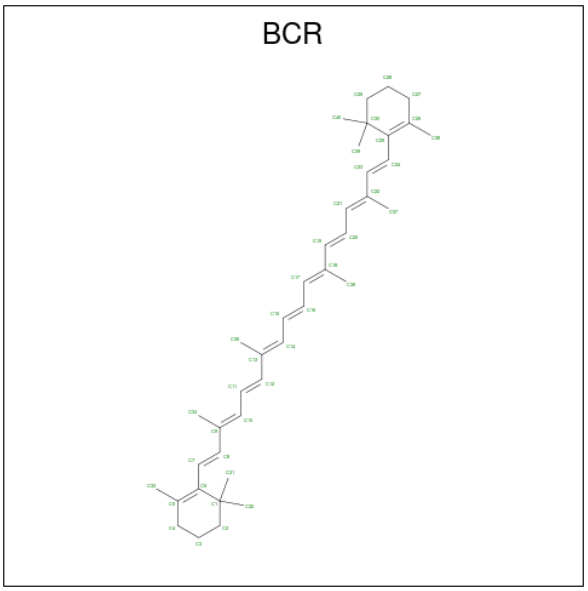
Mol	Chain	Residues	Atoms						AltConf
32	Gg	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	D	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	AA	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	DD	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 34 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	D	1	Total	C	H	0
			96	40	56	
34	H	1	Total	C	H	0
			96	40	56	
34	K	1	Total	C	H	0
			96	40	56	
34	T	1	Total	C	H	0
			96	40	56	
34	a	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	

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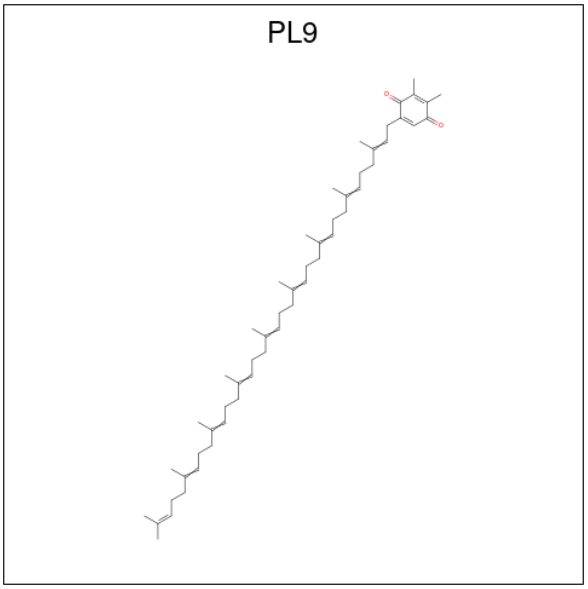
Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total C H 96 40 56	0
34	d	1	Total C H 96 40 56	0
34	h	1	Total C H 96 40 56	0
34	k	1	Total C H 96 40 56	0
34	AA	1	Total C H 96 40 56	0
34	BB	1	Total C H 96 40 56	0
34	BB	1	Total C H 96 40 56	0
34	BB	1	Total C H 96 40 56	0
34	BB	1	Total C H 96 40 56	0
34	CC	1	Total C H 96 40 56	0
34	CC	1	Total C H 96 40 56	0
34	CC	1	Total C H 96 40 56	0
34	DD	1	Total C H 96 40 56	0
34	B	1	Total C H 96 40 56	0
34	B	1	Total C H 96 40 56	0
34	B	1	Total C H 96 40 56	0
34	B	1	Total C H 96 40 56	0
34	KK	1	Total C H 96 40 56	0
34	TT	1	Total C H 96 40 56	0
34	XX	1	Total C H 96 40 56	0
34	Aa	1	Total C H 96 40 56	0

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Mol	Chain	Residues	Atoms	AltConf
34	Bb	1	Total C H 96 40 56	0
34	Bb	1	Total C H 96 40 56	0
34	Bb	1	Total C H 96 40 56	0
34	Cc	1	Total C H 96 40 56	0
34	Cc	1	Total C H 96 40 56	0
34	Cc	1	Total C H 96 40 56	0
34	Dd	1	Total C H 96 40 56	0
34	Hh	1	Total C H 96 40 56	0
34	Kk	1	Total C H 96 40 56	0

- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



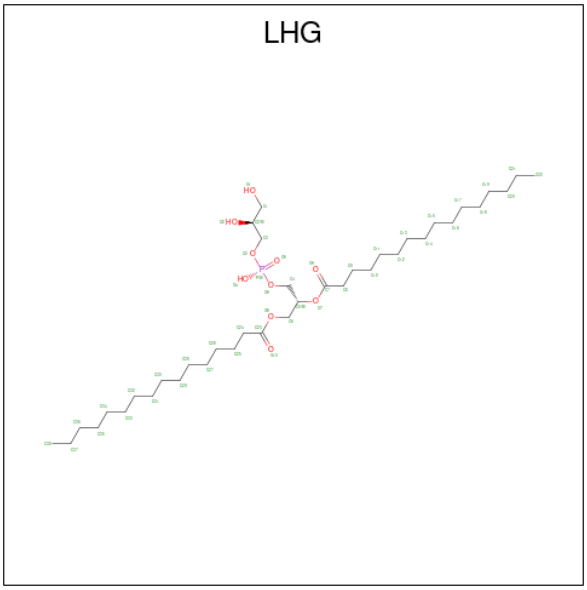
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C O 55 53 2	0

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Mol	Chain	Residues	Atoms	AltConf
35	D	1	Total C O 55 53 2	0
35	d	1	Total C O 55 53 2	0
35	AA	1	Total C O 55 53 2	0
35	DD	1	Total C O 55 53 2	0
35	Dd	1	Total C O 55 53 2	0

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C H O P 72 23 38 10 1	0
36	A	1	Total C H O P 81 26 44 10 1	0
36	A	1	Total C H O P 108 34 63 10 1	0
36	Rr	1	Total C H O P 123 38 74 10 1	0
36	Ss	1	Total C H O P 117 37 69 10 1	0
36	Yy	1	Total C H O P 123 38 74 10 1	0

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Mol	Chain	Residues	Atoms					AltConf
36	44	1	Total	C	H	O	P	0
			33	10	12	10	1	
36	44	1	Total	C	H	O	P	0
			31	8	12	10	1	
36	11	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	22	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	33	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	1	1	Total	C	H	O	P	0
			60	19	30	10	1	
36	3	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	0	1	Total	C	H	O	P	0
			114	36	67	10	1	
36	C	1	Total	C	H	O	P	0
			63	20	32	10	1	
36	D	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	D	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	G	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	J	1	Total	C	H	O	P	0
			51	16	24	10	1	
36	K	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	N	1	Total	C	H	O	P	0
			84	27	46	10	1	
36	Y	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	a	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	d	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	d	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	g	1	Total	C	H	O	P	0
			72	23	38	10	1	

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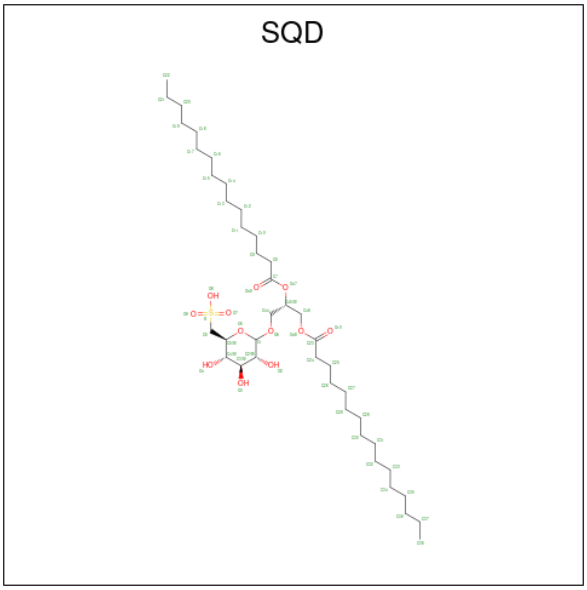
Mol	Chain	Residues	Atoms					AltConf
36	l	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	n	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	r	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	s	1	Total	C	H	O	P	0
			117	37	69	10	1	
36	y	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	4	1	Total	C	H	O	P	0
			31	8	12	10	1	
36	4	1	Total	C	H	O	P	0
			33	10	12	10	1	
36	AA	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	AA	1	Total	C	H	O	P	0
			108	34	63	10	1	
36	BB	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	CC	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	CC	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	DD	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	DD	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	EE	1	Total	C	H	O	P	0
			93	29	53	10	1	
36	GG	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	II	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	JJ	1	Total	C	H	O	P	0
			69	22	36	10	1	
36	KK	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	NN	1	Total	C	H	O	P	0
			84	27	46	10	1	
36	SS	1	Total	C	H	O	P	0
			48	15	22	10	1	

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Mol	Chain	Residues	Atoms					AltConf
36	YY	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	Dd	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	Gg	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	Ll	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Nn	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



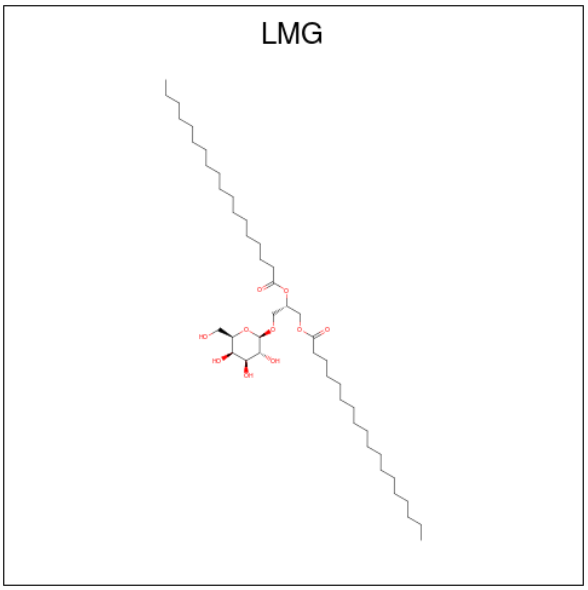
Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	C	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			72	23	36	12	1	

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Mol	Chain	Residues	Atoms					AltConf
37	l	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	AA	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	BB	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	CC	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	B	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	B	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	Aa	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	Ll	1	Total	C	H	O	S	0
			132	41	78	12	1	

- Molecule 38 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



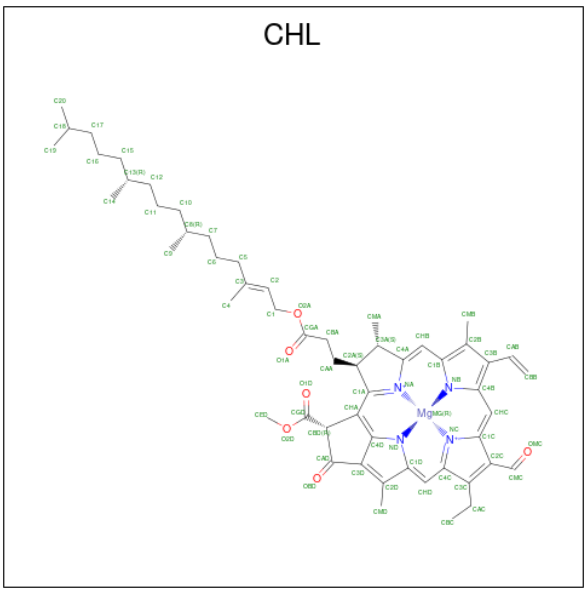
Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	H	O	0
			78	26	42	10	

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Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	H	O	0
			123	41	72	10	
38	F	1	Total	C	H	O	0
			108	36	62	10	
38	W	1	Total	C	H	O	0
			114	38	66	10	
38	a	1	Total	C	H	O	0
			97	33	54	10	
38	b	1	Total	C	H	O	0
			78	26	42	10	
38	b	1	Total	C	H	O	0
			78	26	42	10	
38	c	1	Total	C	H	O	0
			72	24	38	10	
38	j	1	Total	C	H	O	0
			108	36	62	10	
38	m	1	Total	C	H	O	0
			123	41	72	10	
38	AA	1	Total	C	H	O	0
			78	26	42	10	
38	BB	1	Total	C	H	O	0
			105	35	60	10	
38	CC	1	Total	C	H	O	0
			87	29	48	10	
38	DD	1	Total	C	H	O	0
			108	36	62	10	
38	B	1	Total	C	H	O	0
			105	35	60	10	
38	WW	1	Total	C	H	O	0
			114	38	66	10	
38	Aa	1	Total	C	H	O	0
			97	33	54	10	
38	Bb	1	Total	C	H	O	0
			78	26	42	10	
38	Bb	1	Total	C	H	O	0
			78	26	42	10	
38	Cc	1	Total	C	H	O	0
			72	24	38	10	
38	Dd	1	Total	C	H	O	0
			108	36	62	10	
38	Mm	1	Total	C	H	O	0
			123	41	72	10	

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms						AltConf
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	44	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	G	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	G	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	N	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	N	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	R	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	R	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	R	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	S	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	S	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	S	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	S	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Y	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Y	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	Y	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Y	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	g	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	y	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	y	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			86	39	36	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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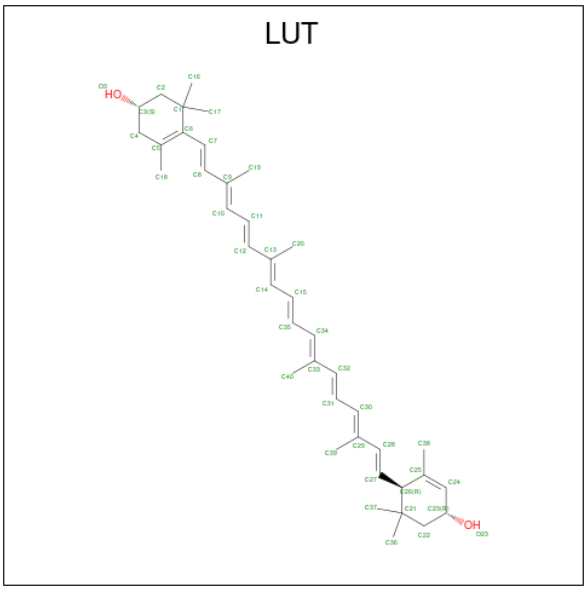
Mol	Chain	Residues	Atoms						AltConf
39	SS	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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



Mol	Chain	Residues	Atoms				AltConf
40	Rr	1	Total	C	H	O	0
			98	40	56	2	
40	Ss	1	Total	C	H	O	0
			98	40	56	2	
40	Ss	1	Total	C	H	O	0
			98	40	56	2	
40	Yy	1	Total	C	H	O	0
			98	40	56	2	
40	Yy	1	Total	C	H	O	0
			98	40	56	2	
40	44	1	Total	C	H	O	0
			98	40	56	2	
40	22	1	Total	C	H	O	0
			98	40	56	2	
40	2	1	Total	C	H	O	0
			98	40	56	2	
40	G	1	Total	C	H	O	0
			98	40	56	2	
40	G	1	Total	C	H	O	0
			98	40	56	2	

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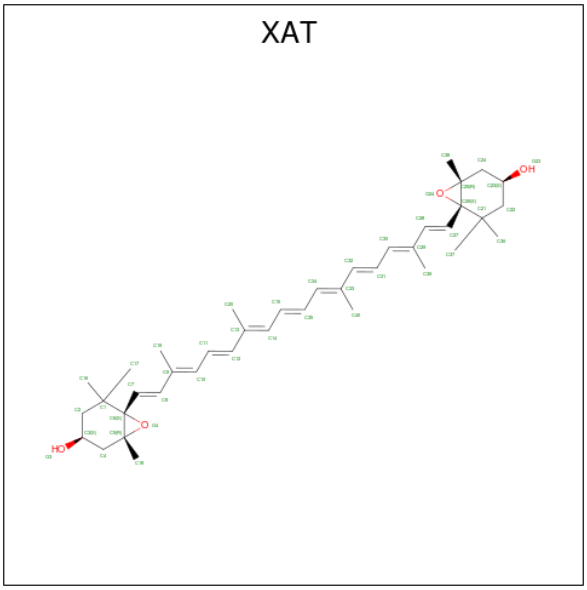
Mol	Chain	Residues	Atoms				AltConf
40	N	1	Total	C	H	O	0
			98	40	56	2	
40	N	1	Total	C	H	O	0
			98	40	56	2	
40	R	1	Total	C	H	O	0
			98	40	56	2	
40	S	1	Total	C	H	O	0
			98	40	56	2	
40	Y	1	Total	C	H	O	0
			98	40	56	2	
40	Y	1	Total	C	H	O	0
			98	40	56	2	
40	g	1	Total	C	H	O	0
			98	40	56	2	
40	g	1	Total	C	H	O	0
			98	40	56	2	
40	n	1	Total	C	H	O	0
			98	40	56	2	
40	n	1	Total	C	H	O	0
			98	40	56	2	
40	r	1	Total	C	H	O	0
			98	40	56	2	
40	s	1	Total	C	H	O	0
			98	40	56	2	
40	s	1	Total	C	H	O	0
			98	40	56	2	
40	y	1	Total	C	H	O	0
			98	40	56	2	
40	y	1	Total	C	H	O	0
			98	40	56	2	
40	4	1	Total	C	H	O	0
			98	40	56	2	
40	GG	1	Total	C	H	O	0
			98	40	56	2	
40	GG	1	Total	C	H	O	0
			98	40	56	2	
40	NN	1	Total	C	H	O	0
			98	40	56	2	
40	NN	1	Total	C	H	O	0
			98	40	56	2	
40	RR	1	Total	C	H	O	0
			98	40	56	2	

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Mol	Chain	Residues	Atoms				AltConf
40	SS	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



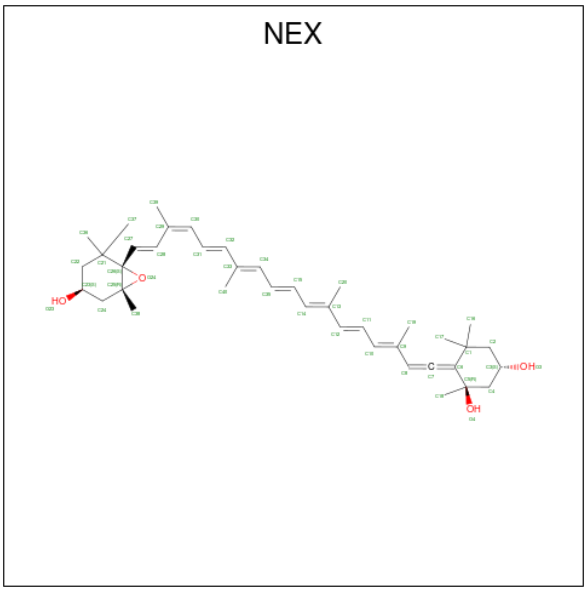
Mol	Chain	Residues	Atoms				AltConf
41	Rr	1	Total	C	H	O	0
			100	40	56	4	
41	Yy	1	Total	C	H	O	0
			100	40	56	4	
41	44	1	Total	C	H	O	0
			100	40	56	4	
41	G	1	Total	C	H	O	0
			100	40	56	4	

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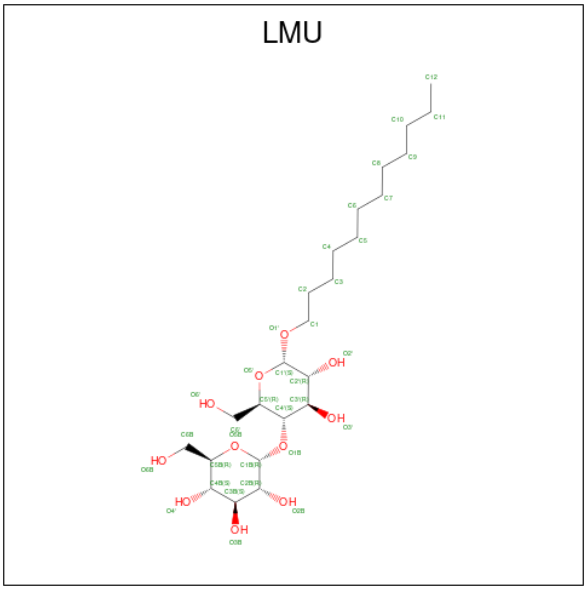
Mol	Chain	Residues	Atoms				AltConf
41	G	1	Total	C	H	O	0
			100	40	56	4	
41	N	1	Total	C	H	O	0
			100	40	56	4	
41	R	1	Total	C	H	O	0
			100	40	56	4	
41	g	1	Total	C	H	O	0
			100	40	56	4	
41	r	1	Total	C	H	O	0
			100	40	56	4	
41	y	1	Total	C	H	O	0
			100	40	56	4	
41	y	1	Total	C	H	O	0
			100	40	56	4	
41	4	1	Total	C	H	O	0
			100	40	56	4	
41	GG	1	Total	C	H	O	0
			100	40	56	4	
41	GG	1	Total	C	H	O	0
			100	40	56	4	
41	NN	1	Total	C	H	O	0
			100	40	56	4	
41	RR	1	Total	C	H	O	0
			100	40	56	4	
41	Gg	1	Total	C	H	O	0
			100	40	56	4	
41	Nn	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 42 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



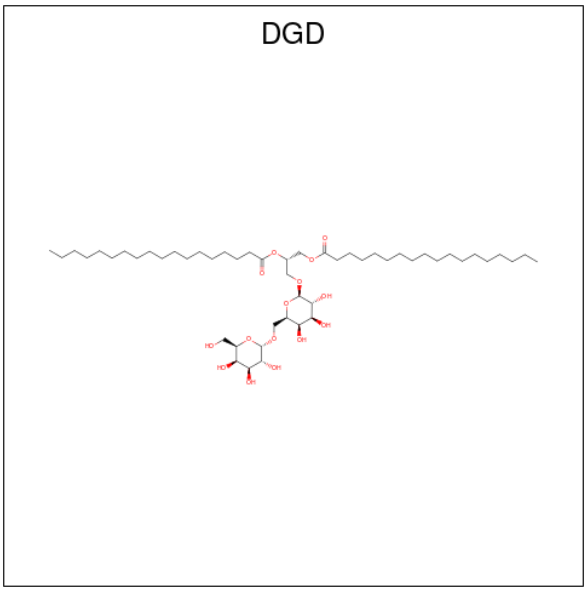
Mol	Chain	Residues	Atoms				AltConf
42	Rr	1	Total	C	H	O	0
			100	40	56	4	
42	Yy	1	Total	C	H	O	0
			100	40	56	4	
42	N	1	Total	C	H	O	0
			100	40	56	4	
42	R	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	g	1	Total	C	H	O	0
			100	40	56	4	
42	n	1	Total	C	H	O	0
			100	40	56	4	
42	y	1	Total	C	H	O	0
			100	40	56	4	
42	NN	1	Total	C	H	O	0
			100	40	56	4	
42	RR	1	Total	C	H	O	0
			100	40	56	4	
42	YY	1	Total	C	H	O	0
			100	40	56	4	
42	Gg	1	Total	C	H	O	0
			100	40	56	4	
42	Nn	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
43	C	1	Total	C	H	O	0
			54	16	27	11	
43	R	1	Total	C	H	O	0
			54	16	27	11	
43	KK	1	Total	C	H	O	0
			54	16	27	11	
43	RR	1	Total	C	H	O	0
			53	16	26	11	

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



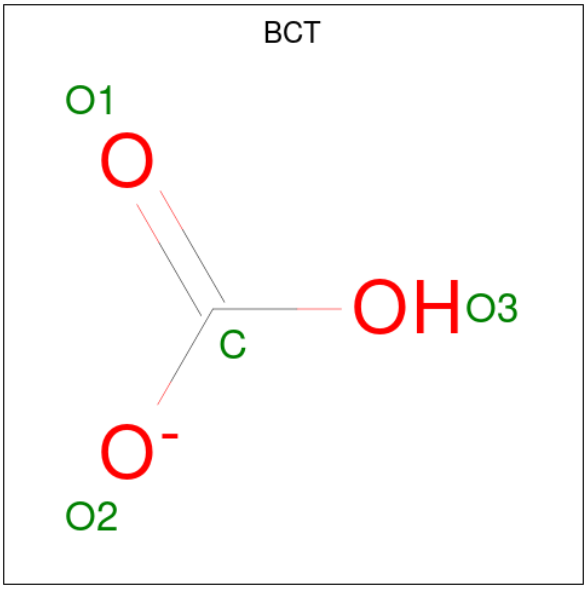
Mol	Chain	Residues	Atoms				AltConf
44	C	1	Total	C	H	O	0
			117	40	62	15	
44	C	1	Total	C	H	O	0
			132	47	70	15	
44	C	1	Total	C	H	O	0
			110	37	58	15	
44	D	1	Total	C	H	O	0
			132	47	70	15	
44	a	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			108	37	56	15	
44	h	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			117	40	62	15	
44	BB	1	Total	C	H	O	0
			121	42	64	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	
44	CC	1	Total	C	H	O	0
			132	47	70	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	

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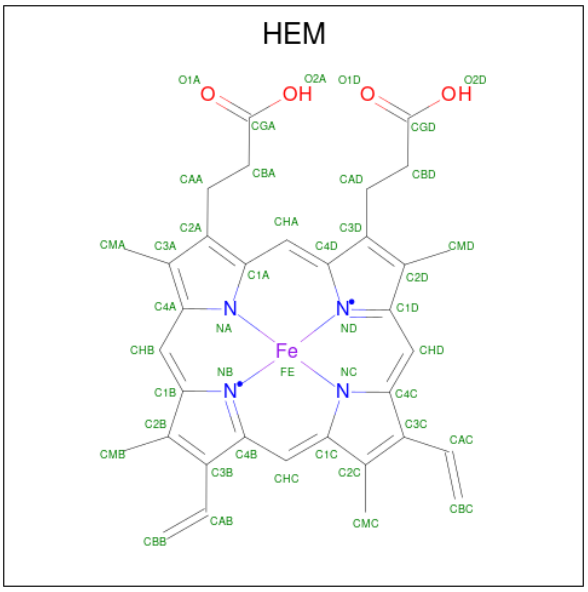
Mol	Chain	Residues	Atoms	AltConf
44	B	1	Total C H O 117 40 62 15	0
44	B	1	Total C H O 121 42 64 15	0
44	Aa	1	Total C H O 117 40 62 15	0
44	Cc	1	Total C H O 117 40 62 15	0
44	Cc	1	Total C H O 108 37 56 15	0
44	Hh	1	Total C H O 132 47 70 15	0

- Molecule 45 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	AltConf
45	D	1	Total C O 4 1 3	0
45	a	1	Total C H O 5 1 1 3	0
45	AA	1	Total C O 4 1 3	0
45	Aa	1	Total C H O 5 1 1 3	0

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
46	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
46	e	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
46	EE	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
46	Ee	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	34.286	Depositor
Minimum map value	-20.735	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	3	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 781 ligands modelled in this entry, 12 are monoatomic - leaving 769 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	SQD	l	102	-	52,54,54	1.11	3 (5%)	62,65,65	1.00	3 (4%)
39	CHL	11	607	-	35,49,74	3.24	8 (22%)	30,83,114	2.05	12 (40%)
39	CHL	r	607	-	44,58,74	2.90	8 (18%)	37,94,114	1.84	13 (35%)
32	CLA	Ss	602	4	53,57,73	1.31	6 (11%)	61,93,113	1.20	4 (6%)
36	LHG	y	320	32	48,48,48	0.92	2 (4%)	51,54,54	0.96	3 (5%)
39	CHL	Gg	309	-	36,50,74	3.17	10 (27%)	29,85,114	1.91	9 (31%)
32	CLA	s	602	4	53,57,73	1.30	6 (11%)	61,93,113	1.18	4 (6%)
36	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
32	CLA	C	513	18	69,73,73	1.16	7 (10%)	82,113,113	1.14	4 (4%)
32	CLA	a	406	1	69,73,73	1.17	9 (13%)	82,113,113	1.12	8 (9%)
32	CLA	SS	309	4	45,49,73	1.41	6 (13%)	54,84,113	1.22	4 (7%)
39	CHL	NN	608	-	36,50,74	3.20	10 (27%)	29,85,114	1.94	9 (31%)
32	CLA	1	602	14	44,48,73	1.44	6 (13%)	51,82,113	1.30	4 (7%)
32	CLA	1	610	36	44,48,73	1.45	5 (11%)	51,82,113	1.27	3 (5%)
32	CLA	d	402	-	69,73,73	1.16	6 (8%)	82,113,113	1.01	4 (4%)
33	PHO	A	407	-	58,69,69	2.15	10 (17%)	55,99,99	1.63	9 (16%)
32	CLA	44	602	11	49,53,73	1.36	8 (16%)	58,89,113	1.21	5 (8%)
32	CLA	11	612	-	44,48,73	1.51	8 (18%)	51,82,113	1.52	9 (17%)
44	DGD	CC	518	-	56,56,67	0.93	2 (3%)	70,70,81	0.95	3 (4%)
36	LHG	D	408	-	42,42,48	1.00	2 (4%)	45,48,54	1.03	2 (4%)
32	CLA	b	606	-	69,73,73	1.15	6 (8%)	82,113,113	1.11	7 (8%)
39	CHL	1	606	-	35,49,74	3.29	8 (22%)	30,83,114	1.89	8 (26%)
42	NEX	Yy	617	-	40,46,46	1.23	3 (7%)	50,70,70	1.94	15 (30%)
32	CLA	Aa	406	1	69,73,73	1.16	8 (11%)	82,113,113	1.11	7 (8%)
32	CLA	3	613	-	44,48,73	1.44	6 (13%)	51,82,113	1.31	4 (7%)
42	NEX	R	617	-	40,46,46	1.25	4 (10%)	50,70,70	1.91	12 (24%)
44	DGD	CC	522	-	56,56,67	0.93	3 (5%)	70,70,81	1.12	5 (7%)
36	LHG	BB	622	-	33,33,48	1.12	2 (6%)	36,39,54	1.02	2 (5%)
32	CLA	C	507	-	69,73,73	1.13	6 (8%)	82,113,113	1.08	6 (7%)
43	LMU	RR	301	-	28,28,36	0.75	0	39,39,47	0.76	0
39	CHL	YY	607	-	37,51,74	3.16	9 (24%)	30,86,114	2.08	12 (40%)
33	PHO	a	409	-	58,69,69	2.18	11 (18%)	55,99,99	1.49	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	XAT	Nn	308	-	41,47,47	1.20	3 (7%)	54,74,74	2.47	13 (24%)
32	CLA	2	611	14	44,48,73	1.45	6 (13%)	51,82,113	1.29	4 (7%)
36	LHG	NN	619	32	37,37,48	1.08	2 (5%)	40,43,54	1.05	2 (5%)
39	CHL	Ss	601	4	46,60,74	2.84	10 (21%)	40,97,114	1.74	13 (32%)
41	XAT	N	617	-	41,47,47	1.17	4 (9%)	54,74,74	2.27	14 (25%)
41	XAT	R	616	-	41,47,47	1.06	2 (4%)	54,74,74	2.19	16 (29%)
44	DGD	D	411	-	63,63,67	0.88	2 (3%)	77,77,81	0.89	3 (3%)
32	CLA	B	620	-	69,73,73	1.15	7 (10%)	82,113,113	1.13	5 (6%)
32	CLA	c	511	18	69,73,73	1.18	5 (7%)	82,113,113	1.04	3 (3%)
32	CLA	y	313	36	46,50,73	1.38	7 (15%)	53,85,113	1.27	4 (7%)
45	BCT	a	413	30	3,3,3	1.14	0	2,3,3	3.88	2 (100%)
32	CLA	D	401	-	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
32	CLA	AA	405	-	69,73,73	1.15	7 (10%)	82,113,113	1.09	5 (6%)
39	CHL	N	601	9	38,52,74	3.14	8 (21%)	31,87,114	1.89	9 (29%)
40	LUT	Rr	614	-	42,43,43	0.93	1 (2%)	51,60,60	1.41	9 (17%)
44	DGD	Aa	401	-	56,56,67	0.96	2 (3%)	70,70,81	0.89	3 (4%)
36	LHG	11	614	32	33,33,48	1.14	2 (6%)	36,39,54	1.13	3 (8%)
44	DGD	C	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	3 (3%)
42	NEX	Rr	616	-	40,46,46	1.23	3 (7%)	50,70,70	2.09	17 (34%)
32	CLA	RR	302	3	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
32	CLA	S	613	-	49,53,73	1.37	7 (14%)	58,89,113	1.17	4 (6%)
39	CHL	S	601	4	46,60,74	2.84	9 (19%)	40,97,114	1.73	11 (27%)
41	XAT	4	314	-	41,47,47	1.04	2 (4%)	54,74,74	2.38	15 (27%)
39	CHL	NN	601	9	38,52,74	3.11	9 (23%)	31,87,114	1.91	9 (29%)
39	CHL	g	609	9	37,51,74	3.10	10 (27%)	30,86,114	1.96	9 (30%)
41	XAT	r	615	-	41,47,47	1.11	3 (7%)	54,74,74	2.30	15 (27%)
32	CLA	3	602	15	44,48,73	1.44	5 (11%)	51,82,113	1.26	4 (7%)
39	CHL	Rr	607	-	44,58,74	2.89	8 (18%)	37,94,114	1.85	13 (35%)
32	CLA	GG	602	9	53,57,73	1.34	5 (9%)	61,93,113	1.36	6 (9%)
32	CLA	Bb	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	6 (7%)
37	SQD	BB	621	-	34,36,54	1.43	4 (11%)	44,47,65	3.79	10 (22%)
32	CLA	S	603	-	49,53,73	1.39	6 (12%)	58,89,113	1.23	4 (6%)
32	CLA	R	609	3	69,73,73	1.16	8 (11%)	82,113,113	1.06	5 (6%)
41	XAT	44	613	-	41,47,47	1.03	2 (4%)	54,74,74	2.28	12 (22%)
32	CLA	g	602	9	53,57,73	1.35	6 (11%)	61,93,113	1.83	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	B	622	-	69,73,73	1.15	6 (8%)	82,113,113	1.16	7 (8%)
40	LUT	GG	615	-	42,43,43	0.94	0	51,60,60	1.49	10 (19%)
42	NEX	Y	617	-	40,46,46	1.25	3 (7%)	50,70,70	1.97	12 (24%)
32	CLA	g	603	-	69,73,73	1.16	6 (8%)	82,113,113	1.01	4 (4%)
32	CLA	Cc	512	-	69,73,73	1.15	8 (11%)	82,113,113	1.09	4 (4%)
39	CHL	Nn	319	9	44,58,74	2.82	12 (27%)	37,94,114	1.83	10 (27%)
32	CLA	N	611	36	53,57,73	1.31	7 (13%)	61,93,113	1.26	6 (9%)
32	CLA	Gg	311	9	53,57,73	1.29	6 (11%)	61,93,113	1.21	5 (8%)
32	CLA	Bb	611	-	69,73,73	1.14	7 (10%)	82,113,113	1.07	4 (4%)
34	BCR	k	101	-	41,41,41	0.91	1 (2%)	56,56,56	1.94	17 (30%)
32	CLA	b	614	-	69,73,73	1.14	6 (8%)	82,113,113	1.09	3 (3%)
39	CHL	3	608	15	35,49,74	3.23	8 (22%)	30,83,114	1.81	8 (26%)
42	NEX	N	618	-	40,46,46	1.25	3 (7%)	50,70,70	2.08	14 (28%)
39	CHL	Y	606	-	38,52,74	3.11	11 (28%)	31,87,114	1.93	8 (25%)
32	CLA	RR	312	3	46,50,73	1.40	5 (10%)	53,85,113	1.17	3 (5%)
32	CLA	Cc	508	-	69,73,73	1.14	7 (10%)	82,113,113	1.17	7 (8%)
32	CLA	YY	604	-	53,57,73	1.30	5 (9%)	61,93,113	1.27	5 (8%)
32	CLA	Y	604	-	53,57,73	1.30	6 (11%)	61,93,113	1.20	5 (8%)
39	CHL	Yy	609	9	60,74,74	2.45	11 (18%)	58,114,114	1.61	9 (15%)
34	BCR	b	619	-	41,41,41	0.90	1 (2%)	56,56,56	1.94	12 (21%)
32	CLA	R	608	3	53,57,73	1.31	7 (13%)	61,93,113	1.28	4 (6%)
32	CLA	N	610	9	69,73,73	1.16	6 (8%)	82,113,113	1.04	6 (7%)
34	BCR	B	614	-	41,41,41	0.98	2 (4%)	56,56,56	1.85	14 (25%)
32	CLA	B	623	-	69,73,73	1.15	6 (8%)	82,113,113	1.03	3 (3%)
33	PHO	Aa	409	-	58,69,69	2.16	11 (18%)	55,99,99	1.50	8 (14%)
35	PL9	A	410	-	55,55,55	4.42	23 (41%)	68,69,69	3.73	38 (55%)
39	CHL	YY	609	9	60,74,74	2.46	10 (16%)	58,114,114	1.51	12 (20%)
32	CLA	Cc	510	-	64,68,73	1.18	6 (9%)	76,107,113	1.05	3 (3%)
39	CHL	G	601	9	60,74,74	2.47	11 (18%)	58,114,114	1.56	13 (22%)
32	CLA	YY	611	36	46,50,73	1.41	9 (19%)	53,85,113	1.26	4 (7%)
42	NEX	n	617	-	40,46,46	1.22	3 (7%)	50,70,70	2.01	12 (24%)
32	CLA	D	405	-	69,73,73	1.15	6 (8%)	82,113,113	1.05	4 (4%)
40	LUT	g	616	-	42,43,43	0.88	1 (2%)	51,60,60	1.58	10 (19%)
32	CLA	Rr	610	36	53,57,73	1.35	6 (11%)	61,93,113	1.24	4 (6%)
34	BCR	DD	405	-	41,41,41	0.85	0	56,56,56	1.94	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	c	502	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	8 (9%)
32	CLA	r	604	-	53,57,73	1.30	5 (9%)	61,93,113	1.21	6 (9%)
42	NEX	y	319	-	40,46,46	1.24	3 (7%)	50,70,70	1.94	12 (24%)
32	CLA	3	610	36	44,48,73	1.45	5 (11%)	51,82,113	1.35	6 (11%)
32	CLA	y	315	9	63,67,73	1.20	6 (9%)	74,105,113	1.14	3 (4%)
39	CHL	S	606	-	36,50,74	3.19	8 (22%)	29,85,114	1.98	10 (34%)
32	CLA	BB	613	-	64,68,73	1.19	6 (9%)	76,107,113	1.14	5 (6%)
34	BCR	CC	516	-	41,41,41	0.97	1 (2%)	56,56,56	1.92	14 (25%)
32	CLA	44	611	-	49,53,73	1.37	5 (10%)	58,89,113	1.22	3 (5%)
32	CLA	Rr	608	3	53,57,73	1.30	6 (11%)	61,93,113	1.19	5 (8%)
34	BCR	C	516	-	41,41,41	0.97	1 (2%)	56,56,56	2.09	18 (32%)
34	BCR	b	618	-	41,41,41	0.91	1 (2%)	56,56,56	1.94	12 (21%)
32	CLA	C	504	-	69,73,73	1.15	7 (10%)	82,113,113	1.20	4 (4%)
32	CLA	r	610	36	53,57,73	1.34	5 (9%)	61,93,113	1.24	4 (6%)
37	SQD	LL	101	-	34,36,54	1.37	3 (8%)	44,47,65	1.12	2 (4%)
44	DGD	C	519	-	56,56,67	0.94	2 (3%)	70,70,81	0.94	3 (4%)
32	CLA	g	611	36	69,73,73	1.17	7 (10%)	82,113,113	1.23	8 (9%)
39	CHL	Nn	316	-	44,58,74	2.86	10 (22%)	37,94,114	1.92	11 (29%)
39	CHL	g	607	-	44,58,74	2.89	11 (25%)	37,94,114	1.75	10 (27%)
46	HEM	Ee	101	21,20	50,50,50	1.42	10 (20%)	67,82,82	1.10	3 (4%)
32	CLA	r	612	3	53,57,73	1.33	5 (9%)	61,93,113	1.24	6 (9%)
38	LMG	CC	520	-	39,39,55	1.07	2 (5%)	47,47,63	0.95	2 (4%)
34	BCR	C	518	-	41,41,41	0.89	0	56,56,56	2.09	14 (25%)
32	CLA	r	602	3	69,73,73	1.16	6 (8%)	82,113,113	1.08	6 (7%)
39	CHL	Nn	311	9	44,58,74	2.90	9 (20%)	37,94,114	1.78	11 (29%)
32	CLA	b	605	-	69,73,73	1.14	6 (8%)	82,113,113	1.09	4 (4%)
41	XAT	Gg	301	-	41,47,47	1.22	4 (9%)	54,74,74	2.46	12 (22%)
42	NEX	Nn	309	-	40,46,46	1.23	3 (7%)	50,70,70	1.99	12 (24%)
32	CLA	22	604	-	44,48,73	1.45	5 (11%)	51,82,113	1.27	4 (7%)
32	CLA	Nn	314	-	53,57,73	1.30	8 (15%)	61,93,113	1.17	6 (9%)
32	CLA	Gg	314	9	44,48,73	1.43	5 (11%)	51,82,113	1.37	5 (9%)
32	CLA	n	610	9	69,73,73	1.16	6 (8%)	82,113,113	1.04	8 (9%)
32	CLA	Cc	515	-	47,51,73	1.36	7 (14%)	55,86,113	1.23	5 (9%)
39	CHL	r	605	3	44,58,74	2.87	9 (20%)	37,94,114	1.94	9 (24%)
35	PL9	Dd	404	-	55,55,55	4.36	21 (38%)	68,69,69	3.81	38 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	33	610	36	44,48,73	1.44	6 (13%)	51,82,113	1.31	5 (9%)
36	LHG	CC	523	-	36,36,48	1.06	2 (5%)	39,42,54	1.05	3 (7%)
32	CLA	2	609	14	44,48,73	1.44	6 (13%)	51,82,113	1.21	3 (5%)
32	CLA	CC	508	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	7 (8%)
32	CLA	d	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	7 (8%)
38	LMG	W	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.06	2 (3%)
32	CLA	11	602	14	44,48,73	1.45	5 (11%)	51,82,113	1.29	5 (9%)
32	CLA	11	611	14	44,48,73	1.45	6 (13%)	51,82,113	1.28	4 (7%)
46	HEM	E	101	21,20	50,50,50	1.40	8 (16%)	67,82,82	1.06	1 (1%)
36	LHG	Nn	310	32	48,48,48	0.95	2 (4%)	51,54,54	1.06	2 (3%)
32	CLA	N	614	-	45,49,73	1.39	7 (15%)	54,84,113	1.18	3 (5%)
36	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.97	3 (5%)
32	CLA	RR	310	36	53,57,73	1.31	4 (7%)	61,93,113	1.17	5 (8%)
40	LUT	r	614	-	42,43,43	0.94	1 (2%)	51,60,60	1.40	8 (15%)
32	CLA	Aa	410	-	64,68,73	1.19	7 (10%)	76,107,113	1.13	7 (9%)
40	LUT	NN	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.34	8 (15%)
32	CLA	B	606	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
32	CLA	y	305	-	53,57,73	1.31	7 (13%)	61,93,113	1.19	3 (4%)
33	PHO	a	408	-	58,69,69	2.18	11 (18%)	55,99,99	1.51	8 (14%)
36	LHG	d	405	-	42,42,48	0.99	2 (4%)	45,48,54	0.98	2 (4%)
32	CLA	YY	602	9	69,73,73	1.16	7 (10%)	82,113,113	1.06	5 (6%)
44	DGD	a	415	-	56,56,67	0.97	3 (5%)	70,70,81	0.90	3 (4%)
32	CLA	Ss	613	-	53,57,73	1.31	6 (11%)	61,93,113	1.17	5 (8%)
32	CLA	r	608	3	53,57,73	1.31	7 (13%)	61,93,113	1.19	5 (8%)
32	CLA	RR	308	3	53,57,73	1.32	7 (13%)	61,93,113	1.29	4 (6%)
36	LHG	EE	101	-	39,39,48	1.05	2 (5%)	42,45,54	0.91	2 (4%)
39	CHL	N	606	-	36,50,74	3.17	11 (30%)	29,85,114	1.97	7 (24%)
29	OEX	A	401	18,1	0,15,15	-	-	-		
39	CHL	11	608	14	35,49,74	3.13	8 (22%)	30,83,114	1.79	8 (26%)
38	LMG	DD	409	-	46,46,55	0.98	2 (4%)	54,54,63	0.89	2 (3%)
39	CHL	33	608	15	35,49,74	3.24	8 (22%)	30,83,114	1.86	9 (30%)
32	CLA	c	501	-	69,73,73	1.14	6 (8%)	82,113,113	1.21	6 (7%)
40	LUT	2	614	-	42,43,43	1.06	4 (9%)	51,60,60	1.71	10 (19%)
32	CLA	B	609	-	64,68,73	1.19	6 (9%)	76,107,113	1.15	5 (6%)
36	LHG	AA	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.90	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	44	603	-	49,53,73	1.38	5 (10%)	58,89,113	1.30	4 (6%)
32	CLA	BB	601	-	69,73,73	1.15	6 (8%)	82,113,113	1.05	6 (7%)
32	CLA	4	305	-	49,53,73	1.36	7 (14%)	58,89,113	1.22	3 (5%)
32	CLA	Cc	506	-	59,63,73	1.23	6 (10%)	70,101,113	1.14	5 (7%)
32	CLA	Nn	312	9	69,73,73	1.15	7 (10%)	82,113,113	1.18	7 (8%)
34	BCR	AA	409	-	41,41,41	1.00	3 (7%)	56,56,56	1.98	13 (23%)
32	CLA	n	603	-	53,57,73	1.30	5 (9%)	61,93,113	1.25	4 (6%)
44	DGD	CC	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.93	3 (3%)
32	CLA	B	610	-	69,73,73	1.15	5 (7%)	82,113,113	1.13	7 (8%)
42	NEX	Y	619	-	40,46,46	1.24	3 (7%)	50,70,70	2.10	17 (34%)
32	CLA	C	503	-	69,73,73	1.15	6 (8%)	82,113,113	1.08	6 (7%)
32	CLA	Yy	614	-	53,57,73	1.29	6 (11%)	61,93,113	1.20	4 (6%)
37	SQD	B	617	-	34,36,54	1.42	4 (11%)	44,47,65	3.78	10 (22%)
32	CLA	11	604	-	44,48,73	1.45	7 (15%)	51,82,113	1.41	7 (13%)
41	XAT	Yy	619	-	41,47,47	1.15	3 (7%)	54,74,74	2.33	18 (33%)
32	CLA	Rr	604	-	53,57,73	1.30	5 (9%)	61,93,113	1.19	7 (11%)
39	CHL	Yy	607	-	37,51,74	3.06	8 (21%)	30,86,114	2.15	12 (40%)
44	DGD	c	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.12	6 (8%)
39	CHL	22	606	-	35,49,74	3.25	8 (22%)	30,83,114	1.84	9 (30%)
39	CHL	33	605	-	35,49,74	3.27	8 (22%)	30,83,114	1.92	10 (33%)
39	CHL	y	307	9	42,56,74	2.91	10 (23%)	36,92,114	1.85	11 (30%)
32	CLA	c	505	-	69,73,73	1.14	7 (10%)	82,113,113	0.99	4 (4%)
32	CLA	33	609	15	44,48,73	1.44	5 (11%)	51,82,113	1.33	5 (9%)
32	CLA	22	609	14	44,48,73	1.44	7 (15%)	51,82,113	1.26	3 (5%)
32	CLA	2	604	-	44,48,73	1.46	6 (13%)	51,82,113	1.33	4 (7%)
40	LUT	S	614	-	42,43,43	0.90	0	51,60,60	1.51	9 (17%)
36	LHG	J	101	-	26,26,48	1.35	2 (7%)	29,32,54	1.40	3 (10%)
39	CHL	44	601	-	39,53,74	3.10	9 (23%)	33,89,114	1.76	8 (24%)
41	XAT	NN	617	-	41,47,47	1.18	5 (12%)	54,74,74	2.26	13 (24%)
32	CLA	Bb	615	-	69,73,73	1.16	5 (7%)	82,113,113	1.10	3 (3%)
39	CHL	3	607	-	35,49,74	3.26	8 (22%)	30,83,114	1.91	10 (33%)
32	CLA	b	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.04	6 (7%)
32	CLA	CC	511	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	5 (6%)
39	CHL	YY	605	9	42,56,74	2.95	9 (21%)	36,92,114	1.82	10 (27%)
39	CHL	GG	607	-	40,54,74	3.00	10 (25%)	34,90,114	1.93	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.92	2 (3%)
40	LUT	s	615	-	42,43,43	0.93	1 (2%)	51,60,60	1.60	13 (25%)
39	CHL	33	607	-	35,49,74	3.27	8 (22%)	30,83,114	1.92	10 (33%)
32	CLA	GG	612	9	53,57,73	1.34	5 (9%)	61,93,113	1.27	5 (8%)
32	CLA	R	603	-	53,57,73	1.31	5 (9%)	61,93,113	1.28	4 (6%)
32	CLA	NN	613	9	53,57,73	1.30	7 (13%)	61,93,113	1.18	3 (4%)
32	CLA	n	613	9	53,57,73	1.32	6 (11%)	61,93,113	1.18	4 (6%)
32	CLA	Ss	603	-	53,57,73	1.33	5 (9%)	61,93,113	1.16	5 (8%)
32	CLA	Ss	610	36	53,57,73	1.32	5 (9%)	61,93,113	1.25	4 (6%)
32	CLA	Y	614	-	53,57,73	1.29	6 (11%)	61,93,113	1.15	6 (9%)
39	CHL	GG	605	9	37,51,74	3.18	8 (21%)	30,86,114	1.89	10 (33%)
32	CLA	SS	303	4	53,57,73	1.30	6 (11%)	61,93,113	1.22	6 (9%)
32	CLA	N	603	-	46,50,73	1.37	6 (13%)	53,85,113	1.24	3 (5%)
33	PHO	AA	407	-	58,69,69	2.16	11 (18%)	55,99,99	1.62	9 (16%)
32	CLA	S	611	4	53,57,73	1.32	5 (9%)	61,93,113	1.30	4 (6%)
39	CHL	Y	607	-	37,51,74	3.14	9 (24%)	30,86,114	2.07	12 (40%)
32	CLA	NN	602	9	69,73,73	1.15	8 (11%)	82,113,113	1.16	7 (8%)
32	CLA	Bb	607	-	69,73,73	1.16	7 (10%)	82,113,113	1.04	4 (4%)
32	CLA	Rr	611	-	53,57,73	1.32	7 (13%)	61,93,113	1.18	4 (6%)
34	BCR	c	515	-	41,41,41	1.02	3 (7%)	56,56,56	1.71	12 (21%)
32	CLA	S	610	-	53,57,73	1.32	6 (11%)	61,93,113	1.27	3 (4%)
32	CLA	Rr	603	-	53,57,73	1.33	7 (13%)	61,93,113	1.23	4 (6%)
32	CLA	G	603	-	69,73,73	1.16	5 (7%)	82,113,113	1.04	4 (4%)
32	CLA	SS	312	4	53,57,73	1.32	5 (9%)	61,93,113	1.26	4 (6%)
34	BCR	BB	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.88	12 (21%)
39	CHL	y	310	-	44,58,74	2.81	11 (25%)	37,94,114	1.77	11 (29%)
35	PL9	d	404	-	55,55,55	4.36	21 (38%)	68,69,69	3.79	38 (55%)
36	LHG	s	616	32	47,47,48	0.96	2 (4%)	50,53,54	0.91	2 (4%)
32	CLA	c	503	-	69,73,73	1.16	6 (8%)	82,113,113	1.05	4 (4%)
42	NEX	g	617	32	40,46,46	1.17	4 (10%)	50,70,70	2.52	17 (34%)
37	SQD	Ll	101	-	52,54,54	1.11	3 (5%)	62,65,65	0.98	3 (4%)
32	CLA	Bb	605	-	69,73,73	1.15	6 (8%)	82,113,113	1.10	4 (4%)
32	CLA	Bb	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.07	6 (7%)
39	CHL	11	605	14	35,49,74	3.29	8 (22%)	30,83,114	1.79	7 (23%)
32	CLA	BB	612	-	69,73,73	1.15	6 (8%)	82,113,113	1.06	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LHG	JJ	101	-	32,32,48	1.13	2 (6%)	35,38,54	1.15	3 (8%)
32	CLA	1	604	-	44,48,73	1.46	7 (15%)	51,82,113	1.36	5 (9%)
36	LHG	KK	101	-	33,33,48	1.12	2 (6%)	36,39,54	1.12	3 (8%)
39	CHL	y	308	-	38,52,74	3.05	11 (28%)	31,87,114	2.02	10 (32%)
39	CHL	1	601	14	35,49,74	3.28	8 (22%)	30,83,114	1.73	7 (23%)
32	CLA	22	610	36	46,50,73	1.41	5 (10%)	53,85,113	1.18	3 (5%)
32	CLA	CC	503	-	69,73,73	1.14	7 (10%)	82,113,113	1.19	7 (8%)
44	DGD	BB	624	-	56,56,67	0.93	2 (3%)	70,70,81	0.99	4 (5%)
32	CLA	C	512	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	5 (6%)
40	LUT	Gg	316	-	42,43,43	0.94	0	51,60,60	1.42	7 (13%)
41	XAT	Rr	615	-	41,47,47	1.12	3 (7%)	54,74,74	2.35	19 (35%)
32	CLA	1	611	14	44,48,73	1.45	5 (11%)	51,82,113	1.33	4 (7%)
32	CLA	n	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.14	5 (8%)
36	LHG	N	619	32	37,37,48	1.07	2 (5%)	40,43,54	1.07	3 (7%)
39	CHL	GG	609	9	37,51,74	3.09	9 (24%)	30,86,114	2.01	11 (36%)
32	CLA	33	603	-	44,48,73	1.45	6 (13%)	51,82,113	1.26	4 (7%)
34	BCR	XX	202	-	41,41,41	0.94	1 (2%)	56,56,56	2.17	17 (30%)
32	CLA	S	608	4	45,49,73	1.43	6 (13%)	54,84,113	1.18	4 (7%)
32	CLA	Y	603	-	53,57,73	1.31	6 (11%)	61,93,113	1.25	4 (6%)
32	CLA	S	609	4	45,49,73	1.41	7 (15%)	54,84,113	1.26	5 (9%)
32	CLA	Y	610	9	69,73,73	1.14	8 (11%)	82,113,113	1.11	7 (8%)
36	LHG	DD	407	-	42,42,48	1.00	2 (4%)	45,48,54	1.04	2 (4%)
32	CLA	11	613	-	44,48,73	1.46	5 (11%)	51,82,113	1.19	3 (5%)
32	CLA	CC	506	-	69,73,73	1.14	7 (10%)	82,113,113	1.12	6 (7%)
32	CLA	A	408	-	64,68,73	1.20	6 (9%)	76,107,113	1.11	6 (7%)
36	LHG	Dd	405	-	42,42,48	0.99	2 (4%)	45,48,54	0.97	2 (4%)
39	CHL	N	609	9	44,58,74	2.83	11 (25%)	37,94,114	1.78	10 (27%)
32	CLA	Yy	612	9	69,73,73	1.14	6 (8%)	82,113,113	1.12	5 (6%)
32	CLA	RR	303	-	53,57,73	1.30	5 (9%)	61,93,113	1.29	3 (4%)
37	SQD	L	102	-	34,36,54	1.37	3 (8%)	44,47,65	1.19	4 (9%)
32	CLA	A	406	-	53,57,73	1.28	7 (13%)	61,93,113	1.19	5 (8%)
39	CHL	Gg	310	9	37,51,74	3.09	8 (21%)	30,86,114	1.94	10 (33%)
34	BCR	Kk	101	-	41,41,41	0.87	0	56,56,56	2.00	13 (23%)
32	CLA	NN	611	36	53,57,73	1.30	6 (11%)	61,93,113	1.28	7 (11%)
40	LUT	Gg	317	-	42,43,43	0.89	1 (2%)	51,60,60	1.58	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CHL	G	609	9	37,51,74	3.06	9 (24%)	30,86,114	1.95	11 (36%)
32	CLA	Bb	609	-	69,73,73	1.14	8 (11%)	82,113,113	1.22	6 (7%)
32	CLA	Nn	302	36	53,57,73	1.31	7 (13%)	61,93,113	1.21	4 (6%)
32	CLA	g	612	9	53,57,73	1.33	6 (11%)	61,93,113	1.22	6 (9%)
39	CHL	g	605	9	37,51,74	3.16	8 (21%)	30,86,114	1.76	9 (30%)
32	CLA	Yy	604	-	53,57,73	1.29	6 (11%)	61,93,113	1.19	4 (6%)
32	CLA	Bb	602	-	69,73,73	1.15	7 (10%)	82,113,113	1.05	5 (6%)
32	CLA	c	508	-	64,68,73	1.19	7 (10%)	76,107,113	1.09	5 (6%)
39	CHL	2	607	-	35,49,74	3.27	8 (22%)	30,83,114	1.88	8 (26%)
39	CHL	r	606	-	44,58,74	2.94	10 (22%)	37,94,114	1.71	10 (27%)
32	CLA	R	613	-	45,49,73	1.41	7 (15%)	54,84,113	1.22	4 (7%)
38	LMG	a	412	-	42,42,55	1.04	2 (4%)	50,50,63	1.11	4 (8%)
39	CHL	Gg	306	9	37,51,74	3.16	8 (21%)	30,86,114	1.76	9 (30%)
36	LHG	YY	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.85	2 (3%)
34	BCR	Bb	619	-	41,41,41	0.92	1 (2%)	56,56,56	2.06	16 (28%)
32	CLA	22	603	-	44,48,73	1.44	6 (13%)	51,82,113	1.29	5 (9%)
40	LUT	GG	616	-	42,43,43	0.95	1 (2%)	51,60,60	1.57	10 (19%)
39	CHL	n	606	-	44,58,74	2.85	11 (25%)	37,94,114	1.94	11 (29%)
32	CLA	b	607	-	69,73,73	1.16	7 (10%)	82,113,113	1.04	5 (6%)
36	LHG	r	616	32	48,48,48	0.97	2 (4%)	51,54,54	0.93	2 (3%)
39	CHL	33	606	-	35,49,74	3.27	9 (25%)	30,83,114	1.91	10 (33%)
44	DGD	BB	625	-	57,57,67	0.91	2 (3%)	70,70,81	0.95	3 (4%)
32	CLA	b	610	-	69,73,73	1.17	7 (10%)	82,113,113	1.08	4 (4%)
40	LUT	4	313	-	42,43,43	0.93	0	51,60,60	1.40	7 (13%)
39	CHL	NN	606	-	36,50,74	3.17	11 (30%)	29,85,114	1.99	7 (24%)
42	NEX	YY	617	-	40,46,46	1.25	3 (7%)	50,70,70	1.95	13 (26%)
38	LMG	BB	619	-	45,45,55	0.99	2 (4%)	53,53,63	0.93	2 (3%)
32	CLA	R	612	3	46,50,73	1.39	6 (13%)	53,85,113	1.17	3 (5%)
32	CLA	G	613	9	44,48,73	1.43	5 (11%)	51,82,113	1.40	6 (11%)
32	CLA	Gg	303	9	53,57,73	1.31	6 (11%)	61,93,113	1.47	7 (11%)
34	BCR	Cc	516	-	41,41,41	0.91	1 (2%)	56,56,56	2.16	19 (33%)
32	CLA	y	306	-	53,57,73	1.29	6 (11%)	61,93,113	1.20	5 (8%)
36	LHG	n	618	32	48,48,48	0.96	2 (4%)	51,54,54	1.02	2 (3%)
32	CLA	Nn	301	9	69,73,73	1.15	7 (10%)	82,113,113	1.07	7 (8%)
32	CLA	44	609	11	49,53,73	1.36	6 (12%)	58,89,113	1.18	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	Cc	504	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	6 (7%)
34	BCR	Aa	411	-	41,41,41	1.01	3 (7%)	56,56,56	1.61	9 (16%)
44	DGD	Cc	519	-	56,56,67	0.92	2 (3%)	70,70,81	1.12	7 (10%)
39	CHL	4	308	-	40,54,74	3.03	10 (25%)	34,90,114	1.86	10 (29%)
32	CLA	G	602	9	53,57,73	1.32	6 (11%)	61,93,113	1.24	6 (9%)
40	LUT	n	615	-	42,43,43	0.97	0	51,60,60	1.29	5 (9%)
36	LHG	II	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.02	2 (5%)
29	OEX	AA	401	18,1	0,15,15	-	-	-		
45	BCT	D	403	30	3,3,3	1.13	0	2,3,3	4.06	2 (100%)
32	CLA	b	615	-	69,73,73	1.16	5 (7%)	82,113,113	1.07	4 (4%)
34	BCR	a	411	-	41,41,41	0.99	3 (7%)	56,56,56	1.65	10 (17%)
32	CLA	S	604	-	53,57,73	1.31	6 (11%)	61,93,113	1.22	5 (8%)
36	LHG	1	614	32	29,29,48	1.21	2 (6%)	32,35,54	1.14	2 (6%)
32	CLA	BB	603	-	69,73,73	1.14	6 (8%)	82,113,113	1.14	5 (6%)
39	CHL	GG	601	9	60,74,74	2.48	11 (18%)	58,114,114	1.53	13 (22%)
32	CLA	n	612	9	53,57,73	1.32	7 (13%)	61,93,113	1.18	5 (8%)
32	CLA	RR	304	-	53,57,73	1.32	7 (13%)	61,93,113	1.30	7 (11%)
36	LHG	0	201	-	46,46,48	0.97	2 (4%)	49,52,54	0.85	2 (4%)
40	LUT	N	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.51	10 (19%)
34	BCR	K	102	-	41,41,41	0.83	0	56,56,56	2.20	19 (33%)
32	CLA	Rr	612	3	53,57,73	1.32	6 (11%)	61,93,113	1.19	4 (6%)
38	LMG	Bb	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.12	6 (13%)
39	CHL	R	606	-	44,58,74	2.89	11 (25%)	37,94,114	1.71	7 (18%)
39	CHL	GG	608	-	36,50,74	3.21	11 (30%)	29,85,114	1.84	9 (31%)
32	CLA	s	608	4	53,57,73	1.31	6 (11%)	61,93,113	1.22	5 (8%)
32	CLA	C	514	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
39	CHL	Ss	606	-	44,58,74	2.90	8 (18%)	37,94,114	1.71	11 (29%)
32	CLA	3	611	15	44,48,73	1.44	6 (13%)	51,82,113	1.27	4 (7%)
32	CLA	g	613	9	44,48,73	1.44	4 (9%)	51,82,113	1.37	6 (11%)
32	CLA	c	510	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	4 (4%)
32	CLA	33	613	-	44,48,73	1.44	6 (13%)	51,82,113	1.33	5 (9%)
34	BCR	Cc	517	-	41,41,41	1.04	3 (7%)	56,56,56	1.79	13 (23%)
36	LHG	AA	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.23	4 (11%)
38	LMG	m	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.83	2 (3%)
41	XAT	g	619	-	41,47,47	1.22	4 (9%)	54,74,74	2.47	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	RR	311	-	53,57,73	1.32	7 (13%)	61,93,113	1.17	3 (4%)
32	CLA	3	604	-	44,48,73	1.45	6 (13%)	51,82,113	1.25	3 (5%)
40	LUT	G	616	-	42,43,43	0.94	0	51,60,60	1.63	11 (21%)
32	CLA	C	506	-	69,73,73	1.15	6 (8%)	82,113,113	1.12	5 (6%)
32	CLA	B	621	-	69,73,73	1.14	7 (10%)	82,113,113	1.09	6 (7%)
32	CLA	Ss	608	4	53,57,73	1.31	6 (11%)	61,93,113	1.25	6 (9%)
32	CLA	GG	604	-	46,50,73	1.39	6 (13%)	53,85,113	1.16	3 (5%)
32	CLA	G	604	-	46,50,73	1.38	6 (13%)	53,85,113	1.15	4 (7%)
32	CLA	b	611	-	69,73,73	1.14	7 (10%)	82,113,113	1.05	4 (4%)
40	LUT	R	615	-	42,43,43	0.90	0	51,60,60	1.63	13 (25%)
32	CLA	Bb	601	-	69,73,73	1.17	8 (11%)	82,113,113	1.18	7 (8%)
33	PHO	Aa	408	-	58,69,69	2.18	11 (18%)	55,99,99	1.52	8 (14%)
46	HEM	EE	102	21,20	50,50,50	1.41	8 (16%)	67,82,82	1.03	0
39	CHL	g	608	-	36,50,74	3.15	11 (30%)	29,85,114	1.93	9 (31%)
37	SQD	L	101	-	52,54,54	1.12	3 (5%)	62,65,65	1.07	3 (4%)
32	CLA	33	612	15	44,48,73	1.44	6 (13%)	51,82,113	1.21	3 (5%)
38	LMG	Mm	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.84	2 (3%)
33	PHO	DD	402	-	58,69,69	2.15	11 (18%)	55,99,99	1.60	7 (12%)
39	CHL	s	607	-	43,57,74	3.00	8 (18%)	37,93,114	1.78	10 (27%)
32	CLA	G	611	36	56,60,73	1.29	6 (10%)	65,97,113	1.17	4 (6%)
32	CLA	NN	610	9	69,73,73	1.15	6 (8%)	82,113,113	1.06	6 (7%)
32	CLA	s	613	-	53,57,73	1.32	6 (11%)	61,93,113	1.18	4 (6%)
36	LHG	g	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.17	3 (8%)
36	LHG	Rr	617	32	48,48,48	0.98	2 (4%)	51,54,54	0.98	2 (3%)
32	CLA	BB	604	-	69,73,73	1.15	6 (8%)	82,113,113	1.05	7 (8%)
39	CHL	Nn	317	-	60,74,74	2.40	11 (18%)	58,114,114	1.65	13 (22%)
32	CLA	GG	614	-	45,49,73	1.40	5 (11%)	54,84,113	1.15	3 (5%)
32	CLA	a	410	-	64,68,73	1.20	8 (12%)	76,107,113	1.13	6 (7%)
34	BCR	BB	617	-	41,41,41	0.98	2 (4%)	56,56,56	1.76	14 (25%)
37	SQD	Aa	413	-	45,47,54	1.20	3 (6%)	55,58,65	1.01	2 (3%)
39	CHL	22	601	14	35,49,74	3.27	9 (25%)	30,83,114	1.86	10 (33%)
38	LMG	b	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.97	2 (4%)
43	LMU	R	618	-	28,28,36	0.77	0	39,39,47	0.99	2 (5%)
39	CHL	SS	302	4	46,60,74	2.84	10 (21%)	40,97,114	1.73	11 (27%)
32	CLA	NN	612	9	46,50,73	1.38	5 (10%)	53,85,113	1.20	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CHL	Nn	315	9	42,56,74	2.91	9 (21%)	36,92,114	2.01	11 (30%)
36	LHG	33	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.11	2 (5%)
29	OEX	Cc	502	18,1	0,15,15	-	-	-		
37	SQD	B	602	-	45,47,54	1.20	3 (6%)	55,58,65	1.02	2 (3%)
32	CLA	b	609	-	69,73,73	1.14	7 (10%)	82,113,113	1.24	6 (7%)
32	CLA	2	602	14	44,48,73	1.45	5 (11%)	51,82,113	1.19	4 (7%)
32	CLA	BB	615	-	45,49,73	1.38	7 (15%)	54,84,113	1.33	7 (12%)
45	BCT	AA	413	30	3,3,3	1.13	0	2,3,3	4.18	2 (100%)
38	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.02	3 (5%)
32	CLA	R	610	36	53,57,73	1.32	6 (11%)	61,93,113	1.14	5 (8%)
39	CHL	y	303	9	60,74,74	2.49	11 (18%)	58,114,114	1.45	10 (17%)
36	LHG	D	410	-	33,33,48	1.12	2 (6%)	36,39,54	1.12	3 (8%)
40	LUT	Ss	615	-	42,43,43	1.00	2 (4%)	51,60,60	1.72	14 (27%)
36	LHG	Yy	618	32	48,48,48	0.92	2 (4%)	51,54,54	1.00	4 (7%)
32	CLA	SS	305	-	53,57,73	1.32	7 (13%)	61,93,113	1.23	4 (6%)
32	CLA	4	312	-	49,53,73	1.37	6 (12%)	58,89,113	1.22	3 (5%)
32	CLA	s	610	36	53,57,73	1.32	6 (11%)	61,93,113	1.25	3 (4%)
40	LUT	Yy	615	-	42,43,43	0.99	1 (2%)	51,60,60	2.12	13 (25%)
32	CLA	11	609	14	44,48,73	1.45	6 (13%)	51,82,113	1.23	4 (7%)
39	CHL	2	608	14	35,49,74	3.26	9 (25%)	30,83,114	1.77	7 (23%)
39	CHL	3	605	-	35,49,74	3.26	9 (25%)	30,83,114	1.92	9 (30%)
32	CLA	1	603	-	44,48,73	1.43	5 (11%)	51,82,113	1.20	3 (5%)
39	CHL	Yy	605	9	42,56,74	2.90	10 (23%)	36,92,114	1.79	10 (27%)
32	CLA	CC	512	18	69,73,73	1.15	7 (10%)	82,113,113	1.11	4 (4%)
32	CLA	22	613	-	44,48,73	1.44	5 (11%)	51,82,113	1.22	3 (5%)
39	CHL	s	601	4	46,60,74	2.84	9 (19%)	40,97,114	1.81	12 (30%)
32	CLA	R	602	3	69,73,73	1.15	8 (11%)	82,113,113	1.14	8 (9%)
36	LHG	3	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
32	CLA	Rr	609	3	69,73,73	1.15	8 (11%)	82,113,113	1.11	6 (7%)
32	CLA	SS	310	4	45,49,73	1.42	6 (13%)	54,84,113	1.19	4 (7%)
39	CHL	y	311	9	60,74,74	2.43	11 (18%)	58,114,114	1.54	10 (17%)
32	CLA	XX	201	-	45,49,73	1.40	6 (13%)	54,84,113	1.20	4 (7%)
34	BCR	Bb	618	-	41,41,41	0.91	1 (2%)	56,56,56	1.95	12 (21%)
34	BCR	CC	515	-	41,41,41	0.99	1 (2%)	56,56,56	2.04	18 (32%)
32	CLA	Cc	503	-	69,73,73	1.14	6 (8%)	82,113,113	1.21	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	LUT	n	616	-	42,43,43	1.00	0	51,60,60	1.53	9 (17%)
32	CLA	Y	612	9	69,73,73	1.18	6 (8%)	82,113,113	1.08	7 (8%)
32	CLA	S	612	4	53,57,73	1.32	5 (9%)	61,93,113	1.17	5 (8%)
32	CLA	b	604	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	5 (6%)
39	CHL	S	605	-	36,50,74	3.18	9 (25%)	29,85,114	2.06	13 (44%)
39	CHL	11	601	14	35,49,74	3.28	8 (22%)	30,83,114	1.72	8 (26%)
32	CLA	BB	610	-	69,73,73	1.14	7 (10%)	82,113,113	1.18	7 (8%)
39	CHL	Gg	302	9	60,74,74	2.51	10 (16%)	58,114,114	1.49	10 (17%)
32	CLA	Gg	315	-	53,57,73	1.30	6 (11%)	61,93,113	1.12	5 (8%)
37	SQD	C	501	-	52,54,54	1.10	3 (5%)	62,65,65	1.04	4 (6%)
32	CLA	YY	610	9	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
32	CLA	s	611	4	53,57,73	1.32	6 (11%)	61,93,113	1.25	6 (9%)
36	LHG	Y	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.86	2 (3%)
32	CLA	NN	604	-	45,49,73	1.39	5 (11%)	54,84,113	1.20	5 (9%)
43	LMU	C	502	-	28,28,36	0.76	0	39,39,47	0.97	1 (2%)
39	CHL	44	606	-	40,54,74	3.03	9 (22%)	34,90,114	1.82	9 (26%)
32	CLA	y	316	-	53,57,73	1.29	6 (11%)	61,93,113	1.19	4 (6%)
37	SQD	AA	412	-	33,35,54	1.38	3 (9%)	43,46,65	1.10	2 (4%)
34	BCR	C	517	-	41,41,41	0.95	1 (2%)	56,56,56	1.90	12 (21%)
39	CHL	2	605	-	35,49,74	3.29	8 (22%)	30,83,114	1.94	11 (36%)
39	CHL	44	608	11	40,54,74	3.05	8 (20%)	34,90,114	1.78	9 (26%)
39	CHL	11	606	-	35,49,74	3.29	8 (22%)	30,83,114	1.94	9 (30%)
39	CHL	n	607	-	60,74,74	2.39	8 (13%)	58,114,114	1.61	12 (20%)
40	LUT	Y	615	-	42,43,43	0.95	1 (2%)	51,60,60	1.87	13 (25%)
40	LUT	YY	615	-	42,43,43	0.96	1 (2%)	51,60,60	1.77	10 (19%)
39	CHL	RR	305	-	44,58,74	2.90	9 (20%)	37,94,114	1.84	12 (32%)
44	DGD	Hh	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.92	2 (2%)
35	PL9	AA	410	-	55,55,55	4.43	24 (43%)	68,69,69	3.67	37 (54%)
32	CLA	Yy	603	-	53,57,73	1.30	6 (11%)	61,93,113	1.27	5 (8%)
32	CLA	y	304	9	69,73,73	1.16	8 (11%)	82,113,113	1.08	4 (4%)
32	CLA	SS	304	-	49,53,73	1.38	5 (10%)	58,89,113	1.23	5 (8%)
34	BCR	BB	620	-	41,41,41	0.86	0	56,56,56	2.01	18 (32%)
39	CHL	S	607	-	37,51,74	3.18	8 (21%)	30,86,114	1.89	10 (33%)
34	BCR	CC	517	-	41,41,41	0.92	1 (2%)	56,56,56	2.02	15 (26%)
32	CLA	y	312	9	69,73,73	1.15	8 (11%)	82,113,113	1.01	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	DD	403	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	7 (8%)
32	CLA	C	508	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	7 (8%)
32	CLA	3	612	15	44,48,73	1.45	6 (13%)	51,82,113	1.21	3 (5%)
32	CLA	GG	603	-	69,73,73	1.15	5 (7%)	82,113,113	1.03	3 (3%)
36	LHG	Ll	102	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	3 (5%)
39	CHL	NN	607	-	60,74,74	2.43	11 (18%)	58,114,114	1.57	11 (18%)
32	CLA	B	618	-	69,73,73	1.15	7 (10%)	82,113,113	1.04	6 (7%)
38	LMG	WW	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.06	2 (3%)
32	CLA	N	604	-	45,49,73	1.39	6 (13%)	54,84,113	1.20	5 (9%)
44	DGD	BB	623	-	63,63,67	0.89	3 (4%)	77,77,81	0.94	2 (2%)
34	BCR	c	516	-	41,41,41	0.92	1 (2%)	56,56,56	2.04	15 (26%)
39	CHL	y	309	-	37,51,74	3.11	10 (27%)	30,86,114	2.00	11 (36%)
32	CLA	Cc	514	-	69,73,73	1.15	6 (8%)	82,113,113	1.12	4 (4%)
32	CLA	c	504	-	59,63,73	1.23	5 (8%)	70,101,113	1.11	4 (5%)
34	BCR	KK	103	-	41,41,41	0.84	0	56,56,56	2.21	19 (33%)
43	LMU	KK	102	-	28,28,36	0.75	0	39,39,47	0.90	1 (2%)
32	CLA	C	515	-	53,57,73	1.29	6 (11%)	61,93,113	1.22	5 (8%)
32	CLA	BB	606	-	69,73,73	1.15	6 (8%)	82,113,113	1.03	3 (3%)
39	CHL	Y	608	-	44,58,74	2.89	11 (25%)	37,94,114	1.84	10 (27%)
32	CLA	B	605	-	69,73,73	1.15	8 (11%)	82,113,113	1.24	8 (9%)
40	LUT	Ss	614	-	42,43,43	1.07	2 (4%)	51,60,60	1.50	11 (21%)
39	CHL	N	607	-	60,74,74	2.43	11 (18%)	58,114,114	1.56	11 (18%)
46	HEM	e	101	21,20	50,50,50	1.43	9 (18%)	67,82,82	1.08	3 (4%)
40	LUT	G	615	-	42,43,43	0.95	0	51,60,60	1.49	7 (13%)
39	CHL	YY	608	-	44,58,74	2.90	11 (25%)	37,94,114	1.84	10 (27%)
32	CLA	n	602	9	69,73,73	1.16	8 (11%)	82,113,113	1.19	9 (10%)
39	CHL	Gg	307	-	37,51,74	3.14	9 (24%)	30,86,114	2.00	9 (30%)
32	CLA	N	612	9	46,50,73	1.39	6 (13%)	53,85,113	1.18	4 (7%)
32	CLA	D	404	-	69,73,73	1.16	7 (10%)	82,113,113	1.17	6 (7%)
42	NEX	Gg	318	-	40,46,46	1.23	4 (10%)	50,70,70	2.23	14 (28%)
34	BCR	Cc	518	-	41,41,41	0.92	1 (2%)	56,56,56	1.92	13 (23%)
32	CLA	33	602	15	44,48,73	1.44	7 (15%)	51,82,113	1.27	4 (7%)
36	LHG	G	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
39	CHL	SS	308	4	43,57,74	2.97	8 (18%)	37,93,114	1.71	8 (21%)
35	PL9	D	407	-	55,55,55	4.35	20 (36%)	68,69,69	3.82	37 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	11	610	36	44,48,73	1.44	6 (13%)	51,82,113	1.27	4 (7%)
36	LHG	4	315	32	20,20,48	1.38	2 (10%)	23,26,54	1.44	2 (8%)
35	PL9	DD	406	-	55,55,55	4.36	21 (38%)	68,69,69	3.78	37 (54%)
39	CHL	22	607	-	35,49,74	3.28	8 (22%)	30,83,114	1.87	7 (23%)
39	CHL	N	605	9	36,50,74	3.17	9 (25%)	29,85,114	1.87	9 (31%)
32	CLA	G	612	9	53,57,73	1.33	7 (13%)	61,93,113	1.21	5 (8%)
32	CLA	g	610	9	53,57,73	1.32	7 (13%)	61,93,113	1.11	5 (8%)
40	LUT	Yy	616	-	42,43,43	0.93	0	51,60,60	1.57	11 (21%)
32	CLA	SS	311	-	53,57,73	1.32	6 (11%)	61,93,113	1.28	4 (6%)
32	CLA	Gg	313	9	53,57,73	1.32	6 (11%)	61,93,113	1.22	5 (8%)
39	CHL	SS	306	4	36,50,74	3.19	9 (25%)	29,85,114	2.13	11 (37%)
32	CLA	Y	611	36	46,50,73	1.37	6 (13%)	53,85,113	1.24	4 (7%)
39	CHL	G	605	9	37,51,74	3.18	8 (21%)	30,86,114	1.87	10 (33%)
39	CHL	22	605	-	35,49,74	3.30	8 (22%)	30,83,114	1.94	11 (36%)
32	CLA	Nn	313	-	53,57,73	1.30	5 (9%)	61,93,113	1.27	4 (6%)
32	CLA	4	311	36	49,53,73	1.37	6 (12%)	58,89,113	1.17	4 (6%)
34	BCR	A	409	-	41,41,41	1.00	3 (7%)	56,56,56	2.00	13 (23%)
39	CHL	Ss	607	-	43,57,74	2.98	9 (20%)	37,93,114	1.78	11 (29%)
32	CLA	r	603	-	53,57,73	1.33	7 (13%)	61,93,113	1.28	4 (6%)
32	CLA	44	604	-	49,53,73	1.35	7 (14%)	58,89,113	1.21	4 (6%)
40	LUT	22	614	-	42,43,43	1.08	4 (9%)	51,60,60	1.69	10 (19%)
40	LUT	SS	315	-	42,43,43	0.99	1 (2%)	51,60,60	1.29	8 (15%)
32	CLA	b	612	-	69,73,73	1.16	6 (8%)	82,113,113	1.17	5 (6%)
32	CLA	Yy	602	9	69,73,73	1.16	7 (10%)	82,113,113	1.10	4 (4%)
32	CLA	Bb	613	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	7 (8%)
39	CHL	Rr	606	-	44,58,74	2.94	10 (22%)	37,94,114	1.67	8 (21%)
32	CLA	Dd	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.13	4 (4%)
39	CHL	4	307	-	40,54,74	3.05	10 (25%)	34,90,114	1.83	9 (26%)
36	LHG	Gg	319	32	33,33,48	1.13	2 (6%)	36,39,54	1.19	3 (8%)
39	CHL	44	607	-	40,54,74	3.03	11 (27%)	34,90,114	1.83	10 (29%)
32	CLA	44	610	36	49,53,73	1.37	6 (12%)	58,89,113	1.16	3 (5%)
38	LMG	b	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.12	6 (13%)
39	CHL	Y	605	9	42,56,74	2.95	9 (21%)	36,92,114	1.81	11 (30%)
32	CLA	NN	603	-	46,50,73	1.36	6 (13%)	53,85,113	1.26	3 (5%)
36	LHG	44	614	32	20,20,48	1.33	2 (10%)	23,26,54	1.55	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	Aa	405	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	5 (6%)
36	LHG	22	615	32	33,33,48	1.14	2 (6%)	36,39,54	0.95	2 (5%)
29	OEX	a	401	18,1	0,15,15	-	-	-		
32	CLA	r	611	-	53,57,73	1.33	5 (9%)	61,93,113	1.13	4 (6%)
32	CLA	33	604	-	44,48,73	1.45	7 (15%)	51,82,113	1.29	4 (7%)
41	XAT	GG	617	-	41,47,47	1.10	3 (7%)	54,74,74	2.29	16 (29%)
38	LMG	F	101	-	46,46,55	0.98	2 (4%)	54,54,63	0.91	2 (3%)
36	LHG	a	414	-	36,36,48	1.07	2 (5%)	39,42,54	0.93	2 (5%)
32	CLA	Gg	312	36	69,73,73	1.15	7 (10%)	82,113,113	1.22	6 (7%)
39	CHL	3	601	15	35,49,74	3.27	8 (22%)	30,83,114	1.71	9 (30%)
32	CLA	Dd	402	-	69,73,73	1.15	7 (10%)	82,113,113	1.06	5 (6%)
34	BCR	c	514	-	41,41,41	0.93	2 (4%)	56,56,56	2.17	18 (32%)
34	BCR	d	403	-	41,41,41	0.89	0	56,56,56	2.05	18 (32%)
41	XAT	y	301	-	41,47,47	1.17	4 (9%)	54,74,74	2.42	17 (31%)
32	CLA	Cc	509	-	69,73,73	1.16	6 (8%)	82,113,113	1.19	5 (6%)
32	CLA	n	611	36	53,57,73	1.31	6 (11%)	61,93,113	1.24	4 (6%)
36	LHG	Dd	406	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
40	LUT	Y	616	-	42,43,43	1.00	0	51,60,60	1.58	11 (21%)
32	CLA	YY	613	9	63,67,73	1.20	6 (9%)	74,105,113	1.09	4 (5%)
40	LUT	Nn	306	-	42,43,43	0.98	1 (2%)	51,60,60	1.30	6 (11%)
32	CLA	33	611	15	44,48,73	1.44	6 (13%)	51,82,113	1.31	4 (7%)
32	CLA	A	405	-	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
32	CLA	a	405	-	69,73,73	1.17	7 (10%)	82,113,113	1.10	4 (4%)
32	CLA	g	614	-	53,57,73	1.31	7 (13%)	61,93,113	1.12	4 (6%)
32	CLA	s	604	-	53,57,73	1.32	6 (11%)	61,93,113	1.15	4 (6%)
32	CLA	Gg	305	-	46,50,73	1.39	7 (15%)	53,85,113	1.20	4 (7%)
32	CLA	Ss	609	4	53,57,73	1.30	7 (13%)	61,93,113	1.17	6 (9%)
32	CLA	R	614	3	53,57,73	1.36	5 (9%)	61,93,113	1.21	4 (6%)
41	XAT	G	617	-	41,47,47	1.12	3 (7%)	54,74,74	2.28	15 (27%)
32	CLA	r	601	3	53,57,73	1.33	6 (11%)	61,93,113	1.15	4 (6%)
39	CHL	Yy	608	-	44,58,74	2.84	11 (25%)	37,94,114	1.79	11 (29%)
34	BCR	h	101	-	41,41,41	1.03	3 (7%)	56,56,56	2.55	23 (41%)
34	BCR	Bb	617	-	41,41,41	1.05	2 (4%)	56,56,56	2.11	17 (30%)
32	CLA	GG	613	9	44,48,73	1.43	5 (11%)	51,82,113	1.45	5 (9%)
39	CHL	R	607	-	44,58,74	2.86	8 (18%)	37,94,114	1.87	11 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	Y	602	9	69,73,73	1.15	8 (11%)	82,113,113	1.08	6 (7%)
32	CLA	3	609	15	44,48,73	1.45	7 (15%)	51,82,113	1.32	5 (9%)
32	CLA	4	310	-	49,53,73	1.36	6 (12%)	58,89,113	1.18	3 (5%)
32	CLA	YY	612	9	62,66,73	1.21	4 (6%)	73,104,113	1.31	11 (15%)
32	CLA	N	613	9	53,57,73	1.30	7 (13%)	61,93,113	1.23	4 (6%)
33	PHO	D	402	-	58,69,69	2.15	10 (17%)	55,99,99	1.56	8 (14%)
32	CLA	44	615	3	53,57,73	1.32	7 (13%)	61,93,113	1.25	3 (4%)
34	BCR	B	613	-	41,41,41	0.98	3 (7%)	56,56,56	1.78	13 (23%)
34	BCR	D	406	-	41,41,41	0.85	0	56,56,56	1.95	16 (28%)
32	CLA	Rr	613	3	53,57,73	1.32	6 (11%)	61,93,113	1.21	4 (6%)
32	CLA	Ss	612	4	53,57,73	1.30	5 (9%)	61,93,113	1.16	4 (6%)
32	CLA	BB	614	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	8 (9%)
39	CHL	44	605	-	40,54,74	3.00	10 (25%)	34,90,114	1.94	11 (32%)
32	CLA	2	612	14	44,48,73	1.44	5 (11%)	51,82,113	1.25	4 (7%)
39	CHL	4	302	-	39,53,74	3.09	9 (23%)	33,89,114	1.79	8 (24%)
38	LMG	j	101	-	46,46,55	0.99	2 (4%)	54,54,63	1.05	4 (7%)
32	CLA	N	602	9	69,73,73	1.14	7 (10%)	82,113,113	1.15	6 (7%)
32	CLA	CC	514	-	53,57,73	1.29	6 (11%)	61,93,113	1.20	4 (6%)
32	CLA	Yy	610	9	69,73,73	1.15	8 (11%)	82,113,113	1.01	4 (4%)
32	CLA	Cc	513	18	69,73,73	1.16	5 (7%)	82,113,113	1.08	5 (6%)
40	LUT	y	318	-	42,43,43	0.92	0	51,60,60	1.55	13 (25%)
39	CHL	Nn	318	-	44,58,74	2.86	10 (22%)	37,94,114	1.75	10 (27%)
44	DGD	B	603	-	57,57,67	0.93	2 (3%)	70,70,81	0.94	4 (5%)
32	CLA	B	611	-	45,49,73	1.38	6 (13%)	54,84,113	1.31	6 (11%)
32	CLA	YY	603	-	53,57,73	1.30	6 (11%)	61,93,113	1.29	4 (6%)
32	CLA	S	602	4	53,57,73	1.29	6 (11%)	61,93,113	1.19	6 (9%)
34	BCR	B	612	-	41,41,41	0.97	1 (2%)	56,56,56	1.77	11 (19%)
32	CLA	BB	607	-	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
38	LMG	c	519	-	34,34,55	1.15	3 (8%)	42,42,63	1.21	6 (14%)
34	BCR	Hh	101	-	41,41,41	1.04	4 (9%)	56,56,56	2.46	23 (41%)
36	LHG	SS	301	-	25,25,48	1.30	2 (8%)	28,31,54	1.04	2 (7%)
39	CHL	YY	606	-	38,52,74	3.09	9 (23%)	31,87,114	1.93	8 (25%)
39	CHL	Yy	606	-	38,52,74	3.06	11 (28%)	31,87,114	2.04	10 (32%)
32	CLA	SS	314	-	53,57,73	1.31	7 (13%)	61,93,113	1.14	5 (8%)
32	CLA	AA	408	-	64,68,73	1.19	6 (9%)	76,107,113	1.12	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	R	601	3	53,57,73	1.33	6 (11%)	61,93,113	1.24	4 (6%)
32	CLA	RR	314	3	53,57,73	1.35	6 (11%)	61,93,113	1.22	5 (8%)
39	CHL	s	606	-	44,58,74	2.91	8 (18%)	37,94,114	1.71	11 (29%)
32	CLA	Bb	610	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	6 (7%)
32	CLA	BB	605	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	7 (8%)
32	CLA	2	603	-	44,48,73	1.45	7 (15%)	51,82,113	1.27	4 (7%)
32	CLA	CC	504	-	69,73,73	1.14	6 (8%)	82,113,113	1.08	5 (6%)
36	LHG	C	522	-	30,30,48	1.17	2 (6%)	33,36,54	1.08	2 (6%)
32	CLA	Cc	507	-	69,73,73	1.15	7 (10%)	82,113,113	1.05	4 (4%)
32	CLA	22	602	14	44,48,73	1.44	7 (15%)	51,82,113	1.22	4 (7%)
32	CLA	B	608	-	69,73,73	1.15	6 (8%)	82,113,113	1.06	4 (4%)
44	DGD	c	518	-	53,53,67	0.95	2 (3%)	67,67,81	0.89	2 (2%)
32	CLA	Ss	604	-	53,57,73	1.33	7 (13%)	61,93,113	1.16	4 (6%)
38	LMG	Aa	412	-	42,42,55	1.05	3 (7%)	50,50,63	1.10	4 (8%)
36	LHG	4	301	32	18,18,48	1.76	3 (16%)	17,22,54	1.50	1 (5%)
39	CHL	1	607	-	35,49,74	3.27	8 (22%)	30,83,114	1.92	10 (33%)
39	CHL	Rr	605	3	44,58,74	2.88	9 (20%)	37,94,114	1.86	9 (24%)
41	XAT	G	619	-	41,47,47	1.20	4 (9%)	54,74,74	2.55	13 (24%)
32	CLA	GG	611	36	56,60,73	1.28	7 (12%)	65,97,113	1.15	3 (4%)
36	LHG	CC	521	-	33,33,48	1.12	2 (6%)	36,39,54	1.05	2 (5%)
39	CHL	G	607	-	40,54,74	3.01	10 (25%)	34,90,114	1.92	10 (29%)
32	CLA	R	611	-	53,57,73	1.31	6 (11%)	61,93,113	1.19	3 (4%)
34	BCR	H	101	-	41,41,41	1.00	2 (4%)	56,56,56	2.19	20 (35%)
39	CHL	N	608	-	36,50,74	3.18	10 (27%)	29,85,114	1.95	9 (31%)
32	CLA	11	603	-	44,48,73	1.45	6 (13%)	51,82,113	1.20	3 (5%)
32	CLA	Nn	303	9	53,57,73	1.32	6 (11%)	61,93,113	1.25	5 (8%)
40	LUT	NN	616	-	42,43,43	0.94	1 (2%)	51,60,60	1.60	10 (19%)
32	CLA	Ss	611	4	53,57,73	1.32	6 (11%)	61,93,113	1.25	7 (11%)
32	CLA	1	612	14	44,48,73	1.45	6 (13%)	51,82,113	1.32	4 (7%)
39	CHL	1	605	14	35,49,74	3.24	7 (20%)	30,83,114	2.03	10 (33%)
32	CLA	g	604	42	46,50,73	1.41	5 (10%)	53,85,113	1.21	3 (5%)
39	CHL	G	608	-	36,50,74	3.22	8 (22%)	29,85,114	1.87	9 (31%)
32	CLA	2	613	-	44,48,73	1.43	6 (13%)	51,82,113	1.25	4 (7%)
32	CLA	C	505	-	69,73,73	1.14	6 (8%)	82,113,113	1.15	6 (7%)
32	CLA	c	506	-	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	Bb	608	-	69,73,73	1.13	6 (8%)	82,113,113	1.10	5 (6%)
37	SQD	LL	102	-	52,54,54	1.12	3 (5%)	62,65,65	1.07	3 (4%)
39	CHL	22	608	14	35,49,74	3.29	8 (22%)	30,83,114	1.78	6 (20%)
32	CLA	GG	610	9	53,57,73	1.31	7 (13%)	61,93,113	1.12	5 (8%)
39	CHL	RR	306	-	44,58,74	2.77	10 (22%)	37,94,114	1.71	11 (29%)
32	CLA	b	613	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	7 (8%)
36	LHG	DD	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.93	2 (3%)
32	CLA	CC	509	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	4 (4%)
32	CLA	BB	609	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	9 (10%)
39	CHL	3	606	-	35,49,74	3.27	9 (25%)	30,83,114	1.86	9 (30%)
32	CLA	DD	404	-	69,73,73	1.15	6 (8%)	82,113,113	1.06	3 (3%)
32	CLA	n	614	-	53,57,73	1.30	5 (9%)	61,93,113	1.13	4 (6%)
32	CLA	Yy	613	9	63,67,73	1.21	7 (11%)	74,105,113	1.16	3 (4%)
32	CLA	1	613	-	44,48,73	1.45	6 (13%)	51,82,113	1.22	4 (7%)
36	LHG	Dd	407	-	36,36,48	1.07	2 (5%)	39,42,54	0.92	2 (5%)
39	CHL	GG	606	-	37,51,74	3.10	8 (21%)	30,86,114	1.96	9 (30%)
45	BCT	Aa	414	30	3,3,3	1.14	0	2,3,3	3.97	2 (100%)
32	CLA	s	609	4	53,57,73	1.29	7 (13%)	61,93,113	1.20	6 (9%)
32	CLA	BB	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	4 (4%)
32	CLA	BB	602	-	69,73,73	1.15	6 (8%)	82,113,113	1.09	7 (8%)
34	BCR	BB	616	-	41,41,41	0.98	1 (2%)	56,56,56	1.91	14 (25%)
32	CLA	c	509	-	69,73,73	1.15	8 (11%)	82,113,113	1.06	5 (6%)
34	BCR	TT	101	-	41,41,41	0.97	1 (2%)	56,56,56	2.05	19 (33%)
39	CHL	Y	609	9	60,74,74	2.42	9 (15%)	58,114,114	1.49	11 (18%)
32	CLA	Cc	511	-	69,73,73	1.15	7 (10%)	82,113,113	1.07	5 (6%)
32	CLA	B	624	-	69,73,73	1.14	7 (10%)	82,113,113	1.15	7 (8%)
37	SQD	A	412	-	33,35,54	1.39	3 (9%)	43,46,65	1.09	3 (6%)
32	CLA	1	609	14	44,48,73	1.44	4 (9%)	51,82,113	1.32	5 (9%)
44	DGD	B	601	-	56,56,67	0.93	2 (3%)	70,70,81	0.98	4 (5%)
39	CHL	RR	307	-	44,58,74	2.86	9 (20%)	37,94,114	1.87	11 (29%)
32	CLA	r	613	3	53,57,73	1.31	7 (13%)	61,93,113	1.21	5 (8%)
32	CLA	Nn	305	-	53,57,73	1.30	5 (9%)	61,93,113	1.15	6 (9%)
32	CLA	Aa	407	-	53,57,73	1.31	8 (15%)	61,93,113	1.28	6 (9%)
32	CLA	22	612	14	44,48,73	1.44	6 (13%)	51,82,113	1.26	3 (5%)
39	CHL	g	601	9	60,74,74	2.49	10 (16%)	58,114,114	1.52	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	22	611	14	44,48,73	1.45	6 (13%)	51,82,113	1.31	4 (7%)
36	LHG	GG	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
32	CLA	R	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.30	6 (9%)
44	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.80	2 (2%)
32	CLA	4	303	11	49,53,73	1.36	5 (10%)	58,89,113	1.20	4 (6%)
32	CLA	s	612	4	53,57,73	1.30	6 (11%)	61,93,113	1.17	4 (6%)
39	CHL	s	605	-	44,58,74	2.89	8 (18%)	37,94,114	1.81	10 (27%)
32	CLA	B	607	-	69,73,73	1.17	8 (11%)	82,113,113	1.11	5 (6%)
32	CLA	RR	313	-	45,49,73	1.41	7 (15%)	54,84,113	1.24	6 (11%)
34	BCR	Dd	403	-	41,41,41	0.88	0	56,56,56	2.05	19 (33%)
39	CHL	G	606	-	37,51,74	3.15	8 (21%)	30,86,114	1.97	8 (26%)
32	CLA	Bb	606	-	69,73,73	1.14	6 (8%)	82,113,113	1.11	7 (8%)
37	SQD	CC	501	-	52,54,54	1.09	4 (7%)	62,65,65	1.19	4 (6%)
40	LUT	N	616	-	42,43,43	0.97	0	51,60,60	1.63	10 (19%)
32	CLA	CC	502	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	6 (7%)
39	CHL	g	606	-	37,51,74	3.14	10 (27%)	30,86,114	2.04	10 (33%)
44	DGD	Cc	520	-	53,53,67	0.96	2 (3%)	67,67,81	0.88	2 (2%)
32	CLA	a	407	-	53,57,73	1.31	7 (13%)	61,93,113	1.25	5 (8%)
34	BCR	b	617	-	41,41,41	1.01	2 (4%)	56,56,56	2.10	16 (28%)
40	LUT	y	317	-	42,43,43	0.97	1 (2%)	51,60,60	2.07	12 (23%)
32	CLA	b	601	-	69,73,73	1.17	8 (11%)	82,113,113	1.17	7 (8%)
32	CLA	Bb	616	-	69,73,73	1.15	7 (10%)	82,113,113	1.10	5 (6%)
38	LMG	Bb	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.96	2 (4%)
39	CHL	2	601	14	35,49,74	3.23	9 (25%)	30,83,114	1.89	10 (33%)
39	CHL	2	606	-	35,49,74	3.26	8 (22%)	30,83,114	1.88	10 (33%)
32	CLA	b	602	-	69,73,73	1.15	6 (8%)	82,113,113	1.08	6 (7%)
40	LUT	s	614	-	42,43,43	1.04	2 (4%)	51,60,60	1.52	10 (19%)
39	CHL	n	605	9	42,56,74	2.92	10 (23%)	36,92,114	1.78	10 (27%)
36	LHG	K	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.09	2 (5%)
32	CLA	CC	513	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	3 (3%)
39	CHL	n	609	9	44,58,74	2.84	11 (25%)	37,94,114	1.87	9 (24%)
39	CHL	4	306	-	40,54,74	2.96	9 (22%)	34,90,114	2.03	9 (26%)
39	CHL	SS	307	-	36,50,74	3.18	8 (22%)	29,85,114	1.97	10 (34%)
32	CLA	Y	613	9	63,67,73	1.20	5 (7%)	74,105,113	1.11	4 (5%)
32	CLA	C	511	-	69,73,73	1.17	8 (11%)	82,113,113	1.13	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CHL	NN	605	9	36,50,74	3.15	9 (25%)	29,85,114	2.03	9 (31%)
38	LMG	B	615	-	45,45,55	0.99	2 (4%)	53,53,63	0.93	2 (3%)
39	CHL	NN	609	9	44,58,74	2.83	11 (25%)	37,94,114	1.77	9 (24%)
39	CHL	Yy	601	9	60,74,74	2.50	11 (18%)	58,114,114	1.44	9 (15%)
32	CLA	y	314	9	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
38	LMG	Cc	501	-	34,34,55	1.15	3 (8%)	42,42,63	1.28	7 (16%)
32	CLA	Rr	602	3	69,73,73	1.17	8 (11%)	82,113,113	1.10	5 (6%)
32	CLA	AA	406	-	53,57,73	1.29	7 (13%)	61,93,113	1.21	6 (9%)
39	CHL	Gg	308	-	44,58,74	2.86	11 (25%)	37,94,114	1.78	10 (27%)
32	CLA	Bb	612	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	5 (6%)
32	CLA	Cc	505	-	69,73,73	1.16	7 (10%)	82,113,113	1.12	6 (7%)
32	CLA	NN	614	-	45,49,73	1.39	6 (13%)	54,84,113	1.19	4 (7%)
32	CLA	Yy	611	36	46,50,73	1.38	7 (15%)	53,85,113	1.28	4 (7%)
32	CLA	CC	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	7 (8%)
41	XAT	y	302	-	41,47,47	1.21	3 (7%)	54,74,74	2.45	17 (31%)
32	CLA	Nn	304	9	53,57,73	1.33	6 (11%)	61,93,113	1.19	4 (6%)
32	CLA	Rr	601	3	53,57,73	1.34	6 (11%)	61,93,113	1.15	4 (6%)
40	LUT	YY	616	-	42,43,43	0.95	0	51,60,60	1.46	9 (17%)
32	CLA	2	610	-	44,48,73	1.44	6 (13%)	51,82,113	1.34	5 (9%)
32	CLA	b	616	-	69,73,73	1.15	7 (10%)	82,113,113	1.09	5 (6%)
32	CLA	c	507	-	69,73,73	1.16	6 (8%)	82,113,113	1.20	5 (6%)
32	CLA	Bb	614	-	69,73,73	1.13	5 (7%)	82,113,113	1.09	3 (3%)
34	BCR	T	101	-	41,41,41	0.96	1 (2%)	56,56,56	2.07	19 (33%)
32	CLA	SS	313	4	53,57,73	1.31	5 (9%)	61,93,113	1.15	5 (8%)
32	CLA	X	201	-	45,49,73	1.41	7 (15%)	54,84,113	1.25	4 (7%)
38	LMG	AA	415	-	36,36,55	1.11	2 (5%)	44,44,63	1.15	3 (6%)
36	LHG	A	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.90	2 (4%)
39	CHL	33	601	15	35,49,74	3.26	8 (22%)	30,83,114	1.77	8 (26%)
32	CLA	CC	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.14	5 (6%)
39	CHL	R	605	-	44,58,74	2.89	10 (22%)	37,94,114	1.79	11 (29%)
32	CLA	s	603	-	53,57,73	1.32	5 (9%)	61,93,113	1.16	4 (6%)
40	LUT	RR	315	-	42,43,43	0.89	1 (2%)	51,60,60	1.60	15 (29%)
32	CLA	c	512	-	69,73,73	1.15	6 (8%)	82,113,113	1.10	4 (4%)
40	LUT	Nn	307	-	42,43,43	1.00	1 (2%)	51,60,60	1.55	8 (15%)
32	CLA	BB	608	-	69,73,73	1.16	7 (10%)	82,113,113	1.08	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	BCR	B	616	-	41,41,41	0.87	0	56,56,56	1.99	19 (33%)
36	LHG	44	616	32	18,18,48	1.76	3 (16%)	17,22,54	1.44	1 (5%)
39	CHL	Ss	605	-	44,58,74	2.88	8 (18%)	37,94,114	1.84	11 (29%)
42	NEX	RR	317	-	40,46,46	1.24	4 (10%)	50,70,70	1.93	13 (26%)
32	CLA	C	509	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
32	CLA	G	610	9	53,57,73	1.33	6 (11%)	61,93,113	1.37	6 (9%)
40	LUT	44	612	-	42,43,43	0.92	0	51,60,60	1.40	7 (13%)
32	CLA	r	609	3	69,73,73	1.15	6 (8%)	82,113,113	1.06	3 (3%)
32	CLA	c	513	-	47,51,73	1.36	7 (14%)	55,86,113	1.24	4 (7%)
36	LHG	A	413	-	36,36,48	1.07	2 (5%)	39,42,54	1.03	3 (7%)
39	CHL	Y	601	9	60,74,74	2.49	11 (18%)	58,114,114	1.50	9 (15%)
32	CLA	B	619	-	69,73,73	1.14	6 (8%)	82,113,113	1.09	6 (7%)
32	CLA	YY	614	-	53,57,73	1.30	7 (13%)	61,93,113	1.18	6 (9%)
39	CHL	YY	601	9	60,74,74	2.49	10 (16%)	58,114,114	1.54	9 (15%)
32	CLA	4	304	-	49,53,73	1.38	6 (12%)	58,89,113	1.37	5 (8%)
39	CHL	4	309	11	40,54,74	3.05	8 (20%)	34,90,114	1.72	8 (23%)
40	LUT	g	615	-	42,43,43	0.95	1 (2%)	51,60,60	1.49	7 (13%)
32	CLA	RR	309	3	69,73,73	1.16	7 (10%)	82,113,113	1.05	5 (6%)
44	DGD	C	523	-	53,53,67	0.94	2 (3%)	67,67,81	0.94	2 (2%)
41	XAT	GG	619	-	41,47,47	1.20	4 (9%)	54,74,74	2.55	12 (22%)
41	XAT	RR	316	-	41,47,47	1.08	2 (4%)	54,74,74	2.21	16 (29%)
32	CLA	DD	401	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
32	CLA	b	608	-	69,73,73	1.14	7 (10%)	82,113,113	1.10	5 (6%)
39	CHL	1	608	14	35,49,74	3.05	7 (20%)	30,83,114	1.79	9 (30%)
32	CLA	CC	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	6 (7%)
38	LMG	A	415	-	36,36,55	1.10	2 (5%)	44,44,63	1.13	3 (6%)
36	LHG	Ss	616	32	47,47,48	0.94	2 (4%)	50,53,54	0.90	2 (4%)
39	CHL	n	601	9	44,58,74	2.91	10 (22%)	37,94,114	1.78	11 (29%)
32	CLA	C	510	-	69,73,73	1.14	7 (10%)	82,113,113	1.15	4 (4%)
32	CLA	B	604	-	69,73,73	1.17	7 (10%)	82,113,113	1.08	4 (4%)
38	LMG	Dd	408	-	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)
42	NEX	NN	618	-	40,46,46	1.21	3 (7%)	50,70,70	2.08	14 (28%)
32	CLA	G	614	-	45,49,73	1.39	5 (11%)	54,84,113	1.14	3 (5%)
32	CLA	3	603	-	44,48,73	1.45	6 (13%)	51,82,113	1.24	4 (7%)
36	LHG	A	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.23	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	Gg	304	-	69,73,73	1.16	5 (7%)	82,113,113	1.03	4 (4%)
39	CHL	n	608	-	44,58,74	2.90	9 (20%)	37,94,114	1.80	10 (27%)

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
39	CHL	r	607	-	3/3/22/26	7/20/118/137	-
39	CHL	11	607	-	3/3/19/26	4/10/104/137	-
37	SQD	l	102	-	-	10/49/69/69	0/1/1/1
32	CLA	Ss	602	4	1/1/16/20	13/20/96/115	-
36	LHG	y	320	32	-	22/53/53/53	-
39	CHL	Gg	309	-	3/3/20/26	2/10/108/137	-
32	CLA	s	602	4	1/1/16/20	12/20/96/115	-
36	LHG	d	406	-	-	11/53/53/53	-
32	CLA	C	513	18	1/1/20/20	14/39/115/115	-
32	CLA	a	406	1	1/1/20/20	8/39/115/115	-
32	CLA	SS	309	4	1/1/14/20	6/10/86/115	-
39	CHL	NN	608	-	3/3/20/26	2/10/108/137	-
32	CLA	1	602	14	1/1/13/20	2/10/82/115	-
32	CLA	1	610	36	1/1/13/20	5/10/82/115	-
32	CLA	d	402	-	1/1/20/20	10/39/115/115	-
33	PHO	A	407	-	-	8/37/103/103	0/5/6/6
32	CLA	44	602	11	1/1/15/20	8/15/91/115	-
32	CLA	11	612	-	1/1/13/20	6/10/82/115	-
44	DGD	CC	518	-	-	10/44/84/95	0/2/2/2
36	LHG	D	408	-	-	12/47/47/53	-
32	CLA	b	606	-	1/1/20/20	9/39/115/115	-
39	CHL	1	606	-	3/3/19/26	2/10/104/137	-
42	NEX	Yy	617	-	-	3/27/83/83	0/3/3/3
32	CLA	Aa	406	1	1/1/20/20	9/39/115/115	-
32	CLA	3	613	-	1/1/13/20	6/10/82/115	-
42	NEX	R	617	-	-	2/27/83/83	0/3/3/3
44	DGD	CC	522	-	-	12/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	BB	622	-	-	8/38/38/53	-
32	CLA	C	507	-	1/1/20/20	11/39/115/115	-
43	LMU	RR	301	-	-	3/13/53/61	0/2/2/2
39	CHL	YY	607	-	3/3/20/26	2/12/110/137	-
33	PHO	a	409	-	-	15/37/103/103	0/5/6/6
41	XAT	Nn	308	-	-	1/31/93/93	0/4/4/4
32	CLA	2	611	14	1/1/13/20	5/10/82/115	-
36	LHG	NN	619	32	-	9/42/42/53	-
39	CHL	Ss	601	4	3/3/23/26	4/23/121/137	-
41	XAT	N	617	-	-	0/31/93/93	0/4/4/4
41	XAT	R	616	-	-	0/31/93/93	0/4/4/4
44	DGD	D	411	-	-	7/51/91/95	0/2/2/2
32	CLA	B	620	-	1/1/20/20	10/39/115/115	-
32	CLA	c	511	18	1/1/20/20	10/39/115/115	-
32	CLA	y	313	36	1/1/14/20	5/12/88/115	-
32	CLA	D	401	-	1/1/20/20	8/39/115/115	-
32	CLA	AA	405	-	1/1/20/20	14/39/115/115	-
39	CHL	N	601	9	3/3/20/26	5/13/111/137	-
40	LUT	Rr	614	-	-	2/29/67/67	0/2/2/2
44	DGD	Aa	401	-	-	9/44/84/95	0/2/2/2
36	LHG	11	614	32	-	16/38/38/53	-
44	DGD	C	520	-	-	4/51/91/95	0/2/2/2
42	NEX	Rr	616	-	-	3/27/83/83	0/3/3/3
32	CLA	RR	302	3	1/1/20/20	17/39/115/115	-
32	CLA	S	613	-	1/1/15/20	2/15/91/115	-
39	CHL	S	601	4	3/3/23/26	7/23/121/137	-
41	XAT	4	314	-	-	0/31/93/93	0/4/4/4
39	CHL	NN	601	9	3/3/20/26	3/13/111/137	-
39	CHL	g	609	9	3/3/20/26	5/12/110/137	-
41	XAT	r	615	-	-	1/31/93/93	0/4/4/4
32	CLA	3	602	15	1/1/13/20	4/10/82/115	-
39	CHL	Rr	607	-	3/3/22/26	7/20/118/137	-
32	CLA	GG	602	9	1/1/16/20	10/20/96/115	-
32	CLA	Bb	604	-	1/1/20/20	7/39/115/115	-
37	SQD	BB	621	-	-	5/31/51/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	S	603	-	1/1/15/20	8/15/91/115	-
32	CLA	R	609	3	1/1/20/20	11/39/115/115	-
41	XAT	44	613	-	-	0/31/93/93	0/4/4/4
32	CLA	g	602	9	-	9/20/96/115	-
32	CLA	B	622	-	1/1/20/20	17/39/115/115	-
40	LUT	GG	615	-	-	2/29/67/67	0/2/2/2
42	NEX	Y	617	-	-	2/27/83/83	0/3/3/3
32	CLA	g	603	-	1/1/20/20	14/39/115/115	-
32	CLA	Cc	512	-	1/1/20/20	12/39/115/115	-
39	CHL	Nn	319	9	3/3/22/26	4/20/118/137	-
32	CLA	N	611	36	1/1/16/20	10/20/96/115	-
32	CLA	Gg	311	9	1/1/16/20	8/20/96/115	-
32	CLA	Bb	611	-	1/1/20/20	7/39/115/115	-
34	BCR	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	b	614	-	1/1/20/20	6/39/115/115	-
39	CHL	3	608	15	3/3/19/26	2/10/104/137	-
42	NEX	N	618	-	-	2/27/83/83	0/3/3/3
39	CHL	Y	606	-	3/3/20/26	4/13/111/137	-
32	CLA	RR	312	3	1/1/14/20	1/12/88/115	-
32	CLA	Cc	508	-	1/1/20/20	18/39/115/115	-
32	CLA	YY	604	-	-	10/20/96/115	-
32	CLA	Y	604	-	-	11/20/96/115	-
39	CHL	Yy	609	9	3/3/26/26	13/39/137/137	-
34	BCR	b	619	-	-	4/29/63/63	0/2/2/2
32	CLA	R	608	3	1/1/16/20	9/20/96/115	-
32	CLA	N	610	9	1/1/20/20	15/39/115/115	-
39	CHL	YY	609	9	3/3/26/26	9/39/137/137	-
32	CLA	B	623	-	1/1/20/20	10/39/115/115	-
33	PHO	Aa	409	-	-	15/37/103/103	0/5/6/6
34	BCR	B	614	-	-	4/29/63/63	0/2/2/2
35	PL9	A	410	-	-	26/53/73/73	0/1/1/1
32	CLA	Cc	510	-	1/1/19/20	6/33/109/115	-
39	CHL	G	601	9	3/3/26/26	12/39/137/137	-
32	CLA	YY	611	36	1/1/14/20	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	n	617	-	-	3/27/83/83	0/3/3/3
32	CLA	D	405	-	1/1/20/20	8/39/115/115	-
40	LUT	g	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Rr	610	36	1/1/16/20	11/20/96/115	-
34	BCR	DD	405	-	-	2/29/63/63	0/2/2/2
32	CLA	c	502	-	1/1/20/20	9/39/115/115	-
32	CLA	r	604	-	1/1/16/20	15/20/96/115	-
42	NEX	y	319	-	-	3/27/83/83	0/3/3/3
32	CLA	3	610	36	1/1/13/20	5/10/82/115	-
32	CLA	y	315	9	1/1/18/20	9/32/108/115	-
39	CHL	S	606	-	3/3/20/26	0/10/108/137	-
32	CLA	BB	613	-	1/1/19/20	6/33/109/115	-
34	BCR	CC	516	-	-	5/29/63/63	0/2/2/2
32	CLA	44	611	-	1/1/15/20	9/15/91/115	-
32	CLA	Rr	608	3	1/1/16/20	13/20/96/115	-
34	BCR	C	516	-	-	6/29/63/63	0/2/2/2
34	BCR	b	618	-	-	4/29/63/63	0/2/2/2
32	CLA	r	610	36	1/1/16/20	9/20/96/115	-
32	CLA	C	504	-	-	11/39/115/115	-
37	SQD	LL	101	-	-	9/31/51/69	0/1/1/1
44	DGD	C	519	-	-	9/44/84/95	0/2/2/2
32	CLA	g	611	36	1/1/20/20	18/39/115/115	-
39	CHL	Nn	316	-	3/3/22/26	3/20/118/137	-
39	CHL	g	607	-	3/3/22/26	7/20/118/137	-
46	HEM	Ee	101	21,20	-	6/14/54/54	-
32	CLA	r	612	3	1/1/16/20	4/20/96/115	-
38	LMG	CC	520	-	-	3/34/54/70	0/1/1/1
34	BCR	C	518	-	-	2/29/63/63	0/2/2/2
32	CLA	r	602	3	1/1/20/20	13/39/115/115	-
39	CHL	Nn	311	9	3/3/22/26	5/20/118/137	-
32	CLA	b	605	-	1/1/20/20	11/39/115/115	-
41	XAT	Gg	301	-	-	1/31/93/93	0/4/4/4
42	NEX	Nn	309	-	-	2/27/83/83	0/3/3/3
32	CLA	22	604	-	1/1/13/20	4/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Nn	314	-	1/1/16/20	4/20/96/115	-
32	CLA	Gg	314	9	1/1/13/20	3/10/82/115	-
32	CLA	n	610	9	1/1/20/20	12/39/115/115	-
32	CLA	Cc	515	-	1/1/14/20	7/13/89/115	-
39	CHL	r	605	3	3/3/22/26	8/20/118/137	-
35	PL9	Dd	404	-	-	28/53/73/73	0/1/1/1
32	CLA	33	610	36	1/1/13/20	4/10/82/115	-
36	LHG	CC	523	-	-	10/41/41/53	-
32	CLA	2	609	14	1/1/13/20	6/10/82/115	-
32	CLA	CC	508	-	1/1/20/20	12/39/115/115	-
32	CLA	d	401	-	-	10/39/115/115	-
38	LMG	W	201	-	-	6/43/63/70	0/1/1/1
32	CLA	11	602	14	1/1/13/20	4/10/82/115	-
32	CLA	11	611	14	1/1/13/20	2/10/82/115	-
46	HEM	E	101	21,20	-	1/14/54/54	-
36	LHG	Nn	310	32	-	14/53/53/53	-
32	CLA	N	614	-	1/1/14/20	4/10/86/115	-
36	LHG	l	101	-	-	12/53/53/53	-
32	CLA	RR	310	36	1/1/16/20	11/20/96/115	-
40	LUT	r	614	-	-	2/29/67/67	0/2/2/2
32	CLA	Aa	410	-	1/1/19/20	10/33/109/115	-
40	LUT	NN	615	-	-	1/29/67/67	0/2/2/2
32	CLA	B	606	-	1/1/20/20	14/39/115/115	-
32	CLA	y	305	-	1/1/16/20	6/20/96/115	-
33	PHO	a	408	-	-	7/37/103/103	0/5/6/6
36	LHG	d	405	-	-	8/47/47/53	-
32	CLA	YY	602	9	1/1/20/20	14/39/115/115	-
44	DGD	a	415	-	-	9/44/84/95	0/2/2/2
32	CLA	Ss	613	-	1/1/16/20	7/20/96/115	-
32	CLA	r	608	3	1/1/16/20	10/20/96/115	-
32	CLA	RR	308	3	1/1/16/20	9/20/96/115	-
36	LHG	EE	101	-	-	7/44/44/53	-
39	CHL	N	606	-	3/3/20/26	0/10/108/137	-
39	CHL	11	608	14	3/3/19/26	2/10/104/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	33	608	15	3/3/19/26	2/10/104/137	-
38	LMG	DD	409	-	-	4/41/61/70	0/1/1/1
32	CLA	c	501	-	1/1/20/20	18/39/115/115	-
40	LUT	2	614	-	-	4/29/67/67	0/2/2/2
32	CLA	B	609	-	1/1/19/20	5/33/109/115	-
36	LHG	AA	414	-	-	9/49/49/53	-
32	CLA	44	603	-	1/1/15/20	11/15/91/115	-
32	CLA	BB	601	-	1/1/20/20	7/39/115/115	-
32	CLA	4	305	-	1/1/15/20	5/15/91/115	-
32	CLA	Cc	506	-	1/1/18/20	8/27/103/115	-
32	CLA	Nn	312	9	1/1/20/20	13/39/115/115	-
34	BCR	AA	409	-	-	5/29/63/63	0/2/2/2
32	CLA	n	603	-	1/1/16/20	9/20/96/115	-
44	DGD	CC	519	-	-	5/51/91/95	0/2/2/2
32	CLA	B	610	-	1/1/20/20	7/39/115/115	-
42	NEX	Y	619	-	-	3/27/83/83	0/3/3/3
32	CLA	C	503	-	1/1/20/20	11/39/115/115	-
32	CLA	Yy	614	-	1/1/16/20	10/20/96/115	-
37	SQD	B	617	-	-	5/31/51/69	0/1/1/1
32	CLA	11	604	-	1/1/13/20	2/10/82/115	-
41	XAT	Yy	619	-	-	3/31/93/93	0/4/4/4
32	CLA	Rr	604	-	1/1/16/20	12/20/96/115	-
39	CHL	Yy	607	-	3/3/20/26	4/12/110/137	-
44	DGD	c	517	-	-	5/44/84/95	0/2/2/2
39	CHL	22	606	-	3/3/19/26	4/10/104/137	-
39	CHL	33	605	-	3/3/19/26	2/10/104/137	-
39	CHL	y	307	9	3/3/21/26	6/18/116/137	-
32	CLA	c	505	-	1/1/20/20	10/39/115/115	-
32	CLA	33	609	15	1/1/13/20	2/10/82/115	-
32	CLA	22	609	14	1/1/13/20	6/10/82/115	-
32	CLA	2	604	-	1/1/13/20	4/10/82/115	-
40	LUT	S	614	-	-	1/29/67/67	0/2/2/2
39	CHL	44	601	-	3/3/21/26	2/13/111/137	-
36	LHG	J	101	-	-	10/30/30/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	XAT	NN	617	-	-	0/31/93/93	0/4/4/4
32	CLA	Bb	615	-	1/1/20/20	13/39/115/115	-
39	CHL	3	607	-	3/3/19/26	2/10/104/137	-
32	CLA	b	603	-	1/1/20/20	16/39/115/115	-
32	CLA	CC	511	-	1/1/20/20	8/39/115/115	-
39	CHL	YY	605	9	3/3/21/26	5/18/116/137	-
39	CHL	GG	607	-	3/3/21/26	4/15/113/137	-
36	LHG	D	409	-	-	5/53/53/53	-
40	LUT	s	615	-	-	2/29/67/67	0/2/2/2
39	CHL	33	607	-	3/3/19/26	2/10/104/137	-
32	CLA	GG	612	9	1/1/16/20	10/20/96/115	-
32	CLA	R	603	-	1/1/16/20	2/20/96/115	-
32	CLA	NN	613	9	1/1/16/20	10/20/96/115	-
32	CLA	n	613	9	1/1/16/20	8/20/96/115	-
32	CLA	Ss	603	-	1/1/16/20	12/20/96/115	-
32	CLA	Ss	610	36	1/1/16/20	9/20/96/115	-
32	CLA	Y	614	-	1/1/16/20	12/20/96/115	-
39	CHL	GG	605	9	3/3/20/26	2/12/110/137	-
32	CLA	SS	303	4	1/1/16/20	12/20/96/115	-
32	CLA	N	603	-	1/1/14/20	4/12/88/115	-
33	PHO	AA	407	-	-	6/37/103/103	0/5/6/6
32	CLA	S	611	4	1/1/16/20	9/20/96/115	-
39	CHL	Y	607	-	3/3/20/26	2/12/110/137	-
32	CLA	NN	602	9	1/1/20/20	13/39/115/115	-
32	CLA	Bb	607	-	1/1/20/20	13/39/115/115	-
32	CLA	Rr	611	-	1/1/16/20	11/20/96/115	-
34	BCR	c	515	-	-	5/29/63/63	0/2/2/2
32	CLA	S	610	-	1/1/16/20	9/20/96/115	-
32	CLA	Rr	603	-	1/1/16/20	7/20/96/115	-
32	CLA	G	603	-	1/1/20/20	13/39/115/115	-
32	CLA	SS	312	4	1/1/16/20	9/20/96/115	-
34	BCR	BB	618	-	-	4/29/63/63	0/2/2/2
39	CHL	y	310	-	3/3/22/26	4/20/118/137	-
35	PL9	d	404	-	-	29/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	s	616	32	-	7/52/52/53	-
32	CLA	c	503	-	1/1/20/20	9/39/115/115	-
42	NEX	g	617	32	-	3/27/83/83	0/3/3/3
37	SQD	Ll	101	-	-	9/49/69/69	0/1/1/1
32	CLA	Bb	605	-	1/1/20/20	12/39/115/115	-
32	CLA	Bb	603	-	1/1/20/20	17/39/115/115	-
39	CHL	11	605	14	3/3/19/26	4/10/104/137	-
32	CLA	BB	612	-	1/1/20/20	10/39/115/115	-
36	LHG	JJ	101	-	-	8/37/37/53	-
32	CLA	1	604	-	1/1/13/20	4/10/82/115	-
36	LHG	KK	101	-	-	8/38/38/53	-
39	CHL	y	308	-	3/3/20/26	2/13/111/137	-
39	CHL	1	601	14	3/3/19/26	2/10/104/137	-
32	CLA	22	610	36	1/1/14/20	7/12/88/115	-
32	CLA	CC	503	-	-	12/39/115/115	-
44	DGD	BB	624	-	-	9/44/84/95	0/2/2/2
32	CLA	C	512	-	1/1/20/20	10/39/115/115	-
40	LUT	Gg	316	-	-	1/29/67/67	0/2/2/2
41	XAT	Rr	615	-	-	3/31/93/93	0/4/4/4
32	CLA	1	611	14	1/1/13/20	2/10/82/115	-
32	CLA	n	604	-	1/1/16/20	6/20/96/115	-
36	LHG	N	619	32	-	9/42/42/53	-
39	CHL	GG	609	9	3/3/20/26	2/12/110/137	-
32	CLA	33	603	-	1/1/13/20	6/10/82/115	-
34	BCR	XX	202	-	-	6/29/63/63	0/2/2/2
32	CLA	S	608	4	1/1/14/20	6/10/86/115	-
32	CLA	Y	603	-	1/1/16/20	10/20/96/115	-
32	CLA	S	609	4	1/1/14/20	2/10/86/115	-
32	CLA	Y	610	9	1/1/20/20	17/39/115/115	-
36	LHG	DD	407	-	-	14/47/47/53	-
32	CLA	11	613	-	1/1/13/20	4/10/82/115	-
32	CLA	CC	506	-	1/1/20/20	14/39/115/115	-
32	CLA	A	408	-	1/1/19/20	7/33/109/115	-
36	LHG	Dd	405	-	-	8/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	N	609	9	3/3/22/26	4/20/118/137	-
32	CLA	Yy	612	9	1/1/20/20	10/39/115/115	-
32	CLA	RR	303	-	1/1/16/20	2/20/96/115	-
37	SQD	L	102	-	-	10/31/51/69	0/1/1/1
32	CLA	A	406	-	1/1/16/20	9/20/96/115	-
39	CHL	Gg	310	9	3/3/20/26	5/12/110/137	-
34	BCR	Kk	101	-	-	4/29/63/63	0/2/2/2
32	CLA	NN	611	36	1/1/16/20	12/20/96/115	-
40	LUT	Gg	317	-	-	1/29/67/67	0/2/2/2
39	CHL	G	609	9	3/3/20/26	2/12/110/137	-
32	CLA	Bb	609	-	1/1/20/20	14/39/115/115	-
32	CLA	Nn	302	36	1/1/16/20	5/20/96/115	-
32	CLA	g	612	9	1/1/16/20	12/20/96/115	-
39	CHL	g	605	9	3/3/20/26	6/12/110/137	-
32	CLA	Yy	604	-	1/1/16/20	10/20/96/115	-
32	CLA	Bb	602	-	1/1/20/20	9/39/115/115	-
32	CLA	c	508	-	1/1/19/20	7/33/109/115	-
39	CHL	2	607	-	3/3/19/26	2/10/104/137	-
39	CHL	r	606	-	3/3/22/26	4/20/118/137	-
32	CLA	R	613	-	1/1/14/20	6/10/86/115	-
39	CHL	Gg	306	9	3/3/20/26	6/12/110/137	-
38	LMG	a	412	-	-	10/37/57/70	0/1/1/1
36	LHG	YY	618	32	-	19/53/53/53	-
34	BCR	Bb	619	-	-	2/29/63/63	0/2/2/2
32	CLA	22	603	-	1/1/13/20	2/10/82/115	-
40	LUT	GG	616	-	-	2/29/67/67	0/2/2/2
39	CHL	n	606	-	3/3/22/26	2/20/118/137	-
32	CLA	b	607	-	1/1/20/20	13/39/115/115	-
36	LHG	r	616	32	-	13/53/53/53	-
39	CHL	33	606	-	3/3/19/26	2/10/104/137	-
44	DGD	BB	625	-	-	3/43/83/95	0/2/2/2
32	CLA	b	610	-	1/1/20/20	11/39/115/115	-
40	LUT	4	313	-	-	2/29/67/67	0/2/2/2
39	CHL	NN	606	-	3/3/20/26	2/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	YY	617	-	-	2/27/83/83	0/3/3/3
38	LMG	BB	619	-	-	10/40/60/70	0/1/1/1
32	CLA	R	612	3	1/1/14/20	3/12/88/115	-
32	CLA	G	613	9	1/1/13/20	5/10/82/115	-
32	CLA	Gg	303	9	-	11/20/96/115	-
34	BCR	Cc	516	-	-	4/29/63/63	0/2/2/2
32	CLA	y	306	-	1/1/16/20	8/20/96/115	-
36	LHG	n	618	32	-	11/53/53/53	-
32	CLA	Nn	301	9	1/1/20/20	11/39/115/115	-
32	CLA	44	609	11	1/1/15/20	6/15/91/115	-
32	CLA	Cc	504	-	-	12/39/115/115	-
34	BCR	Aa	411	-	-	4/29/63/63	0/2/2/2
44	DGD	Cc	519	-	-	9/44/84/95	0/2/2/2
39	CHL	4	308	-	3/3/21/26	6/15/113/137	-
32	CLA	G	602	9	1/1/16/20	9/20/96/115	-
40	LUT	n	615	-	-	1/29/67/67	0/2/2/2
36	LHG	II	101	-	-	10/38/38/53	-
32	CLA	b	615	-	1/1/20/20	13/39/115/115	-
34	BCR	a	411	-	-	4/29/63/63	0/2/2/2
32	CLA	S	604	-	1/1/16/20	8/20/96/115	-
36	LHG	1	614	32	-	7/34/34/53	-
32	CLA	BB	603	-	1/1/20/20	11/39/115/115	-
39	CHL	GG	601	9	3/3/26/26	10/39/137/137	-
32	CLA	n	612	9	1/1/16/20	8/20/96/115	-
32	CLA	RR	304	-	1/1/16/20	8/20/96/115	-
36	LHG	0	201	-	-	9/51/51/53	-
40	LUT	N	615	-	-	1/29/67/67	0/2/2/2
34	BCR	K	102	-	-	5/29/63/63	0/2/2/2
32	CLA	Rr	612	3	1/1/16/20	6/20/96/115	-
39	CHL	GG	608	-	3/3/20/26	4/10/108/137	-
39	CHL	R	606	-	3/3/22/26	10/20/118/137	-
38	LMG	Bb	621	-	-	8/31/51/70	0/1/1/1
32	CLA	s	608	4	1/1/16/20	8/20/96/115	-
32	CLA	C	514	-	1/1/20/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Ss	606	-	3/3/22/26	9/20/118/137	-
32	CLA	3	611	15	1/1/13/20	6/10/82/115	-
32	CLA	g	613	9	1/1/13/20	5/10/82/115	-
32	CLA	c	510	-	1/1/20/20	16/39/115/115	-
32	CLA	33	613	-	1/1/13/20	6/10/82/115	-
34	BCR	Cc	517	-	-	5/29/63/63	0/2/2/2
36	LHG	AA	411	-	-	13/38/38/53	-
38	LMG	m	101	-	-	14/46/66/70	0/1/1/1
41	XAT	g	619	-	-	1/31/93/93	0/4/4/4
32	CLA	RR	311	-	1/1/16/20	8/20/96/115	-
32	CLA	3	604	-	1/1/13/20	3/10/82/115	-
40	LUT	G	616	-	-	2/29/67/67	0/2/2/2
32	CLA	C	506	-	1/1/20/20	10/39/115/115	-
32	CLA	B	621	-	1/1/20/20	13/39/115/115	-
32	CLA	Ss	608	4	1/1/16/20	10/20/96/115	-
32	CLA	GG	604	-	1/1/14/20	4/12/88/115	-
32	CLA	G	604	-	1/1/14/20	7/12/88/115	-
32	CLA	b	611	-	1/1/20/20	7/39/115/115	-
40	LUT	R	615	-	-	0/29/67/67	0/2/2/2
32	CLA	Bb	601	-	1/1/20/20	15/39/115/115	-
33	PHO	Aa	408	-	-	7/37/103/103	0/5/6/6
46	HEM	EE	102	21,20	-	1/14/54/54	-
39	CHL	g	608	-	3/3/20/26	2/10/108/137	-
37	SQD	L	101	-	-	16/49/69/69	0/1/1/1
32	CLA	33	612	15	1/1/13/20	4/10/82/115	-
38	LMG	Mm	101	-	-	11/46/66/70	0/1/1/1
33	PHO	DD	402	-	-	10/37/103/103	0/5/6/6
39	CHL	s	607	-	3/3/22/26	5/19/117/137	-
32	CLA	G	611	36	1/1/17/20	11/24/100/115	-
32	CLA	NN	610	9	1/1/20/20	14/39/115/115	-
32	CLA	s	613	-	1/1/16/20	6/20/96/115	-
36	LHG	g	618	32	-	7/38/38/53	-
36	LHG	Rr	617	32	-	11/53/53/53	-
32	CLA	BB	604	-	1/1/20/20	13/39/115/115	-
39	CHL	Nn	317	-	3/3/26/26	12/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	GG	614	-	1/1/14/20	4/10/86/115	-
32	CLA	a	410	-	1/1/19/20	10/33/109/115	-
34	BCR	BB	617	-	-	4/29/63/63	0/2/2/2
37	SQD	Aa	413	-	-	10/42/62/69	0/1/1/1
39	CHL	22	601	14	3/3/19/26	2/10/104/137	-
38	LMG	b	620	-	-	4/31/51/70	0/1/1/1
43	LMU	R	618	-	-	5/13/53/61	0/2/2/2
39	CHL	SS	302	4	3/3/23/26	7/23/121/137	-
32	CLA	NN	612	9	1/1/14/20	3/12/88/115	-
39	CHL	Nn	315	9	3/3/21/26	6/18/116/137	-
36	LHG	33	614	32	-	10/38/38/53	-
37	SQD	B	602	-	-	10/42/62/69	0/1/1/1
32	CLA	b	609	-	1/1/20/20	17/39/115/115	-
32	CLA	2	602	14	1/1/13/20	6/10/82/115	-
32	CLA	BB	615	-	1/1/14/20	2/10/86/115	-
38	LMG	C	521	-	-	10/46/66/70	0/1/1/1
32	CLA	R	610	36	1/1/16/20	10/20/96/115	-
39	CHL	y	303	9	3/3/26/26	12/39/137/137	-
36	LHG	D	410	-	-	10/38/38/53	-
40	LUT	Ss	615	-	-	0/29/67/67	0/2/2/2
36	LHG	Yy	618	32	-	19/53/53/53	-
32	CLA	SS	305	-	1/1/16/20	8/20/96/115	-
32	CLA	4	312	-	1/1/15/20	9/15/91/115	-
32	CLA	s	610	36	1/1/16/20	9/20/96/115	-
40	LUT	Yy	615	-	-	2/29/67/67	0/2/2/2
32	CLA	11	609	14	1/1/13/20	4/10/82/115	-
39	CHL	2	608	14	3/3/19/26	2/10/104/137	-
39	CHL	3	605	-	3/3/19/26	4/10/104/137	-
32	CLA	1	603	-	1/1/13/20	6/10/82/115	-
39	CHL	Yy	605	9	3/3/21/26	7/18/116/137	-
32	CLA	CC	512	18	1/1/20/20	13/39/115/115	-
32	CLA	22	613	-	1/1/13/20	4/10/82/115	-
39	CHL	s	601	4	3/3/23/26	7/23/121/137	-
32	CLA	R	602	3	1/1/20/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	3	614	32	-	10/38/38/53	-
32	CLA	Rr	609	3	1/1/20/20	11/39/115/115	-
32	CLA	SS	310	4	1/1/14/20	2/10/86/115	-
39	CHL	y	311	9	3/3/26/26	14/39/137/137	-
32	CLA	XX	201	-	1/1/14/20	4/10/86/115	-
34	BCR	Bb	618	-	-	4/29/63/63	0/2/2/2
34	BCR	CC	515	-	-	6/29/63/63	0/2/2/2
32	CLA	Cc	503	-	1/1/20/20	17/39/115/115	-
40	LUT	n	616	-	-	3/29/67/67	0/2/2/2
32	CLA	Y	612	9	1/1/20/20	11/39/115/115	-
32	CLA	S	612	4	1/1/16/20	8/20/96/115	-
32	CLA	b	604	-	1/1/20/20	9/39/115/115	-
39	CHL	S	605	-	3/3/20/26	2/10/108/137	-
39	CHL	11	601	14	3/3/19/26	2/10/104/137	-
32	CLA	BB	610	-	1/1/20/20	13/39/115/115	-
39	CHL	Gg	302	9	3/3/26/26	10/39/137/137	-
32	CLA	Gg	315	-	1/1/16/20	10/20/96/115	-
37	SQD	C	501	-	-	16/49/69/69	0/1/1/1
32	CLA	YY	610	9	1/1/20/20	13/39/115/115	-
32	CLA	s	611	4	1/1/16/20	9/20/96/115	-
36	LHG	Y	618	32	-	18/53/53/53	-
32	CLA	NN	604	-	1/1/14/20	4/10/86/115	-
43	LMU	C	502	-	-	4/13/53/61	0/2/2/2
39	CHL	44	606	-	3/3/21/26	4/15/113/137	-
32	CLA	y	316	-	1/1/16/20	11/20/96/115	-
39	CHL	2	605	-	3/3/19/26	2/10/104/137	-
34	BCR	C	517	-	-	5/29/63/63	0/2/2/2
37	SQD	AA	412	-	-	8/30/50/69	0/1/1/1
39	CHL	44	608	11	3/3/21/26	4/15/113/137	-
39	CHL	11	606	-	3/3/19/26	2/10/104/137	-
39	CHL	n	607	-	3/3/26/26	15/39/137/137	-
40	LUT	Y	615	-	-	4/29/67/67	0/2/2/2
40	LUT	YY	615	-	-	4/29/67/67	0/2/2/2
39	CHL	RR	305	-	3/3/22/26	7/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGD	Hh	102	-	-	12/51/91/95	0/2/2/2
35	PL9	AA	410	-	-	28/53/73/73	0/1/1/1
32	CLA	Yy	603	-	1/1/16/20	6/20/96/115	-
32	CLA	y	304	9	1/1/20/20	12/39/115/115	-
32	CLA	SS	304	-	1/1/15/20	6/15/91/115	-
34	BCR	BB	620	-	-	5/29/63/63	0/2/2/2
39	CHL	S	607	-	3/3/20/26	0/12/110/137	-
34	BCR	CC	517	-	-	2/29/63/63	0/2/2/2
32	CLA	y	312	9	1/1/20/20	13/39/115/115	-
32	CLA	DD	403	-	1/1/20/20	10/39/115/115	-
32	CLA	C	508	-	1/1/20/20	10/39/115/115	-
32	CLA	3	612	15	1/1/13/20	4/10/82/115	-
32	CLA	GG	603	-	1/1/20/20	12/39/115/115	-
36	LHG	Ll	102	-	-	14/53/53/53	-
39	CHL	NN	607	-	3/3/26/26	9/39/137/137	-
32	CLA	B	618	-	1/1/20/20	9/39/115/115	-
38	LMG	WW	201	-	-	7/43/63/70	0/1/1/1
32	CLA	N	604	-	1/1/14/20	4/10/86/115	-
44	DGD	BB	623	-	-	9/51/91/95	0/2/2/2
34	BCR	c	516	-	-	4/29/63/63	0/2/2/2
39	CHL	y	309	-	3/3/20/26	2/12/110/137	-
32	CLA	Cc	514	-	1/1/20/20	9/39/115/115	-
32	CLA	c	504	-	1/1/18/20	7/27/103/115	-
34	BCR	KK	103	-	-	4/29/63/63	0/2/2/2
43	LMU	KK	102	-	-	5/13/53/61	0/2/2/2
32	CLA	C	515	-	1/1/16/20	6/20/96/115	-
32	CLA	BB	606	-	1/1/20/20	10/39/115/115	-
39	CHL	Y	608	-	3/3/22/26	6/20/118/137	-
32	CLA	B	605	-	-	15/39/115/115	-
40	LUT	Ss	614	-	-	2/29/67/67	0/2/2/2
39	CHL	N	607	-	3/3/26/26	10/39/137/137	-
46	HEM	e	101	21,20	-	3/14/54/54	-
40	LUT	G	615	-	-	2/29/67/67	0/2/2/2
39	CHL	YY	608	-	3/3/22/26	7/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	n	602	9	1/1/20/20	14/39/115/115	-
39	CHL	Gg	307	-	3/3/20/26	4/12/110/137	-
32	CLA	N	612	9	1/1/14/20	3/12/88/115	-
32	CLA	D	404	-	1/1/20/20	15/39/115/115	-
42	NEX	Gg	318	-	-	3/27/83/83	0/3/3/3
34	BCR	Cc	518	-	-	3/29/63/63	0/2/2/2
32	CLA	33	602	15	1/1/13/20	4/10/82/115	-
36	LHG	G	618	32	-	6/38/38/53	-
39	CHL	SS	308	4	3/3/22/26	3/19/117/137	-
35	PL9	D	407	-	-	29/53/73/73	0/1/1/1
32	CLA	11	610	36	1/1/13/20	4/10/82/115	-
39	CHL	22	607	-	3/3/19/26	2/10/104/137	-
35	PL9	DD	406	-	-	26/53/73/73	0/1/1/1
36	LHG	4	315	32	-	8/23/23/53	-
39	CHL	N	605	9	3/3/20/26	4/10/108/137	-
32	CLA	G	612	9	1/1/16/20	10/20/96/115	-
32	CLA	g	610	9	1/1/16/20	6/20/96/115	-
40	LUT	Yy	616	-	-	3/29/67/67	0/2/2/2
32	CLA	SS	311	-	1/1/16/20	7/20/96/115	-
32	CLA	Gg	313	9	1/1/16/20	14/20/96/115	-
39	CHL	SS	306	4	3/3/20/26	2/10/108/137	-
32	CLA	Y	611	36	1/1/14/20	5/12/88/115	-
39	CHL	G	605	9	3/3/20/26	2/12/110/137	-
39	CHL	22	605	-	3/3/19/26	2/10/104/137	-
32	CLA	Nn	313	-	1/1/16/20	10/20/96/115	-
32	CLA	4	311	36	1/1/15/20	5/15/91/115	-
39	CHL	Ss	607	-	3/3/22/26	5/19/117/137	-
34	BCR	A	409	-	-	5/29/63/63	0/2/2/2
32	CLA	r	603	-	1/1/16/20	8/20/96/115	-
32	CLA	44	604	-	1/1/15/20	7/15/91/115	-
40	LUT	22	614	-	-	4/29/67/67	0/2/2/2
40	LUT	SS	315	-	-	2/29/67/67	0/2/2/2
32	CLA	b	612	-	1/1/20/20	14/39/115/115	-
32	CLA	Yy	602	9	1/1/20/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Bb	613	-	1/1/20/20	14/39/115/115	-
39	CHL	Rr	606	-	3/3/22/26	5/20/118/137	-
39	CHL	4	307	-	3/3/21/26	4/15/113/137	-
32	CLA	Dd	401	-	-	13/39/115/115	-
36	LHG	Gg	319	32	-	6/38/38/53	-
39	CHL	44	607	-	3/3/21/26	6/15/113/137	-
32	CLA	44	610	36	1/1/15/20	8/15/91/115	-
38	LMG	b	621	-	-	9/31/51/70	0/1/1/1
39	CHL	Y	605	9	3/3/21/26	5/18/116/137	-
32	CLA	NN	603	-	1/1/14/20	4/12/88/115	-
36	LHG	44	614	32	-	8/23/23/53	-
32	CLA	Aa	405	-	1/1/20/20	10/39/115/115	-
36	LHG	22	615	32	-	8/38/38/53	-
32	CLA	r	611	-	1/1/16/20	13/20/96/115	-
32	CLA	33	604	-	1/1/13/20	4/10/82/115	-
41	XAT	GG	617	-	-	2/31/93/93	0/4/4/4
38	LMG	F	101	-	-	3/41/61/70	0/1/1/1
36	LHG	a	414	-	-	3/41/41/53	-
32	CLA	Gg	312	36	1/1/20/20	17/39/115/115	-
39	CHL	3	601	15	3/3/19/26	4/10/104/137	-
32	CLA	Dd	402	-	1/1/20/20	13/39/115/115	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
34	BCR	d	403	-	-	4/29/63/63	0/2/2/2
41	XAT	y	301	-	-	3/31/93/93	0/4/4/4
32	CLA	Cc	509	-	1/1/20/20	12/39/115/115	-
32	CLA	n	611	36	1/1/16/20	7/20/96/115	-
36	LHG	Dd	406	-	-	10/53/53/53	-
40	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
32	CLA	YY	613	9	1/1/18/20	7/32/108/115	-
40	LUT	Nn	306	-	-	1/29/67/67	0/2/2/2
32	CLA	33	611	15	1/1/13/20	6/10/82/115	-
32	CLA	A	405	-	1/1/20/20	13/39/115/115	-
32	CLA	a	405	-	1/1/20/20	13/39/115/115	-
32	CLA	g	614	-	1/1/16/20	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	s	604	-	1/1/16/20	10/20/96/115	-
32	CLA	Gg	305	-	1/1/14/20	5/12/88/115	-
32	CLA	Ss	609	4	1/1/16/20	10/20/96/115	-
32	CLA	R	614	3	-	6/20/96/115	-
41	XAT	G	617	-	-	2/31/93/93	0/4/4/4
32	CLA	r	601	3	1/1/16/20	13/20/96/115	-
39	CHL	Yy	608	-	3/3/22/26	4/20/118/137	-
34	BCR	h	101	-	-	7/29/63/63	0/2/2/2
34	BCR	Bb	617	-	-	5/29/63/63	0/2/2/2
32	CLA	GG	613	9	1/1/13/20	5/10/82/115	-
39	CHL	R	607	-	3/3/22/26	6/20/118/137	-
32	CLA	Y	602	9	1/1/20/20	15/39/115/115	-
32	CLA	3	609	15	1/1/13/20	3/10/82/115	-
32	CLA	4	310	-	1/1/15/20	6/15/91/115	-
32	CLA	YY	612	9	1/1/18/20	10/31/107/115	-
32	CLA	N	613	9	1/1/16/20	9/20/96/115	-
33	PHO	D	402	-	-	9/37/103/103	0/5/6/6
32	CLA	44	615	3	1/1/16/20	10/20/96/115	-
34	BCR	B	613	-	-	4/29/63/63	0/2/2/2
34	BCR	D	406	-	-	2/29/63/63	0/2/2/2
32	CLA	Rr	613	3	1/1/16/20	8/20/96/115	-
32	CLA	Ss	612	4	1/1/16/20	7/20/96/115	-
32	CLA	BB	614	-	1/1/20/20	7/39/115/115	-
39	CHL	44	605	-	3/3/21/26	4/15/113/137	-
32	CLA	2	612	14	1/1/13/20	4/10/82/115	-
39	CHL	4	302	-	3/3/21/26	2/13/111/137	-
38	LMG	j	101	-	-	3/41/61/70	0/1/1/1
32	CLA	N	602	9	1/1/20/20	13/39/115/115	-
32	CLA	CC	514	-	1/1/16/20	6/20/96/115	-
32	CLA	Yy	610	9	1/1/20/20	12/39/115/115	-
32	CLA	Cc	513	18	1/1/20/20	8/39/115/115	-
40	LUT	y	318	-	-	2/29/67/67	0/2/2/2
39	CHL	Nn	318	-	3/3/22/26	6/20/118/137	-
44	DGD	B	603	-	-	6/43/83/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	B	611	-	1/1/14/20	2/10/86/115	-
32	CLA	YY	603	-	1/1/16/20	8/20/96/115	-
32	CLA	S	602	4	1/1/16/20	10/20/96/115	-
34	BCR	B	612	-	-	4/29/63/63	0/2/2/2
32	CLA	BB	607	-	1/1/20/20	11/39/115/115	-
38	LMG	c	519	-	-	7/29/49/70	0/1/1/1
34	BCR	Hh	101	-	-	9/29/63/63	0/2/2/2
39	CHL	YY	606	-	3/3/20/26	4/13/111/137	-
36	LHG	SS	301	-	-	4/30/30/53	-
39	CHL	Yy	606	-	3/3/20/26	2/13/111/137	-
32	CLA	SS	314	-	1/1/16/20	5/20/96/115	-
32	CLA	AA	408	-	1/1/19/20	6/33/109/115	-
32	CLA	R	601	3	1/1/16/20	7/20/96/115	-
32	CLA	RR	314	3	-	9/20/96/115	-
39	CHL	s	606	-	3/3/22/26	9/20/118/137	-
32	CLA	Bb	610	-	1/1/20/20	16/39/115/115	-
32	CLA	BB	605	-	1/1/20/20	14/39/115/115	-
32	CLA	2	603	-	1/1/13/20	4/10/82/115	-
32	CLA	CC	504	-	1/1/20/20	15/39/115/115	-
36	LHG	C	522	-	-	9/35/35/53	-
32	CLA	Cc	507	-	1/1/20/20	10/39/115/115	-
32	CLA	22	602	14	1/1/13/20	4/10/82/115	-
32	CLA	B	608	-	1/1/20/20	11/39/115/115	-
44	DGD	c	518	-	-	8/41/81/95	0/2/2/2
32	CLA	Ss	604	-	1/1/16/20	10/20/96/115	-
38	LMG	Aa	412	-	-	7/37/57/70	0/1/1/1
36	LHG	4	301	32	-	6/21/21/53	-
39	CHL	1	607	-	3/3/19/26	4/10/104/137	-
39	CHL	Rr	605	3	3/3/22/26	7/20/118/137	-
41	XAT	G	619	-	-	1/31/93/93	0/4/4/4
32	CLA	GG	611	36	1/1/17/20	9/24/100/115	-
36	LHG	CC	521	-	-	7/38/38/53	-
39	CHL	G	607	-	3/3/21/26	4/15/113/137	-
32	CLA	R	611	-	1/1/16/20	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	N	608	-	3/3/20/26	2/10/108/137	-
34	BCR	H	101	-	-	3/29/63/63	0/2/2/2
32	CLA	11	603	-	1/1/13/20	4/10/82/115	-
32	CLA	Nn	303	9	1/1/16/20	5/20/96/115	-
40	LUT	NN	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Ss	611	4	1/1/16/20	9/20/96/115	-
32	CLA	1	612	14	1/1/13/20	0/10/82/115	-
39	CHL	1	605	14	3/3/19/26	2/10/104/137	-
32	CLA	g	604	42	1/1/14/20	5/12/88/115	-
39	CHL	G	608	-	3/3/20/26	5/10/108/137	-
32	CLA	2	613	-	1/1/13/20	4/10/82/115	-
32	CLA	C	505	-	1/1/20/20	17/39/115/115	-
32	CLA	c	506	-	1/1/20/20	18/39/115/115	-
32	CLA	Bb	608	-	1/1/20/20	12/39/115/115	-
39	CHL	22	608	14	3/3/19/26	2/10/104/137	-
37	SQD	LL	102	-	-	16/49/69/69	0/1/1/1
32	CLA	GG	610	9	1/1/16/20	6/20/96/115	-
39	CHL	RR	306	-	3/3/21/26	9/20/118/137	-
32	CLA	b	613	-	1/1/20/20	14/39/115/115	-
36	LHG	DD	408	-	-	8/53/53/53	-
32	CLA	CC	509	-	1/1/20/20	11/39/115/115	-
32	CLA	BB	609	-	-	12/39/115/115	-
39	CHL	3	606	-	3/3/19/26	2/10/104/137	-
32	CLA	DD	404	-	1/1/20/20	10/39/115/115	-
32	CLA	n	614	-	1/1/16/20	8/20/96/115	-
32	CLA	Yy	613	9	1/1/18/20	7/32/108/115	-
32	CLA	1	613	-	1/1/13/20	6/10/82/115	-
36	LHG	Dd	407	-	-	3/41/41/53	-
39	CHL	GG	606	-	3/3/20/26	4/12/110/137	-
32	CLA	s	609	4	1/1/16/20	10/20/96/115	-
32	CLA	BB	611	-	1/1/20/20	5/39/115/115	-
32	CLA	BB	602	-	1/1/20/20	17/39/115/115	-
34	BCR	BB	616	-	-	4/29/63/63	0/2/2/2
32	CLA	c	509	-	1/1/20/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Y	609	9	3/3/26/26	10/39/137/137	-
34	BCR	TT	101	-	-	5/29/63/63	0/2/2/2
32	CLA	Cc	511	-	1/1/20/20	15/39/115/115	-
32	CLA	B	624	-	1/1/20/20	11/39/115/115	-
37	SQD	A	412	-	-	6/30/50/69	0/1/1/1
32	CLA	1	609	14	1/1/13/20	4/10/82/115	-
44	DGD	B	601	-	-	7/44/84/95	0/2/2/2
39	CHL	RR	307	-	3/3/22/26	6/20/118/137	-
32	CLA	r	613	3	1/1/16/20	9/20/96/115	-
32	CLA	Nn	305	-	-	9/20/96/115	-
32	CLA	Aa	407	-	1/1/16/20	8/20/96/115	-
32	CLA	22	612	14	1/1/13/20	2/10/82/115	-
39	CHL	g	601	9	3/3/26/26	11/39/137/137	-
32	CLA	22	611	14	1/1/13/20	6/10/82/115	-
36	LHG	GG	618	32	-	6/38/38/53	-
32	CLA	R	604	-	1/1/16/20	8/20/96/115	-
44	DGD	h	102	-	-	8/51/91/95	0/2/2/2
32	CLA	4	303	11	1/1/15/20	8/15/91/115	-
32	CLA	s	612	4	1/1/16/20	7/20/96/115	-
39	CHL	s	605	-	3/3/22/26	9/20/118/137	-
32	CLA	B	607	-	1/1/20/20	7/39/115/115	-
32	CLA	RR	313	-	1/1/14/20	4/10/86/115	-
34	BCR	Dd	403	-	-	4/29/63/63	0/2/2/2
39	CHL	G	606	-	3/3/20/26	4/12/110/137	-
32	CLA	Bb	606	-	1/1/20/20	8/39/115/115	-
37	SQD	CC	501	-	-	13/49/69/69	0/1/1/1
40	LUT	N	616	-	-	2/29/67/67	0/2/2/2
32	CLA	CC	502	-	1/1/20/20	12/39/115/115	-
39	CHL	g	606	-	3/3/20/26	4/12/110/137	-
44	DGD	Cc	520	-	-	9/41/81/95	0/2/2/2
32	CLA	a	407	-	1/1/16/20	6/20/96/115	-
34	BCR	b	617	-	-	4/29/63/63	0/2/2/2
40	LUT	y	317	-	-	3/29/67/67	0/2/2/2
32	CLA	b	601	-	1/1/20/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Bb	616	-	1/1/20/20	12/39/115/115	-
39	CHL	2	601	14	3/3/19/26	2/10/104/137	-
38	LMG	Bb	620	-	-	4/31/51/70	0/1/1/1
39	CHL	2	606	-	3/3/19/26	4/10/104/137	-
32	CLA	b	602	-	1/1/20/20	11/39/115/115	-
40	LUT	s	614	-	-	2/29/67/67	0/2/2/2
39	CHL	n	605	9	3/3/21/26	6/18/116/137	-
36	LHG	K	101	-	-	11/38/38/53	-
32	CLA	CC	513	-	1/1/20/20	9/39/115/115	-
39	CHL	n	609	9	3/3/22/26	4/20/118/137	-
39	CHL	4	306	-	3/3/21/26	4/15/113/137	-
39	CHL	SS	307	-	3/3/20/26	0/10/108/137	-
32	CLA	Y	613	9	1/1/18/20	11/32/108/115	-
32	CLA	C	511	-	1/1/20/20	14/39/115/115	-
39	CHL	NN	605	9	3/3/20/26	4/10/108/137	-
38	LMG	B	615	-	-	8/40/60/70	0/1/1/1
39	CHL	NN	609	9	3/3/22/26	4/20/118/137	-
39	CHL	Yy	601	9	3/3/26/26	12/39/137/137	-
32	CLA	y	314	9	1/1/20/20	12/39/115/115	-
38	LMG	Cc	501	-	-	7/29/49/70	0/1/1/1
32	CLA	Rr	602	3	1/1/20/20	12/39/115/115	-
32	CLA	AA	406	-	1/1/16/20	9/20/96/115	-
39	CHL	Gg	308	-	3/3/22/26	8/20/118/137	-
32	CLA	Bb	612	-	1/1/20/20	15/39/115/115	-
32	CLA	Cc	505	-	1/1/20/20	11/39/115/115	-
32	CLA	Yy	611	36	1/1/14/20	5/12/88/115	-
32	CLA	NN	614	-	1/1/14/20	4/10/86/115	-
32	CLA	CC	507	-	1/1/20/20	10/39/115/115	-
41	XAT	y	302	-	-	1/31/93/93	0/4/4/4
32	CLA	Nn	304	9	1/1/16/20	7/20/96/115	-
32	CLA	Rr	601	3	1/1/16/20	13/20/96/115	-
40	LUT	YY	616	-	-	2/29/67/67	0/2/2/2
32	CLA	2	610	-	1/1/13/20	4/10/82/115	-
32	CLA	b	616	-	1/1/20/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	c	507	-	1/1/20/20	10/39/115/115	-
32	CLA	Bb	614	-	1/1/20/20	7/39/115/115	-
34	BCR	T	101	-	-	3/29/63/63	0/2/2/2
32	CLA	SS	313	4	1/1/16/20	8/20/96/115	-
32	CLA	X	201	-	1/1/14/20	4/10/86/115	-
39	CHL	33	601	15	3/3/19/26	4/10/104/137	-
36	LHG	A	414	-	-	9/49/49/53	-
38	LMG	AA	415	-	-	4/31/51/70	0/1/1/1
32	CLA	CC	510	-	1/1/20/20	14/39/115/115	-
39	CHL	R	605	-	3/3/22/26	7/20/118/137	-
32	CLA	s	603	-	1/1/16/20	12/20/96/115	-
40	LUT	RR	315	-	-	2/29/67/67	0/2/2/2
32	CLA	c	512	-	1/1/20/20	8/39/115/115	-
40	LUT	Nn	307	-	-	2/29/67/67	0/2/2/2
32	CLA	BB	608	-	1/1/20/20	11/39/115/115	-
34	BCR	B	616	-	-	4/29/63/63	0/2/2/2
36	LHG	44	616	32	-	7/21/21/53	-
39	CHL	Ss	605	-	3/3/22/26	11/20/118/137	-
42	NEX	RR	317	-	-	3/27/83/83	0/3/3/3
32	CLA	C	509	-	1/1/20/20	12/39/115/115	-
32	CLA	G	610	9	1/1/16/20	9/20/96/115	-
40	LUT	44	612	-	-	2/29/67/67	0/2/2/2
32	CLA	r	609	3	1/1/20/20	11/39/115/115	-
32	CLA	c	513	-	1/1/14/20	9/13/89/115	-
36	LHG	A	413	-	-	11/41/41/53	-
39	CHL	Y	601	9	3/3/26/26	12/39/137/137	-
32	CLA	B	619	-	1/1/20/20	18/39/115/115	-
32	CLA	YY	614	-	1/1/16/20	12/20/96/115	-
39	CHL	YY	601	9	3/3/26/26	13/39/137/137	-
32	CLA	4	304	-	1/1/15/20	8/15/91/115	-
39	CHL	4	309	11	3/3/21/26	6/15/113/137	-
40	LUT	g	615	-	-	1/29/67/67	0/2/2/2
32	CLA	RR	309	3	1/1/20/20	11/39/115/115	-
44	DGD	C	523	-	-	9/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	XAT	GG	619	-	-	1/31/93/93	0/4/4/4
41	XAT	RR	316	-	-	0/31/93/93	0/4/4/4
32	CLA	DD	401	-	1/1/20/20	8/39/115/115	-
32	CLA	b	608	-	1/1/20/20	10/39/115/115	-
39	CHL	1	608	14	3/3/19/26	2/10/104/137	-
32	CLA	CC	505	-	1/1/20/20	9/39/115/115	-
38	LMG	A	415	-	-	4/31/51/70	0/1/1/1
36	LHG	Ss	616	32	-	7/52/52/53	-
39	CHL	n	601	9	3/3/22/26	5/20/118/137	-
32	CLA	C	510	-	1/1/20/20	10/39/115/115	-
32	CLA	B	604	-	1/1/20/20	10/39/115/115	-
38	LMG	Dd	408	-	-	5/41/61/70	0/1/1/1
42	NEX	NN	618	-	-	2/27/83/83	0/3/3/3
32	CLA	G	614	-	1/1/14/20	4/10/86/115	-
32	CLA	3	603	-	1/1/13/20	6/10/82/115	-
36	LHG	A	411	-	-	11/38/38/53	-
32	CLA	Gg	304	-	1/1/20/20	13/39/115/115	-
39	CHL	n	608	-	3/3/22/26	7/20/118/137	-

All (4369) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	r	606	CHL	C3B-C4B	11.64	1.52	1.41
39	22	605	CHL	C3B-C4B	11.60	1.52	1.41
39	33	607	CHL	C3B-C4B	11.54	1.52	1.41
39	22	606	CHL	C3B-C4B	11.51	1.52	1.41
39	Rr	605	CHL	C3B-C4B	11.50	1.52	1.41
39	2	605	CHL	C3B-C4B	11.50	1.52	1.41
39	3	607	CHL	C3B-C4B	11.48	1.52	1.41
39	2	606	CHL	C3B-C4B	11.48	1.52	1.41
39	11	607	CHL	C3B-C4B	11.47	1.52	1.41
39	Ss	606	CHL	C3B-C4B	11.45	1.52	1.41
39	1	607	CHL	C3B-C4B	11.43	1.52	1.41
39	SS	306	CHL	C3B-C4B	11.43	1.52	1.41
39	s	606	CHL	C3B-C4B	11.42	1.52	1.41
39	4	309	CHL	C3B-C4B	11.40	1.52	1.41
39	s	605	CHL	C3B-C4B	11.39	1.52	1.41
39	33	608	CHL	C3B-C4B	11.37	1.52	1.41
39	Ss	605	CHL	C3B-C4B	11.34	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	r	607	CHL	C3B-C4B	11.34	1.52	1.41
39	s	601	CHL	C3B-C4B	11.29	1.52	1.41
39	NN	605	CHL	C3B-C4B	11.27	1.52	1.41
39	N	605	CHL	C3B-C4B	11.27	1.52	1.41
39	Y	607	CHL	C3B-C4B	11.23	1.52	1.41
39	S	605	CHL	C3B-C4B	11.22	1.52	1.41
39	Rr	607	CHL	C3B-C4B	11.22	1.52	1.41
39	YY	607	CHL	C3B-C4B	11.20	1.52	1.41
39	44	608	CHL	C3B-C4B	11.19	1.52	1.41
39	Yy	609	CHL	C3B-C4B	11.19	1.52	1.41
39	44	605	CHL	C3B-C4B	11.17	1.52	1.41
39	4	306	CHL	C3B-C4B	11.16	1.52	1.41
39	3	601	CHL	C3B-C4B	11.15	1.52	1.41
39	y	309	CHL	C3B-C4B	11.13	1.52	1.41
39	Nn	315	CHL	C3B-C4B	11.13	1.52	1.41
39	R	605	CHL	C3B-C4B	11.11	1.52	1.41
39	r	605	CHL	C3B-C4B	11.11	1.52	1.41
39	Gg	310	CHL	C3B-C4B	11.09	1.52	1.41
39	R	607	CHL	C3B-C4B	11.09	1.52	1.41
39	RR	305	CHL	C3B-C4B	11.08	1.52	1.41
39	33	601	CHL	C3B-C4B	11.08	1.52	1.41
39	11	605	CHL	C3B-C4B	11.06	1.52	1.41
39	G	605	CHL	C3B-C4B	11.05	1.52	1.41
39	GG	609	CHL	C3B-C4B	11.04	1.52	1.41
39	RR	307	CHL	C3B-C4B	11.04	1.52	1.41
39	4	308	CHL	C3B-C4B	11.03	1.52	1.41
39	s	607	CHL	C3B-C4B	11.02	1.52	1.41
39	22	608	CHL	C3B-C4B	11.01	1.52	1.41
39	g	609	CHL	C3B-C4B	11.00	1.52	1.41
39	Nn	311	CHL	C3B-C4B	11.00	1.52	1.41
39	1	601	CHL	C3B-C4B	10.98	1.52	1.41
39	Rr	606	CHL	C3B-C4B	10.96	1.52	1.41
39	1	606	CHL	C3B-C4B	10.95	1.52	1.41
39	22	607	CHL	C3B-C4B	10.95	1.52	1.41
39	N	601	CHL	C3B-C4B	10.94	1.52	1.41
39	11	601	CHL	C3B-C4B	10.94	1.52	1.41
39	G	608	CHL	C3B-C4B	10.94	1.52	1.41
39	33	605	CHL	C3B-C4B	10.93	1.52	1.41
39	Ss	607	CHL	C3B-C4B	10.92	1.52	1.41
39	S	607	CHL	C3B-C4B	10.91	1.52	1.41
39	n	601	CHL	C3B-C4B	10.91	1.52	1.41
39	44	601	CHL	C3B-C4B	10.91	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	605	CHL	C3B-C4B	10.91	1.52	1.41
39	SS	308	CHL	C3B-C4B	10.91	1.52	1.41
39	2	607	CHL	C3B-C4B	10.89	1.52	1.41
39	22	601	CHL	C3B-C4B	10.89	1.52	1.41
39	NN	601	CHL	C3B-C4B	10.89	1.52	1.41
39	3	606	CHL	C3B-C4B	10.88	1.52	1.41
39	g	605	CHL	C3B-C4B	10.88	1.52	1.41
39	Gg	306	CHL	C3B-C4B	10.88	1.52	1.41
35	AA	410	PL9	C23-C24	10.87	1.58	1.33
39	2	608	CHL	C3B-C4B	10.87	1.52	1.41
39	G	609	CHL	C3B-C4B	10.86	1.52	1.41
39	GG	605	CHL	C3B-C4B	10.85	1.52	1.41
39	N	606	CHL	C3B-C4B	10.85	1.52	1.41
39	33	606	CHL	C3B-C4B	10.85	1.52	1.41
39	NN	608	CHL	C3B-C4B	10.84	1.51	1.41
39	1	605	CHL	C3B-C4B	10.83	1.51	1.41
39	4	302	CHL	C3B-C4B	10.82	1.51	1.41
39	S	601	CHL	C3B-C4B	10.82	1.51	1.41
39	Gg	307	CHL	C3B-C4B	10.82	1.51	1.41
39	g	601	CHL	C3B-C4B	10.82	1.51	1.41
39	11	606	CHL	C3B-C4B	10.81	1.51	1.41
39	G	606	CHL	C3B-C4B	10.81	1.51	1.41
39	NN	606	CHL	C3B-C4B	10.81	1.51	1.41
39	Gg	302	CHL	C3B-C4B	10.80	1.51	1.41
39	GG	608	CHL	C3B-C4B	10.80	1.51	1.41
39	3	608	CHL	C3B-C4B	10.80	1.51	1.41
39	n	605	CHL	C3B-C4B	10.78	1.51	1.41
39	Y	605	CHL	C3B-C4B	10.77	1.51	1.41
35	A	410	PL9	C23-C24	10.76	1.57	1.33
39	SS	302	CHL	C3B-C4B	10.76	1.51	1.41
39	Ss	601	CHL	C3B-C4B	10.75	1.51	1.41
39	N	608	CHL	C3B-C4B	10.74	1.51	1.41
39	Y	608	CHL	C3B-C4B	10.74	1.51	1.41
39	YY	608	CHL	C3B-C4B	10.73	1.51	1.41
39	SS	307	CHL	C3B-C4B	10.72	1.51	1.41
39	4	307	CHL	C3B-C4B	10.72	1.51	1.41
39	n	606	CHL	C3B-C4B	10.71	1.51	1.41
39	S	606	CHL	C3B-C4B	10.71	1.51	1.41
39	Y	606	CHL	C3B-C4B	10.70	1.51	1.41
39	YY	605	CHL	C3B-C4B	10.70	1.51	1.41
39	n	608	CHL	C3B-C4B	10.70	1.51	1.41
39	YY	606	CHL	C3B-C4B	10.70	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	606	CHL	C3B-C4B	10.69	1.51	1.41
39	GG	601	CHL	C3B-C4B	10.69	1.51	1.41
39	Nn	316	CHL	C3B-C4B	10.69	1.51	1.41
39	g	607	CHL	C3B-C4B	10.68	1.51	1.41
39	G	601	CHL	C3B-C4B	10.66	1.51	1.41
39	y	308	CHL	C3B-C4B	10.65	1.51	1.41
39	YY	601	CHL	C3B-C4B	10.64	1.51	1.41
39	44	606	CHL	C3B-C4B	10.64	1.51	1.41
39	Gg	309	CHL	C3B-C4B	10.63	1.51	1.41
39	Y	601	CHL	C3B-C4B	10.63	1.51	1.41
39	n	609	CHL	C3B-C4B	10.63	1.51	1.41
39	Nn	318	CHL	C3B-C4B	10.61	1.51	1.41
35	d	404	PL9	C23-C24	10.60	1.57	1.33
35	Dd	404	PL9	C23-C24	10.59	1.57	1.33
39	Yy	606	CHL	C3B-C4B	10.59	1.51	1.41
39	2	601	CHL	C3B-C4B	10.59	1.51	1.41
39	GG	606	CHL	C3B-C4B	10.59	1.51	1.41
39	Yy	605	CHL	C3B-C4B	10.58	1.51	1.41
39	y	307	CHL	C3B-C4B	10.57	1.51	1.41
39	G	607	CHL	C3B-C4B	10.57	1.51	1.41
39	44	607	CHL	C3B-C4B	10.56	1.51	1.41
35	DD	406	PL9	C23-C24	10.56	1.57	1.33
39	Nn	319	CHL	C3B-C4B	10.55	1.51	1.41
39	11	608	CHL	C3B-C4B	10.54	1.51	1.41
35	A	410	PL9	C38-C39	10.54	1.57	1.33
39	Gg	308	CHL	C3B-C4B	10.54	1.51	1.41
35	AA	410	PL9	C38-C39	10.53	1.57	1.33
35	D	407	PL9	C23-C24	10.53	1.57	1.33
39	g	608	CHL	C3B-C4B	10.50	1.51	1.41
39	N	609	CHL	C3B-C4B	10.49	1.51	1.41
39	Yy	608	CHL	C3B-C4B	10.44	1.51	1.41
39	YY	609	CHL	C3B-C4B	10.44	1.51	1.41
39	N	607	CHL	C3B-C4B	10.43	1.51	1.41
39	Yy	601	CHL	C3B-C4B	10.40	1.51	1.41
39	NN	607	CHL	C3B-C4B	10.38	1.51	1.41
39	R	606	CHL	C3B-C4B	10.37	1.51	1.41
39	NN	609	CHL	C3B-C4B	10.37	1.51	1.41
39	GG	607	CHL	C3B-C4B	10.36	1.51	1.41
39	y	310	CHL	C3B-C4B	10.36	1.51	1.41
35	DD	406	PL9	C38-C39	10.36	1.56	1.33
35	d	404	PL9	C38-C39	10.35	1.56	1.33
39	y	303	CHL	C3B-C4B	10.35	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	D	407	PL9	C38-C39	10.33	1.56	1.33
35	Dd	404	PL9	C38-C39	10.30	1.56	1.33
39	Yy	607	CHL	C3B-C4B	10.26	1.51	1.41
35	AA	410	PL9	C18-C19	10.21	1.56	1.33
39	y	311	CHL	C3B-C4B	10.19	1.51	1.41
39	RR	306	CHL	C1B-C2B	10.18	1.51	1.39
39	Nn	317	CHL	C3B-C4B	10.18	1.51	1.41
39	n	607	CHL	C3B-C4B	10.17	1.51	1.41
39	11	606	CHL	C1B-C2B	10.16	1.51	1.39
39	1	605	CHL	C1B-C2B	10.13	1.51	1.39
39	2	607	CHL	C1B-C2B	10.13	1.51	1.39
39	Y	609	CHL	C3B-C4B	10.12	1.51	1.41
35	A	410	PL9	C18-C19	10.12	1.56	1.33
39	1	608	CHL	C3B-C4B	10.11	1.51	1.41
39	33	606	CHL	C1B-C2B	10.10	1.51	1.39
39	3	605	CHL	C1B-C2B	10.09	1.51	1.39
39	22	607	CHL	C1B-C2B	10.07	1.51	1.39
39	y	303	CHL	C1B-C2B	10.06	1.51	1.39
39	Ss	607	CHL	C1B-C2B	10.06	1.51	1.39
39	3	606	CHL	C1B-C2B	10.05	1.51	1.39
39	22	608	CHL	C1B-C2B	10.04	1.51	1.39
39	Y	601	CHL	C1B-C2B	10.03	1.51	1.39
35	Dd	404	PL9	C18-C19	10.03	1.56	1.33
39	Yy	601	CHL	C1B-C2B	10.03	1.51	1.39
39	33	605	CHL	C1B-C2B	10.03	1.51	1.39
39	s	607	CHL	C1B-C2B	10.02	1.51	1.39
39	1	601	CHL	C1B-C2B	10.02	1.51	1.39
39	22	601	CHL	C1B-C2B	10.01	1.51	1.39
39	11	601	CHL	C1B-C2B	10.00	1.51	1.39
39	2	601	CHL	C1B-C2B	10.00	1.51	1.39
35	d	404	PL9	C18-C19	10.00	1.56	1.33
39	YY	601	CHL	C1B-C2B	9.99	1.50	1.39
35	DD	406	PL9	C18-C19	9.98	1.56	1.33
35	D	407	PL9	C18-C19	9.97	1.56	1.33
39	1	606	CHL	C1B-C2B	9.97	1.50	1.39
39	S	606	CHL	C1B-C2B	9.96	1.50	1.39
39	S	607	CHL	C1B-C2B	9.96	1.50	1.39
39	11	605	CHL	C1B-C2B	9.95	1.50	1.39
39	GG	601	CHL	C1B-C2B	9.95	1.50	1.39
39	Y	608	CHL	C1B-C2B	9.93	1.50	1.39
39	YY	608	CHL	C1B-C2B	9.93	1.50	1.39
39	GG	605	CHL	C1B-C2B	9.92	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	608	CHL	C1B-C2B	9.92	1.50	1.39
39	GG	608	CHL	C1B-C2B	9.92	1.50	1.39
39	g	601	CHL	C1B-C2B	9.92	1.50	1.39
39	G	601	CHL	C1B-C2B	9.92	1.50	1.39
39	Ss	601	CHL	C1B-C2B	9.91	1.50	1.39
35	AA	410	PL9	C28-C29	9.90	1.55	1.33
39	NN	608	CHL	C1B-C2B	9.88	1.50	1.39
39	SS	307	CHL	C1B-C2B	9.88	1.50	1.39
39	3	608	CHL	C1B-C2B	9.88	1.50	1.39
39	SS	308	CHL	C1B-C2B	9.87	1.50	1.39
39	44	607	CHL	C1B-C2B	9.87	1.50	1.39
39	Gg	302	CHL	C1B-C2B	9.87	1.50	1.39
39	YY	605	CHL	C1B-C2B	9.86	1.50	1.39
39	n	601	CHL	C1B-C2B	9.86	1.50	1.39
39	n	606	CHL	C1B-C2B	9.85	1.50	1.39
39	N	601	CHL	C1B-C2B	9.85	1.50	1.39
39	2	608	CHL	C1B-C2B	9.84	1.50	1.39
39	Nn	311	CHL	C1B-C2B	9.84	1.50	1.39
39	4	302	CHL	C1B-C2B	9.84	1.50	1.39
39	Y	605	CHL	C1B-C2B	9.83	1.50	1.39
35	A	410	PL9	C28-C29	9.83	1.55	1.33
39	g	606	CHL	C1B-C2B	9.83	1.50	1.39
39	Yy	607	CHL	C1B-C2B	9.83	1.50	1.39
39	44	601	CHL	C1B-C2B	9.81	1.50	1.39
39	SS	302	CHL	C1B-C2B	9.81	1.50	1.39
39	G	605	CHL	C1B-C2B	9.80	1.50	1.39
39	4	307	CHL	C1B-C2B	9.80	1.50	1.39
39	Rr	606	CHL	C1B-C2B	9.80	1.50	1.39
39	N	608	CHL	C1B-C2B	9.79	1.50	1.39
39	y	308	CHL	C1B-C2B	9.79	1.50	1.39
39	Gg	307	CHL	C1B-C2B	9.78	1.50	1.39
39	n	605	CHL	C1B-C2B	9.78	1.50	1.39
39	Nn	316	CHL	C1B-C2B	9.77	1.50	1.39
39	n	608	CHL	C1B-C2B	9.77	1.50	1.39
39	S	601	CHL	C1B-C2B	9.77	1.50	1.39
39	g	607	CHL	C1B-C2B	9.75	1.50	1.39
39	GG	607	CHL	C1B-C2B	9.74	1.50	1.39
39	Y	606	CHL	C1B-C2B	9.72	1.50	1.39
39	Yy	606	CHL	C1B-C2B	9.72	1.50	1.39
39	3	601	CHL	C1B-C2B	9.72	1.50	1.39
39	y	307	CHL	C1B-C2B	9.72	1.50	1.39
39	Gg	309	CHL	C1B-C2B	9.71	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Gg	308	CHL	C1B-C2B	9.71	1.50	1.39
39	33	601	CHL	C1B-C2B	9.71	1.50	1.39
39	YY	609	CHL	C1B-C2B	9.70	1.50	1.39
39	G	607	CHL	C1B-C2B	9.70	1.50	1.39
39	g	608	CHL	C1B-C2B	9.69	1.50	1.39
35	Dd	404	PL9	C28-C29	9.69	1.55	1.33
39	R	606	CHL	C1B-C2B	9.69	1.50	1.39
39	G	606	CHL	C1B-C2B	9.68	1.50	1.39
39	NN	606	CHL	C1B-C2B	9.68	1.50	1.39
39	N	606	CHL	C1B-C2B	9.67	1.50	1.39
35	D	407	PL9	C28-C29	9.67	1.55	1.33
39	Yy	605	CHL	C1B-C2B	9.66	1.50	1.39
35	d	404	PL9	C28-C29	9.66	1.55	1.33
33	a	409	PHO	C1B-C2B	9.66	1.50	1.39
39	YY	606	CHL	C1B-C2B	9.65	1.50	1.39
35	DD	406	PL9	C28-C29	9.65	1.55	1.33
33	a	408	PHO	C1B-C2B	9.65	1.50	1.39
39	y	311	CHL	C1B-C2B	9.65	1.50	1.39
39	NN	607	CHL	C1B-C2B	9.64	1.50	1.39
39	44	606	CHL	C1B-C2B	9.62	1.50	1.39
33	Aa	409	PHO	C1B-C2B	9.62	1.50	1.39
39	Gg	306	CHL	C1B-C2B	9.61	1.50	1.39
39	N	607	CHL	C1B-C2B	9.60	1.50	1.39
33	Aa	408	PHO	C1B-C2B	9.59	1.50	1.39
39	Nn	318	CHL	C1B-C2B	9.59	1.50	1.39
39	Nn	317	CHL	C1B-C2B	9.59	1.50	1.39
39	n	607	CHL	C1B-C2B	9.58	1.50	1.39
39	GG	606	CHL	C1B-C2B	9.57	1.50	1.39
33	AA	407	PHO	C1B-C2B	9.55	1.50	1.39
39	g	605	CHL	C1B-C2B	9.54	1.50	1.39
39	Y	609	CHL	C1B-C2B	9.53	1.50	1.39
39	2	605	CHL	C1B-C2B	9.51	1.50	1.39
39	NN	601	CHL	C1B-C2B	9.51	1.50	1.39
33	A	407	PHO	C1B-C2B	9.50	1.49	1.39
39	1	607	CHL	C1B-C2B	9.49	1.50	1.39
39	Yy	608	CHL	C1B-C2B	9.47	1.50	1.39
39	22	605	CHL	C1B-C2B	9.44	1.50	1.39
35	DD	406	PL9	C33-C34	9.41	1.54	1.33
35	AA	410	PL9	C33-C34	9.41	1.54	1.33
39	3	607	CHL	C1B-C2B	9.41	1.50	1.39
35	A	410	PL9	C33-C34	9.39	1.54	1.33
39	N	609	CHL	C1B-C2B	9.37	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	S	605	CHL	C1B-C2B	9.37	1.50	1.39
33	DD	402	PHO	C1B-C2B	9.37	1.49	1.39
33	D	402	PHO	C1B-C2B	9.37	1.49	1.39
39	Ss	605	CHL	C1B-C2B	9.35	1.50	1.39
35	Dd	404	PL9	C33-C34	9.35	1.54	1.33
39	r	605	CHL	C1B-C2B	9.34	1.50	1.39
39	33	607	CHL	C1B-C2B	9.34	1.50	1.39
35	d	404	PL9	C33-C34	9.34	1.54	1.33
39	s	605	CHL	C1B-C2B	9.34	1.50	1.39
39	s	601	CHL	C1B-C2B	9.29	1.50	1.39
39	NN	609	CHL	C1B-C2B	9.29	1.50	1.39
35	D	407	PL9	C33-C34	9.28	1.54	1.33
39	2	606	CHL	C1B-C2B	9.28	1.50	1.39
39	y	309	CHL	C1B-C2B	9.27	1.50	1.39
39	11	607	CHL	C1B-C2B	9.26	1.50	1.39
39	r	607	CHL	C1B-C2B	9.24	1.50	1.39
39	y	310	CHL	C1B-C2B	9.24	1.50	1.39
35	A	410	PL9	C43-C44	9.22	1.54	1.33
35	AA	410	PL9	C43-C44	9.21	1.54	1.33
39	R	607	CHL	C1B-C2B	9.19	1.50	1.39
39	Rr	607	CHL	C1B-C2B	9.19	1.50	1.39
35	A	410	PL9	C8-C9	9.18	1.54	1.33
35	AA	410	PL9	C8-C9	9.18	1.54	1.33
39	RR	307	CHL	C1B-C2B	9.18	1.50	1.39
39	s	606	CHL	C1B-C2B	9.18	1.50	1.39
35	Dd	404	PL9	C8-C9	9.17	1.54	1.33
39	4	308	CHL	C1B-C2B	9.15	1.50	1.39
35	DD	406	PL9	C8-C9	9.13	1.54	1.33
39	SS	306	CHL	C1B-C2B	9.13	1.50	1.39
39	YY	607	CHL	C1B-C2B	9.13	1.50	1.39
39	33	608	CHL	C1B-C2B	9.13	1.50	1.39
39	Y	607	CHL	C1B-C2B	9.13	1.50	1.39
39	Ss	606	CHL	C1B-C2B	9.12	1.49	1.39
39	N	605	CHL	C1B-C2B	9.11	1.49	1.39
35	D	407	PL9	C8-C9	9.11	1.54	1.33
39	r	606	CHL	C1B-C2B	9.10	1.49	1.39
39	NN	605	CHL	C1B-C2B	9.09	1.49	1.39
35	D	407	PL9	C43-C44	9.08	1.54	1.33
39	11	608	CHL	C1B-C2B	9.08	1.49	1.39
39	RR	305	CHL	C1B-C2B	9.07	1.49	1.39
39	22	606	CHL	C1B-C2B	9.06	1.49	1.39
35	d	404	PL9	C43-C44	9.05	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	DD	406	PL9	C43-C44	9.05	1.53	1.33
35	d	404	PL9	C8-C9	9.04	1.53	1.33
39	44	608	CHL	C1B-C2B	9.03	1.49	1.39
39	n	609	CHL	C1B-C2B	9.02	1.49	1.39
39	Nn	315	CHL	C1B-C2B	9.02	1.49	1.39
35	Dd	404	PL9	C43-C44	8.98	1.53	1.33
39	R	605	CHL	C1B-C2B	8.97	1.49	1.39
39	Nn	319	CHL	C1B-C2B	8.96	1.49	1.39
39	Gg	310	CHL	C1B-C2B	8.96	1.49	1.39
39	4	309	CHL	C1B-C2B	8.95	1.49	1.39
39	g	609	CHL	C1B-C2B	8.95	1.49	1.39
39	Yy	609	CHL	C1B-C2B	8.93	1.49	1.39
39	44	605	CHL	C1B-C2B	8.90	1.49	1.39
39	Rr	605	CHL	C1B-C2B	8.90	1.49	1.39
39	GG	609	CHL	C1B-C2B	8.88	1.49	1.39
39	G	609	CHL	C1B-C2B	8.79	1.49	1.39
33	a	409	PHO	C3B-C4B	8.75	1.50	1.41
39	4	306	CHL	C1B-C2B	8.74	1.49	1.39
33	D	402	PHO	C3B-C4B	8.71	1.50	1.41
39	1	608	CHL	C1B-C2B	8.69	1.49	1.39
33	Aa	408	PHO	C3B-C4B	8.67	1.50	1.41
33	a	408	PHO	C3B-C4B	8.64	1.50	1.41
33	Aa	409	PHO	C3B-C4B	8.61	1.50	1.41
33	DD	402	PHO	C3B-C4B	8.59	1.50	1.41
33	A	407	PHO	C3B-C4B	8.58	1.50	1.41
33	AA	407	PHO	C3B-C4B	8.45	1.50	1.41
39	RR	306	CHL	C3B-C4B	8.43	1.49	1.41
35	A	410	PL9	C13-C14	8.35	1.52	1.33
35	AA	410	PL9	C13-C14	8.35	1.52	1.33
35	Dd	404	PL9	C13-C14	8.29	1.52	1.33
39	11	605	CHL	C1D-C2D	8.24	1.48	1.39
39	22	607	CHL	C1D-C2D	8.23	1.48	1.39
35	d	404	PL9	C13-C14	8.22	1.52	1.33
39	2	608	CHL	C1D-C2D	8.20	1.48	1.39
39	22	608	CHL	C1D-C2D	8.18	1.48	1.39
35	D	407	PL9	C13-C14	8.17	1.51	1.33
35	DD	406	PL9	C13-C14	8.16	1.51	1.33
39	3	606	CHL	C1D-C2D	8.10	1.48	1.39
39	11	606	CHL	C1D-C2D	8.09	1.48	1.39
39	N	601	CHL	C1D-C2D	8.07	1.48	1.39
39	11	601	CHL	C1D-C2D	8.06	1.48	1.39
39	22	605	CHL	C1D-C2D	8.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	33	608	CHL	C1D-C2D	8.04	1.48	1.39
39	s	607	CHL	C1D-C2D	8.03	1.48	1.39
39	33	606	CHL	C1D-C2D	8.03	1.48	1.39
39	2	605	CHL	C1D-C2D	8.02	1.48	1.39
39	1	606	CHL	C1D-C2D	8.01	1.48	1.39
39	n	609	CHL	C1D-C2D	8.00	1.48	1.39
39	3	605	CHL	C1D-C2D	8.00	1.48	1.39
39	R	606	CHL	C1D-C2D	7.99	1.48	1.39
39	33	607	CHL	C1D-C2D	7.98	1.48	1.39
39	2	607	CHL	C1D-C2D	7.98	1.48	1.39
39	33	605	CHL	C1D-C2D	7.98	1.48	1.39
39	2	601	CHL	C1D-C2D	7.98	1.48	1.39
39	44	608	CHL	C1D-C2D	7.98	1.48	1.39
39	NN	601	CHL	C1D-C2D	7.97	1.48	1.39
39	44	601	CHL	C1D-C2D	7.96	1.48	1.39
39	RR	306	CHL	C1D-C2D	7.96	1.48	1.39
39	4	308	CHL	C1D-C2D	7.95	1.48	1.39
39	4	309	CHL	C1D-C2D	7.94	1.48	1.39
39	3	608	CHL	C1D-C2D	7.93	1.48	1.39
39	s	606	CHL	C1D-C2D	7.93	1.48	1.39
39	11	607	CHL	C1D-C2D	7.93	1.48	1.39
39	G	605	CHL	C1D-C2D	7.92	1.48	1.39
39	22	601	CHL	C1D-C2D	7.91	1.48	1.39
39	Ss	607	CHL	C1D-C2D	7.91	1.48	1.39
39	G	608	CHL	C1D-C2D	7.91	1.48	1.39
39	Gg	306	CHL	C1D-C2D	7.91	1.48	1.39
39	r	606	CHL	C1D-C2D	7.91	1.48	1.39
39	3	607	CHL	C1D-C2D	7.91	1.48	1.39
39	GG	605	CHL	C1D-C2D	7.89	1.48	1.39
39	YY	606	CHL	C1D-C2D	7.89	1.48	1.39
39	GG	608	CHL	C1D-C2D	7.89	1.48	1.39
39	G	606	CHL	C1D-C2D	7.88	1.48	1.39
39	RR	305	CHL	C1D-C2D	7.88	1.48	1.39
39	Rr	606	CHL	C1D-C2D	7.87	1.48	1.39
39	4	302	CHL	C1D-C2D	7.87	1.48	1.39
39	1	601	CHL	C1D-C2D	7.86	1.48	1.39
39	Ss	606	CHL	C1D-C2D	7.85	1.48	1.39
39	Nn	319	CHL	C1D-C2D	7.85	1.48	1.39
39	Y	606	CHL	C1D-C2D	7.85	1.48	1.39
39	g	605	CHL	C1D-C2D	7.84	1.48	1.39
39	SS	308	CHL	C1D-C2D	7.84	1.48	1.39
39	22	606	CHL	C1D-C2D	7.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	YY	607	CHL	C1D-C2D	7.82	1.48	1.39
39	Yy	601	CHL	C1D-C2D	7.82	1.48	1.39
39	g	609	CHL	C1D-C2D	7.82	1.48	1.39
39	1	607	CHL	C1D-C2D	7.82	1.48	1.39
39	S	601	CHL	C1D-C2D	7.81	1.48	1.39
39	y	303	CHL	C1D-C2D	7.80	1.48	1.39
39	YY	601	CHL	C1D-C2D	7.80	1.48	1.39
39	2	606	CHL	C1D-C2D	7.79	1.48	1.39
39	s	601	CHL	C1D-C2D	7.79	1.48	1.39
39	44	606	CHL	C1D-C2D	7.79	1.48	1.39
39	S	606	CHL	C1D-C2D	7.78	1.48	1.39
39	44	607	CHL	C1D-C2D	7.78	1.48	1.39
39	n	608	CHL	C1D-C2D	7.77	1.48	1.39
39	3	601	CHL	C1D-C2D	7.77	1.48	1.39
39	4	307	CHL	C1D-C2D	7.77	1.48	1.39
39	g	601	CHL	C1D-C2D	7.76	1.48	1.39
39	SS	302	CHL	C1D-C2D	7.76	1.48	1.39
39	GG	606	CHL	C1D-C2D	7.76	1.48	1.39
39	Y	601	CHL	C1D-C2D	7.75	1.48	1.39
39	S	607	CHL	C1D-C2D	7.75	1.48	1.39
39	G	601	CHL	C1D-C2D	7.74	1.48	1.39
39	1	605	CHL	C1D-C2D	7.74	1.48	1.39
39	GG	609	CHL	C1D-C2D	7.73	1.48	1.39
39	S	605	CHL	C1D-C2D	7.73	1.48	1.39
39	NN	609	CHL	C1D-C2D	7.73	1.48	1.39
39	YY	608	CHL	C1D-C2D	7.72	1.48	1.39
39	g	607	CHL	C1D-C2D	7.72	1.48	1.39
39	GG	601	CHL	C1D-C2D	7.72	1.48	1.39
39	33	601	CHL	C1D-C2D	7.72	1.48	1.39
39	Yy	609	CHL	C1D-C2D	7.71	1.48	1.39
39	NN	608	CHL	C1D-C2D	7.71	1.48	1.39
39	YY	609	CHL	C1D-C2D	7.71	1.48	1.39
39	Y	607	CHL	C1D-C2D	7.71	1.48	1.39
39	N	608	CHL	C1D-C2D	7.70	1.48	1.39
39	44	605	CHL	C1D-C2D	7.70	1.48	1.39
39	YY	605	CHL	C1D-C2D	7.69	1.48	1.39
39	Gg	310	CHL	C1D-C2D	7.69	1.48	1.39
39	Gg	308	CHL	C1D-C2D	7.68	1.48	1.39
39	Gg	302	CHL	C1D-C2D	7.68	1.48	1.39
39	Gg	307	CHL	C1D-C2D	7.68	1.48	1.39
39	G	607	CHL	C1D-C2D	7.67	1.48	1.39
39	Gg	309	CHL	C1D-C2D	7.67	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	605	CHL	C1D-C2D	7.67	1.48	1.39
39	R	605	CHL	C1D-C2D	7.67	1.48	1.39
39	Rr	607	CHL	C1D-C2D	7.67	1.48	1.39
39	SS	306	CHL	C1D-C2D	7.66	1.48	1.39
39	Rr	605	CHL	C1D-C2D	7.65	1.48	1.39
39	N	609	CHL	C1D-C2D	7.65	1.48	1.39
39	Ss	601	CHL	C1D-C2D	7.65	1.48	1.39
39	SS	307	CHL	C1D-C2D	7.65	1.48	1.39
39	GG	607	CHL	C1D-C2D	7.65	1.48	1.39
39	r	607	CHL	C1D-C2D	7.64	1.48	1.39
39	y	311	CHL	C1D-C2D	7.64	1.48	1.39
39	Y	608	CHL	C1D-C2D	7.64	1.48	1.39
39	g	608	CHL	C1D-C2D	7.62	1.48	1.39
39	r	605	CHL	C1D-C2D	7.62	1.48	1.39
39	NN	607	CHL	C1D-C2D	7.62	1.48	1.39
39	Y	609	CHL	C1D-C2D	7.61	1.48	1.39
39	N	607	CHL	C1D-C2D	7.60	1.48	1.39
39	n	605	CHL	C1D-C2D	7.60	1.48	1.39
39	1	608	CHL	C1D-C2D	7.60	1.48	1.39
39	n	601	CHL	C1D-C2D	7.60	1.48	1.39
39	NN	605	CHL	C1D-C2D	7.59	1.48	1.39
39	Yy	606	CHL	C1D-C2D	7.58	1.48	1.39
39	g	606	CHL	C1D-C2D	7.58	1.48	1.39
39	N	606	CHL	C1D-C2D	7.58	1.48	1.39
39	Yy	608	CHL	C1D-C2D	7.56	1.48	1.39
39	11	608	CHL	C1D-C2D	7.56	1.48	1.39
39	s	605	CHL	C1D-C2D	7.56	1.48	1.39
39	y	309	CHL	C1D-C2D	7.55	1.48	1.39
39	Nn	311	CHL	C1D-C2D	7.54	1.48	1.39
39	G	609	CHL	C1D-C2D	7.54	1.48	1.39
39	y	310	CHL	C1D-C2D	7.53	1.48	1.39
39	R	607	CHL	C1D-C2D	7.51	1.48	1.39
39	RR	307	CHL	C1D-C2D	7.50	1.48	1.39
39	Nn	317	CHL	C1D-C2D	7.49	1.48	1.39
39	y	308	CHL	C1D-C2D	7.48	1.48	1.39
39	Nn	315	CHL	C1D-C2D	7.48	1.48	1.39
39	Yy	605	CHL	C1D-C2D	7.47	1.48	1.39
39	n	606	CHL	C1D-C2D	7.47	1.48	1.39
39	y	307	CHL	C1D-C2D	7.47	1.48	1.39
39	NN	606	CHL	C1D-C2D	7.46	1.48	1.39
39	N	605	CHL	C1D-C2D	7.45	1.48	1.39
39	Ss	605	CHL	C1D-C2D	7.44	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Yy	607	CHL	C1D-C2D	7.43	1.48	1.39
39	Nn	316	CHL	C1D-C2D	7.41	1.48	1.39
35	A	410	PL9	C48-C49	7.40	1.54	1.32
39	4	306	CHL	C1D-C2D	7.38	1.48	1.39
35	AA	410	PL9	C48-C49	7.37	1.54	1.32
39	Nn	318	CHL	C1D-C2D	7.37	1.47	1.39
39	n	607	CHL	C1D-C2D	7.36	1.47	1.39
35	A	410	PL9	O1-C4	7.33	1.39	1.23
35	D	407	PL9	C48-C49	7.31	1.54	1.32
35	Dd	404	PL9	O1-C4	7.29	1.39	1.23
35	AA	410	PL9	O1-C4	7.29	1.39	1.23
35	d	404	PL9	C48-C49	7.27	1.54	1.32
35	DD	406	PL9	C48-C49	7.26	1.54	1.32
35	Dd	404	PL9	C48-C49	7.26	1.54	1.32
35	d	404	PL9	O1-C4	7.22	1.39	1.23
35	DD	406	PL9	O1-C4	7.15	1.39	1.23
35	D	407	PL9	O1-C4	7.12	1.39	1.23
35	DD	406	PL9	C3-C4	-6.81	1.38	1.49
35	D	407	PL9	C3-C4	-6.75	1.39	1.49
35	d	404	PL9	C3-C4	-6.70	1.39	1.49
35	Dd	404	PL9	C3-C4	-6.65	1.39	1.49
35	A	410	PL9	C3-C4	-6.30	1.39	1.49
35	AA	410	PL9	C3-C4	-6.25	1.39	1.49
35	Dd	404	PL9	C6-C1	-6.13	1.38	1.48
35	DD	406	PL9	C6-C1	-6.07	1.38	1.48
35	D	407	PL9	C6-C1	-6.06	1.38	1.48
35	d	404	PL9	C6-C1	-6.06	1.38	1.48
36	44	616	LHG	O7-C7	5.84	1.45	1.33
35	A	410	PL9	O2-C1	5.79	1.39	1.24
36	4	301	LHG	O7-C7	5.79	1.45	1.33
35	AA	410	PL9	O2-C1	5.78	1.39	1.24
35	AA	410	PL9	C6-C1	-5.70	1.39	1.48
35	A	410	PL9	C6-C1	-5.70	1.39	1.48
35	Dd	404	PL9	O2-C1	5.67	1.39	1.24
35	d	404	PL9	O2-C1	5.66	1.39	1.24
35	DD	406	PL9	O2-C1	5.63	1.39	1.24
35	D	407	PL9	O2-C1	5.61	1.39	1.24
36	4	315	LHG	O7-C7	4.90	1.46	1.35
36	J	101	LHG	O7-C7	4.83	1.45	1.35
37	BB	621	SQD	O8-S	4.81	1.65	1.47
37	B	617	SQD	O8-S	4.80	1.65	1.47
36	44	614	LHG	O7-C7	4.57	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	306	CHL	C3D-C4D	4.57	1.48	1.41
39	44	608	CHL	C2C-C3C	4.57	1.40	1.36
39	g	605	CHL	C2C-C3C	4.51	1.40	1.36
39	S	607	CHL	C2C-C3C	4.50	1.40	1.36
37	l	102	SQD	O8-S	4.46	1.64	1.47
39	2	606	CHL	C2C-C3C	4.45	1.40	1.36
37	Ll	101	SQD	O8-S	4.45	1.64	1.47
39	22	606	CHL	C2C-C3C	4.45	1.40	1.36
39	1	605	CHL	C2C-C3C	4.44	1.40	1.36
37	Aa	413	SQD	O8-S	4.44	1.63	1.47
39	Gg	306	CHL	C2C-C3C	4.44	1.40	1.36
37	B	602	SQD	O8-S	4.44	1.63	1.47
36	Rr	617	LHG	O7-C7	4.44	1.46	1.34
37	L	102	SQD	O8-S	4.43	1.63	1.47
37	LL	101	SQD	O8-S	4.42	1.63	1.47
39	1	607	CHL	C2C-C3C	4.42	1.40	1.36
39	2	605	CHL	C2C-C3C	4.42	1.40	1.36
37	L	101	SQD	O8-S	4.42	1.63	1.47
37	LL	102	SQD	O8-S	4.42	1.63	1.47
37	A	412	SQD	O8-S	4.41	1.63	1.47
39	33	606	CHL	C3D-C4D	4.41	1.48	1.41
39	3	601	CHL	C2C-C3C	4.40	1.40	1.36
44	a	415	DGD	O1G-C1A	4.39	1.46	1.33
39	s	606	CHL	C2C-C3C	4.39	1.40	1.36
39	SS	308	CHL	C2C-C3C	4.39	1.40	1.36
36	Rr	617	LHG	O8-C23	4.38	1.46	1.33
36	r	616	LHG	O7-C7	4.38	1.46	1.34
36	r	616	LHG	O8-C23	4.37	1.46	1.33
37	C	501	SQD	O8-S	4.37	1.63	1.47
44	Aa	401	DGD	O1G-C1A	4.37	1.46	1.33
39	11	601	CHL	C2C-C3C	4.36	1.40	1.36
39	22	601	CHL	C3D-C4D	4.36	1.48	1.41
37	B	602	SQD	O48-C23	4.36	1.46	1.33
39	1	606	CHL	C2C-C3C	4.35	1.40	1.36
39	33	605	CHL	C3D-C4D	4.35	1.48	1.41
37	Aa	413	SQD	O48-C23	4.35	1.46	1.33
39	N	607	CHL	C3D-C4D	4.35	1.48	1.41
39	S	605	CHL	C3D-C4D	4.35	1.48	1.41
39	SS	306	CHL	C3D-C4D	4.35	1.48	1.41
44	a	415	DGD	O2G-C1B	4.34	1.46	1.34
39	s	606	CHL	C3D-C4D	4.34	1.48	1.41
39	22	605	CHL	C3D-C4D	4.34	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	33	601	CHL	C3D-C4D	4.34	1.48	1.41
37	L	101	SQD	O48-C23	4.34	1.46	1.33
39	R	605	CHL	C2C-C3C	4.34	1.40	1.36
39	Ss	605	CHL	C3D-C4D	4.34	1.48	1.41
39	2	606	CHL	C3D-C4D	4.34	1.48	1.41
39	3	606	CHL	C3D-C4D	4.33	1.48	1.41
39	22	605	CHL	C2C-C3C	4.33	1.40	1.36
39	G	605	CHL	C3D-C4D	4.33	1.48	1.41
37	LL	102	SQD	O48-C23	4.33	1.46	1.33
39	2	601	CHL	C3D-C4D	4.33	1.48	1.41
38	W	201	LMG	O7-C10	4.33	1.46	1.34
39	3	607	CHL	C3D-C4D	4.33	1.48	1.41
36	1	614	LHG	O8-C23	4.33	1.46	1.33
38	WW	201	LMG	O7-C10	4.33	1.46	1.34
39	22	606	CHL	C3D-C4D	4.33	1.48	1.41
39	NN	607	CHL	C3D-C4D	4.33	1.48	1.41
39	2	605	CHL	C3D-C4D	4.32	1.48	1.41
44	C	519	DGD	O1G-C1A	4.32	1.45	1.33
39	S	607	CHL	C3D-C4D	4.32	1.48	1.41
37	BB	621	SQD	O48-C23	4.32	1.45	1.33
44	Hh	102	DGD	O2G-C1B	4.32	1.46	1.34
39	1	605	CHL	C3D-C4D	4.32	1.48	1.41
39	1	606	CHL	C3D-C4D	4.32	1.48	1.41
36	11	614	LHG	O8-C23	4.32	1.45	1.33
44	CC	518	DGD	O1G-C1A	4.32	1.45	1.33
39	S	606	CHL	C3D-C4D	4.32	1.48	1.41
39	11	608	CHL	C3D-C4D	4.32	1.48	1.41
39	1	601	CHL	C3D-C4D	4.31	1.48	1.41
39	r	606	CHL	C3D-C4D	4.31	1.48	1.41
39	11	606	CHL	C3D-C4D	4.31	1.48	1.41
39	44	605	CHL	C3D-C4D	4.31	1.48	1.41
39	22	608	CHL	C3D-C4D	4.31	1.48	1.41
37	AA	412	SQD	O8-S	4.31	1.63	1.47
39	n	607	CHL	C3D-C4D	4.31	1.48	1.41
39	YY	607	CHL	C2C-C3C	4.31	1.40	1.36
44	Aa	401	DGD	O2G-C1B	4.31	1.46	1.34
39	11	606	CHL	C2C-C3C	4.31	1.40	1.36
44	B	603	DGD	O1G-C1A	4.31	1.45	1.33
38	j	101	LMG	O8-C28	4.30	1.45	1.33
36	EE	101	LHG	O7-C7	4.30	1.46	1.34
38	BB	619	LMG	O8-C28	4.30	1.45	1.33
39	1	601	CHL	C2C-C3C	4.30	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	RR	305	CHL	C2C-C3C	4.30	1.40	1.36
39	Ss	606	CHL	C3D-C4D	4.30	1.48	1.41
39	22	601	CHL	C2C-C3C	4.29	1.40	1.36
36	SS	301	LHG	O8-C23	4.29	1.45	1.33
37	B	617	SQD	O48-C23	4.29	1.45	1.33
39	Ss	607	CHL	C3D-C4D	4.29	1.48	1.41
44	Cc	520	DGD	O1G-C1A	4.29	1.45	1.33
39	s	607	CHL	C3D-C4D	4.29	1.48	1.41
39	SS	308	CHL	C3D-C4D	4.29	1.48	1.41
36	Nn	310	LHG	O7-C7	4.29	1.46	1.34
37	A	412	SQD	O48-C23	4.29	1.45	1.33
44	h	102	DGD	O1G-C1A	4.29	1.45	1.33
39	s	607	CHL	C2C-C3C	4.29	1.40	1.36
37	CC	501	SQD	O8-S	4.29	1.63	1.47
38	CC	520	LMG	O8-C28	4.28	1.45	1.33
36	0	201	LHG	O7-C7	4.28	1.46	1.34
38	Aa	412	LMG	O8-C28	4.28	1.45	1.33
38	Bb	621	LMG	O8-C28	4.28	1.45	1.33
39	4	309	CHL	C2C-C3C	4.28	1.40	1.36
36	g	618	LHG	O8-C23	4.28	1.45	1.33
44	h	102	DGD	O2G-C1B	4.28	1.46	1.34
36	n	618	LHG	O7-C7	4.28	1.46	1.34
36	Gg	319	LHG	O8-C23	4.28	1.45	1.33
39	33	601	CHL	C2C-C3C	4.28	1.40	1.36
39	1	607	CHL	C3D-C4D	4.28	1.48	1.41
39	s	605	CHL	C3D-C4D	4.27	1.48	1.41
38	B	615	LMG	O8-C28	4.27	1.45	1.33
44	c	518	DGD	O1G-C1A	4.27	1.45	1.33
38	Dd	408	LMG	O8-C28	4.27	1.45	1.33
38	b	621	LMG	O8-C28	4.27	1.45	1.33
39	Nn	315	CHL	C3D-C4D	4.27	1.48	1.41
44	BB	625	DGD	O1G-C1A	4.27	1.45	1.33
39	2	608	CHL	C3D-C4D	4.27	1.48	1.41
39	N	605	CHL	C3D-C4D	4.27	1.48	1.41
36	3	614	LHG	O8-C23	4.26	1.45	1.33
39	GG	605	CHL	C3D-C4D	4.26	1.48	1.41
39	3	605	CHL	C3D-C4D	4.26	1.48	1.41
36	n	618	LHG	O8-C23	4.26	1.45	1.33
36	NN	619	LHG	O8-C23	4.26	1.45	1.33
39	SS	307	CHL	C3D-C4D	4.26	1.48	1.41
36	Ll	102	LHG	O8-C23	4.26	1.45	1.33
39	Ss	606	CHL	C2C-C3C	4.26	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	102	SQD	O48-C23	4.26	1.45	1.33
44	C	519	DGD	O2G-C1B	4.26	1.46	1.34
36	G	618	LHG	O8-C23	4.26	1.45	1.33
38	m	101	LMG	O7-C10	4.26	1.46	1.34
37	LL	101	SQD	O48-C23	4.26	1.45	1.33
44	BB	624	DGD	O1G-C1A	4.26	1.45	1.33
36	D	410	LHG	O8-C23	4.26	1.45	1.33
39	1	608	CHL	C3D-C4D	4.26	1.48	1.41
36	22	615	LHG	O8-C23	4.26	1.45	1.33
39	GG	607	CHL	C3D-C4D	4.26	1.48	1.41
39	4	302	CHL	C3D-C4D	4.25	1.48	1.41
37	AA	412	SQD	O48-C23	4.25	1.45	1.33
39	33	605	CHL	C2C-C3C	4.25	1.40	1.36
39	33	607	CHL	C3D-C4D	4.25	1.48	1.41
36	GG	618	LHG	O8-C23	4.25	1.45	1.33
44	B	601	DGD	O1G-C1A	4.25	1.45	1.33
39	G	607	CHL	C3D-C4D	4.25	1.48	1.41
38	A	415	LMG	O8-C28	4.25	1.45	1.33
39	44	601	CHL	C3D-C4D	4.25	1.48	1.41
39	Rr	606	CHL	C3D-C4D	4.25	1.48	1.41
36	s	616	LHG	O8-C23	4.24	1.45	1.33
37	Ll	101	SQD	O48-C23	4.24	1.45	1.33
39	4	307	CHL	C3D-C4D	4.24	1.48	1.41
39	11	601	CHL	C3D-C4D	4.24	1.48	1.41
39	2	607	CHL	C3D-C4D	4.24	1.48	1.41
36	22	615	LHG	O7-C7	4.24	1.46	1.34
38	W	201	LMG	O8-C28	4.24	1.45	1.33
39	3	607	CHL	C2C-C3C	4.24	1.40	1.36
39	GG	601	CHL	C3D-C4D	4.24	1.48	1.41
39	G	601	CHL	C3D-C4D	4.24	1.48	1.41
37	l	102	SQD	O48-C23	4.23	1.45	1.33
38	AA	415	LMG	O8-C28	4.23	1.45	1.33
36	NN	619	LHG	O7-C7	4.23	1.46	1.34
38	b	620	LMG	O8-C28	4.23	1.45	1.33
36	BB	622	LHG	O7-C7	4.23	1.46	1.34
39	Ss	601	CHL	C3D-C4D	4.23	1.48	1.41
38	Mm	101	LMG	O7-C10	4.23	1.46	1.34
39	44	606	CHL	C2C-C3C	4.23	1.40	1.36
36	Nn	310	LHG	O8-C23	4.23	1.45	1.33
38	F	101	LMG	O8-C28	4.23	1.45	1.33
39	S	601	CHL	C3D-C4D	4.23	1.48	1.41
36	KK	101	LHG	O8-C23	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	22	607	CHL	C3D-C4D	4.22	1.48	1.41
36	33	614	LHG	O8-C23	4.22	1.45	1.33
38	DD	409	LMG	O8-C28	4.22	1.45	1.33
36	N	619	LHG	O7-C7	4.22	1.46	1.34
39	33	607	CHL	C2C-C3C	4.22	1.40	1.36
44	D	411	DGD	O1G-C1A	4.22	1.45	1.33
36	AA	414	LHG	O7-C7	4.22	1.46	1.34
39	RR	305	CHL	C3D-C4D	4.22	1.48	1.41
38	a	412	LMG	O8-C28	4.22	1.45	1.33
36	A	414	LHG	O7-C7	4.22	1.46	1.34
39	Y	605	CHL	C3D-C4D	4.22	1.48	1.41
36	II	101	LHG	O8-C23	4.21	1.45	1.33
44	BB	623	DGD	O2G-C1B	4.21	1.46	1.34
38	WW	201	LMG	O8-C28	4.21	1.45	1.33
38	Bb	620	LMG	O7-C10	4.21	1.46	1.34
36	D	408	LHG	O8-C23	4.21	1.45	1.33
39	33	608	CHL	C3D-C4D	4.20	1.47	1.41
39	NN	605	CHL	C3D-C4D	4.20	1.47	1.41
38	Bb	620	LMG	O8-C28	4.20	1.45	1.33
36	EE	101	LHG	O8-C23	4.20	1.45	1.33
36	K	101	LHG	O8-C23	4.20	1.45	1.33
39	g	605	CHL	C3D-C4D	4.20	1.47	1.41
38	c	519	LMG	O8-C28	4.20	1.45	1.33
36	11	614	LHG	O7-C7	4.20	1.46	1.34
39	3	601	CHL	C3D-C4D	4.20	1.47	1.41
39	NN	609	CHL	C3D-C4D	4.20	1.47	1.41
39	Nn	311	CHL	C2C-C3C	4.20	1.40	1.36
44	Hh	102	DGD	O1G-C1A	4.20	1.45	1.33
39	44	606	CHL	C3D-C4D	4.20	1.47	1.41
39	SS	302	CHL	C3D-C4D	4.20	1.47	1.41
39	Y	607	CHL	C2C-C3C	4.20	1.40	1.36
39	YY	605	CHL	C3D-C4D	4.19	1.47	1.41
36	33	614	LHG	O7-C7	4.19	1.46	1.34
39	Yy	606	CHL	C3D-C4D	4.19	1.47	1.41
39	YY	607	CHL	C3D-C4D	4.19	1.47	1.41
36	0	201	LHG	O8-C23	4.19	1.45	1.33
36	CC	521	LHG	O8-C23	4.19	1.45	1.33
36	1	614	LHG	O7-C7	4.19	1.46	1.34
39	11	607	CHL	C3D-C4D	4.19	1.47	1.41
39	g	601	CHL	C3D-C4D	4.19	1.47	1.41
39	GG	605	CHL	C2C-C3C	4.19	1.40	1.36
36	DD	407	LHG	O8-C23	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	607	CHL	C3D-C4D	4.19	1.47	1.41
39	11	605	CHL	C3D-C4D	4.19	1.47	1.41
36	SS	301	LHG	O7-C7	4.19	1.46	1.34
44	C	523	DGD	O1G-C1A	4.18	1.45	1.33
39	Gg	310	CHL	C3D-C4D	4.18	1.47	1.41
39	n	601	CHL	C3D-C4D	4.18	1.47	1.41
38	DD	409	LMG	O7-C10	4.18	1.46	1.34
39	Nn	311	CHL	C3D-C4D	4.18	1.47	1.41
36	A	411	LHG	O7-C7	4.18	1.46	1.34
36	a	414	LHG	O7-C7	4.18	1.46	1.34
38	Mm	101	LMG	O8-C28	4.18	1.45	1.33
39	Y	607	CHL	C3D-C4D	4.18	1.47	1.41
39	Rr	607	CHL	C2C-C3C	4.18	1.40	1.36
36	N	619	LHG	O8-C23	4.17	1.45	1.33
39	Y	606	CHL	C3D-C4D	4.17	1.47	1.41
39	r	607	CHL	C3D-C4D	4.17	1.47	1.41
36	l	101	LHG	O8-C23	4.17	1.45	1.33
38	F	101	LMG	O7-C10	4.17	1.46	1.34
36	d	405	LHG	O8-C23	4.17	1.45	1.33
39	33	606	CHL	C2C-C3C	4.17	1.40	1.36
36	A	411	LHG	O8-C23	4.17	1.45	1.33
39	y	307	CHL	C3D-C4D	4.17	1.47	1.41
44	CC	522	DGD	O1G-C1A	4.17	1.45	1.33
38	Cc	501	LMG	O8-C28	4.17	1.45	1.33
38	b	620	LMG	O7-C10	4.17	1.46	1.34
39	Yy	605	CHL	C3D-C4D	4.17	1.47	1.41
36	K	101	LHG	O7-C7	4.17	1.46	1.34
36	Dd	407	LHG	O7-C7	4.17	1.46	1.34
38	m	101	LMG	O8-C28	4.16	1.45	1.33
39	y	311	CHL	C3D-C4D	4.16	1.47	1.41
36	BB	622	LHG	O8-C23	4.16	1.45	1.33
39	Yy	607	CHL	C3D-C4D	4.16	1.47	1.41
39	Rr	607	CHL	C3D-C4D	4.16	1.47	1.41
39	G	608	CHL	C2C-C3C	4.16	1.40	1.36
38	C	521	LMG	O8-C28	4.16	1.45	1.33
39	g	609	CHL	C3D-C4D	4.16	1.47	1.41
36	s	616	LHG	O7-C7	4.16	1.46	1.34
39	N	609	CHL	C3D-C4D	4.16	1.47	1.41
39	y	308	CHL	C3D-C4D	4.16	1.47	1.41
44	BB	623	DGD	O1G-C1A	4.16	1.45	1.33
36	C	522	LHG	O8-C23	4.16	1.45	1.33
36	II	101	LHG	O7-C7	4.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	608	CHL	C3D-C4D	4.15	1.47	1.41
39	y	309	CHL	C3D-C4D	4.15	1.47	1.41
44	C	520	DGD	O1G-C1A	4.15	1.45	1.33
39	RR	307	CHL	C3D-C4D	4.15	1.47	1.41
39	Nn	316	CHL	C3D-C4D	4.15	1.47	1.41
36	AA	411	LHG	O8-C23	4.15	1.45	1.33
39	Gg	306	CHL	C3D-C4D	4.15	1.47	1.41
39	Y	608	CHL	C3D-C4D	4.15	1.47	1.41
38	AA	415	LMG	O7-C10	4.15	1.46	1.34
39	R	606	CHL	C2C-C3C	4.15	1.40	1.36
39	R	606	CHL	C3D-C4D	4.15	1.47	1.41
36	AA	411	LHG	O7-C7	4.14	1.46	1.34
39	g	606	CHL	C3D-C4D	4.14	1.47	1.41
39	R	605	CHL	C3D-C4D	4.14	1.47	1.41
37	Ll	101	SQD	O47-C7	4.14	1.46	1.34
44	CC	518	DGD	O2G-C1B	4.14	1.46	1.34
36	A	413	LHG	O7-C7	4.14	1.46	1.34
39	Gg	308	CHL	C3D-C4D	4.14	1.47	1.41
39	4	307	CHL	C2C-C3C	4.14	1.40	1.36
36	JJ	101	LHG	O7-C7	4.14	1.46	1.34
39	Gg	307	CHL	C3D-C4D	4.14	1.47	1.41
39	Nn	317	CHL	C3D-C4D	4.14	1.47	1.41
39	n	606	CHL	C3D-C4D	4.14	1.47	1.41
39	Ss	605	CHL	C2C-C3C	4.14	1.40	1.36
38	A	415	LMG	O7-C10	4.14	1.46	1.34
39	y	310	CHL	C3D-C4D	4.14	1.47	1.41
37	l	102	SQD	O47-C7	4.14	1.46	1.34
36	J	101	LHG	O8-C23	4.13	1.45	1.33
38	Aa	412	LMG	O7-C10	4.13	1.46	1.34
39	44	607	CHL	C3D-C4D	4.13	1.47	1.41
36	Dd	405	LHG	O8-C23	4.13	1.45	1.33
39	YY	608	CHL	C3D-C4D	4.13	1.47	1.41
44	C	520	DGD	O2G-C1B	4.13	1.45	1.34
39	SS	307	CHL	C2C-C3C	4.13	1.40	1.36
38	CC	520	LMG	O7-C10	4.13	1.45	1.34
36	d	406	LHG	O8-C23	4.13	1.45	1.33
44	Cc	519	DGD	O1G-C1A	4.13	1.45	1.33
39	s	601	CHL	C3D-C4D	4.13	1.47	1.41
36	AA	414	LHG	O8-C23	4.13	1.45	1.33
36	A	413	LHG	O8-C23	4.13	1.45	1.33
39	n	608	CHL	C3D-C4D	4.13	1.47	1.41
36	Ss	616	LHG	O8-C23	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	GG	618	LHG	O7-C7	4.12	1.45	1.34
39	NN	608	CHL	C3D-C4D	4.12	1.47	1.41
39	n	608	CHL	C2C-C3C	4.12	1.40	1.36
36	KK	101	LHG	O7-C7	4.12	1.45	1.34
39	GG	609	CHL	C3D-C4D	4.12	1.47	1.41
36	D	408	LHG	O7-C7	4.12	1.45	1.34
39	4	308	CHL	C3D-C4D	4.12	1.47	1.41
39	YY	609	CHL	C2C-C3C	4.12	1.40	1.36
36	Y	618	LHG	O7-C7	4.12	1.45	1.34
39	G	606	CHL	C3D-C4D	4.12	1.47	1.41
39	n	601	CHL	C2C-C3C	4.12	1.40	1.36
36	JJ	101	LHG	O8-C23	4.12	1.45	1.33
36	y	320	LHG	O8-C23	4.12	1.45	1.33
39	s	601	CHL	C2C-C3C	4.11	1.40	1.36
44	c	517	DGD	O1G-C1A	4.11	1.45	1.33
39	G	608	CHL	C3D-C4D	4.11	1.47	1.41
36	A	414	LHG	O8-C23	4.11	1.45	1.33
33	D	402	PHO	C1D-C2D	4.11	1.44	1.39
36	YY	618	LHG	O8-C23	4.11	1.45	1.33
39	N	608	CHL	C3D-C4D	4.11	1.47	1.41
36	a	414	LHG	O8-C23	4.10	1.45	1.33
39	n	609	CHL	C3D-C4D	4.10	1.47	1.41
44	CC	519	DGD	O1G-C1A	4.10	1.45	1.33
39	Nn	319	CHL	C3D-C4D	4.10	1.47	1.41
39	Y	609	CHL	C3D-C4D	4.10	1.47	1.41
39	YY	601	CHL	C3D-C4D	4.10	1.47	1.41
39	YY	609	CHL	C3D-C4D	4.10	1.47	1.41
36	g	618	LHG	O7-C7	4.10	1.45	1.34
44	D	411	DGD	O2G-C1B	4.10	1.45	1.34
39	r	605	CHL	C3D-C4D	4.10	1.47	1.41
44	B	603	DGD	O2G-C1B	4.10	1.45	1.34
39	N	605	CHL	C2C-C3C	4.10	1.40	1.36
36	Ss	616	LHG	O7-C7	4.10	1.45	1.34
39	g	607	CHL	C3D-C4D	4.10	1.47	1.41
36	G	618	LHG	O7-C7	4.10	1.45	1.34
36	Y	618	LHG	O8-C23	4.10	1.45	1.33
44	CC	519	DGD	O2G-C1B	4.10	1.45	1.34
36	CC	521	LHG	O7-C7	4.09	1.45	1.34
36	Dd	406	LHG	O8-C23	4.09	1.45	1.33
39	Gg	309	CHL	C3D-C4D	4.09	1.47	1.41
36	DD	407	LHG	O7-C7	4.09	1.45	1.34
39	GG	606	CHL	C3D-C4D	4.09	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Dd	407	LHG	O8-C23	4.09	1.45	1.33
39	NN	606	CHL	C3D-C4D	4.09	1.47	1.41
39	GG	608	CHL	C3D-C4D	4.09	1.47	1.41
39	g	608	CHL	C3D-C4D	4.08	1.47	1.41
38	a	412	LMG	O7-C10	4.08	1.45	1.34
36	Yy	618	LHG	O8-C23	4.08	1.45	1.33
33	a	408	PHO	C1D-C2D	4.08	1.44	1.39
37	B	617	SQD	O47-C7	4.08	1.45	1.34
36	3	614	LHG	O7-C7	4.08	1.45	1.34
36	YY	618	LHG	O7-C7	4.08	1.45	1.34
36	Gg	319	LHG	O7-C7	4.08	1.45	1.34
36	CC	523	LHG	O7-C7	4.08	1.45	1.34
39	GG	608	CHL	C2C-C3C	4.08	1.40	1.36
39	RR	306	CHL	C3D-C4D	4.08	1.47	1.41
37	BB	621	SQD	O47-C7	4.08	1.45	1.34
39	YY	606	CHL	C3D-C4D	4.07	1.47	1.41
39	22	608	CHL	C2C-C3C	4.07	1.40	1.36
39	Yy	609	CHL	C3D-C4D	4.07	1.47	1.41
36	d	406	LHG	O7-C7	4.07	1.45	1.34
39	r	607	CHL	C2C-C3C	4.07	1.40	1.36
39	Nn	315	CHL	C2C-C3C	4.07	1.40	1.36
39	44	608	CHL	C3D-C4D	4.07	1.47	1.41
44	Cc	520	DGD	O2G-C1B	4.07	1.45	1.34
39	Yy	601	CHL	C3D-C4D	4.07	1.47	1.41
36	d	405	LHG	O7-C7	4.07	1.45	1.34
39	N	601	CHL	C3D-C4D	4.07	1.47	1.41
33	Aa	408	PHO	C1D-C2D	4.06	1.44	1.39
39	s	605	CHL	C2C-C3C	4.06	1.40	1.36
39	4	309	CHL	C3D-C4D	4.06	1.47	1.41
39	N	606	CHL	C3D-C4D	4.06	1.47	1.41
37	C	501	SQD	O47-C7	4.06	1.45	1.34
36	C	522	LHG	O7-C7	4.06	1.45	1.34
37	AA	412	SQD	O47-C7	4.06	1.45	1.34
38	Dd	408	LMG	O7-C10	4.06	1.45	1.34
39	Yy	608	CHL	C3D-C4D	4.06	1.47	1.41
44	c	518	DGD	O2G-C1B	4.06	1.45	1.34
44	BB	625	DGD	O2G-C1B	4.06	1.45	1.34
38	B	615	LMG	O7-C10	4.05	1.45	1.34
39	Rr	605	CHL	C3D-C4D	4.05	1.47	1.41
39	Y	601	CHL	C3D-C4D	4.05	1.47	1.41
38	j	101	LMG	O7-C10	4.05	1.45	1.34
36	Dd	405	LHG	O7-C7	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	609	CHL	C3D-C4D	4.05	1.47	1.41
37	B	602	SQD	O47-C7	4.05	1.45	1.34
44	C	523	DGD	O2G-C1B	4.05	1.45	1.34
36	D	409	LHG	O7-C7	4.04	1.45	1.34
37	L	102	SQD	O47-C7	4.04	1.45	1.34
36	l	101	LHG	O7-C7	4.04	1.45	1.34
39	Ss	607	CHL	C2C-C3C	4.04	1.40	1.36
36	CC	523	LHG	O8-C23	4.04	1.45	1.33
37	LL	101	SQD	O47-C7	4.04	1.45	1.34
36	Dd	406	LHG	O7-C7	4.04	1.45	1.34
39	2	607	CHL	C2C-C3C	4.04	1.40	1.36
39	Nn	318	CHL	C2C-C3C	4.04	1.40	1.36
36	D	410	LHG	O7-C7	4.03	1.45	1.34
37	L	101	SQD	O47-C7	4.03	1.45	1.34
39	r	606	CHL	C2C-C3C	4.03	1.40	1.36
39	NN	608	CHL	C2C-C3C	4.03	1.40	1.36
39	y	303	CHL	C3D-C4D	4.03	1.47	1.41
38	c	519	LMG	O7-C10	4.03	1.45	1.34
37	Aa	413	SQD	O47-C7	4.02	1.45	1.34
37	LL	102	SQD	O47-C7	4.02	1.45	1.34
38	Bb	621	LMG	O7-C10	4.02	1.45	1.34
37	CC	501	SQD	O47-C7	4.02	1.45	1.34
37	A	412	SQD	O47-C7	4.02	1.45	1.34
38	BB	619	LMG	O7-C10	4.02	1.45	1.34
38	Cc	501	LMG	O7-C10	4.02	1.45	1.34
38	b	621	LMG	O7-C10	4.02	1.45	1.34
39	44	601	CHL	C2C-C3C	4.01	1.40	1.36
37	C	501	SQD	O48-C23	4.01	1.45	1.33
39	NN	601	CHL	C3D-C4D	4.01	1.47	1.41
44	c	517	DGD	O2G-C1B	4.01	1.45	1.34
39	SS	302	CHL	C2C-C3C	4.01	1.40	1.36
36	Ll	102	LHG	O7-C7	4.01	1.45	1.34
36	DD	408	LHG	O8-C23	4.01	1.45	1.33
39	S	606	CHL	C2C-C3C	4.00	1.40	1.36
36	DD	408	LHG	O7-C7	4.00	1.45	1.34
39	n	605	CHL	C3D-C4D	4.00	1.47	1.41
37	CC	501	SQD	O48-C23	4.00	1.45	1.33
39	Gg	302	CHL	C3D-C4D	3.99	1.47	1.41
44	Cc	519	DGD	O2G-C1B	3.99	1.45	1.34
44	BB	624	DGD	O2G-C1B	3.99	1.45	1.34
39	R	607	CHL	C2C-C3C	3.99	1.40	1.36
36	D	409	LHG	O8-C23	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	605	CHL	C2C-C3C	3.98	1.40	1.36
39	2	601	CHL	C2C-C3C	3.97	1.40	1.36
39	4	308	CHL	C2C-C3C	3.97	1.40	1.36
33	DD	402	PHO	C1D-C2D	3.97	1.43	1.39
39	4	302	CHL	C2C-C3C	3.97	1.40	1.36
33	a	409	PHO	C1D-C2D	3.97	1.43	1.39
39	Ss	601	CHL	C2C-C3C	3.97	1.40	1.36
38	C	521	LMG	O7-C10	3.97	1.45	1.34
44	B	601	DGD	O2G-C1B	3.96	1.45	1.34
39	2	608	CHL	C2C-C3C	3.96	1.40	1.36
33	Aa	409	PHO	C1D-C2D	3.96	1.43	1.39
39	Yy	607	CHL	C2C-C3C	3.95	1.40	1.36
39	Rr	606	CHL	C2C-C3C	3.95	1.40	1.36
39	44	607	CHL	C2C-C3C	3.95	1.40	1.36
39	RR	306	CHL	C2C-C3C	3.95	1.40	1.36
39	33	608	CHL	C2C-C3C	3.95	1.40	1.36
39	11	607	CHL	C2C-C3C	3.94	1.40	1.36
39	RR	307	CHL	C2C-C3C	3.94	1.40	1.36
39	11	605	CHL	C2C-C3C	3.93	1.40	1.36
39	11	608	CHL	C2C-C3C	3.93	1.40	1.36
39	S	601	CHL	C2C-C3C	3.92	1.40	1.36
36	y	320	LHG	O7-C7	3.92	1.45	1.34
39	g	606	CHL	C2C-C3C	3.91	1.40	1.36
36	Yy	618	LHG	O7-C7	3.91	1.45	1.34
39	3	605	CHL	C2C-C3C	3.91	1.40	1.36
39	g	608	CHL	C2C-C3C	3.90	1.40	1.36
39	Gg	302	CHL	C2C-C3C	3.89	1.40	1.36
39	Y	606	CHL	C2C-C3C	3.89	1.40	1.36
39	NN	605	CHL	C2C-C3C	3.89	1.40	1.36
39	Y	609	CHL	C2C-C3C	3.89	1.40	1.36
33	A	407	PHO	C1D-C2D	3.88	1.43	1.39
39	Rr	605	CHL	C2C-C3C	3.88	1.40	1.36
39	Gg	309	CHL	C2C-C3C	3.88	1.40	1.36
39	3	606	CHL	C2C-C3C	3.88	1.40	1.36
39	y	307	CHL	C2C-C3C	3.87	1.40	1.36
39	G	605	CHL	C2C-C3C	3.87	1.40	1.36
39	Y	605	CHL	C2C-C3C	3.87	1.40	1.36
42	Y	617	NEX	C7-C6	-3.86	1.26	1.30
39	G	609	CHL	C2C-C3C	3.86	1.40	1.36
39	YY	608	CHL	C2C-C3C	3.85	1.40	1.36
39	Gg	307	CHL	C2C-C3C	3.84	1.40	1.36
39	22	607	CHL	C2C-C3C	3.84	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Nn	318	CHL	C3D-C4D	3.83	1.47	1.41
39	GG	609	CHL	C2C-C3C	3.83	1.40	1.36
42	R	617	NEX	C7-C6	-3.82	1.26	1.30
39	g	607	CHL	C2C-C3C	3.82	1.40	1.36
33	AA	407	PHO	C1D-C2D	3.82	1.43	1.39
39	3	608	CHL	C2C-C3C	3.82	1.40	1.36
42	Y	619	NEX	C7-C6	-3.81	1.26	1.30
42	y	319	NEX	C7-C6	-3.81	1.26	1.30
42	YY	617	NEX	C7-C6	-3.81	1.26	1.30
39	N	601	CHL	C2C-C3C	3.80	1.40	1.36
39	YY	605	CHL	C2C-C3C	3.80	1.40	1.36
39	y	311	CHL	C2C-C3C	3.80	1.40	1.36
44	CC	522	DGD	O2G-C1B	3.79	1.45	1.34
39	N	608	CHL	C2C-C3C	3.79	1.40	1.36
32	g	612	CLA	C1D-ND	3.79	1.42	1.37
42	NN	618	NEX	C7-C8	-3.79	1.25	1.31
42	Nn	309	NEX	C7-C6	-3.79	1.26	1.30
39	G	606	CHL	C2C-C3C	3.79	1.40	1.36
32	GG	612	CLA	C1D-ND	3.79	1.42	1.37
39	S	605	CHL	C2C-C3C	3.78	1.40	1.36
39	r	605	CHL	C2C-C3C	3.78	1.40	1.36
39	Yy	601	CHL	C2C-C3C	3.77	1.40	1.36
39	NN	601	CHL	C2C-C3C	3.77	1.40	1.36
32	1	609	CLA	C1D-ND	3.77	1.42	1.37
39	y	303	CHL	C2C-C3C	3.76	1.40	1.36
42	RR	317	NEX	C7-C6	-3.76	1.26	1.30
32	r	610	CLA	C1D-ND	3.76	1.42	1.37
39	44	605	CHL	C2C-C3C	3.75	1.40	1.36
42	Rr	616	NEX	C7-C6	-3.75	1.26	1.30
42	N	618	NEX	C7-C8	-3.75	1.25	1.31
39	Gg	308	CHL	C2C-C3C	3.74	1.40	1.36
33	a	409	PHO	C4D-CHA	3.73	1.45	1.39
39	Nn	317	CHL	C2C-C3C	3.73	1.40	1.36
39	SS	306	CHL	C2C-C3C	3.73	1.40	1.36
33	a	408	PHO	C4D-CHA	3.73	1.45	1.39
32	r	601	CLA	C1D-ND	3.72	1.42	1.37
32	G	612	CLA	C1D-ND	3.72	1.42	1.37
39	N	606	CHL	C1A-CHA	-3.72	1.35	1.40
33	Aa	408	PHO	C4D-CHA	3.72	1.45	1.39
39	GG	607	CHL	C2C-C3C	3.72	1.40	1.36
39	NN	609	CHL	C2C-C3C	3.72	1.40	1.36
32	S	608	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	610	CLA	C1D-ND	3.71	1.42	1.37
39	NN	606	CHL	C1A-CHA	-3.71	1.35	1.40
39	Yy	605	CHL	C2C-C3C	3.71	1.40	1.36
39	y	310	CHL	C2C-C3C	3.70	1.40	1.36
33	AA	407	PHO	C4D-CHA	3.70	1.45	1.39
42	Yy	617	NEX	C7-C6	-3.70	1.26	1.30
39	Yy	608	CHL	C2C-C3C	3.69	1.39	1.36
32	3	609	CLA	C1D-ND	3.69	1.42	1.37
32	Rr	601	CLA	C1D-ND	3.69	1.42	1.37
32	1	612	CLA	C1D-ND	3.69	1.42	1.37
33	Aa	409	PHO	C4D-CHA	3.68	1.45	1.39
39	YY	606	CHL	C1A-CHA	-3.68	1.35	1.40
39	G	607	CHL	C2C-C3C	3.68	1.39	1.36
32	YY	612	CLA	C1D-ND	3.68	1.42	1.37
32	Aa	406	CLA	C1D-ND	3.68	1.42	1.37
39	Gg	302	CHL	C1A-CHA	-3.67	1.35	1.40
42	YY	617	NEX	C7-C8	-3.67	1.25	1.31
32	G	611	CLA	C1D-ND	3.66	1.42	1.37
33	DD	402	PHO	C4D-CHA	3.66	1.45	1.39
32	d	401	CLA	C1D-ND	3.66	1.42	1.37
39	GG	606	CHL	C2C-C3C	3.66	1.39	1.36
42	Y	617	NEX	C7-C8	-3.66	1.26	1.31
32	Rr	602	CLA	C1D-ND	3.65	1.42	1.37
32	3	610	CLA	C1D-ND	3.65	1.42	1.37
39	R	605	CHL	C1A-CHA	-3.64	1.35	1.40
32	33	609	CLA	C1D-ND	3.64	1.42	1.37
32	1	611	CLA	C1D-ND	3.64	1.42	1.37
32	11	604	CLA	C1D-ND	3.63	1.42	1.37
32	11	613	CLA	C1D-ND	3.63	1.42	1.37
32	1	603	CLA	C1D-ND	3.63	1.42	1.37
39	Y	608	CHL	C2C-C3C	3.63	1.39	1.36
32	r	612	CLA	C1D-ND	3.62	1.42	1.37
33	A	407	PHO	C4D-CHA	3.62	1.45	1.39
39	N	609	CHL	C2C-C3C	3.62	1.39	1.36
32	R	614	CLA	C1D-ND	3.62	1.42	1.37
42	Y	619	NEX	C7-C8	-3.61	1.26	1.31
32	S	609	CLA	C1D-ND	3.61	1.42	1.37
32	22	610	CLA	C1D-ND	3.61	1.42	1.37
32	RR	312	CLA	C1D-ND	3.61	1.42	1.37
39	RR	305	CHL	C1A-CHA	-3.61	1.35	1.40
39	g	609	CHL	C2C-C3C	3.60	1.39	1.36
32	11	609	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Rr	610	CLA	C1D-ND	3.60	1.42	1.37
32	33	604	CLA	C1D-ND	3.59	1.42	1.37
32	3	604	CLA	C1D-ND	3.59	1.42	1.37
42	g	617	NEX	C7-C8	-3.59	1.26	1.31
39	n	607	CHL	C2C-C3C	3.59	1.39	1.36
39	N	607	CHL	C2C-C3C	3.59	1.39	1.36
42	Nn	309	NEX	C7-C8	-3.59	1.26	1.31
32	R	614	CLA	C4B-NB	3.58	1.42	1.37
39	n	609	CHL	C2C-C3C	3.58	1.39	1.36
39	NN	607	CHL	C2C-C3C	3.58	1.39	1.36
42	n	617	NEX	C7-C8	-3.58	1.26	1.31
39	Gg	310	CHL	C2C-C3C	3.58	1.39	1.36
32	S	603	CLA	C1D-ND	3.58	1.42	1.37
32	44	615	CLA	C1D-ND	3.57	1.42	1.37
32	g	611	CLA	C1D-ND	3.57	1.42	1.37
32	s	613	CLA	C1D-ND	3.57	1.42	1.37
39	Nn	316	CHL	C2C-C3C	3.57	1.39	1.36
39	g	601	CHL	C2C-C3C	3.57	1.39	1.36
32	22	602	CLA	C1D-ND	3.56	1.42	1.37
32	s	610	CLA	C1D-ND	3.56	1.42	1.37
32	2	610	CLA	C1D-ND	3.56	1.42	1.37
32	33	610	CLA	C1D-ND	3.56	1.42	1.37
42	n	617	NEX	C7-C6	-3.56	1.26	1.30
32	GG	613	CLA	C1D-ND	3.56	1.42	1.37
32	2	612	CLA	C1D-ND	3.56	1.42	1.37
39	G	601	CHL	C2C-C3C	3.56	1.39	1.36
32	Ss	611	CLA	C1D-ND	3.56	1.42	1.37
32	3	612	CLA	C1D-ND	3.56	1.42	1.37
39	G	606	CHL	C1A-CHA	-3.55	1.36	1.40
32	11	602	CLA	C1D-ND	3.55	1.42	1.37
42	RR	317	NEX	C7-C8	-3.55	1.26	1.31
32	3	611	CLA	C1D-ND	3.55	1.42	1.37
39	GG	606	CHL	C1A-CHA	-3.55	1.36	1.40
32	Gg	314	CLA	C1D-ND	3.55	1.42	1.37
32	1	604	CLA	C1D-ND	3.55	1.42	1.37
32	1	613	CLA	C1D-ND	3.55	1.42	1.37
32	SS	309	CLA	C1D-ND	3.55	1.42	1.37
32	Ss	613	CLA	C1D-ND	3.55	1.42	1.37
39	Yy	601	CHL	C1A-CHA	-3.54	1.36	1.40
32	Dd	401	CLA	C1D-ND	3.54	1.42	1.37
32	SS	310	CLA	C1D-ND	3.54	1.42	1.37
33	D	402	PHO	C4D-CHA	3.54	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	601	CHL	C2C-C3C	3.54	1.39	1.36
32	r	611	CLA	C1D-ND	3.54	1.42	1.37
32	r	609	CLA	C1D-ND	3.54	1.42	1.37
32	Ss	610	CLA	C1D-ND	3.53	1.42	1.37
32	n	610	CLA	C1D-ND	3.53	1.42	1.37
32	22	611	CLA	C1D-ND	3.53	1.42	1.37
32	2	611	CLA	C1D-ND	3.53	1.42	1.37
39	y	309	CHL	C2C-C3C	3.53	1.39	1.36
42	Rr	616	NEX	C7-C8	-3.52	1.26	1.31
32	Rr	611	CLA	C1D-ND	3.52	1.42	1.37
32	11	611	CLA	C1D-ND	3.52	1.42	1.37
32	Rr	610	CLA	C4B-NB	3.52	1.42	1.37
46	Ee	101	HEM	FE-NB	3.52	2.05	1.94
32	2	604	CLA	C1D-ND	3.52	1.42	1.37
42	y	319	NEX	C7-C8	-3.51	1.26	1.31
32	Ss	603	CLA	C1D-ND	3.51	1.42	1.37
39	Y	606	CHL	C1A-CHA	-3.51	1.36	1.40
32	2	609	CLA	C1D-ND	3.51	1.42	1.37
32	2	603	CLA	C1D-ND	3.51	1.42	1.37
39	YY	601	CHL	C2C-C3C	3.51	1.39	1.36
32	33	611	CLA	C1D-ND	3.51	1.42	1.37
42	R	617	NEX	C7-C8	-3.51	1.26	1.31
39	y	303	CHL	C1A-CHA	-3.51	1.36	1.40
32	SS	313	CLA	C1D-ND	3.50	1.42	1.37
39	NN	601	CHL	C1A-CHA	-3.50	1.36	1.40
39	YY	606	CHL	C2C-C3C	3.50	1.39	1.36
32	RR	314	CLA	C4B-NB	3.50	1.42	1.37
32	r	611	CLA	C4B-NB	3.50	1.42	1.37
32	33	613	CLA	C1D-ND	3.50	1.42	1.37
32	G	610	CLA	C4B-NB	3.50	1.42	1.37
32	3	602	CLA	C1D-ND	3.50	1.42	1.37
32	S	612	CLA	C1D-ND	3.50	1.42	1.37
32	c	511	CLA	C1D-ND	3.50	1.42	1.37
32	3	609	CLA	C4B-NB	3.50	1.42	1.37
32	Aa	410	CLA	C1D-ND	3.50	1.42	1.37
39	4	306	CHL	C2C-C3C	3.50	1.39	1.36
39	GG	601	CHL	C2C-C3C	3.49	1.39	1.36
32	44	610	CLA	C1D-ND	3.49	1.42	1.37
35	A	410	PL9	C7-C3	3.49	1.55	1.51
32	3	603	CLA	C1D-ND	3.49	1.42	1.37
32	Ss	604	CLA	C1D-ND	3.49	1.42	1.37
32	Nn	303	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	613	CLA	C1D-ND	3.49	1.42	1.37
32	33	612	CLA	C1D-ND	3.49	1.42	1.37
32	a	410	CLA	C1D-ND	3.49	1.42	1.37
32	11	603	CLA	C1D-ND	3.48	1.42	1.37
32	2	602	CLA	C1D-ND	3.48	1.42	1.37
32	3	604	CLA	C4B-NB	3.48	1.42	1.37
32	n	612	CLA	C1D-ND	3.48	1.42	1.37
39	N	608	CHL	C1A-CHA	-3.48	1.36	1.40
32	R	613	CLA	C1D-ND	3.48	1.42	1.37
32	r	603	CLA	C1D-ND	3.48	1.42	1.37
32	R	612	CLA	C1D-ND	3.48	1.42	1.37
32	22	604	CLA	C1D-ND	3.48	1.42	1.37
32	R	601	CLA	C1D-ND	3.48	1.42	1.37
35	AA	410	PL9	C7-C3	3.48	1.55	1.51
32	N	614	CLA	C1D-ND	3.48	1.42	1.37
32	22	613	CLA	C1D-ND	3.47	1.42	1.37
32	33	603	CLA	C1D-ND	3.47	1.42	1.37
32	22	609	CLA	C1D-ND	3.47	1.42	1.37
32	Cc	506	CLA	C1D-ND	3.47	1.42	1.37
32	1	610	CLA	C1D-ND	3.47	1.42	1.37
32	s	611	CLA	C1D-ND	3.47	1.42	1.37
32	SS	310	CLA	C4B-NB	3.47	1.42	1.37
32	Bb	615	CLA	C1D-ND	3.47	1.42	1.37
32	RR	311	CLA	C1D-ND	3.47	1.42	1.37
39	NN	608	CHL	C1A-CHA	-3.47	1.36	1.40
32	Rr	613	CLA	C1D-ND	3.46	1.42	1.37
32	YY	604	CLA	C1D-ND	3.46	1.42	1.37
39	Nn	318	CHL	C1A-CHA	-3.46	1.36	1.40
39	1	608	CHL	C2C-C3C	3.46	1.39	1.36
39	g	607	CHL	C1A-CHA	-3.46	1.36	1.40
32	S	611	CLA	C1D-ND	3.46	1.42	1.37
39	N	601	CHL	C1A-CHA	-3.46	1.36	1.40
39	Nn	319	CHL	C2C-C3C	3.46	1.39	1.36
32	22	613	CLA	C4B-NB	3.46	1.42	1.37
39	n	608	CHL	C1A-CHA	-3.46	1.36	1.40
32	Rr	612	CLA	C1D-ND	3.46	1.42	1.37
32	b	613	CLA	C1D-ND	3.46	1.42	1.37
32	r	602	CLA	C1D-ND	3.46	1.42	1.37
32	RR	308	CLA	C1D-ND	3.46	1.42	1.37
32	33	602	CLA	C1D-ND	3.45	1.42	1.37
32	s	604	CLA	C1D-ND	3.45	1.42	1.37
32	N	612	CLA	C1D-ND	3.45	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	604	CLA	C1D-ND	3.45	1.42	1.37
32	SS	312	CLA	C1D-ND	3.45	1.42	1.37
32	Bb	613	CLA	C1D-ND	3.45	1.42	1.37
32	g	614	CLA	C1D-ND	3.45	1.42	1.37
32	RR	310	CLA	C1D-ND	3.45	1.42	1.37
32	22	603	CLA	C1D-ND	3.44	1.42	1.37
32	R	610	CLA	C1D-ND	3.44	1.42	1.37
32	NN	614	CLA	C1D-ND	3.44	1.42	1.37
32	CC	505	CLA	C1D-ND	3.44	1.42	1.37
32	GG	610	CLA	C1D-ND	3.44	1.42	1.37
32	1	602	CLA	C1D-ND	3.44	1.42	1.37
32	Rr	604	CLA	C1D-ND	3.44	1.42	1.37
32	Gg	313	CLA	C1D-ND	3.43	1.42	1.37
32	R	608	CLA	C1D-ND	3.43	1.42	1.37
32	Nn	305	CLA	C1D-ND	3.43	1.42	1.37
32	Y	604	CLA	C1D-ND	3.43	1.42	1.37
32	b	615	CLA	C1D-ND	3.43	1.42	1.37
42	Yy	617	NEX	C7-C8	-3.43	1.26	1.31
32	44	603	CLA	C1D-ND	3.43	1.42	1.37
32	11	610	CLA	C4B-NB	3.43	1.42	1.37
32	RR	304	CLA	C4B-NB	3.42	1.42	1.37
32	s	603	CLA	C1D-ND	3.42	1.42	1.37
32	RR	302	CLA	C1D-ND	3.42	1.42	1.37
32	Cc	513	CLA	C1D-ND	3.42	1.42	1.37
32	R	611	CLA	C1D-ND	3.42	1.42	1.37
32	a	407	CLA	C1D-ND	3.42	1.42	1.37
32	N	610	CLA	C1D-ND	3.42	1.42	1.37
32	SS	311	CLA	C1D-ND	3.42	1.42	1.37
32	C	511	CLA	C1D-ND	3.42	1.42	1.37
32	b	601	CLA	C1D-ND	3.42	1.42	1.37
32	Rr	603	CLA	C1D-ND	3.42	1.42	1.37
32	g	603	CLA	C1D-ND	3.42	1.42	1.37
32	r	608	CLA	C1D-ND	3.42	1.42	1.37
32	4	304	CLA	C1D-ND	3.41	1.42	1.37
32	11	603	CLA	C4B-NB	3.41	1.42	1.37
32	S	613	CLA	C1D-ND	3.41	1.42	1.37
32	n	614	CLA	C1D-ND	3.41	1.42	1.37
32	RR	313	CLA	C1D-ND	3.41	1.42	1.37
32	g	602	CLA	C1D-ND	3.41	1.42	1.37
32	RR	314	CLA	C1D-ND	3.41	1.42	1.37
32	Aa	405	CLA	C1D-ND	3.41	1.42	1.37
32	Rr	609	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	604	CLA	C1D-ND	3.41	1.42	1.37
32	b	606	CLA	C1D-ND	3.41	1.42	1.37
32	44	611	CLA	C1D-ND	3.41	1.42	1.37
32	2	613	CLA	C1D-ND	3.41	1.42	1.37
32	Bb	603	CLA	C1D-ND	3.41	1.42	1.37
32	Nn	302	CLA	C1D-ND	3.41	1.42	1.37
32	Ss	602	CLA	C1D-ND	3.40	1.42	1.37
32	G	603	CLA	C1D-ND	3.40	1.42	1.37
32	Gg	315	CLA	C1D-ND	3.40	1.42	1.37
32	c	510	CLA	C1D-ND	3.40	1.42	1.37
32	Cc	512	CLA	C1D-ND	3.40	1.42	1.37
32	B	604	CLA	C1D-ND	3.40	1.42	1.37
32	r	613	CLA	C1D-ND	3.40	1.42	1.37
32	G	614	CLA	C1D-ND	3.40	1.42	1.37
32	GG	614	CLA	C1D-ND	3.40	1.42	1.37
32	BB	608	CLA	C1D-ND	3.40	1.42	1.37
32	22	612	CLA	C1D-ND	3.40	1.42	1.37
32	C	508	CLA	C1D-ND	3.40	1.42	1.37
32	11	610	CLA	C1D-ND	3.39	1.42	1.37
32	BB	612	CLA	C1D-ND	3.39	1.42	1.37
32	1	609	CLA	C4B-NB	3.39	1.42	1.37
32	A	408	CLA	C1D-ND	3.39	1.42	1.37
32	C	515	CLA	C1D-ND	3.39	1.42	1.37
32	y	304	CLA	C1D-ND	3.39	1.42	1.37
32	Cc	510	CLA	C1D-ND	3.39	1.42	1.37
32	S	604	CLA	C1D-ND	3.39	1.42	1.37
32	s	608	CLA	C1D-ND	3.39	1.42	1.37
32	NN	612	CLA	C1D-ND	3.39	1.42	1.37
32	SS	304	CLA	C1D-ND	3.39	1.42	1.37
32	g	604	CLA	C1D-ND	3.39	1.42	1.37
32	SS	314	CLA	C1D-ND	3.38	1.42	1.37
39	Yy	609	CHL	C2C-C3C	3.38	1.39	1.36
32	4	311	CLA	C1D-ND	3.38	1.42	1.37
32	SS	305	CLA	C1D-ND	3.38	1.42	1.37
32	Gg	304	CLA	C1D-ND	3.38	1.42	1.37
32	C	509	CLA	C1D-ND	3.38	1.42	1.37
32	y	305	CLA	C1D-ND	3.38	1.42	1.37
32	4	312	CLA	C1D-ND	3.38	1.42	1.37
32	CC	514	CLA	C1D-ND	3.38	1.42	1.37
32	Gg	312	CLA	C1D-ND	3.38	1.42	1.37
32	n	611	CLA	C1D-ND	3.38	1.42	1.37
32	Bb	604	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	YY	607	CHL	C1A-CHA	-3.38	1.36	1.40
32	Bb	601	CLA	C1D-ND	3.37	1.42	1.37
32	1	610	CLA	C4B-NB	3.37	1.42	1.37
32	YY	612	CLA	C4B-NB	3.37	1.42	1.37
32	B	609	CLA	C1D-ND	3.37	1.42	1.37
32	c	513	CLA	C1D-ND	3.37	1.42	1.37
32	BB	609	CLA	C1D-ND	3.37	1.42	1.37
32	C	506	CLA	C1D-ND	3.37	1.42	1.37
32	b	603	CLA	C1D-ND	3.37	1.42	1.37
32	s	603	CLA	C4B-NB	3.37	1.42	1.37
39	GG	608	CHL	C1A-CHA	-3.37	1.36	1.40
32	11	604	CLA	C4B-NB	3.37	1.42	1.37
32	N	602	CLA	C1D-ND	3.37	1.42	1.37
32	g	610	CLA	C1D-ND	3.37	1.42	1.37
32	Gg	311	CLA	C1D-ND	3.37	1.42	1.37
32	3	603	CLA	C4B-NB	3.37	1.42	1.37
32	Rr	608	CLA	C1D-ND	3.37	1.42	1.37
32	YY	602	CLA	C1D-ND	3.36	1.42	1.37
32	11	609	CLA	C4B-NB	3.36	1.42	1.37
39	YY	608	CHL	C1A-CHA	-3.36	1.36	1.40
32	G	602	CLA	C1D-ND	3.36	1.42	1.37
32	Ss	603	CLA	C4B-NB	3.36	1.42	1.37
32	33	604	CLA	C4B-NB	3.36	1.42	1.37
32	Y	614	CLA	C1D-ND	3.36	1.42	1.37
39	44	608	CHL	C1A-CHA	-3.36	1.36	1.40
32	B	608	CLA	C1D-ND	3.36	1.42	1.37
39	GG	605	CHL	C1A-CHA	-3.36	1.36	1.40
32	G	613	CLA	C1D-ND	3.36	1.42	1.37
32	C	512	CLA	C1D-ND	3.36	1.42	1.37
39	g	609	CHL	C1A-CHA	-3.36	1.36	1.40
32	CC	508	CLA	C1D-ND	3.36	1.42	1.37
32	CC	510	CLA	C1D-ND	3.36	1.42	1.37
32	GG	604	CLA	C1D-ND	3.35	1.42	1.37
32	Nn	312	CLA	C1D-ND	3.35	1.42	1.37
32	4	310	CLA	C1D-ND	3.35	1.42	1.37
32	B	623	CLA	C1D-ND	3.35	1.42	1.37
46	e	101	HEM	FE-NB	3.35	2.05	1.94
32	Bb	606	CLA	C1D-ND	3.35	1.42	1.37
32	a	406	CLA	C1D-ND	3.35	1.42	1.37
32	c	508	CLA	C1D-ND	3.35	1.42	1.37
32	NN	610	CLA	C1D-ND	3.35	1.42	1.37
32	Cc	515	CLA	C1D-ND	3.35	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Yy	602	CLA	C1D-ND	3.35	1.42	1.37
32	Bb	616	CLA	C1D-ND	3.35	1.42	1.37
32	22	610	CLA	C4B-NB	3.35	1.42	1.37
32	Cc	504	CLA	C1D-ND	3.35	1.42	1.37
39	g	601	CHL	C1A-CHA	-3.35	1.36	1.40
32	Ss	609	CLA	C1D-ND	3.35	1.42	1.37
32	s	609	CLA	C1D-ND	3.35	1.42	1.37
32	CC	507	CLA	C1D-ND	3.35	1.42	1.37
32	1	604	CLA	C4B-NB	3.35	1.42	1.37
32	c	504	CLA	C1D-ND	3.35	1.42	1.37
32	Yy	603	CLA	C1D-ND	3.34	1.42	1.37
32	C	510	CLA	C1D-ND	3.34	1.42	1.37
39	Rr	606	CHL	C1A-CHA	-3.34	1.36	1.40
39	R	606	CHL	C1A-CHA	-3.34	1.36	1.40
32	2	602	CLA	C4B-NB	3.34	1.42	1.37
32	RR	303	CLA	C1D-ND	3.34	1.42	1.37
32	Bb	607	CLA	C1D-ND	3.34	1.42	1.37
32	Ss	608	CLA	C1D-ND	3.34	1.42	1.37
32	c	512	CLA	C1D-ND	3.34	1.42	1.37
39	SS	302	CHL	C1A-CHA	-3.34	1.36	1.40
39	Gg	308	CHL	C1A-CHA	-3.34	1.36	1.40
32	R	610	CLA	C4B-NB	3.34	1.42	1.37
32	4	305	CLA	C1D-ND	3.34	1.42	1.37
39	n	606	CHL	C2C-C3C	3.34	1.39	1.36
32	c	501	CLA	C1D-ND	3.33	1.42	1.37
32	c	503	CLA	C1D-ND	3.33	1.42	1.37
32	Y	610	CLA	C1D-ND	3.33	1.42	1.37
32	Y	612	CLA	C1D-ND	3.33	1.42	1.37
32	4	303	CLA	C1D-ND	3.33	1.42	1.37
36	4	301	LHG	O8-C23	3.33	1.46	1.33
32	BB	601	CLA	C1D-ND	3.33	1.42	1.37
32	CC	511	CLA	C1D-ND	3.33	1.42	1.37
39	S	601	CHL	C1A-CHA	-3.33	1.36	1.40
39	4	308	CHL	C1A-CHA	-3.33	1.36	1.40
32	CC	512	CLA	C1D-ND	3.33	1.42	1.37
32	a	405	CLA	C1D-ND	3.32	1.42	1.37
32	b	611	CLA	C1D-ND	3.32	1.42	1.37
32	1	611	CLA	C4B-NB	3.32	1.42	1.37
32	g	610	CLA	C4B-NB	3.32	1.42	1.37
32	AA	408	CLA	C1D-ND	3.32	1.42	1.37
32	11	613	CLA	C4B-NB	3.32	1.42	1.37
32	2	609	CLA	C4B-NB	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	602	CLA	C1D-ND	3.32	1.42	1.37
32	C	514	CLA	C1D-ND	3.32	1.42	1.37
32	GG	603	CLA	C1D-ND	3.32	1.42	1.37
39	g	608	CHL	C1A-CHA	-3.32	1.36	1.40
32	Rr	602	CLA	C4B-NB	3.32	1.42	1.37
32	NN	604	CLA	C1D-ND	3.32	1.42	1.37
32	R	604	CLA	C4B-NB	3.32	1.42	1.37
32	B	618	CLA	C1D-ND	3.32	1.42	1.37
32	g	613	CLA	C1D-ND	3.32	1.42	1.37
39	NN	606	CHL	C2C-C3C	3.32	1.39	1.36
32	3	612	CLA	C4B-NB	3.32	1.42	1.37
32	d	402	CLA	C1D-ND	3.32	1.42	1.37
39	Gg	307	CHL	C1A-CHA	-3.32	1.36	1.40
32	Y	603	CLA	C1D-ND	3.32	1.42	1.37
32	c	502	CLA	C1D-ND	3.32	1.42	1.37
32	YY	614	CLA	C1D-ND	3.32	1.42	1.37
32	D	405	CLA	C1D-ND	3.31	1.42	1.37
32	b	616	CLA	C1D-ND	3.31	1.42	1.37
39	G	605	CHL	C1A-CHA	-3.31	1.36	1.40
39	N	606	CHL	C2C-C3C	3.31	1.39	1.36
32	Nn	314	CLA	C1D-ND	3.31	1.42	1.37
32	Yy	612	CLA	C1D-ND	3.31	1.42	1.37
32	R	609	CLA	C1D-ND	3.31	1.42	1.37
32	44	609	CLA	C1D-ND	3.31	1.42	1.37
32	22	604	CLA	C4B-NB	3.31	1.42	1.37
32	b	607	CLA	C1D-ND	3.31	1.42	1.37
39	YY	601	CHL	C1A-CHA	-3.31	1.36	1.40
32	YY	611	CLA	CMD-C2D	-3.31	1.44	1.50
32	s	612	CLA	C1D-ND	3.31	1.42	1.37
32	CC	509	CLA	C1D-ND	3.31	1.42	1.37
32	Cc	509	CLA	C1D-ND	3.31	1.42	1.37
32	BB	610	CLA	C1D-ND	3.31	1.42	1.37
32	BB	613	CLA	C1D-ND	3.30	1.42	1.37
32	Cc	503	CLA	C1D-ND	3.30	1.42	1.37
32	D	404	CLA	C1D-ND	3.30	1.42	1.37
32	b	614	CLA	C1D-ND	3.30	1.42	1.37
32	N	604	CLA	C1D-ND	3.30	1.42	1.37
36	44	616	LHG	O8-C23	3.30	1.45	1.33
32	Yy	614	CLA	C1D-ND	3.30	1.42	1.37
32	Bb	614	CLA	C1D-ND	3.30	1.42	1.37
39	4	309	CHL	C1A-CHA	-3.30	1.36	1.40
32	B	604	CLA	C4B-NB	3.30	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	33	609	CLA	C4B-NB	3.30	1.42	1.37
39	s	607	CHL	C1A-CHA	-3.30	1.36	1.40
39	Gg	306	CHL	C1A-CHA	-3.30	1.36	1.40
39	Y	608	CHL	C1A-CHA	-3.30	1.36	1.40
32	33	603	CLA	C4B-NB	3.30	1.42	1.37
32	s	602	CLA	C1D-ND	3.30	1.42	1.37
32	RR	304	CLA	C1D-ND	3.30	1.42	1.37
32	22	609	CLA	C4B-NB	3.29	1.42	1.37
32	X	201	CLA	C1D-ND	3.29	1.42	1.37
32	R	603	CLA	C1D-ND	3.29	1.42	1.37
32	Cc	511	CLA	C1D-ND	3.29	1.42	1.37
32	Cc	514	CLA	C1D-ND	3.29	1.42	1.37
39	G	601	CHL	C1A-CHA	-3.29	1.36	1.40
39	Y	601	CHL	C1A-CHA	-3.29	1.36	1.40
32	S	610	CLA	C1D-ND	3.29	1.42	1.37
32	y	312	CLA	C1D-ND	3.29	1.42	1.37
32	B	605	CLA	C1D-ND	3.29	1.42	1.37
32	y	314	CLA	C1D-ND	3.29	1.42	1.37
32	R	604	CLA	C1D-ND	3.29	1.42	1.37
32	c	506	CLA	C1D-ND	3.29	1.42	1.37
32	Aa	407	CLA	C1D-ND	3.29	1.42	1.37
32	b	610	CLA	C1D-ND	3.29	1.42	1.37
39	Nn	319	CHL	C1A-CHA	-3.29	1.36	1.40
39	44	601	CHL	C1A-CHA	-3.29	1.36	1.40
39	Gg	309	CHL	C1A-CHA	-3.29	1.36	1.40
32	XX	201	CLA	C1D-ND	3.28	1.42	1.37
42	Gg	318	NEX	C7-C6	-3.28	1.26	1.30
32	R	602	CLA	C1D-ND	3.28	1.42	1.37
39	n	609	CHL	C1A-CHA	-3.28	1.36	1.40
32	RR	309	CLA	C1D-ND	3.28	1.42	1.37
32	1	612	CLA	C4B-NB	3.28	1.42	1.37
32	Bb	611	CLA	C1D-ND	3.28	1.42	1.37
32	G	604	CLA	C1D-ND	3.28	1.42	1.37
32	N	611	CLA	C1D-ND	3.28	1.42	1.37
32	Ss	612	CLA	C4B-NB	3.28	1.42	1.37
39	4	302	CHL	C1A-CHA	-3.28	1.36	1.40
32	Ss	612	CLA	C1D-ND	3.28	1.42	1.37
32	s	604	CLA	C4B-NB	3.28	1.42	1.37
32	y	316	CLA	C1D-ND	3.28	1.42	1.37
39	Yy	606	CHL	C2C-C3C	3.28	1.39	1.36
32	CC	504	CLA	C1D-ND	3.28	1.42	1.37
32	Gg	303	CLA	C1D-ND	3.28	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	XX	201	CLA	C4B-NB	3.28	1.42	1.37
39	SS	308	CHL	C1A-CHA	-3.27	1.36	1.40
32	YY	610	CLA	C1D-ND	3.27	1.42	1.37
39	Rr	605	CHL	C1A-CHA	-3.27	1.36	1.40
32	33	602	CLA	C4B-NB	3.27	1.42	1.37
32	Gg	305	CLA	C1D-ND	3.27	1.42	1.37
32	c	509	CLA	C1D-ND	3.27	1.42	1.37
32	Bb	609	CLA	C1D-ND	3.27	1.42	1.37
32	b	605	CLA	C1D-ND	3.27	1.42	1.37
32	BB	606	CLA	C1D-ND	3.27	1.42	1.37
35	d	404	PL9	C7-C3	3.27	1.55	1.51
32	44	604	CLA	C1D-ND	3.26	1.42	1.37
32	Dd	402	CLA	C1D-ND	3.26	1.42	1.37
32	C	505	CLA	C1D-ND	3.26	1.42	1.37
32	y	306	CLA	C1D-ND	3.26	1.42	1.37
32	YY	603	CLA	C1D-ND	3.26	1.42	1.37
32	Nn	301	CLA	C1D-ND	3.26	1.42	1.37
32	2	604	CLA	C4B-NB	3.26	1.42	1.37
32	y	315	CLA	C4B-NB	3.26	1.42	1.37
32	B	606	CLA	C1D-ND	3.26	1.42	1.37
32	Bb	605	CLA	C1D-ND	3.26	1.42	1.37
32	SS	303	CLA	C1D-ND	3.26	1.42	1.37
32	BB	615	CLA	C1D-ND	3.26	1.42	1.37
39	s	601	CHL	C1A-CHA	-3.26	1.36	1.40
32	B	619	CLA	C1D-ND	3.26	1.42	1.37
32	2	611	CLA	C4B-NB	3.25	1.42	1.37
32	N	611	CLA	C4B-NB	3.25	1.42	1.37
32	C	513	CLA	C1D-ND	3.25	1.42	1.37
32	r	603	CLA	C4B-NB	3.25	1.42	1.37
32	3	611	CLA	C4B-NB	3.25	1.42	1.37
32	r	608	CLA	C4B-NB	3.25	1.42	1.37
32	33	612	CLA	C4B-NB	3.25	1.42	1.37
39	g	605	CHL	C1A-CHA	-3.25	1.36	1.40
46	EE	102	HEM	FE-NC	3.25	2.05	1.95
32	Bb	610	CLA	C1D-ND	3.25	1.42	1.37
32	Bb	612	CLA	C1D-ND	3.25	1.42	1.37
39	44	606	CHL	C1A-CHA	-3.25	1.36	1.40
32	BB	605	CLA	C1D-ND	3.25	1.42	1.37
32	g	604	CLA	C4B-NB	3.24	1.42	1.37
32	GG	602	CLA	C1D-ND	3.24	1.42	1.37
32	Yy	610	CLA	C1D-ND	3.24	1.42	1.37
32	3	613	CLA	C4B-NB	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Yy	606	CHL	C1A-CHA	-3.24	1.36	1.40
32	S	608	CLA	C4B-NB	3.24	1.42	1.37
32	CC	513	CLA	C1D-ND	3.24	1.42	1.37
32	c	507	CLA	C1D-ND	3.24	1.42	1.37
35	DD	406	PL9	C7-C3	3.24	1.55	1.51
32	C	504	CLA	C1D-ND	3.24	1.42	1.37
32	C	503	CLA	C1D-ND	3.24	1.42	1.37
32	Yy	604	CLA	C1D-ND	3.24	1.42	1.37
32	11	612	CLA	CMD-C2D	-3.23	1.44	1.50
32	n	602	CLA	C1D-ND	3.23	1.42	1.37
32	Cc	508	CLA	C1D-ND	3.23	1.42	1.37
32	Ss	604	CLA	C4B-NB	3.23	1.42	1.37
32	Cc	507	CLA	C1D-ND	3.23	1.42	1.37
32	s	602	CLA	C4B-NB	3.23	1.42	1.37
32	NN	602	CLA	C1D-ND	3.23	1.42	1.37
32	Y	602	CLA	C1D-ND	3.23	1.42	1.37
32	n	603	CLA	C1D-ND	3.23	1.42	1.37
39	44	607	CHL	C1A-CHA	-3.23	1.36	1.40
32	44	602	CLA	C1D-ND	3.23	1.42	1.37
32	g	602	CLA	C1B-C2B	3.23	1.50	1.43
32	Nn	302	CLA	C4B-NB	3.23	1.42	1.37
32	CC	502	CLA	C1D-ND	3.23	1.42	1.37
32	r	601	CLA	C4B-NB	3.23	1.42	1.37
32	D	401	CLA	C1D-ND	3.23	1.42	1.37
32	11	611	CLA	C4B-NB	3.23	1.42	1.37
35	D	407	PL9	C7-C3	3.23	1.55	1.51
42	Gg	318	NEX	C7-C8	-3.22	1.26	1.31
39	GG	609	CHL	C1A-CHA	-3.22	1.36	1.40
32	22	611	CLA	C4B-NB	3.22	1.42	1.37
32	b	609	CLA	C1D-ND	3.22	1.42	1.37
32	Rr	611	CLA	C4B-NB	3.22	1.42	1.37
32	1	613	CLA	C4B-NB	3.22	1.42	1.37
32	Gg	305	CLA	C4B-NB	3.22	1.42	1.37
32	DD	403	CLA	C1D-ND	3.22	1.42	1.37
39	G	609	CHL	C1A-CHA	-3.22	1.36	1.40
32	2	603	CLA	C4B-NB	3.22	1.42	1.37
42	N	618	NEX	C7-C6	-3.22	1.26	1.30
35	Dd	404	PL9	C7-C3	3.22	1.55	1.51
32	33	613	CLA	C4B-NB	3.21	1.42	1.37
32	NN	611	CLA	C1D-ND	3.21	1.42	1.37
32	a	406	CLA	C4B-NB	3.21	1.42	1.37
39	Yy	608	CHL	C1A-CHA	-3.21	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	620	CLA	C1D-ND	3.21	1.42	1.37
32	SS	309	CLA	C4B-NB	3.21	1.42	1.37
39	YY	605	CHL	C1A-CHA	-3.21	1.36	1.40
32	b	604	CLA	C1D-ND	3.21	1.42	1.37
32	22	602	CLA	C4B-NB	3.21	1.42	1.37
32	g	602	CLA	C4B-NB	3.21	1.42	1.37
32	B	611	CLA	C1D-ND	3.21	1.42	1.37
32	R	601	CLA	C4B-NB	3.21	1.42	1.37
32	Nn	304	CLA	C1D-ND	3.21	1.42	1.37
32	S	604	CLA	C4B-NB	3.21	1.42	1.37
32	RR	310	CLA	C4B-NB	3.21	1.42	1.37
32	Nn	313	CLA	C1D-ND	3.21	1.42	1.37
32	1	602	CLA	C4B-NB	3.21	1.42	1.37
32	Cc	505	CLA	C1D-ND	3.20	1.42	1.37
32	DD	404	CLA	C1D-ND	3.20	1.42	1.37
32	B	622	CLA	C1D-ND	3.20	1.42	1.37
32	NN	613	CLA	C1D-ND	3.20	1.42	1.37
32	GG	602	CLA	C1B-C2B	3.20	1.50	1.43
32	BB	614	CLA	C1D-ND	3.20	1.42	1.37
32	s	612	CLA	C4B-NB	3.20	1.42	1.37
32	44	615	CLA	C4B-NB	3.20	1.42	1.37
32	n	613	CLA	C1D-ND	3.20	1.42	1.37
46	E	101	HEM	FE-NC	3.20	2.05	1.95
32	BB	603	CLA	C1D-ND	3.20	1.42	1.37
39	GG	607	CHL	C1A-CHA	-3.20	1.36	1.40
32	s	611	CLA	C4B-NB	3.20	1.42	1.37
32	g	604	CLA	C1B-C2B	3.20	1.50	1.43
32	Rr	603	CLA	C4B-NB	3.19	1.42	1.37
32	B	610	CLA	C1D-ND	3.19	1.42	1.37
32	GG	602	CLA	C4B-NB	3.19	1.42	1.37
32	S	603	CLA	C4B-NB	3.19	1.42	1.37
32	Nn	303	CLA	C4B-NB	3.19	1.42	1.37
32	Y	611	CLA	C1D-ND	3.19	1.42	1.37
32	A	406	CLA	C1D-ND	3.19	1.42	1.37
32	y	315	CLA	C1D-ND	3.19	1.42	1.37
32	b	612	CLA	C1D-ND	3.18	1.42	1.37
32	DD	401	CLA	C1D-ND	3.18	1.42	1.37
32	NN	611	CLA	C4B-NB	3.18	1.42	1.37
32	d	402	CLA	C4B-NB	3.18	1.42	1.37
39	Y	607	CHL	C1A-CHA	-3.18	1.36	1.40
32	Ss	611	CLA	C4B-NB	3.18	1.42	1.37
32	g	613	CLA	C4B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AA	405	CLA	C1D-ND	3.18	1.42	1.37
32	3	602	CLA	C4B-NB	3.18	1.42	1.37
32	N	613	CLA	C4B-NB	3.18	1.42	1.37
32	r	613	CLA	C4B-NB	3.18	1.42	1.37
32	Rr	608	CLA	C4B-NB	3.18	1.42	1.37
32	c	505	CLA	C1D-ND	3.18	1.42	1.37
32	33	611	CLA	C4B-NB	3.18	1.42	1.37
32	B	624	CLA	C1D-ND	3.18	1.42	1.37
32	2	612	CLA	C4B-NB	3.18	1.42	1.37
32	R	602	CLA	C4B-NB	3.18	1.42	1.37
32	A	405	CLA	C1D-ND	3.18	1.42	1.37
32	C	507	CLA	C1D-ND	3.18	1.42	1.37
32	b	610	CLA	C4B-NB	3.17	1.42	1.37
32	G	602	CLA	C4B-NB	3.17	1.42	1.37
32	X	201	CLA	C4B-NB	3.17	1.42	1.37
32	r	610	CLA	C4B-NB	3.17	1.42	1.37
32	BB	602	CLA	C1D-ND	3.17	1.42	1.37
32	Yy	613	CLA	C4B-NB	3.17	1.42	1.37
32	SS	305	CLA	C4B-NB	3.17	1.42	1.37
32	N	612	CLA	C4B-NB	3.17	1.42	1.37
39	Gg	310	CHL	C1A-CHA	-3.17	1.36	1.40
32	GG	604	CLA	C4B-NB	3.17	1.42	1.37
32	YY	604	CLA	C4B-NB	3.17	1.42	1.37
32	Yy	611	CLA	C1D-ND	3.16	1.42	1.37
32	Yy	613	CLA	C1D-ND	3.16	1.42	1.37
32	4	304	CLA	C4B-NB	3.16	1.42	1.37
32	Gg	314	CLA	C4B-NB	3.16	1.42	1.37
32	22	612	CLA	C4B-NB	3.16	1.42	1.37
32	11	612	CLA	C1D-ND	3.16	1.42	1.37
32	Nn	304	CLA	C4B-NB	3.16	1.42	1.37
32	y	313	CLA	C1D-ND	3.16	1.42	1.37
32	Rr	601	CLA	C4B-NB	3.15	1.42	1.37
32	11	602	CLA	C4B-NB	3.15	1.42	1.37
32	RR	302	CLA	C4B-NB	3.15	1.42	1.37
32	n	612	CLA	C4B-NB	3.15	1.42	1.37
39	Ss	607	CHL	C1A-CHA	-3.15	1.36	1.40
32	BB	604	CLA	C1D-ND	3.15	1.42	1.37
32	NN	614	CLA	C4B-NB	3.15	1.42	1.37
32	33	610	CLA	C4B-NB	3.15	1.42	1.37
39	g	606	CHL	C1A-CHA	-3.15	1.36	1.40
32	SS	304	CLA	C4B-NB	3.15	1.42	1.37
32	D	405	CLA	C4B-NB	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	307	CHL	C1A-CHA	-3.15	1.36	1.40
32	Ss	602	CLA	C4B-NB	3.15	1.42	1.37
32	Bb	607	CLA	C4B-NB	3.15	1.42	1.37
32	SS	311	CLA	C4B-NB	3.14	1.42	1.37
39	GG	601	CHL	C1A-CHA	-3.14	1.36	1.40
32	y	313	CLA	C4B-NB	3.14	1.42	1.37
32	n	613	CLA	C4B-NB	3.14	1.42	1.37
32	CC	503	CLA	C1D-ND	3.14	1.42	1.37
32	S	612	CLA	C1B-C2B	3.14	1.50	1.43
39	y	308	CHL	C2C-C3C	3.14	1.39	1.36
32	G	612	CLA	C4B-NB	3.14	1.42	1.37
32	y	316	CLA	C4B-NB	3.14	1.42	1.37
32	b	602	CLA	C1D-ND	3.14	1.42	1.37
32	n	611	CLA	C4B-NB	3.14	1.42	1.37
32	Bb	602	CLA	C1D-ND	3.14	1.42	1.37
32	44	610	CLA	C4B-NB	3.14	1.42	1.37
32	d	401	CLA	C4B-NB	3.14	1.42	1.37
32	NN	612	CLA	C4B-NB	3.14	1.42	1.37
32	4	303	CLA	C4B-NB	3.14	1.42	1.37
32	Rr	613	CLA	C4B-NB	3.13	1.42	1.37
32	S	609	CLA	C4B-NB	3.13	1.42	1.37
32	4	310	CLA	C4B-NB	3.13	1.42	1.37
32	BB	607	CLA	C1D-ND	3.13	1.42	1.37
32	GG	610	CLA	C4B-NB	3.13	1.42	1.37
46	Ee	101	HEM	CAB-C3B	3.13	1.55	1.47
32	GG	611	CLA	C4B-NB	3.13	1.42	1.37
32	Gg	303	CLA	C4B-NB	3.13	1.42	1.37
32	44	602	CLA	C4B-NB	3.13	1.42	1.37
32	4	311	CLA	C4B-NB	3.13	1.42	1.37
39	y	309	CHL	C1A-CHA	-3.13	1.36	1.40
32	G	611	CLA	C4B-NB	3.13	1.42	1.37
32	Y	613	CLA	C1D-ND	3.13	1.42	1.37
32	S	611	CLA	C4B-NB	3.12	1.42	1.37
32	GG	612	CLA	C4B-NB	3.12	1.42	1.37
32	BB	604	CLA	C4B-NB	3.12	1.42	1.37
32	Nn	301	CLA	C4B-NB	3.12	1.42	1.37
32	AA	406	CLA	C1D-ND	3.12	1.42	1.37
32	BB	611	CLA	C1D-ND	3.12	1.42	1.37
39	r	607	CHL	C1A-CHA	-3.12	1.36	1.40
32	22	603	CLA	C4B-NB	3.12	1.42	1.37
32	Y	610	CLA	C4B-NB	3.12	1.42	1.37
32	R	613	CLA	C4B-NB	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	608	CLA	C4B-NB	3.12	1.42	1.37
32	Bb	610	CLA	C4B-NB	3.12	1.42	1.37
32	GG	613	CLA	C4B-NB	3.12	1.42	1.37
32	Bb	608	CLA	C1D-ND	3.12	1.42	1.37
32	N	614	CLA	C4B-NB	3.12	1.42	1.37
46	e	101	HEM	FE-ND	3.12	2.04	1.94
39	Rr	607	CHL	C1A-CHA	-3.11	1.36	1.40
32	YY	613	CLA	C1D-ND	3.11	1.42	1.37
32	Rr	612	CLA	C4B-NB	3.11	1.42	1.37
32	c	511	CLA	C4B-NB	3.11	1.42	1.37
32	b	607	CLA	C4B-NB	3.11	1.41	1.37
32	c	510	CLA	C4B-NB	3.11	1.41	1.37
32	BB	608	CLA	C4B-NB	3.11	1.41	1.37
32	B	621	CLA	C1D-ND	3.11	1.41	1.37
32	N	604	CLA	C4B-NB	3.11	1.41	1.37
32	N	613	CLA	C1D-ND	3.11	1.41	1.37
32	Y	612	CLA	C4B-NB	3.11	1.41	1.37
32	Nn	313	CLA	C4B-NB	3.11	1.41	1.37
32	44	609	CLA	C4B-NB	3.11	1.41	1.37
32	YY	610	CLA	C4B-NB	3.11	1.41	1.37
32	r	612	CLA	C4B-NB	3.11	1.41	1.37
32	Gg	315	CLA	C4B-NB	3.11	1.41	1.37
32	RR	311	CLA	C4B-NB	3.11	1.41	1.37
32	S	612	CLA	C4B-NB	3.11	1.41	1.37
32	b	601	CLA	C4B-NB	3.11	1.41	1.37
32	b	615	CLA	C4B-NB	3.11	1.41	1.37
32	Dd	401	CLA	C4B-NB	3.11	1.41	1.37
39	YY	609	CHL	C1A-CHA	-3.10	1.36	1.40
32	G	604	CLA	C4B-NB	3.10	1.41	1.37
32	R	609	CLA	C4B-NB	3.10	1.41	1.37
32	2	610	CLA	C4B-NB	3.10	1.41	1.37
39	Ss	601	CHL	C1A-CHA	-3.10	1.36	1.40
32	Bb	601	CLA	C4B-NB	3.10	1.41	1.37
39	G	607	CHL	C1A-CHA	-3.10	1.36	1.40
32	S	602	CLA	C4B-NB	3.09	1.41	1.37
32	r	602	CLA	C4B-NB	3.09	1.41	1.37
32	Gg	312	CLA	C4B-NB	3.09	1.41	1.37
39	Y	609	CHL	C1A-CHA	-3.09	1.36	1.40
46	e	101	HEM	CAB-C3B	3.09	1.55	1.47
32	SS	313	CLA	C1B-C2B	3.09	1.50	1.43
39	3	601	CHL	C1A-CHA	-3.09	1.35	1.39
32	Y	614	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	RR	313	CLA	C4B-NB	3.09	1.41	1.37
32	Y	602	CLA	C4B-NB	3.09	1.41	1.37
32	G	613	CLA	C4B-NB	3.09	1.41	1.37
32	NN	604	CLA	C4B-NB	3.09	1.41	1.37
39	y	308	CHL	C1A-CHA	-3.09	1.36	1.40
32	N	610	CLA	C4B-NB	3.09	1.41	1.37
32	4	312	CLA	C4B-NB	3.09	1.41	1.37
32	Dd	402	CLA	C4B-NB	3.09	1.41	1.37
32	CC	506	CLA	C1D-ND	3.09	1.41	1.37
32	RR	309	CLA	C4B-NB	3.09	1.41	1.37
46	EE	102	HEM	FE-NA	3.08	2.05	1.95
32	b	608	CLA	C1D-ND	3.08	1.41	1.37
39	SS	307	CHL	C1A-CHA	-3.08	1.36	1.40
32	B	606	CLA	C4B-NB	3.08	1.41	1.37
39	r	606	CHL	C1A-CHA	-3.08	1.36	1.40
32	Y	611	CLA	C4B-NB	3.08	1.41	1.37
32	NN	613	CLA	C4B-NB	3.08	1.41	1.37
39	n	601	CHL	C1A-CHA	-3.08	1.36	1.40
32	2	613	CLA	C4B-NB	3.08	1.41	1.37
32	Y	604	CLA	C4B-NB	3.08	1.41	1.37
32	g	614	CLA	C4B-NB	3.08	1.41	1.37
32	NN	610	CLA	C4B-NB	3.08	1.41	1.37
32	GG	614	CLA	C4B-NB	3.08	1.41	1.37
32	Ss	608	CLA	C4B-NB	3.08	1.41	1.37
32	G	614	CLA	C4B-NB	3.08	1.41	1.37
32	SS	313	CLA	C4B-NB	3.08	1.41	1.37
32	BB	615	CLA	C4B-NB	3.08	1.41	1.37
32	R	603	CLA	C4B-NB	3.07	1.41	1.37
46	EE	102	HEM	CAC-C3C	3.07	1.55	1.47
39	G	608	CHL	C1A-CHA	-3.07	1.36	1.40
32	GG	613	CLA	C1B-C2B	3.07	1.50	1.43
32	Ss	613	CLA	C4B-NB	3.07	1.41	1.37
32	NN	613	CLA	C1B-C2B	3.07	1.50	1.43
32	Ss	610	CLA	C4B-NB	3.07	1.41	1.37
32	Cc	513	CLA	C4B-NB	3.07	1.41	1.37
32	11	612	CLA	C1B-C2B	3.07	1.50	1.43
32	Rr	604	CLA	C4B-NB	3.07	1.41	1.37
32	RR	312	CLA	C4B-NB	3.07	1.41	1.37
46	Ee	101	HEM	FE-ND	3.07	2.04	1.94
32	S	610	CLA	C4B-NB	3.07	1.41	1.37
39	33	601	CHL	C1A-CHA	-3.07	1.35	1.39
32	A	408	CLA	C4B-NB	3.06	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	610	CLA	C4B-NB	3.06	1.41	1.37
32	Cc	511	CLA	C4B-NB	3.06	1.41	1.37
32	CC	510	CLA	C4B-NB	3.06	1.41	1.37
32	YY	602	CLA	C4B-NB	3.06	1.41	1.37
32	1	603	CLA	C4B-NB	3.06	1.41	1.37
32	DD	404	CLA	C4B-NB	3.06	1.41	1.37
39	N	605	CHL	C1A-CHA	-3.06	1.36	1.40
32	GG	611	CLA	C1D-ND	3.06	1.41	1.37
32	s	610	CLA	C4B-NB	3.06	1.41	1.37
32	r	609	CLA	C4B-NB	3.06	1.41	1.37
32	SS	312	CLA	C4B-NB	3.06	1.41	1.37
32	YY	603	CLA	C4B-NB	3.06	1.41	1.37
32	a	407	CLA	C4B-NB	3.05	1.41	1.37
32	b	603	CLA	C4B-NB	3.05	1.41	1.37
39	y	310	CHL	C1A-CHA	-3.05	1.36	1.40
46	e	101	HEM	CAC-C3C	3.05	1.55	1.47
32	Yy	610	CLA	C4B-NB	3.05	1.41	1.37
32	Nn	305	CLA	C4B-NB	3.05	1.41	1.37
32	Rr	604	CLA	C1B-C2B	3.05	1.50	1.43
32	G	602	CLA	C1B-C2B	3.05	1.50	1.43
32	C	506	CLA	C4B-NB	3.05	1.41	1.37
32	Y	613	CLA	C4B-NB	3.05	1.41	1.37
32	4	305	CLA	C4B-NB	3.05	1.41	1.37
39	1	608	CHL	C1A-CHA	-3.05	1.35	1.39
32	Yy	614	CLA	C4B-NB	3.05	1.41	1.37
32	b	602	CLA	C4B-NB	3.05	1.41	1.37
32	BB	606	CLA	C4B-NB	3.05	1.41	1.37
32	Rr	609	CLA	C4B-NB	3.05	1.41	1.37
32	a	410	CLA	C4B-NB	3.05	1.41	1.37
32	g	612	CLA	C4B-NB	3.05	1.41	1.37
32	G	611	CLA	C1B-C2B	3.05	1.50	1.43
46	Ee	101	HEM	CAC-C3C	3.05	1.55	1.47
32	SS	303	CLA	C4B-NB	3.05	1.41	1.37
32	R	612	CLA	C4B-NB	3.04	1.41	1.37
39	Yy	609	CHL	C1A-CHA	-3.04	1.36	1.40
32	n	604	CLA	C4B-NB	3.04	1.41	1.37
32	Aa	407	CLA	C4B-NB	3.04	1.41	1.37
32	n	614	CLA	C4B-NB	3.04	1.41	1.37
32	Cc	505	CLA	C4B-NB	3.04	1.41	1.37
32	R	608	CLA	C4B-NB	3.04	1.41	1.37
32	YY	614	CLA	C4B-NB	3.04	1.41	1.37
32	Gg	303	CLA	C1B-C2B	3.04	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	603	CLA	C4B-NB	3.04	1.41	1.37
32	c	508	CLA	C4B-NB	3.04	1.41	1.37
32	3	610	CLA	C4B-NB	3.03	1.41	1.37
32	C	503	CLA	C4B-NB	3.03	1.41	1.37
32	B	621	CLA	C4B-NB	3.03	1.41	1.37
39	Yy	605	CHL	C1A-CHA	-3.03	1.36	1.40
32	s	613	CLA	C4B-NB	3.03	1.41	1.37
32	B	611	CLA	C4B-NB	3.03	1.41	1.37
32	44	603	CLA	C4B-NB	3.03	1.41	1.37
32	C	511	CLA	C4B-NB	3.03	1.41	1.37
32	Cc	512	CLA	C4B-NB	3.03	1.41	1.37
32	BB	613	CLA	C1B-C2B	3.03	1.50	1.43
32	G	610	CLA	C1B-C2B	3.02	1.50	1.43
32	r	604	CLA	C1B-C2B	3.02	1.50	1.43
32	44	611	CLA	C4B-NB	3.02	1.41	1.37
32	B	610	CLA	C4B-NB	3.02	1.41	1.37
32	Cc	507	CLA	C4B-NB	3.02	1.41	1.37
39	RR	307	CHL	C1A-CHA	-3.02	1.36	1.40
32	AA	408	CLA	C4B-NB	3.02	1.41	1.37
32	g	613	CLA	C1B-C2B	3.02	1.50	1.43
32	Bb	602	CLA	C4B-NB	3.02	1.41	1.37
32	RR	303	CLA	C4B-NB	3.02	1.41	1.37
32	C	513	CLA	C4B-NB	3.02	1.41	1.37
32	R	611	CLA	C4B-NB	3.02	1.41	1.37
32	c	504	CLA	C1B-C2B	3.02	1.50	1.43
32	c	509	CLA	C4B-NB	3.01	1.41	1.37
32	3	613	CLA	C1B-C2B	3.01	1.50	1.43
32	B	611	CLA	C1B-C2B	3.01	1.50	1.43
32	NN	602	CLA	C4B-NB	3.01	1.41	1.37
32	2	610	CLA	C1B-C2B	3.01	1.50	1.43
32	Yy	611	CLA	C4B-NB	3.01	1.41	1.37
32	n	603	CLA	C4B-NB	3.01	1.41	1.37
32	1	603	CLA	C1B-C2B	3.01	1.50	1.43
32	y	304	CLA	C4B-NB	3.01	1.41	1.37
32	Bb	604	CLA	C4B-NB	3.01	1.41	1.37
32	Ss	609	CLA	C4B-NB	3.01	1.41	1.37
32	BB	610	CLA	C4B-NB	3.01	1.41	1.37
46	E	101	HEM	CAC-C3C	3.00	1.55	1.47
32	b	608	CLA	C4B-NB	3.00	1.41	1.37
32	CC	505	CLA	C4B-NB	3.00	1.41	1.37
32	RR	308	CLA	C4B-NB	3.00	1.41	1.37
39	Y	605	CHL	C1A-CHA	-3.00	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	611	CLA	C4B-NB	3.00	1.41	1.37
32	s	609	CLA	C4B-NB	3.00	1.41	1.37
32	Gg	305	CLA	C1B-C2B	3.00	1.50	1.43
32	b	611	CLA	C4B-NB	3.00	1.41	1.37
32	NN	603	CLA	C1D-ND	3.00	1.41	1.37
32	n	602	CLA	C4B-NB	3.00	1.41	1.37
32	Cc	510	CLA	C4B-NB	3.00	1.41	1.37
32	CC	509	CLA	C4B-NB	2.99	1.41	1.37
46	E	101	HEM	CAB-C3B	2.99	1.55	1.47
32	B	623	CLA	C4B-NB	2.99	1.41	1.37
32	BB	614	CLA	C4B-NB	2.99	1.41	1.37
32	RR	312	CLA	C1B-C2B	2.99	1.50	1.43
32	B	609	CLA	C1B-C2B	2.99	1.50	1.43
46	e	101	HEM	FE-NA	2.99	2.05	1.95
32	Y	603	CLA	C4B-NB	2.99	1.41	1.37
32	C	514	CLA	C4B-NB	2.99	1.41	1.37
32	Bb	615	CLA	C4B-NB	2.99	1.41	1.37
32	y	312	CLA	C4B-NB	2.99	1.41	1.37
32	SS	314	CLA	C4B-NB	2.99	1.41	1.37
32	Aa	410	CLA	C4B-NB	2.99	1.41	1.37
39	SS	306	CHL	C1A-CHA	-2.99	1.36	1.40
39	S	606	CHL	C1A-CHA	-2.98	1.36	1.40
32	N	602	CLA	C4B-NB	2.98	1.41	1.37
32	N	603	CLA	C1D-ND	2.98	1.41	1.37
46	e	101	HEM	FE-NC	2.98	2.05	1.95
32	b	614	CLA	C4B-NB	2.98	1.41	1.37
32	c	505	CLA	C4B-NB	2.98	1.41	1.37
39	y	311	CHL	C1A-CHA	-2.98	1.36	1.40
32	A	406	CLA	C4B-NB	2.98	1.41	1.37
32	G	603	CLA	C4B-NB	2.98	1.41	1.37
32	3	610	CLA	C1B-C2B	2.98	1.50	1.43
32	n	604	CLA	C1B-C2B	2.98	1.50	1.43
32	Gg	311	CLA	C4B-NB	2.98	1.41	1.37
32	b	606	CLA	C4B-NB	2.98	1.41	1.37
32	Aa	406	CLA	C4B-NB	2.98	1.41	1.37
46	E	101	HEM	FE-NA	2.98	2.05	1.95
32	1	611	CLA	C1B-C2B	2.97	1.50	1.43
46	EE	102	HEM	CAB-C3B	2.97	1.55	1.47
32	Cc	515	CLA	C4B-NB	2.97	1.41	1.37
32	C	510	CLA	C4B-NB	2.97	1.41	1.37
32	YY	613	CLA	C4B-NB	2.97	1.41	1.37
39	3	608	CHL	C1A-CHA	-2.97	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	GG	603	CLA	C4B-NB	2.96	1.41	1.37
32	G	604	CLA	C1B-C2B	2.96	1.50	1.43
32	b	604	CLA	C4B-NB	2.96	1.41	1.37
41	y	301	XAT	C26-C27	2.96	1.55	1.50
39	R	607	CHL	C1A-CHA	-2.96	1.36	1.40
32	Bb	603	CLA	C4B-NB	2.96	1.41	1.37
32	S	613	CLA	C4B-NB	2.96	1.41	1.37
32	CC	512	CLA	C4B-NB	2.96	1.41	1.37
32	Yy	602	CLA	C4B-NB	2.96	1.41	1.37
32	A	405	CLA	C1B-C2B	2.96	1.50	1.43
32	BB	613	CLA	C4B-NB	2.96	1.41	1.37
32	r	612	CLA	C1B-C2B	2.96	1.50	1.43
32	Gg	304	CLA	C4B-NB	2.95	1.41	1.37
32	Nn	314	CLA	C4B-NB	2.95	1.41	1.37
32	C	507	CLA	C4B-NB	2.95	1.41	1.37
32	44	604	CLA	C4B-NB	2.95	1.41	1.37
39	r	605	CHL	C1A-CHA	-2.95	1.36	1.40
32	C	505	CLA	C4B-NB	2.95	1.41	1.37
32	c	503	CLA	C4B-NB	2.95	1.41	1.37
32	AA	406	CLA	C4B-NB	2.95	1.41	1.37
32	BB	602	CLA	C4B-NB	2.95	1.41	1.37
32	33	613	CLA	C1B-C2B	2.95	1.50	1.43
46	Ee	101	HEM	FE-NA	2.95	2.04	1.95
32	BB	601	CLA	C4B-NB	2.95	1.41	1.37
32	B	622	CLA	C4B-NB	2.95	1.41	1.37
32	g	603	CLA	C4B-NB	2.95	1.41	1.37
32	Gg	313	CLA	C4B-NB	2.94	1.41	1.37
39	y	307	CHL	C1A-CHA	-2.94	1.36	1.40
39	NN	605	CHL	C1A-CHA	-2.94	1.36	1.40
32	CC	506	CLA	C4B-NB	2.94	1.41	1.37
32	D	405	CLA	C1B-C2B	2.94	1.50	1.43
32	3	609	CLA	C1B-C2B	2.94	1.50	1.43
32	r	604	CLA	C4B-NB	2.94	1.41	1.37
32	CC	513	CLA	C4B-NB	2.94	1.41	1.37
39	11	605	CHL	C1A-CHA	-2.94	1.36	1.39
32	BB	612	CLA	C4B-NB	2.93	1.41	1.37
46	EE	102	HEM	FE-ND	2.93	2.03	1.94
39	1	601	CHL	C1A-CHA	-2.93	1.36	1.39
39	2	608	CHL	C1A-CHA	-2.93	1.36	1.39
32	Yy	604	CLA	C4B-NB	2.93	1.41	1.37
39	RR	306	CHL	C1A-CHA	-2.93	1.36	1.40
32	c	504	CLA	C4B-NB	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	515	CLA	C4B-NB	2.92	1.41	1.37
39	44	605	CHL	C1A-CHA	-2.92	1.36	1.40
32	c	502	CLA	C4B-NB	2.92	1.41	1.37
32	Y	611	CLA	C1B-C2B	2.92	1.50	1.43
46	E	101	HEM	FE-ND	2.92	2.03	1.94
32	Bb	616	CLA	C4B-NB	2.91	1.41	1.37
32	B	607	CLA	C1D-ND	2.91	1.41	1.37
32	B	619	CLA	C4B-NB	2.91	1.41	1.37
32	Cc	503	CLA	C1B-C2B	2.91	1.50	1.43
32	Bb	611	CLA	C4B-NB	2.91	1.41	1.37
32	1	609	CLA	C1B-C2B	2.91	1.50	1.43
32	NN	603	CLA	C4B-NB	2.91	1.41	1.37
32	YY	611	CLA	C4B-NB	2.91	1.41	1.37
32	C	512	CLA	C4B-NB	2.91	1.41	1.37
32	Cc	503	CLA	C4B-NB	2.91	1.41	1.37
39	33	608	CHL	C1A-CHA	-2.91	1.36	1.39
32	Cc	506	CLA	C1B-C2B	2.91	1.49	1.43
39	Nn	316	CHL	C1A-CHA	-2.90	1.36	1.40
32	3	612	CLA	C1B-C2B	2.90	1.49	1.43
32	b	616	CLA	C4B-NB	2.90	1.41	1.37
32	C	508	CLA	C4B-NB	2.90	1.41	1.37
32	B	607	CLA	C4B-NB	2.90	1.41	1.37
32	b	605	CLA	C4B-NB	2.90	1.41	1.37
32	B	620	CLA	C4B-NB	2.90	1.41	1.37
32	c	501	CLA	C4B-NB	2.90	1.41	1.37
32	b	612	CLA	C4B-NB	2.90	1.41	1.37
32	CC	504	CLA	C4B-NB	2.90	1.41	1.37
32	y	315	CLA	C1B-C2B	2.90	1.49	1.43
32	Gg	314	CLA	C1B-C2B	2.90	1.49	1.43
32	c	513	CLA	C4B-NB	2.89	1.41	1.37
32	Rr	612	CLA	C1B-C2B	2.89	1.49	1.43
32	B	609	CLA	C4B-NB	2.89	1.41	1.37
32	22	603	CLA	C1B-C2B	2.89	1.49	1.43
32	2	611	CLA	C1B-C2B	2.89	1.49	1.43
32	c	506	CLA	C4B-NB	2.89	1.41	1.37
32	AA	405	CLA	C4B-NB	2.89	1.41	1.37
32	BB	605	CLA	C4B-NB	2.89	1.41	1.37
39	n	606	CHL	C1A-CHA	-2.89	1.36	1.40
32	A	405	CLA	C4B-NB	2.88	1.41	1.37
32	Cc	508	CLA	C4B-NB	2.88	1.41	1.37
39	Gg	302	CHL	CMD-C2D	-2.88	1.45	1.51
32	y	306	CLA	C4B-NB	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Bb	614	CLA	C4B-NB	2.88	1.41	1.37
32	B	618	CLA	C4B-NB	2.88	1.41	1.37
32	B	624	CLA	C4B-NB	2.88	1.41	1.37
46	EE	102	HEM	FE-NB	2.88	2.03	1.94
32	CC	507	CLA	C4B-NB	2.88	1.41	1.37
32	Bb	605	CLA	C4B-NB	2.88	1.41	1.37
32	2	613	CLA	C1B-C2B	2.88	1.49	1.43
36	4	301	LHG	O7-C5	-2.87	1.42	1.46
32	33	610	CLA	C1B-C2B	2.87	1.49	1.43
32	D	401	CLA	C4B-NB	2.87	1.41	1.37
32	Nn	303	CLA	C1B-C2B	2.87	1.49	1.43
32	Bb	606	CLA	C4B-NB	2.87	1.41	1.37
32	CC	502	CLA	C4B-NB	2.87	1.41	1.37
46	E	101	HEM	FE-NB	2.87	2.03	1.94
32	DD	401	CLA	C4B-NB	2.87	1.41	1.37
32	Cc	504	CLA	C4B-NB	2.87	1.41	1.37
32	Nn	305	CLA	C1B-C2B	2.87	1.49	1.43
32	b	613	CLA	C4B-NB	2.86	1.41	1.37
32	Cc	514	CLA	C4B-NB	2.86	1.41	1.37
35	A	410	PL9	C36-C34	2.86	1.57	1.51
39	11	606	CHL	C1A-CHA	-2.86	1.36	1.39
32	n	614	CLA	C1B-C2B	2.86	1.49	1.43
32	Bb	614	CLA	C1B-C2B	2.86	1.49	1.43
39	22	607	CHL	C1A-CHA	-2.86	1.36	1.39
32	a	405	CLA	C4B-NB	2.86	1.41	1.37
32	BB	612	CLA	C1B-C2B	2.86	1.49	1.43
32	GG	604	CLA	C1B-C2B	2.86	1.49	1.43
32	S	611	CLA	C1B-C2B	2.86	1.49	1.43
39	S	607	CHL	C1A-CHA	-2.86	1.36	1.40
32	r	610	CLA	C1B-C2B	2.86	1.49	1.43
36	44	616	LHG	O7-C5	-2.85	1.42	1.46
39	NN	606	CHL	CMD-C2D	-2.85	1.45	1.51
32	Aa	405	CLA	C4B-NB	2.85	1.41	1.37
32	G	613	CLA	C1B-C2B	2.85	1.49	1.43
32	Bb	612	CLA	C4B-NB	2.85	1.41	1.37
39	S	605	CHL	C1A-CHA	-2.85	1.36	1.40
39	1	606	CHL	C1A-CHA	-2.85	1.36	1.39
32	CC	511	CLA	C4B-NB	2.85	1.41	1.37
39	11	601	CHL	C1A-CHA	-2.85	1.36	1.39
32	BB	609	CLA	C4B-NB	2.85	1.41	1.37
32	33	612	CLA	C1B-C2B	2.85	1.49	1.43
32	B	605	CLA	C4B-NB	2.85	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	608	CLA	C4B-NB	2.85	1.41	1.37
32	b	614	CLA	C1B-C2B	2.85	1.49	1.43
32	YY	611	CLA	C1B-C2B	2.84	1.49	1.43
32	22	611	CLA	C1B-C2B	2.84	1.49	1.43
32	DD	404	CLA	C1B-C2B	2.84	1.49	1.43
32	n	612	CLA	C1B-C2B	2.84	1.49	1.43
32	AA	405	CLA	C1B-C2B	2.84	1.49	1.43
32	DD	403	CLA	C4B-NB	2.84	1.41	1.37
39	22	608	CHL	C1A-CHA	-2.84	1.36	1.39
39	NN	609	CHL	C1A-CHA	-2.84	1.36	1.40
32	c	512	CLA	C4B-NB	2.83	1.41	1.37
32	GG	614	CLA	C1B-C2B	2.83	1.49	1.43
32	Cc	509	CLA	C4B-NB	2.83	1.41	1.37
32	Y	613	CLA	C1B-C2B	2.83	1.49	1.43
32	Bb	613	CLA	C4B-NB	2.83	1.41	1.37
32	22	602	CLA	C1B-C2B	2.83	1.49	1.43
32	NN	612	CLA	C1B-C2B	2.83	1.49	1.43
32	11	613	CLA	C1B-C2B	2.83	1.49	1.43
32	s	604	CLA	C1B-C2B	2.83	1.49	1.43
32	Ss	613	CLA	C1B-C2B	2.82	1.49	1.43
35	AA	410	PL9	C36-C34	2.82	1.57	1.51
32	RR	314	CLA	C1B-C2B	2.82	1.49	1.43
32	Bb	608	CLA	C4B-NB	2.82	1.41	1.37
32	22	612	CLA	C1B-C2B	2.82	1.49	1.43
32	BB	603	CLA	C4B-NB	2.82	1.41	1.37
32	Y	604	CLA	C1B-C2B	2.82	1.49	1.43
32	N	611	CLA	C1B-C2B	2.82	1.49	1.43
32	22	604	CLA	C1B-C2B	2.82	1.49	1.43
32	b	605	CLA	C1B-C2B	2.82	1.49	1.43
32	Aa	405	CLA	C1B-C2B	2.82	1.49	1.43
32	G	614	CLA	C1B-C2B	2.81	1.49	1.43
32	XX	201	CLA	C1B-C2B	2.81	1.49	1.43
32	Yy	603	CLA	C4B-NB	2.81	1.41	1.37
32	1	613	CLA	C1B-C2B	2.81	1.49	1.43
32	a	405	CLA	C1B-C2B	2.81	1.49	1.43
32	4	311	CLA	C1B-C2B	2.81	1.49	1.43
32	Ss	612	CLA	C1B-C2B	2.81	1.49	1.43
32	YY	604	CLA	C1B-C2B	2.81	1.49	1.43
32	22	613	CLA	C1B-C2B	2.81	1.49	1.43
32	y	305	CLA	C4B-NB	2.81	1.41	1.37
32	c	507	CLA	C4B-NB	2.81	1.41	1.37
39	2	607	CHL	C1A-CHA	-2.81	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	604	CLA	C1B-C2B	2.81	1.49	1.43
32	3	611	CLA	C1B-C2B	2.80	1.49	1.43
39	33	607	CHL	C1A-CHA	-2.80	1.36	1.39
32	s	613	CLA	C1B-C2B	2.80	1.49	1.43
32	C	509	CLA	C4B-NB	2.80	1.41	1.37
32	11	604	CLA	C1B-C2B	2.80	1.49	1.43
32	GG	610	CLA	C1B-C2B	2.80	1.49	1.43
32	CC	514	CLA	C4B-NB	2.80	1.41	1.37
32	s	612	CLA	C1B-C2B	2.80	1.49	1.43
32	11	609	CLA	C1B-C2B	2.80	1.49	1.43
32	2	603	CLA	C1B-C2B	2.80	1.49	1.43
32	R	612	CLA	C1B-C2B	2.80	1.49	1.43
32	b	607	CLA	C1B-C2B	2.79	1.49	1.43
32	11	612	CLA	C4B-NB	2.79	1.41	1.37
32	BB	611	CLA	C4B-NB	2.79	1.41	1.37
32	Bb	615	CLA	C1B-C2B	2.79	1.49	1.43
32	Nn	302	CLA	C1B-C2B	2.79	1.49	1.43
39	s	605	CHL	C1A-CHA	-2.79	1.36	1.40
32	NN	604	CLA	C1B-C2B	2.79	1.49	1.43
32	D	404	CLA	C4B-NB	2.79	1.41	1.37
32	c	501	CLA	C1B-C2B	2.79	1.49	1.43
32	NN	611	CLA	C1B-C2B	2.79	1.49	1.43
32	S	604	CLA	C1B-C2B	2.79	1.49	1.43
32	Nn	314	CLA	C1B-C2B	2.79	1.49	1.43
32	Bb	605	CLA	C1B-C2B	2.79	1.49	1.43
39	Nn	311	CHL	C1A-CHA	-2.78	1.36	1.40
32	GG	611	CLA	C1B-C2B	2.78	1.49	1.43
32	1	610	CLA	C1B-C2B	2.78	1.49	1.43
32	B	608	CLA	C1B-C2B	2.78	1.49	1.43
32	RR	313	CLA	C1B-C2B	2.78	1.49	1.43
32	BB	607	CLA	C4B-NB	2.78	1.41	1.37
39	11	608	CHL	C1A-CHA	-2.78	1.36	1.39
32	33	609	CLA	C1B-C2B	2.78	1.49	1.43
32	2	604	CLA	C1B-C2B	2.77	1.49	1.43
32	B	623	CLA	C1B-C2B	2.77	1.49	1.43
32	1	602	CLA	C1B-C2B	2.77	1.49	1.43
32	Cc	505	CLA	C1B-C2B	2.77	1.49	1.43
35	d	404	PL9	C36-C34	2.77	1.57	1.51
32	Rr	601	CLA	C1B-C2B	2.77	1.49	1.43
32	Yy	613	CLA	C1B-C2B	2.77	1.49	1.43
32	44	610	CLA	C1B-C2B	2.77	1.49	1.43
32	4	312	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	513	CLA	C1B-C2B	2.77	1.49	1.43
32	BB	615	CLA	C1B-C2B	2.77	1.49	1.43
32	C	504	CLA	C1B-C2B	2.77	1.49	1.43
32	44	609	CLA	C1B-C2B	2.76	1.49	1.43
32	SS	309	CLA	C1B-C2B	2.76	1.49	1.43
32	3	602	CLA	C1B-C2B	2.76	1.49	1.43
32	R	614	CLA	C1B-C2B	2.76	1.49	1.43
32	BB	611	CLA	CMD-C2D	-2.76	1.45	1.50
32	Ss	602	CLA	C1B-C2B	2.76	1.49	1.43
32	RR	303	CLA	C1B-C2B	2.76	1.49	1.43
35	DD	406	PL9	C36-C34	2.76	1.57	1.51
32	N	612	CLA	C1B-C2B	2.76	1.49	1.43
32	Cc	506	CLA	C4B-NB	2.76	1.41	1.37
32	S	609	CLA	C1B-C2B	2.76	1.49	1.43
39	N	609	CHL	C1A-CHA	-2.76	1.36	1.40
32	R	603	CLA	C1B-C2B	2.76	1.49	1.43
39	N	606	CHL	CMD-C2D	-2.76	1.46	1.51
32	s	610	CLA	C1B-C2B	2.76	1.49	1.43
32	Nn	313	CLA	C1B-C2B	2.76	1.49	1.43
32	1	604	CLA	C1B-C2B	2.75	1.49	1.43
32	c	503	CLA	C1B-C2B	2.75	1.49	1.43
32	44	611	CLA	C1B-C2B	2.75	1.49	1.43
32	n	611	CLA	C1B-C2B	2.75	1.49	1.43
32	S	602	CLA	C1B-C2B	2.75	1.49	1.43
32	SS	312	CLA	C1B-C2B	2.75	1.49	1.43
32	Yy	604	CLA	C1B-C2B	2.75	1.49	1.43
32	11	610	CLA	C1B-C2B	2.75	1.49	1.43
32	33	603	CLA	C1B-C2B	2.75	1.49	1.43
32	SS	303	CLA	C1B-C2B	2.75	1.49	1.43
39	22	606	CHL	C1A-CHA	-2.75	1.36	1.39
32	Yy	612	CLA	C4B-NB	2.75	1.41	1.37
32	y	313	CLA	C1B-C2B	2.75	1.49	1.43
41	Yy	619	XAT	C26-C27	2.75	1.55	1.50
32	Bb	607	CLA	C1B-C2B	2.75	1.49	1.43
32	11	602	CLA	C1B-C2B	2.75	1.49	1.43
32	n	603	CLA	C1B-C2B	2.75	1.49	1.43
35	D	407	PL9	C36-C34	2.75	1.57	1.51
35	Dd	404	PL9	C36-C34	2.74	1.57	1.51
32	3	603	CLA	C1B-C2B	2.74	1.49	1.43
39	Rr	605	CHL	CMD-C2D	-2.74	1.46	1.51
32	CC	503	CLA	C1B-C2B	2.74	1.49	1.43
32	33	611	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	608	CLA	C1B-C2B	2.74	1.49	1.43
32	Gg	313	CLA	C1B-C2B	2.74	1.49	1.43
32	Rr	613	CLA	C1B-C2B	2.74	1.49	1.43
32	y	306	CLA	C1B-C2B	2.74	1.49	1.43
39	33	606	CHL	C1A-CHA	-2.74	1.36	1.39
32	Ss	608	CLA	C1B-C2B	2.74	1.49	1.43
32	44	604	CLA	C1B-C2B	2.74	1.49	1.43
39	22	601	CHL	C1A-CHA	-2.73	1.36	1.39
32	Yy	611	CLA	C1B-C2B	2.73	1.49	1.43
35	AA	410	PL9	C21-C19	2.73	1.56	1.51
32	r	613	CLA	C1B-C2B	2.73	1.49	1.43
32	CC	513	CLA	C1B-C2B	2.73	1.49	1.43
32	R	613	CLA	C1B-C2B	2.73	1.49	1.43
39	2	606	CHL	C1A-CHA	-2.73	1.36	1.39
32	B	607	CLA	CMD-C2D	-2.73	1.45	1.50
32	2	612	CLA	C1B-C2B	2.73	1.49	1.43
32	BB	606	CLA	C1B-C2B	2.73	1.49	1.43
32	SS	304	CLA	C1B-C2B	2.73	1.49	1.43
32	4	304	CLA	C1B-C2B	2.73	1.49	1.43
32	YY	613	CLA	C1B-C2B	2.73	1.49	1.43
32	22	610	CLA	C1B-C2B	2.73	1.49	1.43
32	CC	503	CLA	C4B-NB	2.72	1.41	1.37
39	NN	601	CHL	CMD-C2D	-2.72	1.46	1.51
39	N	607	CHL	C1A-CHA	-2.72	1.36	1.40
42	NN	618	NEX	C7-C6	-2.72	1.27	1.30
32	RR	304	CLA	C1B-C2B	2.72	1.49	1.43
39	1	608	CHL	CMD-C2D	-2.72	1.46	1.51
39	2	605	CHL	C1A-CHA	-2.72	1.36	1.39
32	C	504	CLA	C4B-NB	2.72	1.41	1.37
39	22	605	CHL	C1A-CHA	-2.72	1.36	1.39
32	y	314	CLA	C4B-NB	2.72	1.41	1.37
32	r	602	CLA	C1B-C2B	2.72	1.49	1.43
39	NN	607	CHL	C1A-CHA	-2.72	1.36	1.40
32	r	608	CLA	C1B-C2B	2.72	1.49	1.43
32	S	603	CLA	C1B-C2B	2.71	1.49	1.43
32	B	618	CLA	C1B-C2B	2.71	1.49	1.43
32	S	610	CLA	C1B-C2B	2.71	1.49	1.43
32	b	616	CLA	C1B-C2B	2.71	1.49	1.43
32	n	610	CLA	C1B-C2B	2.71	1.49	1.43
32	r	609	CLA	C1B-C2B	2.71	1.49	1.43
32	C	505	CLA	C1B-C2B	2.71	1.49	1.43
32	Gg	312	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	611	CLA	C1B-C2B	2.71	1.49	1.43
32	s	603	CLA	C1B-C2B	2.71	1.49	1.43
39	R	605	CHL	CMD-C2D	-2.71	1.46	1.51
32	44	603	CLA	C1B-C2B	2.71	1.49	1.43
32	1	612	CLA	C1B-C2B	2.70	1.49	1.43
32	R	611	CLA	C1B-C2B	2.70	1.49	1.43
32	Gg	304	CLA	C1B-C2B	2.70	1.49	1.43
32	Ss	610	CLA	C1B-C2B	2.70	1.49	1.43
32	4	305	CLA	C1B-C2B	2.70	1.49	1.43
32	s	608	CLA	C1B-C2B	2.70	1.49	1.43
39	Nn	316	CHL	CMD-C2D	-2.70	1.46	1.51
32	Yy	614	CLA	C1B-C2B	2.70	1.49	1.43
32	RR	311	CLA	C1B-C2B	2.70	1.49	1.43
32	SS	314	CLA	C1B-C2B	2.70	1.49	1.43
32	Nn	312	CLA	C4B-NB	2.70	1.41	1.37
32	g	614	CLA	C1B-C2B	2.69	1.49	1.43
32	r	601	CLA	C1B-C2B	2.69	1.49	1.43
32	b	601	CLA	C1B-C2B	2.69	1.49	1.43
32	c	511	CLA	C1B-C2B	2.69	1.49	1.43
32	Nn	301	CLA	C1B-C2B	2.69	1.49	1.43
32	Ss	603	CLA	C1B-C2B	2.69	1.49	1.43
39	y	303	CHL	CMD-C2D	-2.69	1.46	1.51
32	c	506	CLA	C1B-C2B	2.69	1.49	1.43
32	c	505	CLA	C1B-C2B	2.69	1.49	1.43
32	s	611	CLA	C1B-C2B	2.69	1.49	1.43
39	3	607	CHL	C1A-CHA	-2.69	1.36	1.39
32	b	602	CLA	C1B-C2B	2.69	1.49	1.43
32	Nn	312	CLA	C1B-C2B	2.68	1.49	1.43
32	S	613	CLA	C1B-C2B	2.68	1.49	1.43
32	GG	603	CLA	C1B-C2B	2.68	1.49	1.43
32	11	611	CLA	C1B-C2B	2.68	1.49	1.43
33	AA	407	PHO	CAC-C3C	-2.68	1.47	1.51
32	4	303	CLA	C1B-C2B	2.68	1.49	1.43
32	SS	305	CLA	C1B-C2B	2.68	1.49	1.43
32	Bb	611	CLA	C1B-C2B	2.68	1.49	1.43
32	YY	602	CLA	C1B-C2B	2.68	1.49	1.43
32	Rr	609	CLA	C1B-C2B	2.68	1.49	1.43
39	3	606	CHL	C1A-CHA	-2.68	1.36	1.39
32	b	611	CLA	C1B-C2B	2.68	1.49	1.43
32	Rr	608	CLA	C1B-C2B	2.68	1.49	1.43
32	S	608	CLA	C1B-C2B	2.68	1.49	1.43
32	NN	614	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	609	CHL	CMD-C2D	-2.67	1.46	1.51
32	N	614	CLA	C1B-C2B	2.67	1.49	1.43
39	44	607	CHL	CMD-C2D	-2.67	1.46	1.51
39	SS	306	CHL	CHC-C1C	2.67	1.44	1.39
32	BB	601	CLA	C1B-C2B	2.67	1.49	1.43
33	AA	407	PHO	CMC-C2C	-2.67	1.46	1.50
32	2	609	CLA	C1B-C2B	2.67	1.49	1.43
32	CC	504	CLA	C1B-C2B	2.67	1.49	1.43
32	Ss	611	CLA	C1B-C2B	2.67	1.49	1.43
32	c	513	CLA	C1B-C2B	2.67	1.49	1.43
32	Y	603	CLA	C1B-C2B	2.67	1.49	1.43
32	Bb	616	CLA	C1B-C2B	2.66	1.49	1.43
39	n	607	CHL	CMD-C2D	-2.66	1.46	1.51
39	NN	609	CHL	CMD-C2D	-2.66	1.46	1.51
32	CC	512	CLA	C1B-C2B	2.66	1.49	1.43
32	Y	602	CLA	C1B-C2B	2.66	1.49	1.43
32	d	402	CLA	C1B-C2B	2.66	1.49	1.43
32	Gg	315	CLA	C1B-C2B	2.66	1.49	1.43
32	Rr	611	CLA	C1B-C2B	2.66	1.49	1.43
40	22	614	LUT	C32-C33	2.66	1.51	1.46
32	Yy	602	CLA	C1B-C2B	2.66	1.49	1.43
32	N	613	CLA	C1B-C2B	2.66	1.49	1.43
32	Nn	304	CLA	C1B-C2B	2.66	1.49	1.43
32	C	514	CLA	C1B-C2B	2.66	1.49	1.43
32	C	515	CLA	C1B-C2B	2.66	1.49	1.43
32	b	604	CLA	C1B-C2B	2.66	1.49	1.43
32	33	602	CLA	C1B-C2B	2.66	1.49	1.43
32	YY	603	CLA	C1B-C2B	2.66	1.49	1.43
32	c	502	CLA	C1B-C2B	2.65	1.49	1.43
39	RR	307	CHL	CMD-C2D	-2.65	1.46	1.51
32	Ss	609	CLA	C1B-C2B	2.65	1.49	1.43
39	RR	306	CHL	CMD-C2D	-2.65	1.46	1.51
32	y	304	CLA	C1B-C2B	2.65	1.49	1.43
32	b	609	CLA	C4B-NB	2.65	1.41	1.37
32	G	603	CLA	C1B-C2B	2.65	1.49	1.43
32	s	609	CLA	C1B-C2B	2.65	1.49	1.43
32	g	603	CLA	C1B-C2B	2.65	1.49	1.43
32	GG	612	CLA	C1B-C2B	2.64	1.49	1.43
33	A	407	PHO	CMC-C2C	-2.64	1.46	1.50
32	44	602	CLA	C1B-C2B	2.64	1.49	1.43
32	y	316	CLA	C1B-C2B	2.64	1.49	1.43
33	Aa	409	PHO	CMC-C2C	-2.64	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Bb	601	CLA	C1B-C2B	2.64	1.49	1.43
32	Rr	603	CLA	C1B-C2B	2.64	1.49	1.43
32	B	621	CLA	C1B-C2B	2.64	1.49	1.43
32	s	602	CLA	C1B-C2B	2.64	1.49	1.43
39	r	605	CHL	CMD-C2D	-2.64	1.46	1.51
32	CC	506	CLA	C1B-C2B	2.64	1.49	1.43
32	CC	514	CLA	C1B-C2B	2.64	1.49	1.43
33	D	402	PHO	CMD-C2D	-2.64	1.46	1.51
33	A	407	PHO	CMD-C2D	-2.63	1.46	1.51
33	AA	407	PHO	CMD-C2D	-2.63	1.46	1.51
32	4	310	CLA	C1B-C2B	2.63	1.49	1.43
39	Nn	317	CHL	C1A-CHA	-2.63	1.37	1.40
33	a	408	PHO	CMC-C2C	-2.63	1.46	1.50
32	33	604	CLA	C1B-C2B	2.63	1.49	1.43
39	YY	609	CHL	CMD-C2D	-2.63	1.46	1.51
32	B	620	CLA	C1B-C2B	2.63	1.49	1.43
32	G	612	CLA	C1B-C2B	2.63	1.49	1.43
32	Cc	507	CLA	C1B-C2B	2.63	1.49	1.43
39	NN	605	CHL	CMD-C2D	-2.63	1.46	1.51
39	1	601	CHL	CMD-C2D	-2.63	1.46	1.51
32	R	602	CLA	C1B-C2B	2.63	1.49	1.43
32	Bb	602	CLA	C1B-C2B	2.62	1.49	1.43
33	AA	407	PHO	CMB-C2B	-2.62	1.46	1.51
32	B	610	CLA	C1B-C2B	2.62	1.49	1.43
39	2	601	CHL	C1A-CHA	-2.62	1.36	1.39
32	b	612	CLA	C1B-C2B	2.62	1.49	1.43
32	R	608	CLA	C1B-C2B	2.62	1.49	1.43
32	3	604	CLA	C1B-C2B	2.62	1.49	1.43
32	Gg	311	CLA	C1B-C2B	2.62	1.49	1.43
33	DD	402	PHO	CMC-C2C	-2.62	1.46	1.50
33	Aa	408	PHO	CAC-C3C	-2.62	1.47	1.51
39	Y	609	CHL	CMD-C2D	-2.62	1.46	1.51
32	c	508	CLA	C1B-C2B	2.62	1.49	1.43
32	b	615	CLA	C1B-C2B	2.62	1.49	1.43
32	g	612	CLA	C1B-C2B	2.62	1.49	1.43
32	SS	310	CLA	C1B-C2B	2.62	1.49	1.43
39	33	605	CHL	C1A-CHA	-2.62	1.36	1.39
39	Yy	609	CHL	CMD-C2D	-2.62	1.46	1.51
32	C	509	CLA	C1B-C2B	2.62	1.49	1.43
32	a	406	CLA	C1B-C2B	2.62	1.49	1.43
32	Cc	513	CLA	C1B-C2B	2.61	1.49	1.43
39	N	601	CHL	CMD-C2D	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	401	CLA	C1B-C2B	2.61	1.49	1.43
32	BB	614	CLA	C1B-C2B	2.61	1.49	1.43
32	CC	509	CLA	C1B-C2B	2.61	1.49	1.43
32	B	605	CLA	C1B-C2B	2.61	1.49	1.43
39	11	608	CHL	CMD-C2D	-2.61	1.46	1.51
39	Nn	317	CHL	CMD-C2D	-2.61	1.46	1.51
32	Yy	603	CLA	C1B-C2B	2.61	1.49	1.43
32	Dd	402	CLA	C1B-C2B	2.61	1.49	1.43
39	Nn	319	CHL	CMD-C2D	-2.61	1.46	1.51
32	Cc	510	CLA	C1B-C2B	2.61	1.49	1.43
32	Cc	504	CLA	C1B-C2B	2.61	1.49	1.43
39	g	606	CHL	CMD-C2D	-2.61	1.46	1.51
32	CC	508	CLA	C4B-NB	2.61	1.41	1.37
32	Bb	612	CLA	C1B-C2B	2.61	1.49	1.43
32	Bb	604	CLA	C1B-C2B	2.61	1.49	1.43
33	Aa	408	PHO	CMC-C2C	-2.61	1.46	1.50
32	y	305	CLA	C1B-C2B	2.61	1.49	1.43
32	r	603	CLA	C1B-C2B	2.61	1.49	1.43
32	Cc	515	CLA	C1B-C2B	2.61	1.49	1.43
32	44	615	CLA	C1B-C2B	2.61	1.49	1.43
32	Yy	612	CLA	C1B-C2B	2.60	1.49	1.43
39	N	607	CHL	CMD-C2D	-2.60	1.46	1.51
39	y	310	CHL	CMD-C2D	-2.60	1.46	1.51
32	B	606	CLA	C1B-C2B	2.60	1.49	1.43
39	Yy	607	CHL	CMD-C2D	-2.60	1.46	1.51
32	2	602	CLA	C1B-C2B	2.60	1.49	1.43
32	C	503	CLA	C1B-C2B	2.60	1.49	1.43
32	n	613	CLA	C1B-C2B	2.60	1.49	1.43
39	Nn	311	CHL	CMD-C2D	-2.60	1.46	1.51
32	B	604	CLA	C1B-C2B	2.60	1.49	1.43
39	Rr	607	CHL	CMD-C2D	-2.60	1.46	1.51
39	Yy	608	CHL	CMD-C2D	-2.60	1.46	1.51
32	Rr	602	CLA	C1B-C2B	2.60	1.49	1.43
33	a	408	PHO	CMD-C2D	-2.60	1.46	1.51
32	Cc	511	CLA	C1B-C2B	2.60	1.49	1.43
32	Aa	410	CLA	C1B-C2B	2.60	1.49	1.43
42	g	617	NEX	C28-C29	2.60	1.51	1.46
36	4	315	LHG	O8-C23	2.60	1.45	1.33
39	S	601	CHL	CMD-C2D	-2.59	1.46	1.51
32	11	603	CLA	C1B-C2B	2.59	1.49	1.43
32	CC	508	CLA	C1B-C2B	2.59	1.49	1.43
39	Y	606	CHL	CMD-C2D	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	y	307	CHL	CMD-C2D	-2.59	1.46	1.51
39	4	307	CHL	CMD-C2D	-2.59	1.46	1.51
39	y	309	CHL	CMD-C2D	-2.59	1.46	1.51
39	g	609	CHL	CMD-C2D	-2.59	1.46	1.51
32	b	606	CLA	C1B-C2B	2.59	1.49	1.43
39	YY	606	CHL	CMD-C2D	-2.59	1.46	1.51
39	N	605	CHL	CMD-C2D	-2.59	1.46	1.51
32	Bb	609	CLA	C4B-NB	2.59	1.41	1.37
32	c	507	CLA	C1B-C2B	2.59	1.49	1.43
32	A	408	CLA	C1B-C2B	2.59	1.49	1.43
32	RR	308	CLA	C1B-C2B	2.59	1.49	1.43
39	N	608	CHL	CMD-C2D	-2.59	1.46	1.51
32	R	604	CLA	C1B-C2B	2.59	1.49	1.43
39	n	605	CHL	CMD-C2D	-2.59	1.46	1.51
32	Dd	401	CLA	C1B-C2B	2.59	1.49	1.43
32	Cc	508	CLA	C1B-C2B	2.58	1.49	1.43
39	Nn	318	CHL	CMD-C2D	-2.58	1.46	1.51
33	DD	402	PHO	CMD-C2D	-2.58	1.46	1.51
33	D	402	PHO	CMC-C2C	-2.58	1.46	1.50
32	YY	614	CLA	C1B-C2B	2.58	1.49	1.43
39	YY	601	CHL	CMD-C2D	-2.58	1.46	1.51
32	C	510	CLA	C1B-C2B	2.58	1.49	1.43
32	Y	614	CLA	C1B-C2B	2.58	1.49	1.43
39	s	601	CHL	CMD-C2D	-2.58	1.46	1.51
39	y	311	CHL	CMD-C2D	-2.58	1.46	1.51
33	a	409	PHO	CMD-C2D	-2.58	1.46	1.51
32	BB	610	CLA	C1B-C2B	2.58	1.49	1.43
32	a	410	CLA	C1B-C2B	2.58	1.49	1.43
39	Nn	315	CHL	CMD-C2D	-2.58	1.46	1.51
39	Gg	309	CHL	CMD-C2D	-2.58	1.46	1.51
32	Bb	606	CLA	C1B-C2B	2.58	1.49	1.43
39	44	606	CHL	CMD-C2D	-2.58	1.46	1.51
39	n	609	CHL	CMD-C2D	-2.58	1.46	1.51
32	Bb	609	CLA	C1B-C2B	2.58	1.49	1.43
39	R	607	CHL	CMD-C2D	-2.58	1.46	1.51
39	3	605	CHL	C1A-CHA	-2.58	1.36	1.39
33	A	407	PHO	CAC-C3C	-2.58	1.47	1.51
32	D	404	CLA	C1B-C2B	2.58	1.49	1.43
39	g	608	CHL	CMD-C2D	-2.57	1.46	1.51
39	GG	601	CHL	CMD-C2D	-2.57	1.46	1.51
32	11	612	CLA	MG-NC	2.57	2.12	2.06
32	CC	505	CLA	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	601	CHL	CMD-C2D	-2.57	1.46	1.51
32	b	609	CLA	C1B-C2B	2.57	1.49	1.43
39	n	606	CHL	CMD-C2D	-2.57	1.46	1.51
39	Y	605	CHL	CMD-C2D	-2.57	1.46	1.51
39	GG	607	CHL	CMD-C2D	-2.57	1.46	1.51
39	SS	307	CHL	CMD-C2D	-2.57	1.46	1.51
39	G	607	CHL	CMD-C2D	-2.57	1.46	1.51
39	Yy	605	CHL	CMD-C2D	-2.57	1.46	1.51
35	A	410	PL9	C21-C19	2.57	1.56	1.51
39	r	607	CHL	CMD-C2D	-2.57	1.46	1.51
33	a	409	PHO	CMC-C2C	-2.57	1.46	1.50
39	Y	607	CHL	CMD-C2D	-2.57	1.46	1.51
39	Ss	601	CHL	CMD-C2D	-2.57	1.46	1.51
32	BB	609	CLA	C1B-C2B	2.57	1.49	1.43
32	Ss	604	CLA	C1B-C2B	2.57	1.49	1.43
32	N	610	CLA	C1B-C2B	2.57	1.49	1.43
39	Ss	605	CHL	CMD-C2D	-2.57	1.46	1.51
39	y	308	CHL	CMD-C2D	-2.57	1.46	1.51
39	Gg	307	CHL	CMD-C2D	-2.57	1.46	1.51
32	NN	603	CLA	C1B-C2B	2.57	1.49	1.43
39	SS	302	CHL	CMD-C2D	-2.57	1.46	1.51
32	C	511	CLA	C1B-C2B	2.57	1.49	1.43
32	SS	311	CLA	C1B-C2B	2.57	1.49	1.43
39	NN	607	CHL	CMD-C2D	-2.57	1.46	1.51
32	BB	607	CLA	C1B-C2B	2.56	1.49	1.43
39	G	609	CHL	CMD-C2D	-2.56	1.46	1.51
39	NN	608	CHL	CMD-C2D	-2.56	1.46	1.51
39	R	606	CHL	CMD-C2D	-2.56	1.46	1.51
32	C	506	CLA	C1B-C2B	2.56	1.49	1.43
39	Yy	601	CHL	CMD-C2D	-2.56	1.46	1.51
39	S	606	CHL	CMD-C2D	-2.56	1.46	1.51
39	Gg	310	CHL	CMD-C2D	-2.56	1.46	1.51
33	A	407	PHO	CMB-C2B	-2.56	1.46	1.51
32	Cc	509	CLA	C1B-C2B	2.56	1.49	1.43
39	4	308	CHL	CMD-C2D	-2.56	1.46	1.51
41	Gg	301	XAT	C32-C33	2.56	1.51	1.46
39	YY	608	CHL	CMD-C2D	-2.56	1.46	1.51
33	Aa	409	PHO	CMD-C2D	-2.56	1.46	1.51
36	44	614	LHG	O8-C23	2.55	1.45	1.33
39	33	608	CHL	CMD-C2D	-2.55	1.46	1.51
39	11	607	CHL	C1A-CHA	-2.55	1.36	1.39
32	N	602	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	608	CHL	CMD-C2D	-2.55	1.46	1.51
39	GG	609	CHL	CMD-C2D	-2.55	1.46	1.51
32	Cc	514	CLA	C1B-C2B	2.55	1.49	1.43
32	X	201	CLA	C1B-C2B	2.55	1.49	1.43
33	Aa	408	PHO	CMB-C2B	-2.55	1.46	1.51
32	Cc	512	CLA	C1B-C2B	2.55	1.49	1.43
46	Ee	101	HEM	FE-NC	2.55	2.03	1.95
32	BB	603	CLA	C1B-C2B	2.55	1.49	1.43
32	RR	302	CLA	C1B-C2B	2.55	1.49	1.43
32	c	510	CLA	C1B-C2B	2.55	1.49	1.43
39	Y	608	CHL	CMD-C2D	-2.55	1.46	1.51
39	g	605	CHL	CMD-C2D	-2.55	1.46	1.51
33	DD	402	PHO	CMB-C2B	-2.55	1.46	1.51
32	y	314	CLA	C1B-C2B	2.54	1.49	1.43
33	a	408	PHO	CAC-C3C	-2.54	1.47	1.51
39	SS	306	CHL	CMD-C2D	-2.54	1.46	1.51
32	C	507	CLA	C1B-C2B	2.54	1.49	1.43
39	g	607	CHL	CMD-C2D	-2.54	1.46	1.51
32	N	603	CLA	C1B-C2B	2.54	1.49	1.43
32	CC	510	CLA	C1B-C2B	2.54	1.49	1.43
41	Nn	308	XAT	O24-C25	-2.54	1.42	1.46
39	s	606	CHL	C1A-CHA	-2.54	1.37	1.40
35	A	410	PL9	C41-C39	2.54	1.56	1.51
39	Gg	306	CHL	CMD-C2D	-2.54	1.46	1.51
39	33	607	CHL	CMD-C2D	-2.54	1.46	1.51
39	g	601	CHL	CMD-C2D	-2.54	1.46	1.51
39	YY	607	CHL	CMD-C2D	-2.54	1.46	1.51
39	4	309	CHL	CMD-C2D	-2.54	1.46	1.51
33	a	408	PHO	CMB-C2B	-2.54	1.46	1.51
39	G	606	CHL	CMD-C2D	-2.54	1.46	1.51
39	GG	606	CHL	CMD-C2D	-2.54	1.46	1.51
39	n	601	CHL	CMD-C2D	-2.54	1.46	1.51
32	a	407	CLA	C1B-C2B	2.54	1.49	1.43
32	BB	605	CLA	C1B-C2B	2.54	1.49	1.43
39	GG	608	CHL	CMD-C2D	-2.53	1.46	1.51
39	Y	607	CHL	CBD-CGD	-2.53	1.49	1.52
39	11	601	CHL	CMD-C2D	-2.53	1.46	1.51
39	y	310	CHL	CMB-C2B	-2.53	1.46	1.51
33	Aa	408	PHO	CMD-C2D	-2.53	1.46	1.51
39	1	607	CHL	CMD-C2D	-2.53	1.46	1.51
39	Yy	606	CHL	CMD-C2D	-2.53	1.46	1.51
41	g	619	XAT	C32-C33	2.53	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	502	CLA	C1B-C2B	2.53	1.49	1.43
32	R	610	CLA	C1B-C2B	2.53	1.49	1.43
39	44	608	CHL	CMD-C2D	-2.53	1.46	1.51
32	RR	310	CLA	C1B-C2B	2.53	1.49	1.43
39	Gg	308	CHL	CMD-C2D	-2.53	1.46	1.51
32	c	512	CLA	C1B-C2B	2.52	1.49	1.43
39	2	608	CHL	CMD-C2D	-2.52	1.46	1.51
39	YY	605	CHL	CMD-C2D	-2.52	1.46	1.51
42	g	617	NEX	O24-C25	-2.52	1.43	1.46
39	1	607	CHL	C1A-CHA	-2.52	1.36	1.39
32	Y	612	CLA	C1B-C2B	2.52	1.49	1.43
39	3	608	CHL	CMD-C2D	-2.52	1.46	1.51
32	B	622	CLA	C1B-C2B	2.52	1.49	1.43
39	S	605	CHL	CMD-C2D	-2.52	1.46	1.51
32	n	602	CLA	C1B-C2B	2.52	1.49	1.43
39	s	605	CHL	CMD-C2D	-2.52	1.46	1.51
32	B	624	CLA	C1B-C2B	2.52	1.49	1.43
32	2	602	CLA	C3B-C4B	2.52	1.50	1.42
39	YY	607	CHL	CBD-CGD	-2.51	1.49	1.52
39	11	607	CHL	CMD-C2D	-2.51	1.46	1.51
32	YY	610	CLA	C1B-C2B	2.51	1.49	1.43
39	G	608	CHL	CMD-C2D	-2.51	1.46	1.51
32	Rr	610	CLA	C1B-C2B	2.51	1.49	1.43
39	33	605	CHL	CMD-C2D	-2.51	1.46	1.51
39	44	601	CHL	CMD-C2D	-2.51	1.46	1.51
32	YY	611	CLA	MG-ND	-2.51	2.00	2.05
32	YY	612	CLA	C1B-C2B	2.51	1.49	1.43
39	4	306	CHL	CMD-C2D	-2.51	1.46	1.51
39	Ss	605	CHL	C1A-CHA	-2.51	1.37	1.40
39	G	605	CHL	CMD-C2D	-2.51	1.46	1.51
39	SS	308	CHL	CMD-C2D	-2.50	1.46	1.51
35	AA	410	PL9	C41-C39	2.50	1.56	1.51
32	NN	602	CLA	C1B-C2B	2.50	1.49	1.43
32	c	509	CLA	C1B-C2B	2.50	1.49	1.43
32	AA	408	CLA	C1B-C2B	2.50	1.49	1.43
39	4	309	CHL	CHC-C1C	2.50	1.44	1.39
39	3	601	CHL	CMD-C2D	-2.50	1.46	1.51
39	1	606	CHL	CMD-C2D	-2.50	1.46	1.51
39	2	607	CHL	CMD-C2D	-2.50	1.46	1.51
39	4	302	CHL	CMD-C2D	-2.50	1.46	1.51
39	Ss	606	CHL	C1A-CHA	-2.50	1.37	1.40
39	Yy	601	CHL	CBD-CGD	-2.50	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	312	CLA	C1B-C2B	2.50	1.49	1.43
39	3	607	CHL	CMD-C2D	-2.50	1.46	1.51
39	2	606	CHL	CMD-C2D	-2.50	1.46	1.51
39	s	606	CHL	CMD-C2D	-2.50	1.46	1.51
32	Aa	406	CLA	C1B-C2B	2.50	1.49	1.43
32	B	619	CLA	C1B-C2B	2.50	1.49	1.43
39	22	605	CHL	CMD-C2D	-2.50	1.46	1.51
39	Rr	606	CHL	CMD-C2D	-2.50	1.46	1.51
39	S	607	CHL	CMD-C2D	-2.49	1.46	1.51
39	1	605	CHL	CMD-C2D	-2.49	1.46	1.51
39	33	601	CHL	CMD-C2D	-2.49	1.46	1.51
32	A	406	CLA	C1B-C2B	2.49	1.49	1.43
32	22	609	CLA	C1B-C2B	2.49	1.49	1.43
39	s	607	CHL	CHC-C1C	2.49	1.44	1.39
33	DD	402	PHO	CAC-C3C	-2.49	1.47	1.51
39	44	605	CHL	CMD-C2D	-2.49	1.46	1.51
32	RR	309	CLA	C1B-C2B	2.49	1.49	1.43
32	NN	610	CLA	C1B-C2B	2.49	1.49	1.43
42	Gg	318	NEX	C28-C29	2.49	1.51	1.46
32	Bb	610	CLA	C1B-C2B	2.49	1.49	1.43
39	22	601	CHL	CMD-C2D	-2.49	1.46	1.51
35	AA	410	PL9	C7-C8	2.49	1.54	1.50
39	11	606	CHL	CMD-C2D	-2.49	1.46	1.51
32	g	611	CLA	C1B-C2B	2.48	1.49	1.43
32	Y	610	CLA	C1B-C2B	2.48	1.49	1.43
32	g	610	CLA	C1B-C2B	2.48	1.48	1.43
32	Aa	407	CLA	C1B-C2B	2.48	1.48	1.43
39	Ss	606	CHL	CMD-C2D	-2.48	1.46	1.51
39	3	605	CHL	CMD-C2D	-2.48	1.46	1.51
39	3	606	CHL	CMD-C2D	-2.48	1.46	1.51
33	D	402	PHO	CMB-C2B	-2.48	1.46	1.51
39	Rr	606	CHL	CBD-CGD	-2.48	1.49	1.52
32	b	610	CLA	C1B-C2B	2.48	1.48	1.43
39	r	606	CHL	CMD-C2D	-2.48	1.46	1.51
39	G	601	CHL	CMD-C2D	-2.48	1.46	1.51
32	Ss	611	CLA	C3B-C4B	2.47	1.49	1.42
39	GG	605	CHL	CMD-C2D	-2.47	1.46	1.51
32	C	508	CLA	C1B-C2B	2.47	1.48	1.43
39	22	606	CHL	CMD-C2D	-2.47	1.46	1.51
32	C	512	CLA	C1B-C2B	2.47	1.48	1.43
39	Ss	607	CHL	CMD-C2D	-2.47	1.46	1.51
32	YY	612	CLA	C3B-C4B	2.47	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	605	CHL	CMD-C2D	-2.47	1.46	1.51
39	n	607	CHL	C1A-CHA	-2.47	1.37	1.40
32	X	201	CLA	C3B-C4B	2.47	1.49	1.42
32	BB	604	CLA	C1B-C2B	2.46	1.48	1.43
32	CC	507	CLA	C1B-C2B	2.46	1.48	1.43
39	s	607	CHL	CMD-C2D	-2.46	1.46	1.51
32	SS	310	CLA	C3B-C4B	2.46	1.49	1.42
32	R	609	CLA	C1B-C2B	2.46	1.48	1.43
32	n	612	CLA	C3B-C4B	2.46	1.49	1.42
33	D	402	PHO	CAC-C3C	-2.46	1.47	1.51
39	2	601	CHL	CMD-C2D	-2.46	1.46	1.51
39	22	607	CHL	CMD-C2D	-2.46	1.46	1.51
39	Ss	606	CHL	CHC-C1C	2.46	1.44	1.39
39	Nn	315	CHL	C1A-CHA	-2.46	1.37	1.40
39	33	606	CHL	CMD-C2D	-2.45	1.46	1.51
39	22	608	CHL	CMD-C2D	-2.45	1.46	1.51
39	Yy	607	CHL	C1A-CHA	-2.45	1.37	1.40
35	DD	406	PL9	C21-C19	2.45	1.56	1.51
32	Bb	608	CLA	C1B-C2B	2.45	1.48	1.43
32	b	608	CLA	CMB-C2B	-2.45	1.45	1.50
34	Hh	101	BCR	C19-C18	2.45	1.51	1.46
32	XX	201	CLA	C3B-C4B	2.45	1.49	1.42
32	YY	611	CLA	C1D-ND	2.45	1.41	1.37
39	Y	601	CHL	CBD-CGD	-2.45	1.49	1.52
32	b	613	CLA	C1B-C2B	2.45	1.48	1.43
40	2	614	LUT	C32-C33	2.44	1.51	1.46
32	AA	406	CLA	C1B-C2B	2.44	1.48	1.43
32	B	607	CLA	C1B-C2B	2.44	1.48	1.43
39	r	606	CHL	CHC-C1C	2.44	1.44	1.39
41	y	302	XAT	O4-C5	-2.44	1.43	1.46
32	n	602	CLA	CHC-C1C	2.44	1.43	1.38
32	BB	611	CLA	C1B-C2B	2.44	1.48	1.43
32	BB	602	CLA	C1B-C2B	2.43	1.48	1.43
41	Nn	308	XAT	O4-C5	-2.43	1.43	1.46
39	g	605	CHL	CHC-C1C	2.43	1.44	1.39
34	h	101	BCR	C19-C18	2.43	1.51	1.46
39	11	605	CHL	CMD-C2D	-2.43	1.46	1.51
32	3	604	CLA	C3B-C4B	2.42	1.49	1.42
34	H	101	BCR	C8-C9	2.42	1.51	1.46
39	RR	305	CHL	CMD-C2D	-2.42	1.46	1.51
39	Rr	605	CHL	CHC-C1C	2.42	1.44	1.39
42	Gg	318	NEX	O24-C25	-2.42	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	606	CHL	CHC-C1C	2.42	1.44	1.39
39	Yy	608	CHL	CMB-C2B	-2.42	1.46	1.51
32	s	611	CLA	C3B-C4B	2.42	1.49	1.42
39	Gg	306	CHL	CHC-C1C	2.42	1.44	1.39
39	G	605	CHL	CHC-C1C	2.42	1.44	1.39
41	y	302	XAT	O24-C25	-2.41	1.43	1.46
39	y	303	CHL	CBD-CGD	-2.41	1.49	1.52
32	R	604	CLA	C3B-C4B	2.41	1.49	1.42
41	Rr	615	XAT	O24-C25	-2.41	1.43	1.46
41	G	619	XAT	C32-C33	2.41	1.51	1.46
32	CC	511	CLA	C1B-C2B	2.41	1.48	1.43
32	BB	612	CLA	C3B-C4B	2.41	1.49	1.42
33	Aa	409	PHO	CMB-C2B	-2.41	1.46	1.51
32	1	610	CLA	C3B-C4B	2.40	1.49	1.42
39	GG	607	CHL	CBD-CGD	-2.40	1.49	1.52
40	Y	615	LUT	C22-C21	-2.40	1.51	1.54
32	c	511	CLA	CMB-C2B	-2.40	1.45	1.50
39	s	606	CHL	CHC-C1C	2.40	1.43	1.39
35	A	410	PL9	C7-C8	2.39	1.54	1.50
32	g	602	CLA	CMB-C2B	-2.39	1.45	1.50
32	B	604	CLA	CHC-C1C	2.39	1.43	1.38
39	SS	308	CHL	CHC-C1C	2.39	1.43	1.39
35	D	407	PL9	C21-C19	2.39	1.56	1.51
32	b	603	CLA	C1B-C2B	2.39	1.48	1.43
39	4	307	CHL	CHC-C1C	2.39	1.43	1.39
32	D	404	CLA	CMD-C2D	-2.39	1.45	1.50
33	a	409	PHO	CMB-C2B	-2.38	1.46	1.51
32	44	609	CLA	C3B-C4B	2.38	1.49	1.42
32	c	502	CLA	CMD-C2D	-2.38	1.45	1.50
32	b	612	CLA	CMD-C2D	-2.38	1.45	1.50
39	Y	609	CHL	CMB-C2B	-2.38	1.46	1.51
39	2	605	CHL	CHC-C1C	2.38	1.43	1.39
32	a	406	CLA	MG-NA	2.38	2.11	2.06
39	22	605	CHL	CHC-C1C	2.38	1.43	1.39
39	33	607	CHL	CHC-C1C	2.38	1.43	1.39
32	Bb	613	CLA	C1B-C2B	2.38	1.48	1.43
39	Ss	607	CHL	CHC-C1C	2.38	1.43	1.39
32	n	613	CLA	CMB-C2B	-2.38	1.45	1.50
33	a	409	PHO	CAC-C3C	-2.38	1.47	1.51
32	11	610	CLA	C3B-C4B	2.38	1.49	1.42
39	SS	306	CHL	CAC-C3C	-2.37	1.47	1.51
41	RR	316	XAT	O4-C5	-2.37	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	11	603	CLA	C3B-C4B	2.37	1.49	1.42
39	g	606	CHL	CBD-CGD	-2.37	1.49	1.52
32	CC	506	CLA	CMD-C2D	-2.37	1.45	1.50
32	R	614	CLA	CMD-C2D	-2.37	1.45	1.50
39	Rr	606	CHL	CAC-C3C	-2.37	1.47	1.51
32	33	609	CLA	C3B-C4B	2.37	1.49	1.42
39	NN	606	CHL	CHC-C1C	2.37	1.43	1.39
39	YY	606	CHL	CHC-C1C	2.37	1.43	1.39
32	r	603	CLA	C3B-C4B	2.37	1.49	1.42
32	Yy	610	CLA	C3B-C4B	2.37	1.49	1.42
32	BB	609	CLA	C3B-C4B	2.36	1.49	1.42
41	NN	617	XAT	O4-C5	-2.36	1.43	1.46
32	Y	610	CLA	C3B-C4B	2.36	1.49	1.42
32	DD	401	CLA	CMB-C2B	-2.36	1.45	1.50
32	R	609	CLA	C3B-C4B	2.36	1.49	1.42
39	RR	306	CHL	CAC-C3C	-2.36	1.47	1.51
32	S	608	CLA	C3B-C4B	2.36	1.49	1.42
39	Rr	606	CHL	CHC-C1C	2.36	1.43	1.39
35	DD	406	PL9	C5-C4	-2.36	1.39	1.47
39	r	606	CHL	CBD-CGD	-2.36	1.49	1.52
32	Rr	603	CLA	C3B-C4B	2.36	1.49	1.42
39	44	608	CHL	CHC-C1C	2.35	1.43	1.39
39	GG	608	CHL	CHC-C1C	2.35	1.43	1.39
32	Rr	611	CLA	C3B-C4B	2.35	1.49	1.42
39	44	606	CHL	CHC-C1C	2.35	1.43	1.39
32	AA	408	CLA	C3B-C4B	2.35	1.49	1.42
39	NN	601	CHL	CAC-C3C	-2.35	1.47	1.51
32	n	602	CLA	C3B-C4B	2.35	1.49	1.42
32	1	604	CLA	C3B-C4B	2.35	1.49	1.42
32	Gg	311	CLA	CHC-C1C	2.35	1.43	1.38
35	Dd	404	PL9	C21-C19	2.35	1.56	1.51
32	g	610	CLA	CHC-C1C	2.35	1.43	1.38
35	d	404	PL9	C21-C19	2.35	1.56	1.51
39	33	601	CHL	CHC-C1C	2.35	1.43	1.39
32	11	611	CLA	C3B-C4B	2.35	1.49	1.42
32	y	314	CLA	CMD-C2D	-2.35	1.46	1.50
32	Yy	610	CLA	C1B-C2B	2.35	1.48	1.43
39	Nn	318	CHL	CHC-C1C	2.35	1.43	1.39
32	Cc	515	CLA	C3B-C4B	2.35	1.49	1.42
32	N	613	CLA	CMB-C2B	-2.35	1.46	1.50
32	r	611	CLA	C3B-C4B	2.35	1.49	1.42
32	R	610	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	609	CLA	C3B-C4B	2.34	1.49	1.42
39	YY	601	CHL	CAC-C3C	-2.34	1.47	1.51
41	N	617	XAT	O4-C5	-2.34	1.43	1.46
32	NN	612	CLA	C3B-C4B	2.34	1.49	1.42
41	R	616	XAT	O24-C25	-2.34	1.43	1.46
39	G	608	CHL	CHC-C1C	2.34	1.43	1.39
32	b	608	CLA	C1B-C2B	2.34	1.48	1.43
32	22	602	CLA	C3B-C4B	2.34	1.49	1.42
39	y	311	CHL	CMB-C2B	-2.34	1.46	1.51
32	b	609	CLA	CHC-C1C	2.34	1.43	1.38
32	DD	403	CLA	C1B-C2B	2.34	1.48	1.43
32	Bb	603	CLA	C1B-C2B	2.34	1.48	1.43
41	GG	619	XAT	C32-C33	2.34	1.51	1.46
32	b	610	CLA	C3B-C4B	2.34	1.49	1.42
32	B	607	CLA	CMB-C2B	-2.34	1.46	1.50
42	g	617	NEX	C7-C6	-2.34	1.27	1.30
32	RR	310	CLA	C3B-C4B	2.34	1.49	1.42
39	NN	609	CHL	CMB-C2B	-2.34	1.47	1.51
33	D	402	PHO	C4D-ND	-2.33	1.35	1.38
32	1	613	CLA	C3B-C4B	2.33	1.49	1.42
39	1	606	CHL	CHC-C1C	2.33	1.43	1.39
32	c	509	CLA	C3B-C4B	2.33	1.49	1.42
35	Dd	404	PL9	C7-C8	2.33	1.54	1.50
32	CC	511	CLA	C3B-C4B	2.33	1.49	1.42
41	Gg	301	XAT	O4-C5	-2.33	1.43	1.46
35	DD	406	PL9	C41-C39	2.33	1.56	1.51
34	Bb	617	BCR	C12-C13	2.33	1.50	1.46
39	SS	302	CHL	CHC-C1C	2.33	1.43	1.39
32	Nn	303	CLA	C3B-C4B	2.33	1.49	1.42
39	S	607	CHL	CHC-C1C	2.33	1.43	1.39
35	D	407	PL9	C41-C39	2.33	1.56	1.51
32	Cc	511	CLA	C3B-C4B	2.33	1.49	1.42
32	C	507	CLA	CMD-C2D	-2.33	1.46	1.50
35	D	407	PL9	C5-C4	-2.33	1.39	1.47
32	a	410	CLA	C3B-C4B	2.33	1.49	1.42
32	B	604	CLA	C3B-C4B	2.33	1.49	1.42
32	A	408	CLA	C3B-C4B	2.32	1.49	1.42
41	RR	316	XAT	O24-C25	-2.32	1.43	1.46
41	R	616	XAT	O4-C5	-2.32	1.43	1.46
39	4	302	CHL	CHC-C1C	2.32	1.43	1.39
32	C	503	CLA	CMD-C2D	-2.32	1.46	1.50
32	BB	608	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	11	613	CLA	C3B-C4B	2.32	1.49	1.42
32	D	401	CLA	C1B-C2B	2.32	1.48	1.43
32	GG	610	CLA	CHC-C1C	2.32	1.43	1.38
39	Yy	601	CHL	CAC-C3C	-2.32	1.47	1.51
39	G	606	CHL	CHC-C1C	2.32	1.43	1.39
32	Ss	603	CLA	C3B-C4B	2.32	1.49	1.42
32	b	603	CLA	C3B-C4B	2.32	1.49	1.42
32	GG	610	CLA	C3B-C4B	2.32	1.49	1.42
39	Nn	316	CHL	CHC-C1C	2.32	1.43	1.39
39	44	601	CHL	CHC-C1C	2.32	1.43	1.39
39	11	607	CHL	CHC-C1C	2.32	1.43	1.39
39	S	601	CHL	CHC-C1C	2.32	1.43	1.39
35	Dd	404	PL9	C5-C4	-2.32	1.39	1.47
32	y	312	CLA	C3B-C4B	2.32	1.49	1.42
39	11	606	CHL	CHC-C1C	2.32	1.43	1.39
39	N	605	CHL	CBD-CGD	-2.32	1.49	1.52
32	RR	304	CLA	C3B-C4B	2.31	1.49	1.42
39	y	303	CHL	CAC-C3C	-2.31	1.47	1.51
32	33	604	CLA	C3B-C4B	2.31	1.49	1.42
32	g	610	CLA	C3B-C4B	2.31	1.49	1.42
35	d	404	PL9	C5-C4	-2.31	1.39	1.47
32	Ss	609	CLA	CMC-C2C	-2.31	1.46	1.50
32	D	401	CLA	CMB-C2B	-2.31	1.46	1.50
32	c	501	CLA	CMD-C2D	-2.31	1.46	1.50
39	3	601	CHL	CHC-C1C	2.31	1.43	1.39
32	RR	314	CLA	CMD-C2D	-2.31	1.46	1.50
41	r	615	XAT	O24-C25	-2.31	1.43	1.46
32	RR	309	CLA	C3B-C4B	2.31	1.49	1.42
32	CC	503	CLA	CMD-C2D	-2.31	1.46	1.50
32	B	605	CLA	C3B-C4B	2.31	1.49	1.42
32	44	609	CLA	CHC-C1C	2.31	1.43	1.38
35	DD	406	PL9	C7-C8	2.31	1.54	1.50
39	r	605	CHL	CHC-C1C	2.31	1.43	1.39
32	r	601	CLA	C3B-C4B	2.30	1.49	1.42
32	SS	310	CLA	CHC-C1C	2.30	1.43	1.38
32	BB	602	CLA	CMD-C2D	-2.30	1.46	1.50
32	S	603	CLA	C3B-C4B	2.30	1.49	1.42
39	n	608	CHL	CHC-C1C	2.30	1.43	1.39
40	22	614	LUT	C12-C13	2.30	1.50	1.46
39	G	607	CHL	CBD-CGD	-2.30	1.49	1.52
35	AA	410	PL9	C5-C4	-2.30	1.39	1.47
39	44	605	CHL	CHC-C1C	2.30	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	607	CHL	CHC-C1C	2.30	1.43	1.39
32	2	612	CLA	C3B-C4B	2.30	1.49	1.42
32	11	602	CLA	C3B-C4B	2.30	1.49	1.42
39	44	607	CHL	CHC-C1C	2.30	1.43	1.39
39	Yy	609	CHL	CMB-C2B	-2.30	1.47	1.51
32	Gg	311	CLA	C3B-C4B	2.30	1.49	1.42
39	3	607	CHL	CHC-C1C	2.30	1.43	1.39
39	SS	307	CHL	CHC-C1C	2.30	1.43	1.39
32	s	608	CLA	C3B-C4B	2.30	1.49	1.42
39	4	308	CHL	CHC-C1C	2.30	1.43	1.39
32	Yy	610	CLA	CHC-C1C	2.30	1.43	1.38
44	CC	522	DGD	O3G-C1D	2.30	1.44	1.40
32	B	608	CLA	CMD-C2D	-2.29	1.46	1.50
39	NN	609	CHL	CHC-C1C	2.29	1.43	1.39
32	33	610	CLA	C3B-C4B	2.29	1.49	1.42
32	N	612	CLA	C3B-C4B	2.29	1.49	1.42
39	Y	606	CHL	CHC-C1C	2.29	1.43	1.39
32	Nn	304	CLA	CMB-C2B	-2.29	1.46	1.50
32	Rr	601	CLA	C3B-C4B	2.29	1.49	1.42
32	c	513	CLA	C3B-C4B	2.29	1.49	1.42
39	Y	601	CHL	CAC-C3C	-2.29	1.47	1.51
39	NN	608	CHL	CHC-C1C	2.29	1.43	1.39
32	R	601	CLA	CMB-C2B	-2.29	1.46	1.50
32	R	609	CLA	CHC-C1C	2.29	1.43	1.38
39	R	606	CHL	CHC-C1C	2.29	1.43	1.39
40	Ss	614	LUT	C32-C33	2.29	1.50	1.46
32	R	614	CLA	C3B-C4B	2.29	1.49	1.42
32	n	611	CLA	C3B-C4B	2.29	1.49	1.42
32	Aa	406	CLA	C3B-C4B	2.29	1.49	1.42
39	3	605	CHL	CHC-C1C	2.29	1.43	1.39
32	y	312	CLA	CHC-C1C	2.29	1.43	1.38
32	BB	602	CLA	CMB-C2B	-2.29	1.46	1.50
33	Aa	409	PHO	CAC-C3C	-2.29	1.47	1.51
32	44	615	CLA	C3B-C4B	2.29	1.49	1.42
32	B	619	CLA	CMD-C2D	-2.29	1.46	1.50
32	Cc	507	CLA	CMD-C2D	-2.29	1.46	1.50
39	22	608	CHL	CHC-C1C	2.29	1.43	1.39
40	Ss	614	LUT	C8-C9	2.29	1.50	1.46
32	Y	612	CLA	C3B-C4B	2.29	1.49	1.42
34	AA	409	BCR	C8-C9	2.29	1.50	1.46
39	YY	607	CHL	CHC-C1C	2.29	1.43	1.39
32	SS	312	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	601	CLA	CMC-C2C	-2.29	1.46	1.50
32	Bb	610	CLA	CMB-C2B	-2.29	1.46	1.50
32	Rr	608	CLA	C3B-C4B	2.29	1.49	1.42
32	Nn	313	CLA	C3B-C4B	2.29	1.49	1.42
32	BB	612	CLA	CMD-C2D	-2.29	1.46	1.50
39	1	607	CHL	CHC-C1C	2.29	1.43	1.39
32	GG	612	CLA	C3B-C4B	2.29	1.49	1.42
32	NN	610	CLA	C3B-C4B	2.28	1.49	1.42
32	S	610	CLA	CMD-C2D	-2.28	1.46	1.50
32	Y	613	CLA	CMD-C2D	-2.28	1.46	1.50
39	YY	601	CHL	CBD-CGD	-2.28	1.49	1.52
32	Y	612	CLA	CMD-C2D	-2.28	1.46	1.50
32	a	406	CLA	CMD-C2D	-2.28	1.46	1.50
32	N	610	CLA	C3B-C4B	2.28	1.49	1.42
32	c	510	CLA	C3B-C4B	2.28	1.49	1.42
32	y	305	CLA	CMD-C2D	-2.28	1.46	1.50
39	RR	305	CHL	CAC-C3C	-2.28	1.47	1.51
32	N	610	CLA	CHC-C1C	2.28	1.43	1.38
32	B	608	CLA	C3B-C4B	2.28	1.49	1.42
39	N	608	CHL	CHC-C1C	2.28	1.43	1.39
32	S	611	CLA	C3B-C4B	2.28	1.49	1.42
32	a	405	CLA	CMD-C2D	-2.28	1.46	1.50
32	Bb	609	CLA	CHC-C1C	2.28	1.43	1.38
32	11	604	CLA	C3B-C4B	2.28	1.49	1.42
41	g	619	XAT	O24-C25	-2.28	1.43	1.46
32	22	610	CLA	C3B-C4B	2.28	1.49	1.42
32	SS	311	CLA	C3B-C4B	2.28	1.49	1.42
40	Ss	615	LUT	C8-C9	2.28	1.50	1.46
32	Cc	505	CLA	CMD-C2D	-2.28	1.46	1.50
32	Rr	613	CLA	C3B-C4B	2.28	1.49	1.42
32	YY	610	CLA	C3B-C4B	2.28	1.49	1.42
32	N	611	CLA	C3B-C4B	2.28	1.49	1.42
32	RR	303	CLA	C3B-C4B	2.28	1.49	1.42
32	CC	502	CLA	CMD-C2D	-2.27	1.46	1.50
32	Bb	601	CLA	CMC-C2C	-2.27	1.46	1.50
39	Gg	302	CHL	CAC-C3C	-2.27	1.47	1.51
32	s	603	CLA	C3B-C4B	2.27	1.49	1.42
32	C	512	CLA	C3B-C4B	2.27	1.49	1.42
39	GG	605	CHL	CHC-C1C	2.27	1.43	1.39
32	d	401	CLA	CMD-C2D	-2.27	1.46	1.50
32	GG	611	CLA	CMD-C2D	-2.27	1.46	1.50
39	R	605	CHL	CHC-C1C	2.27	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BB	616	BCR	C30-C25	-2.27	1.50	1.53
32	SS	312	CLA	CMD-C2D	-2.27	1.46	1.50
32	g	612	CLA	C3B-C4B	2.27	1.49	1.42
35	d	404	PL9	C7-C8	2.27	1.54	1.50
39	33	605	CHL	CHC-C1C	2.27	1.43	1.39
32	RR	309	CLA	CHC-C1C	2.27	1.43	1.38
35	d	404	PL9	C41-C39	2.27	1.56	1.51
32	BB	606	CLA	CMD-C2D	-2.27	1.46	1.50
39	N	609	CHL	CHC-C1C	2.27	1.43	1.39
32	r	613	CLA	C3B-C4B	2.27	1.49	1.42
32	Bb	607	CLA	CMD-C2D	-2.27	1.46	1.50
32	BB	604	CLA	CMB-C2B	-2.27	1.46	1.50
32	R	602	CLA	C3B-C4B	2.27	1.49	1.42
40	y	317	LUT	C22-C21	-2.27	1.52	1.54
39	Ss	601	CHL	CHC-C1C	2.27	1.43	1.39
32	Bb	612	CLA	CMD-C2D	-2.27	1.46	1.50
39	Rr	607	CHL	CHC-C1C	2.27	1.43	1.39
32	c	508	CLA	C3B-C4B	2.27	1.49	1.42
32	1	611	CLA	C3B-C4B	2.27	1.49	1.42
32	33	603	CLA	C3B-C4B	2.27	1.49	1.42
32	33	612	CLA	C3B-C4B	2.27	1.49	1.42
32	R	608	CLA	C3B-C4B	2.27	1.49	1.42
32	RR	314	CLA	C3B-C4B	2.27	1.49	1.42
39	GG	606	CHL	CHC-C1C	2.27	1.43	1.39
32	S	611	CLA	CMD-C2D	-2.27	1.46	1.50
33	DD	402	PHO	C4D-ND	-2.27	1.35	1.38
32	1	612	CLA	C3B-C4B	2.27	1.49	1.42
32	11	612	CLA	CHC-C1C	2.27	1.43	1.38
32	3	612	CLA	C3B-C4B	2.27	1.49	1.42
32	RR	302	CLA	CMB-C2B	-2.27	1.46	1.50
32	RR	308	CLA	C3B-C4B	2.27	1.49	1.42
32	Cc	512	CLA	C3B-C4B	2.26	1.49	1.42
32	NN	602	CLA	CHC-C1C	2.26	1.43	1.38
39	22	606	CHL	CHC-C1C	2.26	1.43	1.39
35	A	410	PL9	C5-C4	-2.26	1.39	1.47
32	D	404	CLA	CMC-C2C	-2.26	1.46	1.50
32	Rr	610	CLA	C3B-C4B	2.26	1.49	1.42
32	2	609	CLA	C3B-C4B	2.26	1.49	1.42
32	b	609	CLA	C3B-C4B	2.26	1.49	1.42
39	2	606	CHL	CHC-C1C	2.26	1.43	1.39
32	BB	611	CLA	CMB-C2B	-2.26	1.46	1.50
35	D	407	PL9	C7-C8	2.26	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Ss	604	CLA	C3B-C4B	2.26	1.49	1.42
39	Y	608	CHL	CHC-C1C	2.26	1.43	1.39
32	NN	602	CLA	C3B-C4B	2.26	1.49	1.42
32	Bb	603	CLA	CMD-C2D	-2.26	1.46	1.50
32	Rr	602	CLA	C3B-C4B	2.26	1.49	1.42
32	c	507	CLA	CMD-C2D	-2.26	1.46	1.50
39	g	609	CHL	CHC-C1C	2.26	1.43	1.39
41	Gg	301	XAT	O24-C25	-2.26	1.43	1.46
32	3	613	CLA	C3B-C4B	2.26	1.49	1.42
32	c	513	CLA	CMD-C2D	-2.26	1.46	1.50
41	GG	617	XAT	O4-C5	-2.26	1.43	1.46
39	2	607	CHL	CHC-C1C	2.26	1.43	1.39
32	BB	613	CLA	C3B-C4B	2.26	1.49	1.42
40	Yy	615	LUT	C22-C21	-2.26	1.52	1.54
32	DD	403	CLA	CMD-C2D	-2.26	1.46	1.50
32	YY	613	CLA	CMD-C2D	-2.26	1.46	1.50
32	BB	614	CLA	CMD-C2D	-2.26	1.46	1.50
32	Bb	608	CLA	CMB-C2B	-2.26	1.46	1.50
32	22	612	CLA	C3B-C4B	2.26	1.49	1.42
39	Gg	309	CHL	CMB-C2B	-2.26	1.47	1.51
32	3	603	CLA	C3B-C4B	2.26	1.49	1.42
42	NN	618	NEX	O24-C25	-2.26	1.43	1.46
32	BB	608	CLA	CMD-C2D	-2.25	1.46	1.50
32	BB	604	CLA	C3B-C4B	2.25	1.49	1.42
32	CC	513	CLA	CMD-C2D	-2.25	1.46	1.50
41	G	617	XAT	O4-C5	-2.25	1.43	1.46
34	BB	617	BCR	C23-C22	2.25	1.50	1.46
32	R	601	CLA	C1B-C2B	2.25	1.48	1.43
32	B	609	CLA	C3B-C4B	2.25	1.49	1.42
32	Bb	610	CLA	C3B-C4B	2.25	1.49	1.42
32	AA	405	CLA	CMD-C2D	-2.25	1.46	1.50
32	s	602	CLA	C3B-C4B	2.25	1.49	1.42
32	b	616	CLA	C3B-C4B	2.25	1.49	1.42
39	g	608	CHL	CMB-C2B	-2.25	1.47	1.51
32	B	621	CLA	CMB-C2B	-2.25	1.46	1.50
32	Aa	405	CLA	CMD-C2D	-2.25	1.46	1.50
41	g	619	XAT	O4-C5	-2.25	1.43	1.46
32	SS	304	CLA	C3B-C4B	2.25	1.49	1.42
32	Aa	406	CLA	MG-NA	2.25	2.11	2.06
41	y	301	XAT	O4-C5	-2.25	1.43	1.46
32	B	606	CLA	CMB-C2B	-2.25	1.46	1.50
32	B	623	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	s	614	LUT	C8-C9	2.25	1.50	1.46
39	NN	609	CHL	CAC-C3C	-2.25	1.47	1.51
32	Yy	612	CLA	CMD-C2D	-2.25	1.46	1.50
32	Ss	608	CLA	C3B-C4B	2.25	1.49	1.42
32	44	610	CLA	C3B-C4B	2.25	1.49	1.42
33	AA	407	PHO	C4D-ND	-2.25	1.35	1.38
39	R	605	CHL	CAC-C3C	-2.25	1.47	1.51
32	NN	611	CLA	C3B-C4B	2.25	1.49	1.42
39	s	601	CHL	CHC-C1C	2.25	1.43	1.39
41	Yy	619	XAT	O4-C5	-2.25	1.43	1.46
32	b	603	CLA	CMD-C2D	-2.25	1.46	1.50
32	Bb	603	CLA	C3B-C4B	2.25	1.49	1.42
32	C	511	CLA	C3B-C4B	2.25	1.49	1.42
32	CC	510	CLA	C3B-C4B	2.25	1.49	1.42
41	44	613	XAT	O24-C25	-2.25	1.43	1.46
39	g	606	CHL	CHC-C1C	2.25	1.43	1.39
39	r	607	CHL	CHC-C1C	2.25	1.43	1.39
32	B	624	CLA	CMB-C2B	-2.25	1.46	1.50
32	33	613	CLA	C3B-C4B	2.24	1.49	1.42
32	Rr	613	CLA	CMD-C2D	-2.24	1.46	1.50
42	Y	617	NEX	O24-C25	-2.24	1.43	1.46
32	22	611	CLA	C3B-C4B	2.24	1.49	1.42
32	d	401	CLA	C3B-C4B	2.24	1.49	1.42
32	Bb	601	CLA	C3B-C4B	2.24	1.49	1.42
32	BB	610	CLA	CMD-C2D	-2.24	1.46	1.50
32	G	612	CLA	C3B-C4B	2.24	1.49	1.42
32	s	609	CLA	C3B-C4B	2.24	1.49	1.42
39	R	607	CHL	CHC-C1C	2.24	1.43	1.39
39	Gg	302	CHL	CHC-C1C	2.24	1.43	1.39
32	N	614	CLA	C3B-C4B	2.24	1.49	1.42
32	BB	601	CLA	C3B-C4B	2.24	1.49	1.42
32	R	603	CLA	CMD-C2D	-2.24	1.46	1.50
32	NN	610	CLA	CHC-C1C	2.24	1.43	1.38
42	N	618	NEX	O24-C25	-2.24	1.43	1.46
32	22	603	CLA	C3B-C4B	2.24	1.49	1.42
39	RR	305	CHL	CHC-C1C	2.24	1.43	1.39
32	Dd	401	CLA	CMD-C2D	-2.24	1.46	1.50
32	SS	309	CLA	C3B-C4B	2.24	1.49	1.42
39	Gg	307	CHL	CHC-C1C	2.24	1.43	1.39
32	b	601	CLA	C3B-C4B	2.24	1.49	1.42
32	b	612	CLA	C3B-C4B	2.24	1.49	1.42
32	YY	614	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	311	CLA	C3B-C4B	2.24	1.49	1.42
39	Y	607	CHL	CHC-C1C	2.24	1.43	1.39
34	AA	409	BCR	C12-C13	2.24	1.50	1.46
39	n	609	CHL	CBD-CGD	-2.24	1.49	1.52
32	Rr	610	CLA	CMB-C2B	-2.24	1.46	1.50
32	Ss	609	CLA	C3B-C4B	2.24	1.49	1.42
32	22	609	CLA	C3B-C4B	2.24	1.49	1.42
32	NN	614	CLA	C3B-C4B	2.24	1.49	1.42
34	H	101	BCR	C19-C18	2.24	1.50	1.46
32	CC	508	CLA	CMD-C2D	-2.24	1.46	1.50
32	DD	401	CLA	C1B-C2B	2.24	1.48	1.43
33	A	407	PHO	C4D-ND	-2.24	1.35	1.38
32	N	603	CLA	C3B-C4B	2.23	1.49	1.42
34	A	409	BCR	C8-C9	2.23	1.50	1.46
32	Aa	410	CLA	C3B-C4B	2.23	1.49	1.42
32	Cc	503	CLA	CMD-C2D	-2.23	1.46	1.50
39	y	308	CHL	CAC-C3C	-2.23	1.47	1.51
32	R	603	CLA	C3B-C4B	2.23	1.49	1.42
39	y	308	CHL	CHC-C1C	2.23	1.43	1.39
32	2	602	CLA	CHC-C1C	2.23	1.43	1.38
32	d	401	CLA	CMC-C2C	-2.23	1.46	1.50
41	44	613	XAT	O4-C5	-2.23	1.43	1.46
39	NN	606	CHL	CBD-CGD	-2.23	1.49	1.52
32	C	514	CLA	CMD-C2D	-2.23	1.46	1.50
32	CC	507	CLA	CMD-C2D	-2.23	1.46	1.50
32	Bb	614	CLA	CMD-C2D	-2.23	1.46	1.50
32	Bb	614	CLA	C3B-C4B	2.23	1.49	1.42
32	Cc	508	CLA	C3B-C4B	2.23	1.49	1.42
32	Gg	315	CLA	C3B-C4B	2.23	1.49	1.42
32	r	613	CLA	CMD-C2D	-2.23	1.46	1.50
32	RR	304	CLA	CMD-C2D	-2.23	1.46	1.50
32	2	613	CLA	C3B-C4B	2.23	1.49	1.42
32	2	611	CLA	C3B-C4B	2.23	1.49	1.42
32	3	611	CLA	C3B-C4B	2.23	1.49	1.42
32	1	602	CLA	C3B-C4B	2.23	1.49	1.42
32	N	602	CLA	C3B-C4B	2.23	1.49	1.42
32	GG	602	CLA	CMB-C2B	-2.23	1.46	1.50
32	4	305	CLA	C3B-C4B	2.23	1.49	1.42
32	Nn	302	CLA	C3B-C4B	2.23	1.49	1.42
39	S	605	CHL	CHC-C1C	2.23	1.43	1.39
32	NN	604	CLA	C3B-C4B	2.23	1.49	1.42
32	BB	605	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Bb	612	CLA	CMB-C2B	-2.23	1.46	1.50
32	r	602	CLA	C3B-C4B	2.23	1.49	1.42
32	r	608	CLA	C3B-C4B	2.23	1.49	1.42
34	c	515	BCR	C12-C13	2.23	1.50	1.46
32	Yy	613	CLA	CMD-C2D	-2.23	1.46	1.50
32	B	604	CLA	CMD-C2D	-2.22	1.46	1.50
40	2	614	LUT	C12-C13	2.22	1.50	1.46
32	Bb	613	CLA	CMD-C2D	-2.22	1.46	1.50
32	b	614	CLA	CMD-C2D	-2.22	1.46	1.50
32	a	406	CLA	C3B-C4B	2.22	1.49	1.42
42	YY	617	NEX	O24-C25	-2.22	1.43	1.46
32	C	510	CLA	CMD-C2D	-2.22	1.46	1.50
39	n	609	CHL	CMB-C2B	-2.22	1.47	1.51
32	g	611	CLA	C3B-C4B	2.22	1.49	1.42
32	CC	509	CLA	C3B-C4B	2.22	1.49	1.42
32	C	508	CLA	CMB-C2B	-2.22	1.46	1.50
39	33	608	CHL	CHC-C1C	2.22	1.43	1.39
39	Gg	309	CHL	CHC-C1C	2.22	1.43	1.39
32	3	610	CLA	C3B-C4B	2.22	1.49	1.42
32	Gg	313	CLA	C3B-C4B	2.22	1.49	1.42
32	b	612	CLA	CMB-C2B	-2.22	1.46	1.50
39	S	606	CHL	CHC-C1C	2.22	1.43	1.39
32	CC	509	CLA	CMD-C2D	-2.22	1.46	1.50
39	Yy	609	CHL	CHC-C1C	2.22	1.43	1.39
32	C	509	CLA	CMD-C2D	-2.22	1.46	1.50
32	Cc	509	CLA	CMD-C2D	-2.22	1.46	1.50
32	22	602	CLA	CHC-C1C	2.22	1.42	1.38
32	4	310	CLA	C3B-C4B	2.22	1.49	1.42
32	B	618	CLA	CMD-C2D	-2.22	1.46	1.50
41	GG	619	XAT	O4-C5	-2.22	1.43	1.46
32	33	611	CLA	C3B-C4B	2.22	1.49	1.42
32	CC	502	CLA	CMB-C2B	-2.22	1.46	1.50
34	Aa	411	BCR	C12-C13	2.22	1.50	1.46
32	33	602	CLA	C3B-C4B	2.22	1.49	1.42
32	11	612	CLA	CMB-C2B	-2.22	1.46	1.50
32	BB	603	CLA	CMD-C2D	-2.22	1.46	1.50
32	B	610	CLA	CMD-C2D	-2.22	1.46	1.50
32	Bb	611	CLA	CMD-C2D	-2.22	1.46	1.50
32	C	510	CLA	C3B-C4B	2.22	1.49	1.42
32	Y	614	CLA	CMD-C2D	-2.22	1.46	1.50
32	y	315	CLA	CMD-C2D	-2.22	1.46	1.50
32	b	614	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	604	CLA	C3B-C4B	2.22	1.49	1.42
34	Hh	101	BCR	C23-C22	2.22	1.50	1.46
32	BB	604	CLA	CMD-C2D	-2.22	1.46	1.50
32	Gg	314	CLA	C3B-C4B	2.22	1.49	1.42
32	g	610	CLA	CMB-C2B	-2.21	1.46	1.50
34	B	613	BCR	C23-C22	2.21	1.50	1.46
32	Ss	602	CLA	C3B-C4B	2.21	1.49	1.42
34	Cc	517	BCR	C12-C13	2.21	1.50	1.46
32	DD	401	CLA	CMD-C2D	-2.21	1.46	1.50
42	y	319	NEX	O24-C25	-2.21	1.43	1.46
32	Ss	613	CLA	C3B-C4B	2.21	1.49	1.42
32	Bb	615	CLA	CMD-C2D	-2.21	1.46	1.50
39	N	608	CHL	CBD-CGD	-2.21	1.49	1.52
32	Cc	510	CLA	C3B-C4B	2.21	1.49	1.42
39	YY	608	CHL	CHC-C1C	2.21	1.43	1.39
39	Nn	315	CHL	CHC-C1C	2.21	1.43	1.39
32	Aa	410	CLA	CMD-C2D	-2.21	1.46	1.50
32	n	610	CLA	CHC-C1C	2.21	1.42	1.38
39	N	609	CHL	CMB-C2B	-2.21	1.47	1.51
32	44	611	CLA	C3B-C4B	2.21	1.49	1.42
32	Yy	611	CLA	C3B-C4B	2.21	1.49	1.42
39	Gg	308	CHL	CHC-C1C	2.21	1.43	1.39
32	C	504	CLA	CMD-C2D	-2.21	1.46	1.50
32	g	602	CLA	MG-NB	-2.21	2.01	2.05
32	3	609	CLA	CHC-C1C	2.21	1.42	1.38
40	s	614	LUT	C32-C33	2.21	1.50	1.46
32	n	610	CLA	C3B-C4B	2.21	1.49	1.42
39	n	605	CHL	C1A-CHA	-2.21	1.37	1.40
32	D	401	CLA	CMD-C2D	-2.21	1.46	1.50
32	Gg	312	CLA	C3B-C4B	2.21	1.49	1.42
32	Rr	609	CLA	C3B-C4B	2.21	1.49	1.42
32	Dd	402	CLA	C3B-C4B	2.21	1.49	1.42
32	C	513	CLA	CMD-C2D	-2.21	1.46	1.50
39	22	601	CHL	CHC-C1C	2.21	1.43	1.39
41	r	615	XAT	C6-C7	2.21	1.54	1.50
32	C	505	CLA	CMD-C2D	-2.21	1.46	1.50
32	XX	201	CLA	CMD-C2D	-2.21	1.46	1.50
39	Yy	606	CHL	CAC-C3C	-2.21	1.47	1.51
32	b	610	CLA	CMB-C2B	-2.21	1.46	1.50
32	BB	610	CLA	CMB-C2B	-2.21	1.46	1.50
41	G	617	XAT	C32-C33	2.21	1.50	1.46
39	g	601	CHL	CBD-CGD	-2.21	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	YY	610	CLA	CHC-C1C	2.21	1.42	1.38
32	r	603	CLA	CMD-C2D	-2.21	1.46	1.50
39	r	606	CHL	CAC-C3C	-2.21	1.47	1.51
32	b	613	CLA	CMD-C2D	-2.21	1.46	1.50
32	YY	603	CLA	CMD-C2D	-2.21	1.46	1.50
40	2	614	LUT	C8-C9	2.21	1.50	1.46
32	r	609	CLA	C3B-C4B	2.21	1.49	1.42
32	B	609	CLA	CMD-C2D	-2.21	1.46	1.50
39	N	609	CHL	CAC-C3C	-2.21	1.47	1.51
32	B	622	CLA	CMD-C2D	-2.21	1.46	1.50
32	c	505	CLA	CMD-C2D	-2.21	1.46	1.50
32	y	304	CLA	CMD-C2D	-2.20	1.46	1.50
39	n	606	CHL	CHC-C1C	2.20	1.43	1.39
32	Aa	407	CLA	CMD-C2D	-2.20	1.46	1.50
39	3	606	CHL	CHC-C1C	2.20	1.43	1.39
32	N	604	CLA	C3B-C4B	2.20	1.49	1.42
32	Bb	609	CLA	C3B-C4B	2.20	1.49	1.42
32	4	310	CLA	CHC-C1C	2.20	1.42	1.38
32	G	610	CLA	CMB-C2B	-2.20	1.46	1.50
39	Gg	310	CHL	CHC-C1C	2.20	1.43	1.39
32	GG	602	CLA	CMD-C2D	-2.20	1.46	1.50
32	y	304	CLA	C3B-C4B	2.20	1.49	1.42
32	4	312	CLA	C3B-C4B	2.20	1.49	1.42
32	Nn	301	CLA	CMC-C2C	-2.20	1.46	1.50
32	Bb	616	CLA	C3B-C4B	2.20	1.49	1.42
39	Yy	608	CHL	CHC-C1C	2.20	1.43	1.39
32	B	611	CLA	CMD-C2D	-2.20	1.46	1.50
32	SS	304	CLA	CMD-C2D	-2.20	1.46	1.50
32	Aa	406	CLA	CMD-C2D	-2.20	1.46	1.50
32	Yy	603	CLA	CMD-C2D	-2.20	1.46	1.50
32	N	610	CLA	CMD-C2D	-2.20	1.46	1.50
32	n	610	CLA	CMD-C2D	-2.20	1.46	1.50
32	2	610	CLA	C3B-C4B	2.20	1.49	1.42
32	s	610	CLA	C3B-C4B	2.20	1.49	1.42
32	33	609	CLA	CHC-C1C	2.20	1.42	1.38
35	Dd	404	PL9	C41-C39	2.20	1.55	1.51
32	c	502	CLA	C3B-C4B	2.20	1.49	1.42
32	d	402	CLA	C3B-C4B	2.20	1.49	1.42
32	GG	604	CLA	C3B-C4B	2.20	1.49	1.42
39	Yy	609	CHL	CBD-CGD	-2.20	1.49	1.52
32	BB	613	CLA	CMD-C2D	-2.20	1.46	1.50
32	2	603	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	617	BCR	C12-C13	2.20	1.50	1.46
40	NN	615	LUT	C22-C21	-2.20	1.52	1.54
32	b	604	CLA	CMD-C2D	-2.20	1.46	1.50
39	1	601	CHL	CHC-C1C	2.20	1.43	1.39
39	g	608	CHL	CHC-C1C	2.20	1.43	1.39
32	22	613	CLA	C3B-C4B	2.20	1.49	1.42
32	n	603	CLA	C3B-C4B	2.20	1.49	1.42
32	G	602	CLA	CMB-C2B	-2.20	1.46	1.50
32	c	503	CLA	CMD-C2D	-2.20	1.46	1.50
32	RR	303	CLA	CMD-C2D	-2.20	1.46	1.50
39	Y	605	CHL	CHC-C1C	2.20	1.43	1.39
42	Nn	309	NEX	O24-C25	-2.20	1.43	1.46
44	BB	623	DGD	O3G-C1D	2.20	1.43	1.40
32	3	602	CLA	C3B-C4B	2.19	1.49	1.42
32	Y	610	CLA	CHC-C1C	2.19	1.42	1.38
34	Aa	411	BCR	C8-C9	2.19	1.50	1.46
32	A	405	CLA	CMD-C2D	-2.19	1.46	1.50
32	X	201	CLA	CMB-C2B	-2.19	1.46	1.50
32	Bb	604	CLA	CMD-C2D	-2.19	1.46	1.50
39	y	309	CHL	CHC-C1C	2.19	1.43	1.39
32	S	609	CLA	C3B-C4B	2.19	1.49	1.42
32	BB	601	CLA	CMD-C2D	-2.19	1.46	1.50
32	RR	311	CLA	C3B-C4B	2.19	1.49	1.42
32	C	506	CLA	CMB-C2B	-2.19	1.46	1.50
39	Yy	608	CHL	CBD-CGD	-2.19	1.49	1.52
32	CC	510	CLA	CMD-C2D	-2.19	1.46	1.50
32	r	602	CLA	CHC-C1C	2.19	1.42	1.38
32	Yy	602	CLA	C3B-C4B	2.19	1.49	1.42
34	Bb	619	BCR	C23-C22	2.19	1.50	1.46
32	C	503	CLA	CMB-C2B	-2.19	1.46	1.50
32	R	604	CLA	CMD-C2D	-2.19	1.46	1.50
32	C	508	CLA	C3B-C4B	2.19	1.49	1.42
32	y	313	CLA	C3B-C4B	2.19	1.49	1.42
32	4	303	CLA	C3B-C4B	2.19	1.49	1.42
32	B	622	CLA	CMB-C2B	-2.19	1.46	1.50
39	y	303	CHL	CMB-C2B	-2.19	1.47	1.51
39	2	608	CHL	CHC-C1C	2.19	1.43	1.39
32	CC	511	CLA	CHC-C1C	2.19	1.42	1.38
39	GG	601	CHL	CAC-C3C	-2.19	1.47	1.51
32	DD	403	CLA	C3B-C4B	2.19	1.49	1.42
32	44	603	CLA	C3B-C4B	2.19	1.49	1.42
32	YY	614	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Rr	611	CLA	CMD-C2D	-2.19	1.46	1.50
32	g	613	CLA	CMD-C2D	-2.19	1.46	1.50
34	A	409	BCR	C12-C13	2.19	1.50	1.46
32	Nn	314	CLA	C3B-C4B	2.19	1.49	1.42
39	22	607	CHL	CHC-C1C	2.19	1.43	1.39
39	Yy	606	CHL	CBD-CGD	-2.19	1.49	1.52
32	B	606	CLA	CMD-C2D	-2.19	1.46	1.50
32	Cc	513	CLA	CMB-C2B	-2.19	1.46	1.50
39	RR	307	CHL	CHC-C1C	2.19	1.43	1.39
32	CC	507	CLA	C3B-C4B	2.19	1.49	1.42
32	SS	314	CLA	C3B-C4B	2.19	1.49	1.42
32	DD	403	CLA	CMC-C2C	-2.19	1.46	1.50
39	11	601	CHL	CHC-C1C	2.18	1.43	1.39
32	Bb	603	CLA	CMB-C2B	-2.18	1.46	1.50
32	B	619	CLA	CMB-C2B	-2.18	1.46	1.50
32	Aa	406	CLA	CMB-C2B	-2.18	1.46	1.50
32	C	506	CLA	C3B-C4B	2.18	1.49	1.42
32	BB	607	CLA	CMD-C2D	-2.18	1.46	1.50
32	22	604	CLA	C3B-C4B	2.18	1.49	1.42
32	2	604	CLA	C3B-C4B	2.18	1.49	1.42
32	AA	406	CLA	C3B-C4B	2.18	1.49	1.42
32	SS	305	CLA	C3B-C4B	2.18	1.49	1.42
32	R	602	CLA	CHC-C1C	2.18	1.42	1.38
33	AA	407	PHO	C3B-C2B	-2.18	1.37	1.40
32	CC	503	CLA	C3B-C4B	2.18	1.49	1.42
39	NN	605	CHL	CHC-C1C	2.18	1.43	1.39
32	BB	605	CLA	CMB-C2B	-2.18	1.46	1.50
32	b	607	CLA	CMD-C2D	-2.18	1.46	1.50
33	a	408	PHO	C4D-ND	-2.18	1.35	1.38
39	y	308	CHL	CBD-CGD	-2.18	1.49	1.52
32	B	607	CLA	C3B-C4B	2.18	1.49	1.42
32	Y	602	CLA	CHC-C1C	2.18	1.42	1.38
32	D	404	CLA	C3B-C4B	2.18	1.49	1.42
32	b	611	CLA	CMD-C2D	-2.18	1.46	1.50
32	d	402	CLA	CMB-C2B	-2.18	1.46	1.50
39	s	605	CHL	CHC-C1C	2.18	1.43	1.39
32	Y	603	CLA	C3B-C4B	2.18	1.49	1.42
39	g	608	CHL	CBD-CGD	-2.18	1.49	1.52
32	S	604	CLA	C3B-C4B	2.18	1.49	1.42
39	n	609	CHL	CHC-C1C	2.18	1.43	1.39
32	Nn	301	CLA	C3B-C4B	2.18	1.49	1.42
32	BB	615	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	44	605	CHL	CBD-CGD	-2.18	1.49	1.52
32	B	610	CLA	C3B-C4B	2.18	1.49	1.42
32	Cc	505	CLA	C3B-C4B	2.18	1.49	1.42
34	a	411	BCR	C8-C9	2.18	1.50	1.46
32	y	316	CLA	C3B-C4B	2.18	1.49	1.42
32	S	613	CLA	C3B-C4B	2.18	1.49	1.42
32	C	508	CLA	CMD-C2D	-2.18	1.46	1.50
32	GG	611	CLA	C3B-C4B	2.18	1.49	1.42
39	YY	609	CHL	CMB-C2B	-2.18	1.47	1.51
32	Yy	602	CLA	CMD-C2D	-2.18	1.46	1.50
32	r	612	CLA	C3B-C4B	2.18	1.49	1.42
41	Rr	615	XAT	C6-C7	2.18	1.54	1.50
39	G	607	CHL	CHC-C1C	2.18	1.43	1.39
39	Nn	311	CHL	CHC-C1C	2.18	1.43	1.39
39	Nn	319	CHL	CMB-C2B	-2.18	1.47	1.51
32	44	602	CLA	C3B-C4B	2.18	1.49	1.42
39	N	609	CHL	CBD-CGD	-2.18	1.49	1.52
32	NN	603	CLA	C3B-C4B	2.18	1.49	1.42
32	c	510	CLA	CMD-C2D	-2.18	1.46	1.50
32	b	603	CLA	CHC-C1C	2.18	1.42	1.38
32	YY	602	CLA	CHC-C1C	2.18	1.42	1.38
32	YY	602	CLA	C3B-C4B	2.18	1.49	1.42
32	Yy	614	CLA	C3B-C4B	2.17	1.49	1.42
32	G	614	CLA	C3B-C4B	2.17	1.49	1.42
32	a	407	CLA	C3B-C4B	2.17	1.49	1.42
32	Nn	312	CLA	CMD-C2D	-2.17	1.46	1.50
32	b	616	CLA	CMD-C2D	-2.17	1.46	1.50
32	DD	404	CLA	CMD-C2D	-2.17	1.46	1.50
32	Ss	612	CLA	C3B-C4B	2.17	1.49	1.42
32	11	609	CLA	C3B-C4B	2.17	1.49	1.42
32	Bb	612	CLA	C3B-C4B	2.17	1.49	1.42
32	CC	508	CLA	CMB-C2B	-2.17	1.46	1.50
32	C	507	CLA	C3B-C4B	2.17	1.49	1.42
32	YY	603	CLA	C3B-C4B	2.17	1.49	1.42
32	X	201	CLA	CMD-C2D	-2.17	1.46	1.50
32	CC	504	CLA	CMD-C2D	-2.17	1.46	1.50
32	C	511	CLA	CMD-C2D	-2.17	1.46	1.50
32	a	406	CLA	CMB-C2B	-2.17	1.46	1.50
32	Cc	504	CLA	CMD-C2D	-2.17	1.46	1.50
39	Nn	319	CHL	CBD-CGD	-2.17	1.49	1.52
32	Ss	610	CLA	C3B-C4B	2.17	1.49	1.42
32	Bb	616	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	33	606	CHL	CHC-C1C	2.17	1.43	1.39
32	B	618	CLA	C3B-C4B	2.17	1.49	1.42
37	CC	501	SQD	O6-C1	2.17	1.43	1.40
32	Gg	312	CLA	CHC-C1C	2.17	1.42	1.38
32	G	613	CLA	C3B-C4B	2.17	1.49	1.42
32	y	304	CLA	CHC-C1C	2.17	1.42	1.38
32	Nn	304	CLA	C3B-C4B	2.17	1.49	1.42
40	22	614	LUT	C8-C9	2.17	1.50	1.46
39	Nn	318	CHL	CBD-CGD	-2.17	1.49	1.52
32	C	509	CLA	CMB-C2B	-2.17	1.46	1.50
32	Cc	512	CLA	CMD-C2D	-2.17	1.46	1.50
42	Yy	617	NEX	O24-C25	-2.17	1.43	1.46
32	s	613	CLA	C3B-C4B	2.17	1.49	1.42
39	RR	306	CHL	CMB-C2B	-2.17	1.47	1.51
32	c	505	CLA	C3B-C4B	2.17	1.49	1.42
32	B	620	CLA	CMD-C2D	-2.17	1.46	1.50
32	Y	602	CLA	C3B-C4B	2.17	1.49	1.42
41	4	314	XAT	O4-C5	-2.17	1.43	1.46
32	Yy	614	CLA	CMD-C2D	-2.17	1.46	1.50
39	y	310	CHL	CHC-C1C	2.17	1.43	1.39
32	S	610	CLA	C3B-C4B	2.17	1.49	1.42
32	B	622	CLA	C3B-C4B	2.17	1.49	1.42
32	N	602	CLA	CHC-C1C	2.17	1.42	1.38
32	S	602	CLA	C3B-C4B	2.17	1.49	1.42
32	c	503	CLA	C3B-C4B	2.17	1.49	1.42
32	b	615	CLA	CMD-C2D	-2.17	1.46	1.50
32	CC	507	CLA	MG-NB	-2.17	2.01	2.05
32	R	611	CLA	C3B-C4B	2.17	1.49	1.42
32	g	614	CLA	C3B-C4B	2.17	1.49	1.42
32	n	614	CLA	C3B-C4B	2.17	1.49	1.42
39	4	306	CHL	C1A-CHA	-2.17	1.37	1.40
32	y	305	CLA	CMB-C2B	-2.17	1.46	1.50
32	C	503	CLA	C3B-C4B	2.16	1.49	1.42
32	NN	603	CLA	CMB-C2B	-2.16	1.46	1.50
32	44	604	CLA	C3B-C4B	2.16	1.49	1.42
35	AA	410	PL9	C37-C38	2.16	1.57	1.50
32	11	604	CLA	CHC-C1C	2.16	1.42	1.38
32	c	506	CLA	C3B-C4B	2.16	1.49	1.42
32	G	611	CLA	C3B-C4B	2.16	1.49	1.42
32	B	621	CLA	C3B-C4B	2.16	1.49	1.42
39	y	311	CHL	CBD-CGD	-2.16	1.49	1.52
39	4	306	CHL	CHC-C1C	2.16	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	614	CLA	C3B-C4B	2.16	1.49	1.42
39	Yy	601	CHL	CMB-C2B	-2.16	1.47	1.51
39	GG	608	CHL	CBD-CGD	-2.16	1.49	1.52
32	R	608	CLA	CMD-C2D	-2.16	1.46	1.50
32	Bb	604	CLA	C3B-C4B	2.16	1.49	1.42
32	YY	604	CLA	C3B-C4B	2.16	1.49	1.42
32	CC	512	CLA	CMD-C2D	-2.16	1.46	1.50
32	GG	614	CLA	C3B-C4B	2.16	1.49	1.42
39	4	308	CHL	CAC-C3C	-2.16	1.47	1.51
32	g	611	CLA	CMB-C2B	-2.16	1.46	1.50
34	h	101	BCR	C8-C9	2.16	1.50	1.46
34	B	614	BCR	C23-C22	2.16	1.50	1.46
42	n	617	NEX	O24-C25	-2.16	1.43	1.46
42	RR	317	NEX	O24-C25	-2.16	1.43	1.46
32	S	608	CLA	CHC-C1C	2.16	1.42	1.38
32	Cc	508	CLA	CMD-C2D	-2.16	1.46	1.50
32	BB	614	CLA	C3B-C4B	2.16	1.49	1.42
32	RR	308	CLA	CMD-C2D	-2.16	1.46	1.50
39	NN	607	CHL	CBD-CGD	-2.16	1.49	1.52
32	C	514	CLA	C3B-C4B	2.16	1.49	1.42
32	R	602	CLA	CMD-C2D	-2.16	1.46	1.50
32	Dd	401	CLA	C3B-C4B	2.16	1.49	1.42
32	Cc	507	CLA	C3B-C4B	2.16	1.49	1.42
32	Y	603	CLA	CMD-C2D	-2.16	1.46	1.50
32	Yy	611	CLA	CMD-C2D	-2.16	1.46	1.50
32	Cc	513	CLA	C3B-C4B	2.16	1.49	1.42
39	2	601	CHL	CHC-C1C	2.16	1.43	1.39
32	Yy	603	CLA	CMB-C2B	-2.16	1.46	1.50
32	G	603	CLA	CMD-C2D	-2.16	1.46	1.50
32	c	511	CLA	C3B-C4B	2.16	1.49	1.42
32	Y	604	CLA	C3B-C4B	2.16	1.49	1.42
32	Bb	609	CLA	CMD-C2D	-2.16	1.46	1.50
32	s	608	CLA	CHC-C1C	2.16	1.42	1.38
32	CC	514	CLA	CMD-C2D	-2.16	1.46	1.50
32	n	602	CLA	CMD-C2D	-2.15	1.46	1.50
32	n	611	CLA	CMD-C2D	-2.15	1.46	1.50
32	Gg	314	CLA	CMD-C2D	-2.15	1.46	1.50
32	R	601	CLA	C3B-C4B	2.15	1.49	1.42
35	A	410	PL9	C37-C38	2.15	1.57	1.50
39	Nn	316	CHL	CBD-CGD	-2.15	1.49	1.52
32	G	604	CLA	C3B-C4B	2.15	1.49	1.42
32	AA	408	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Cc	510	CLA	CMD-C2D	-2.15	1.46	1.50
38	WW	201	LMG	O1-C1	2.15	1.43	1.40
32	n	603	CLA	CMD-C2D	-2.15	1.46	1.50
32	Bb	606	CLA	CMD-C2D	-2.15	1.46	1.50
34	h	101	BCR	C23-C22	2.15	1.50	1.46
32	CC	514	CLA	C3B-C4B	2.15	1.49	1.42
32	y	316	CLA	CMD-C2D	-2.15	1.46	1.50
32	1	604	CLA	CHC-C1C	2.15	1.42	1.38
32	S	609	CLA	CHC-C1C	2.15	1.42	1.38
32	Bb	610	CLA	CMD-C2D	-2.15	1.46	1.50
39	N	605	CHL	CHC-C1C	2.15	1.43	1.39
32	R	610	CLA	CMD-C2D	-2.15	1.46	1.50
32	SS	303	CLA	C3B-C4B	2.15	1.49	1.42
32	C	512	CLA	CMD-C2D	-2.15	1.46	1.50
32	b	605	CLA	CMD-C2D	-2.15	1.46	1.50
39	y	307	CHL	CHC-C1C	2.15	1.43	1.39
39	y	310	CHL	CBD-CGD	-2.15	1.49	1.52
32	BB	606	CLA	C3B-C4B	2.15	1.49	1.42
33	a	409	PHO	C3D-C4D	2.15	1.44	1.41
32	c	507	CLA	C3B-C4B	2.15	1.49	1.42
39	R	606	CHL	CAC-C3C	-2.15	1.48	1.51
32	N	613	CLA	C3B-C4B	2.15	1.49	1.42
32	CC	507	CLA	CMB-C2B	-2.15	1.46	1.50
32	Bb	605	CLA	CMD-C2D	-2.15	1.46	1.50
32	Nn	301	CLA	CHC-C1C	2.15	1.42	1.38
32	A	406	CLA	C3B-C4B	2.15	1.49	1.42
32	Yy	604	CLA	CMB-C2B	-2.15	1.46	1.50
32	Nn	303	CLA	CMD-C2D	-2.15	1.46	1.50
32	Cc	504	CLA	C3B-C4B	2.15	1.49	1.42
32	2	604	CLA	CMD-C2D	-2.15	1.46	1.50
32	s	613	CLA	CMD-C2D	-2.15	1.46	1.50
32	Cc	511	CLA	CMD-C2D	-2.15	1.46	1.50
38	Cc	501	LMG	O1-C1	2.15	1.43	1.40
32	AA	405	CLA	CMB-C2B	-2.15	1.46	1.50
32	Aa	407	CLA	CMB-C2B	-2.15	1.46	1.50
32	4	304	CLA	C3B-C4B	2.15	1.49	1.42
32	b	613	CLA	CMB-C2B	-2.15	1.46	1.50
32	DD	403	CLA	CMB-C2B	-2.15	1.46	1.50
32	Dd	402	CLA	CMB-C2B	-2.15	1.46	1.50
32	C	504	CLA	C3B-C4B	2.15	1.49	1.42
32	YY	611	CLA	MG-NB	-2.14	2.01	2.05
32	Yy	613	CLA	C3B-C4B	2.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	505	CLA	C3B-C4B	2.14	1.49	1.42
32	Rr	613	CLA	CMB-C2B	-2.14	1.46	1.50
32	B	624	CLA	CMD-C2D	-2.14	1.46	1.50
32	SS	313	CLA	CMD-C2D	-2.14	1.46	1.50
38	c	519	LMG	O1-C1	2.14	1.43	1.40
35	AA	410	PL9	C26-C24	2.14	1.55	1.51
32	g	611	CLA	CHC-C1C	2.14	1.42	1.38
32	N	612	CLA	CMD-C2D	-2.14	1.46	1.50
32	r	604	CLA	CMD-C2D	-2.14	1.46	1.50
32	c	512	CLA	CMD-C2D	-2.14	1.46	1.50
32	NN	610	CLA	CMD-C2D	-2.14	1.46	1.50
39	Gg	309	CHL	CBD-CGD	-2.14	1.49	1.52
33	Aa	408	PHO	C4D-ND	-2.14	1.35	1.38
32	a	407	CLA	CMB-C2B	-2.14	1.46	1.50
32	y	312	CLA	CMD-C2D	-2.14	1.46	1.50
32	Bb	613	CLA	CMB-C2B	-2.14	1.46	1.50
32	b	604	CLA	C3B-C4B	2.14	1.49	1.42
32	C	513	CLA	CMB-C2B	-2.14	1.46	1.50
32	b	609	CLA	CMD-C2D	-2.14	1.46	1.50
41	N	617	XAT	O24-C25	-2.14	1.43	1.46
32	Rr	608	CLA	CMD-C2D	-2.14	1.46	1.50
32	b	604	CLA	CMB-C2B	-2.14	1.46	1.50
32	CC	505	CLA	CMB-C2B	-2.14	1.46	1.50
32	NN	613	CLA	CMD-C2D	-2.14	1.46	1.50
39	S	605	CHL	CAC-C3C	-2.14	1.48	1.51
35	AA	410	PL9	C42-C43	2.14	1.56	1.50
32	SS	309	CLA	CMD-C2D	-2.14	1.46	1.50
46	e	101	HEM	CMC-C2C	2.14	1.55	1.50
40	RR	315	LUT	C22-C21	-2.14	1.52	1.54
32	R	609	CLA	CMD-C2D	-2.14	1.46	1.50
32	R	612	CLA	CMD-C2D	-2.14	1.46	1.50
32	CC	505	CLA	CMD-C2D	-2.14	1.46	1.50
32	XX	201	CLA	CHC-C1C	2.14	1.42	1.38
32	CC	509	CLA	CMB-C2B	-2.14	1.46	1.50
41	G	619	XAT	O24-C25	-2.14	1.43	1.46
40	N	615	LUT	C22-C21	-2.14	1.52	1.54
32	Rr	612	CLA	C3B-C4B	2.14	1.49	1.42
39	G	601	CHL	CAC-C3C	-2.14	1.48	1.51
39	n	601	CHL	CAC-C3C	-2.14	1.48	1.51
32	Rr	603	CLA	CMD-C2D	-2.14	1.46	1.50
32	c	508	CLA	CMD-C2D	-2.14	1.46	1.50
32	g	614	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	303	CLA	CMD-C2D	-2.14	1.46	1.50
32	Nn	305	CLA	C3B-C4B	2.14	1.49	1.42
39	N	608	CHL	CMB-C2B	-2.14	1.47	1.51
41	GG	617	XAT	C32-C33	2.14	1.50	1.46
32	RR	313	CLA	C3B-C4B	2.14	1.49	1.42
32	Ss	609	CLA	CHC-C1C	2.14	1.42	1.38
32	A	406	CLA	CMD-C2D	-2.14	1.46	1.50
32	N	603	CLA	CMB-C2B	-2.14	1.46	1.50
32	RR	309	CLA	CMD-C2D	-2.14	1.46	1.50
39	NN	609	CHL	CBD-CGD	-2.14	1.49	1.52
32	b	615	CLA	C3B-C4B	2.14	1.49	1.42
32	BB	602	CLA	C3B-C4B	2.14	1.49	1.42
32	a	410	CLA	CMD-C2D	-2.14	1.46	1.50
32	s	611	CLA	CMD-C2D	-2.14	1.46	1.50
32	BB	615	CLA	C3B-C4B	2.14	1.49	1.42
39	4	306	CHL	CBD-CGD	-2.14	1.49	1.52
32	g	602	CLA	CMD-C2D	-2.14	1.46	1.50
32	Ss	602	CLA	CMD-C2D	-2.14	1.46	1.50
32	n	604	CLA	CMD-C2D	-2.14	1.46	1.50
32	Cc	504	CLA	CHC-C1C	2.14	1.42	1.38
39	Yy	606	CHL	CHC-C1C	2.14	1.43	1.39
32	A	408	CLA	CMD-C2D	-2.13	1.46	1.50
32	GG	603	CLA	CMD-C2D	-2.13	1.46	1.50
32	Gg	313	CLA	CMD-C2D	-2.13	1.46	1.50
32	Ss	611	CLA	CMD-C2D	-2.13	1.46	1.50
32	Y	611	CLA	C3B-C4B	2.13	1.49	1.42
32	BB	607	CLA	CMB-C2B	-2.13	1.46	1.50
32	Nn	314	CLA	CMD-C2D	-2.13	1.46	1.50
32	AA	406	CLA	CMB-C2B	-2.13	1.46	1.50
32	GG	613	CLA	CMD-C2D	-2.13	1.46	1.50
32	YY	613	CLA	C3B-C4B	2.13	1.49	1.42
39	y	309	CHL	CBD-CGD	-2.13	1.49	1.52
32	44	611	CLA	CMD-C2D	-2.13	1.46	1.50
32	N	604	CLA	CMD-C2D	-2.13	1.46	1.50
32	b	606	CLA	CMB-C2B	-2.13	1.46	1.50
32	Nn	301	CLA	CMD-C2D	-2.13	1.46	1.50
32	CC	502	CLA	C3B-C4B	2.13	1.49	1.42
39	1	605	CHL	CHC-C1C	2.13	1.43	1.39
32	2	613	CLA	CMD-C2D	-2.13	1.46	1.50
32	RR	312	CLA	CMD-C2D	-2.13	1.46	1.50
32	C	515	CLA	C3B-C4B	2.13	1.49	1.42
32	44	609	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AA	406	CLA	CMD-C2D	-2.13	1.46	1.50
32	Yy	602	CLA	CHC-C1C	2.13	1.42	1.38
32	G	610	CLA	MG-NC	2.13	2.11	2.06
32	r	611	CLA	CMD-C2D	-2.13	1.46	1.50
32	c	506	CLA	CMD-C2D	-2.13	1.46	1.50
32	Gg	304	CLA	CMD-C2D	-2.13	1.46	1.50
32	Aa	407	CLA	C3B-C4B	2.13	1.48	1.42
42	R	617	NEX	O24-C25	-2.13	1.43	1.46
32	NN	611	CLA	CHC-C1C	2.13	1.42	1.38
32	C	510	CLA	CMB-C2B	-2.13	1.46	1.50
39	g	601	CHL	CHC-C1C	2.13	1.43	1.39
32	a	405	CLA	CMB-C2B	-2.13	1.46	1.50
32	RR	302	CLA	CMD-C2D	-2.13	1.46	1.50
32	R	613	CLA	C3B-C4B	2.13	1.48	1.42
35	A	410	PL9	C42-C43	2.13	1.56	1.50
32	Gg	304	CLA	C3B-C4B	2.13	1.48	1.42
32	n	612	CLA	CMD-C2D	-2.13	1.46	1.50
32	b	602	CLA	CMD-C2D	-2.13	1.46	1.50
32	C	508	CLA	MG-NB	-2.13	2.01	2.05
32	S	612	CLA	CMD-C2D	-2.13	1.46	1.50
32	Bb	615	CLA	C3B-C4B	2.13	1.48	1.42
39	Nn	318	CHL	CMB-C2B	-2.13	1.47	1.51
39	Ss	607	CHL	CBD-CGD	-2.13	1.49	1.52
39	Y	608	CHL	CBD-CGD	-2.13	1.49	1.52
32	BB	603	CLA	CMB-C2B	-2.13	1.46	1.50
32	s	609	CLA	CHC-C1C	2.13	1.42	1.38
32	Rr	609	CLA	CMD-C2D	-2.13	1.46	1.50
32	Ss	608	CLA	CMD-C2D	-2.13	1.46	1.50
32	G	602	CLA	CMD-C2D	-2.13	1.46	1.50
32	Bb	602	CLA	C3B-C4B	2.13	1.48	1.42
32	b	606	CLA	CMD-C2D	-2.13	1.46	1.50
32	b	606	CLA	C3B-C4B	2.13	1.48	1.42
39	Y	608	CHL	CMB-C2B	-2.13	1.47	1.51
32	BB	603	CLA	CMC-C2C	-2.13	1.46	1.50
32	C	504	CLA	CHC-C1C	2.13	1.42	1.38
32	G	603	CLA	C3B-C4B	2.13	1.48	1.42
32	NN	612	CLA	CMD-C2D	-2.12	1.46	1.50
32	r	610	CLA	C3B-C4B	2.12	1.48	1.42
32	y	315	CLA	C3B-C4B	2.12	1.48	1.42
32	B	619	CLA	C3B-C4B	2.12	1.48	1.42
46	Ee	101	HEM	CMC-C2C	2.12	1.55	1.50
32	Bb	613	CLA	C3B-C4B	2.12	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	405	CLA	CMD-C2D	-2.12	1.46	1.50
32	BB	605	CLA	C3B-C4B	2.12	1.48	1.42
39	YY	608	CHL	CMB-C2B	-2.12	1.47	1.51
32	N	611	CLA	CHC-C1C	2.12	1.42	1.38
32	SS	309	CLA	CHC-C1C	2.12	1.42	1.38
32	Yy	610	CLA	CMD-C2D	-2.12	1.46	1.50
32	CC	513	CLA	C3B-C4B	2.12	1.48	1.42
32	b	607	CLA	C3B-C4B	2.12	1.48	1.42
32	CC	511	CLA	CMD-C2D	-2.12	1.46	1.50
32	NN	603	CLA	CMD-C2D	-2.12	1.46	1.50
32	RR	308	CLA	CMB-C2B	-2.12	1.46	1.50
32	SS	311	CLA	CMB-C2B	-2.12	1.46	1.50
32	Cc	514	CLA	CMD-C2D	-2.12	1.46	1.50
41	NN	617	XAT	O24-C25	-2.12	1.43	1.46
32	C	511	CLA	CMB-C2B	-2.12	1.46	1.50
32	Nn	302	CLA	CHC-C1C	2.12	1.42	1.38
32	Ss	604	CLA	CMB-C2B	-2.12	1.46	1.50
32	44	602	CLA	CMD-C2D	-2.12	1.46	1.50
41	G	619	XAT	O4-C5	-2.12	1.43	1.46
32	Rr	604	CLA	CMD-C2D	-2.12	1.46	1.50
32	r	612	CLA	CMD-C2D	-2.12	1.46	1.50
32	CC	503	CLA	CHC-C1C	2.12	1.42	1.38
32	Nn	314	CLA	CHC-C1C	2.12	1.42	1.38
32	2	604	CLA	CMB-C2B	-2.12	1.46	1.50
32	g	603	CLA	C3B-C4B	2.12	1.48	1.42
32	RR	302	CLA	C3B-C4B	2.12	1.48	1.42
32	s	608	CLA	CMD-C2D	-2.12	1.46	1.50
32	y	313	CLA	CMD-C2D	-2.12	1.46	1.50
33	DD	402	PHO	C3B-C2B	-2.12	1.37	1.40
32	Bb	603	CLA	CMC-C2C	-2.12	1.46	1.50
32	Gg	303	CLA	CMD-C2D	-2.12	1.46	1.50
34	k	101	BCR	C1-C6	-2.12	1.51	1.53
32	3	613	CLA	CMD-C2D	-2.12	1.46	1.50
32	X	201	CLA	CHC-C1C	2.12	1.42	1.38
32	g	604	CLA	CMD-C2D	-2.12	1.46	1.50
33	Aa	408	PHO	C3B-C2B	-2.12	1.37	1.40
39	N	601	CHL	CAC-C3C	-2.12	1.48	1.51
41	G	617	XAT	O24-C25	-2.12	1.43	1.46
32	s	612	CLA	C3B-C4B	2.12	1.48	1.42
32	Cc	506	CLA	CMD-C2D	-2.12	1.46	1.50
39	NN	601	CHL	CHC-C4B	-2.12	1.36	1.39
32	C	506	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	512	CLA	CMB-C2B	-2.12	1.46	1.50
32	CC	512	CLA	CMB-C2B	-2.12	1.46	1.50
32	g	603	CLA	CMD-C2D	-2.12	1.46	1.50
32	g	610	CLA	CMD-C2D	-2.11	1.46	1.50
32	B	620	CLA	CMC-C2C	-2.11	1.46	1.50
32	C	512	CLA	CHC-C1C	2.11	1.42	1.38
32	b	613	CLA	C3B-C4B	2.11	1.48	1.42
32	S	602	CLA	CMD-C2D	-2.11	1.46	1.50
32	SS	303	CLA	CMD-C2D	-2.11	1.46	1.50
32	CC	507	CLA	CHC-C1C	2.11	1.42	1.38
32	Bb	611	CLA	C3B-C4B	2.11	1.48	1.42
32	c	509	CLA	CMD-C2D	-2.11	1.46	1.50
32	R	608	CLA	CHC-C1C	2.11	1.42	1.38
32	Cc	515	CLA	CMD-C2D	-2.11	1.46	1.50
32	Rr	602	CLA	CMB-C2B	-2.11	1.46	1.50
32	22	603	CLA	CMD-C2D	-2.11	1.46	1.50
32	RR	304	CLA	CMB-C2B	-2.11	1.46	1.50
32	44	610	CLA	CMD-C2D	-2.11	1.46	1.50
41	GG	619	XAT	C12-C13	2.11	1.50	1.46
32	NN	604	CLA	CMD-C2D	-2.11	1.46	1.50
39	Nn	319	CHL	CHC-C1C	2.11	1.43	1.39
32	22	609	CLA	CMB-C2B	-2.11	1.46	1.50
32	BB	607	CLA	C3B-C4B	2.11	1.48	1.42
39	NN	608	CHL	CBD-CGD	-2.11	1.49	1.52
32	Rr	603	CLA	CMB-C2B	-2.11	1.46	1.50
32	4	304	CLA	CMD-C2D	-2.11	1.46	1.50
32	Bb	602	CLA	CMD-C2D	-2.11	1.46	1.50
32	B	623	CLA	C3B-C4B	2.11	1.48	1.42
32	2	603	CLA	CMD-C2D	-2.11	1.46	1.50
32	BB	611	CLA	C3B-C4B	2.11	1.48	1.42
32	C	515	CLA	CMB-C2B	-2.11	1.46	1.50
32	R	608	CLA	CMB-C2B	-2.11	1.46	1.50
32	Y	610	CLA	CMD-C2D	-2.11	1.46	1.50
32	a	407	CLA	CMD-C2D	-2.11	1.46	1.50
32	r	602	CLA	CMD-C2D	-2.11	1.46	1.50
32	C	508	CLA	CHC-C1C	2.11	1.42	1.38
32	CC	506	CLA	C3B-C4B	2.11	1.48	1.42
32	4	312	CLA	CMD-C2D	-2.11	1.46	1.50
32	Bb	604	CLA	CMB-C2B	-2.11	1.46	1.50
34	C	516	BCR	C12-C13	2.11	1.50	1.46
32	4	310	CLA	CMD-C2D	-2.11	1.46	1.50
32	Bb	606	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	DD	406	PL9	C37-C38	2.11	1.56	1.50
32	YY	610	CLA	CMD-C2D	-2.11	1.46	1.50
32	Cc	514	CLA	C3B-C4B	2.11	1.48	1.42
41	NN	617	XAT	C32-C33	2.11	1.50	1.46
32	Cc	509	CLA	C3B-C4B	2.11	1.48	1.42
32	b	602	CLA	CMB-C2B	-2.11	1.46	1.50
32	B	624	CLA	CMC-C2C	-2.11	1.46	1.50
32	Bb	606	CLA	CMB-C2B	-2.11	1.46	1.50
32	n	604	CLA	CHC-C1C	2.11	1.42	1.38
32	CC	512	CLA	C3B-C4B	2.11	1.48	1.42
32	33	613	CLA	CMD-C2D	-2.11	1.46	1.50
32	C	515	CLA	CMD-C2D	-2.11	1.46	1.50
32	Y	603	CLA	CMB-C2B	-2.11	1.46	1.50
32	b	611	CLA	C3B-C4B	2.11	1.48	1.42
32	Bb	607	CLA	C3B-C4B	2.11	1.48	1.42
32	C	505	CLA	C3B-C4B	2.11	1.48	1.42
32	S	610	CLA	CMB-C2B	-2.11	1.46	1.50
32	r	608	CLA	CMD-C2D	-2.11	1.46	1.50
32	Cc	503	CLA	C3B-C4B	2.11	1.48	1.42
32	n	612	CLA	CMC-C2C	-2.11	1.46	1.50
32	B	621	CLA	CMD-C2D	-2.11	1.46	1.50
32	GG	612	CLA	CMB-C2B	-2.10	1.46	1.50
32	Bb	605	CLA	CMB-C2B	-2.10	1.46	1.50
32	Rr	602	CLA	CHC-C1C	2.10	1.42	1.38
39	Y	601	CHL	CMB-C2B	-2.10	1.47	1.51
32	s	604	CLA	C3B-C4B	2.10	1.48	1.42
32	44	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	B	620	CLA	CMB-C2B	-2.10	1.46	1.50
37	BB	621	SQD	O6-C1	2.10	1.43	1.40
32	DD	401	CLA	C3B-C4B	2.10	1.48	1.42
32	C	513	CLA	C3B-C4B	2.10	1.48	1.42
39	N	606	CHL	CBD-CGD	-2.10	1.49	1.52
32	BB	608	CLA	CHC-C1C	2.10	1.42	1.38
32	Rr	602	CLA	CMD-C2D	-2.10	1.46	1.50
32	Y	611	CLA	CMD-C2D	-2.10	1.46	1.50
32	22	611	CLA	CMD-C2D	-2.10	1.46	1.50
32	BB	609	CLA	CMB-C2B	-2.10	1.46	1.50
32	b	608	CLA	CMD-C2D	-2.10	1.46	1.50
32	4	311	CLA	CMD-C2D	-2.10	1.46	1.50
32	B	605	CLA	CMB-C2B	-2.10	1.46	1.50
39	4	307	CHL	CMB-C2B	-2.10	1.47	1.51
32	Bb	601	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Gg	315	CLA	CMD-C2D	-2.10	1.46	1.50
32	Nn	312	CLA	CMB-C2B	-2.10	1.46	1.50
32	BB	611	CLA	MG-NB	-2.10	2.01	2.05
32	SS	311	CLA	CMD-C2D	-2.10	1.46	1.50
39	Y	608	CHL	CAC-C3C	-2.10	1.48	1.51
41	y	301	XAT	C28-C29	2.10	1.50	1.46
32	CC	510	CLA	CMB-C2B	-2.10	1.46	1.50
40	r	614	LUT	C22-C21	-2.10	1.52	1.54
39	n	608	CHL	CMB-C2B	-2.10	1.47	1.51
32	Cc	504	CLA	CMB-C2B	-2.10	1.46	1.50
32	Dd	402	CLA	CMD-C2D	-2.10	1.46	1.50
32	c	506	CLA	CHC-C1C	2.10	1.42	1.38
32	GG	611	CLA	CHC-C1C	2.10	1.42	1.38
34	Bb	617	BCR	C19-C18	2.10	1.50	1.46
39	n	601	CHL	CHC-C1C	2.10	1.43	1.39
32	Cc	515	CLA	CHC-C1C	2.10	1.42	1.38
34	B	612	BCR	C30-C25	-2.10	1.51	1.53
39	2	601	CHL	CMB-C2B	-2.10	1.47	1.51
41	y	302	XAT	C12-C13	2.10	1.50	1.46
39	Yy	609	CHL	CAC-C3C	-2.10	1.48	1.51
33	DD	402	PHO	C3D-C4D	2.10	1.44	1.41
39	GG	607	CHL	CHC-C1C	2.10	1.43	1.39
32	Y	613	CLA	C3B-C4B	2.10	1.48	1.42
32	SS	314	CLA	CHC-C1C	2.10	1.42	1.38
32	44	615	CLA	CMD-C2D	-2.10	1.46	1.50
32	BB	609	CLA	CMD-C2D	-2.10	1.46	1.50
39	Nn	319	CHL	CAC-C3C	-2.10	1.48	1.51
40	YY	615	LUT	C22-C21	-2.10	1.52	1.54
32	RR	311	CLA	CMD-C2D	-2.10	1.46	1.50
39	y	307	CHL	CAC-C3C	-2.10	1.48	1.51
32	N	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	y	306	CLA	CMB-C2B	-2.10	1.46	1.50
32	Nn	312	CLA	C3B-C4B	2.10	1.48	1.42
32	Ss	613	CLA	CHC-C1C	2.10	1.42	1.38
32	A	406	CLA	CMB-C2B	-2.09	1.46	1.50
32	s	604	CLA	CMB-C2B	-2.09	1.46	1.50
46	EE	102	HEM	C2A-C3A	-2.09	1.33	1.38
39	g	601	CHL	CAC-C3C	-2.09	1.48	1.51
39	G	601	CHL	CBD-CGD	-2.09	1.49	1.52
39	2	608	CHL	CMB-C2B	-2.09	1.47	1.51
32	11	613	CLA	CHC-C1C	2.09	1.42	1.38
32	S	609	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	YY	614	CLA	CMB-C2B	-2.09	1.46	1.50
32	c	504	CLA	CMD-C2D	-2.09	1.46	1.50
39	Ss	601	CHL	CBD-CGD	-2.09	1.49	1.52
32	c	513	CLA	CHC-C1C	2.09	1.42	1.38
32	G	612	CLA	CMD-C2D	-2.09	1.46	1.50
32	Y	604	CLA	CMD-C2D	-2.09	1.46	1.50
39	G	601	CHL	CHC-C1C	2.09	1.43	1.39
32	c	512	CLA	CMB-C2B	-2.09	1.46	1.50
32	Cc	511	CLA	CMB-C2B	-2.09	1.46	1.50
32	D	404	CLA	CHC-C1C	2.09	1.42	1.38
32	44	602	CLA	CMB-C2B	-2.09	1.46	1.50
32	G	613	CLA	CMD-C2D	-2.09	1.46	1.50
32	b	601	CLA	CHC-C1C	2.09	1.42	1.38
32	NN	602	CLA	CMD-C2D	-2.09	1.46	1.50
32	CC	504	CLA	C3B-C4B	2.09	1.48	1.42
32	Gg	305	CLA	C3B-C4B	2.09	1.48	1.42
34	B	613	BCR	C19-C18	2.09	1.50	1.46
32	R	611	CLA	CMD-C2D	-2.09	1.46	1.50
32	Gg	312	CLA	CMB-C2B	-2.09	1.46	1.50
32	DD	403	CLA	CHC-C1C	2.09	1.42	1.38
32	y	304	CLA	CMB-C2B	-2.09	1.46	1.50
32	RR	309	CLA	CMB-C2B	-2.09	1.46	1.50
32	RR	313	CLA	CMD-C2D	-2.09	1.46	1.50
32	Nn	313	CLA	CMD-C2D	-2.09	1.46	1.50
41	GG	619	XAT	O24-C25	-2.09	1.43	1.46
32	B	624	CLA	C3B-C4B	2.09	1.48	1.42
32	R	602	CLA	CMC-C2C	-2.09	1.46	1.50
32	g	612	CLA	CMD-C2D	-2.09	1.46	1.50
32	4	305	CLA	CMD-C2D	-2.09	1.46	1.50
34	b	618	BCR	C23-C22	2.09	1.50	1.46
32	22	609	CLA	CMD-C2D	-2.09	1.46	1.50
32	r	603	CLA	CMB-C2B	-2.09	1.46	1.50
32	YY	604	CLA	CMD-C2D	-2.09	1.46	1.50
39	Yy	605	CHL	CMB-C2B	-2.09	1.47	1.51
39	Yy	605	CHL	CHC-C1C	2.09	1.43	1.39
32	1	604	CLA	CMD-C2D	-2.09	1.46	1.50
32	1	611	CLA	CMD-C2D	-2.09	1.46	1.50
32	SS	314	CLA	CMB-C2B	-2.09	1.46	1.50
34	Hh	101	BCR	C7-C6	2.09	1.52	1.45
32	Cc	507	CLA	CMB-C2B	-2.09	1.46	1.50
32	Aa	405	CLA	CMB-C2B	-2.09	1.46	1.50
32	Ss	613	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	605	CLA	CMC-C2C	-2.09	1.46	1.50
32	NN	613	CLA	CMB-C2B	-2.09	1.46	1.50
32	2	610	CLA	CHC-C1C	2.09	1.42	1.38
32	c	502	CLA	CHC-C1C	2.09	1.42	1.38
32	n	613	CLA	C3B-C4B	2.09	1.48	1.42
32	2	610	CLA	CMD-C2D	-2.09	1.46	1.50
41	N	617	XAT	C12-C13	2.09	1.50	1.46
32	1	609	CLA	CMD-C2D	-2.08	1.46	1.50
32	1	613	CLA	CHC-C1C	2.08	1.42	1.38
32	CC	510	CLA	CHC-C1C	2.08	1.42	1.38
41	Rr	615	XAT	O4-C5	-2.08	1.43	1.46
39	YY	601	CHL	CMB-C2B	-2.08	1.47	1.51
40	SS	315	LUT	C32-C33	2.08	1.50	1.46
32	Yy	603	CLA	C3B-C4B	2.08	1.48	1.42
32	R	613	CLA	CMD-C2D	-2.08	1.46	1.50
32	r	613	CLA	CMB-C2B	-2.08	1.46	1.50
32	22	610	CLA	CHC-C1C	2.08	1.42	1.38
41	NN	617	XAT	C12-C13	2.08	1.50	1.46
32	c	503	CLA	CMB-C2B	-2.08	1.46	1.50
40	g	616	LUT	C8-C9	2.08	1.50	1.46
32	A	405	CLA	CMB-C2B	-2.08	1.46	1.50
32	G	610	CLA	CMD-C2D	-2.08	1.46	1.50
32	N	602	CLA	CMD-C2D	-2.08	1.46	1.50
32	C	514	CLA	CMB-C2B	-2.08	1.46	1.50
32	s	602	CLA	CMD-C2D	-2.08	1.46	1.50
32	DD	404	CLA	CMB-C2B	-2.08	1.46	1.50
32	s	602	CLA	CHC-C1C	2.08	1.42	1.38
32	Bb	603	CLA	CHC-C1C	2.08	1.42	1.38
32	d	402	CLA	CMD-C2D	-2.08	1.46	1.50
32	GG	604	CLA	CMD-C2D	-2.08	1.46	1.50
39	GG	609	CHL	CHC-C1C	2.08	1.43	1.39
32	33	612	CLA	CMD-C2D	-2.08	1.46	1.50
32	b	601	CLA	CMD-C2D	-2.08	1.46	1.50
32	c	512	CLA	C3B-C4B	2.08	1.48	1.42
32	y	304	CLA	CMC-C2C	-2.08	1.46	1.50
32	2	613	CLA	CHC-C1C	2.08	1.42	1.38
32	NN	614	CLA	CHC-C1C	2.08	1.42	1.38
32	Yy	610	CLA	CMC-C2C	-2.08	1.46	1.50
34	TT	101	BCR	C12-C13	2.08	1.50	1.46
39	YY	608	CHL	CAC-C3C	-2.08	1.48	1.51
39	44	606	CHL	CMB-C2B	-2.08	1.47	1.51
32	SS	313	CLA	C3B-C4B	2.08	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Nn	312	CLA	CHC-C1C	2.08	1.42	1.38
39	YY	606	CHL	CAC-C3C	-2.08	1.48	1.51
39	Gg	302	CHL	CBD-CGD	-2.08	1.49	1.52
32	g	604	CLA	CMB-C2B	-2.08	1.46	1.50
39	GG	601	CHL	CBD-CGD	-2.08	1.49	1.52
32	D	405	CLA	CMB-C2B	-2.08	1.46	1.50
32	Y	614	CLA	CMB-C2B	-2.08	1.46	1.50
32	n	613	CLA	CMD-C2D	-2.08	1.46	1.50
39	Y	605	CHL	CMB-C2B	-2.08	1.47	1.51
32	3	611	CLA	CMD-C2D	-2.08	1.46	1.50
32	S	604	CLA	CMD-C2D	-2.08	1.46	1.50
32	s	610	CLA	CMD-C2D	-2.08	1.46	1.50
32	c	505	CLA	CMC-C2C	-2.08	1.46	1.50
32	r	609	CLA	CMD-C2D	-2.08	1.46	1.50
32	Cc	510	CLA	CMB-C2B	-2.08	1.46	1.50
39	YY	605	CHL	CHC-C1C	2.08	1.43	1.39
32	n	611	CLA	CHC-C1C	2.08	1.42	1.38
32	Bb	601	CLA	CHC-C1C	2.08	1.42	1.38
32	c	509	CLA	CMB-C2B	-2.08	1.46	1.50
32	B	611	CLA	C3B-C4B	2.08	1.48	1.42
32	11	603	CLA	CHC-C1C	2.08	1.42	1.38
32	s	609	CLA	CMC-C2C	-2.08	1.46	1.50
32	DD	404	CLA	C3B-C4B	2.08	1.48	1.42
39	4	302	CHL	CMB-C2B	-2.07	1.47	1.51
32	BB	608	CLA	CMB-C2B	-2.07	1.46	1.50
32	Gg	311	CLA	CMD-C2D	-2.07	1.46	1.50
32	C	511	CLA	CHC-C1C	2.07	1.42	1.38
39	NN	607	CHL	CHC-C1C	2.07	1.43	1.39
40	NN	615	LUT	C12-C13	2.07	1.50	1.46
33	Aa	409	PHO	C3B-C2B	-2.07	1.37	1.40
32	Ss	612	CLA	CMD-C2D	-2.07	1.46	1.50
32	Yy	602	CLA	CMB-C2B	-2.07	1.46	1.50
32	R	601	CLA	CMD-C2D	-2.07	1.46	1.50
32	SS	314	CLA	CMD-C2D	-2.07	1.46	1.50
41	4	314	XAT	O24-C25	-2.07	1.43	1.46
42	Rr	616	NEX	O24-C25	-2.07	1.43	1.46
32	BB	607	CLA	CMC-C2C	-2.07	1.46	1.50
32	2	611	CLA	CHC-C1C	2.07	1.42	1.38
32	RR	308	CLA	CHC-C1C	2.07	1.42	1.38
33	a	408	PHO	C3D-C4D	2.07	1.44	1.41
32	G	612	CLA	CMB-C2B	-2.07	1.46	1.50
32	b	601	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	504	CLA	CMB-C2B	-2.07	1.46	1.50
39	44	607	CHL	CMB-C2B	-2.07	1.47	1.51
35	A	410	PL9	C31-C29	2.07	1.55	1.51
32	Ss	603	CLA	CMD-C2D	-2.07	1.46	1.50
32	n	602	CLA	CMB-C2B	-2.07	1.46	1.50
32	GG	610	CLA	CMD-C2D	-2.07	1.46	1.50
32	YY	602	CLA	CMD-C2D	-2.07	1.46	1.50
32	Nn	302	CLA	CMD-C2D	-2.07	1.46	1.50
41	Nn	308	XAT	C12-C13	2.07	1.50	1.46
38	Aa	412	LMG	O1-C1	2.07	1.43	1.40
32	Ss	602	CLA	CHC-C1C	2.07	1.42	1.38
39	R	606	CHL	CMB-C2B	-2.07	1.47	1.51
32	Ss	610	CLA	CMD-C2D	-2.07	1.46	1.50
32	1	603	CLA	CMD-C2D	-2.07	1.46	1.50
32	YY	611	CLA	CHC-C1C	2.07	1.42	1.38
32	Aa	406	CLA	CHC-C1C	2.07	1.42	1.38
46	e	101	HEM	CMB-C2B	2.07	1.55	1.50
32	NN	611	CLA	CMD-C2D	-2.07	1.46	1.50
39	Nn	319	CHL	MG-NB	-2.07	2.01	2.05
34	BB	618	BCR	C23-C22	2.07	1.50	1.46
32	D	401	CLA	C3B-C4B	2.07	1.48	1.42
32	YY	603	CLA	CMB-C2B	-2.07	1.46	1.50
32	4	311	CLA	CHC-C1C	2.07	1.42	1.38
40	Rr	614	LUT	C22-C21	-2.07	1.52	1.54
32	2	603	CLA	CMB-C2B	-2.07	1.46	1.50
32	s	603	CLA	CMD-C2D	-2.07	1.46	1.50
32	SS	303	CLA	CMB-C2B	-2.07	1.46	1.50
32	Dd	401	CLA	CMC-C2C	-2.07	1.46	1.50
32	Yy	604	CLA	CMD-C2D	-2.07	1.46	1.50
32	Y	602	CLA	CMB-C2B	-2.07	1.46	1.50
32	c	501	CLA	CMB-C2B	-2.07	1.46	1.50
32	Cc	508	CLA	CHC-C1C	2.07	1.42	1.38
32	BB	610	CLA	C3B-C4B	2.07	1.48	1.42
33	a	408	PHO	C3B-C2B	-2.07	1.37	1.40
32	a	410	CLA	CMB-C2B	-2.07	1.46	1.50
32	s	612	CLA	CMD-C2D	-2.07	1.46	1.50
32	33	612	CLA	CHC-C1C	2.07	1.42	1.38
32	Bb	609	CLA	MG-NB	-2.07	2.01	2.05
32	c	504	CLA	C3B-C4B	2.07	1.48	1.42
32	R	604	CLA	CMB-C2B	-2.07	1.46	1.50
32	Aa	410	CLA	CMB-C2B	-2.07	1.46	1.50
35	d	404	PL9	C37-C38	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	R	602	CLA	CMB-C2B	-2.07	1.46	1.50
32	Nn	304	CLA	CMD-C2D	-2.07	1.46	1.50
39	y	310	CHL	CAC-C3C	-2.07	1.48	1.51
41	G	619	XAT	C12-C13	2.07	1.50	1.46
32	11	612	CLA	MG-NA	2.07	2.11	2.06
32	Bb	601	CLA	CMB-C2B	-2.07	1.46	1.50
39	YY	608	CHL	CBD-CGD	-2.07	1.49	1.52
34	T	101	BCR	C12-C13	2.07	1.50	1.46
32	S	608	CLA	CMD-C2D	-2.07	1.46	1.50
32	BB	609	CLA	CMC-C2C	-2.07	1.46	1.50
32	Bb	608	CLA	CMD-C2D	-2.07	1.46	1.50
32	11	611	CLA	CHC-C1C	2.07	1.42	1.38
32	Rr	612	CLA	CMD-C2D	-2.07	1.46	1.50
32	11	609	CLA	CMD-C2D	-2.07	1.46	1.50
32	n	602	CLA	CMC-C2C	-2.07	1.46	1.50
32	GG	614	CLA	CMD-C2D	-2.07	1.46	1.50
32	R	612	CLA	C3B-C4B	2.07	1.48	1.42
34	c	516	BCR	C23-C22	2.07	1.50	1.46
34	Cc	517	BCR	C8-C9	2.07	1.50	1.46
32	AA	406	CLA	CHC-C1C	2.07	1.42	1.38
42	Y	619	NEX	O24-C25	-2.07	1.43	1.46
32	Y	612	CLA	CMB-C2B	-2.07	1.46	1.50
32	GG	604	CLA	CMB-C2B	-2.07	1.46	1.50
32	Gg	315	CLA	CMB-C2B	-2.07	1.46	1.50
39	R	606	CHL	CBD-CGD	-2.06	1.49	1.52
39	Yy	601	CHL	CHC-C1C	2.06	1.43	1.39
39	n	605	CHL	CHC-C1C	2.06	1.43	1.39
46	E	101	HEM	CMB-C2B	2.06	1.55	1.50
32	y	306	CLA	CMD-C2D	-2.06	1.46	1.50
39	n	605	CHL	CMB-C2B	-2.06	1.47	1.51
32	r	604	CLA	C3B-C4B	2.06	1.48	1.42
32	3	612	CLA	CMD-C2D	-2.06	1.46	1.50
32	C	509	CLA	CMC-C2C	-2.06	1.46	1.50
32	Bb	610	CLA	CMC-C2C	-2.06	1.46	1.50
34	Cc	518	BCR	C23-C22	2.06	1.50	1.46
32	S	603	CLA	CMD-C2D	-2.06	1.46	1.50
39	4	307	CHL	CBD-CGD	-2.06	1.49	1.52
32	Rr	609	CLA	CHC-C1C	2.06	1.42	1.38
32	b	602	CLA	C3B-C4B	2.06	1.48	1.42
32	44	602	CLA	CHC-C1C	2.06	1.42	1.38
39	N	607	CHL	CHC-C1C	2.06	1.43	1.39
32	G	611	CLA	CHC-C1C	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	SS	310	CLA	CMD-C2D	-2.06	1.46	1.50
40	NN	616	LUT	C8-C9	2.06	1.50	1.46
32	44	604	CLA	CMD-C2D	-2.06	1.46	1.50
32	CC	512	CLA	CMC-C2C	-2.06	1.46	1.50
32	B	618	CLA	CMC-C2C	-2.06	1.46	1.50
32	S	612	CLA	C3B-C4B	2.06	1.48	1.42
32	Rr	601	CLA	CHC-C1C	2.06	1.42	1.38
32	RR	304	CLA	CHC-C1C	2.06	1.42	1.38
32	c	501	CLA	C3B-C4B	2.06	1.48	1.42
33	Aa	409	PHO	C4D-ND	-2.06	1.35	1.38
32	s	613	CLA	CHC-C1C	2.06	1.42	1.38
32	Yy	610	CLA	CMB-C2B	-2.06	1.46	1.50
32	22	604	CLA	CMD-C2D	-2.06	1.46	1.50
41	GG	617	XAT	O24-C25	-2.06	1.43	1.46
32	3	604	CLA	CHC-C1C	2.06	1.42	1.38
32	b	605	CLA	CMB-C2B	-2.06	1.46	1.50
32	AA	408	CLA	CMB-C2B	-2.06	1.46	1.50
32	Bb	608	CLA	CMC-C2C	-2.06	1.46	1.50
32	Dd	401	CLA	CMB-C2B	-2.06	1.46	1.50
39	GG	609	CHL	CMB-C2B	-2.06	1.47	1.51
32	Ss	608	CLA	CHC-C1C	2.06	1.42	1.38
32	r	609	CLA	CHC-C1C	2.06	1.42	1.38
32	CC	506	CLA	CMB-C2B	-2.06	1.46	1.50
39	Ss	601	CHL	CMB-C2B	-2.06	1.47	1.51
32	a	405	CLA	C3B-C4B	2.06	1.48	1.42
39	GG	601	CHL	CHC-C1C	2.06	1.43	1.39
32	s	604	CLA	CMD-C2D	-2.06	1.46	1.50
32	SS	305	CLA	CMD-C2D	-2.06	1.46	1.50
32	C	509	CLA	C3B-C4B	2.06	1.48	1.42
32	B	620	CLA	C3B-C4B	2.06	1.48	1.42
32	11	602	CLA	CHC-C1C	2.06	1.42	1.38
32	22	611	CLA	CHC-C1C	2.06	1.42	1.38
32	Gg	305	CLA	CHC-C1C	2.06	1.42	1.38
32	YY	611	CLA	C3B-C4B	2.06	1.48	1.42
34	CC	516	BCR	C12-C13	2.06	1.50	1.46
32	1	612	CLA	CMB-C2B	-2.06	1.46	1.50
32	B	604	CLA	CMB-C2B	-2.06	1.46	1.50
32	B	607	CLA	CMC-C2C	-2.06	1.46	1.50
32	Cc	505	CLA	CMB-C2B	-2.06	1.46	1.50
39	Yy	608	CHL	CAC-C3C	-2.06	1.48	1.51
39	Gg	308	CHL	CAC-C3C	-2.06	1.48	1.51
32	33	611	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	614	CLA	CMD-C2D	-2.06	1.46	1.50
32	Bb	602	CLA	CMC-C2C	-2.06	1.46	1.50
39	Yy	607	CHL	CMB-C2B	-2.06	1.47	1.51
32	11	603	CLA	CMD-C2D	-2.06	1.46	1.50
38	W	201	LMG	O1-C1	2.06	1.43	1.40
32	33	604	CLA	CMB-C2B	-2.05	1.46	1.50
32	g	612	CLA	CMB-C2B	-2.05	1.46	1.50
32	y	313	CLA	CMB-C2B	-2.05	1.46	1.50
39	3	608	CHL	CHC-C1C	2.05	1.43	1.39
39	N	607	CHL	CBD-CGD	-2.05	1.49	1.52
39	Gg	308	CHL	CBD-CGD	-2.05	1.49	1.52
32	R	611	CLA	CMB-C2B	-2.05	1.46	1.50
39	Y	606	CHL	CMB-C2B	-2.05	1.47	1.51
39	11	605	CHL	CHC-C1C	2.05	1.43	1.39
32	Yy	604	CLA	C3B-C4B	2.05	1.48	1.42
32	CC	509	CLA	CMC-C2C	-2.05	1.46	1.50
32	Nn	314	CLA	CMB-C2B	-2.05	1.46	1.50
32	Yy	611	CLA	CHC-C1C	2.05	1.42	1.38
32	B	621	CLA	CMC-C2C	-2.05	1.46	1.50
32	RR	311	CLA	CMB-C2B	-2.05	1.46	1.50
32	1	602	CLA	CHC-C1C	2.05	1.42	1.38
32	3	609	CLA	CMC-C2C	-2.05	1.46	1.50
32	b	604	CLA	CMC-C2C	-2.05	1.46	1.50
32	RR	302	CLA	CHC-C1C	2.05	1.42	1.38
39	Nn	315	CHL	CAC-C3C	-2.05	1.48	1.51
32	33	603	CLA	CMD-C2D	-2.05	1.46	1.50
32	y	306	CLA	C3B-C4B	2.05	1.48	1.42
32	B	606	CLA	C3B-C4B	2.05	1.48	1.42
32	44	604	CLA	CMB-C2B	-2.05	1.46	1.50
32	11	610	CLA	CMD-C2D	-2.05	1.46	1.50
32	s	611	CLA	CHC-C1C	2.05	1.42	1.38
39	G	609	CHL	CMB-C2B	-2.05	1.47	1.51
32	RR	312	CLA	C3B-C4B	2.05	1.48	1.42
32	CC	511	CLA	CMB-C2B	-2.05	1.46	1.50
32	CC	511	CLA	CMC-C2C	-2.05	1.46	1.50
39	Y	606	CHL	CBD-CGD	-2.05	1.49	1.52
32	R	610	CLA	CHC-C1C	2.05	1.42	1.38
32	Cc	506	CLA	C3B-C4B	2.05	1.48	1.42
32	33	604	CLA	CMD-C2D	-2.05	1.46	1.50
32	C	510	CLA	CMC-C2C	-2.05	1.46	1.50
32	s	609	CLA	CMD-C2D	-2.05	1.46	1.50
32	Bb	616	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	606	CHL	CAC-C3C	-2.05	1.48	1.51
32	b	603	CLA	CMC-C2C	-2.05	1.46	1.50
32	b	616	CLA	CMC-C2C	-2.05	1.46	1.50
32	CC	514	CLA	CMB-C2B	-2.05	1.46	1.50
32	N	614	CLA	CHC-C1C	2.05	1.42	1.38
34	AA	409	BCR	C19-C18	2.05	1.50	1.46
32	r	601	CLA	CHC-C1C	2.05	1.42	1.38
39	NN	607	CHL	CMB-C2B	-2.05	1.47	1.51
32	Ss	604	CLA	CMD-C2D	-2.05	1.46	1.50
32	Yy	611	CLA	CMB-C2B	-2.05	1.46	1.50
32	Yy	613	CLA	CMC-C2C	-2.05	1.46	1.50
32	Bb	605	CLA	C3B-C4B	2.05	1.48	1.42
32	4	305	CLA	CMB-C2B	-2.05	1.46	1.50
32	Bb	616	CLA	CMB-C2B	-2.05	1.46	1.50
32	Nn	303	CLA	CMC-C2C	-2.05	1.46	1.50
39	Y	606	CHL	CAC-C3C	-2.05	1.48	1.51
35	DD	406	PL9	C42-C43	2.05	1.56	1.50
32	b	605	CLA	C3B-C4B	2.05	1.48	1.42
32	Bb	607	CLA	CMB-C2B	-2.05	1.46	1.50
32	G	604	CLA	CHC-C1C	2.05	1.42	1.38
32	DD	401	CLA	CHC-C1C	2.05	1.42	1.38
39	YY	605	CHL	CMB-C2B	-2.05	1.47	1.51
32	Yy	612	CLA	CMB-C2B	-2.05	1.46	1.50
32	3	609	CLA	CMD-C2D	-2.05	1.46	1.50
39	YY	609	CHL	CAC-C3C	-2.05	1.48	1.51
32	G	604	CLA	CMD-C2D	-2.05	1.46	1.50
32	b	607	CLA	CMB-C2B	-2.05	1.46	1.50
39	g	609	CHL	CAC-C3C	-2.05	1.48	1.51
32	CC	510	CLA	CMC-C2C	-2.05	1.46	1.50
39	NN	605	CHL	CAC-C3C	-2.05	1.48	1.51
32	S	613	CLA	CMB-C2B	-2.05	1.46	1.50
32	Bb	611	CLA	CMB-C2B	-2.05	1.46	1.50
32	33	613	CLA	CHC-C1C	2.05	1.42	1.38
46	Ee	101	HEM	CMB-C2B	2.05	1.55	1.50
32	22	612	CLA	CHC-C1C	2.05	1.42	1.38
39	n	606	CHL	CBD-CGD	-2.05	1.49	1.52
32	2	603	CLA	CHC-C1C	2.05	1.42	1.38
32	b	607	CLA	CMC-C2C	-2.04	1.46	1.50
39	3	605	CHL	CAC-C3C	-2.04	1.48	1.51
32	a	410	CLA	CHC-C1C	2.04	1.42	1.38
39	22	601	CHL	CMB-C2B	-2.04	1.47	1.51
32	Rr	612	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	602	CLA	CMC-C2C	-2.04	1.46	1.50
32	c	505	CLA	CMB-C2B	-2.04	1.46	1.50
32	BB	615	CLA	CMB-C2B	-2.04	1.46	1.50
32	BB	615	CLA	CMC-C2C	-2.04	1.46	1.50
39	Ss	605	CHL	CHC-C1C	2.04	1.43	1.39
32	Rr	602	CLA	CMC-C2C	-2.04	1.46	1.50
32	33	604	CLA	CHC-C1C	2.04	1.42	1.38
32	b	603	CLA	CMB-C2B	-2.04	1.46	1.50
32	B	611	CLA	CMC-C2C	-2.04	1.46	1.50
34	a	411	BCR	C12-C13	2.04	1.50	1.46
34	c	515	BCR	C8-C9	2.04	1.50	1.46
32	CC	502	CLA	CHC-C1C	2.04	1.42	1.38
39	Gg	307	CHL	CMB-C2B	-2.04	1.47	1.51
32	Gg	312	CLA	CMD-C2D	-2.04	1.46	1.50
40	N	615	LUT	C12-C13	2.04	1.50	1.46
32	R	609	CLA	CMC-C2C	-2.04	1.46	1.50
32	c	510	CLA	CMB-C2B	-2.04	1.46	1.50
32	g	611	CLA	CMD-C2D	-2.04	1.46	1.50
32	Bb	609	CLA	CMB-C2B	-2.04	1.46	1.50
32	Cc	515	CLA	CMB-C2B	-2.04	1.46	1.50
41	y	301	XAT	C12-C13	2.04	1.50	1.46
39	RR	307	CHL	CBD-CGD	-2.04	1.49	1.52
39	NN	607	CHL	CAC-C3C	-2.04	1.48	1.51
46	E	101	HEM	C2A-C3A	-2.04	1.33	1.38
32	2	609	CLA	CMB-C2B	-2.04	1.46	1.50
35	Dd	404	PL9	C37-C38	2.04	1.56	1.50
39	G	609	CHL	CHC-C1C	2.04	1.43	1.39
32	Cc	509	CLA	CMB-C2B	-2.04	1.46	1.50
35	A	410	PL9	C26-C24	2.04	1.55	1.51
32	Bb	612	CLA	MG-NB	-2.04	2.01	2.05
32	AA	405	CLA	C3B-C4B	2.04	1.48	1.42
32	22	602	CLA	CMD-C2D	-2.04	1.46	1.50
32	33	602	CLA	CMB-C2B	-2.04	1.46	1.50
32	s	612	CLA	CMB-C2B	-2.04	1.46	1.50
32	RR	313	CLA	CMB-C2B	-2.04	1.46	1.50
32	n	612	CLA	MG-NA	2.04	2.11	2.06
39	Yy	605	CHL	CBD-CGD	-2.04	1.49	1.52
32	S	613	CLA	CHC-C1C	2.04	1.42	1.38
32	N	613	CLA	MG-ND	-2.04	2.01	2.05
32	N	602	CLA	CMB-C2B	-2.04	1.46	1.50
32	r	601	CLA	CMD-C2D	-2.04	1.46	1.50
32	NN	602	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	44	602	CLA	CMC-C2C	-2.04	1.46	1.50
39	GG	608	CHL	CAC-C3C	-2.04	1.48	1.51
39	RR	306	CHL	CBD-CGD	-2.04	1.49	1.52
34	a	411	BCR	C23-C22	2.04	1.50	1.46
40	g	615	LUT	C12-C13	2.04	1.50	1.46
32	Aa	407	CLA	CHC-C1C	2.04	1.42	1.38
32	R	613	CLA	CMB-C2B	-2.04	1.46	1.50
32	b	609	CLA	CMB-C2B	-2.04	1.46	1.50
39	y	303	CHL	CHC-C1C	2.04	1.43	1.39
35	D	407	PL9	C42-C43	2.04	1.56	1.50
39	n	606	CHL	CMB-C2B	-2.04	1.47	1.51
32	Gg	305	CLA	CMD-C2D	-2.04	1.46	1.50
32	R	609	CLA	CMB-C2B	-2.04	1.46	1.50
32	Y	610	CLA	CMB-C2B	-2.04	1.46	1.50
32	b	614	CLA	CMC-C2C	-2.04	1.46	1.50
32	CC	506	CLA	CMC-C2C	-2.04	1.46	1.50
39	n	607	CHL	CMB-C2B	-2.04	1.47	1.51
39	NN	608	CHL	CMB-C2B	-2.04	1.47	1.51
33	Aa	409	PHO	C3D-C4D	2.04	1.44	1.41
39	N	607	CHL	CAC-C3C	-2.04	1.48	1.51
32	C	513	CLA	CMC-C2C	-2.04	1.46	1.50
32	B	605	CLA	CMD-C2D	-2.04	1.46	1.50
32	B	607	CLA	MG-NB	-2.04	2.01	2.05
39	g	607	CHL	CBD-CGD	-2.04	1.49	1.52
39	YY	609	CHL	CBD-CGD	-2.04	1.49	1.52
32	Rr	604	CLA	C3B-C4B	2.04	1.48	1.42
39	Y	609	CHL	CAC-C3C	-2.04	1.48	1.51
35	AA	410	PL9	C31-C29	2.04	1.55	1.51
39	y	307	CHL	CMB-C2B	-2.04	1.47	1.51
39	g	609	CHL	CBD-CGD	-2.04	1.49	1.52
34	CC	515	BCR	C12-C13	2.04	1.50	1.46
32	D	405	CLA	C3B-C4B	2.04	1.48	1.42
32	c	509	CLA	CHC-C1C	2.04	1.42	1.38
32	b	611	CLA	CMB-C2B	-2.04	1.46	1.50
32	Rr	611	CLA	CHC-C1C	2.04	1.42	1.38
32	y	313	CLA	CHC-C1C	2.04	1.42	1.38
32	N	614	CLA	CMD-C2D	-2.04	1.46	1.50
32	RR	313	CLA	CHC-C1C	2.04	1.42	1.38
32	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
32	4	304	CLA	CMB-C2B	-2.03	1.46	1.50
32	Cc	514	CLA	CMB-C2B	-2.03	1.46	1.50
46	e	101	HEM	CMA-C3A	2.03	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	613	CLA	CHC-C1C	2.03	1.42	1.38
32	33	602	CLA	CMD-C2D	-2.03	1.46	1.50
32	A	405	CLA	C3B-C4B	2.03	1.48	1.42
32	Ss	604	CLA	CHC-C1C	2.03	1.42	1.38
32	N	611	CLA	CMD-C2D	-2.03	1.46	1.50
32	y	305	CLA	CMC-C2C	-2.03	1.46	1.50
39	Nn	317	CHL	CHC-C1C	2.03	1.43	1.39
32	Y	602	CLA	CMD-C2D	-2.03	1.46	1.50
32	CC	503	CLA	CMB-C2B	-2.03	1.46	1.50
39	R	605	CHL	CBD-CGD	-2.03	1.49	1.52
32	33	611	CLA	CMB-C2B	-2.03	1.46	1.50
32	3	603	CLA	CMD-C2D	-2.03	1.46	1.50
32	c	508	CLA	CMB-C2B	-2.03	1.46	1.50
32	NN	613	CLA	MG-ND	-2.03	2.01	2.05
32	YY	602	CLA	CMB-C2B	-2.03	1.46	1.50
32	BB	601	CLA	CHC-C1C	2.03	1.42	1.38
39	y	311	CHL	CHC-C1C	2.03	1.43	1.39
32	Cc	512	CLA	CMB-C2B	-2.03	1.46	1.50
32	33	602	CLA	CHC-C1C	2.03	1.42	1.38
32	3	612	CLA	CHC-C1C	2.03	1.42	1.38
39	g	607	CHL	CMB-C2B	-2.03	1.47	1.51
39	Nn	317	CHL	CBD-CGD	-2.03	1.49	1.52
32	11	604	CLA	CMB-C2B	-2.03	1.46	1.50
32	2	611	CLA	CMD-C2D	-2.03	1.46	1.50
32	C	505	CLA	CMB-C2B	-2.03	1.46	1.50
32	Gg	313	CLA	CMB-C2B	-2.03	1.46	1.50
34	Cc	516	BCR	C23-C22	2.03	1.50	1.46
32	G	612	CLA	CMC-C2C	-2.03	1.46	1.50
32	Cc	507	CLA	CMC-C2C	-2.03	1.46	1.50
32	Nn	305	CLA	CMD-C2D	-2.03	1.46	1.50
34	c	514	BCR	C23-C22	2.03	1.50	1.46
32	BB	606	CLA	CMC-C2C	-2.03	1.46	1.50
39	Y	601	CHL	CHC-C1C	2.03	1.43	1.39
41	Yy	619	XAT	C12-C13	2.03	1.50	1.46
32	44	610	CLA	CHC-C1C	2.03	1.42	1.38
32	a	407	CLA	CHC-C1C	2.03	1.42	1.38
39	SS	302	CHL	CBD-CGD	-2.03	1.49	1.52
32	c	507	CLA	CMB-C2B	-2.03	1.46	1.50
32	NN	614	CLA	CMD-C2D	-2.03	1.46	1.50
41	NN	617	XAT	C28-C29	2.03	1.50	1.46
33	A	407	PHO	C3B-C2B	-2.03	1.37	1.40
32	CC	502	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	608	CLA	C3B-C4B	2.03	1.48	1.42
32	33	603	CLA	CHC-C1C	2.03	1.42	1.38
40	Nn	307	LUT	C22-C21	-2.03	1.52	1.54
32	CC	502	CLA	CMC-C2C	-2.03	1.46	1.50
32	YY	613	CLA	CMB-C2B	-2.03	1.46	1.50
39	44	607	CHL	CBD-CGD	-2.03	1.50	1.52
32	YY	614	CLA	CHC-C1C	2.03	1.42	1.38
32	Aa	410	CLA	CHC-C1C	2.03	1.42	1.38
32	B	609	CLA	CMB-C2B	-2.03	1.46	1.50
32	Gg	305	CLA	CMB-C2B	-2.03	1.46	1.50
32	b	610	CLA	CHC-C1C	2.03	1.42	1.38
39	GG	608	CHL	CMB-C2B	-2.03	1.47	1.51
32	Yy	614	CLA	CMB-C2B	-2.03	1.46	1.50
32	s	610	CLA	CMB-C2B	-2.03	1.46	1.50
32	S	603	CLA	CHC-C1C	2.03	1.42	1.38
32	Y	611	CLA	CHC-C1C	2.03	1.42	1.38
32	Bb	611	CLA	CMC-C2C	-2.03	1.46	1.50
32	2	609	CLA	CHC-C1C	2.03	1.42	1.38
34	BB	617	BCR	C19-C18	2.03	1.50	1.46
32	Rr	611	CLA	CMB-C2B	-2.03	1.46	1.50
32	C	507	CLA	CMB-C2B	-2.03	1.46	1.50
32	G	611	CLA	CMD-C2D	-2.03	1.46	1.50
39	SS	302	CHL	CMB-C2B	-2.02	1.47	1.51
32	1	602	CLA	CMD-C2D	-2.02	1.46	1.50
32	3	610	CLA	CMD-C2D	-2.02	1.46	1.50
39	N	606	CHL	CAC-C3C	-2.02	1.48	1.51
32	44	604	CLA	CHC-C1C	2.02	1.42	1.38
34	b	619	BCR	C23-C22	2.02	1.50	1.46
32	GG	603	CLA	C3B-C4B	2.02	1.48	1.42
32	SS	305	CLA	CHC-C1C	2.02	1.42	1.38
32	Gg	303	CLA	C3B-C4B	2.02	1.48	1.42
32	Rr	609	CLA	CMC-C2C	-2.02	1.46	1.50
32	33	610	CLA	CMD-C2D	-2.02	1.46	1.50
32	4	312	CLA	CMB-C2B	-2.02	1.46	1.50
32	B	605	CLA	MG-NB	-2.02	2.01	2.05
39	Nn	316	CHL	CMB-C2B	-2.02	1.47	1.51
39	n	601	CHL	CBD-CGD	-2.02	1.50	1.52
32	22	613	CLA	CMD-C2D	-2.02	1.46	1.50
32	BB	610	CLA	CMC-C2C	-2.02	1.46	1.50
41	N	617	XAT	C28-C29	2.02	1.50	1.46
32	R	604	CLA	CHC-C1C	2.02	1.42	1.38
39	n	609	CHL	CAC-C3C	-2.02	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	316	CLA	CMB-C2B	-2.02	1.46	1.50
39	NN	606	CHL	CMB-C2B	-2.02	1.47	1.51
39	Nn	317	CHL	CMB-C2B	-2.02	1.47	1.51
32	11	610	CLA	CHC-C1C	2.02	1.42	1.38
35	d	404	PL9	C42-C43	2.02	1.56	1.50
32	y	314	CLA	C3B-C4B	2.02	1.48	1.42
32	A	405	CLA	CMC-C2C	-2.02	1.46	1.50
32	11	611	CLA	CMD-C2D	-2.02	1.46	1.50
32	n	614	CLA	CMD-C2D	-2.02	1.46	1.50
32	CC	507	CLA	CMC-C2C	-2.02	1.46	1.50
32	YY	610	CLA	CMB-C2B	-2.02	1.46	1.50
39	N	607	CHL	CMB-C2B	-2.02	1.47	1.51
34	A	409	BCR	C19-C18	2.02	1.50	1.46
39	g	607	CHL	CAC-C3C	-2.02	1.48	1.51
32	Rr	601	CLA	CMD-C2D	-2.02	1.46	1.50
32	GG	611	CLA	CMB-C2B	-2.02	1.46	1.50
32	Bb	602	CLA	CMB-C2B	-2.02	1.46	1.50
32	Gg	303	CLA	CMB-C2B	-2.02	1.46	1.50
39	S	601	CHL	CMB-C2B	-2.02	1.47	1.51
32	NN	613	CLA	C3B-C4B	2.02	1.48	1.42
34	c	514	BCR	C12-C13	2.02	1.50	1.46
32	3	603	CLA	CHC-C1C	2.02	1.42	1.38
33	D	402	PHO	C3B-C2B	-2.02	1.37	1.40
32	1	604	CLA	CMB-C2B	-2.02	1.46	1.50
33	a	409	PHO	C4D-ND	-2.02	1.35	1.38
32	3	611	CLA	CHC-C1C	2.02	1.42	1.38
32	Cc	505	CLA	CHC-C1C	2.02	1.42	1.38
37	B	617	SQD	O6-C1	2.02	1.43	1.40
41	g	619	XAT	C28-C29	2.02	1.50	1.46
32	4	305	CLA	CHC-C1C	2.02	1.42	1.38
32	g	614	CLA	CMB-C2B	-2.02	1.46	1.50
34	XX	202	BCR	C23-C22	2.02	1.50	1.46
32	Ss	609	CLA	CMB-C2B	-2.02	1.46	1.50
39	g	606	CHL	CMB-C2B	-2.02	1.47	1.51
39	g	608	CHL	CAC-C3C	-2.02	1.48	1.51
39	n	605	CHL	CAC-C3C	-2.02	1.48	1.51
32	Aa	405	CLA	C3B-C4B	2.02	1.48	1.42
32	R	613	CLA	CHC-C1C	2.02	1.42	1.38
32	C	504	CLA	CMB-C2B	-2.02	1.46	1.50
32	c	509	CLA	CMC-C2C	-2.02	1.46	1.50
40	Gg	317	LUT	C8-C9	2.02	1.50	1.46
39	Yy	606	CHL	CMB-C2B	-2.02	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	44	601	CHL	CMB-C2B	-2.02	1.47	1.51
32	r	603	CLA	CHC-C1C	2.02	1.42	1.38
39	Nn	311	CHL	CBD-CGD	-2.02	1.50	1.52
32	Rr	609	CLA	CMB-C2B	-2.02	1.46	1.50
32	22	602	CLA	CMC-C2C	-2.02	1.46	1.50
40	Ss	615	LUT	C7-C6	2.02	1.52	1.45
32	Bb	604	CLA	CMC-C2C	-2.02	1.46	1.50
44	a	415	DGD	O5D-C1E	2.02	1.43	1.40
39	GG	601	CHL	CMB-C2B	-2.02	1.47	1.51
32	33	610	CLA	CHC-C1C	2.02	1.42	1.38
32	Cc	503	CLA	CMC-C2C	-2.02	1.46	1.50
32	N	613	CLA	CMD-C2D	-2.02	1.46	1.50
32	c	510	CLA	CMC-C2C	-2.02	1.46	1.50
32	BB	614	CLA	CMB-C2B	-2.02	1.46	1.50
32	1	613	CLA	CMD-C2D	-2.02	1.46	1.50
34	Hh	101	BCR	C8-C9	2.02	1.50	1.46
32	A	408	CLA	CMB-C2B	-2.02	1.46	1.50
32	S	609	CLA	CMB-C2B	-2.02	1.46	1.50
32	B	623	CLA	CMB-C2B	-2.02	1.46	1.50
33	a	409	PHO	C3B-C2B	-2.02	1.37	1.40
34	Bb	618	BCR	C23-C22	2.02	1.50	1.46
32	c	508	CLA	CHC-C1C	2.01	1.42	1.38
32	1	610	CLA	CMD-C2D	-2.01	1.46	1.50
32	B	608	CLA	CMC-C2C	-2.01	1.46	1.50
32	22	612	CLA	CMD-C2D	-2.01	1.46	1.50
32	AA	405	CLA	CMC-C2C	-2.01	1.46	1.50
32	Cc	506	CLA	CMB-C2B	-2.01	1.46	1.50
46	Ee	101	HEM	CMA-C3A	2.01	1.54	1.50
34	c	515	BCR	C19-C18	2.01	1.50	1.46
39	44	605	CHL	CAC-C3C	-2.01	1.48	1.51
32	a	406	CLA	CHC-C4B	-2.01	1.34	1.39
35	AA	410	PL9	C22-C23	2.01	1.56	1.50
32	A	406	CLA	CMC-C2C	-2.01	1.46	1.50
32	y	312	CLA	CMB-C2B	-2.01	1.46	1.50
32	Nn	302	CLA	CMB-C2B	-2.01	1.46	1.50
40	GG	616	LUT	C8-C9	2.01	1.50	1.46
32	BB	612	CLA	CMC-C2C	-2.01	1.46	1.50
32	B	606	CLA	CMC-C2C	-2.01	1.46	1.50
32	SS	305	CLA	CMB-C2B	-2.01	1.46	1.50
32	Bb	613	CLA	CHC-C1C	2.01	1.42	1.38
39	y	311	CHL	CAC-C3C	-2.01	1.48	1.51
32	c	502	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	315	CLA	CMC-C2C	-2.01	1.46	1.50
34	B	614	BCR	C19-C18	2.01	1.50	1.46
32	3	602	CLA	CMB-C2B	-2.01	1.46	1.50
32	Cc	508	CLA	CMB-C2B	-2.01	1.46	1.50
39	s	601	CHL	CAC-C3C	-2.01	1.48	1.51
32	y	314	CLA	CMA-C3A	-2.01	1.48	1.53
32	Yy	612	CLA	C3B-C4B	2.01	1.48	1.42
34	b	617	BCR	C19-C18	2.01	1.50	1.46
46	EE	102	HEM	CMB-C2B	2.01	1.54	1.50
32	B	618	CLA	CMB-C2B	-2.01	1.46	1.50
32	GG	610	CLA	CMC-C2C	-2.01	1.46	1.50
39	44	607	CHL	CAC-C3C	-2.01	1.48	1.51
41	Gg	301	XAT	C28-C29	2.01	1.50	1.46
35	Dd	404	PL9	C42-C43	2.01	1.56	1.50
32	N	604	CLA	CMB-C2B	-2.01	1.46	1.50
32	c	506	CLA	CMC-C2C	-2.01	1.46	1.50
32	c	513	CLA	CMB-C2B	-2.01	1.46	1.50
32	CC	508	CLA	CMC-C2C	-2.01	1.46	1.50
39	y	309	CHL	CAC-C3C	-2.01	1.48	1.51
34	Aa	411	BCR	C23-C22	2.01	1.50	1.46
32	Rr	608	CLA	CMB-C2B	-2.01	1.46	1.50
32	a	406	CLA	CMC-C2C	-2.01	1.46	1.50
32	22	603	CLA	CHC-C1C	2.01	1.42	1.38
32	g	603	CLA	CMB-C2B	-2.01	1.46	1.50
32	y	312	CLA	CMC-C2C	-2.01	1.46	1.50
39	33	606	CHL	CMB-C2B	-2.01	1.47	1.51
32	N	614	CLA	CMB-C2B	-2.01	1.46	1.50
32	Cc	512	CLA	CMC-C2C	-2.01	1.46	1.50
33	AA	407	PHO	C3D-C4D	2.01	1.44	1.41
33	Aa	408	PHO	C3D-C4D	2.01	1.44	1.41
32	3	613	CLA	CHC-C1C	2.01	1.42	1.38
32	RR	311	CLA	CHC-C1C	2.01	1.42	1.38
32	Yy	613	CLA	CMB-C2B	-2.01	1.46	1.50
41	r	615	XAT	O4-C5	-2.01	1.43	1.46
32	S	602	CLA	CHC-C1C	2.01	1.42	1.38
34	B	613	BCR	C12-C13	2.01	1.50	1.46
39	GG	607	CHL	CMB-C2B	-2.01	1.47	1.51
32	RR	302	CLA	MG-NB	-2.01	2.01	2.05
32	a	410	CLA	CMC-C2C	-2.01	1.46	1.50
32	Nn	314	CLA	CMC-C2C	-2.01	1.46	1.50
32	y	305	CLA	C3B-C4B	2.01	1.48	1.42
39	G	601	CHL	CMB-C2B	-2.01	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	612	CLA	CMC-C2C	-2.01	1.46	1.50
40	Nn	306	LUT	C22-C21	-2.01	1.52	1.54
39	3	606	CHL	CAC-C3C	-2.01	1.48	1.51
32	Y	610	CLA	CMC-C2C	-2.01	1.46	1.50
40	2	614	LUT	C28-C29	2.01	1.50	1.46
32	44	615	CLA	CHC-C1C	2.01	1.42	1.38
39	Gg	308	CHL	CMB-C2B	-2.01	1.47	1.51
32	R	612	CLA	CMB-C2B	-2.01	1.46	1.50
32	r	610	CLA	CMD-C2D	-2.01	1.46	1.50
34	C	517	BCR	C12-C13	2.01	1.50	1.46
32	Cc	512	CLA	CHC-C1C	2.01	1.42	1.38
32	y	314	CLA	CMB-C2B	-2.01	1.46	1.50
32	YY	611	CLA	CMB-C2B	-2.01	1.46	1.50
32	Cc	511	CLA	CMC-C2C	-2.01	1.46	1.50
32	S	604	CLA	CHC-C1C	2.01	1.42	1.38
34	CC	517	BCR	C19-C18	2.01	1.50	1.46
32	n	604	CLA	CMC-C2C	-2.01	1.46	1.50
32	CC	505	CLA	CMC-C2C	-2.01	1.46	1.50
32	CC	505	CLA	CHC-C1C	2.01	1.42	1.38
32	3	604	CLA	CMB-C2B	-2.01	1.46	1.50
44	h	102	DGD	O5D-C1E	2.01	1.43	1.40
32	2	612	CLA	CHC-C1C	2.01	1.42	1.38
32	Bb	607	CLA	CHC-C1C	2.01	1.42	1.38
39	Nn	317	CHL	CAC-C3C	-2.01	1.48	1.51
46	Ee	101	HEM	CMD-C2D	2.00	1.54	1.50
32	Rr	610	CLA	CMD-C2D	-2.00	1.46	1.50
32	C	511	CLA	CMC-C2C	-2.00	1.46	1.50
32	NN	602	CLA	CMC-C2C	-2.00	1.46	1.50
39	y	308	CHL	CMB-C2B	-2.00	1.47	1.51
42	R	617	NEX	C12-C13	2.00	1.50	1.46
42	RR	317	NEX	C12-C13	2.00	1.50	1.46
32	CC	513	CLA	CMB-C2B	-2.00	1.46	1.50
39	r	605	CHL	CAC-C3C	-2.00	1.48	1.51
39	NN	606	CHL	CAC-C3C	-2.00	1.48	1.51
40	22	614	LUT	C28-C29	2.00	1.50	1.46
32	N	611	CLA	CMB-C2B	-2.00	1.46	1.50
32	b	608	CLA	CMC-C2C	-2.00	1.46	1.50
32	BB	613	CLA	CMC-C2C	-2.00	1.46	1.50
32	Ss	611	CLA	CHC-C1C	2.00	1.42	1.38
39	Rr	605	CHL	CAC-C3C	-2.00	1.48	1.51
32	C	512	CLA	CMC-C2C	-2.00	1.46	1.50
32	22	609	CLA	CHC-C1C	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	611	CLA	CMC-C2C	-2.00	1.46	1.50
32	GG	613	CLA	C3B-C4B	2.00	1.48	1.42
32	1	603	CLA	C3B-C4B	2.00	1.48	1.42
32	11	604	CLA	CMD-C2D	-2.00	1.46	1.50
32	RR	314	CLA	CMB-C2B	-2.00	1.46	1.50
32	G	602	CLA	C3B-C4B	2.00	1.48	1.42
32	r	608	CLA	CHC-C1C	2.00	1.42	1.38
32	Dd	402	CLA	CHC-C1C	2.00	1.42	1.38
34	Cc	517	BCR	C19-C18	2.00	1.50	1.46
32	S	613	CLA	CMD-C2D	-2.00	1.46	1.50
32	a	405	CLA	CMC-C2C	-2.00	1.46	1.50
32	b	616	CLA	CMB-C2B	-2.00	1.46	1.50
32	Rr	603	CLA	CHC-C1C	2.00	1.42	1.38
32	Y	604	CLA	CHC-C1C	2.00	1.42	1.38
32	g	614	CLA	CHC-C1C	2.00	1.42	1.38
40	s	615	LUT	C8-C9	2.00	1.50	1.46
32	r	608	CLA	CMB-C2B	-2.00	1.46	1.50
39	11	608	CHL	CAC-C3C	-2.00	1.48	1.51
39	4	308	CHL	CBD-CGD	-2.00	1.50	1.52
39	G	607	CHL	CMB-C2B	-2.00	1.47	1.51
32	d	401	CLA	CHC-C1C	2.00	1.42	1.38
32	44	615	CLA	CMC-C2C	-2.00	1.46	1.50
32	1	612	CLA	CMD-C2D	-2.00	1.46	1.50
39	N	606	CHL	CMB-C2B	-2.00	1.47	1.51
32	Aa	407	CLA	MG-NB	-2.00	2.01	2.05
32	11	609	CLA	CHC-C1C	2.00	1.42	1.38

All (5348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BB	621	SQD	O9-S-C6	-15.25	83.99	106.76
37	B	617	SQD	O9-S-C6	-15.19	84.07	106.76
41	G	619	XAT	O24-C25-C24	11.36	124.14	113.49
41	GG	619	XAT	O24-C25-C24	11.33	124.11	113.49
37	BB	621	SQD	O8-S-O9	-11.31	83.10	111.40
37	B	617	SQD	O8-S-O9	-11.30	83.12	111.40
41	g	619	XAT	O24-C25-C24	11.05	123.85	113.49
41	Gg	301	XAT	O24-C25-C24	10.89	123.69	113.49
41	Nn	308	XAT	O24-C25-C24	10.36	123.20	113.49
37	B	617	SQD	O9-S-O7	-9.66	82.39	113.82
37	BB	621	SQD	O9-S-O7	-9.64	82.47	113.82
35	Dd	404	PL9	C7-C8-C9	-9.55	110.38	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	d	404	PL9	C7-C8-C9	-9.30	110.81	126.83
41	y	302	XAT	O24-C25-C24	9.23	122.14	113.49
35	D	407	PL9	C7-C8-C9	-9.13	111.11	126.83
35	DD	406	PL9	C7-C8-C9	-9.07	111.21	126.83
40	Yy	615	LUT	C1-C6-C5	-9.06	110.26	122.64
41	GG	619	XAT	O4-C5-C4	8.83	121.77	113.49
41	y	301	XAT	O24-C25-C38	8.72	124.79	115.05
41	NN	617	XAT	O24-C25-C24	8.69	121.63	113.49
35	AA	410	PL9	C7-C8-C9	-8.61	112.00	126.83
35	A	410	PL9	C7-C8-C9	-8.56	112.08	126.83
41	G	619	XAT	O4-C5-C4	8.47	121.43	113.49
41	Gg	301	XAT	O4-C5-C4	8.45	121.41	113.49
41	44	613	XAT	O4-C5-C4	8.45	121.41	113.49
41	g	619	XAT	O4-C5-C4	8.32	121.28	113.49
41	N	617	XAT	O24-C25-C24	8.19	121.17	113.49
37	B	617	SQD	O7-S-C6	8.02	118.73	106.76
37	BB	621	SQD	O7-S-C6	8.00	118.70	106.76
41	44	613	XAT	O24-C25-C24	7.99	120.98	113.49
41	4	314	XAT	O24-C25-C24	7.95	120.94	113.49
42	Gg	318	NEX	O24-C25-C24	7.76	120.77	113.49
40	y	317	LUT	C1-C6-C5	-7.50	112.39	122.64
41	GG	617	XAT	O24-C25-C24	7.39	120.42	113.49
32	g	602	CLA	C4A-NA-C1A	7.38	110.05	106.68
41	4	314	XAT	O4-C5-C4	7.36	120.39	113.49
41	G	617	XAT	O24-C25-C24	7.34	120.37	113.49
42	g	617	NEX	O24-C25-C24	7.29	120.33	113.49
35	Dd	404	PL9	C37-C38-C39	-7.26	111.01	127.62
35	D	407	PL9	C37-C38-C39	-7.20	111.14	127.62
33	DD	402	PHO	C4D-CHA-CBD	-7.18	105.01	108.45
41	r	615	XAT	O4-C5-C4	7.18	120.22	113.49
35	d	404	PL9	C37-C38-C39	-7.18	111.19	127.62
35	d	404	PL9	C22-C23-C24	-7.13	111.31	127.62
35	DD	406	PL9	C37-C38-C39	-7.12	111.32	127.62
34	h	101	BCR	C32-C1-C6	7.12	121.41	110.24
35	Dd	404	PL9	C22-C23-C24	-7.09	111.39	127.62
34	Hh	101	BCR	C32-C1-C6	7.09	121.36	110.24
35	d	404	PL9	C12-C13-C14	-7.09	111.39	127.62
35	A	410	PL9	C22-C23-C24	-7.08	111.41	127.62
35	Dd	404	PL9	C42-C43-C44	-7.02	111.56	127.62
41	G	617	XAT	O4-C5-C4	6.98	120.03	113.49
34	XX	202	BCR	C1-C6-C5	-6.97	113.11	122.64
35	D	407	PL9	C32-C33-C34	-6.96	111.70	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	GG	617	XAT	O4-C5-C4	6.95	120.00	113.49
42	Y	617	NEX	O24-C25-C24	6.95	120.00	113.49
35	Dd	404	PL9	C12-C13-C14	-6.94	111.74	127.62
35	D	407	PL9	C17-C18-C19	-6.93	111.76	127.62
34	KK	103	BCR	C30-C25-C26	-6.91	113.20	122.64
35	d	404	PL9	C42-C43-C44	-6.91	111.81	127.62
42	g	617	NEX	C39-C29-C30	-6.87	111.68	122.82
35	d	404	PL9	C27-C28-C29	-6.87	111.90	127.62
35	Dd	404	PL9	C27-C28-C29	-6.84	111.97	127.62
35	d	404	PL9	C17-C18-C19	-6.84	111.98	127.62
34	K	102	BCR	C30-C25-C26	-6.84	113.30	122.64
35	A	410	PL9	C17-C18-C19	-6.82	112.01	127.62
39	Nn	316	CHL	C1B-CHB-C4A	6.82	125.71	121.32
35	D	407	PL9	C27-C28-C29	-6.82	112.02	127.62
35	AA	410	PL9	C32-C33-C34	-6.81	112.04	127.62
42	Rr	616	NEX	O24-C25-C24	6.79	119.86	113.49
35	DD	406	PL9	C32-C33-C34	-6.79	112.08	127.62
35	DD	406	PL9	C17-C18-C19	-6.79	112.08	127.62
35	D	407	PL9	C22-C23-C24	-6.79	112.09	127.62
42	Y	619	NEX	O24-C25-C24	6.78	119.85	113.49
39	G	601	CHL	C1B-CHB-C4A	6.77	125.68	121.32
34	b	617	BCR	C28-C27-C26	-6.77	101.99	114.06
32	CC	507	CLA	C4A-NA-C1A	6.74	109.75	106.68
35	D	407	PL9	C12-C13-C14	-6.73	112.21	127.62
35	DD	406	PL9	C22-C23-C24	-6.73	112.23	127.62
39	n	606	CHL	C1B-CHB-C4A	6.72	125.65	121.32
35	A	410	PL9	C32-C33-C34	-6.72	112.24	127.62
35	A	410	PL9	C27-C28-C29	-6.71	112.27	127.62
35	Dd	404	PL9	C17-C18-C19	-6.70	112.29	127.62
33	Aa	409	PHO	C4D-CHA-CBD	-6.69	105.24	108.45
35	AA	410	PL9	C12-C13-C14	-6.69	112.30	127.62
39	y	308	CHL	C1B-CHB-C4A	6.69	125.63	121.32
35	D	407	PL9	C42-C43-C44	-6.69	112.32	127.62
35	DD	406	PL9	C12-C13-C14	-6.68	112.33	127.62
33	a	409	PHO	C4D-CHA-CBD	-6.67	105.25	108.45
34	c	514	BCR	C3-C4-C5	-6.67	102.16	114.06
35	A	410	PL9	C12-C13-C14	-6.66	112.37	127.62
35	DD	406	PL9	C27-C28-C29	-6.65	112.41	127.62
39	Yy	606	CHL	C1B-CHB-C4A	6.61	125.57	121.32
35	DD	406	PL9	C42-C43-C44	-6.59	112.54	127.62
34	C	518	BCR	C3-C4-C5	-6.57	102.34	114.06
35	A	410	PL9	C42-C43-C44	-6.56	112.61	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	402	PHO	C4D-CHA-CBD	-6.55	105.31	108.45
32	C	508	CLA	C4A-NA-C1A	6.55	109.67	106.68
41	Rr	615	XAT	O4-C5-C18	6.52	122.34	115.05
35	AA	410	PL9	C37-C38-C39	-6.52	112.71	127.62
35	A	410	PL9	C37-C38-C39	-6.51	112.72	127.62
39	SS	306	CHL	C1B-CHB-C4A	6.50	125.50	121.32
37	B	617	SQD	O8-S-C6	6.48	118.48	105.97
35	AA	410	PL9	C42-C43-C44	-6.48	112.80	127.62
34	Cc	516	BCR	C28-C27-C26	-6.45	102.55	114.06
33	Aa	408	PHO	C4D-CHA-CBD	-6.44	105.37	108.45
33	A	407	PHO	C4D-CHA-CBD	-6.43	105.37	108.45
42	N	618	NEX	O24-C25-C24	6.43	119.52	113.49
37	BB	621	SQD	O8-S-C6	6.43	118.39	105.97
35	AA	410	PL9	C22-C23-C24	-6.43	112.91	127.62
33	a	408	PHO	C4D-CHA-CBD	-6.43	105.37	108.45
35	AA	410	PL9	C17-C18-C19	-6.43	112.92	127.62
42	YY	617	NEX	O24-C25-C24	6.41	119.50	113.49
35	d	404	PL9	C32-C33-C34	-6.40	112.97	127.62
32	GG	602	CLA	C4A-NA-C1A	6.39	109.59	106.68
39	Yy	607	CHL	C1B-CHB-C4A	6.38	125.43	121.32
33	AA	407	PHO	C4D-CHA-CBD	-6.37	105.40	108.45
34	c	514	BCR	C28-C27-C26	-6.34	102.75	114.06
34	Kk	101	BCR	C1-C6-C5	-6.33	113.99	122.64
34	CC	517	BCR	C3-C4-C5	-6.32	102.79	114.06
42	NN	618	NEX	O24-C25-C24	6.30	119.39	113.49
39	S	606	CHL	C1B-CHB-C4A	6.29	125.37	121.32
32	CC	502	CLA	C4A-NA-C1A	6.28	109.55	106.68
39	NN	606	CHL	C1B-CHB-C4A	6.27	125.36	121.32
39	g	606	CHL	C1B-CHB-C4A	6.27	125.36	121.32
34	b	619	BCR	C3-C4-C5	-6.26	102.89	114.06
32	R	608	CLA	C4A-NA-C1A	6.26	109.53	106.68
39	11	606	CHL	C1B-CHB-C4A	6.25	125.34	121.32
39	YY	601	CHL	C1B-CHB-C4A	6.24	125.33	121.32
39	33	606	CHL	C1B-CHB-C4A	6.23	125.33	121.32
39	GG	601	CHL	C1B-CHB-C4A	6.23	125.33	121.32
34	c	516	BCR	C3-C4-C5	-6.23	102.95	114.06
34	AA	409	BCR	C28-C27-C26	-6.22	102.96	114.06
35	AA	410	PL9	C27-C28-C29	-6.22	113.39	127.62
39	SS	307	CHL	C1B-CHB-C4A	6.21	125.32	121.32
35	Dd	404	PL9	C32-C33-C34	-6.18	113.48	127.62
39	YY	608	CHL	C1B-CHB-C4A	6.17	125.30	121.32
34	Bb	617	BCR	C28-C27-C26	-6.17	103.05	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Yy	619	XAT	O24-C25-C38	6.17	121.94	115.05
39	1	606	CHL	C1B-CHB-C4A	6.16	125.29	121.32
34	C	517	BCR	C3-C4-C5	-6.16	103.07	114.06
41	y	301	XAT	O4-C5-C4	6.14	119.25	113.49
34	A	409	BCR	C28-C27-C26	-6.13	103.12	114.06
32	b	609	CLA	C4A-NA-C1A	6.12	109.47	106.68
41	Nn	308	XAT	O4-C5-C4	6.12	119.23	113.49
39	GG	607	CHL	C1B-CHB-C4A	6.12	125.26	121.32
39	G	607	CHL	C1B-CHB-C4A	6.12	125.26	121.32
34	h	101	BCR	C28-C27-C26	-6.11	103.16	114.06
39	N	606	CHL	C1B-CHB-C4A	6.10	125.25	121.32
34	Bb	619	BCR	C3-C4-C5	-6.09	103.19	114.06
41	Yy	619	XAT	O24-C25-C24	6.06	119.17	113.49
39	Y	608	CHL	C1B-CHB-C4A	6.06	125.22	121.32
41	r	615	XAT	O24-C25-C24	6.06	119.17	113.49
42	n	617	NEX	O24-C25-C24	6.04	119.15	113.49
34	DD	405	BCR	C28-C27-C26	-6.04	103.29	114.06
39	NN	608	CHL	C1B-CHB-C4A	6.04	125.21	121.32
32	RR	308	CLA	C4A-NA-C1A	6.02	109.43	106.68
39	Ss	607	CHL	C1B-CHB-C4A	6.01	125.19	121.32
39	n	608	CHL	C1B-CHB-C4A	6.01	125.19	121.32
39	N	608	CHL	C1B-CHB-C4A	6.01	125.19	121.32
39	4	306	CHL	C1B-CHB-C4A	6.01	125.19	121.32
39	Y	606	CHL	C1B-CHB-C4A	6.00	125.18	121.32
39	s	607	CHL	C1B-CHB-C4A	5.99	125.18	121.32
39	g	608	CHL	C1B-CHB-C4A	5.99	125.18	121.32
39	2	607	CHL	C1B-CHB-C4A	5.99	125.17	121.32
34	TT	101	BCR	C28-C27-C26	-5.99	103.38	114.06
39	33	605	CHL	C1B-CHB-C4A	5.98	125.17	121.32
39	Nn	318	CHL	C1B-CHB-C4A	5.98	125.17	121.32
39	22	607	CHL	C1B-CHB-C4A	5.97	125.16	121.32
39	3	605	CHL	C1B-CHB-C4A	5.96	125.16	121.32
41	N	617	XAT	O4-C5-C4	5.96	119.08	113.49
34	h	101	BCR	C1-C6-C5	-5.96	114.50	122.64
34	D	406	BCR	C28-C27-C26	-5.93	103.47	114.06
34	Hh	101	BCR	C28-C27-C26	-5.93	103.48	114.06
39	Gg	307	CHL	C1B-CHB-C4A	5.93	125.14	121.32
39	g	601	CHL	C1B-CHB-C4A	5.92	125.13	121.32
39	Gg	309	CHL	C1B-CHB-C4A	5.92	125.13	121.32
39	R	607	CHL	C1B-CHB-C4A	5.90	125.12	121.32
39	n	607	CHL	C1B-CHB-C4A	5.90	125.12	121.32
39	NN	607	CHL	C1B-CHB-C4A	5.89	125.11	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	NN	617	XAT	O4-C5-C4	5.88	119.00	113.49
34	Cc	518	BCR	C30-C25-C26	-5.87	114.61	122.64
39	S	601	CHL	C1B-CHB-C4A	5.86	125.09	121.32
39	SS	302	CHL	C1B-CHB-C4A	5.86	125.09	121.32
39	Ss	601	CHL	C1B-CHB-C4A	5.85	125.09	121.32
39	Yy	608	CHL	C1B-CHB-C4A	5.84	125.08	121.32
32	C	504	CLA	C4A-NA-C1A	5.83	109.34	106.68
34	Bb	618	BCR	C28-C27-C26	-5.83	103.67	114.06
34	C	518	BCR	C28-C27-C26	-5.81	103.69	114.06
34	b	618	BCR	C28-C27-C26	-5.81	103.69	114.06
39	RR	307	CHL	C1B-CHB-C4A	5.81	125.06	121.32
39	N	607	CHL	C1B-CHB-C4A	5.80	125.05	121.32
34	CC	516	BCR	C30-C25-C26	-5.79	114.72	122.64
34	CC	516	BCR	C3-C4-C5	-5.76	103.79	114.06
39	Nn	311	CHL	C1B-CHB-C4A	5.75	125.02	121.32
39	Nn	317	CHL	C1B-CHB-C4A	5.75	125.02	121.32
39	2	601	CHL	C1B-CHB-C4A	5.73	125.01	121.32
32	RR	304	CLA	C4A-NA-C1A	5.72	109.29	106.68
35	AA	410	PL9	C10-C9-C8	-5.72	108.94	123.63
41	Rr	615	XAT	O24-C25-C24	5.71	118.84	113.49
39	22	601	CHL	C1B-CHB-C4A	5.71	124.99	121.32
39	Gg	308	CHL	C1B-CHB-C4A	5.71	124.99	121.32
39	Gg	302	CHL	C1B-CHB-C4A	5.70	124.99	121.32
34	K	102	BCR	C3-C4-C5	-5.69	103.90	114.06
36	4	301	LHG	O7-C7-O9	-5.69	118.41	125.70
39	Y	607	CHL	C1B-CHB-C4A	5.68	124.98	121.32
35	AA	410	PL9	C15-C14-C13	-5.68	109.04	123.63
39	4	302	CHL	C1B-CHB-C4A	5.67	124.97	121.32
34	C	517	BCR	C30-C25-C26	-5.67	114.89	122.64
35	d	404	PL9	C45-C44-C43	-5.67	109.06	123.63
39	y	307	CHL	C1B-CHB-C4A	5.67	124.97	121.32
34	Cc	516	BCR	C3-C4-C5	-5.67	103.95	114.06
42	Nn	309	NEX	O24-C25-C24	5.66	118.80	113.49
39	y	310	CHL	C1B-CHB-C4A	5.66	124.96	121.32
39	S	605	CHL	C1B-CHB-C4A	5.65	124.96	121.32
39	YY	605	CHL	C1B-CHB-C4A	5.65	124.96	121.32
39	YY	607	CHL	C1B-CHB-C4A	5.65	124.96	121.32
35	Dd	404	PL9	C10-C9-C8	-5.65	109.12	123.63
34	BB	620	BCR	C28-C27-C26	-5.64	103.99	114.06
39	g	607	CHL	C1B-CHB-C4A	5.64	124.95	121.32
32	R	604	CLA	C4A-NA-C1A	5.64	109.25	106.68
35	A	410	PL9	C10-C9-C8	-5.63	109.16	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	r	605	CHL	C1B-CHB-C4A	5.63	124.94	121.32
35	d	404	PL9	C10-C9-C8	-5.63	109.18	123.63
39	G	606	CHL	C1B-CHB-C4A	5.62	124.94	121.32
35	A	410	PL9	C45-C44-C43	-5.62	109.19	123.63
41	y	302	XAT	O4-C5-C4	5.62	118.76	113.49
35	DD	406	PL9	C15-C14-C13	-5.61	109.21	123.63
35	D	407	PL9	C15-C14-C13	-5.61	109.22	123.63
35	Dd	404	PL9	C45-C44-C43	-5.61	109.22	123.63
35	Dd	404	PL9	C15-C14-C13	-5.61	109.23	123.63
35	D	407	PL9	C10-C9-C8	-5.60	109.24	123.63
39	Yy	605	CHL	C1B-CHB-C4A	5.60	124.92	121.32
34	CC	515	BCR	C30-C25-C26	-5.60	114.99	122.64
32	S	611	CLA	C4A-NA-C1A	5.59	109.23	106.68
39	y	311	CHL	C1B-CHB-C4A	5.59	124.92	121.32
35	D	407	PL9	C45-C44-C43	-5.59	109.27	123.63
34	T	101	BCR	C28-C27-C26	-5.59	104.09	114.06
35	AA	410	PL9	C45-C44-C43	-5.58	109.29	123.63
39	N	601	CHL	C1B-CHB-C4A	5.58	124.91	121.32
32	g	602	CLA	CGD-CBD-CAD	-5.58	92.79	110.85
32	Gg	303	CLA	C4A-NA-C1A	5.57	109.22	106.68
39	2	605	CHL	C1B-CHB-C4A	5.57	124.91	121.32
32	Bb	609	CLA	C4A-NA-C1A	5.56	109.22	106.68
39	YY	606	CHL	C1B-CHB-C4A	5.56	124.90	121.32
36	44	616	LHG	O7-C7-O9	-5.56	118.57	125.70
39	Y	601	CHL	C1B-CHB-C4A	5.56	124.90	121.32
35	d	404	PL9	C15-C14-C13	-5.56	109.35	123.63
39	2	608	CHL	C1B-CHB-C4A	5.56	124.90	121.32
39	44	607	CHL	C1B-CHB-C4A	5.55	124.90	121.32
39	GG	606	CHL	C1B-CHB-C4A	5.55	124.89	121.32
32	n	611	CLA	C4A-NA-C1A	5.55	109.21	106.68
35	DD	406	PL9	C45-C44-C43	-5.55	109.37	123.63
34	Hh	101	BCR	C1-C6-C5	-5.55	115.06	122.64
40	Y	616	LUT	C1-C6-C5	-5.53	115.08	122.64
39	y	309	CHL	C1B-CHB-C4A	5.53	124.88	121.32
34	CC	517	BCR	C28-C27-C26	-5.52	104.21	114.06
32	C	509	CLA	C4A-NA-C1A	5.52	109.20	106.68
34	k	101	BCR	C33-C5-C6	-5.52	118.46	124.48
39	1	607	CHL	C1B-CHB-C4A	5.51	124.87	121.32
39	s	601	CHL	C1B-CHB-C4A	5.51	124.87	121.32
32	S	610	CLA	C4A-NA-C1A	5.51	109.19	106.68
39	3	606	CHL	C1B-CHB-C4A	5.50	124.86	121.32
32	Ss	610	CLA	C4A-NA-C1A	5.50	109.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	R	617	NEX	O24-C25-C24	5.49	118.64	113.49
34	c	516	BCR	C30-C25-C26	-5.48	115.14	122.64
34	Dd	403	BCR	C30-C25-C26	-5.48	115.14	122.64
39	44	601	CHL	C1B-CHB-C4A	5.48	124.85	121.32
34	B	616	BCR	C28-C27-C26	-5.48	104.29	114.06
34	XX	202	BCR	C28-C27-C26	-5.47	104.30	114.06
34	b	619	BCR	C28-C27-C26	-5.47	104.31	114.06
39	3	608	CHL	C1B-CHB-C4A	5.46	124.83	121.32
45	AA	413	BCT	O2-C-O1	5.45	133.61	119.68
41	Yy	619	XAT	O4-C5-C4	5.45	118.59	113.49
32	R	603	CLA	C4A-NA-C1A	5.44	109.16	106.68
32	B	605	CLA	C4A-NA-C1A	5.44	109.16	106.68
35	A	410	PL9	C15-C14-C13	-5.44	109.65	123.63
35	DD	406	PL9	C16-C14-C13	-5.44	108.96	121.17
39	Rr	607	CHL	C1B-CHB-C4A	5.43	124.82	121.32
39	S	607	CHL	C1B-CHB-C4A	5.43	124.82	121.32
39	Y	605	CHL	C1B-CHB-C4A	5.43	124.82	121.32
39	y	303	CHL	C1B-CHB-C4A	5.43	124.81	121.32
34	d	403	BCR	C30-C25-C26	-5.43	115.22	122.64
34	C	516	BCR	C30-C25-C26	-5.43	115.22	122.64
35	DD	406	PL9	C10-C9-C8	-5.43	109.69	123.63
35	D	407	PL9	C16-C14-C13	-5.42	108.99	121.17
34	KK	103	BCR	C3-C4-C5	-5.42	104.38	114.06
32	CC	508	CLA	C4A-NA-C1A	5.42	109.15	106.68
42	RR	317	NEX	O24-C25-C24	5.41	118.56	113.49
41	Rr	615	XAT	O4-C5-C4	5.41	118.56	113.49
34	BB	616	BCR	C3-C4-C5	-5.41	104.42	114.06
34	KK	103	BCR	C28-C27-C26	-5.40	104.42	114.06
32	s	610	CLA	C4A-NA-C1A	5.39	109.14	106.68
34	Aa	411	BCR	C3-C4-C5	-5.39	104.45	114.06
39	2	606	CHL	C1B-CHB-C4A	5.39	124.79	121.32
32	Cc	503	CLA	C4A-NA-C1A	5.37	109.13	106.68
32	Bb	612	CLA	C4A-NA-C1A	5.36	109.13	106.68
39	n	609	CHL	C1B-CHB-C4A	5.36	124.77	121.32
35	Dd	404	PL9	C46-C44-C43	-5.36	109.13	121.17
34	Dd	403	BCR	C1-C6-C5	-5.36	115.31	122.64
32	RR	303	CLA	C4A-NA-C1A	5.35	109.12	106.68
35	D	407	PL9	C35-C34-C33	-5.35	109.88	123.63
39	GG	605	CHL	C1B-CHB-C4A	5.35	124.77	121.32
34	a	411	BCR	C3-C4-C5	-5.35	104.51	114.06
34	A	409	BCR	C3-C4-C5	-5.35	104.51	114.06
42	Gg	318	NEX	C39-C29-C30	-5.35	114.15	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Cc	509	CLA	C4A-NA-C1A	5.35	109.12	106.68
32	c	507	CLA	C4A-NA-C1A	5.34	109.11	106.68
34	b	617	BCR	C36-C18-C19	5.33	126.23	118.09
35	d	404	PL9	C46-C44-C43	-5.33	109.21	121.17
39	22	608	CHL	C1B-CHB-C4A	5.32	124.74	121.32
39	n	601	CHL	C1B-CHB-C4A	5.31	124.74	121.32
32	SS	311	CLA	C4A-NA-C1A	5.31	109.10	106.68
39	G	605	CHL	C1B-CHB-C4A	5.31	124.74	121.32
32	NN	611	CLA	C4A-NA-C1A	5.30	109.10	106.68
35	D	407	PL9	C46-C44-C43	-5.30	109.27	121.17
35	d	404	PL9	C11-C9-C8	-5.30	109.27	121.17
39	G	608	CHL	C1B-CHB-C4A	5.28	124.72	121.32
32	G	610	CLA	C4A-NA-C1A	5.28	109.09	106.68
39	GG	608	CHL	C1B-CHB-C4A	5.28	124.72	121.32
42	g	617	NEX	C27-C28-C29	5.27	133.71	125.53
32	Bb	601	CLA	C4A-NA-C1A	5.27	109.08	106.68
39	r	607	CHL	C1B-CHB-C4A	5.27	124.71	121.32
34	Bb	617	BCR	C30-C25-C26	-5.27	115.44	122.64
35	D	407	PL9	C11-C9-C8	-5.27	109.34	121.17
39	22	605	CHL	C1B-CHB-C4A	5.26	124.71	121.32
34	Bb	617	BCR	C36-C18-C19	5.26	126.12	118.09
35	A	410	PL9	C11-C9-C8	-5.26	109.36	121.17
34	H	101	BCR	C28-C27-C26	-5.25	104.69	114.06
35	DD	406	PL9	C11-C9-C8	-5.25	109.39	121.17
39	3	607	CHL	C1B-CHB-C4A	5.24	124.69	121.32
34	b	618	BCR	C3-C4-C5	-5.24	104.72	114.06
39	33	607	CHL	C1B-CHB-C4A	5.23	124.69	121.32
39	1	601	CHL	C1B-CHB-C4A	5.23	124.69	121.32
35	D	407	PL9	C40-C39-C38	-5.23	110.20	123.63
35	DD	406	PL9	C46-C44-C43	-5.23	109.44	121.17
32	4	304	CLA	C4A-NA-C1A	5.23	109.06	106.68
32	BB	609	CLA	C4A-NA-C1A	5.23	109.06	106.68
35	DD	406	PL9	C30-C29-C28	-5.22	110.22	123.63
45	D	403	BCT	O2-C-O1	5.21	133.01	119.68
32	Nn	302	CLA	C4A-NA-C1A	5.21	109.06	106.68
34	BB	617	BCR	C3-C4-C5	-5.21	104.77	114.06
34	AA	409	BCR	C3-C4-C5	-5.20	104.78	114.06
39	Yy	601	CHL	C1B-CHB-C4A	5.20	124.67	121.32
39	4	307	CHL	C1B-CHB-C4A	5.20	124.67	121.32
32	CC	503	CLA	C4A-NA-C1A	5.20	109.05	106.68
35	Dd	404	PL9	C40-C39-C38	-5.20	110.28	123.63
32	y	313	CLA	C4A-NA-C1A	5.19	109.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	613	BCR	C3-C4-C5	-5.19	104.81	114.06
32	Gg	312	CLA	C4A-NA-C1A	5.18	109.04	106.68
39	G	609	CHL	C1B-CHB-C4A	5.18	124.66	121.32
39	Nn	315	CHL	C1B-CHB-C4A	5.18	124.66	121.32
39	Y	609	CHL	C1B-CHB-C4A	5.18	124.65	121.32
39	44	606	CHL	C1B-CHB-C4A	5.18	124.65	121.32
34	k	101	BCR	C1-C6-C5	-5.17	115.57	122.64
34	Bb	618	BCR	C3-C4-C5	-5.17	104.84	114.06
45	Aa	414	BCT	O2-C-O1	5.17	132.89	119.68
35	AA	410	PL9	C35-C34-C33	-5.16	110.38	123.63
35	DD	406	PL9	C40-C39-C38	-5.16	110.38	123.63
32	YY	604	CLA	C4A-NA-C1A	5.16	109.03	106.68
40	Nn	307	LUT	C1-C6-C5	-5.16	115.59	122.64
32	r	610	CLA	C4A-NA-C1A	5.15	109.03	106.68
41	R	616	XAT	O24-C25-C24	5.15	118.32	113.49
34	d	403	BCR	C1-C6-C5	-5.15	115.60	122.64
35	A	410	PL9	C16-C14-C13	-5.15	109.61	121.17
35	d	404	PL9	C40-C39-C38	-5.14	110.44	123.63
32	N	611	CLA	C4A-NA-C1A	5.14	109.02	106.68
39	11	607	CHL	C1B-CHB-C4A	5.13	124.63	121.32
32	YY	611	CLA	C4A-NA-C1A	5.13	109.02	106.68
35	A	410	PL9	C46-C44-C43	-5.13	109.65	121.17
40	y	317	LUT	C18-C5-C6	5.12	130.08	124.48
35	AA	410	PL9	C46-C44-C43	-5.12	109.67	121.17
32	Bb	604	CLA	C4A-NA-C1A	5.12	109.02	106.68
32	Yy	611	CLA	C4A-NA-C1A	5.12	109.01	106.68
32	r	612	CLA	C4A-NA-C1A	5.12	109.01	106.68
39	44	605	CHL	C1B-CHB-C4A	5.11	124.61	121.32
35	AA	410	PL9	C16-C14-C13	-5.11	109.70	121.17
35	Dd	404	PL9	C16-C14-C13	-5.10	109.72	121.17
34	Bb	619	BCR	C30-C25-C26	-5.10	115.67	122.64
35	DD	406	PL9	C35-C34-C33	-5.10	110.54	123.63
32	Rr	610	CLA	C4A-NA-C1A	5.08	109.00	106.68
32	b	612	CLA	C4A-NA-C1A	5.07	108.99	106.68
34	B	612	BCR	C3-C4-C5	-5.06	105.03	114.06
39	YY	609	CHL	C1B-CHB-C4A	5.06	124.58	121.32
35	A	410	PL9	C25-C24-C23	-5.06	110.63	123.63
32	g	611	CLA	C4A-NA-C1A	5.06	108.99	106.68
35	Dd	404	PL9	C35-C34-C33	-5.06	110.64	123.63
34	XX	202	BCR	C3-C4-C5	-5.05	105.05	114.06
35	d	404	PL9	C35-C34-C33	-5.05	110.65	123.63
35	D	407	PL9	C20-C19-C18	-5.04	110.68	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	YY	603	CLA	C4A-NA-C1A	5.04	108.98	106.68
35	D	407	PL9	C30-C29-C28	-5.04	110.68	123.63
32	b	601	CLA	C4A-NA-C1A	5.04	108.98	106.68
35	DD	406	PL9	C20-C19-C18	-5.04	110.69	123.63
41	Rr	615	XAT	O24-C25-C38	5.03	120.67	115.05
41	RR	316	XAT	O24-C25-C38	5.03	120.67	115.05
32	G	602	CLA	C4A-NA-C1A	5.03	108.97	106.68
35	Dd	404	PL9	C36-C34-C33	-5.03	109.88	121.17
35	D	407	PL9	C25-C24-C23	-5.02	110.73	123.63
32	Ss	602	CLA	C4A-NA-C1A	5.01	108.97	106.68
32	r	603	CLA	C4A-NA-C1A	5.01	108.97	106.68
39	SS	308	CHL	C1B-CHB-C4A	5.00	124.54	121.32
35	d	404	PL9	C20-C19-C18	-5.00	110.79	123.63
35	A	410	PL9	C35-C34-C33	-5.00	110.79	123.63
36	4	315	LHG	O7-C7-C8	5.00	120.00	111.09
39	Nn	319	CHL	C1B-CHB-C4A	5.00	124.54	121.32
41	Yy	619	XAT	O4-C5-C18	5.00	120.63	115.05
32	Yy	603	CLA	C4A-NA-C1A	5.00	108.96	106.68
32	GG	613	CLA	C4A-NA-C1A	5.00	108.96	106.68
35	DD	406	PL9	C25-C24-C23	-4.99	110.81	123.63
39	Rr	605	CHL	C1B-CHB-C4A	4.99	124.53	121.32
42	g	617	NEX	C8-C7-C6	-4.97	171.79	177.66
45	a	413	BCT	O2-C-O1	4.97	132.39	119.68
39	11	601	CHL	C1B-CHB-C4A	4.97	124.52	121.32
32	C	512	CLA	C4A-NA-C1A	4.97	108.94	106.68
39	Nn	315	CHL	O2D-CGD-CBD	4.96	116.40	110.95
40	Ss	615	LUT	C1-C6-C5	-4.96	115.86	122.64
32	b	604	CLA	C4A-NA-C1A	4.96	108.94	106.68
32	B	609	CLA	C4A-NA-C1A	4.96	108.94	106.68
35	D	407	PL9	C36-C34-C33	-4.96	110.04	121.17
32	Aa	407	CLA	C4A-NA-C1A	4.96	108.94	106.68
42	y	319	NEX	O24-C25-C38	4.96	120.59	115.05
34	d	403	BCR	C3-C4-C5	-4.95	105.22	114.06
41	RR	316	XAT	C18-C5-C6	-4.95	114.15	122.30
35	A	410	PL9	C20-C19-C18	-4.95	110.91	123.63
32	Y	611	CLA	C4A-NA-C1A	4.95	108.94	106.68
32	BB	613	CLA	C4A-NA-C1A	4.94	108.94	106.68
34	K	102	BCR	C28-C27-C26	-4.94	105.24	114.06
32	CC	509	CLA	C4A-NA-C1A	4.94	108.93	106.68
35	AA	410	PL9	C11-C9-C8	-4.94	110.07	121.17
35	A	410	PL9	C30-C29-C28	-4.94	110.95	123.63
32	c	510	CLA	C4A-NA-C1A	4.93	108.93	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Dd	404	PL9	C11-C9-C8	-4.93	110.11	121.17
39	NN	601	CHL	C1B-CHB-C4A	4.93	124.49	121.32
32	GG	611	CLA	C4A-NA-C1A	4.92	108.92	106.68
36	J	101	LHG	O7-C7-C8	4.92	119.86	111.09
39	Ss	605	CHL	C1B-CHB-C4A	4.92	124.49	121.32
39	1	605	CHL	O2D-CGD-CBD	4.92	116.35	110.95
34	BB	616	BCR	C30-C25-C26	-4.92	115.92	122.64
35	Dd	404	PL9	C20-C19-C18	-4.92	111.00	123.63
32	S	604	CLA	C4A-NA-C1A	4.91	108.92	106.68
41	r	615	XAT	O4-C5-C18	4.91	120.54	115.05
35	D	407	PL9	C21-C19-C18	-4.91	110.14	121.17
35	AA	410	PL9	C40-C39-C38	-4.91	111.02	123.63
39	s	605	CHL	C1B-CHB-C4A	4.91	124.48	121.32
41	RR	316	XAT	O24-C25-C24	4.91	118.09	113.49
32	y	315	CLA	C4A-NA-C1A	4.90	108.92	106.68
34	h	101	BCR	C31-C1-C6	-4.90	102.56	110.24
35	Dd	404	PL9	C25-C24-C23	-4.89	111.06	123.63
34	Dd	403	BCR	C3-C4-C5	-4.89	105.33	114.06
32	Bb	610	CLA	C4A-NA-C1A	4.89	108.91	106.68
40	G	616	LUT	C1-C6-C5	-4.89	115.95	122.64
35	AA	410	PL9	C20-C19-C18	-4.89	111.07	123.63
32	B	607	CLA	C4A-NA-C1A	4.89	108.91	106.68
35	Dd	404	PL9	C31-C29-C28	-4.88	110.20	121.17
41	R	616	XAT	C18-C5-C6	-4.88	114.27	122.30
35	DD	406	PL9	C21-C19-C18	-4.87	110.22	121.17
32	y	306	CLA	C4A-NA-C1A	4.87	108.90	106.68
32	B	611	CLA	C4A-NA-C1A	4.87	108.90	106.68
40	G	615	LUT	C1-C6-C5	-4.87	115.99	122.64
39	r	605	CHL	O2D-CGD-CBD	4.86	116.29	110.95
35	A	410	PL9	C40-C39-C38	-4.86	111.14	123.63
35	d	404	PL9	C25-C24-C23	-4.86	111.15	123.63
35	d	404	PL9	C16-C14-C13	-4.86	110.26	121.17
32	B	608	CLA	C4A-NA-C1A	4.86	108.89	106.68
36	44	614	LHG	O7-C7-C8	4.86	119.75	111.09
34	h	101	BCR	C1-C6-C7	4.85	128.80	115.65
32	DD	404	CLA	C4A-NA-C1A	4.85	108.89	106.68
32	G	611	CLA	C4A-NA-C1A	4.84	108.89	106.68
32	44	603	CLA	C4A-NA-C1A	4.84	108.89	106.68
34	Cc	518	BCR	C3-C4-C5	-4.84	105.43	114.06
34	Cc	517	BCR	C30-C25-C26	-4.84	116.03	122.64
39	R	606	CHL	C1B-CHB-C4A	4.83	124.43	121.32
32	BB	612	CLA	C4A-NA-C1A	4.83	108.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Hh	102	DGD	O2G-C1B-C2B	4.83	121.93	111.48
34	B	614	BCR	C1-C6-C5	-4.83	116.04	122.64
32	2	604	CLA	C4A-NA-C1A	4.83	108.88	106.68
41	r	615	XAT	O24-C25-C38	4.82	120.44	115.05
34	H	101	BCR	C34-C9-C8	4.82	125.45	118.09
32	Yy	613	CLA	C4A-NA-C1A	4.82	108.88	106.68
32	C	511	CLA	C4A-NA-C1A	4.82	108.88	106.68
34	Kk	101	BCR	C4-C5-C6	-4.81	116.20	122.70
34	Bb	619	BCR	C28-C27-C26	-4.81	105.48	114.06
35	AA	410	PL9	C30-C29-C28	-4.81	111.27	123.63
32	CC	505	CLA	C4A-NA-C1A	4.81	108.87	106.68
32	CC	510	CLA	C4A-NA-C1A	4.81	108.87	106.68
32	S	603	CLA	C4A-NA-C1A	4.81	108.87	106.68
35	AA	410	PL9	C25-C24-C23	-4.81	111.29	123.63
39	g	605	CHL	C1B-CHB-C4A	4.80	124.41	121.32
32	22	612	CLA	C4A-NA-C1A	4.80	108.87	106.68
32	Bb	613	CLA	C4A-NA-C1A	4.80	108.87	106.68
39	N	605	CHL	C1B-CHB-C4A	4.80	124.41	121.32
32	X	201	CLA	C4A-NA-C1A	4.80	108.87	106.68
32	d	401	CLA	C4A-NA-C1A	4.80	108.87	106.68
32	C	510	CLA	C4A-NA-C1A	4.79	108.86	106.68
32	Nn	313	CLA	C4A-NA-C1A	4.79	108.86	106.68
32	C	506	CLA	C4A-NA-C1A	4.78	108.86	106.68
34	b	617	BCR	C30-C25-C26	-4.78	116.10	122.64
32	Cc	504	CLA	C4A-NA-C1A	4.78	108.86	106.68
32	b	613	CLA	C4A-NA-C1A	4.78	108.86	106.68
35	Dd	404	PL9	C30-C29-C28	-4.77	111.37	123.63
39	Yy	609	CHL	CMB-C2B-C3B	4.77	134.22	124.68
39	Gg	306	CHL	C1B-CHB-C4A	4.77	124.39	121.32
41	RR	316	XAT	O4-C5-C4	4.76	117.95	113.49
35	d	404	PL9	C30-C29-C28	-4.76	111.40	123.63
35	d	404	PL9	C36-C34-C33	-4.76	110.48	121.17
41	R	616	XAT	O4-C5-C4	4.76	117.95	113.49
32	Bb	611	CLA	C4A-NA-C1A	4.76	108.85	106.68
32	g	602	CLA	O2D-CGD-CBD	4.75	119.54	111.23
32	44	615	CLA	C4A-NA-C1A	4.75	108.85	106.68
32	Cc	511	CLA	C4A-NA-C1A	4.75	108.85	106.68
33	AA	407	PHO	C2B-C1B-NB	-4.75	106.00	109.43
32	BB	611	CLA	C4A-NA-C1A	4.75	108.85	106.68
41	R	616	XAT	O24-C25-C38	4.75	120.36	115.05
40	n	616	LUT	C1-C6-C5	-4.75	116.15	122.64
40	Y	615	LUT	C1-C6-C5	-4.74	116.15	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	g	604	CLA	C4A-NA-C1A	4.74	108.84	106.68
41	N	617	XAT	C40-C33-C32	4.73	125.32	118.09
39	33	601	CHL	C1B-CHB-C4A	4.73	124.37	121.32
35	d	404	PL9	C31-C29-C28	-4.73	110.55	121.17
32	Dd	401	CLA	C4A-NA-C1A	4.73	108.83	106.68
32	33	609	CLA	C3A-C2A-C1A	-4.73	101.47	106.30
42	Yy	617	NEX	O24-C25-C38	4.72	120.33	115.05
41	N	617	XAT	O4-C5-C18	4.71	120.31	115.05
34	Hh	101	BCR	C1-C6-C7	4.70	128.40	115.65
32	c	501	CLA	C4A-NA-C1A	4.70	108.82	106.68
41	NN	617	XAT	O4-C5-C18	4.70	120.30	115.05
39	22	606	CHL	C1B-CHB-C4A	4.69	124.34	121.32
32	D	405	CLA	C4A-NA-C1A	4.69	108.82	106.68
32	Y	604	CLA	C4A-NA-C1A	4.68	108.81	106.68
41	RR	316	XAT	O4-C5-C18	4.67	120.27	115.05
32	S	612	CLA	C4A-NA-C1A	4.67	108.81	106.68
32	BB	610	CLA	C4A-NA-C1A	4.67	108.81	106.68
33	A	407	PHO	C2B-C1B-NB	-4.66	106.06	109.43
32	SS	305	CLA	C4A-NA-C1A	4.66	108.80	106.68
32	22	604	CLA	C4A-NA-C1A	4.65	108.80	106.68
32	XX	201	CLA	C4A-NA-C1A	4.65	108.80	106.68
39	Rr	606	CHL	C1B-CHB-C4A	4.65	124.31	121.32
34	BB	618	BCR	C1-C6-C5	-4.64	116.29	122.64
32	C	514	CLA	C4A-NA-C1A	4.64	108.80	106.68
32	c	513	CLA	C4A-NA-C1A	4.64	108.80	106.68
32	s	602	CLA	C4A-NA-C1A	4.64	108.80	106.68
32	a	407	CLA	C4A-NA-C1A	4.63	108.79	106.68
32	SS	312	CLA	C4A-NA-C1A	4.63	108.79	106.68
35	Dd	404	PL9	C21-C19-C18	-4.63	110.77	121.17
32	1	611	CLA	C3A-C2A-C1A	-4.63	101.57	106.30
34	BB	617	BCR	C36-C18-C19	4.63	125.16	118.09
35	d	404	PL9	C21-C19-C18	-4.63	110.78	121.17
34	B	614	BCR	C33-C5-C6	-4.62	119.44	124.48
40	Yy	616	LUT	C1-C6-C5	-4.62	116.33	122.64
35	AA	410	PL9	C36-C34-C33	-4.62	110.80	121.17
32	GG	612	CLA	C4A-NA-C1A	4.62	108.78	106.68
40	22	614	LUT	C1-C6-C5	-4.62	116.33	122.64
34	Kk	101	BCR	C34-C9-C8	4.61	125.13	118.09
32	b	610	CLA	C4A-NA-C1A	4.61	108.78	106.68
32	CC	513	CLA	C4A-NA-C1A	4.61	108.78	106.68
39	Yy	609	CHL	C1B-CHB-C4A	4.61	124.29	121.32
32	Gg	305	CLA	C4A-NA-C1A	4.61	108.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	511	CLA	C4A-NA-C1A	4.60	108.78	106.68
35	DD	406	PL9	C31-C29-C28	-4.60	110.84	121.17
40	Y	615	LUT	C18-C5-C6	-4.60	119.47	124.48
32	Cc	513	CLA	C4A-NA-C1A	4.60	108.78	106.68
42	Yy	617	NEX	O24-C25-C24	4.60	117.80	113.49
41	G	619	XAT	C20-C13-C12	4.59	125.11	118.09
42	Gg	318	NEX	C16-C1-C6	4.59	114.58	110.47
32	SS	304	CLA	C4A-NA-C1A	4.59	108.77	106.68
41	Nn	308	XAT	C40-C33-C32	4.59	125.10	118.09
32	BB	603	CLA	C4A-NA-C1A	4.59	108.77	106.68
34	B	613	BCR	C36-C18-C19	4.58	125.09	118.09
39	1	605	CHL	C1B-CHB-C4A	4.58	124.27	121.32
32	2	612	CLA	C4A-NA-C1A	4.58	108.77	106.68
32	BB	615	CLA	C4A-NA-C1A	4.58	108.77	106.68
35	A	410	PL9	C41-C39-C38	-4.58	110.89	121.17
42	y	319	NEX	O24-C25-C24	4.58	117.78	113.49
32	22	610	CLA	C4A-NA-C1A	4.57	108.77	106.68
35	D	407	PL9	C41-C39-C38	-4.57	110.90	121.17
32	Y	603	CLA	C4A-NA-C1A	4.57	108.77	106.68
32	GG	604	CLA	C4A-NA-C1A	4.57	108.77	106.68
32	3	609	CLA	C3A-C2A-C1A	-4.57	101.62	106.30
39	g	609	CHL	C1B-CHB-C4A	4.57	124.26	121.32
34	H	101	BCR	C3-C4-C5	-4.57	105.91	114.06
32	Yy	604	CLA	C4A-NA-C1A	4.56	108.76	106.68
32	r	613	CLA	C4A-NA-C1A	4.56	108.76	106.68
35	AA	410	PL9	C47-C48-C49	-4.56	112.44	127.64
42	Yy	617	NEX	C38-C25-C26	-4.56	114.80	122.30
39	4	308	CHL	C1B-CHB-C4A	4.56	124.25	121.32
32	11	604	CLA	C4A-NA-C1A	4.55	108.76	106.68
35	AA	410	PL9	C41-C39-C38	-4.55	110.96	121.17
35	A	410	PL9	C26-C24-C23	-4.55	110.96	121.17
32	n	603	CLA	C4A-NA-C1A	4.54	108.75	106.68
36	AA	411	LHG	O7-C7-C8	4.54	121.31	111.48
35	A	410	PL9	C47-C48-C49	-4.54	112.50	127.64
32	Bb	616	CLA	C4A-NA-C1A	4.54	108.75	106.68
34	BB	618	BCR	C33-C5-C6	-4.54	119.53	124.48
39	33	608	CHL	C1B-CHB-C4A	4.53	124.24	121.32
32	c	506	CLA	C4A-NA-C1A	4.53	108.75	106.68
34	TT	101	BCR	C36-C18-C19	4.52	125.00	118.09
36	A	411	LHG	O7-C7-C8	4.52	121.26	111.48
39	GG	609	CHL	C1B-CHB-C4A	4.52	124.23	121.32
42	NN	618	NEX	C40-C33-C32	4.52	124.99	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Ss	608	CLA	C4A-NA-C1A	4.51	108.74	106.68
32	1	604	CLA	C4A-NA-C1A	4.51	108.73	106.68
32	Bb	615	CLA	C4A-NA-C1A	4.51	108.73	106.68
35	D	407	PL9	C26-C24-C23	-4.50	111.06	121.17
41	R	616	XAT	O4-C5-C18	4.50	120.08	115.05
34	CC	517	BCR	C1-C6-C5	-4.50	116.49	122.64
32	b	616	CLA	C4A-NA-C1A	4.50	108.73	106.68
35	A	410	PL9	C21-C19-C18	-4.49	111.08	121.17
32	s	604	CLA	C4A-NA-C1A	4.49	108.73	106.68
32	Cc	508	CLA	C4A-NA-C1A	4.49	108.73	106.68
41	R	616	XAT	C38-C25-C26	-4.49	114.92	122.30
32	SS	313	CLA	C4A-NA-C1A	4.48	108.72	106.68
42	Gg	318	NEX	C20-C13-C12	4.48	124.94	118.09
35	D	407	PL9	C31-C29-C28	-4.48	111.11	121.17
40	GG	616	LUT	C1-C6-C5	-4.48	116.51	122.64
35	A	410	PL9	C36-C34-C33	-4.48	111.11	121.17
41	RR	316	XAT	C38-C25-C26	-4.47	114.94	122.30
35	DD	406	PL9	C47-C48-C49	-4.47	112.73	127.64
34	DD	405	BCR	C1-C6-C5	-4.47	116.53	122.64
32	3	610	CLA	C4A-NA-C1A	4.47	108.72	106.68
39	NN	605	CHL	C1B-CHB-C4A	4.47	124.20	121.32
32	CC	511	CLA	C4A-NA-C1A	4.46	108.72	106.68
40	g	616	LUT	C1-C6-C5	-4.46	116.55	122.64
32	BB	605	CLA	C4A-NA-C1A	4.46	108.71	106.68
42	y	319	NEX	C38-C25-C26	-4.46	114.97	122.30
41	y	302	XAT	C40-C33-C32	4.46	124.89	118.09
41	NN	617	XAT	C18-C5-C6	-4.46	114.97	122.30
40	YY	615	LUT	C18-C5-C6	-4.45	119.63	124.48
35	D	407	PL9	C47-C48-C49	-4.45	112.80	127.64
32	Cc	505	CLA	C4A-NA-C1A	4.45	108.71	106.68
34	T	101	BCR	C36-C18-C19	4.45	124.88	118.09
32	Rr	613	CLA	C4A-NA-C1A	4.45	108.71	106.68
35	DD	406	PL9	C36-C34-C33	-4.44	111.20	121.17
34	BB	618	BCR	C28-C27-C26	-4.44	106.14	114.06
32	4	312	CLA	C4A-NA-C1A	4.44	108.70	106.68
32	c	509	CLA	C4A-NA-C1A	4.44	108.70	106.68
41	y	301	XAT	O4-C5-C18	4.44	120.01	115.05
42	N	618	NEX	C40-C33-C32	4.44	124.87	118.09
41	y	302	XAT	O4-C5-C18	4.44	120.00	115.05
41	N	617	XAT	C18-C5-C6	-4.43	115.00	122.30
32	b	605	CLA	C4A-NA-C1A	4.43	108.70	106.68
34	D	406	BCR	C1-C6-C5	-4.43	116.58	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	YY	616	LUT	C1-C6-C5	-4.43	116.59	122.64
44	BB	623	DGD	O2G-C1B-C2B	4.43	121.06	111.48
41	y	302	XAT	C18-C5-C6	-4.43	115.02	122.30
32	Nn	314	CLA	C4A-NA-C1A	4.42	108.69	106.68
35	Dd	404	PL9	C47-C48-C49	-4.42	112.91	127.64
35	Dd	404	PL9	C26-C24-C23	-4.42	111.25	121.17
34	T	101	BCR	C1-C6-C5	-4.41	116.60	122.64
42	R	617	NEX	O24-C25-C38	4.41	119.98	115.05
35	d	404	PL9	C26-C24-C23	-4.41	111.26	121.17
32	B	606	CLA	C4A-NA-C1A	4.41	108.69	106.68
32	BB	614	CLA	C4A-NA-C1A	4.41	108.69	106.68
34	B	612	BCR	C30-C25-C26	-4.41	116.61	122.64
41	GG	619	XAT	C20-C13-C12	4.41	124.82	118.09
32	3	602	CLA	C4A-NA-C1A	4.40	108.69	106.68
32	Bb	605	CLA	C4A-NA-C1A	4.40	108.69	106.68
35	DD	406	PL9	C41-C39-C38	-4.40	111.30	121.17
34	Cc	518	BCR	C28-C27-C26	-4.39	106.22	114.06
42	RR	317	NEX	C38-C25-C26	-4.39	115.08	122.30
32	b	611	CLA	C4A-NA-C1A	4.39	108.68	106.68
32	44	604	CLA	C4A-NA-C1A	4.39	108.68	106.68
32	C	513	CLA	C4A-NA-C1A	4.39	108.68	106.68
32	Aa	405	CLA	C4A-NA-C1A	4.39	108.68	106.68
32	S	609	CLA	C4A-NA-C1A	4.38	108.68	106.68
35	d	404	PL9	C47-C48-C49	-4.38	113.03	127.64
32	R	611	CLA	C4A-NA-C1A	4.38	108.68	106.68
36	Nn	310	LHG	O7-C7-C8	4.38	120.95	111.48
32	A	406	CLA	C4A-NA-C1A	4.38	108.67	106.68
42	RR	317	NEX	O24-C25-C38	4.37	119.94	115.05
34	Bb	619	BCR	C36-C18-C19	4.36	124.75	118.09
32	4	305	CLA	C4A-NA-C1A	4.36	108.67	106.68
32	B	622	CLA	C4A-NA-C1A	4.36	108.67	106.68
34	c	516	BCR	C28-C27-C26	-4.35	106.29	114.06
35	d	404	PL9	C41-C39-C38	-4.35	111.39	121.17
32	Cc	506	CLA	C4A-NA-C1A	4.35	108.66	106.68
32	Nn	303	CLA	C4A-NA-C1A	4.35	108.66	106.68
35	DD	406	PL9	C26-C24-C23	-4.35	111.41	121.17
34	H	101	BCR	C8-C7-C6	-4.35	115.39	127.00
35	Dd	404	PL9	C41-C39-C38	-4.34	111.42	121.17
39	n	605	CHL	O2D-CGD-CBD	4.34	115.72	110.95
33	DD	402	PHO	C2B-C1B-NB	-4.34	106.29	109.43
42	g	617	NEX	C39-C29-C28	4.34	124.72	118.09
40	N	616	LUT	C1-C6-C5	-4.34	116.70	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	NN	616	LUT	C1-C6-C5	-4.34	116.70	122.64
32	N	613	CLA	C4A-NA-C1A	4.34	108.66	106.68
41	G	617	XAT	C26-C27-C28	-4.34	116.82	125.99
34	C	518	BCR	C1-C6-C5	-4.33	116.71	122.64
42	n	617	NEX	C40-C33-C32	4.33	124.70	118.09
40	YY	615	LUT	C1-C6-C5	-4.33	116.72	122.64
32	44	611	CLA	C4A-NA-C1A	4.32	108.65	106.68
32	3	612	CLA	C4A-NA-C1A	4.32	108.65	106.68
41	G	617	XAT	C38-C25-C26	-4.32	115.19	122.30
32	a	405	CLA	C4A-NA-C1A	4.32	108.65	106.68
34	Hh	101	BCR	C31-C1-C6	-4.32	103.47	110.24
42	Nn	309	NEX	C38-C25-C26	-4.32	115.20	122.30
40	2	614	LUT	C3-C4-C5	-4.32	101.43	112.18
32	s	612	CLA	C4A-NA-C1A	4.32	108.65	106.68
42	Gg	318	NEX	C27-C28-C29	4.31	132.22	125.53
35	A	410	PL9	C31-C29-C28	-4.31	111.49	121.17
32	Rr	603	CLA	C4A-NA-C1A	4.31	108.64	106.68
41	Rr	615	XAT	C38-C25-C26	-4.31	115.21	122.30
39	NN	609	CHL	C1B-CHB-C4A	4.31	124.09	121.32
40	g	615	LUT	C1-C6-C5	-4.31	116.75	122.64
42	Yy	617	NEX	C26-C27-C28	-4.31	116.89	125.99
32	Rr	612	CLA	C4A-NA-C1A	4.30	108.64	106.68
34	B	614	BCR	C28-C27-C26	-4.30	106.38	114.06
38	Cc	501	LMG	O7-C10-C11	4.30	120.79	111.48
42	R	617	NEX	C38-C25-C26	-4.30	115.22	122.30
32	Ss	612	CLA	C4A-NA-C1A	4.30	108.64	106.68
42	Y	619	NEX	C20-C13-C12	4.30	124.65	118.09
32	R	612	CLA	C4A-NA-C1A	4.29	108.64	106.68
32	G	613	CLA	C3A-C2A-C1A	-4.29	101.91	106.30
32	Gg	314	CLA	C4A-NA-C1A	4.29	108.64	106.68
34	BB	620	BCR	C33-C5-C6	-4.29	119.80	124.48
32	Bb	614	CLA	C4A-NA-C1A	4.29	108.63	106.68
36	Yy	618	LHG	O7-C7-C8	4.29	120.75	111.48
32	33	610	CLA	C4A-NA-C1A	4.28	108.63	106.68
32	NN	603	CLA	C4A-NA-C1A	4.28	108.63	106.68
38	c	519	LMG	O7-C10-C11	4.28	120.75	111.48
39	NN	605	CHL	O2D-CGD-CBD	4.28	115.65	110.95
40	GG	615	LUT	C1-C6-C5	-4.28	116.79	122.64
44	c	517	DGD	O2G-C1B-C2B	4.28	120.73	111.48
41	4	314	XAT	C40-C33-C32	4.27	124.62	118.09
40	2	614	LUT	C1-C6-C5	-4.27	116.80	122.64
32	RR	312	CLA	C4A-NA-C1A	4.27	108.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	409	BCR	C30-C25-C26	-4.27	116.80	122.64
34	b	619	BCR	C36-C18-C19	4.27	124.61	118.09
41	GG	617	XAT	C26-C27-C28	-4.27	116.97	125.99
32	SS	309	CLA	C4A-NA-C1A	4.27	108.62	106.68
42	Rr	616	NEX	C20-C13-C12	4.26	124.60	118.09
35	AA	410	PL9	C31-C29-C28	-4.26	111.61	121.17
32	2	609	CLA	C4A-NA-C1A	4.25	108.62	106.68
34	Cc	517	BCR	C33-C5-C6	-4.25	119.85	124.48
40	Gg	317	LUT	C3-C4-C5	-4.25	101.60	112.18
32	D	401	CLA	C4A-NA-C1A	4.25	108.62	106.68
41	Nn	308	XAT	O4-C5-C18	4.25	119.80	115.05
41	GG	617	XAT	C38-C25-C26	-4.25	115.31	122.30
35	AA	410	PL9	C26-C24-C23	-4.25	111.64	121.17
32	B	610	CLA	C4A-NA-C1A	4.25	108.62	106.68
32	11	612	CLA	C3A-C2A-C1A	-4.24	101.96	106.30
33	D	402	PHO	C2B-C1B-NB	-4.24	106.36	109.43
32	b	607	CLA	C4A-NA-C1A	4.24	108.61	106.68
32	AA	405	CLA	C4A-NA-C1A	4.24	108.61	106.68
32	SS	303	CLA	C4A-NA-C1A	4.24	108.61	106.68
41	4	314	XAT	C18-C5-C6	-4.23	115.33	122.30
32	RR	302	CLA	C4A-NA-C1A	4.23	108.61	106.68
41	Yy	619	XAT	C18-C5-C6	-4.23	115.33	122.30
32	Ss	613	CLA	C4A-NA-C1A	4.23	108.61	106.68
32	1	602	CLA	C4A-NA-C1A	4.23	108.61	106.68
32	y	305	CLA	C4A-NA-C1A	4.23	108.61	106.68
32	Ss	604	CLA	C4A-NA-C1A	4.22	108.61	106.68
32	Cc	512	CLA	C4A-NA-C1A	4.22	108.61	106.68
36	g	618	LHG	O7-C7-C8	4.22	120.61	111.48
35	AA	410	PL9	C21-C19-C18	-4.22	111.69	121.17
32	b	614	CLA	C4A-NA-C1A	4.22	108.60	106.68
41	Nn	308	XAT	C18-C5-C6	-4.22	115.36	122.30
33	Aa	408	PHO	C2B-C1B-NB	-4.21	106.38	109.43
32	A	405	CLA	C4A-NA-C1A	4.21	108.60	106.68
34	c	515	BCR	C38-C26-C25	-4.21	119.89	124.48
32	s	608	CLA	C4A-NA-C1A	4.21	108.60	106.68
32	22	602	CLA	C4A-NA-C1A	4.20	108.60	106.68
32	Bb	607	CLA	C4A-NA-C1A	4.20	108.59	106.68
39	1	608	CHL	CMB-C2B-C3B	4.20	133.07	124.68
34	C	516	BCR	C1-C6-C5	-4.20	116.90	122.64
44	CC	522	DGD	O2G-C1B-C2B	4.20	120.56	111.48
36	Gg	319	LHG	O7-C7-C8	4.19	120.56	111.48
32	CC	514	CLA	C4A-NA-C1A	4.19	108.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	Nn	309	NEX	O24-C25-C38	4.19	119.73	115.05
32	A	408	CLA	C4A-NA-C1A	4.19	108.59	106.68
32	1	612	CLA	C4A-NA-C1A	4.18	108.59	106.68
42	g	617	NEX	C20-C13-C12	4.18	124.47	118.09
32	n	614	CLA	C4A-NA-C1A	4.18	108.59	106.68
34	D	406	BCR	C1-C6-C7	4.18	126.98	115.65
33	a	408	PHO	C2B-C1B-NB	-4.18	106.41	109.43
42	n	617	NEX	C26-C27-C28	-4.18	117.16	125.99
32	AA	406	CLA	C4A-NA-C1A	4.18	108.58	106.68
32	RR	313	CLA	C4A-NA-C1A	4.18	108.58	106.68
42	y	319	NEX	C26-C27-C28	-4.17	117.18	125.99
34	DD	405	BCR	C1-C6-C7	4.16	126.94	115.65
41	4	314	XAT	C38-C25-C26	-4.16	115.45	122.30
32	NN	613	CLA	C4A-NA-C1A	4.16	108.58	106.68
34	CC	517	BCR	C1-C6-C7	4.16	126.93	115.65
41	Yy	619	XAT	C40-C33-C32	4.16	124.44	118.09
41	y	301	XAT	C18-C5-C6	-4.16	115.46	122.30
32	n	604	CLA	C4A-NA-C1A	4.15	108.57	106.68
42	NN	618	NEX	C38-C25-C26	-4.15	115.47	122.30
36	n	618	LHG	O7-C7-C8	4.14	120.45	111.48
42	n	617	NEX	C38-C25-C26	-4.14	115.48	122.30
32	Dd	402	CLA	C4A-NA-C1A	4.14	108.57	106.68
34	Bb	618	BCR	C36-C18-C19	4.14	124.42	118.09
32	NN	612	CLA	C4A-NA-C1A	4.14	108.57	106.68
41	N	617	XAT	C38-C25-C26	-4.14	115.49	122.30
32	YY	602	CLA	C4A-NA-C1A	4.14	108.57	106.68
42	Nn	309	NEX	C26-C27-C28	-4.14	117.25	125.99
34	TT	101	BCR	C1-C6-C5	-4.13	116.99	122.64
34	C	518	BCR	C1-C6-C7	4.13	126.84	115.65
32	Yy	602	CLA	C4A-NA-C1A	4.13	108.56	106.68
32	11	613	CLA	C4A-NA-C1A	4.13	108.56	106.68
32	D	404	CLA	C4A-NA-C1A	4.12	108.56	106.68
41	G	617	XAT	C18-C5-C6	-4.12	115.52	122.30
32	4	311	CLA	C4A-NA-C1A	4.12	108.56	106.68
32	Rr	611	CLA	C4A-NA-C1A	4.12	108.56	106.68
32	G	604	CLA	C4A-NA-C1A	4.12	108.56	106.68
40	y	318	LUT	C1-C6-C5	-4.11	117.01	122.64
32	s	613	CLA	C4A-NA-C1A	4.11	108.56	106.68
32	AA	408	CLA	C4A-NA-C1A	4.11	108.56	106.68
34	Cc	516	BCR	C36-C18-C19	4.11	124.37	118.09
40	Y	615	LUT	C36-C21-C26	4.11	115.77	109.55
32	RR	311	CLA	C4A-NA-C1A	4.11	108.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	YY	617	NEX	C38-C25-C26	-4.10	115.55	122.30
39	11	605	CHL	C1B-CHB-C4A	4.10	123.96	121.32
32	c	503	CLA	C4A-NA-C1A	4.10	108.55	106.68
40	s	615	LUT	C3-C4-C5	-4.10	101.96	112.18
34	AA	409	BCR	C30-C25-C26	-4.10	117.03	122.64
39	Gg	310	CHL	C1B-CHB-C4A	4.10	123.96	121.32
40	RR	315	LUT	C1-C6-C5	-4.10	117.03	122.64
32	CC	512	CLA	C4A-NA-C1A	4.10	108.55	106.68
40	y	317	LUT	C4-C5-C6	-4.10	112.34	120.76
32	33	602	CLA	C4A-NA-C1A	4.09	108.55	106.68
32	2	611	CLA	C4A-NA-C1A	4.09	108.55	106.68
34	c	515	BCR	C33-C5-C6	-4.09	120.02	124.48
32	44	602	CLA	C4A-NA-C1A	4.09	108.55	106.68
32	c	502	CLA	C4A-NA-C1A	4.09	108.55	106.68
32	DD	401	CLA	C4A-NA-C1A	4.09	108.55	106.68
32	NN	604	CLA	C4A-NA-C1A	4.09	108.54	106.68
32	RR	310	CLA	C4A-NA-C1A	4.09	108.54	106.68
36	Ll	102	LHG	O7-C7-C8	4.08	120.32	111.48
32	B	620	CLA	C4A-NA-C1A	4.08	108.54	106.68
41	y	301	XAT	C39-C29-C28	4.08	124.33	118.09
34	D	406	BCR	C30-C25-C26	-4.08	117.06	122.64
32	Gg	314	CLA	C3A-C2A-C1A	-4.08	102.13	106.30
36	D	408	LHG	O7-C7-C8	4.08	120.30	111.48
32	11	602	CLA	C4A-NA-C1A	4.08	108.54	106.68
32	N	602	CLA	C4A-NA-C1A	4.08	108.54	106.68
32	c	504	CLA	C4A-NA-C1A	4.08	108.54	106.68
34	B	616	BCR	C33-C5-C6	-4.07	120.04	124.48
44	Cc	519	DGD	O2G-C1B-C2B	4.07	120.29	111.48
42	N	618	NEX	C38-C25-C26	-4.07	115.60	122.30
42	Y	617	NEX	C38-C25-C26	-4.07	115.60	122.30
34	c	515	BCR	C1-C6-C5	-4.07	117.07	122.64
41	GG	617	XAT	C18-C5-C6	-4.07	115.60	122.30
32	33	612	CLA	C4A-NA-C1A	4.07	108.54	106.68
40	S	614	LUT	C18-C5-C6	-4.07	120.04	124.48
32	C	515	CLA	C4A-NA-C1A	4.07	108.53	106.68
32	G	613	CLA	C4A-NA-C1A	4.07	108.53	106.68
34	BB	620	BCR	C1-C6-C5	-4.06	117.08	122.64
36	y	320	LHG	O7-C7-C8	4.06	120.27	111.48
34	BB	616	BCR	C27-C26-C25	-4.06	117.22	122.70
32	1	613	CLA	C4A-NA-C1A	4.06	108.53	106.68
36	DD	407	LHG	O7-C7-C8	4.06	120.26	111.48
32	N	604	CLA	C4A-NA-C1A	4.06	108.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Hh	101	BCR	C3-C4-C5	-4.06	106.83	114.06
34	B	616	BCR	C1-C6-C5	-4.05	117.10	122.64
40	NN	616	LUT	C3-C4-C5	-4.05	102.10	112.18
32	2	610	CLA	C4A-NA-C1A	4.05	108.53	106.68
32	N	603	CLA	C4A-NA-C1A	4.04	108.52	106.68
34	a	411	BCR	C1-C6-C5	-4.04	117.11	122.64
38	W	201	LMG	O7-C10-C11	4.04	120.22	111.48
36	44	614	LHG	C5-O7-C7	-4.04	110.71	117.85
32	y	304	CLA	C4A-NA-C1A	4.04	108.52	106.68
42	Y	619	NEX	C38-C25-C26	-4.04	115.66	122.30
36	GG	618	LHG	O7-C7-C8	4.04	120.21	111.48
41	NN	617	XAT	C38-C25-C26	-4.03	115.66	122.30
42	Nn	309	NEX	C20-C13-C12	4.03	124.25	118.09
32	22	611	CLA	C4A-NA-C1A	4.03	108.52	106.68
41	44	613	XAT	C6-C7-C8	-4.03	117.47	125.99
44	D	411	DGD	O2G-C1B-C2B	4.03	120.19	111.48
32	BB	607	CLA	C4A-NA-C1A	4.02	108.52	106.68
41	r	615	XAT	C38-C25-C26	-4.02	115.68	122.30
39	RR	306	CHL	C1B-CHB-C4A	4.02	123.91	121.32
37	CC	501	SQD	O47-C7-C8	4.02	120.18	111.48
42	Rr	616	NEX	C38-C25-C26	-4.02	115.68	122.30
39	N	609	CHL	C1B-CHB-C4A	4.02	123.91	121.32
40	Ss	615	LUT	C16-C1-C6	4.02	116.55	110.24
34	b	618	BCR	C36-C18-C19	4.02	124.22	118.09
34	DD	405	BCR	C30-C25-C26	-4.02	117.15	122.64
34	XX	202	BCR	C36-C18-C19	4.02	124.22	118.09
41	Rr	615	XAT	C20-C13-C12	4.01	124.22	118.09
36	KK	101	LHG	O7-C7-C8	4.01	120.17	111.48
34	Hh	101	BCR	C2-C1-C6	4.01	116.27	110.44
41	R	616	XAT	C6-C7-C8	-4.01	117.51	125.99
32	Bb	608	CLA	C4A-NA-C1A	4.01	108.51	106.68
32	Cc	514	CLA	C4A-NA-C1A	4.01	108.51	106.68
36	11	614	LHG	O7-C7-C8	4.00	120.14	111.48
32	G	610	CLA	C1D-ND-C4D	-4.00	103.50	106.31
32	B	604	CLA	C4A-NA-C1A	4.00	108.50	106.68
38	AA	415	LMG	O7-C10-C11	4.00	120.13	111.48
36	N	619	LHG	O7-C7-C8	4.00	120.13	111.48
38	Dd	408	LMG	O7-C10-C11	4.00	120.12	111.48
42	n	617	NEX	C20-C13-C12	3.99	124.19	118.09
34	T	101	BCR	C33-C5-C6	-3.99	120.13	124.48
35	Dd	404	PL9	C51-C49-C48	-3.99	110.68	122.66
36	NN	619	LHG	O7-C7-C8	3.99	120.11	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	AA	410	PL9	C7-C3-C4	3.98	120.19	116.91
37	BB	621	SQD	O47-C7-C8	3.98	120.09	111.48
34	CC	515	BCR	C1-C6-C5	-3.98	117.20	122.64
42	YY	617	NEX	C20-C13-C12	3.98	124.17	118.09
34	B	612	BCR	C36-C18-C19	3.98	124.16	118.09
32	S	602	CLA	C4A-NA-C1A	3.97	108.49	106.68
32	b	606	CLA	C4A-NA-C1A	3.97	108.49	106.68
32	g	602	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
38	A	415	LMG	O7-C10-C11	3.97	120.07	111.48
34	Cc	517	BCR	C1-C6-C5	-3.97	117.21	122.64
44	BB	625	DGD	O2G-C1B-C2B	3.97	120.06	111.48
32	b	615	CLA	C4A-NA-C1A	3.96	108.49	106.68
35	d	404	PL9	C51-C49-C48	-3.96	110.77	122.66
38	WW	201	LMG	O7-C10-C11	3.96	120.05	111.48
41	44	613	XAT	C18-C5-C6	-3.96	115.79	122.30
34	BB	616	BCR	C1-C6-C5	-3.96	117.23	122.64
34	B	613	BCR	C1-C6-C5	-3.96	117.23	122.64
32	R	613	CLA	C4A-NA-C1A	3.95	108.48	106.68
39	11	608	CHL	C1B-CHB-C4A	3.95	123.87	121.32
42	Y	617	NEX	C20-C13-C12	3.95	124.13	118.09
38	C	521	LMG	O7-C10-C11	3.95	120.03	111.48
42	Nn	309	NEX	C40-C33-C32	3.95	124.12	118.09
35	D	407	PL9	C51-C49-C48	-3.95	110.80	122.66
34	T	101	BCR	C15-C16-C17	-3.95	115.44	123.52
32	B	623	CLA	C4A-NA-C1A	3.95	108.48	106.68
38	j	101	LMG	O7-C10-C11	3.94	120.01	111.48
34	TT	101	BCR	C15-C16-C17	-3.94	115.45	123.52
34	A	409	BCR	C29-C30-C25	3.94	116.16	110.44
36	33	614	LHG	O7-C7-C8	3.94	120.00	111.48
32	33	604	CLA	C4A-NA-C1A	3.93	108.47	106.68
34	h	101	BCR	C8-C9-C10	3.93	125.19	119.01
32	YY	613	CLA	C4A-NA-C1A	3.93	108.47	106.68
44	B	603	DGD	O2G-C1B-C2B	3.93	119.98	111.48
40	s	615	LUT	C1-C6-C5	-3.93	117.27	122.64
36	D	410	LHG	O7-C7-C8	3.92	119.97	111.48
32	44	609	CLA	C4A-NA-C1A	3.92	108.47	106.68
35	DD	406	PL9	C51-C49-C48	-3.92	110.90	122.66
34	c	514	BCR	C30-C25-C26	-3.92	117.28	122.64
32	Cc	515	CLA	C4A-NA-C1A	3.91	108.46	106.68
36	G	618	LHG	O7-C7-C8	3.91	119.94	111.48
37	B	617	SQD	O47-C7-C8	3.91	119.94	111.48
40	22	614	LUT	C20-C13-C14	-3.91	116.48	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	22	614	LUT	C12-C13-C14	3.91	125.16	119.01
34	CC	515	BCR	C8-C9-C10	3.91	125.15	119.01
32	Y	613	CLA	C4A-NA-C1A	3.91	108.46	106.68
32	CC	504	CLA	C4A-NA-C1A	3.91	108.46	106.68
35	DD	406	PL9	C50-C49-C48	-3.90	110.95	122.66
39	N	609	CHL	O2D-CGD-CBD	3.90	115.23	110.95
32	2	610	CLA	C3A-C2A-C1A	-3.90	102.31	106.30
32	33	603	CLA	C4A-NA-C1A	3.90	108.46	106.68
34	BB	616	BCR	C36-C18-C19	3.90	124.04	118.09
32	Aa	410	CLA	C4A-NA-C1A	3.90	108.46	106.68
41	R	616	XAT	C39-C29-C28	3.89	124.04	118.09
36	Rr	617	LHG	O7-C7-C8	3.89	119.91	111.48
40	Y	615	LUT	C1-C6-C7	3.89	126.21	115.65
35	D	407	PL9	C50-C49-C48	-3.89	110.97	122.66
32	R	614	CLA	C4A-NA-C1A	3.89	108.45	106.68
32	RR	314	CLA	C4A-NA-C1A	3.89	108.45	106.68
37	LL	102	SQD	O47-C7-C8	3.89	119.89	111.48
40	YY	615	LUT	C1-C6-C7	3.89	126.19	115.65
39	3	601	CHL	C1B-CHB-C4A	3.89	123.82	121.32
33	Aa	409	PHO	C2B-C1B-NB	-3.89	106.62	109.43
32	BB	606	CLA	C4A-NA-C1A	3.88	108.45	106.68
39	r	606	CHL	C1B-CHB-C4A	3.88	123.82	121.32
32	C	505	CLA	C4A-NA-C1A	3.88	108.45	106.68
32	c	508	CLA	C4A-NA-C1A	3.88	108.45	106.68
42	N	618	NEX	C16-C1-C6	3.88	113.94	110.47
41	4	314	XAT	C39-C29-C28	3.87	124.00	118.09
32	22	609	CLA	C4A-NA-C1A	3.87	108.44	106.68
34	KK	103	BCR	C34-C9-C8	3.87	124.00	118.09
42	n	617	NEX	O24-C25-C38	3.87	119.37	115.05
36	D	409	LHG	O7-C7-C8	3.87	119.85	111.48
42	g	617	NEX	C16-C1-C6	3.87	113.93	110.47
44	CC	519	DGD	O2G-C1B-C2B	3.87	119.85	111.48
39	NN	609	CHL	O2D-CGD-CBD	3.87	115.20	110.95
32	s	611	CLA	C4A-NA-C1A	3.86	108.44	106.68
32	Gg	313	CLA	C4A-NA-C1A	3.86	108.44	106.68
37	l	102	SQD	O47-C7-C8	3.86	119.83	111.48
39	Yy	607	CHL	O2D-CGD-O1D	-3.86	116.34	123.85
33	a	409	PHO	C2B-C1B-NB	-3.85	106.64	109.43
36	K	101	LHG	O7-C7-C8	3.85	119.82	111.48
32	r	608	CLA	C4A-NA-C1A	3.85	108.44	106.68
36	r	616	LHG	O7-C7-C8	3.85	119.81	111.48
41	G	619	XAT	C18-C5-C6	-3.85	115.97	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	K	102	BCR	C37-C22-C23	3.85	123.97	118.09
32	r	611	CLA	C4A-NA-C1A	3.85	108.44	106.68
34	C	516	BCR	C8-C9-C10	3.85	125.06	119.01
32	22	603	CLA	C4A-NA-C1A	3.84	108.43	106.68
44	BB	624	DGD	O2G-C1B-C2B	3.84	119.80	111.48
32	Nn	305	CLA	C4A-NA-C1A	3.84	108.43	106.68
34	Cc	516	BCR	C30-C25-C26	-3.84	117.39	122.64
37	L	101	SQD	O47-C7-C8	3.84	119.78	111.48
39	n	605	CHL	C1B-CHB-C4A	3.84	123.79	121.32
34	AA	409	BCR	C23-C22-C21	3.84	125.04	119.01
38	Bb	621	LMG	O7-C10-C11	3.83	119.78	111.48
35	Dd	404	PL9	C50-C49-C48	-3.83	111.15	122.66
41	NN	617	XAT	C40-C33-C32	3.83	123.94	118.09
34	BB	618	BCR	C30-C25-C26	-3.83	117.40	122.64
34	AA	409	BCR	C29-C30-C25	3.83	116.00	110.44
35	d	404	PL9	C50-C49-C48	-3.83	111.16	122.66
38	b	621	LMG	O7-C10-C11	3.83	119.77	111.48
34	A	409	BCR	C23-C22-C21	3.83	125.03	119.01
34	BB	618	BCR	C36-C18-C19	3.83	123.93	118.09
36	DD	408	LHG	O7-C7-C8	3.83	119.76	111.48
34	b	617	BCR	C1-C6-C5	-3.83	117.41	122.64
34	BB	617	BCR	C1-C6-C5	-3.83	117.41	122.64
34	h	101	BCR	C2-C1-C6	3.83	116.00	110.44
34	Hh	101	BCR	C8-C9-C10	3.83	125.03	119.01
32	a	410	CLA	C4A-NA-C1A	3.82	108.42	106.68
34	C	516	BCR	C1-C6-C7	3.82	126.01	115.65
42	Yy	617	NEX	C20-C13-C12	3.82	123.92	118.09
41	y	302	XAT	C20-C13-C12	3.82	123.92	118.09
44	B	601	DGD	O2G-C1B-C2B	3.82	119.74	111.48
32	B	621	CLA	C4A-NA-C1A	3.81	108.42	106.68
34	B	614	BCR	C36-C18-C19	3.81	123.90	118.09
32	Ss	609	CLA	C4A-NA-C1A	3.81	108.42	106.68
35	AA	410	PL9	C51-C49-C48	-3.81	111.24	122.66
36	1	614	LHG	O7-C7-C8	3.80	119.71	111.48
34	Cc	516	BCR	C30-C25-C24	3.80	125.96	115.65
32	R	610	CLA	C4A-NA-C1A	3.80	108.41	106.68
39	4	306	CHL	CMB-C2B-C3B	3.80	132.27	124.68
41	GG	619	XAT	C18-C5-C6	-3.80	116.05	122.30
32	NN	614	CLA	C4A-NA-C1A	3.80	108.41	106.68
32	d	402	CLA	C4A-NA-C1A	3.79	108.41	106.68
32	Rr	601	CLA	C4A-NA-C1A	3.79	108.41	106.68
32	Rr	609	CLA	C4A-NA-C1A	3.79	108.41	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	410	PL9	C50-C49-C48	-3.79	111.29	122.66
32	Y	602	CLA	C4A-NA-C1A	3.78	108.40	106.68
36	JJ	101	LHG	O7-C7-C8	3.78	119.66	111.48
34	C	516	BCR	C33-C5-C6	-3.78	120.36	124.48
39	22	606	CHL	CMB-C2B-C3B	3.78	132.23	124.68
32	3	613	CLA	C3A-C2A-C1A	-3.78	102.44	106.30
36	3	614	LHG	O7-C7-C8	3.77	119.64	111.48
41	RR	316	XAT	C6-C7-C8	-3.77	118.02	125.99
37	Ll	101	SQD	O47-C7-C8	3.77	119.64	111.48
34	Bb	617	BCR	C1-C6-C5	-3.77	117.49	122.64
41	GG	617	XAT	O4-C5-C18	3.77	119.26	115.05
32	3	604	CLA	C4A-NA-C1A	3.77	108.40	106.68
42	g	617	NEX	C26-C27-C28	3.77	133.96	125.99
34	C	518	BCR	C36-C18-C19	3.77	123.84	118.09
34	c	514	BCR	C30-C25-C24	3.77	125.86	115.65
32	s	603	CLA	C4A-NA-C1A	3.77	108.40	106.68
32	33	613	CLA	C4A-NA-C1A	3.76	108.40	106.68
34	d	403	BCR	C38-C26-C25	-3.76	120.38	124.48
32	2	603	CLA	C4A-NA-C1A	3.76	108.39	106.68
32	Bb	606	CLA	C4A-NA-C1A	3.76	108.39	106.68
39	SS	306	CHL	C1C-CHC-C4B	3.76	129.53	116.07
44	C	520	DGD	O2G-C1B-C2B	3.76	119.61	111.48
39	Rr	605	CHL	C1C-CHC-C4B	3.76	129.52	116.07
32	c	512	CLA	C4A-NA-C1A	3.76	108.39	106.68
34	k	101	BCR	C3-C4-C5	-3.76	107.35	114.06
40	2	614	LUT	C20-C13-C14	-3.76	116.73	122.82
34	TT	101	BCR	C33-C5-C6	-3.75	120.39	124.48
44	C	519	DGD	O2G-C1B-C2B	3.75	119.60	111.48
40	N	616	LUT	C36-C21-C26	3.75	115.23	109.55
32	Ss	611	CLA	C4A-NA-C1A	3.75	108.39	106.68
40	Gg	317	LUT	C1-C6-C5	-3.75	117.51	122.64
34	Bb	618	BCR	C1-C6-C5	-3.75	117.52	122.64
34	Cc	516	BCR	C8-C9-C10	3.75	124.90	119.01
32	C	503	CLA	C4A-NA-C1A	3.75	108.39	106.68
38	Aa	412	LMG	O7-C10-C11	3.75	119.58	111.48
35	A	410	PL9	C51-C49-C48	-3.75	111.42	122.66
35	AA	410	PL9	C50-C49-C48	-3.74	111.42	122.66
34	b	618	BCR	C30-C25-C26	-3.74	117.52	122.64
34	Bb	617	BCR	C33-C5-C6	-3.74	120.40	124.48
35	A	410	PL9	C15-C14-C16	-3.74	108.73	115.23
41	44	613	XAT	C38-C25-C26	-3.74	116.14	122.30
32	2	613	CLA	C3A-C2A-C1A	-3.74	102.47	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	g	619	XAT	C18-C5-C6	-3.74	116.15	122.30
41	G	617	XAT	O4-C5-C18	3.73	119.22	115.05
34	KK	103	BCR	C27-C26-C25	-3.73	117.66	122.70
35	Dd	404	PL9	C15-C14-C16	-3.73	108.75	115.23
34	b	618	BCR	C37-C22-C23	3.73	123.78	118.09
42	YY	617	NEX	O24-C25-C38	3.73	119.21	115.05
32	g	613	CLA	C4A-NA-C1A	3.72	108.38	106.68
32	Rr	608	CLA	C4A-NA-C1A	3.72	108.38	106.68
42	NN	618	NEX	C20-C13-C12	3.72	123.77	118.09
32	SS	314	CLA	C4A-NA-C1A	3.72	108.38	106.68
34	c	514	BCR	C36-C18-C19	3.72	123.77	118.09
34	Aa	411	BCR	C1-C6-C5	-3.72	117.56	122.64
32	4	303	CLA	C4A-NA-C1A	3.72	108.37	106.68
34	Bb	618	BCR	C37-C22-C23	3.71	123.76	118.09
39	YY	607	CHL	O2D-CGD-CBD	3.71	115.03	110.95
39	r	605	CHL	C1C-CHC-C4B	3.71	129.35	116.07
32	NN	602	CLA	C4A-NA-C1A	3.71	108.37	106.68
34	Cc	517	BCR	C36-C18-C19	3.71	123.75	118.09
36	Dd	406	LHG	O7-C7-C8	3.71	119.50	111.48
42	Rr	616	NEX	O24-C25-C38	3.70	119.19	115.05
40	YY	615	LUT	C3-C4-C5	-3.70	102.96	112.18
34	Kk	101	BCR	C30-C25-C26	-3.70	117.58	122.64
34	c	515	BCR	C30-C25-C26	-3.70	117.59	122.64
32	S	613	CLA	C4A-NA-C1A	3.70	108.36	106.68
32	CC	506	CLA	C4A-NA-C1A	3.70	108.36	106.68
32	g	613	CLA	C3A-C2A-C1A	-3.69	102.52	106.30
36	C	522	LHG	O7-C7-C8	3.69	119.47	111.48
34	Dd	403	BCR	C36-C18-C19	3.69	123.73	118.09
32	11	611	CLA	C4A-NA-C1A	3.69	108.36	106.68
34	Dd	403	BCR	C38-C26-C25	-3.69	120.46	124.48
34	h	101	BCR	C3-C4-C5	-3.69	107.48	114.06
39	r	606	CHL	C1C-CHC-C4B	3.68	129.25	116.07
40	Yy	615	LUT	C4-C5-C6	-3.68	113.19	120.76
32	3	603	CLA	C4A-NA-C1A	3.68	108.36	106.68
39	s	606	CHL	C1C-CHC-C4B	3.68	129.24	116.07
39	Ss	606	CHL	C1C-CHC-C4B	3.68	129.24	116.07
34	d	403	BCR	C36-C18-C19	3.68	123.71	118.09
42	Y	619	NEX	O24-C25-C38	3.68	119.16	115.05
32	3	611	CLA	C3A-C2A-C1A	-3.68	102.54	106.30
36	l	101	LHG	O7-C7-C8	3.68	119.44	111.48
32	r	609	CLA	C4A-NA-C1A	3.67	108.35	106.68
42	Y	617	NEX	C39-C29-C30	-3.67	116.88	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	33	608	CHL	CMB-C2B-C3B	3.67	132.01	124.68
40	g	616	LUT	C3-C4-C5	-3.66	103.06	112.18
32	BB	608	CLA	C4A-NA-C1A	3.66	108.35	106.68
36	d	406	LHG	O7-C7-C8	3.66	119.40	111.48
34	B	614	BCR	C37-C22-C23	3.66	123.68	118.09
35	DD	406	PL9	C10-C9-C11	-3.66	108.88	115.23
39	y	311	CHL	O2D-CGD-CBD	3.66	114.97	110.95
41	GG	619	XAT	C35-C15-C14	-3.66	116.04	123.52
39	R	605	CHL	C1C-CHC-C4B	3.66	129.15	116.07
32	Ss	603	CLA	C4A-NA-C1A	3.66	108.35	106.68
39	11	608	CHL	C1C-CHC-C4B	3.66	129.15	116.07
39	RR	305	CHL	C1C-CHC-C4B	3.66	129.15	116.07
39	Gg	310	CHL	C1C-CHC-C4B	3.65	129.15	116.07
34	c	514	BCR	C37-C22-C23	3.65	123.67	118.09
32	YY	612	CLA	C4A-NA-C1A	3.65	108.35	106.68
39	Ss	605	CHL	C1C-CHC-C4B	3.65	129.14	116.07
36	CC	523	LHG	O7-C7-C8	3.65	119.38	111.48
34	Bb	618	BCR	C30-C25-C26	-3.65	117.65	122.64
39	3	601	CHL	C1C-CHC-C4B	3.65	129.13	116.07
41	G	619	XAT	C35-C15-C14	-3.65	116.05	123.52
34	CC	515	BCR	C3-C4-C5	-3.65	107.55	114.06
39	R	607	CHL	C1C-CHC-C4B	3.65	129.12	116.07
34	KK	103	BCR	C1-C6-C5	-3.65	117.66	122.64
42	YY	617	NEX	C39-C29-C30	-3.64	116.91	122.82
34	CC	515	BCR	C1-C6-C7	3.64	125.53	115.65
34	c	515	BCR	C36-C18-C19	3.64	123.65	118.09
32	Nn	304	CLA	C4A-NA-C1A	3.64	108.34	106.68
39	RR	307	CHL	C1C-CHC-C4B	3.64	129.08	116.07
44	CC	518	DGD	O2G-C1B-C2B	3.63	119.34	111.48
39	44	605	CHL	C1C-CHC-C4B	3.63	129.07	116.07
37	C	501	SQD	O47-C7-C8	3.63	119.34	111.48
41	Gg	301	XAT	C18-C5-C6	-3.63	116.32	122.30
40	Gg	316	LUT	C3-C4-C5	-3.63	103.15	112.18
40	2	614	LUT	C12-C13-C14	3.63	124.71	119.01
41	r	615	XAT	C20-C13-C12	3.63	123.63	118.09
39	4	309	CHL	C1C-CHC-C4B	3.62	129.04	116.07
41	Yy	619	XAT	C39-C29-C28	3.62	123.62	118.09
34	Cc	516	BCR	C37-C22-C23	3.62	123.62	118.09
39	44	608	CHL	C1C-CHC-C4B	3.62	129.02	116.07
41	y	301	XAT	C40-C33-C32	3.62	123.61	118.09
32	22	613	CLA	C4A-NA-C1A	3.62	108.33	106.68
39	r	607	CHL	C1C-CHC-C4B	3.61	129.00	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	c	518	DGD	O2G-C1B-C2B	3.61	119.30	111.48
36	A	413	LHG	O7-C7-C8	3.61	119.29	111.48
35	A	410	PL9	C7-C3-C4	3.61	119.88	116.91
34	k	101	BCR	C37-C22-C23	3.61	123.60	118.09
34	H	101	BCR	C38-C26-C25	-3.61	120.54	124.48
34	CC	517	BCR	C36-C18-C19	3.61	123.60	118.09
34	XX	202	BCR	C4-C5-C6	-3.61	117.83	122.70
32	DD	403	CLA	C4A-NA-C1A	3.61	108.33	106.68
39	NN	605	CHL	C1C-CHC-C4B	3.61	128.97	116.07
39	g	609	CHL	C1C-CHC-C4B	3.61	128.97	116.07
34	KK	103	BCR	C37-C22-C23	3.60	123.59	118.09
42	RR	317	NEX	C39-C29-C30	-3.60	116.98	122.82
32	BB	602	CLA	C4A-NA-C1A	3.60	108.32	106.68
42	y	319	NEX	C40-C33-C32	3.60	123.59	118.09
39	s	605	CHL	C1C-CHC-C4B	3.60	128.95	116.07
32	1	604	CLA	C3A-C2A-C1A	-3.60	102.62	106.30
34	B	616	BCR	C29-C30-C25	3.60	115.67	110.44
42	NN	618	NEX	C39-C29-C30	-3.60	116.99	122.82
34	Cc	517	BCR	C38-C26-C25	-3.60	120.56	124.48
32	GG	614	CLA	C4A-NA-C1A	3.59	108.32	106.68
39	n	609	CHL	O2D-CGD-CBD	3.59	114.89	110.95
32	YY	614	CLA	C4A-NA-C1A	3.59	108.32	106.68
40	Ss	614	LUT	C1-C6-C5	-3.59	117.73	122.64
39	s	606	CHL	C1B-CHB-C4A	3.59	123.63	121.32
39	Nn	311	CHL	CHA-C1A-C2A	-3.59	124.89	133.31
39	N	605	CHL	C1C-CHC-C4B	3.59	128.90	116.07
39	YY	606	CHL	CHA-C1A-C2A	-3.58	124.89	133.31
37	LL	101	SQD	O47-C7-C8	3.58	119.23	111.48
34	b	617	BCR	C33-C5-C6	-3.58	120.58	124.48
41	4	314	XAT	C6-C7-C8	-3.58	118.42	125.99
34	H	101	BCR	C30-C25-C26	-3.58	117.75	122.64
42	NN	618	NEX	O24-C25-C38	3.57	119.04	115.05
34	c	516	BCR	C33-C5-C6	-3.57	120.58	124.48
34	H	101	BCR	C1-C6-C5	-3.57	117.75	122.64
32	33	613	CLA	C3A-C2A-C1A	-3.57	102.65	106.30
34	BB	618	BCR	C37-C22-C23	3.57	123.55	118.09
34	C	517	BCR	C36-C18-C19	3.57	123.54	118.09
39	33	608	CHL	C1C-CHC-C4B	3.57	128.85	116.07
32	GG	613	CLA	C3A-C2A-C1A	-3.57	102.65	106.30
36	CC	521	LHG	O7-C7-C8	3.57	119.20	111.48
34	b	618	BCR	C1-C6-C5	-3.57	117.76	122.64
32	Cc	507	CLA	C4A-NA-C1A	3.57	108.31	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	GG	609	CHL	C1C-CHC-C4B	3.57	128.84	116.07
39	GG	609	CHL	CMB-C2B-C3B	3.57	131.81	124.68
39	44	608	CHL	C1B-CHB-C4A	3.56	123.62	121.32
35	DD	406	PL9	C45-C44-C46	-3.56	109.04	115.23
32	44	610	CLA	C4A-NA-C1A	3.56	108.30	106.68
32	B	624	CLA	C4A-NA-C1A	3.56	108.30	106.68
38	CC	520	LMG	O7-C10-C11	3.56	119.19	111.48
39	Nn	315	CHL	C1C-CHC-C4B	3.56	128.81	116.07
41	y	302	XAT	C38-C25-C26	-3.56	116.44	122.30
41	G	617	XAT	O24-C25-C38	3.56	119.03	115.05
39	S	605	CHL	C1C-CHC-C4B	3.56	128.80	116.07
39	Y	607	CHL	O2D-CGD-CBD	3.56	114.86	110.95
39	33	601	CHL	C1C-CHC-C4B	3.56	128.80	116.07
39	1	608	CHL	C1C-CHC-C4B	3.56	128.79	116.07
32	r	601	CLA	C4A-NA-C1A	3.56	108.30	106.68
36	II	101	LHG	O7-C7-C8	3.56	119.17	111.48
34	CC	516	BCR	C36-C18-C19	3.55	123.52	118.09
39	Rr	607	CHL	C1C-CHC-C4B	3.55	128.78	116.07
39	44	605	CHL	CMB-C2B-C3B	3.55	131.78	124.68
39	33	607	CHL	C1C-CHC-C4B	3.55	128.76	116.07
39	Y	606	CHL	CHA-C1A-C2A	-3.55	124.98	133.31
39	y	309	CHL	C1C-CHC-C4B	3.55	128.76	116.07
39	RR	305	CHL	C1B-CHB-C4A	3.55	123.60	121.32
41	g	619	XAT	C35-C15-C14	-3.54	116.27	123.52
42	g	617	NEX	C35-C15-C14	-3.54	116.27	123.52
36	Y	618	LHG	O7-C7-C8	3.54	119.15	111.48
32	n	613	CLA	C4A-NA-C1A	3.54	108.30	106.68
40	YY	615	LUT	C36-C21-C26	3.54	114.91	109.55
39	Yy	609	CHL	O2D-CGD-CBD	3.54	114.84	110.95
38	Mm	101	LMG	O7-C10-C11	3.54	119.14	111.48
32	Cc	510	CLA	C4A-NA-C1A	3.54	108.29	106.68
42	Y	617	NEX	O24-C25-C38	3.54	119.00	115.05
32	1	609	CLA	C1D-ND-C4D	-3.54	103.83	106.31
44	h	102	DGD	O2G-C1B-C2B	3.54	119.13	111.48
34	c	516	BCR	C36-C18-C19	3.53	123.49	118.09
34	BB	620	BCR	C36-C18-C19	3.53	123.49	118.09
42	y	319	NEX	C20-C13-C12	3.53	123.49	118.09
34	BB	620	BCR	C30-C25-C26	-3.53	117.81	122.64
40	N	615	LUT	C1-C6-C5	-3.53	117.81	122.64
34	B	616	BCR	C30-C25-C26	-3.53	117.81	122.64
32	Aa	410	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
40	Ss	615	LUT	C19-C9-C8	3.53	123.48	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	N	618	NEX	O24-C25-C38	3.53	118.99	115.05
37	L	102	SQD	O47-C7-C8	3.53	119.11	111.48
32	11	610	CLA	C4A-NA-C1A	3.53	108.29	106.68
34	h	101	BCR	C30-C25-C26	-3.53	117.82	122.64
39	G	609	CHL	C1C-CHC-C4B	3.53	128.69	116.07
38	Bb	620	LMG	O7-C10-C11	3.53	119.11	111.48
39	Nn	315	CHL	O2D-CGD-O1D	-3.53	116.98	123.85
38	b	620	LMG	O7-C10-C11	3.52	119.11	111.48
42	N	618	NEX	C39-C29-C30	-3.52	117.11	122.82
35	Dd	404	PL9	C45-C44-C46	-3.52	109.11	115.23
39	Gg	302	CHL	CHA-C1A-C2A	-3.52	125.04	133.31
42	Y	619	NEX	C39-C29-C30	-3.52	117.11	122.82
44	Cc	520	DGD	O2G-C1B-C2B	3.52	119.10	111.48
39	22	606	CHL	C1C-CHC-C4B	3.52	128.67	116.07
32	3	613	CLA	C4A-NA-C1A	3.52	108.28	106.68
41	Gg	301	XAT	C35-C15-C14	-3.52	116.32	123.52
39	22	605	CHL	C1C-CHC-C4B	3.52	128.65	116.07
32	11	604	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
32	N	614	CLA	C4A-NA-C1A	3.52	108.28	106.68
38	F	101	LMG	O7-C10-C11	3.52	119.09	111.48
39	2	606	CHL	C1C-CHC-C4B	3.51	128.64	116.07
32	22	603	CLA	C3A-C2A-C1A	-3.51	102.71	106.30
39	n	601	CHL	CHA-C1A-C2A	-3.51	125.06	133.31
39	4	306	CHL	C1C-CHC-C4B	3.51	128.63	116.07
34	BB	617	BCR	C37-C22-C23	3.51	123.45	118.09
32	G	612	CLA	C4A-NA-C1A	3.51	108.28	106.68
34	CC	516	BCR	C1-C6-C5	-3.51	117.84	122.64
35	D	407	PL9	C15-C14-C16	-3.51	109.14	115.23
34	c	514	BCR	C8-C9-C10	3.51	124.52	119.01
35	D	407	PL9	C45-C44-C46	-3.50	109.15	115.23
41	y	302	XAT	C19-C9-C8	3.50	123.44	118.09
39	Nn	319	CHL	C1C-CHC-C4B	3.50	128.59	116.07
41	RR	316	XAT	C39-C29-C28	3.50	123.43	118.09
39	s	601	CHL	C1C-CHC-C4B	3.50	128.58	116.07
42	N	618	NEX	C20-C13-C12	3.50	123.43	118.09
39	YY	605	CHL	CHA-C1A-C2A	-3.50	125.10	133.31
39	2	605	CHL	C1C-CHC-C4B	3.49	128.57	116.07
39	3	607	CHL	C1C-CHC-C4B	3.49	128.57	116.07
39	4	309	CHL	CMB-C2B-C3B	3.49	131.66	124.68
32	CC	508	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
39	SS	308	CHL	C1C-CHC-C4B	3.49	128.57	116.07
39	11	608	CHL	CMB-C2B-C3B	3.49	131.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	3	609	CLA	C4A-NA-C1A	3.49	108.27	106.68
39	Ss	606	CHL	C1B-CHB-C4A	3.49	123.57	121.32
39	Yy	609	CHL	C1C-CHC-C4B	3.49	128.54	116.07
39	4	307	CHL	C1C-CHC-C4B	3.48	128.54	116.07
34	C	516	BCR	C36-C18-C19	3.48	123.41	118.09
39	Gg	307	CHL	CHA-C1A-C2A	-3.48	125.12	133.31
39	1	607	CHL	C1C-CHC-C4B	3.48	128.53	116.07
32	Y	612	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
39	YY	607	CHL	C1C-CHC-C4B	3.48	128.52	116.07
40	y	317	LUT	C17-C1-C6	-3.48	104.78	110.24
38	m	101	LMG	O7-C10-C11	3.48	119.01	111.48
39	3	606	CHL	C1C-CHC-C4B	3.48	128.52	116.07
39	Y	607	CHL	C1C-CHC-C4B	3.48	128.51	116.07
39	4	308	CHL	C1C-CHC-C4B	3.48	128.51	116.07
32	N	612	CLA	C4A-NA-C1A	3.48	108.27	106.68
41	GG	617	XAT	O24-C25-C38	3.48	118.93	115.05
39	RR	305	CHL	O2D-CGD-CBD	3.48	114.77	110.95
40	s	614	LUT	C1-C6-C5	-3.47	117.89	122.64
42	NN	618	NEX	C16-C1-C6	3.47	113.58	110.47
34	B	613	BCR	C37-C22-C23	3.47	123.39	118.09
39	11	605	CHL	O2D-CGD-O1D	-3.47	117.09	123.85
39	Rr	606	CHL	C1C-CHC-C4B	3.47	128.49	116.07
39	44	606	CHL	C1C-CHC-C4B	3.47	128.48	116.07
40	44	612	LUT	C3-C4-C5	-3.47	103.54	112.18
32	11	609	CLA	C4A-NA-C1A	3.47	108.26	106.68
44	C	523	DGD	O2G-C1B-C2B	3.47	118.98	111.48
34	BB	620	BCR	C29-C30-C25	3.47	115.47	110.44
39	1	605	CHL	C1C-CHC-C4B	3.47	128.47	116.07
32	Gg	311	CLA	C4A-NA-C1A	3.47	108.26	106.68
40	R	615	LUT	C1-C6-C5	-3.47	117.90	122.64
39	S	607	CHL	C1C-CHC-C4B	3.46	128.47	116.07
32	33	611	CLA	C4A-NA-C1A	3.46	108.26	106.68
39	Gg	310	CHL	CMB-C2B-C3B	3.46	131.60	124.68
39	Nn	317	CHL	C1C-CHC-C4B	3.46	128.46	116.07
39	r	605	CHL	O2D-CGD-O1D	-3.46	117.11	123.85
32	B	618	CLA	C4A-NA-C1A	3.46	108.26	106.68
39	NN	607	CHL	O2D-CGD-CBD	3.46	114.75	110.95
39	Nn	317	CHL	C1-C2-C3	-3.46	120.53	126.20
38	a	412	LMG	O7-C10-C11	3.46	118.97	111.48
41	G	617	XAT	C28-C29-C30	3.46	124.45	119.01
42	Nn	309	NEX	C39-C29-C30	-3.46	117.21	122.82
38	DD	409	LMG	O7-C10-C11	3.46	118.96	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	4	306	CHL	C4D-CHA-CBD	-3.46	105.48	108.97
39	2	606	CHL	CMB-C2B-C3B	3.46	131.59	124.68
42	NN	618	NEX	C26-C27-C28	-3.45	118.69	125.99
39	g	601	CHL	CHA-C1A-C2A	-3.45	125.20	133.31
40	s	614	LUT	C1-C6-C7	3.45	125.02	115.65
41	Rr	615	XAT	C19-C9-C8	3.45	123.36	118.09
32	33	611	CLA	C3A-C2A-C1A	-3.45	102.77	106.30
37	Aa	413	SQD	O47-C7-C8	3.45	118.95	111.48
39	g	609	CHL	CHA-C1A-C2A	-3.45	125.20	133.31
42	Yy	617	NEX	C39-C29-C30	-3.45	117.22	122.82
35	d	404	PL9	C45-C44-C46	-3.45	109.24	115.23
39	N	607	CHL	O2D-CGD-CBD	3.45	114.74	110.95
35	Dd	404	PL9	C10-C9-C11	-3.45	109.24	115.23
34	B	612	BCR	C1-C6-C5	-3.45	117.92	122.64
32	1	612	CLA	C3A-C2A-C1A	-3.45	102.77	106.30
41	RR	316	XAT	C40-C33-C32	3.45	123.35	118.09
39	n	609	CHL	CMB-C2B-C3B	3.45	131.57	124.68
35	d	404	PL9	C15-C14-C16	-3.45	109.25	115.23
34	Cc	518	BCR	C37-C22-C23	3.45	123.35	118.09
42	RR	317	NEX	C20-C13-C12	3.44	123.35	118.09
32	R	602	CLA	C4A-NA-C1A	3.44	108.25	106.68
38	B	615	LMG	O7-C10-C11	3.44	118.92	111.48
39	n	607	CHL	C1C-CHC-C4B	3.44	128.38	116.07
36	Ss	616	LHG	O7-C7-C8	3.44	118.92	111.48
32	C	506	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
39	NN	605	CHL	CMB-C2B-C3B	3.43	131.55	124.68
32	Nn	312	CLA	C4A-NA-C1A	3.43	108.25	106.68
35	DD	406	PL9	C15-C14-C16	-3.43	109.27	115.23
32	R	609	CLA	C4A-NA-C1A	3.43	108.24	106.68
34	A	409	BCR	C1-C6-C5	-3.43	117.95	122.64
39	g	606	CHL	CHA-C1A-C2A	-3.43	125.26	133.31
34	B	613	BCR	C30-C25-C26	-3.43	117.95	122.64
39	Gg	310	CHL	CHA-C1A-C2A	-3.43	125.26	133.31
32	R	601	CLA	C4A-NA-C1A	3.43	108.24	106.68
34	Cc	518	BCR	C36-C18-C19	3.43	123.32	118.09
39	R	605	CHL	CMB-C2B-C3B	3.43	131.53	124.68
39	G	607	CHL	C1C-CHC-C4B	3.43	128.33	116.07
39	NN	607	CHL	C1C-CHC-C4B	3.43	128.33	116.07
32	Nn	312	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
36	s	616	LHG	O7-C7-C8	3.42	118.89	111.48
34	B	614	BCR	C30-C25-C26	-3.42	117.96	122.64
39	n	609	CHL	C1C-CHC-C4B	3.42	128.32	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	606	CHL	C1C-CHC-C4B	3.42	128.32	116.07
39	SS	307	CHL	C1C-CHC-C4B	3.42	128.32	116.07
32	C	509	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
41	y	301	XAT	C38-C25-C26	-3.42	116.67	122.30
39	GG	607	CHL	C1C-CHC-C4B	3.42	128.31	116.07
42	N	618	NEX	C26-C27-C28	-3.42	118.77	125.99
39	N	609	CHL	C1C-CHC-C4B	3.42	128.29	116.07
34	h	101	BCR	C36-C18-C19	3.41	123.30	118.09
39	NN	609	CHL	C1C-CHC-C4B	3.41	128.28	116.07
39	1	606	CHL	C1C-CHC-C4B	3.41	128.28	116.07
34	d	403	BCR	C37-C22-C23	3.41	123.30	118.09
44	Aa	401	DGD	O2G-C1B-C2B	3.41	118.86	111.48
34	C	516	BCR	C3-C4-C5	-3.41	107.97	114.06
42	R	617	NEX	C39-C29-C30	-3.41	117.29	122.82
40	Yy	615	LUT	C3-C4-C5	-3.41	103.69	112.18
34	Cc	518	BCR	C33-C5-C6	-3.41	120.77	124.48
39	44	608	CHL	CMB-C2B-C3B	3.41	131.49	124.68
39	N	607	CHL	C1C-CHC-C4B	3.41	128.26	116.07
40	N	616	LUT	C3-C4-C5	-3.41	103.70	112.18
42	Rr	616	NEX	C39-C29-C30	-3.40	117.30	122.82
32	Yy	614	CLA	C4A-NA-C1A	3.40	108.23	106.68
39	n	605	CHL	C1C-CHC-C4B	3.40	128.25	116.07
44	a	415	DGD	O2G-C1B-C2B	3.40	118.84	111.48
32	N	602	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
42	y	319	NEX	C39-C29-C30	-3.40	117.30	122.82
39	Y	605	CHL	C1C-CHC-C4B	3.40	128.24	116.07
39	NN	606	CHL	C1C-CHC-C4B	3.40	128.24	116.07
39	11	601	CHL	C1C-CHC-C4B	3.40	128.24	116.07
39	y	307	CHL	CHA-C1A-C2A	-3.40	125.32	133.31
39	Rr	605	CHL	CMB-C2B-C3B	3.40	131.48	124.68
34	K	102	BCR	C34-C9-C8	3.40	123.28	118.09
39	YY	609	CHL	C1C-CHC-C4B	3.40	128.24	116.07
39	1	601	CHL	C1C-CHC-C4B	3.40	128.24	116.07
39	22	608	CHL	C1C-CHC-C4B	3.40	128.24	116.07
35	AA	410	PL9	C10-C9-C11	-3.40	109.33	115.23
39	g	606	CHL	C1C-CHC-C4B	3.40	128.24	116.07
39	YY	606	CHL	C1C-CHC-C4B	3.40	128.24	116.07
40	Y	615	LUT	C3-C4-C5	-3.40	103.72	112.18
39	y	307	CHL	C1C-CHC-C4B	3.40	128.23	116.07
32	s	609	CLA	C4A-NA-C1A	3.40	108.23	106.68
34	Bb	619	BCR	C37-C22-C23	3.40	123.28	118.09
32	B	619	CLA	C4A-NA-C1A	3.40	108.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	SS	302	CHL	C1C-CHC-C4B	3.39	128.21	116.07
39	YY	605	CHL	C1C-CHC-C4B	3.39	128.20	116.07
34	B	616	BCR	C36-C18-C19	3.39	123.27	118.09
32	33	609	CLA	C4A-NA-C1A	3.39	108.23	106.68
39	r	606	CHL	CMB-C2B-C3B	3.39	131.46	124.68
36	a	414	LHG	O7-C7-C8	3.39	118.82	111.48
34	K	102	BCR	C1-C6-C5	-3.39	118.00	122.64
38	BB	619	LMG	O7-C10-C11	3.39	118.81	111.48
34	BB	620	BCR	C3-C4-C5	-3.39	108.01	114.06
34	H	101	BCR	C29-C30-C25	3.39	115.36	110.44
37	B	602	SQD	O47-C7-C8	3.39	118.81	111.48
32	2	611	CLA	C3A-C2A-C1A	-3.39	102.83	106.30
39	Y	605	CHL	CHA-C1A-C2A	-3.39	125.35	133.31
39	Nn	319	CHL	CHA-C1A-C2A	-3.39	125.36	133.31
39	Gg	307	CHL	C1C-CHC-C4B	3.39	128.19	116.07
39	Yy	605	CHL	C1C-CHC-C4B	3.38	128.18	116.07
39	S	601	CHL	C1C-CHC-C4B	3.38	128.18	116.07
32	2	603	CLA	C3A-C2A-C1A	-3.38	102.84	106.30
32	Bb	613	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
32	a	410	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
40	4	313	LUT	C3-C4-C5	-3.38	103.76	112.18
39	N	606	CHL	C1C-CHC-C4B	3.38	128.17	116.07
39	Rr	605	CHL	O2D-CGD-CBD	3.38	114.66	110.95
39	Yy	607	CHL	O2D-CGD-CBD	3.38	114.66	110.95
39	1	605	CHL	O2D-CGD-O1D	-3.38	117.27	123.85
39	y	311	CHL	C1C-CHC-C4B	3.38	128.15	116.07
39	Y	606	CHL	C1C-CHC-C4B	3.38	128.15	116.07
34	Kk	101	BCR	C37-C22-C23	3.38	123.25	118.09
39	G	609	CHL	CHA-C1A-C2A	-3.38	125.38	133.31
39	GG	606	CHL	C1C-CHC-C4B	3.38	128.15	116.07
39	n	605	CHL	O2D-CGD-O1D	-3.38	117.28	123.85
32	C	510	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
32	n	602	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
39	Nn	318	CHL	C1C-CHC-C4B	3.37	128.14	116.07
39	s	605	CHL	CMB-C2B-C3B	3.37	131.42	124.68
39	n	609	CHL	CHA-C1A-C2A	-3.37	125.39	133.31
39	Y	608	CHL	C1C-CHC-C4B	3.37	128.12	116.07
39	Ss	606	CHL	CMB-C2B-C3B	3.37	131.41	124.68
39	Nn	311	CHL	C1C-CHC-C4B	3.37	128.12	116.07
39	r	607	CHL	CMB-C2B-C3B	3.37	131.41	124.68
39	11	607	CHL	C1C-CHC-C4B	3.37	128.12	116.07
35	D	407	PL9	C10-C9-C11	-3.37	109.39	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	y	307	CHL	O2D-CGD-O1D	-3.37	117.30	123.85
39	Rr	607	CHL	CMB-C2B-C3B	3.36	131.41	124.68
39	r	607	CHL	CHA-C1A-C2A	-3.36	125.41	133.31
32	DD	403	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
34	H	101	BCR	C23-C22-C21	3.36	124.30	119.01
39	Y	609	CHL	C1C-CHC-C4B	3.36	128.10	116.07
39	Yy	605	CHL	CHA-C1A-C2A	-3.36	125.42	133.31
32	11	610	CLA	C3A-C2A-C1A	-3.36	102.86	106.30
32	1	610	CLA	C4A-NA-C1A	3.36	108.21	106.68
39	YY	608	CHL	C1C-CHC-C4B	3.36	128.08	116.07
32	NN	602	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
39	G	606	CHL	C1C-CHC-C4B	3.35	128.07	116.07
34	Kk	101	BCR	C38-C26-C25	-3.35	120.82	124.48
35	A	410	PL9	C45-C44-C46	-3.35	109.41	115.23
34	k	101	BCR	C38-C26-C25	-3.35	120.83	124.48
41	y	302	XAT	C39-C29-C28	3.35	123.21	118.09
32	CC	509	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
39	Ss	605	CHL	CMB-C2B-C3B	3.35	131.38	124.68
39	Yy	608	CHL	C1C-CHC-C4B	3.35	128.06	116.07
39	SS	302	CHL	CHA-C1A-C2A	-3.35	125.44	133.31
34	Aa	411	BCR	C36-C18-C19	3.35	123.20	118.09
39	n	608	CHL	C1C-CHC-C4B	3.35	128.05	116.07
34	Hh	101	BCR	C30-C25-C26	-3.35	118.06	122.64
39	GG	606	CHL	CHA-C1A-C2A	-3.35	125.45	133.31
34	CC	515	BCR	C36-C18-C19	3.35	123.20	118.09
39	NN	608	CHL	C1C-CHC-C4B	3.34	128.04	116.07
32	33	610	CLA	C3A-C2A-C1A	-3.34	102.88	106.30
39	Gg	309	CHL	C1C-CHC-C4B	3.34	128.04	116.07
34	b	617	BCR	C37-C22-C23	3.34	123.20	118.09
39	N	608	CHL	C1C-CHC-C4B	3.34	128.03	116.07
39	11	605	CHL	C1C-CHC-C4B	3.34	128.03	116.07
39	n	601	CHL	C1C-CHC-C4B	3.34	128.03	116.07
41	GG	617	XAT	C28-C29-C30	3.34	124.27	119.01
39	Ss	601	CHL	C1C-CHC-C4B	3.34	128.03	116.07
34	B	616	BCR	C37-C22-C23	3.34	123.19	118.09
39	S	601	CHL	CHA-C1A-C2A	-3.34	125.46	133.31
34	BB	617	BCR	C30-C25-C26	-3.34	118.07	122.64
40	4	313	LUT	C1-C6-C5	-3.34	118.07	122.64
39	NN	601	CHL	C1C-CHC-C4B	3.34	128.02	116.07
37	CC	501	SQD	O9-S-C6	3.34	111.74	106.76
32	RR	309	CLA	C4A-NA-C1A	3.34	108.20	106.68
34	H	101	BCR	C2-C1-C6	3.34	115.29	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	22	611	CLA	C3A-C2A-C1A	-3.34	102.89	106.30
39	G	606	CHL	CHA-C1A-C2A	-3.33	125.48	133.31
32	CC	505	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
39	SS	306	CHL	CMB-C2B-C3B	3.33	131.34	124.68
39	Gg	308	CHL	C1C-CHC-C4B	3.33	128.00	116.07
34	CC	515	BCR	C27-C26-C25	-3.33	118.20	122.70
39	y	310	CHL	C1C-CHC-C4B	3.33	127.99	116.07
39	G	601	CHL	CHA-C1A-C2A	-3.33	125.48	133.31
32	BB	601	CLA	C4A-NA-C1A	3.33	108.20	106.68
39	GG	607	CHL	O2D-CGD-CBD	3.33	114.61	110.95
33	D	402	PHO	C3B-C4B-NB	-3.33	105.30	107.46
40	GG	616	LUT	C3-C4-C5	-3.33	103.90	112.18
39	22	607	CHL	C1C-CHC-C4B	3.32	127.97	116.07
44	CC	522	DGD	C2G-O2G-C1B	-3.32	109.84	117.80
39	Nn	316	CHL	C1C-CHC-C4B	3.32	127.97	116.07
34	AA	409	BCR	C1-C6-C5	-3.32	118.09	122.64
36	BB	622	LHG	O7-C7-C8	3.32	118.67	111.48
39	N	601	CHL	C1C-CHC-C4B	3.32	127.96	116.07
39	GG	601	CHL	CHA-C1A-C2A	-3.32	125.50	133.31
32	b	613	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
39	2	608	CHL	C1C-CHC-C4B	3.32	127.96	116.07
34	Dd	403	BCR	C37-C22-C23	3.32	123.16	118.09
39	3	605	CHL	C1C-CHC-C4B	3.32	127.95	116.07
32	Cc	515	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
32	BB	605	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
39	G	609	CHL	CMB-C2B-C3B	3.32	131.31	124.68
39	g	607	CHL	C1C-CHC-C4B	3.32	127.94	116.07
39	S	607	CHL	CHA-C1A-C2A	-3.32	125.52	133.31
34	Bb	617	BCR	C27-C26-C25	-3.31	118.22	122.70
32	1	609	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
39	g	608	CHL	C1C-CHC-C4B	3.31	127.92	116.07
32	n	602	CLA	C4A-NA-C1A	3.31	108.19	106.68
34	C	517	BCR	C1-C6-C5	-3.31	118.11	122.64
39	2	607	CHL	C1C-CHC-C4B	3.31	127.91	116.07
37	AA	412	SQD	O47-C7-C8	3.31	118.64	111.48
39	Yy	607	CHL	C1C-CHC-C4B	3.31	127.91	116.07
35	A	410	PL9	C10-C9-C11	-3.31	109.49	115.23
39	GG	609	CHL	CHA-C1A-C2A	-3.31	125.54	133.31
40	G	616	LUT	C3-C4-C5	-3.31	103.94	112.18
39	44	607	CHL	C1C-CHC-C4B	3.31	127.90	116.07
36	YY	618	LHG	O7-C7-C8	3.31	118.63	111.48
39	Nn	315	CHL	CMB-C2B-C3B	3.30	131.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	33	606	CHL	C1C-CHC-C4B	3.30	127.88	116.07
34	B	616	BCR	C27-C26-C25	-3.30	118.25	122.70
35	d	404	PL9	C10-C9-C11	-3.30	109.50	115.23
39	Gg	302	CHL	C1C-CHC-C4B	3.30	127.86	116.07
36	d	405	LHG	O7-C7-C8	3.29	118.61	111.48
39	11	606	CHL	C1C-CHC-C4B	3.29	127.86	116.07
32	YY	604	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
40	44	612	LUT	C1-C6-C5	-3.29	118.14	122.64
41	Nn	308	XAT	C39-C29-C28	3.29	123.12	118.09
32	BB	610	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
34	BB	620	BCR	C37-C22-C23	3.29	123.11	118.09
32	G	614	CLA	C4A-NA-C1A	3.29	108.18	106.68
32	SS	310	CLA	C4A-NA-C1A	3.29	108.18	106.68
39	GG	601	CHL	C1C-CHC-C4B	3.29	127.84	116.07
35	AA	410	PL9	C45-C44-C46	-3.29	109.52	115.23
32	b	602	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
44	CC	522	DGD	O3G-C1D-C2D	3.29	113.27	108.27
33	A	407	PHO	O1D-CGD-CBD	3.29	129.71	124.72
40	N	615	LUT	C3-C4-C5	-3.29	104.00	112.18
39	4	309	CHL	O2D-CGD-CBD	3.28	114.56	110.95
42	R	617	NEX	C20-C13-C12	3.28	123.10	118.09
39	YY	607	CHL	CMB-C2B-C3B	3.28	131.24	124.68
39	Nn	319	CHL	CMB-C2B-C3B	3.28	131.24	124.68
39	11	605	CHL	O2D-CGD-CBD	3.28	114.55	110.95
39	g	601	CHL	C1C-CHC-C4B	3.28	127.81	116.07
34	a	411	BCR	C36-C18-C19	3.28	123.10	118.09
39	s	606	CHL	CMB-C2B-C3B	3.28	131.23	124.68
34	H	101	BCR	C34-C9-C10	-3.28	117.51	122.82
41	N	617	XAT	C40-C33-C34	-3.28	117.51	122.82
39	Yy	606	CHL	C1C-CHC-C4B	3.27	127.79	116.07
32	Gg	303	CLA	C1D-ND-C4D	-3.27	104.02	106.31
42	Gg	318	NEX	C35-C15-C14	-3.27	116.82	123.52
39	G	601	CHL	C1C-CHC-C4B	3.27	127.78	116.07
40	Ss	614	LUT	C1-C6-C7	3.27	124.53	115.65
39	4	307	CHL	O2D-CGD-CBD	3.27	114.54	110.95
39	g	609	CHL	CMB-C2B-C3B	3.27	131.22	124.68
39	33	605	CHL	C1C-CHC-C4B	3.27	127.77	116.07
32	Nn	301	CLA	C4A-NA-C1A	3.27	108.17	106.68
39	YY	609	CHL	O2D-CGD-CBD	3.27	114.54	110.95
40	NN	616	LUT	C36-C21-C26	3.27	114.49	109.55
39	G	605	CHL	C1C-CHC-C4B	3.27	127.76	116.07
41	y	301	XAT	C19-C9-C8	3.27	123.08	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Y	607	CHL	CMB-C2B-C3B	3.27	131.21	124.68
33	AA	407	PHO	O1D-CGD-CBD	3.27	129.68	124.72
41	NN	617	XAT	C20-C13-C12	3.27	123.08	118.09
39	n	606	CHL	C1C-CHC-C4B	3.26	127.75	116.07
39	33	607	CHL	CMB-C2B-C3B	3.26	131.21	124.68
39	s	607	CHL	C1C-CHC-C4B	3.26	127.75	116.07
32	B	622	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
39	2	601	CHL	C1C-CHC-C4B	3.26	127.74	116.07
42	n	617	NEX	C39-C29-C30	-3.26	117.53	122.82
36	Dd	407	LHG	O7-C7-C8	3.26	118.54	111.48
40	Yy	615	LUT	C1-C6-C7	3.26	124.49	115.65
41	44	613	XAT	O24-C25-C38	3.26	118.69	115.05
32	y	314	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
39	S	605	CHL	CMB-C2B-C3B	3.25	131.18	124.68
39	g	606	CHL	O2D-CGD-CBD	3.25	114.52	110.95
32	1	610	CLA	C3A-C2A-C1A	-3.25	102.97	106.30
32	B	605	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
39	11	606	CHL	O2D-CGD-CBD	3.25	114.52	110.95
32	Gg	304	CLA	C4A-NA-C1A	3.25	108.16	106.68
41	Nn	308	XAT	C38-C25-C26	-3.25	116.96	122.30
39	Nn	318	CHL	CHA-C1A-C2A	-3.25	125.68	133.31
32	BB	609	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
39	YY	609	CHL	CHA-C1A-C2A	-3.25	125.68	133.31
39	Rr	607	CHL	CHA-C1A-C2A	-3.25	125.69	133.31
41	r	615	XAT	C39-C29-C28	3.24	123.04	118.09
39	y	308	CHL	C1C-CHC-C4B	3.24	127.67	116.07
32	Gg	315	CLA	C4A-NA-C1A	3.24	108.16	106.68
34	b	619	BCR	C37-C22-C23	3.24	123.04	118.09
39	n	608	CHL	CHA-C1A-C2A	-3.24	125.70	133.31
39	Y	609	CHL	CHA-C1A-C2A	-3.24	125.70	133.31
32	Yy	612	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
39	3	608	CHL	C1C-CHC-C4B	3.24	127.65	116.07
39	22	601	CHL	C1C-CHC-C4B	3.23	127.64	116.07
32	BB	601	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
39	GG	608	CHL	C1C-CHC-C4B	3.23	127.63	116.07
34	Bb	617	BCR	C37-C22-C23	3.23	123.02	118.09
34	Kk	101	BCR	C3-C4-C5	-3.23	108.30	114.06
32	C	505	CLA	C4-C3-C5	3.23	120.83	115.23
42	YY	617	NEX	C26-C27-C28	-3.23	119.17	125.99
40	Ss	614	LUT	C35-C15-C14	-3.23	116.92	123.52
40	Yy	615	LUT	C18-C5-C4	3.23	120.35	114.42
41	g	619	XAT	C38-C25-C26	-3.22	117.00	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	408	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
40	S	614	LUT	C3-C4-C5	-3.22	104.15	112.18
41	Gg	301	XAT	C38-C25-C26	-3.22	117.00	122.30
32	Yy	612	CLA	C4A-NA-C1A	3.22	108.15	106.68
32	B	618	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
40	s	614	LUT	C35-C15-C14	-3.22	116.93	123.52
34	Bb	617	BCR	C40-C30-C25	3.22	115.29	110.24
34	Bb	617	BCR	C37-C22-C21	-3.22	117.60	122.82
39	Ss	607	CHL	C1C-CHC-C4B	3.22	127.58	116.07
39	G	608	CHL	C1C-CHC-C4B	3.22	127.58	116.07
32	y	316	CLA	C4A-NA-C1A	3.22	108.15	106.68
35	AA	410	PL9	C15-C14-C16	-3.22	109.65	115.23
39	RR	305	CHL	CMB-C2B-C3B	3.22	131.11	124.68
34	Bb	619	BCR	C40-C30-C25	-3.22	105.20	110.24
39	11	607	CHL	CMB-C2B-C3B	3.21	131.10	124.68
39	4	308	CHL	CMB-C2B-C3B	3.21	131.10	124.68
32	g	612	CLA	C4A-NA-C1A	3.21	108.14	106.68
32	3	610	CLA	C3A-C2A-C1A	-3.21	103.01	106.30
32	AA	408	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
34	BB	620	BCR	C27-C26-C25	-3.21	118.36	122.70
32	1	609	CLA	C3A-C2A-C1A	-3.21	103.02	106.30
34	k	101	BCR	C30-C25-C26	-3.21	118.25	122.64
42	Rr	616	NEX	C28-C29-C30	3.21	124.06	119.01
39	R	606	CHL	C1C-CHC-C4B	3.21	127.55	116.07
34	b	619	BCR	C1-C6-C5	-3.21	118.25	122.64
39	Y	601	CHL	C1C-CHC-C4B	3.21	127.54	116.07
32	11	602	CLA	C3A-C2A-C1A	-3.21	103.02	106.30
39	s	605	CHL	CHA-C1A-C2A	-3.21	125.78	133.31
32	D	404	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
42	Y	619	NEX	C2-C1-C6	3.20	112.33	109.21
39	GG	605	CHL	C1C-CHC-C4B	3.20	127.53	116.07
34	TT	101	BCR	C38-C26-C25	-3.20	120.99	124.48
39	GG	607	CHL	CHA-C1A-C2A	-3.20	125.79	133.31
34	Bb	619	BCR	C1-C6-C5	-3.20	118.27	122.64
39	Rr	605	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
39	44	606	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
32	B	606	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
32	Aa	407	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
39	Ss	605	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
44	c	517	DGD	O1G-C1A-C2A	3.20	121.58	111.83
32	33	613	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
39	4	302	CHL	C1C-CHC-C4B	3.19	127.50	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	605	CHL	CHA-C1A-C2A	-3.19	125.81	133.31
39	N	605	CHL	CMB-C2B-C3B	3.19	131.06	124.68
39	s	601	CHL	CMB-C2B-C3B	3.19	131.06	124.68
32	a	406	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
34	h	101	BCR	C35-C13-C12	3.19	122.95	118.09
44	Cc	519	DGD	O1G-C1A-C2A	3.18	121.54	111.83
36	Dd	405	LHG	O7-C7-C8	3.18	118.37	111.48
32	Y	614	CLA	C4A-NA-C1A	3.18	108.13	106.68
39	Y	607	CHL	CHA-C1A-C2A	-3.18	125.83	133.31
32	33	602	CLA	C3A-C2A-C1A	-3.18	103.05	106.30
39	RR	307	CHL	CHA-C1A-C2A	-3.18	125.84	133.31
39	R	605	CHL	C1B-CHB-C4A	3.18	123.37	121.32
39	YY	601	CHL	C1C-CHC-C4B	3.17	127.42	116.07
34	T	101	BCR	C33-C5-C4	3.17	120.36	113.60
39	Yy	601	CHL	C1C-CHC-C4B	3.17	127.41	116.07
32	1	603	CLA	C4A-NA-C1A	3.17	108.12	106.68
32	GG	603	CLA	C4A-NA-C1A	3.17	108.12	106.68
39	NN	605	CHL	O2D-CGD-O1D	-3.17	117.68	123.85
44	D	411	DGD	O1G-C1A-C2A	3.17	121.49	111.83
44	B	603	DGD	O1G-C1A-C2A	3.17	121.49	111.83
34	H	101	BCR	C32-C1-C6	-3.17	105.28	110.24
39	YY	607	CHL	CHA-C1A-C2A	-3.17	125.87	133.31
34	C	516	BCR	C38-C26-C25	-3.16	121.03	124.48
41	N	617	XAT	O24-C25-C38	3.16	118.58	115.05
41	g	619	XAT	O4-C5-C18	3.16	118.58	115.05
39	44	601	CHL	C1C-CHC-C4B	3.16	127.38	116.07
39	G	607	CHL	CHA-C1A-C2A	-3.16	125.88	133.31
33	D	402	PHO	O1D-CGD-CBD	3.16	129.52	124.72
39	y	303	CHL	O2D-CGD-CBD	3.16	114.42	110.95
40	G	615	LUT	C3-C4-C5	-3.16	104.31	112.18
32	33	604	CLA	C3A-C2A-C1A	-3.16	103.07	106.30
40	YY	615	LUT	C18-C5-C4	3.16	120.23	114.42
32	AA	406	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
32	YY	612	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
40	g	615	LUT	C3-C4-C5	-3.16	104.32	112.18
32	YY	610	CLA	C4A-NA-C1A	3.15	108.12	106.68
41	Gg	301	XAT	O4-C5-C18	3.15	118.57	115.05
34	k	101	BCR	C33-C5-C4	3.15	120.32	113.60
42	RR	317	NEX	C26-C27-C28	-3.15	119.33	125.99
39	RR	306	CHL	C1C-CHC-C4B	3.15	127.34	116.07
41	y	301	XAT	O24-C25-C24	3.15	116.44	113.49
32	2	604	CLA	C3A-C2A-C1A	-3.15	103.08	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	BB	607	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
32	GG	610	CLA	C4A-NA-C1A	3.15	108.12	106.68
39	y	309	CHL	CMB-C2B-C3B	3.15	130.98	124.68
41	Nn	308	XAT	C19-C9-C8	3.15	122.90	118.09
39	4	307	CHL	CHA-C1A-C2A	-3.15	125.91	133.31
39	R	607	CHL	CHA-C1A-C2A	-3.15	125.91	133.31
32	YY	612	CLA	C2A-C1A-CHA	3.15	129.33	123.87
32	CC	512	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
39	Nn	319	CHL	O2D-CGD-CBD	3.15	114.40	110.95
34	T	101	BCR	C37-C22-C23	3.15	122.89	118.09
34	BB	618	BCR	C38-C26-C25	-3.15	121.05	124.48
39	GG	605	CHL	CHA-C1A-C2A	-3.14	125.92	133.31
41	44	613	XAT	C26-C27-C28	-3.14	119.34	125.99
39	Yy	601	CHL	O2D-CGD-CBD	3.14	114.40	110.95
32	4	310	CLA	C4A-NA-C1A	3.14	108.11	106.68
32	11	609	CLA	C3A-C2A-C1A	-3.14	103.09	106.30
32	1	603	CLA	C3A-C2A-C1A	-3.14	103.09	106.30
33	Aa	409	PHO	O1D-CGD-CBD	3.14	129.49	124.72
39	1	606	CHL	O2D-CGD-CBD	3.14	114.40	110.95
39	2	605	CHL	CMB-C2B-C3B	3.14	130.96	124.68
32	BB	604	CLA	C4A-NA-C1A	3.13	108.11	106.68
34	Dd	403	BCR	C28-C27-C26	-3.13	108.47	114.06
39	11	607	CHL	C2A-C1A-CHA	3.13	127.03	121.84
36	A	414	LHG	O7-C7-C8	3.13	118.25	111.48
34	d	403	BCR	C28-C27-C26	-3.13	108.47	114.06
39	Yy	606	CHL	CHA-C1A-C2A	-3.13	125.96	133.31
32	g	603	CLA	C4A-NA-C1A	3.13	108.11	106.68
39	3	607	CHL	CMB-C2B-C3B	3.13	130.94	124.68
39	YY	605	CHL	O2D-CGD-CBD	3.13	114.39	110.95
40	Nn	307	LUT	C26-C27-C28	-3.13	119.71	124.58
41	Rr	615	XAT	C6-C7-C8	-3.13	119.38	125.99
36	Rr	617	LHG	O8-C23-C24	3.13	121.37	111.83
39	22	605	CHL	CMB-C2B-C3B	3.13	130.93	124.68
34	b	617	BCR	C15-C16-C17	-3.12	117.13	123.52
34	h	101	BCR	C38-C26-C25	-3.12	121.08	124.48
32	3	611	CLA	C4A-NA-C1A	3.12	108.10	106.68
32	C	513	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
32	11	603	CLA	C3A-C2A-C1A	-3.12	103.11	106.30
34	A	409	BCR	C36-C18-C19	3.12	122.85	118.09
40	Yy	615	LUT	C17-C1-C6	-3.12	105.35	110.24
39	Y	605	CHL	O2D-CGD-O1D	-3.12	117.78	123.85
32	CC	502	CLA	O2D-CGD-O1D	-3.12	117.78	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	g	614	CLA	C4A-NA-C1A	3.12	108.10	106.68
39	YY	608	CHL	CHA-C1A-C2A	-3.12	125.99	133.31
39	44	605	CHL	CHA-C1A-C2A	-3.12	125.99	133.31
32	3	603	CLA	C3A-C2A-C1A	-3.12	103.11	106.30
42	Gg	318	NEX	C26-C27-C28	3.11	132.58	125.99
32	4	303	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
32	Aa	406	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
44	BB	625	DGD	O1G-C1A-C2A	3.11	121.33	111.83
33	a	409	PHO	O1D-CGD-CBD	3.11	129.44	124.72
32	B	620	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
32	Bb	602	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
39	G	608	CHL	O2D-CGD-O1D	-3.11	117.79	123.85
41	g	619	XAT	C20-C13-C12	3.11	122.84	118.09
39	Ss	606	CHL	O2D-CGD-O1D	-3.11	117.80	123.85
36	EE	101	LHG	O7-C7-C8	3.11	118.20	111.48
39	YY	608	CHL	O2D-CGD-CBD	3.11	114.36	110.95
39	y	303	CHL	C1C-CHC-C4B	3.11	127.19	116.07
39	1	607	CHL	CMB-C2B-C3B	3.11	130.89	124.68
32	C	507	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
42	Rr	616	NEX	C26-C27-C28	-3.11	119.43	125.99
38	C	521	LMG	C8-O7-C10	-3.11	110.36	117.80
32	Bb	610	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
37	A	412	SQD	O47-C7-C8	3.10	118.20	111.48
32	Dd	401	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
32	R	604	CLA	O2D-CGD-CBD	3.10	116.65	111.23
32	a	407	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
32	BB	615	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
32	CC	509	CLA	O2D-CGD-CBD	3.10	116.65	111.23
36	CC	523	LHG	O8-C23-C24	3.10	121.29	111.83
39	n	605	CHL	CHA-C1A-C2A	-3.10	126.03	133.31
32	b	608	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
34	D	406	BCR	C37-C22-C23	3.10	122.82	118.09
32	1	602	CLA	C3A-C2A-C1A	-3.10	103.13	106.30
32	s	609	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
32	C	510	CLA	O2D-CGD-CBD	3.10	116.64	111.23
32	2	602	CLA	C4A-NA-C1A	3.09	108.09	106.68
34	b	617	BCR	C36-C18-C17	-3.09	117.80	122.82
40	Yy	615	LUT	C36-C21-C26	3.09	114.23	109.55
42	g	617	NEX	C17-C1-C6	-3.09	107.70	110.47
42	R	617	NEX	C26-C27-C28	-3.09	119.46	125.99
36	0	201	LHG	O7-C7-C8	3.09	118.17	111.48
32	c	502	CLA	O2D-CGD-O1D	-3.09	117.83	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	y	311	CHL	CHA-C1A-C2A	-3.09	126.06	133.31
34	Cc	516	BCR	C1-C6-C5	-3.09	118.42	122.64
32	d	401	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
41	4	314	XAT	O24-C25-C38	3.08	118.50	115.05
42	R	617	NEX	C28-C29-C30	3.08	123.86	119.01
41	4	314	XAT	C26-C27-C28	-3.08	119.47	125.99
34	k	101	BCR	C36-C18-C19	3.08	122.79	118.09
32	33	603	CLA	C3A-C2A-C1A	-3.08	103.15	106.30
34	C	516	BCR	C31-C1-C6	3.07	115.06	110.24
34	AA	409	BCR	C36-C18-C19	3.07	122.78	118.09
34	b	617	BCR	C27-C26-C25	-3.07	118.55	122.70
40	R	615	LUT	C17-C1-C6	-3.07	105.42	110.24
42	YY	617	NEX	C28-C29-C30	3.07	123.84	119.01
32	R	612	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
39	y	308	CHL	CHA-C1A-C2A	-3.07	126.09	133.31
34	Bb	617	BCR	C36-C18-C17	-3.07	117.84	122.82
42	Y	619	NEX	C26-C27-C28	-3.07	119.50	125.99
39	Y	608	CHL	O2D-CGD-CBD	3.07	114.32	110.95
34	D	406	BCR	C33-C5-C6	-3.07	121.13	124.48
32	1	609	CLA	C4A-NA-C1A	3.07	108.08	106.68
41	Rr	615	XAT	C26-C27-C28	-3.07	119.51	125.99
39	SS	308	CHL	CHA-C1A-C2A	-3.07	126.10	133.31
40	Rr	614	LUT	C3-C4-C5	-3.07	104.54	112.18
41	r	615	XAT	C19-C9-C8	3.07	122.77	118.09
34	T	101	BCR	C38-C26-C25	-3.07	121.14	124.48
34	XX	202	BCR	C32-C1-C6	3.07	115.05	110.24
32	Bb	615	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
32	11	604	CLA	O2D-CGD-CBD	3.06	116.59	111.23
39	r	605	CHL	CHA-C1A-C2A	-3.06	126.11	133.31
39	RR	307	CHL	CMB-C2B-C3B	3.06	130.81	124.68
32	3	604	CLA	C3A-C2A-C1A	-3.06	103.17	106.30
34	Kk	101	BCR	C36-C18-C19	3.06	122.77	118.09
40	Y	615	LUT	C18-C5-C4	3.06	120.05	114.42
42	Yy	617	NEX	C40-C33-C32	3.06	122.77	118.09
37	L	101	SQD	O48-C23-C24	3.06	121.17	111.83
42	Gg	318	NEX	C39-C29-C28	3.06	122.76	118.09
40	y	317	LUT	C3-C4-C5	-3.06	104.56	112.18
33	DD	402	PHO	O1D-CGD-CBD	3.06	129.36	124.72
32	Ss	611	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
32	CC	506	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
34	DD	405	BCR	C33-C5-C6	-3.06	121.15	124.48
42	Y	619	NEX	C28-C29-C30	3.06	123.82	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Cc	504	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
33	DD	402	PHO	C3B-C4B-NB	-3.06	105.47	107.46
41	GG	619	XAT	C38-C25-C26	-3.06	117.27	122.30
36	22	615	LHG	O7-C7-C8	3.06	118.09	111.48
38	a	412	LMG	O8-C28-C29	3.06	121.16	111.83
32	R	604	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
41	g	619	XAT	C6-C7-C8	-3.05	119.53	125.99
34	d	403	BCR	C38-C26-C27	3.05	120.11	113.60
32	RR	312	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
34	b	617	BCR	C37-C22-C21	-3.05	117.87	122.82
36	A	413	LHG	O8-C23-C24	3.05	121.14	111.83
32	B	611	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
39	Y	608	CHL	CHA-C1A-C2A	-3.05	126.15	133.31
32	g	610	CLA	C4A-NA-C1A	3.05	108.07	106.68
42	Y	617	NEX	C26-C27-C28	-3.05	119.55	125.99
32	3	609	CLA	C1D-ND-C4D	-3.05	104.17	106.31
33	A	407	PHO	C3B-C4B-NB	-3.04	105.48	107.46
39	GG	609	CHL	O2D-CGD-O1D	-3.04	117.92	123.85
39	s	606	CHL	O2D-CGD-O1D	-3.04	117.92	123.85
37	LL	102	SQD	O48-C23-C24	3.04	121.11	111.83
41	GG	617	XAT	C40-C33-C32	3.04	122.73	118.09
34	K	102	BCR	C33-C5-C6	-3.04	121.17	124.48
36	AA	411	LHG	C5-O7-C7	-3.04	110.52	117.80
44	B	601	DGD	C2G-O2G-C1B	-3.04	110.52	117.80
39	n	606	CHL	O2D-CGD-CBD	3.04	114.28	110.95
39	44	608	CHL	O2D-CGD-CBD	3.04	114.28	110.95
40	R	615	LUT	C26-C27-C28	-3.04	119.85	124.58
34	Dd	403	BCR	C38-C26-C27	3.04	120.07	113.60
32	S	609	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
32	Bb	612	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
42	Y	617	NEX	C28-C29-C30	3.04	123.78	119.01
44	BB	624	DGD	O1G-C1A-C2A	3.03	121.09	111.83
41	G	619	XAT	O4-C5-C18	3.03	118.44	115.05
34	Bb	617	BCR	C15-C16-C17	-3.03	117.31	123.52
41	Gg	301	XAT	C6-C7-C8	-3.03	119.58	125.99
34	h	101	BCR	C29-C30-C25	3.03	114.84	110.44
34	XX	202	BCR	C29-C30-C25	3.03	114.84	110.44
44	c	517	DGD	C2G-O2G-C1B	-3.03	110.55	117.80
39	Yy	609	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
32	CC	503	CLA	CBA-CAA-C2A	3.03	122.80	113.79
39	44	606	CHL	O2D-CGD-CBD	3.03	114.27	110.95
32	C	505	CLA	O2D-CGD-O1D	-3.03	117.95	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	516	BCR	C27-C26-C25	-3.03	118.62	122.70
39	Nn	317	CHL	CHA-C1A-C2A	-3.02	126.20	133.31
32	c	501	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
34	b	619	BCR	C29-C30-C25	3.02	114.83	110.44
32	B	624	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
32	Rr	604	CLA	C4A-NA-C1A	3.02	108.06	106.68
34	C	517	BCR	C27-C26-C25	-3.02	118.63	122.70
42	Y	619	NEX	C17-C1-C6	-3.02	107.77	110.47
34	CC	515	BCR	C38-C26-C27	3.02	120.03	113.60
32	B	607	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
32	Gg	311	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
41	G	619	XAT	C38-C25-C26	-3.01	117.34	122.30
44	B	601	DGD	O1G-C1A-C2A	3.01	121.02	111.83
40	y	317	LUT	C36-C21-C26	3.01	114.11	109.55
33	AA	407	PHO	C3B-C4B-NB	-3.01	105.50	107.46
39	1	606	CHL	O2D-CGD-O1D	-3.01	117.99	123.85
32	A	406	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
34	c	516	BCR	C37-C22-C23	3.00	122.68	118.09
32	s	611	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
32	3	613	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
32	Nn	314	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
32	r	604	CLA	C4A-NA-C1A	3.00	108.05	106.68
41	y	302	XAT	C40-C33-C34	-3.00	117.95	122.82
32	BB	602	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
40	SS	315	LUT	C1-C6-C5	-3.00	118.54	122.64
41	Gg	301	XAT	C20-C13-C12	3.00	122.67	118.09
40	g	615	LUT	C26-C27-C28	-3.00	119.91	124.58
40	r	614	LUT	C3-C4-C5	-3.00	104.71	112.18
41	r	615	XAT	C18-C5-C6	-3.00	117.37	122.30
32	BB	611	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
44	BB	623	DGD	O1G-C1A-C2A	2.99	120.97	111.83
39	R	607	CHL	CMB-C2B-C3B	2.99	130.67	124.68
44	CC	519	DGD	O1G-C1A-C2A	2.99	120.96	111.83
39	NN	607	CHL	CHA-C1A-C2A	-2.99	126.28	133.31
39	Y	601	CHL	O2D-CGD-CBD	2.99	114.23	110.95
37	B	602	SQD	O48-C23-C24	2.99	120.96	111.83
32	c	513	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
42	NN	618	NEX	C28-C29-C30	2.99	123.72	119.01
36	AA	414	LHG	O7-C7-C8	2.99	117.95	111.48
32	n	612	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
32	n	604	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
32	BB	603	CLA	O2D-CGD-O1D	-2.99	118.03	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	n	617	NEX	C15-C35-C34	-2.99	117.40	123.52
32	C	514	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
44	C	520	DGD	O1G-C1A-C2A	2.99	120.94	111.83
34	CC	517	BCR	C29-C30-C25	2.99	114.78	110.44
40	R	615	LUT	C19-C9-C8	2.99	122.65	118.09
42	g	617	NEX	C37-C21-C36	-2.98	103.03	107.37
32	b	601	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
40	Ss	615	LUT	C35-C15-C14	-2.98	117.42	123.52
32	11	611	CLA	C3A-C2A-C1A	-2.98	103.25	106.30
34	CC	515	BCR	C31-C1-C6	2.98	114.92	110.24
40	RR	315	LUT	C26-C27-C28	-2.98	119.94	124.58
38	Aa	412	LMG	O8-C28-C29	2.98	120.92	111.83
40	Rr	614	LUT	C1-C6-C5	-2.98	118.56	122.64
37	BB	621	SQD	C45-O47-C7	-2.98	110.66	117.80
32	S	608	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
32	CC	511	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
32	Bb	601	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
39	s	601	CHL	CHA-C1A-C2A	-2.98	126.32	133.31
41	r	615	XAT	C26-C27-C28	-2.97	119.70	125.99
39	R	605	CHL	O2D-CGD-CBD	2.97	114.21	110.95
34	b	618	BCR	C29-C30-C25	2.97	114.76	110.44
32	S	608	CLA	C4A-NA-C1A	2.97	108.03	106.68
36	DD	407	LHG	O8-C23-C24	2.97	120.90	111.83
39	44	605	CHL	O2D-CGD-O1D	-2.97	118.06	123.85
32	G	610	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
40	n	615	LUT	C17-C1-C6	-2.97	105.58	110.24
41	GG	617	XAT	C6-C7-C8	-2.97	119.71	125.99
32	2	610	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
32	G	603	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
32	Y	604	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
34	Bb	619	BCR	C29-C30-C25	2.97	114.75	110.44
39	y	311	CHL	O2D-CGD-O1D	-2.97	118.07	123.85
32	22	612	CLA	C3A-C2A-C1A	-2.97	103.26	106.30
32	G	603	CLA	C4A-NA-C1A	2.97	108.03	106.68
32	1	613	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
32	BB	606	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
32	11	613	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
32	Yy	604	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
32	b	610	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
39	n	607	CHL	C4D-CHA-CBD	-2.96	105.98	108.97
32	Gg	313	CLA	CHB-C4A-NA	2.96	128.68	124.40
34	K	102	BCR	C16-C15-C14	-2.96	117.45	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	614	LUT	C1-C6-C5	-2.96	118.59	122.64
40	s	615	LUT	C26-C27-C28	-2.96	119.97	124.58
32	B	619	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
32	b	602	CLA	C4A-NA-C1A	2.96	108.03	106.68
32	33	604	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
36	A	411	LHG	C5-O7-C7	-2.96	110.71	117.80
44	BB	624	DGD	C2G-O2G-C1B	-2.96	110.71	117.80
34	TT	101	BCR	C33-C5-C4	2.96	119.91	113.60
32	Cc	514	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
39	44	607	CHL	O2D-CGD-O1D	-2.96	118.09	123.85
36	d	405	LHG	O8-C23-C24	2.96	120.85	111.83
32	CC	513	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
40	G	616	LUT	C19-C9-C8	2.96	122.60	118.09
36	D	408	LHG	O8-C23-C24	2.96	120.85	111.83
40	s	615	LUT	C35-C15-C14	-2.96	117.47	123.52
39	G	607	CHL	O2D-CGD-CBD	2.96	114.19	110.95
39	11	606	CHL	O2D-CGD-O1D	-2.96	118.09	123.85
39	Gg	306	CHL	C1C-CHC-C4B	2.96	126.64	116.07
32	BB	614	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
32	Bb	615	CLA	CHB-C4A-NA	2.95	128.66	124.40
40	y	318	LUT	C36-C21-C26	2.95	114.02	109.55
39	g	605	CHL	C1C-CHC-C4B	2.95	126.64	116.07
32	33	602	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
32	C	515	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
34	C	516	BCR	C38-C26-C27	2.95	119.89	113.60
39	y	309	CHL	CHA-C1A-C2A	-2.95	126.37	133.31
42	g	617	NEX	C38-C25-C26	-2.95	117.44	122.30
32	11	604	CLA	C3A-C2A-C1A	-2.95	103.28	106.30
39	N	607	CHL	CHA-C1A-C2A	-2.95	126.38	133.31
40	G	616	LUT	C26-C27-C28	-2.95	119.99	124.58
40	n	616	LUT	C26-C27-C28	-2.95	119.99	124.58
37	AA	412	SQD	O48-C23-C24	2.95	120.10	111.15
32	C	503	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
37	C	501	SQD	O48-C23-C24	2.95	120.82	111.83
32	22	609	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
32	r	612	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
34	c	514	BCR	C1-C6-C5	-2.94	118.61	122.64
34	C	516	BCR	C37-C22-C23	2.94	122.59	118.09
32	22	613	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
36	3	614	LHG	C5-O7-C7	-2.94	110.75	117.80
39	G	606	CHL	O2D-CGD-CBD	2.94	114.18	110.95
32	c	507	CLA	O2D-CGD-O1D	-2.94	118.12	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	RR	306	CHL	O2D-CGD-CBD	2.94	114.18	110.95
32	33	611	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
34	Cc	517	BCR	C38-C26-C27	2.94	119.86	113.60
32	1	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
37	BB	621	SQD	O8-S-O7	2.94	118.75	111.40
34	C	518	BCR	C29-C30-C25	2.94	114.70	110.44
32	n	611	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
37	B	617	SQD	C45-O47-C7	-2.94	110.77	117.80
34	B	612	BCR	C27-C26-C25	-2.94	118.74	122.70
34	CC	515	BCR	C37-C22-C23	2.94	122.57	118.09
32	r	604	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
32	4	310	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
32	CC	504	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
32	Bb	606	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
32	b	606	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
34	Hh	101	BCR	C29-C30-C25	2.93	114.70	110.44
32	Bb	604	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
42	RR	317	NEX	C28-C29-C30	2.93	123.62	119.01
36	r	616	LHG	O8-C23-C24	2.93	120.78	111.83
42	Nn	309	NEX	C15-C35-C34	-2.93	117.52	123.52
34	Hh	101	BCR	C38-C26-C25	-2.93	121.28	124.48
32	b	614	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
39	4	308	CHL	O2D-CGD-CBD	2.93	114.17	110.95
32	b	615	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	Bb	614	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	Cc	503	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
34	b	619	BCR	C30-C25-C26	-2.93	118.63	122.64
32	c	512	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
32	y	312	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
32	Nn	302	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
42	Rr	616	NEX	C17-C1-C6	-2.93	107.85	110.47
46	e	101	HEM	C3B-C2B-C1B	2.92	108.61	106.41
34	B	616	BCR	C3-C4-C5	-2.92	108.84	114.06
35	D	407	PL9	C20-C19-C21	-2.92	110.15	115.23
41	Rr	615	XAT	C18-C5-C6	-2.92	117.49	122.30
32	Bb	603	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	B	609	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	3	602	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	b	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	Cc	507	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
39	N	609	CHL	O2D-CGD-O1D	-2.92	118.16	123.85
42	y	319	NEX	C28-C29-C30	2.92	123.60	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	YY	615	LUT	C26-C27-C28	-2.92	120.03	124.58
40	Nn	306	LUT	C17-C1-C6	-2.92	105.66	110.24
36	Dd	405	LHG	O8-C23-C24	2.92	120.74	111.83
32	b	611	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
39	4	308	CHL	O2D-CGD-O1D	-2.92	118.17	123.85
34	T	101	BCR	C30-C25-C26	-2.92	118.65	122.64
40	r	614	LUT	C1-C6-C5	-2.92	118.65	122.64
34	Cc	518	BCR	C1-C6-C5	-2.92	118.65	122.64
32	Nn	303	CLA	CHB-C4A-NA	2.92	128.61	124.40
41	y	301	XAT	C24-C23-C22	-2.92	105.34	110.79
32	Ss	612	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
34	DD	405	BCR	C37-C22-C23	2.91	122.54	118.09
40	GG	616	LUT	C19-C9-C8	2.91	122.54	118.09
34	B	613	BCR	C38-C26-C25	-2.91	121.31	124.48
44	Cc	519	DGD	C2G-O2G-C1B	-2.91	110.82	117.80
32	22	613	CLA	C3A-C2A-C1A	-2.91	103.32	106.30
39	44	607	CHL	O2D-CGD-CBD	2.91	114.15	110.95
36	Nn	310	LHG	O8-C23-C24	2.91	120.71	111.83
36	J	101	LHG	C5-O7-C7	-2.91	112.70	117.85
39	Y	608	CHL	O2D-CGD-O1D	-2.91	118.18	123.85
37	Aa	413	SQD	O48-C23-C24	2.91	120.71	111.83
40	Gg	316	LUT	C1-C6-C5	-2.91	118.66	122.64
32	Rr	601	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	b	615	CLA	CHB-C4A-NA	2.91	128.60	124.40
32	3	611	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	Rr	609	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
34	Bb	618	BCR	C29-C30-C25	2.91	114.66	110.44
42	N	618	NEX	C28-C29-C30	2.91	123.58	119.01
32	1	610	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
32	RR	302	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
35	DD	406	PL9	C20-C19-C21	-2.91	110.18	115.23
32	c	509	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
32	n	610	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
39	Yy	606	CHL	O2D-CGD-CBD	2.91	114.14	110.95
42	g	617	NEX	C28-C29-C30	2.91	123.58	119.01
34	c	514	BCR	C2-C1-C6	2.91	114.66	110.44
41	y	301	XAT	C36-C21-C22	-2.91	103.86	108.97
34	B	612	BCR	C15-C16-C17	-2.90	117.58	123.52
32	R	601	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
34	XX	202	BCR	C37-C22-C23	2.90	122.52	118.09
32	b	604	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	Rr	602	CLA	O2D-CGD-O1D	-2.90	118.20	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	602	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	GG	613	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	Nn	303	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	GG	610	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
34	KK	103	BCR	C40-C30-C25	2.90	114.79	110.24
39	GG	606	CHL	O2D-CGD-CBD	2.90	114.13	110.95
39	NN	601	CHL	O2D-CGD-CBD	2.90	114.13	110.95
39	Nn	317	CHL	O2D-CGD-CBD	2.90	114.13	110.95
32	11	602	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	Cc	509	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	3	602	CLA	C3A-C2A-C1A	-2.90	103.34	106.30
32	c	505	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
32	Ss	602	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
32	R	603	CLA	CHB-C4A-NA	2.90	128.58	124.40
39	Yy	609	CHL	O2D-CGD-O1D	-2.89	118.21	123.85
39	N	605	CHL	O2D-CGD-CBD	2.89	114.13	110.95
39	RR	305	CHL	O2D-CGD-O1D	-2.89	118.22	123.85
39	Gg	302	CHL	O2D-CGD-O1D	-2.89	118.22	123.85
34	B	612	BCR	C37-C22-C23	2.89	122.51	118.09
46	Ee	101	HEM	C3B-C2B-C1B	2.89	108.58	106.41
32	Yy	613	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
37	B	617	SQD	O8-S-O7	2.89	118.63	111.40
32	Rr	604	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	R	602	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
34	XX	202	BCR	C30-C25-C26	-2.89	118.69	122.64
32	C	512	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
41	Nn	308	XAT	C20-C13-C12	2.89	122.50	118.09
32	Nn	313	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
34	CC	515	BCR	C28-C27-C26	-2.89	108.90	114.06
40	2	614	LUT	C16-C1-C6	2.89	114.78	110.24
32	Bb	605	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	S	611	CLA	CHB-C4A-NA	2.89	128.57	124.40
39	N	608	CHL	O2D-CGD-O1D	-2.89	118.22	123.85
37	L	102	SQD	O48-C23-C24	2.89	120.64	111.83
40	Y	616	LUT	C18-C5-C6	-2.89	121.33	124.48
34	BB	616	BCR	C15-C16-C17	-2.89	117.61	123.52
32	Bb	616	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
33	Aa	408	PHO	O1D-CGD-CBD	2.89	129.10	124.72
40	NN	615	LUT	C3-C4-C5	-2.89	104.99	112.18
34	T	101	BCR	C29-C30-C25	2.89	114.63	110.44
32	b	605	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
32	g	614	CLA	O2D-CGD-O1D	-2.89	118.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	R	615	LUT	C16-C1-C6	2.89	114.77	110.24
40	44	612	LUT	C26-C27-C28	-2.89	120.09	124.58
32	r	604	CLA	O2A-CGA-O1A	-2.89	116.41	123.63
32	c	510	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
32	11	610	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
40	YY	616	LUT	C3-C4-C5	-2.88	105.00	112.18
32	1	613	CLA	C3A-C2A-C1A	-2.88	103.35	106.30
39	g	609	CHL	O2D-CGD-O1D	-2.88	118.24	123.85
32	c	507	CLA	CHB-C4A-NA	2.88	128.56	124.40
32	2	602	CLA	C3A-C2A-C1A	-2.88	103.35	106.30
32	BB	614	CLA	CHB-C4A-NA	2.88	128.56	124.40
39	Ss	601	CHL	CHA-C1A-C2A	-2.88	126.54	133.31
32	33	612	CLA	C3A-C2A-C1A	-2.88	103.35	106.30
39	Yy	605	CHL	O2D-CGD-O1D	-2.88	118.24	123.85
42	N	618	NEX	C15-C35-C34	-2.88	117.63	123.52
39	33	607	CHL	O2D-CGD-CBD	2.88	114.11	110.95
32	r	601	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
39	NN	601	CHL	O2D-CGD-O1D	-2.88	118.25	123.85
32	4	304	CLA	CHB-C4A-NA	2.88	128.55	124.40
32	B	623	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
32	C	507	CLA	C4A-NA-C1A	2.88	107.99	106.68
32	b	609	CLA	C3B-C4B-NB	-2.88	107.96	110.53
32	SS	312	CLA	CHB-C4A-NA	2.87	128.55	124.40
42	Y	619	NEX	C15-C35-C34	-2.87	117.64	123.52
41	Nn	308	XAT	C40-C33-C34	-2.87	118.16	122.82
39	s	607	CHL	CHA-C1A-C2A	-2.87	126.56	133.31
41	44	613	XAT	C35-C15-C14	-2.87	117.64	123.52
41	NN	617	XAT	O24-C25-C38	2.87	118.26	115.05
40	Nn	306	LUT	C26-C27-C28	-2.87	120.11	124.58
32	3	604	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
32	SS	309	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
39	GG	608	CHL	O2D-CGD-O1D	-2.87	118.26	123.85
39	N	607	CHL	O2D-CGD-O1D	-2.87	118.26	123.85
32	1	603	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
32	Rr	602	CLA	C4A-NA-C1A	2.87	107.99	106.68
42	y	319	NEX	C15-C35-C34	-2.87	117.65	123.52
36	G	618	LHG	C5-O7-C7	-2.87	110.93	117.80
32	NN	610	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
32	Bb	611	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
40	s	615	LUT	C16-C1-C6	2.87	114.74	110.24
39	Y	609	CHL	O2D-CGD-CBD	2.87	114.10	110.95
32	g	611	CLA	O2D-CGD-O1D	-2.87	118.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	TT	101	BCR	C30-C25-C26	-2.87	118.72	122.64
32	y	306	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
32	S	610	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
32	DD	404	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
39	NN	608	CHL	O2D-CGD-O1D	-2.87	118.27	123.85
33	a	408	PHO	O1D-CGD-CBD	2.87	129.07	124.72
39	n	607	CHL	CHA-C1A-C2A	-2.87	126.58	133.31
42	Gg	318	NEX	C36-C21-C26	2.86	117.78	110.05
32	RR	303	CLA	CHB-C4A-NA	2.86	128.53	124.40
34	BB	616	BCR	C38-C26-C27	2.86	119.70	113.60
34	T	101	BCR	C15-C14-C13	-2.86	123.26	127.28
34	Cc	516	BCR	C2-C1-C6	2.86	114.60	110.44
37	LL	101	SQD	O48-C23-C24	2.86	120.56	111.83
39	N	601	CHL	CHA-C1A-C2A	-2.86	126.59	133.31
39	G	606	CHL	O2D-CGD-O1D	-2.86	118.28	123.85
32	11	611	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
32	R	609	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
39	NN	609	CHL	O2D-CGD-O1D	-2.86	118.28	123.85
41	Nn	308	XAT	C6-C7-C8	-2.86	119.95	125.99
39	Ss	605	CHL	O2D-CGD-CBD	2.86	114.09	110.95
41	y	302	XAT	C6-C7-C8	-2.86	119.95	125.99
39	Gg	310	CHL	O2D-CGD-O1D	-2.86	118.28	123.85
42	Yy	617	NEX	C28-C29-C30	2.86	123.51	119.01
39	Nn	316	CHL	O2D-CGD-CBD	2.86	114.09	110.95
39	Ss	607	CHL	CHA-C1A-C2A	-2.86	126.60	133.31
39	33	601	CHL	O2D-CGD-O1D	-2.86	118.29	123.85
32	3	612	CLA	C3A-C2A-C1A	-2.86	103.38	106.30
34	BB	616	BCR	C28-C27-C26	-2.86	108.96	114.06
34	Cc	517	BCR	C33-C5-C4	2.86	119.69	113.60
34	C	516	BCR	C27-C26-C25	-2.85	118.85	122.70
34	c	515	BCR	C33-C5-C4	2.85	119.68	113.60
32	N	602	CLA	O2D-CGD-CBD	2.85	116.22	111.23
34	c	515	BCR	C24-C23-C22	-2.85	122.02	126.23
39	n	609	CHL	O2D-CGD-O1D	-2.85	118.30	123.85
41	Yy	619	XAT	C36-C21-C22	-2.85	103.96	108.97
37	A	412	SQD	O48-C23-C24	2.85	119.80	111.15
32	B	610	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
38	AA	415	LMG	O8-C28-C29	2.85	120.52	111.83
32	n	603	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
41	GG	619	XAT	O4-C5-C18	2.85	118.23	115.05
32	22	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
32	Rr	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
39	Ss	605	CHL	O2D-CGD-O1D	-2.85	118.31	123.85
38	b	620	LMG	O8-C28-C29	2.85	120.52	111.83
32	CC	510	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
40	Yy	616	LUT	C7-C8-C9	-2.85	122.02	126.23
32	Ss	609	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
32	RR	304	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
32	b	608	CLA	C4A-NA-C1A	2.85	107.98	106.68
40	s	614	LUT	C19-C9-C8	2.84	122.43	118.09
34	Hh	101	BCR	C36-C18-C19	2.84	122.43	118.09
32	S	602	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
34	C	518	BCR	C30-C25-C26	-2.84	118.75	122.64
32	4	305	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
39	YY	601	CHL	O2D-CGD-CBD	2.84	114.07	110.95
36	BB	622	LHG	O8-C23-C24	2.84	120.50	111.83
34	h	101	BCR	C16-C15-C14	-2.84	117.70	123.52
32	BB	613	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
39	YY	605	CHL	O2D-CGD-O1D	-2.84	118.32	123.85
35	d	404	PL9	C7-C3-C4	2.84	119.25	116.91
35	Dd	404	PL9	C7-C3-C4	2.84	119.25	116.91
32	YY	603	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
34	CC	516	BCR	C27-C26-C25	-2.84	118.86	122.70
39	Rr	606	CHL	CHA-C1A-C2A	-2.84	126.64	133.31
32	g	602	CLA	C1D-ND-C4D	-2.84	104.32	106.31
32	B	610	CLA	CHB-C4A-NA	2.84	128.50	124.40
32	22	602	CLA	C3A-C2A-C1A	-2.84	103.40	106.30
39	s	605	CHL	O2D-CGD-O1D	-2.84	118.32	123.85
40	GG	616	LUT	C26-C27-C28	-2.84	120.16	124.58
39	G	605	CHL	O2D-CGD-O1D	-2.84	118.32	123.85
41	G	619	XAT	C6-C7-C8	-2.84	119.99	125.99
32	b	603	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
40	4	313	LUT	C26-C27-C28	-2.84	120.17	124.58
32	s	613	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
32	Cc	510	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
32	Aa	406	CLA	C1D-ND-C4D	-2.84	104.32	106.31
39	YY	601	CHL	CHA-C1A-C2A	-2.84	126.65	133.31
42	n	617	NEX	C28-C29-C30	2.84	123.47	119.01
32	2	611	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
39	Rr	605	CHL	O2D-CGD-O1D	-2.84	118.33	123.85
39	3	601	CHL	O2D-CGD-O1D	-2.84	118.33	123.85
38	A	415	LMG	O8-C28-C29	2.84	120.48	111.83
32	44	604	CLA	O2D-CGD-O1D	-2.83	118.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	22	610	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
32	D	405	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
34	c	516	BCR	C1-C6-C5	-2.83	118.76	122.64
34	c	516	BCR	C2-C1-C6	2.83	114.55	110.44
39	3	605	CHL	O2D-CGD-O1D	-2.83	118.33	123.85
32	C	514	CLA	CHB-C4A-NA	2.83	128.49	124.40
39	Nn	316	CHL	CHA-C1A-C2A	-2.83	126.66	133.31
32	y	315	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
34	AA	409	BCR	C2-C1-C6	2.83	114.55	110.44
39	4	302	CHL	CHA-C1A-C2A	-2.83	126.66	133.31
32	c	511	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
34	h	101	BCR	C36-C18-C17	-2.83	118.23	122.82
32	1	611	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
42	R	617	NEX	C15-C35-C34	-2.83	117.73	123.52
32	44	603	CLA	CHB-C4A-NA	2.83	128.48	124.40
40	Yy	615	LUT	C26-C27-C28	-2.83	120.18	124.58
32	Bb	608	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
34	H	101	BCR	C37-C22-C23	-2.83	113.77	118.09
32	SS	305	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
42	Y	619	NEX	C5-C6-C1	2.83	122.50	119.70
32	NN	603	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
34	Bb	619	BCR	C36-C18-C17	-2.83	118.24	122.82
41	r	615	XAT	C40-C33-C32	2.83	122.41	118.09
32	RR	309	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
39	NN	601	CHL	C3C-C4C-NC	-2.82	107.75	114.65
33	D	402	PHO	O2D-CGD-O1D	-2.82	118.35	123.85
34	h	101	BCR	C11-C10-C9	-2.82	123.32	127.28
35	AA	410	PL9	C7-C3-C2	-2.82	120.06	123.39
32	R	614	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
39	Yy	606	CHL	O2D-CGD-O1D	-2.82	118.35	123.85
32	S	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
42	RR	317	NEX	C15-C35-C34	-2.82	117.75	123.52
39	GG	605	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
39	GG	606	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
41	4	314	XAT	O4-C5-C18	2.82	118.20	115.05
34	Cc	517	BCR	C24-C23-C22	-2.82	122.06	126.23
32	b	603	CLA	C3B-C4B-NB	-2.82	108.01	110.53
32	S	611	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
39	NN	607	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
39	RR	307	CHL	O2D-CGD-CBD	2.82	114.04	110.95
32	N	610	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
32	Y	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	YY	608	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
39	Gg	309	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
39	N	601	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
42	Nn	309	NEX	C28-C29-C30	2.82	123.44	119.01
32	NN	611	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
41	Yy	619	XAT	C6-C7-C8	-2.82	120.04	125.99
39	r	607	CHL	O2D-CGD-O1D	-2.82	118.37	123.85
40	G	616	LUT	C36-C21-C26	2.81	113.81	109.55
39	YY	601	CHL	O2D-CGD-O1D	-2.81	118.37	123.85
39	s	601	CHL	O2D-CGD-O1D	-2.81	118.37	123.85
32	Nn	301	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
39	Yy	607	CHL	O1D-CGD-CBD	2.81	128.99	124.72
32	NN	604	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
32	Gg	315	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
42	Rr	616	NEX	C2-C1-C6	2.81	111.94	109.21
40	GG	615	LUT	C26-C27-C28	-2.81	120.20	124.58
32	SS	312	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
41	Gg	301	XAT	C39-C29-C28	2.81	122.38	118.09
32	11	603	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
39	33	608	CHL	O2D-CGD-CBD	2.81	114.03	110.95
32	SS	310	CLA	C3B-C4B-NB	-2.81	108.02	110.53
36	n	618	LHG	O8-C23-C24	2.81	120.40	111.83
39	R	607	CHL	O2D-CGD-CBD	2.81	114.03	110.95
32	N	604	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
39	Nn	315	CHL	CHA-C1A-C2A	-2.81	126.72	133.31
40	y	317	LUT	C26-C27-C28	-2.80	120.21	124.58
32	Yy	612	CLA	CHB-C4A-NA	2.80	128.45	124.40
36	SS	301	LHG	O8-C23-C24	2.80	120.39	111.83
32	GG	612	CLA	CHB-C4A-NA	2.80	128.45	124.40
32	y	316	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
32	YY	610	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
39	g	608	CHL	O2D-CGD-O1D	-2.80	118.39	123.85
39	GG	601	CHL	O2D-CGD-O1D	-2.80	118.39	123.85
34	Bb	617	BCR	C33-C5-C4	2.80	119.57	113.60
39	S	605	CHL	O2D-CGD-O1D	-2.80	118.39	123.85
44	a	415	DGD	O5D-C1E-C2E	2.80	112.53	108.27
39	G	601	CHL	O2D-CGD-O1D	-2.80	118.40	123.85
42	Y	617	NEX	C40-C33-C32	2.80	122.37	118.09
32	Rr	610	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
32	44	615	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
41	RR	316	XAT	C26-C27-C28	-2.80	120.07	125.99
35	Dd	404	PL9	C20-C19-C21	-2.80	110.37	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Gg	312	CLA	CBA-CAA-C2A	2.80	122.12	113.79
39	R	606	CHL	O2D-CGD-CBD	2.80	114.02	110.95
32	G	614	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
39	2	605	CHL	O2D-CGD-O1D	-2.80	118.40	123.85
32	Rr	604	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
35	D	407	PL9	C40-C39-C41	-2.80	110.37	115.23
34	A	409	BCR	C2-C1-C6	2.80	114.50	110.44
34	b	617	BCR	C40-C30-C25	2.80	114.63	110.24
32	SS	304	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
39	SS	306	CHL	O2D-CGD-O1D	-2.80	118.40	123.85
34	BB	616	BCR	C37-C22-C23	2.80	122.36	118.09
39	RR	306	CHL	C3C-C4C-NC	-2.80	107.81	114.65
32	22	604	CLA	C3A-C2A-C1A	-2.80	103.44	106.30
32	Aa	405	CLA	CHB-C4A-NA	2.80	128.44	124.40
32	B	624	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
32	11	603	CLA	C4A-NA-C1A	2.80	107.95	106.68
32	R	608	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
39	33	605	CHL	O2D-CGD-O1D	-2.80	118.40	123.85
32	c	508	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
36	s	616	LHG	O8-C23-C24	2.80	120.36	111.83
32	Gg	314	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
39	3	606	CHL	O2D-CGD-O1D	-2.79	118.41	123.85
37	CC	501	SQD	O48-C23-C24	2.79	120.36	111.83
32	44	609	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
32	s	612	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
32	r	613	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
39	s	605	CHL	O2D-CGD-CBD	2.79	114.02	110.95
34	Cc	518	BCR	C27-C26-C25	-2.79	118.93	122.70
32	c	501	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
32	g	611	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
32	YY	603	CLA	CHB-C4A-NA	2.79	128.43	124.40
32	Rr	611	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
39	44	606	CHL	O2D-CGD-O1D	-2.79	118.41	123.85
39	22	601	CHL	O2D-CGD-O1D	-2.79	118.41	123.85
32	NN	613	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
39	22	605	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
34	B	614	BCR	C3-C4-C5	-2.79	109.08	114.06
32	22	604	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	Yy	614	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
44	h	102	DGD	O1G-C1A-C2A	2.79	120.34	111.83
39	n	606	CHL	CHA-C1A-C2A	-2.79	126.76	133.31
32	C	504	CLA	O2D-CGD-O1D	-2.79	118.42	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Yy	602	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
35	d	404	PL9	C20-C19-C21	-2.79	110.39	115.23
32	Rr	603	CLA	CHB-C4A-NA	2.79	128.42	124.40
32	GG	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	RR	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
39	G	609	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
39	N	608	CHL	O2D-CGD-CBD	2.79	114.01	110.95
34	TT	101	BCR	C19-C18-C17	-2.79	114.62	119.01
32	N	613	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
39	Nn	317	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
39	S	607	CHL	O2D-CGD-O1D	-2.79	118.43	123.85
34	KK	103	BCR	C30-C25-C24	2.79	123.20	115.65
34	TT	101	BCR	C15-C14-C13	-2.79	123.37	127.28
39	33	608	CHL	O2D-CGD-O1D	-2.79	118.43	123.85
39	Yy	608	CHL	CHA-C1A-C2A	-2.78	126.77	133.31
32	c	503	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
32	11	609	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
32	22	612	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
39	RR	306	CHL	OMC-CMC-C2C	-2.78	120.29	125.12
39	s	601	CHL	O2D-CGD-CBD	2.78	114.00	110.95
32	3	612	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
39	Y	605	CHL	O1D-CGD-CBD	2.78	128.94	124.72
34	CC	516	BCR	C38-C26-C25	-2.78	121.45	124.48
32	CC	508	CLA	O2D-CGD-CBD	2.78	116.09	111.23
32	y	314	CLA	CHB-C4A-NA	2.78	128.41	124.40
39	S	601	CHL	O2D-CGD-O1D	-2.78	118.43	123.85
32	1	604	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
40	Gg	316	LUT	C17-C1-C6	-2.78	105.88	110.24
42	Rr	616	NEX	C15-C35-C34	-2.78	117.83	123.52
32	b	603	CLA	C4A-NA-C1A	2.78	107.95	106.68
40	22	614	LUT	C15-C35-C34	2.78	129.21	123.52
32	r	610	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
32	S	612	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
36	Gg	319	LHG	O8-C23-C24	2.78	120.31	111.83
34	B	614	BCR	C33-C5-C4	2.78	119.52	113.60
44	Aa	401	DGD	O5D-C1E-C2E	2.78	112.49	108.27
32	11	612	CLA	C4A-NA-C1A	2.78	107.95	106.68
42	Rr	616	NEX	C40-C33-C32	2.78	122.33	118.09
41	G	617	XAT	C39-C29-C28	-2.78	113.85	118.09
32	b	616	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
39	4	306	CHL	O2D-CGD-O1D	-2.78	118.45	123.85
32	g	612	CLA	CHB-C4A-NA	2.78	128.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Rr	602	CLA	C1D-ND-C4D	-2.77	104.36	106.31
32	GG	604	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
40	Yy	616	LUT	C19-C9-C8	2.77	122.33	118.09
32	Cc	513	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
39	33	607	CHL	O2D-CGD-O1D	-2.77	118.45	123.85
32	NN	602	CLA	C3B-C4B-NB	-2.77	108.05	110.53
34	K	102	BCR	C27-C26-C25	-2.77	118.96	122.70
32	Bb	602	CLA	C4A-NA-C1A	2.77	107.94	106.68
39	22	608	CHL	O2D-CGD-O1D	-2.77	118.45	123.85
34	CC	517	BCR	C30-C25-C26	-2.77	118.85	122.64
32	c	504	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
32	Cc	512	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
34	BB	620	BCR	C16-C15-C14	-2.77	117.85	123.52
41	R	616	XAT	C26-C27-C28	-2.77	120.13	125.99
34	D	406	BCR	C36-C18-C19	2.77	122.32	118.09
36	4	315	LHG	C5-O7-C7	-2.77	112.95	117.85
32	r	602	CLA	C4A-NA-C1A	2.77	107.94	106.68
39	N	609	CHL	CMB-C2B-C3B	2.77	130.22	124.68
32	Rr	608	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
39	R	606	CHL	O2D-CGD-O1D	-2.77	118.46	123.85
35	A	410	PL9	C25-C24-C26	-2.77	110.42	115.23
32	44	610	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
39	Nn	319	CHL	O2D-CGD-O1D	-2.77	118.46	123.85
32	N	602	CLA	CHB-C4A-NA	2.77	128.39	124.40
40	22	614	LUT	C36-C21-C26	2.77	113.74	109.55
39	11	601	CHL	O2D-CGD-O1D	-2.77	118.46	123.85
40	n	616	LUT	C3-C4-C5	-2.77	105.29	112.18
41	G	617	XAT	C20-C13-C12	2.77	122.31	118.09
32	C	511	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
34	Aa	411	BCR	C2-C1-C6	2.77	114.46	110.44
40	N	615	LUT	C26-C27-C28	-2.77	120.28	124.58
33	Aa	408	PHO	C3B-C4B-NB	-2.76	105.66	107.46
42	NN	618	NEX	C15-C35-C34	-2.76	117.86	123.52
40	NN	615	LUT	C26-C27-C28	-2.76	120.28	124.58
34	XX	202	BCR	C7-C8-C9	-2.76	122.15	126.23
32	g	604	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
39	Gg	307	CHL	O2D-CGD-O1D	-2.76	118.47	123.85
34	T	101	BCR	C3-C4-C5	-2.76	109.13	114.06
32	N	603	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
39	YY	609	CHL	O2D-CGD-O1D	-2.76	118.47	123.85
39	n	607	CHL	O2D-CGD-CBD	2.76	113.98	110.95
39	Gg	308	CHL	O2D-CGD-CBD	2.76	113.98	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	GG	612	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	Bb	603	CLA	C4A-NA-C1A	2.76	107.94	106.68
39	RR	305	CHL	CHA-C1A-C2A	-2.76	126.83	133.31
34	TT	101	BCR	C29-C30-C25	2.76	114.45	110.44
34	c	515	BCR	C15-C16-C17	-2.76	117.88	123.52
32	r	609	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
33	a	408	PHO	O2D-CGD-O1D	-2.76	118.48	123.85
38	Bb	620	LMG	O8-C28-C29	2.76	120.25	111.83
32	Ss	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
34	B	614	BCR	C38-C26-C25	-2.76	121.47	124.48
34	Cc	517	BCR	C15-C16-C17	-2.76	117.88	123.52
32	r	603	CLA	CHB-C4A-NA	2.76	128.38	124.40
39	R	605	CHL	O2D-CGD-O1D	-2.76	118.48	123.85
35	DD	406	PL9	C40-C39-C41	-2.76	110.44	115.23
32	CC	508	CLA	CHB-C4A-NA	2.76	128.38	124.40
39	1	607	CHL	O2D-CGD-O1D	-2.76	118.48	123.85
39	g	605	CHL	O2D-CGD-O1D	-2.76	118.48	123.85
34	Bb	619	BCR	C27-C26-C25	-2.76	118.98	122.70
39	4	309	CHL	C1B-CHB-C4A	2.75	123.09	121.32
32	G	604	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
36	JJ	101	LHG	O8-C23-C24	2.75	120.23	111.83
34	Hh	101	BCR	C34-C9-C8	-2.75	113.88	118.09
32	Y	602	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
39	33	606	CHL	O2D-CGD-O1D	-2.75	118.49	123.85
39	2	607	CHL	O2D-CGD-O1D	-2.75	118.49	123.85
39	n	601	CHL	O2D-CGD-O1D	-2.75	118.49	123.85
35	D	407	PL9	C35-C34-C36	-2.75	110.45	115.23
39	Y	601	CHL	CHA-C1A-C2A	-2.75	126.84	133.31
36	d	406	LHG	O8-C23-C24	2.75	120.22	111.83
34	K	102	BCR	C40-C30-C25	2.75	114.56	110.24
32	CC	513	CLA	CHB-C4A-NA	2.75	128.37	124.40
41	y	301	XAT	C6-C7-C8	-2.75	120.18	125.99
39	NN	608	CHL	O2D-CGD-CBD	2.75	113.97	110.95
39	4	306	CHL	CHA-C1A-C2A	-2.75	126.85	133.31
32	RR	314	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
39	11	607	CHL	O2D-CGD-O1D	-2.75	118.50	123.85
40	GG	615	LUT	C3-C4-C5	-2.75	105.33	112.18
32	2	609	CLA	C3A-C2A-C1A	-2.75	103.49	106.30
36	g	618	LHG	O8-C23-C24	2.75	120.22	111.83
39	y	310	CHL	CHA-C1A-C2A	-2.75	126.85	133.31
39	Gg	306	CHL	O2D-CGD-O1D	-2.75	118.50	123.85
34	a	411	BCR	C2-C1-C6	2.75	114.43	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	22	614	LUT	C38-C25-C24	-2.75	116.86	123.36
32	G	612	CLA	CHB-C4A-NA	2.75	128.37	124.40
39	Rr	607	CHL	O2D-CGD-O1D	-2.75	118.50	123.85
32	Gg	303	CLA	CHD-C1D-ND	-2.75	120.94	124.80
32	r	608	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
34	CC	516	BCR	C38-C26-C27	2.75	119.45	113.60
32	33	612	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
32	SS	303	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
33	Aa	409	PHO	O2D-CGD-O1D	-2.74	118.50	123.85
32	g	612	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
39	Nn	311	CHL	O2D-CGD-O1D	-2.74	118.51	123.85
32	44	603	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	G	612	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	Cc	511	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	Gg	305	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	Gg	312	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
33	Aa	408	PHO	O2D-CGD-O1D	-2.74	118.51	123.85
32	RR	304	CLA	O2D-CGD-CBD	2.74	116.02	111.23
32	Ss	613	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
32	4	304	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
32	SS	311	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
36	Dd	406	LHG	O8-C23-C24	2.74	120.18	111.83
39	Nn	315	CHL	C4D-CHA-CBD	-2.74	106.21	108.97
32	Y	611	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
32	s	604	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
39	S	606	CHL	O2D-CGD-O1D	-2.74	118.52	123.85
39	SS	302	CHL	O2D-CGD-O1D	-2.74	118.52	123.85
40	g	616	LUT	C26-C27-C28	-2.74	120.32	124.58
40	GG	616	LUT	C36-C21-C26	2.74	113.69	109.55
32	33	609	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
34	Aa	411	BCR	C37-C22-C23	2.74	122.27	118.09
40	Gg	316	LUT	C26-C27-C28	-2.74	120.32	124.58
33	a	409	PHO	O2D-CGD-O1D	-2.74	118.52	123.85
38	b	621	LMG	O8-C28-C29	2.73	120.17	111.83
40	y	318	LUT	C7-C8-C9	-2.73	122.19	126.23
39	1	605	CHL	C2A-C3A-C4A	-2.73	101.75	103.53
39	Y	609	CHL	O2D-CGD-O1D	-2.73	118.53	123.85
32	c	501	CLA	C4-C3-C5	2.73	119.97	115.23
34	BB	617	BCR	C15-C16-C17	-2.73	117.93	123.52
34	C	517	BCR	C38-C26-C27	2.73	119.42	113.60
34	a	411	BCR	C37-C22-C23	2.73	122.26	118.09
32	Rr	603	CLA	O2D-CGD-O1D	-2.73	118.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Ss	614	LUT	C36-C21-C26	2.73	113.68	109.55
39	g	607	CHL	O2D-CGD-O1D	-2.73	118.53	123.85
39	N	609	CHL	C3C-C4C-NC	-2.73	107.97	114.65
32	2	612	CLA	C3A-C2A-C1A	-2.73	103.51	106.30
38	Bb	621	LMG	O8-C28-C29	2.73	120.16	111.83
44	Hh	102	DGD	O1G-C1A-C2A	2.73	120.16	111.83
32	22	603	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
32	R	611	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
32	Rr	612	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
39	RR	306	CHL	O2D-CGD-O1D	-2.73	118.54	123.85
39	Gg	308	CHL	CHA-C1A-C2A	-2.73	126.90	133.31
36	AA	414	LHG	O8-C23-C24	2.73	120.15	111.83
32	GG	614	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
39	22	607	CHL	O2D-CGD-O1D	-2.73	118.54	123.85
39	y	309	CHL	O2D-CGD-CBD	2.73	113.94	110.95
39	n	607	CHL	O2D-CGD-O1D	-2.73	118.54	123.85
39	NN	601	CHL	CHA-C1A-C2A	-2.73	126.91	133.31
39	g	601	CHL	O2D-CGD-O1D	-2.73	118.54	123.85
32	Nn	312	CLA	O2D-CGD-CBD	2.73	116.00	111.23
40	Ss	615	LUT	C18-C5-C6	2.73	127.46	124.48
32	N	614	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
32	Cc	506	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
39	1	608	CHL	C1B-CHB-C4A	2.73	123.08	121.32
39	3	605	CHL	O2D-CGD-CBD	2.72	113.94	110.95
39	22	606	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
32	N	612	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
32	SS	313	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
39	NN	609	CHL	C3C-C4C-NC	-2.72	107.99	114.65
34	K	102	BCR	C30-C25-C24	2.72	123.04	115.65
40	R	615	LUT	C3-C4-C5	-2.72	105.40	112.18
34	BB	618	BCR	C3-C4-C5	-2.72	109.20	114.06
32	Cc	505	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
35	Dd	404	PL9	C35-C34-C36	-2.72	110.50	115.23
39	y	307	CHL	O1D-CGD-CBD	2.72	128.85	124.72
39	g	607	CHL	O2D-CGD-CBD	2.72	113.94	110.95
39	1	601	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
39	Gg	308	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
32	Y	603	CLA	CHB-C4A-NA	2.72	128.33	124.40
32	Gg	303	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
32	Cc	508	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
32	NN	602	CLA	O2D-CGD-CBD	2.72	115.99	111.23
32	n	612	CLA	CHB-C4A-NA	2.72	128.33	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Hh	101	BCR	C16-C15-C14	-2.72	117.95	123.52
34	Kk	101	BCR	C33-C5-C4	2.72	119.39	113.60
34	B	616	BCR	C33-C5-C4	2.72	119.39	113.60
39	2	601	CHL	O2D-CGD-O1D	-2.72	118.56	123.85
34	CC	515	BCR	C38-C26-C25	-2.72	121.52	124.48
32	n	612	CLA	C4A-NA-C1A	2.72	107.92	106.68
32	2	604	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
39	RR	307	CHL	O2D-CGD-O1D	-2.71	118.56	123.85
32	N	611	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
32	y	313	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
34	b	619	BCR	C36-C18-C17	-2.71	118.42	122.82
32	r	611	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
36	J	101	LHG	O8-C23-C24	2.71	120.11	111.83
32	b	609	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
32	r	602	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
32	G	611	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
32	n	602	CLA	C3B-C4B-NB	-2.71	108.11	110.53
42	R	617	NEX	C17-C1-C6	-2.71	108.05	110.47
39	Yy	607	CHL	CHA-C1A-C2A	-2.71	126.95	133.31
39	3	608	CHL	O2D-CGD-O1D	-2.71	118.58	123.85
39	R	607	CHL	O2D-CGD-O1D	-2.71	118.58	123.85
38	Cc	501	LMG	C4-C3-C2	2.71	115.58	110.83
32	G	613	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
32	B	622	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
34	BB	618	BCR	C33-C5-C4	2.70	119.36	113.60
32	2	603	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
39	Nn	318	CHL	O2D-CGD-O1D	-2.70	118.59	123.85
32	D	404	CLA	CHB-C4A-NA	2.70	128.30	124.40
32	Bb	616	CLA	CHB-C4A-NA	2.70	128.30	124.40
40	Nn	306	LUT	C36-C21-C26	2.70	113.64	109.55
32	YY	611	CLA	C3B-C4B-NB	-2.70	108.12	110.53
39	SS	308	CHL	O2D-CGD-O1D	-2.70	118.59	123.85
32	C	509	CLA	CHB-C4A-NA	2.70	128.30	124.40
41	GG	619	XAT	C6-C7-C8	-2.70	120.28	125.99
32	11	613	CLA	C3A-C2A-C1A	-2.70	103.54	106.30
39	4	307	CHL	O2D-CGD-O1D	-2.70	118.59	123.85
40	Gg	317	LUT	C26-C27-C28	-2.70	120.38	124.58
32	B	608	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
32	G	610	CLA	CHB-C4A-NA	2.70	128.29	124.40
32	RR	310	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
42	NN	618	NEX	C11-C10-C9	-2.70	123.49	127.28
34	C	517	BCR	C15-C16-C17	-2.70	118.00	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	506	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
32	YY	611	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
36	3	614	LHG	O8-C23-C24	2.70	120.06	111.83
32	33	610	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
40	Gg	317	LUT	C17-C1-C6	-2.70	106.02	110.24
39	y	303	CHL	CHA-C1A-C2A	-2.70	126.98	133.31
39	33	605	CHL	O2D-CGD-CBD	2.69	113.91	110.95
32	Gg	313	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
32	S	604	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
32	4	312	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
32	Cc	509	CLA	CHB-C4A-NA	2.69	128.28	124.40
32	Y	610	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
39	y	308	CHL	O2D-CGD-O1D	-2.69	118.61	123.85
32	NN	612	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
32	YY	613	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
32	YY	604	CLA	O2D-CGD-CBD	2.69	115.93	111.23
39	s	607	CHL	O2D-CGD-O1D	-2.69	118.61	123.85
32	NN	610	CLA	C4A-NA-C1A	2.69	107.91	106.68
39	n	606	CHL	O2D-CGD-O1D	-2.69	118.62	123.85
32	C	504	CLA	CBA-CAA-C2A	2.69	121.79	113.79
34	BB	617	BCR	C36-C18-C17	-2.69	118.47	122.82
32	AA	405	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
39	GG	605	CHL	O2D-CGD-CBD	2.68	113.90	110.95
34	H	101	BCR	C16-C15-C14	-2.68	118.03	123.52
40	22	614	LUT	C3-C4-C5	-2.68	105.50	112.18
32	CC	511	CLA	C3B-C4B-NB	-2.68	108.13	110.53
39	R	606	CHL	C3C-C4C-NC	-2.68	108.09	114.65
39	Yy	601	CHL	CHA-C1A-C2A	-2.68	127.01	133.31
32	g	610	CLA	C3B-C4B-NB	-2.68	108.14	110.53
37	CC	501	SQD	C45-O47-C7	-2.68	111.38	117.80
35	AA	410	PL9	C25-C24-C26	-2.68	110.57	115.23
39	N	607	CHL	C4D-CHA-CBD	-2.68	106.26	108.97
41	G	617	XAT	C6-C7-C8	-2.68	120.33	125.99
34	B	613	BCR	C15-C16-C17	-2.68	118.03	123.52
39	g	605	CHL	O2D-CGD-CBD	2.68	113.89	110.95
32	CC	511	CLA	CHB-C4A-NA	2.68	128.27	124.40
32	11	612	CLA	CBC-CAC-C3C	2.68	119.68	112.42
32	RR	311	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
40	n	616	LUT	C7-C8-C9	-2.68	122.27	126.23
32	Ss	610	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
36	11	614	LHG	O8-C23-C24	2.68	120.00	111.83
32	CC	502	CLA	CHB-C4A-NA	2.68	128.26	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Ss	615	LUT	C26-C27-C28	-2.68	120.42	124.58
32	DD	401	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
44	Cc	519	DGD	O6D-C5D-C6D	2.68	112.00	106.69
39	2	606	CHL	O2D-CGD-O1D	-2.68	118.64	123.85
42	Y	617	NEX	C15-C35-C34	-2.67	118.05	123.52
40	Nn	307	LUT	C36-C21-C26	2.67	113.59	109.55
39	NN	606	CHL	O2D-CGD-O1D	-2.67	118.64	123.85
39	g	609	CHL	O2D-CGD-CBD	2.67	113.88	110.95
39	Gg	307	CHL	O2D-CGD-CBD	2.67	113.88	110.95
40	2	614	LUT	C36-C21-C26	2.67	113.59	109.55
32	D	401	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
39	Y	601	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
39	3	607	CHL	O2D-CGD-CBD	2.67	113.88	110.95
34	TT	101	BCR	C24-C23-C22	-2.67	122.28	126.23
32	Bb	613	CLA	CHB-C4A-NA	2.67	128.25	124.40
39	y	309	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
41	Yy	619	XAT	C38-C25-C26	-2.67	117.91	122.30
32	SS	310	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
39	2	608	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
34	KK	103	BCR	C16-C15-C14	-2.67	118.06	123.52
32	B	605	CLA	C3B-C4B-NB	-2.67	108.15	110.53
32	CC	514	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
40	Rr	614	LUT	C26-C27-C28	-2.67	120.42	124.58
32	YY	614	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
39	3	607	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
34	C	518	BCR	C37-C22-C23	2.67	122.17	118.09
32	Y	612	CLA	CHB-C4A-NA	2.67	128.25	124.40
39	n	608	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
32	r	602	CLA	C1D-ND-C4D	-2.67	104.44	106.31
32	XX	201	CLA	CMA-C3A-C2A	-2.67	110.11	116.23
39	3	608	CHL	O2D-CGD-CBD	2.67	113.88	110.95
39	NN	607	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
32	3	610	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
39	YY	606	CHL	O2D-CGD-O1D	-2.67	118.66	123.85
35	D	407	PL9	C25-C24-C26	-2.67	110.60	115.23
39	4	309	CHL	O2D-CGD-O1D	-2.67	118.66	123.85
34	B	613	BCR	C36-C18-C17	-2.67	118.50	122.82
39	SS	307	CHL	O2D-CGD-O1D	-2.67	118.66	123.85
36	Y	618	LHG	O8-C23-C24	2.67	119.96	111.83
34	CC	516	BCR	C15-C16-C17	-2.67	118.07	123.52
33	a	408	PHO	C3B-C4B-NB	-2.67	105.73	107.46
40	Nn	307	LUT	C19-C9-C8	2.66	122.16	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	410	PL9	C7-C3-C2	-2.66	120.25	123.39
41	Yy	619	XAT	C24-C23-C22	-2.66	105.81	110.79
40	n	616	LUT	C36-C21-C26	2.66	113.58	109.55
32	BB	612	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
32	a	405	CLA	CHB-C4A-NA	2.66	128.24	124.40
34	C	516	BCR	C28-C27-C26	-2.66	109.31	114.06
32	YY	612	CLA	C2C-C1C-NC	2.66	112.77	109.98
32	Y	614	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
34	C	517	BCR	C28-C27-C26	-2.66	109.32	114.06
44	CC	518	DGD	O1G-C1A-C2A	2.66	119.94	111.83
32	R	610	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
39	11	607	CHL	O2D-CGD-CBD	2.66	113.86	110.95
39	N	601	CHL	O2D-CGD-CBD	2.66	113.86	110.95
39	s	601	CHL	C1-C2-C3	-2.66	121.84	126.20
41	R	616	XAT	C35-C15-C14	-2.66	118.08	123.52
32	Bb	609	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
39	Yy	605	CHL	O1D-CGD-CBD	2.66	128.75	124.72
32	YY	612	CLA	O2A-CGA-O1A	-2.66	116.99	123.63
41	GG	617	XAT	C39-C29-C28	-2.66	114.03	118.09
39	1	607	CHL	O2D-CGD-CBD	2.65	113.86	110.95
32	Yy	611	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
32	Yy	603	CLA	CHB-C4A-NA	2.65	128.23	124.40
40	2	614	LUT	C19-C9-C8	2.65	122.14	118.09
39	11	607	CHL	C3C-C4C-NC	-2.65	108.17	114.65
44	Aa	401	DGD	O1G-C1A-C2A	2.65	119.92	111.83
39	YY	607	CHL	OMC-CMC-C2C	-2.65	120.52	125.12
36	A	414	LHG	O8-C23-C24	2.65	119.91	111.83
44	a	415	DGD	O1G-C1A-C2A	2.65	119.91	111.83
32	Bb	609	CLA	C3B-C4B-NB	-2.65	108.17	110.53
34	B	616	BCR	C16-C15-C14	-2.65	118.10	123.52
43	C	502	LMU	C1B-O1B-C4'	-2.65	111.70	117.98
39	Gg	306	CHL	OMC-CMC-C2C	-2.65	120.52	125.12
41	g	619	XAT	C39-C29-C28	2.65	122.13	118.09
34	CC	515	BCR	C34-C9-C8	-2.65	114.04	118.09
39	4	308	CHL	C3C-C4C-NC	-2.65	108.18	114.65
32	CC	507	CLA	CBA-CAA-C2A	2.65	121.67	113.79
32	b	616	CLA	CHB-C4A-NA	2.65	128.22	124.40
32	s	608	CLA	CHB-C4A-NA	2.65	128.22	124.40
32	BB	608	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
32	RR	313	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
39	Ss	601	CHL	O2D-CGD-O1D	-2.65	118.70	123.85
33	DD	402	PHO	O2D-CGD-O1D	-2.64	118.70	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Gg	306	CHL	O2D-CGD-CBD	2.64	113.85	110.95
44	CC	522	DGD	O1G-C1A-C2A	2.64	119.90	111.83
34	TT	101	BCR	C3-C4-C5	-2.64	109.34	114.06
39	1	608	CHL	O2D-CGD-O1D	-2.64	118.70	123.85
32	B	604	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
35	Dd	404	PL9	C30-C29-C31	-2.64	110.64	115.23
39	44	608	CHL	O2D-CGD-O1D	-2.64	118.71	123.85
34	H	101	BCR	C20-C21-C22	-2.64	123.58	127.28
32	Bb	603	CLA	C3B-C4B-NB	-2.64	108.17	110.53
32	44	611	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
40	Yy	616	LUT	C36-C21-C26	2.64	113.54	109.55
39	44	601	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
32	Yy	610	CLA	C3B-C4B-NB	-2.64	108.17	110.53
32	c	501	CLA	C6-C5-C3	2.64	119.90	113.47
39	33	606	CHL	OMC-CMC-C2C	-2.64	120.54	125.12
32	BB	607	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
34	d	403	BCR	C4-C5-C6	-2.64	119.14	122.70
32	Ss	608	CLA	CHB-C4A-NA	2.64	128.21	124.40
32	22	609	CLA	C3A-C2A-C1A	-2.64	103.61	106.30
32	C	509	CLA	O2D-CGD-CBD	2.63	115.83	111.23
32	GG	602	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
32	g	602	CLA	CHC-C4B-NB	2.63	128.00	124.05
39	R	605	CHL	CHA-C1A-C2A	-2.63	127.12	133.31
32	Cc	514	CLA	CHB-C4A-NA	2.63	128.20	124.40
32	Gg	304	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
32	AA	408	CLA	C3B-C4B-NB	-2.63	108.18	110.53
32	RR	309	CLA	C3B-C4B-NB	-2.63	108.18	110.53
38	j	101	LMG	O8-C28-C29	2.63	119.85	111.83
39	11	608	CHL	CMD-C2D-C3D	2.63	129.94	124.68
39	Nn	316	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
39	33	605	CHL	OMC-CMC-C2C	-2.63	120.56	125.12
32	BB	612	CLA	CHB-C4A-NA	2.63	128.19	124.40
39	G	605	CHL	O2D-CGD-CBD	2.63	113.83	110.95
35	DD	406	PL9	C35-C34-C36	-2.63	110.67	115.23
32	NN	602	CLA	CHB-C4A-NA	2.63	128.19	124.40
32	RR	311	CLA	CHB-C4A-NA	2.63	128.19	124.40
32	C	508	CLA	CBA-CAA-C2A	2.63	121.60	113.79
34	T	101	BCR	C19-C18-C17	-2.63	114.88	119.01
39	y	307	CHL	O2D-CGD-CBD	2.62	113.83	110.95
32	Y	613	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
42	YY	617	NEX	C15-C35-C34	-2.62	118.15	123.52
39	Y	607	CHL	OMC-CMC-C2C	-2.62	120.56	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	DD	405	BCR	C29-C30-C25	2.62	114.25	110.44
39	YY	609	CHL	OMC-CMC-C2C	-2.62	120.57	125.12
40	RR	315	LUT	C19-C9-C8	2.62	122.09	118.09
39	R	605	CHL	C3C-C4C-NC	-2.62	108.24	114.65
32	11	612	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
41	NN	617	XAT	C6-C7-C8	-2.62	120.45	125.99
38	Dd	408	LMG	O8-C28-C29	2.62	119.83	111.83
34	Hh	101	BCR	C11-C10-C9	-2.62	123.60	127.28
39	y	311	CHL	OMC-CMC-C2C	-2.62	120.57	125.12
35	A	410	PL9	C35-C34-C36	-2.62	110.68	115.23
39	1	608	CHL	CMD-C2D-C3D	2.62	129.91	124.68
39	N	601	CHL	C3C-C4C-NC	-2.62	108.25	114.65
40	s	614	LUT	C8-C9-C10	-2.62	114.89	119.01
32	R	609	CLA	C3B-C4B-NB	-2.62	108.19	110.53
39	Yy	607	CHL	OMC-CMC-C2C	-2.62	120.58	125.12
32	s	610	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
32	NN	614	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
32	b	613	CLA	CHB-C4A-NA	2.61	128.17	124.40
34	C	516	BCR	C34-C9-C8	-2.61	114.10	118.09
32	Nn	312	CLA	CHB-C4A-NA	2.61	128.17	124.40
32	s	602	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
32	Aa	405	CLA	CAC-C3C-C4C	2.61	128.19	124.79
34	Dd	403	BCR	C4-C5-C6	-2.61	119.17	122.70
40	2	614	LUT	C38-C25-C24	-2.61	117.18	123.36
40	Gg	317	LUT	C36-C21-C26	2.61	113.50	109.55
39	22	608	CHL	O2D-CGD-CBD	2.61	113.81	110.95
32	Dd	402	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
36	CC	521	LHG	O8-C23-C24	2.61	119.79	111.83
32	y	312	CLA	CHB-C4A-NA	2.61	128.17	124.40
32	2	609	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
32	CC	503	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
40	r	614	LUT	C26-C27-C28	-2.61	120.52	124.58
39	r	606	CHL	C3C-C4C-NC	-2.61	108.28	114.65
39	s	606	CHL	O2D-CGD-CBD	2.61	113.81	110.95
32	c	505	CLA	C4A-NA-C1A	2.61	107.87	106.68
36	II	101	LHG	O8-C23-C24	2.61	119.78	111.83
32	BB	608	CLA	CAA-C2A-C1A	-2.61	103.44	111.97
34	CC	516	BCR	C28-C27-C26	-2.60	109.41	114.06
40	N	616	LUT	C19-C9-C8	2.60	122.06	118.09
39	y	308	CHL	O2D-CGD-CBD	2.60	113.81	110.95
32	d	402	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
40	N	616	LUT	C26-C27-C28	-2.60	120.53	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	r	615	XAT	C6-C7-C8	-2.60	120.49	125.99
32	BB	609	CLA	C3B-C4B-NB	-2.60	108.21	110.53
34	Bb	618	BCR	C15-C16-C17	-2.60	118.20	123.52
39	33	601	CHL	O2D-CGD-CBD	2.60	113.80	110.95
34	Aa	411	BCR	C30-C25-C26	-2.60	119.08	122.64
32	XX	201	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
32	R	611	CLA	CHB-C4A-NA	2.60	128.15	124.40
32	r	603	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
39	n	606	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
32	g	603	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
40	n	615	LUT	C26-C27-C28	-2.60	120.54	124.58
40	s	615	LUT	C17-C1-C6	-2.60	106.17	110.24
34	Kk	101	BCR	C16-C15-C14	-2.60	118.21	123.52
39	Ss	607	CHL	O2D-CGD-O1D	-2.60	118.79	123.85
39	2	605	CHL	O2D-CGD-CBD	2.60	113.80	110.95
34	c	514	BCR	C34-C9-C8	-2.60	114.12	118.09
32	y	304	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
32	n	602	CLA	O2D-CGD-CBD	2.60	115.77	111.23
34	b	617	BCR	C33-C5-C4	2.60	119.13	113.60
39	Y	601	CHL	C3C-C4C-NC	-2.59	108.31	114.65
36	Ss	616	LHG	O8-C23-C24	2.59	119.75	111.83
40	SS	315	LUT	C3-C4-C5	-2.59	105.72	112.18
34	c	516	BCR	C8-C7-C6	-2.59	120.07	127.00
34	DD	405	BCR	C36-C18-C19	2.59	122.05	118.09
34	a	411	BCR	C30-C25-C26	-2.59	119.10	122.64
36	AA	411	LHG	O8-C23-C24	2.59	119.73	111.83
32	Y	612	CLA	CED-O2D-CGD	2.59	121.79	115.92
36	YY	618	LHG	O8-C23-C24	2.59	119.73	111.83
40	N	615	LUT	C17-C1-C6	-2.59	106.19	110.24
37	l	102	SQD	O48-C23-C24	2.59	119.72	111.83
32	GG	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
39	2	607	CHL	O2D-CGD-CBD	2.59	113.79	110.95
40	G	615	LUT	C36-C21-C26	2.59	113.46	109.55
42	N	618	NEX	C11-C10-C9	-2.59	123.65	127.28
32	R	613	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
32	BB	602	CLA	CHB-C4A-NA	2.58	128.13	124.40
35	Dd	404	PL9	C40-C39-C41	-2.58	110.74	115.23
32	X	201	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
40	y	318	LUT	C19-C9-C8	2.58	122.03	118.09
32	Nn	305	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
32	44	611	CLA	CHB-C4A-NA	2.58	128.13	124.40
34	CC	517	BCR	C37-C22-C23	2.58	122.03	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	605	CHL	O2D-CGD-CBD	2.58	113.78	110.95
39	Ss	606	CHL	C3C-C4C-NC	-2.58	108.34	114.65
39	g	607	CHL	CHA-C1A-C2A	-2.58	127.25	133.31
41	Nn	308	XAT	C15-C35-C34	-2.58	118.24	123.52
34	D	406	BCR	C3-C4-C5	-2.58	109.45	114.06
40	Y	616	LUT	C40-C33-C32	2.58	122.03	118.09
39	g	609	CHL	C3C-C4C-NC	-2.58	108.35	114.65
39	G	608	CHL	O1D-CGD-CBD	2.58	128.63	124.72
36	GG	618	LHG	C5-O7-C7	-2.58	111.63	117.80
32	3	603	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
37	B	617	SQD	O48-C23-C24	2.58	119.69	111.83
39	44	608	CHL	OMC-CMC-C2C	-2.58	120.64	125.12
32	B	619	CLA	CHB-C4A-NA	2.58	128.12	124.40
32	C	508	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
40	S	614	LUT	C18-C5-C4	2.58	119.16	114.42
41	Rr	615	XAT	C39-C29-C28	2.57	122.02	118.09
39	44	608	CHL	CHA-C1A-C2A	-2.57	127.27	133.31
32	Ss	603	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
39	RR	305	CHL	C3C-C4C-NC	-2.57	108.36	114.65
39	Nn	316	CHL	O2D-CGD-O1D	-2.57	118.84	123.85
32	NN	611	CLA	CHB-C4A-NA	2.57	128.11	124.40
34	TT	101	BCR	C37-C22-C23	2.57	122.02	118.09
39	N	606	CHL	O2D-CGD-O1D	-2.57	118.84	123.85
39	YY	601	CHL	C3C-C4C-NC	-2.57	108.36	114.65
32	CC	507	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
32	B	611	CLA	CHB-C4A-NA	2.57	128.11	124.40
40	Y	615	LUT	C21-C26-C27	-2.57	109.87	112.83
34	K	102	BCR	C36-C18-C19	2.57	122.01	118.09
39	s	606	CHL	C3C-C4C-NC	-2.57	108.37	114.65
37	BB	621	SQD	O48-C23-C24	2.57	119.66	111.83
32	N	610	CLA	C4A-NA-C1A	2.57	107.85	106.68
32	2	612	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
32	c	512	CLA	CHB-C4A-NA	2.57	128.10	124.40
32	RR	309	CLA	CHB-C4A-NA	2.56	128.10	124.40
36	G	618	LHG	O8-C23-C24	2.56	119.65	111.83
35	d	404	PL9	C40-C39-C41	-2.56	110.78	115.23
42	Gg	318	NEX	C28-C29-C30	2.56	123.04	119.01
40	Gg	316	LUT	C36-C21-C26	2.56	113.43	109.55
32	g	610	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
40	Nn	307	LUT	C3-C4-C5	-2.56	105.80	112.18
42	Yy	617	NEX	C15-C35-C34	-2.56	118.28	123.52
32	Yy	610	CLA	CHB-C4A-NA	2.56	128.09	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	3	601	CHL	O2D-CGD-CBD	2.56	113.76	110.95
39	g	605	CHL	OMC-CMC-C2C	-2.56	120.68	125.12
36	A	411	LHG	O8-C23-C24	2.56	119.63	111.83
35	AA	410	PL9	C30-C29-C31	-2.56	110.79	115.23
32	c	504	CLA	CHB-C4A-NA	2.56	128.09	124.40
39	Nn	317	CHL	C4D-CHA-CBD	-2.56	106.39	108.97
39	SS	308	CHL	O2D-CGD-CBD	2.56	113.75	110.95
39	Yy	608	CHL	O2D-CGD-O1D	-2.55	118.88	123.85
32	r	610	CLA	CHB-C4A-NA	2.55	128.09	124.40
32	4	312	CLA	CHB-C4A-NA	2.55	128.09	124.40
32	Cc	506	CLA	CHB-C4A-NA	2.55	128.09	124.40
34	DD	405	BCR	C3-C4-C5	-2.55	109.50	114.06
39	g	606	CHL	O2D-CGD-O1D	-2.55	118.88	123.85
39	4	306	CHL	O2D-CGD-CBD	2.55	113.75	110.95
32	R	609	CLA	CHB-C4A-NA	2.55	128.09	124.40
38	WW	201	LMG	O8-C28-C29	2.55	119.62	111.83
38	W	201	LMG	O8-C28-C29	2.55	119.62	111.83
40	N	616	LUT	C15-C35-C34	-2.55	118.30	123.52
35	AA	410	PL9	C35-C34-C36	-2.55	110.80	115.23
42	YY	617	NEX	C40-C33-C32	2.55	121.98	118.09
39	Rr	606	CHL	C3C-C4C-NC	-2.55	108.42	114.65
39	N	609	CHL	C4D-CHA-CBD	-2.55	106.40	108.97
34	BB	617	BCR	C38-C26-C25	-2.55	121.70	124.48
41	G	617	XAT	C40-C33-C32	2.55	121.98	118.09
39	YY	607	CHL	O2D-CGD-O1D	-2.55	118.89	123.85
40	s	615	LUT	C19-C9-C8	2.55	121.98	118.09
32	R	604	CLA	CHB-C4A-NA	2.55	128.08	124.40
32	DD	401	CLA	O2D-CGD-CBD	2.55	115.68	111.23
36	33	614	LHG	O8-C23-C24	2.55	119.60	111.83
41	N	617	XAT	C6-C7-C8	-2.55	120.61	125.99
32	s	608	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
40	NN	616	LUT	C19-C9-C8	2.54	121.97	118.09
37	Ll	101	SQD	O48-C23-C24	2.54	119.59	111.83
32	Bb	607	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
40	Ss	615	LUT	C17-C1-C6	-2.54	106.26	110.24
32	GG	610	CLA	CHB-C4A-NA	2.54	128.07	124.40
32	s	603	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
41	RR	316	XAT	C35-C15-C14	-2.54	118.32	123.52
34	Bb	617	BCR	C24-C23-C22	-2.54	122.47	126.23
40	4	313	LUT	C36-C21-C26	2.54	113.39	109.55
39	Ss	606	CHL	O2D-CGD-CBD	2.54	113.74	110.95
36	K	101	LHG	O8-C23-C24	2.54	119.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	22	601	CHL	O2D-CGD-CBD	2.54	113.74	110.95
36	KK	101	LHG	O8-C23-C24	2.54	119.58	111.83
32	R	613	CLA	CAC-C3C-C4C	2.54	128.09	124.79
40	2	614	LUT	C17-C1-C6	-2.54	106.26	110.24
32	b	607	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
39	NN	601	CHL	CMB-C2B-C3B	2.54	129.75	124.68
44	C	519	DGD	O1G-C1A-C2A	2.54	119.57	111.83
32	c	501	CLA	CHB-C4A-NA	2.54	128.06	124.40
32	BB	601	CLA	C3B-C4B-NB	-2.54	108.27	110.53
40	GG	615	LUT	C36-C21-C26	2.54	113.39	109.55
32	A	405	CLA	CHB-C4A-NA	2.54	128.06	124.40
32	B	609	CLA	C1-C2-C3	-2.53	122.04	126.20
34	b	618	BCR	C15-C16-C17	-2.53	118.33	123.52
40	Ss	615	LUT	C38-C25-C24	-2.53	117.36	123.36
39	Rr	605	CHL	C3C-C4C-NC	-2.53	108.46	114.65
39	22	605	CHL	C2A-C1A-CHA	2.53	126.04	121.84
32	c	513	CLA	CHB-C4A-NA	2.53	128.05	124.40
39	g	608	CHL	O2D-CGD-CBD	2.53	113.73	110.95
39	s	607	CHL	O2D-CGD-CBD	2.53	113.73	110.95
32	GG	611	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
32	YY	614	CLA	CHB-C4A-NA	2.53	128.05	124.40
39	RR	306	CHL	C3D-C4D-CHA	2.53	112.39	108.54
32	YY	604	CLA	CHB-C4A-NA	2.53	128.05	124.40
39	3	606	CHL	O2D-CGD-CBD	2.53	113.73	110.95
35	d	404	PL9	C30-C29-C31	-2.53	110.84	115.23
32	CC	509	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	GG	603	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	S	613	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
32	DD	403	CLA	CHB-C4A-NA	2.53	128.05	124.40
39	Yy	601	CHL	O2D-CGD-O1D	-2.53	118.93	123.85
39	22	607	CHL	O2D-CGD-CBD	2.53	113.72	110.95
32	C	510	CLA	CHB-C4A-NA	2.53	128.05	124.40
40	Gg	317	LUT	C16-C1-C6	2.53	114.21	110.24
32	g	613	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
32	Nn	304	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
32	CC	510	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	SS	304	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	n	602	CLA	CHB-C4A-NA	2.53	128.04	124.40
32	b	604	CLA	C4-C3-C5	2.53	119.61	115.23
33	A	407	PHO	O2D-CGD-O1D	-2.53	118.93	123.85
32	s	611	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
40	RR	315	LUT	C15-C35-C34	-2.53	118.35	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	DD	406	PL9	C30-C29-C31	-2.52	110.85	115.23
38	C	521	LMG	O8-C28-C29	2.52	119.53	111.83
34	C	517	BCR	C38-C26-C25	-2.52	121.73	124.48
32	X	201	CLA	CMA-C3A-C2A	-2.52	110.45	116.23
39	Yy	601	CHL	C3C-C4C-NC	-2.52	108.49	114.65
32	BB	607	CLA	CHB-C4A-NA	2.52	128.04	124.40
39	Y	606	CHL	O2D-CGD-O1D	-2.52	118.94	123.85
41	Yy	619	XAT	C40-C33-C34	-2.52	118.73	122.82
39	33	608	CHL	C3C-C4C-NC	-2.52	108.49	114.65
40	NN	616	LUT	C38-C25-C24	-2.52	117.40	123.36
41	4	314	XAT	C35-C15-C14	-2.52	118.37	123.52
34	K	102	BCR	C7-C8-C9	-2.52	122.51	126.23
39	GG	605	CHL	OMC-CMC-C2C	-2.52	120.75	125.12
36	C	522	LHG	O8-C23-C24	2.52	119.51	111.83
39	Gg	309	CHL	O2D-CGD-CBD	2.52	113.71	110.95
39	11	608	CHL	O2D-CGD-O1D	-2.52	118.95	123.85
39	y	303	CHL	C3C-C4C-NC	-2.52	108.50	114.65
32	y	305	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
32	y	312	CLA	C4A-NA-C1A	2.52	107.83	106.68
32	Bb	606	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
32	y	312	CLA	C3B-C4B-NB	-2.52	108.28	110.53
42	Rr	616	NEX	C20-C13-C14	-2.52	118.74	122.82
32	GG	613	CLA	CAC-C3C-C4C	2.52	128.06	124.79
32	BB	615	CLA	CAA-C2A-C3A	-2.52	110.46	116.23
32	C	504	CLA	CHB-C4A-NA	2.52	128.03	124.40
32	B	607	CLA	CHB-C4A-NA	2.52	128.03	124.40
39	Nn	311	CHL	O2D-CGD-CBD	2.52	113.71	110.95
39	Gg	310	CHL	C3C-C4C-NC	-2.51	108.50	114.65
32	Bb	604	CLA	C4-C3-C5	2.51	119.59	115.23
38	CC	520	LMG	O8-C28-C29	2.51	119.50	111.83
42	Y	619	NEX	C20-C13-C14	-2.51	118.74	122.82
42	Nn	309	NEX	C20-C13-C14	-2.51	118.74	122.82
32	y	305	CLA	CHB-C4A-NA	2.51	128.03	124.40
39	3	606	CHL	C3C-C4C-NC	-2.51	108.51	114.65
39	44	605	CHL	C4D-CHA-CBD	-2.51	106.43	108.97
32	g	613	CLA	CHC-C4B-NB	2.51	127.82	124.05
39	GG	608	CHL	C3C-C4C-NC	-2.51	108.51	114.65
32	BB	604	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
32	33	603	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
40	Y	615	LUT	C26-C27-C28	-2.51	120.67	124.58
32	AA	405	CLA	CHB-C4A-NA	2.51	128.02	124.40
35	AA	410	PL9	C53-C6-C1	2.51	120.42	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	44	605	CHL	O2D-CGD-CBD	2.51	113.70	110.95
34	CC	516	BCR	C24-C23-C22	-2.51	122.52	126.23
40	Yy	616	LUT	C3-C4-C5	-2.51	105.93	112.18
39	S	601	CHL	O2D-CGD-CBD	2.51	113.70	110.95
32	Yy	603	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
32	B	608	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	Cc	515	CLA	CHB-C4A-NA	2.51	128.02	124.40
39	11	605	CHL	C3C-C4C-NC	-2.51	108.52	114.65
35	A	410	PL9	C53-C6-C1	2.51	120.41	115.28
32	Ss	611	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
32	SS	314	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
36	y	320	LHG	O8-C23-C24	2.51	119.47	111.83
32	YY	602	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
41	Rr	615	XAT	O4-C5-C6	-2.51	56.94	58.93
40	Y	616	LUT	C18-C5-C4	2.50	119.03	114.42
32	b	612	CLA	CHB-C4A-NA	2.50	128.01	124.40
32	DD	401	CLA	CHB-C4A-NA	2.50	128.01	124.40
41	Rr	615	XAT	C16-C1-C2	-2.50	104.57	108.97
34	D	406	BCR	C29-C30-C25	2.50	114.07	110.44
39	n	607	CHL	O2A-CGA-O1A	-2.50	117.37	123.63
32	NN	610	CLA	C3B-C4B-NB	-2.50	108.30	110.53
39	Gg	302	CHL	C3C-C4C-NC	-2.50	108.54	114.65
32	G	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
32	SS	311	CLA	CHB-C4A-NA	2.50	128.01	124.40
34	KK	103	BCR	C36-C18-C19	2.50	121.91	118.09
32	G	602	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
32	CC	506	CLA	CAC-C3C-C4C	2.50	128.04	124.79
40	g	616	LUT	C19-C9-C8	2.50	121.91	118.09
39	Y	607	CHL	O2D-CGD-O1D	-2.50	118.98	123.85
32	C	512	CLA	C3B-C4B-NB	-2.50	108.30	110.53
36	1	614	LHG	O8-C23-C24	2.50	119.45	111.83
34	b	619	BCR	C2-C1-C6	2.50	114.07	110.44
39	r	606	CHL	C3D-C4D-CHA	2.50	112.33	108.54
38	Cc	501	LMG	C1-C2-C3	2.50	115.26	110.01
39	RR	307	CHL	C4D-CHA-CBD	-2.50	106.45	108.97
35	DD	406	PL9	C53-C6-C1	2.50	120.39	115.28
32	B	619	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
38	AA	415	LMG	C8-O7-C10	-2.50	111.82	117.80
32	b	606	CLA	CHB-C4A-NA	2.50	128.00	124.40
36	N	619	LHG	O8-C23-C24	2.50	119.44	111.83
34	XX	202	BCR	C1-C6-C7	2.49	122.42	115.65
32	C	512	CLA	CHB-C4A-NA	2.49	128.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	S	603	CLA	CHB-C4A-NA	2.49	128.00	124.40
39	YY	606	CHL	C3C-C4C-NC	-2.49	108.56	114.65
40	Gg	317	LUT	C19-C9-C8	2.49	121.90	118.09
32	N	611	CLA	CHB-C4A-NA	2.49	128.00	124.40
39	22	605	CHL	O2D-CGD-CBD	2.49	113.69	110.95
36	Gg	319	LHG	C5-O7-C7	-2.49	111.83	117.80
32	Cc	503	CLA	CHB-C4A-NA	2.49	128.00	124.40
39	Y	608	CHL	C3C-C4C-NC	-2.49	108.56	114.65
32	X	201	CLA	C3B-C4B-NB	-2.49	108.31	110.53
32	11	612	CLA	C1D-ND-C4D	-2.49	104.56	106.31
42	Rr	616	NEX	C5-C6-C1	2.49	122.17	119.70
40	N	616	LUT	C7-C8-C9	-2.49	122.55	126.23
39	Ss	605	CHL	C4D-CHA-CBD	-2.49	106.46	108.97
32	22	602	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
32	3	609	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
40	N	615	LUT	C20-C13-C12	2.49	121.89	118.09
34	C	516	BCR	C11-C10-C9	-2.49	123.79	127.28
39	y	303	CHL	O2D-CGD-O1D	-2.49	119.00	123.85
34	Dd	403	BCR	C27-C26-C25	-2.49	119.34	122.70
34	Bb	619	BCR	C2-C1-C6	2.49	114.05	110.44
32	C	511	CLA	CHB-C4A-NA	2.49	127.99	124.40
32	BB	615	CLA	CHB-C4A-NA	2.49	127.99	124.40
39	G	608	CHL	C3C-C4C-NC	-2.49	108.57	114.65
39	2	601	CHL	O2D-CGD-CBD	2.49	113.68	110.95
34	h	101	BCR	C38-C26-C27	2.49	118.90	113.60
32	RR	314	CLA	O2D-CGD-CBD	2.49	115.58	111.23
32	Rr	609	CLA	CHB-C4A-NA	2.49	127.99	124.40
35	A	410	PL9	C20-C19-C21	-2.48	110.92	115.23
39	r	607	CHL	O2D-CGD-CBD	2.48	113.68	110.95
32	n	613	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
32	BB	605	CLA	C1-C2-C3	-2.48	122.13	126.20
39	N	609	CHL	C3D-C4D-CHA	2.48	112.31	108.54
32	b	601	CLA	C1-C2-C3	-2.48	122.13	126.20
39	G	601	CHL	O2D-CGD-CBD	2.48	113.67	110.95
39	Y	606	CHL	O2D-CGD-CBD	2.48	113.67	110.95
39	n	607	CHL	C1-C2-C3	-2.48	122.13	126.20
34	CC	516	BCR	C37-C22-C23	2.48	121.88	118.09
32	Gg	303	CLA	C3B-C4B-NB	-2.48	108.31	110.53
39	Yy	609	CHL	C3C-C4C-NC	-2.48	108.59	114.65
33	AA	407	PHO	O2D-CGD-O1D	-2.48	119.02	123.85
39	n	608	CHL	O2D-CGD-CBD	2.48	113.67	110.95
32	s	603	CLA	CHB-C4A-NA	2.48	127.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	614	LUT	C26-C27-C28	-2.48	120.72	124.58
32	Y	610	CLA	CAA-C2A-C1A	-2.48	103.86	111.97
39	SS	308	CHL	C3C-C4C-NC	-2.48	108.60	114.65
32	4	311	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
32	BB	605	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
41	y	301	XAT	O24-C25-C26	-2.48	56.97	58.93
39	22	607	CHL	C3C-C4C-NC	-2.47	108.60	114.65
39	g	601	CHL	C3C-C4C-NC	-2.47	108.61	114.65
32	Ss	609	CLA	CHB-C4A-NA	2.47	127.97	124.40
32	r	613	CLA	CHB-C4A-NA	2.47	127.97	124.40
42	g	617	NEX	C36-C21-C26	2.47	116.72	110.05
41	r	615	XAT	C16-C1-C2	-2.47	104.62	108.97
39	Yy	609	CHL	C4D-CHA-CBD	-2.47	106.48	108.97
33	a	409	PHO	C3B-C4B-NB	-2.47	105.85	107.46
41	Rr	615	XAT	C4-C3-C2	-2.47	106.17	110.79
42	RR	317	NEX	C17-C1-C6	-2.47	108.26	110.47
40	RR	315	LUT	C7-C8-C9	-2.47	122.58	126.23
32	b	606	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
32	Yy	614	CLA	CHB-C4A-NA	2.47	127.96	124.40
39	GG	609	CHL	O1D-CGD-CBD	2.47	128.47	124.72
39	44	607	CHL	C3C-C4C-NC	-2.47	108.62	114.65
34	Cc	517	BCR	C27-C26-C25	-2.47	119.37	122.70
41	GG	617	XAT	C20-C13-C12	2.47	121.86	118.09
32	a	410	CLA	C3B-C4B-NB	-2.47	108.33	110.53
39	NN	606	CHL	O1D-CGD-CBD	2.47	128.46	124.72
32	D	401	CLA	CHB-C4A-NA	2.46	127.96	124.40
39	11	601	CHL	O2D-CGD-CBD	2.46	113.65	110.95
32	a	410	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
32	RR	314	CLA	CAC-C3C-C4C	2.46	128.00	124.79
32	Cc	508	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	DD	401	CLA	C3B-C4B-NB	-2.46	108.33	110.53
39	44	601	CHL	C3C-C4C-NC	-2.46	108.63	114.65
40	s	614	LUT	C38-C25-C24	-2.46	117.53	123.36
39	Ss	606	CHL	O1D-CGD-CBD	2.46	128.46	124.72
39	GG	608	CHL	O1D-CGD-CBD	2.46	128.46	124.72
39	r	606	CHL	C4D-CHA-CBD	-2.46	106.48	108.97
39	y	311	CHL	C4D-CHA-CBD	-2.46	106.48	108.97
34	H	101	BCR	C33-C5-C6	2.46	127.17	124.48
39	GG	601	CHL	C3C-C4C-NC	-2.46	108.64	114.65
32	N	610	CLA	C3B-C4B-NB	-2.46	108.33	110.53
32	Yy	610	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
32	n	614	CLA	O2D-CGD-O1D	-2.46	119.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Cc	508	CLA	C4-C3-C5	2.46	119.50	115.23
32	CC	507	CLA	CHB-C4A-NA	2.46	127.95	124.40
39	Gg	308	CHL	C3C-C4C-NC	-2.46	108.64	114.65
32	AA	408	CLA	C1-C2-C3	-2.46	122.17	126.20
32	c	506	CLA	C4-C3-C5	2.46	119.50	115.23
39	YY	606	CHL	O2D-CGD-CBD	2.46	113.65	110.95
32	44	604	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	BB	601	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
36	NN	619	LHG	O8-C23-C24	2.46	119.33	111.83
40	g	615	LUT	C36-C21-C26	2.46	113.27	109.55
40	Yy	616	LUT	C26-C27-C28	-2.46	120.75	124.58
32	44	602	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
32	NN	612	CLA	CHB-C4A-NA	2.46	127.95	124.40
39	SS	302	CHL	O2D-CGD-CBD	2.46	113.65	110.95
34	Kk	101	BCR	C34-C9-C10	-2.46	118.84	122.82
32	N	602	CLA	C3B-C4B-NB	-2.46	108.34	110.53
40	SS	315	LUT	C35-C15-C14	-2.46	118.49	123.52
40	YY	615	LUT	C35-C15-C14	-2.46	118.49	123.52
32	BB	613	CLA	C1-C2-C3	-2.46	122.17	126.20
34	B	613	BCR	C33-C5-C6	-2.46	121.81	124.48
32	y	316	CLA	CHB-C4A-NA	2.46	127.94	124.40
34	C	518	BCR	C27-C26-C25	-2.45	119.39	122.70
39	YY	609	CHL	C3C-C4C-NC	-2.45	108.65	114.65
37	L	102	SQD	O9-S-C6	2.45	110.42	106.76
34	d	403	BCR	C27-C26-C25	-2.45	119.39	122.70
39	g	607	CHL	C3C-C4C-NC	-2.45	108.66	114.65
32	NN	602	CLA	CAC-C3C-C4C	2.45	127.98	124.79
40	SS	315	LUT	C38-C25-C24	-2.45	117.56	123.36
32	Gg	311	CLA	CHB-C4A-NA	2.45	127.94	124.40
42	n	617	NEX	C20-C13-C14	-2.45	118.84	122.82
42	Gg	318	NEX	C38-C25-C26	-2.45	118.27	122.30
40	n	615	LUT	C36-C21-C26	2.45	113.26	109.55
32	R	602	CLA	CHB-C4A-NA	2.45	127.94	124.40
32	BB	615	CLA	O2D-CGD-CBD	2.45	115.51	111.23
32	B	605	CLA	O2D-CGD-CBD	2.45	115.51	111.23
40	Ss	615	LUT	C20-C13-C12	2.45	121.83	118.09
32	B	611	CLA	CAA-C2A-C3A	-2.45	110.61	116.23
32	Rr	601	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	C	503	CLA	CHB-C4A-NA	2.45	127.93	124.40
35	D	407	PL9	C7-C3-C4	2.45	118.93	116.91
32	Cc	505	CLA	C3B-C4B-NB	-2.45	108.34	110.53
39	4	309	CHL	C3C-C4C-NC	-2.45	108.67	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	RR	310	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	c	506	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	a	405	CLA	CAC-C3C-C4C	2.45	127.97	124.79
32	Ss	608	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
39	4	302	CHL	C3C-C4C-NC	-2.44	108.67	114.65
39	SS	306	CHL	C3C-C4C-NC	-2.44	108.67	114.65
36	EE	101	LHG	O8-C23-C24	2.44	119.29	111.83
35	d	404	PL9	C35-C34-C36	-2.44	110.99	115.23
36	GG	618	LHG	O8-C23-C24	2.44	119.28	111.83
34	B	612	BCR	C2-C1-C6	2.44	113.99	110.44
34	T	101	BCR	C4-C5-C6	-2.44	119.40	122.70
36	Yy	618	LHG	O8-C23-C24	2.44	119.28	111.83
32	CC	510	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
32	Aa	406	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
39	GG	601	CHL	O2D-CGD-CBD	2.44	113.63	110.95
44	c	517	DGD	O6D-C5D-C6D	2.44	111.53	106.69
32	y	306	CLA	CHB-C4A-NA	2.44	127.92	124.40
39	R	607	CHL	C4D-CHA-CBD	-2.44	106.51	108.97
42	Rr	616	NEX	C32-C33-C34	-2.44	115.17	119.01
35	D	407	PL9	C53-C6-C1	2.44	120.27	115.28
34	Cc	516	BCR	C11-C10-C9	-2.44	123.86	127.28
39	G	601	CHL	C3C-C4C-NC	-2.44	108.69	114.65
32	r	602	CLA	CHB-C4A-NA	2.44	127.92	124.40
42	Nn	309	NEX	C32-C33-C34	-2.44	115.17	119.01
32	y	315	CLA	CHB-C4A-NA	2.44	127.92	124.40
39	G	606	CHL	C3C-C4C-NC	-2.44	108.69	114.65
34	C	517	BCR	C24-C23-C22	-2.44	122.63	126.23
34	k	101	BCR	C16-C15-C14	-2.44	118.53	123.52
40	s	615	LUT	C20-C13-C12	2.44	121.81	118.09
32	Rr	612	CLA	CHB-C4A-NA	2.44	127.91	124.40
39	Gg	302	CHL	O2D-CGD-CBD	2.43	113.62	110.95
33	Aa	409	PHO	C3B-C4B-NB	-2.43	105.88	107.46
32	YY	610	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
34	Dd	403	BCR	C33-C5-C4	2.43	118.78	113.60
32	Rr	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
32	Y	614	CLA	CHB-C4A-NA	2.43	127.91	124.40
32	RR	304	CLA	CHB-C4A-NA	2.43	127.91	124.40
39	Gg	306	CHL	C3C-C4C-NC	-2.43	108.71	114.65
33	A	407	PHO	CMB-C2B-C3B	2.43	129.54	124.68
34	C	517	BCR	C37-C22-C23	2.43	121.80	118.09
32	Bb	606	CLA	CHB-C4A-NA	2.43	127.91	124.40
35	Dd	404	PL9	C53-C6-C1	2.43	120.26	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Cc	517	BCR	C3-C4-C5	-2.43	109.72	114.06
32	Nn	301	CLA	CHB-C4A-NA	2.43	127.91	124.40
39	r	605	CHL	C3C-C4C-NC	-2.43	108.71	114.65
40	Ss	614	LUT	C38-C25-C24	-2.43	117.61	123.36
32	N	612	CLA	CHB-C4A-NA	2.43	127.91	124.40
39	33	607	CHL	C3C-C4C-NC	-2.43	108.71	114.65
32	BB	602	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
39	Ss	601	CHL	C3C-C4C-NC	-2.43	108.72	114.65
39	y	309	CHL	C3C-C4C-NC	-2.43	108.72	114.65
39	3	605	CHL	C3C-C4C-NC	-2.43	108.72	114.65
32	D	404	CLA	O2D-CGD-CBD	2.43	115.47	111.23
36	Dd	407	LHG	O8-C23-C24	2.43	119.23	111.83
32	Yy	602	CLA	CHB-C4A-NA	2.43	127.90	124.40
42	RR	317	NEX	C11-C10-C9	-2.43	123.88	127.28
34	Hh	101	BCR	C12-C13-C14	-2.43	115.19	119.01
32	A	408	CLA	CHB-C4A-NA	2.43	127.90	124.40
41	44	613	XAT	C12-C13-C14	-2.43	115.19	119.01
32	BB	605	CLA	CHB-C4A-NA	2.43	127.90	124.40
38	A	415	LMG	C8-O7-C10	-2.43	111.99	117.80
32	Gg	304	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
34	D	406	BCR	C38-C26-C25	-2.42	121.84	124.48
32	b	602	CLA	O1D-CGD-CBD	2.42	129.30	124.52
32	r	601	CLA	CHB-C4A-NA	2.42	127.90	124.40
40	Y	615	LUT	C35-C15-C14	-2.42	118.56	123.52
39	GG	609	CHL	C3C-C4C-NC	-2.42	108.73	114.65
32	y	313	CLA	C3B-C4B-NB	-2.42	108.37	110.53
40	y	318	LUT	C38-C25-C24	-2.42	117.63	123.36
32	NN	610	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
39	Ss	607	CHL	C3C-C4C-NC	-2.42	108.73	114.65
32	C	511	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
39	4	307	CHL	C3C-C4C-NC	-2.42	108.73	114.65
39	Yy	608	CHL	C3C-C4C-NC	-2.42	108.74	114.65
39	44	608	CHL	C3C-C4C-NC	-2.42	108.74	114.65
32	11	604	CLA	CHB-C4A-NA	2.42	127.89	124.40
32	Aa	410	CLA	CHB-C4A-NA	2.42	127.89	124.40
39	YY	607	CHL	C3C-C4C-NC	-2.42	108.74	114.65
35	D	407	PL9	C30-C29-C31	-2.42	111.03	115.23
32	r	609	CLA	CHB-C4A-NA	2.42	127.89	124.40
35	d	404	PL9	C53-C6-C1	2.42	120.23	115.28
32	2	602	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
41	y	302	XAT	C15-C35-C34	-2.42	118.57	123.52
32	B	620	CLA	O2A-CGA-O1A	-2.42	117.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	44	606	CHL	C3C-C4C-NC	-2.42	108.74	114.65
39	y	310	CHL	C3C-C4C-NC	-2.42	108.74	114.65
39	1	605	CHL	C4D-CHA-CBD	-2.42	106.53	108.97
32	Aa	406	CLA	O2D-CGD-CBD	2.42	115.45	111.23
32	XX	201	CLA	C3B-C4B-NB	-2.42	108.37	110.53
39	Yy	607	CHL	C4D-CHA-CBD	-2.42	106.53	108.97
32	Ss	603	CLA	CHB-C4A-NA	2.41	127.89	124.40
34	A	409	BCR	C27-C26-C25	-2.41	119.44	122.70
39	NN	609	CHL	C3D-C4D-CHA	2.41	112.21	108.54
39	33	606	CHL	C3C-C4C-NC	-2.41	108.75	114.65
39	3	607	CHL	C3C-C4C-NC	-2.41	108.75	114.65
39	GG	606	CHL	C3C-C4C-NC	-2.41	108.75	114.65
32	NN	613	CLA	CHB-C4A-NA	2.41	127.88	124.40
39	RR	305	CHL	CAA-CBA-CGA	-2.41	106.36	113.21
42	Gg	318	NEX	C12-C13-C14	-2.41	115.22	119.01
35	DD	406	PL9	C25-C24-C26	-2.41	111.04	115.23
32	C	508	CLA	CHB-C4A-NA	2.41	127.88	124.40
35	A	410	PL9	C40-C39-C41	-2.41	111.04	115.23
39	GG	609	CHL	O2D-CGD-CBD	2.41	113.59	110.95
39	NN	605	CHL	C4D-CHA-CBD	-2.41	106.54	108.97
32	CC	502	CLA	C3B-C4B-NB	-2.41	108.38	110.53
39	Ss	605	CHL	CMD-C2D-C3D	2.41	129.50	124.68
40	s	615	LUT	C38-C25-C24	-2.41	117.66	123.36
32	RR	313	CLA	CAC-C3C-C4C	2.41	127.92	124.79
40	Ss	615	LUT	C12-C13-C14	-2.41	115.22	119.01
32	RR	303	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
32	a	406	CLA	O2D-CGD-CBD	2.41	115.44	111.23
40	2	614	LUT	C15-C35-C34	2.41	128.45	123.52
39	YY	608	CHL	C3C-C4C-NC	-2.41	108.77	114.65
32	Nn	314	CLA	C3B-C4B-NB	-2.41	108.38	110.53
32	BB	608	CLA	CHB-C4A-NA	2.41	127.87	124.40
39	Rr	606	CHL	C3D-C4D-CHA	2.41	112.20	108.54
32	s	613	CLA	CHB-C4A-NA	2.41	127.87	124.40
40	G	616	LUT	C20-C13-C12	2.41	121.76	118.09
36	l	101	LHG	O8-C23-C24	2.41	119.17	111.83
39	22	605	CHL	C3C-C4C-NC	-2.41	108.77	114.65
39	R	605	CHL	CAA-CBA-CGA	-2.41	106.38	113.21
32	C	505	CLA	C6-C5-C3	2.41	119.33	113.47
32	Cc	508	CLA	C3B-C4B-NB	-2.41	108.38	110.53
40	Ss	614	LUT	C8-C9-C10	-2.41	115.23	119.01
39	22	608	CHL	C3C-C4C-NC	-2.40	108.77	114.65
34	BB	620	BCR	C12-C13-C14	-2.40	115.23	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Y	609	CHL	OMC-CMC-C2C	-2.40	120.95	125.12
39	Ss	606	CHL	C3D-C4D-CHA	2.40	112.19	108.54
32	a	410	CLA	CHB-C4A-NA	2.40	127.87	124.40
32	R	614	CLA	O2D-CGD-CBD	2.40	115.43	111.23
32	Y	610	CLA	CHB-C4A-NA	2.40	127.87	124.40
40	s	614	LUT	C12-C13-C14	-2.40	115.23	119.01
32	B	611	CLA	O2D-CGD-CBD	2.40	115.43	111.23
34	DD	405	BCR	C33-C5-C4	2.40	118.71	113.60
39	s	601	CHL	C3C-C4C-NC	-2.40	108.79	114.65
39	Yy	606	CHL	C3C-C4C-NC	-2.40	108.79	114.65
44	C	523	DGD	O1G-C1A-C2A	2.40	119.15	111.83
39	NN	609	CHL	C4D-CHA-CBD	-2.40	106.55	108.97
32	Ss	613	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	B	622	CLA	CHB-C4A-NA	2.40	127.86	124.40
34	d	403	BCR	C33-C5-C4	2.40	118.71	113.60
32	S	610	CLA	CHB-C4A-NA	2.40	127.86	124.40
42	Yy	617	NEX	C32-C33-C34	-2.40	115.24	119.01
32	g	603	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
32	Cc	511	CLA	CHB-C4A-NA	2.40	127.86	124.40
39	3	608	CHL	C3C-C4C-NC	-2.40	108.79	114.65
40	y	318	LUT	C20-C13-C12	2.40	121.75	118.09
34	BB	620	BCR	C33-C5-C4	2.40	118.70	113.60
39	g	608	CHL	C3C-C4C-NC	-2.40	108.80	114.65
39	N	605	CHL	O2D-CGD-O1D	-2.40	119.19	123.85
32	3	613	CLA	CHB-C4A-NA	2.40	127.86	124.40
39	NN	605	CHL	C3C-C4C-NC	-2.40	108.80	114.65
32	Aa	406	CLA	CHB-C4A-NA	2.39	127.86	124.40
32	Bb	612	CLA	CHB-C4A-NA	2.39	127.85	124.40
39	Nn	311	CHL	C4D-CHA-CBD	-2.39	106.55	108.97
39	2	601	CHL	C3C-C4C-NC	-2.39	108.80	114.65
32	B	605	CLA	CHB-C4A-NA	2.39	127.85	124.40
39	s	606	CHL	C3D-C4D-CHA	2.39	112.18	108.54
39	N	606	CHL	C3C-C4C-NC	-2.39	108.80	114.65
39	11	605	CHL	O1D-CGD-CBD	2.39	128.35	124.72
39	Y	607	CHL	C3C-C4C-NC	-2.39	108.80	114.65
39	Gg	309	CHL	C3C-C4C-NC	-2.39	108.80	114.65
32	A	408	CLA	C1-C2-C3	-2.39	122.28	126.20
45	D	403	BCT	O3-C-O1	-2.39	113.56	119.68
36	JJ	101	LHG	C5-O7-C7	-2.39	112.08	117.80
39	g	605	CHL	C3C-C4C-NC	-2.39	108.81	114.65
46	e	101	HEM	C1B-NB-C4B	2.39	108.04	105.21
39	Rr	607	CHL	O1D-CGD-CBD	2.39	128.35	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BB	621	SQD	O5-C5-C4	-2.39	105.39	109.70
39	G	608	CHL	O2D-CGD-CBD	2.39	113.57	110.95
39	4	309	CHL	C3D-C4D-CHA	2.39	112.17	108.54
40	YY	616	LUT	C19-C9-C8	2.39	121.74	118.09
39	s	606	CHL	CHA-C1A-C2A	-2.39	127.70	133.31
32	33	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
41	R	616	XAT	C8-C9-C10	-2.39	115.25	119.01
32	GG	613	CLA	CHB-C4A-NA	2.39	127.84	124.40
39	Ss	605	CHL	C3D-C4D-CHA	2.39	112.17	108.54
40	Y	615	LUT	C38-C25-C24	-2.39	117.71	123.36
32	a	406	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
39	G	607	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
42	R	617	NEX	C11-C10-C9	-2.39	123.93	127.28
32	AA	408	CLA	CHB-C4A-NA	2.39	127.84	124.40
32	BB	613	CLA	CHB-C4A-NA	2.39	127.84	124.40
34	D	406	BCR	C33-C5-C4	2.38	118.68	113.60
32	A	408	CLA	C3B-C4B-NB	-2.38	108.40	110.53
32	Cc	504	CLA	C3B-C4B-NB	-2.38	108.40	110.53
32	r	604	CLA	CHB-C4A-NA	2.38	127.84	124.40
32	BB	610	CLA	CHB-C4A-NA	2.38	127.84	124.40
32	AA	405	CLA	CAC-C3C-C4C	2.38	127.89	124.79
32	B	618	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
32	c	506	CLA	C3B-C4B-NB	-2.38	108.40	110.53
34	Dd	403	BCR	C33-C5-C6	-2.38	121.88	124.48
34	BB	620	BCR	C24-C23-C22	-2.38	122.71	126.23
32	11	612	CLA	CHC-C4B-NB	2.38	127.62	124.05
32	SS	313	CLA	CHB-C4A-NA	2.38	127.84	124.40
32	Yy	602	CLA	C3B-C4B-NB	-2.38	108.40	110.53
39	n	605	CHL	C4D-CHA-CBD	-2.38	106.56	108.97
32	Gg	311	CLA	C3B-C4B-NB	-2.38	108.40	110.53
34	Hh	101	BCR	C36-C18-C17	-2.38	118.96	122.82
39	n	607	CHL	C3D-C4D-CHA	2.38	112.16	108.54
32	BB	604	CLA	C3B-C4B-NB	-2.38	108.41	110.53
32	Bb	601	CLA	C3B-C4B-NB	-2.38	108.41	110.53
34	BB	616	BCR	C2-C1-C6	2.38	113.89	110.44
34	A	409	BCR	C40-C30-C25	-2.38	106.51	110.24
34	BB	617	BCR	C33-C5-C6	-2.38	121.89	124.48
32	Y	611	CLA	CHB-C4A-NA	2.38	127.83	124.40
39	RR	306	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
39	r	607	CHL	O2A-CGA-O1A	-2.38	117.68	123.63
39	4	302	CHL	O2D-CGD-O1D	-2.38	118.69	124.08
39	11	606	CHL	C3C-C4C-NC	-2.38	108.84	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	r	614	LUT	C19-C9-C8	2.38	121.72	118.09
41	G	617	XAT	C35-C15-C14	-2.38	118.66	123.52
34	c	515	BCR	C39-C30-C25	-2.38	106.52	110.24
32	Aa	407	CLA	C3B-C4B-NB	-2.38	108.41	110.53
39	3	601	CHL	C3D-C4D-CHA	2.38	112.15	108.54
32	BB	611	CLA	CHB-C4A-NA	2.38	127.83	124.40
39	Nn	319	CHL	C3C-C4C-NC	-2.38	108.84	114.65
41	y	302	XAT	C26-C27-C28	-2.38	120.97	125.99
32	Y	602	CLA	CHB-C4A-NA	2.37	127.83	124.40
32	Bb	614	CLA	CHB-C4A-NA	2.37	127.83	124.40
40	R	615	LUT	C15-C35-C34	-2.37	118.66	123.52
34	Bb	619	BCR	C33-C5-C6	-2.37	121.89	124.48
42	RR	317	NEX	C32-C33-C34	-2.37	115.27	119.01
34	c	516	BCR	C29-C30-C25	2.37	113.89	110.44
32	Rr	613	CLA	CHB-C4A-NA	2.37	127.83	124.40
32	r	602	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
32	a	406	CLA	CHD-C1D-ND	-2.37	121.46	124.80
34	KK	103	BCR	C33-C5-C6	-2.37	121.89	124.48
39	2	608	CHL	C3C-C4C-NC	-2.37	108.85	114.65
39	Gg	307	CHL	C3C-C4C-NC	-2.37	108.85	114.65
34	B	612	BCR	C28-C27-C26	-2.37	109.82	114.06
32	c	508	CLA	CHB-C4A-NA	2.37	127.83	124.40
32	B	621	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
32	Aa	405	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
32	BB	603	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
36	g	618	LHG	C5-O7-C7	-2.37	112.12	117.80
32	BB	609	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	n	602	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
32	RR	302	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
32	Aa	410	CLA	C3B-C4B-NB	-2.37	108.41	110.53
39	s	607	CHL	C3C-C4C-NC	-2.37	108.86	114.65
35	Dd	404	PL9	C25-C24-C26	-2.37	111.11	115.23
32	RR	302	CLA	O2D-CGD-CBD	2.37	115.37	111.23
39	G	607	CHL	C3C-C4C-NC	-2.37	108.86	114.65
36	22	615	LHG	O8-C23-C24	2.37	119.06	111.83
38	c	519	LMG	O8-C28-C29	2.37	119.06	111.83
41	Gg	301	XAT	C31-C30-C29	-2.37	123.95	127.28
39	n	601	CHL	C4D-CHA-CBD	-2.37	106.58	108.97
39	n	605	CHL	C3C-C4C-NC	-2.37	108.86	114.65
32	S	609	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	Y	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	s	604	CLA	CHB-C4A-NA	2.37	127.82	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	44	601	CHL	O2D-CGD-O1D	-2.37	118.71	124.08
41	y	301	XAT	C38-C25-C24	-2.37	111.58	114.24
32	Bb	609	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
32	BB	609	CLA	O2D-CGD-CBD	2.37	115.37	111.23
39	Y	609	CHL	C1-C2-C3	-2.37	122.32	126.20
39	n	609	CHL	C3C-C4C-NC	-2.37	108.86	114.65
34	h	101	BCR	C27-C26-C25	-2.37	119.50	122.70
32	Yy	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	n	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	BB	609	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
39	NN	607	CHL	C3C-C4C-NC	-2.37	108.87	114.65
36	SS	301	LHG	O7-C7-C8	2.37	119.62	110.93
41	GG	617	XAT	C35-C15-C14	-2.37	118.68	123.52
32	y	304	CLA	C3B-C4B-NB	-2.37	108.42	110.53
39	11	607	CHL	C2A-C3A-C4A	-2.37	101.99	103.53
32	S	612	CLA	CHB-C4A-NA	2.37	127.81	124.40
32	y	304	CLA	CHB-C4A-NA	2.37	127.81	124.40
43	R	618	LMU	C1-O1'-C1'	2.36	117.72	113.68
38	a	412	LMG	C8-O7-C10	-2.36	112.14	117.80
32	Aa	410	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
40	22	614	LUT	C19-C9-C8	2.36	121.70	118.09
39	N	607	CHL	C3C-C4C-NC	-2.36	108.87	114.65
39	GG	607	CHL	C3C-C4C-NC	-2.36	108.87	114.65
32	BB	609	CLA	CAC-C3C-C4C	2.36	127.86	124.79
32	B	605	CLA	CAC-C3C-C4C	2.36	127.86	124.79
39	2	605	CHL	C3C-C4C-NC	-2.36	108.88	114.65
34	c	515	BCR	C3-C4-C5	-2.36	109.84	114.06
39	2	607	CHL	C3C-C4C-NC	-2.36	108.88	114.65
32	C	507	CLA	CAC-C3C-C4C	2.36	127.86	124.79
34	CC	515	BCR	C11-C10-C9	-2.36	123.97	127.28
39	SS	306	CHL	O2D-CGD-CBD	2.36	113.54	110.95
39	r	606	CHL	CHA-C1A-C2A	-2.36	127.76	133.31
39	n	605	CHL	C3D-C4D-CHA	2.36	112.13	108.54
32	YY	610	CLA	C3B-C4B-NB	-2.36	108.42	110.53
39	G	609	CHL	O1D-CGD-CBD	2.36	128.30	124.72
40	g	616	LUT	C36-C21-C26	2.36	113.12	109.55
32	D	405	CLA	CHB-C4A-NA	2.36	127.81	124.40
41	Yy	619	XAT	C38-C25-C24	-2.36	111.59	114.24
32	Nn	301	CLA	CAC-C3C-C4C	2.36	127.86	124.79
32	Aa	407	CLA	CHB-C4A-NA	2.36	127.80	124.40
40	S	614	LUT	C38-C25-C24	-2.36	117.78	123.36
39	33	605	CHL	C3C-C4C-NC	-2.36	108.89	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	AA	410	PL9	C20-C19-C21	-2.36	111.14	115.23
32	SS	303	CLA	CHB-C4A-NA	2.36	127.80	124.40
32	D	401	CLA	C3B-C4B-NB	-2.36	108.43	110.53
40	N	615	LUT	C12-C13-C14	-2.36	115.30	119.01
39	2	608	CHL	O2D-CGD-CBD	2.36	113.53	110.95
34	AA	409	BCR	C37-C22-C23	-2.36	114.49	118.09
32	r	612	CLA	CHB-C4A-NA	2.36	127.80	124.40
34	C	518	BCR	C24-C23-C22	-2.36	122.75	126.23
34	CC	516	BCR	C40-C30-C25	2.35	113.94	110.24
40	n	615	LUT	C15-C35-C34	-2.35	118.70	123.52
32	R	610	CLA	C3B-C4B-NB	-2.35	108.43	110.53
40	NN	615	LUT	C20-C13-C12	2.35	121.69	118.09
34	Cc	516	BCR	C34-C9-C8	-2.35	114.49	118.09
32	2	613	CLA	CHB-C4A-NA	2.35	127.80	124.40
32	B	605	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
39	g	601	CHL	O2D-CGD-CBD	2.35	113.53	110.95
39	G	608	CHL	C4C-CHD-C1D	2.35	124.48	116.07
39	s	605	CHL	C3D-C4D-CHA	2.35	112.11	108.54
39	n	601	CHL	O2D-CGD-CBD	2.35	113.53	110.95
32	Cc	508	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
39	Gg	310	CHL	O2D-CGD-CBD	2.35	113.53	110.95
39	NN	606	CHL	C3C-C4C-NC	-2.35	108.91	114.65
41	G	619	XAT	C39-C29-C28	2.35	121.68	118.09
32	S	602	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
39	NN	605	CHL	C3D-C4D-CHA	2.35	112.11	108.54
32	YY	602	CLA	CHB-C4A-NA	2.35	127.79	124.40
39	GG	607	CHL	C4D-CHA-CBD	-2.35	106.60	108.97
39	Y	606	CHL	C3C-C4C-NC	-2.35	108.91	114.65
34	b	617	BCR	C3-C4-C5	-2.35	109.87	114.06
39	Ss	607	CHL	CMD-C2D-C3D	2.35	129.38	124.68
32	A	405	CLA	CAC-C3C-C4C	2.35	127.84	124.79
35	DD	406	PL9	C7-C3-C4	2.35	118.84	116.91
34	DD	405	BCR	C38-C26-C25	-2.35	121.92	124.48
40	Ss	615	LUT	C8-C9-C10	-2.35	115.32	119.01
42	Y	619	NEX	C32-C33-C34	-2.35	115.32	119.01
39	R	606	CHL	C4C-CHD-C1D	2.35	124.47	116.07
32	R	602	CLA	C3B-C4B-NB	-2.35	108.44	110.53
32	Bb	607	CLA	C3B-C4B-NB	-2.35	108.44	110.53
32	N	613	CLA	CHB-C4A-NA	2.35	127.79	124.40
34	C	518	BCR	C7-C6-C5	-2.35	116.15	121.56
38	Cc	501	LMG	O8-C28-C29	2.35	118.99	111.83
32	CC	514	CLA	CHB-C4A-NA	2.35	127.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Rr	602	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
39	33	601	CHL	CMD-C2D-C3D	2.34	129.37	124.68
39	S	605	CHL	C3C-C4C-NC	-2.34	108.92	114.65
32	Gg	304	CLA	CHB-C4A-NA	2.34	127.78	124.40
32	B	623	CLA	CHB-C4A-NA	2.34	127.78	124.40
32	b	601	CLA	C3B-C4B-NB	-2.34	108.44	110.53
32	CC	502	CLA	CBA-CAA-C2A	2.34	120.77	113.79
35	d	404	PL9	C25-C24-C26	-2.34	111.16	115.23
32	BB	611	CLA	C3B-C4B-NB	-2.34	108.44	110.53
32	a	406	CLA	C1D-ND-C4D	-2.34	104.67	106.31
40	Rr	614	LUT	C15-C35-C34	-2.34	118.73	123.52
32	Gg	315	CLA	CHB-C4A-NA	2.34	127.78	124.40
34	Dd	403	BCR	C1-C6-C7	2.34	122.00	115.65
40	S	614	LUT	C15-C35-C34	-2.34	118.73	123.52
39	1	605	CHL	C3C-C4C-NC	-2.34	108.93	114.65
32	Gg	312	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
39	G	607	CHL	C4D-CHA-CBD	-2.34	106.61	108.97
40	G	616	LUT	C35-C15-C14	-2.34	118.73	123.52
39	N	608	CHL	C3C-C4C-NC	-2.34	108.93	114.65
34	c	516	BCR	C15-C16-C17	-2.34	118.73	123.52
39	Rr	607	CHL	O2A-CGA-O1A	-2.34	117.78	123.63
38	a	412	LMG	O1-C1-C2	2.34	111.83	108.27
39	RR	305	CHL	C3D-C4D-CHA	2.34	112.09	108.54
43	KK	102	LMU	C1'-O5'-C5'	2.34	118.29	113.72
41	r	615	XAT	O4-C5-C6	-2.34	57.08	58.93
33	D	402	PHO	CMB-C2B-C3B	2.34	129.36	124.68
36	0	201	LHG	O8-C23-C24	2.34	118.97	111.83
32	B	618	CLA	O2D-CGD-CBD	2.34	115.32	111.23
34	CC	516	BCR	C2-C1-C6	2.34	113.83	110.44
44	CC	518	DGD	O6D-C5D-C6D	2.34	111.33	106.69
39	1	606	CHL	C3C-C4C-NC	-2.34	108.94	114.65
39	s	605	CHL	C3C-C4C-NC	-2.34	108.94	114.65
32	B	604	CLA	C3B-C4B-NB	-2.34	108.44	110.53
39	n	606	CHL	C3C-C4C-NC	-2.34	108.94	114.65
32	C	507	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
32	Nn	304	CLA	CHB-C4A-NA	2.34	127.77	124.40
32	B	606	CLA	CHB-C4A-NA	2.33	127.77	124.40
42	N	618	NEX	C15-C14-C13	-2.33	124.00	127.28
36	D	410	LHG	O8-C23-C24	2.33	118.95	111.83
39	N	601	CHL	C4C-CHD-C1D	2.33	124.42	116.07
34	DD	405	BCR	C27-C26-C25	-2.33	119.55	122.70
32	SS	303	CLA	O2A-CGA-O1A	-2.33	117.79	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	R	616	XAT	C24-C23-C22	-2.33	106.43	110.79
39	s	606	CHL	O1D-CGD-CBD	2.33	128.26	124.72
39	1	605	CHL	C3D-C4D-CHA	2.33	112.08	108.54
39	s	605	CHL	C4D-CHA-CBD	-2.33	106.61	108.97
40	n	616	LUT	C19-C9-C8	2.33	121.65	118.09
34	Cc	518	BCR	C15-C16-C17	-2.33	118.75	123.52
42	Y	617	NEX	C17-C1-C6	-2.33	108.39	110.47
32	DD	401	CLA	CAA-CBA-CGA	-2.33	106.59	113.21
41	y	302	XAT	C20-C13-C14	-2.33	119.04	122.82
39	Yy	606	CHL	C4D-CHA-CBD	-2.33	106.62	108.97
39	G	605	CHL	C3C-C4C-NC	-2.33	108.95	114.65
39	3	607	CHL	C2A-C1A-CHA	2.33	125.71	121.84
40	N	615	LUT	C38-C25-C24	-2.33	117.85	123.36
32	4	305	CLA	CHB-C4A-NA	2.33	127.76	124.40
39	Nn	317	CHL	C3D-C4D-CHA	2.33	112.08	108.54
40	y	318	LUT	C40-C33-C32	2.33	121.65	118.09
32	Yy	611	CLA	C3B-C4B-NB	-2.33	108.45	110.53
39	33	606	CHL	O2D-CGD-CBD	2.33	113.50	110.95
32	Cc	506	CLA	CAC-C3C-C4C	2.33	127.82	124.79
39	YY	605	CHL	C3C-C4C-NC	-2.33	108.96	114.65
32	c	506	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
41	N	617	XAT	C36-C21-C22	-2.33	104.88	108.97
32	Bb	609	CLA	C1-C2-C3	-2.33	122.39	126.20
39	N	607	CHL	C1-C2-C3	-2.33	122.39	126.20
34	b	617	BCR	C39-C30-C25	-2.33	106.59	110.24
39	n	601	CHL	C3C-C4C-NC	-2.33	108.97	114.65
39	y	311	CHL	C3C-C4C-NC	-2.33	108.97	114.65
40	Ss	614	LUT	C12-C13-C14	-2.33	115.35	119.01
32	44	615	CLA	CHB-C4A-NA	2.33	127.76	124.40
32	Aa	406	CLA	CHD-C1D-ND	-2.33	121.53	124.80
32	A	405	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
34	C	518	BCR	C4-C5-C6	-2.33	119.56	122.70
34	CC	517	BCR	C4-C5-C6	-2.33	119.56	122.70
45	a	413	BCT	O3-C-O1	-2.32	113.73	119.68
39	S	606	CHL	C3C-C4C-NC	-2.32	108.97	114.65
32	S	608	CLA	C3B-C4B-NB	-2.32	108.45	110.53
34	CC	515	BCR	C2-C3-C4	-2.32	106.17	111.28
39	2	605	CHL	C2A-C1A-CHA	2.32	125.69	121.84
39	NN	608	CHL	C3C-C4C-NC	-2.32	108.97	114.65
32	n	610	CLA	C4A-NA-C1A	2.32	107.74	106.68
32	SS	314	CLA	C3B-C4B-NB	-2.32	108.46	110.53
39	y	310	CHL	C4C-CHD-C1D	2.32	124.38	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	GG	619	XAT	C12-C13-C14	-2.32	115.36	119.01
34	BB	620	BCR	C35-C13-C12	2.32	121.64	118.09
40	Gg	317	LUT	C15-C35-C34	-2.32	118.77	123.52
32	4	304	CLA	CAC-C3C-C4C	2.32	127.81	124.79
32	RR	302	CLA	C1-C2-C3	-2.32	122.39	126.20
34	h	101	BCR	C4-C5-C6	-2.32	119.57	122.70
41	N	617	XAT	C15-C35-C34	-2.32	118.77	123.52
39	n	608	CHL	C3C-C4C-NC	-2.32	108.98	114.65
40	Rr	614	LUT	C38-C25-C24	-2.32	117.87	123.36
40	GG	616	LUT	C35-C15-C14	-2.32	118.77	123.52
34	b	617	BCR	C24-C23-C22	-2.32	122.80	126.23
32	R	601	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
40	y	317	LUT	C1-C2-C3	2.32	118.68	113.59
32	BB	614	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
32	B	609	CLA	CHB-C4A-NA	2.32	127.75	124.40
32	r	613	CLA	C3B-C4B-NB	-2.32	108.46	110.53
32	N	610	CLA	CHB-C4A-NA	2.32	127.75	124.40
32	b	604	CLA	CHB-C4A-NA	2.32	127.75	124.40
32	b	609	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
39	Yy	608	CHL	C4C-CHD-C1D	2.32	124.36	116.07
39	y	310	CHL	O1D-CGD-CBD	2.32	128.24	124.72
40	Gg	317	LUT	C38-C25-C24	-2.32	117.88	123.36
40	Rr	614	LUT	C19-C9-C8	2.32	121.63	118.09
39	Yy	607	CHL	C4C-CHD-C1D	2.32	124.36	116.07
40	N	616	LUT	C16-C1-C6	2.32	113.88	110.24
40	Y	616	LUT	C26-C27-C28	-2.32	120.97	124.58
39	GG	605	CHL	C3C-C4C-NC	-2.32	108.99	114.65
40	Nn	307	LUT	C15-C35-C34	-2.32	118.78	123.52
39	R	606	CHL	C3D-C4D-CHA	2.32	112.06	108.54
40	S	614	LUT	C19-C9-C8	2.31	121.62	118.09
32	s	609	CLA	CHB-C4A-NA	2.31	127.74	124.40
32	Cc	513	CLA	C1-C2-C3	-2.31	122.41	126.20
32	Dd	402	CLA	C3B-C4B-NB	-2.31	108.46	110.53
32	g	602	CLA	CED-O2D-CGD	-2.31	110.67	115.92
32	CC	504	CLA	CHB-C4A-NA	2.31	127.74	124.40
39	44	601	CHL	C4C-CHD-C1D	2.31	124.35	116.07
39	NN	607	CHL	C1-C2-C3	-2.31	122.41	126.20
32	B	624	CLA	CHB-C4A-NA	2.31	127.74	124.40
32	Bb	604	CLA	CHB-C4A-NA	2.31	127.74	124.40
39	Y	605	CHL	C3C-C4C-NC	-2.31	109.00	114.65
32	s	602	CLA	CHB-C4A-NA	2.31	127.74	124.40
32	BB	606	CLA	CHB-C4A-NA	2.31	127.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Nn	305	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
40	Y	616	LUT	C15-C35-C34	-2.31	118.79	123.52
39	NN	601	CHL	C4C-CHD-C1D	2.31	124.34	116.07
32	C	515	CLA	CHB-C4A-NA	2.31	127.73	124.40
40	R	615	LUT	C32-C33-C34	-2.31	115.37	119.01
39	4	308	CHL	C4C-CHD-C1D	2.31	124.34	116.07
39	Ss	606	CHL	C4D-CHA-CBD	-2.31	106.64	108.97
42	YY	617	NEX	C17-C1-C6	-2.31	108.40	110.47
40	Nn	307	LUT	C7-C8-C9	-2.31	122.82	126.23
39	N	607	CHL	C3D-C4D-CHA	2.31	112.05	108.54
34	TT	101	BCR	C4-C5-C6	-2.31	119.58	122.70
34	Cc	516	BCR	C36-C18-C17	-2.31	119.07	122.82
32	CC	506	CLA	CHB-C4A-NA	2.31	127.73	124.40
39	y	310	CHL	O2D-CGD-O1D	-2.31	119.35	123.85
39	Y	609	CHL	C3C-C4C-NC	-2.31	109.00	114.65
32	Nn	313	CLA	CHB-C4A-NA	2.31	127.73	124.40
40	n	616	LUT	C38-C25-C24	-2.31	117.90	123.36
44	Cc	519	DGD	C6E-C5E-C4E	-2.31	107.35	113.02
32	RR	314	CLA	CHB-C4A-NA	2.31	127.73	124.40
39	1	607	CHL	C3C-C4C-NC	-2.31	109.01	114.65
32	N	610	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
40	Yy	616	LUT	C38-C25-C24	-2.31	117.90	123.36
32	S	604	CLA	CHB-C4A-NA	2.31	127.73	124.40
32	c	509	CLA	CHB-C4A-NA	2.31	127.73	124.40
34	Hh	101	BCR	C2-C3-C4	-2.31	106.20	111.28
39	Nn	317	CHL	O2A-CGA-O1A	-2.31	117.86	123.63
34	XX	202	BCR	C16-C15-C14	-2.31	118.80	123.52
41	g	619	XAT	C31-C30-C29	-2.31	124.04	127.28
39	44	605	CHL	O1D-CGD-CBD	2.31	128.22	124.72
32	d	401	CLA	CHB-C4A-NA	2.31	127.73	124.40
41	g	619	XAT	C12-C13-C14	-2.31	115.38	119.01
32	Rr	611	CLA	CHB-C4A-NA	2.31	127.73	124.40
32	SS	303	CLA	C3B-C4B-NB	-2.31	108.47	110.53
39	YY	601	CHL	C4C-CHD-C1D	2.30	124.31	116.07
39	Gg	306	CHL	C4C-CHD-C1D	2.30	124.31	116.07
39	r	606	CHL	O2D-CGD-O1D	-2.30	119.36	123.85
32	c	503	CLA	C3B-C4B-NB	-2.30	108.47	110.53
39	g	606	CHL	C3C-C4C-NC	-2.30	109.02	114.65
38	Bb	621	LMG	O1-C1-C2	2.30	111.77	108.27
34	XX	202	BCR	C31-C1-C6	-2.30	106.63	110.24
39	Yy	607	CHL	C3D-C4D-CHA	2.30	112.04	108.54
36	DD	408	LHG	O8-C23-C24	2.30	118.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Rr	606	CHL	CMD-C2D-C3D	2.30	129.29	124.68
41	Yy	619	XAT	O24-C25-C26	-2.30	57.10	58.93
39	Y	608	CHL	C4C-CHD-C1D	2.30	124.31	116.07
39	GG	608	CHL	C4C-CHD-C1D	2.30	124.31	116.07
32	Ss	602	CLA	CHB-C4A-NA	2.30	127.72	124.40
32	Rr	602	CLA	CHB-C4A-NA	2.30	127.72	124.40
32	n	610	CLA	CHB-C4A-NA	2.30	127.72	124.40
39	SS	308	CHL	C3D-C4D-CHA	2.30	112.04	108.54
34	K	102	BCR	C16-C17-C18	-2.30	124.05	127.28
39	1	601	CHL	O2D-CGD-CBD	2.30	113.47	110.95
32	33	609	CLA	CHB-C4A-NA	2.30	127.72	124.40
32	b	614	CLA	CHB-C4A-NA	2.30	127.72	124.40
32	YY	612	CLA	CHB-C4A-NA	2.30	127.72	124.40
34	B	614	BCR	C36-C18-C17	-2.30	119.09	122.82
38	b	621	LMG	C8-O7-C10	-2.30	112.29	117.80
39	Nn	315	CHL	C3C-C4C-NC	-2.30	109.03	114.65
32	Y	604	CLA	CHB-C4A-NA	2.30	127.72	124.40
32	1	604	CLA	C3B-C4B-NB	-2.30	108.48	110.53
32	2	610	CLA	C3B-C4B-NB	-2.30	108.48	110.53
34	Cc	517	BCR	C37-C22-C23	2.30	121.60	118.09
40	Nn	306	LUT	C38-C25-C24	-2.30	117.92	123.36
32	DD	403	CLA	O2D-CGD-CBD	2.30	115.25	111.23
39	NN	607	CHL	C3D-C4D-CHA	2.30	112.03	108.54
32	g	614	CLA	CHB-C4A-NA	2.30	127.72	124.40
32	Cc	503	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
32	33	610	CLA	CHD-C1D-ND	-2.30	121.57	124.80
36	D	409	LHG	O8-C23-C24	2.30	118.84	111.83
32	Y	612	CLA	O2D-CGD-CBD	2.30	115.25	111.23
39	n	608	CHL	O2A-CGA-O1A	-2.30	117.88	123.63
39	4	309	CHL	CHA-C1A-C2A	-2.30	127.91	133.31
32	SS	309	CLA	C3B-C4B-NB	-2.30	108.48	110.53
39	s	607	CHL	C4C-CHD-C1D	2.30	124.29	116.07
42	Y	619	NEX	C8-C7-C6	-2.30	174.95	177.66
39	R	607	CHL	C3C-C4C-NC	-2.30	109.04	114.65
32	S	602	CLA	CHB-C4A-NA	2.30	127.71	124.40
32	b	605	CLA	CHB-C4A-NA	2.30	127.71	124.40
39	GG	607	CHL	O2D-CGD-O1D	-2.30	119.38	123.85
32	BB	602	CLA	C3B-C4B-NB	-2.30	108.48	110.53
32	B	607	CLA	C3B-C4B-NB	-2.30	108.48	110.53
39	44	607	CHL	C4C-CHD-C1D	2.30	124.28	116.07
41	Yy	619	XAT	C20-C13-C12	2.30	121.59	118.09
32	4	310	CLA	CHB-C4A-NA	2.30	127.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	RR	315	LUT	C3-C4-C5	-2.29	106.46	112.18
39	4	307	CHL	C3D-C4D-CHA	2.29	112.03	108.54
32	Y	610	CLA	CBA-CAA-C2A	2.29	120.62	113.79
32	BB	601	CLA	O2D-CGD-CBD	2.29	115.24	111.23
32	Nn	301	CLA	C3B-C4B-NB	-2.29	108.48	110.53
39	Y	601	CHL	C4C-CHD-C1D	2.29	124.28	116.07
39	y	308	CHL	C3C-C4C-NC	-2.29	109.04	114.65
40	RR	315	LUT	C32-C33-C34	-2.29	115.40	119.01
40	G	615	LUT	C38-C25-C24	-2.29	117.93	123.36
42	y	319	NEX	C32-C33-C34	-2.29	115.40	119.01
34	A	409	BCR	C37-C22-C23	-2.29	114.58	118.09
32	GG	602	CLA	C3B-C4B-NB	-2.29	108.48	110.53
39	Yy	606	CHL	C4C-CHD-C1D	2.29	124.27	116.07
32	S	613	CLA	CHB-C4A-NA	2.29	127.71	124.40
38	b	621	LMG	O1-C1-C2	2.29	111.75	108.27
39	11	607	CHL	C4C-CHD-C1D	2.29	124.27	116.07
32	g	603	CLA	CHB-C4A-NA	2.29	127.71	124.40
32	g	602	CLA	CHD-C1D-ND	-2.29	121.58	124.80
32	B	622	CLA	C1-C2-C3	-2.29	122.44	126.20
42	n	617	NEX	C15-C14-C13	-2.29	124.06	127.28
34	Dd	403	BCR	C15-C16-C17	-2.29	118.83	123.52
32	Dd	402	CLA	CHB-C4A-NA	2.29	127.71	124.40
39	SS	307	CHL	C3C-C4C-NC	-2.29	109.05	114.65
42	Y	617	NEX	C32-C33-C34	-2.29	115.41	119.01
39	S	601	CHL	C3C-C4C-NC	-2.29	109.05	114.65
45	AA	413	BCT	O3-C-O1	-2.29	113.82	119.68
40	y	317	LUT	C38-C25-C24	-2.29	117.94	123.36
39	44	607	CHL	CHA-C1A-C2A	-2.29	127.93	133.31
32	A	406	CLA	CHB-C4A-NA	2.29	127.70	124.40
34	KK	103	BCR	C2-C1-C6	2.29	113.76	110.44
39	YY	608	CHL	C4C-CHD-C1D	2.29	124.26	116.07
32	CC	505	CLA	CHB-C4A-NA	2.29	127.70	124.40
34	K	102	BCR	C23-C22-C21	-2.29	115.41	119.01
32	YY	610	CLA	CHB-C4A-NA	2.29	127.70	124.40
34	K	102	BCR	C38-C26-C27	2.29	118.47	113.60
39	2	601	CHL	C2A-C1A-CHA	2.29	125.63	121.84
32	BB	604	CLA	C6-C5-C3	2.29	119.04	113.47
39	Yy	607	CHL	C3C-C4C-NC	-2.29	109.06	114.65
32	Y	602	CLA	C3B-C4B-NB	-2.29	108.49	110.53
39	N	606	CHL	O1D-CGD-CBD	2.29	128.19	124.72
39	Nn	318	CHL	O1D-CGD-CBD	2.29	128.19	124.72
39	44	608	CHL	C3D-C4D-CHA	2.29	112.01	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Gg	308	CHL	O2A-CGA-O1A	-2.29	117.91	123.63
39	R	605	CHL	CMD-C2D-C3D	2.28	129.25	124.68
40	Y	616	LUT	C36-C21-C26	2.28	113.00	109.55
32	B	618	CLA	C3B-C4B-NB	-2.28	108.49	110.53
39	y	303	CHL	C4C-CHD-C1D	2.28	124.24	116.07
32	RR	304	CLA	CED-O2D-CGD	2.28	121.10	115.92
40	g	616	LUT	C38-C25-C24	-2.28	117.96	123.36
32	s	602	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
39	y	310	CHL	C3D-C4D-CHA	2.28	112.01	108.54
34	d	403	BCR	C33-C5-C6	-2.28	121.99	124.48
32	B	610	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
32	AA	406	CLA	CHB-C4A-NA	2.28	127.69	124.40
39	Ss	601	CHL	O2A-CGA-O1A	-2.28	117.92	123.63
37	B	617	SQD	O5-C5-C4	-2.28	105.59	109.70
32	22	611	CLA	CHB-C4A-NA	2.28	127.69	124.40
32	Bb	610	CLA	CHB-C4A-NA	2.28	127.69	124.40
39	4	302	CHL	C4C-CHD-C1D	2.28	124.23	116.07
32	R	602	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
39	Nn	315	CHL	C3D-C4D-CHA	2.28	112.01	108.54
32	44	602	CLA	CHB-C4A-NA	2.28	127.69	124.40
41	RR	316	XAT	C24-C23-C22	-2.28	106.52	110.79
32	Cc	508	CLA	C1-C2-C3	-2.28	122.46	126.20
32	C	513	CLA	CHB-C4A-NA	2.28	127.69	124.40
38	m	101	LMG	O8-C28-C29	2.28	118.79	111.83
39	Yy	609	CHL	C3D-C4D-CHA	2.28	112.00	108.54
39	33	601	CHL	C3D-C4D-CHA	2.28	112.00	108.54
34	XX	202	BCR	C36-C18-C17	-2.28	119.12	122.82
32	CC	512	CLA	C3B-C4B-NB	-2.28	108.50	110.53
34	BB	620	BCR	C20-C21-C22	-2.28	124.08	127.28
39	YY	607	CHL	C4C-CHD-C1D	2.28	124.22	116.07
34	AA	409	BCR	C20-C21-C22	-2.28	124.08	127.28
39	g	605	CHL	C4C-CHD-C1D	2.28	124.22	116.07
32	Y	602	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
36	a	414	LHG	O8-C23-C24	2.28	118.78	111.83
39	GG	607	CHL	C3D-C4D-CHA	2.28	112.00	108.54
39	RR	307	CHL	C3C-C4C-NC	-2.28	109.09	114.65
39	Gg	308	CHL	C4C-CHD-C1D	2.28	124.21	116.07
34	C	517	BCR	C2-C1-C6	2.28	113.75	110.44
32	g	611	CLA	CHB-C4A-NA	2.28	127.68	124.40
39	Y	607	CHL	C4C-CHD-C1D	2.28	124.21	116.07
39	y	309	CHL	C4C-CHD-C1D	2.28	124.21	116.07
40	N	616	LUT	C17-C1-C6	-2.28	106.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	g	615	LUT	C17-C1-C6	-2.28	106.67	110.24
34	c	516	BCR	C33-C5-C4	2.28	118.45	113.60
40	NN	615	LUT	C38-C25-C24	-2.28	117.98	123.36
39	2	606	CHL	O2D-CGD-CBD	2.28	113.45	110.95
39	Gg	310	CHL	O1D-CGD-CBD	2.27	128.17	124.72
40	N	615	LUT	C18-C5-C6	-2.27	122.00	124.48
39	g	607	CHL	C4C-CHD-C1D	2.27	124.21	116.07
32	s	613	CLA	C3B-C4B-NB	-2.27	108.50	110.53
34	B	616	BCR	C16-C17-C18	-2.27	124.09	127.28
39	g	608	CHL	C4C-CHD-C1D	2.27	124.20	116.07
32	SS	309	CLA	CHB-C4A-NA	2.27	127.68	124.40
39	NN	608	CHL	C4C-CHD-C1D	2.27	124.20	116.07
39	y	308	CHL	C4D-CHA-CBD	-2.27	106.67	108.97
40	r	614	LUT	C38-C25-C24	-2.27	117.98	123.36
42	n	617	NEX	C32-C33-C34	-2.27	115.44	119.01
32	Dd	401	CLA	CHB-C4A-NA	2.27	127.68	124.40
32	4	303	CLA	O2D-CGD-CBD	2.27	115.20	111.23
32	Nn	301	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
32	BB	609	CLA	C5-C3-C2	2.27	126.27	121.17
33	DD	402	PHO	CMB-C2B-C3B	2.27	129.22	124.68
32	YY	602	CLA	C3B-C4B-NB	-2.27	108.50	110.53
40	N	615	LUT	C15-C35-C34	-2.27	118.87	123.52
39	S	607	CHL	O2D-CGD-CBD	2.27	113.44	110.95
36	Yy	618	LHG	C5-O7-C7	-2.27	112.36	117.80
34	Hh	101	BCR	C4-C5-C6	-2.27	119.64	122.70
40	R	615	LUT	C20-C13-C12	2.27	121.56	118.09
39	Ss	601	CHL	C4C-CHD-C1D	2.27	124.19	116.07
39	22	605	CHL	C4C-CHD-C1D	2.27	124.19	116.07
39	n	606	CHL	C4C-CHD-C1D	2.27	124.19	116.07
39	Yy	608	CHL	C3D-C4D-CHA	2.27	111.99	108.54
34	T	101	BCR	C23-C22-C21	-2.27	115.44	119.01
39	R	605	CHL	C3D-C4D-CHA	2.27	111.99	108.54
34	c	514	BCR	C29-C30-C25	2.27	113.73	110.44
34	Bb	617	BCR	C39-C30-C25	-2.27	106.69	110.24
34	c	514	BCR	C11-C10-C9	-2.27	124.10	127.28
34	D	406	BCR	C27-C26-C25	-2.27	119.64	122.70
32	b	607	CLA	CHB-C4A-NA	2.27	127.67	124.40
32	RR	304	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
34	CC	517	BCR	C7-C6-C5	-2.27	116.33	121.56
32	SS	305	CLA	CHB-C4A-NA	2.27	127.67	124.40
41	NN	617	XAT	C40-C33-C34	-2.27	119.14	122.82
39	n	606	CHL	C3D-C4D-CHA	2.27	111.98	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	YY	613	CLA	CHB-C4A-NA	2.27	127.67	124.40
32	n	604	CLA	C3B-C4B-NB	-2.27	108.51	110.53
39	1	607	CHL	C2A-C1A-CHA	2.26	125.60	121.84
40	Ss	614	LUT	C16-C1-C6	2.26	113.79	110.24
40	n	615	LUT	C38-C25-C24	-2.26	118.00	123.36
39	4	306	CHL	C3D-C4D-CHA	2.26	111.98	108.54
39	22	601	CHL	C3C-C4C-NC	-2.26	109.12	114.65
39	Nn	317	CHL	C3C-C4C-NC	-2.26	109.12	114.65
39	Nn	316	CHL	C3D-C4D-CHA	2.26	111.98	108.54
34	D	406	BCR	C7-C6-C5	-2.26	116.34	121.56
32	C	503	CLA	C3B-C4B-NB	-2.26	108.51	110.53
32	YY	614	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
34	H	101	BCR	C24-C23-C22	-2.26	122.89	126.23
39	44	606	CHL	C3D-C4D-CHA	2.26	111.98	108.54
39	11	606	CHL	C4C-CHD-C1D	2.26	124.16	116.07
39	Gg	302	CHL	O1D-CGD-CBD	2.26	128.15	124.72
39	Yy	601	CHL	C4C-CHD-C1D	2.26	124.16	116.07
39	Ss	601	CHL	O2D-CGD-CBD	2.26	113.43	110.95
39	s	601	CHL	C4C-CHD-C1D	2.26	124.16	116.07
32	RR	302	CLA	CHB-C4A-NA	2.26	127.66	124.40
39	R	607	CHL	C3D-C4D-CHA	2.26	111.98	108.54
32	c	509	CLA	C3B-C4B-NB	-2.26	108.51	110.53
32	Cc	507	CLA	C3B-C4B-NB	-2.26	108.51	110.53
32	C	508	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
39	Ss	606	CHL	CHA-C1A-C2A	-2.26	128.00	133.31
32	b	603	CLA	CHB-C4A-NA	2.26	127.66	124.40
39	22	606	CHL	O2D-CGD-CBD	2.26	113.43	110.95
39	Yy	605	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
40	SS	315	LUT	C18-C5-C6	-2.26	122.02	124.48
35	A	410	PL9	C30-C29-C31	-2.26	111.31	115.23
39	S	605	CHL	C3D-C4D-CHA	2.26	111.97	108.54
32	Ss	610	CLA	CHB-C4A-NA	2.26	127.66	124.40
39	Rr	607	CHL	C3C-C4C-NC	-2.26	109.13	114.65
39	Gg	309	CHL	C4C-CHD-C1D	2.26	124.15	116.07
40	YY	616	LUT	C26-C27-C28	-2.26	121.07	124.58
32	R	603	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
41	Rr	615	XAT	C24-C23-C22	-2.26	106.57	110.79
32	C	508	CLA	C3B-C4B-NB	-2.26	108.52	110.53
39	g	607	CHL	O2A-CGA-O1A	-2.26	117.98	123.63
40	R	615	LUT	C36-C21-C26	2.26	112.96	109.55
34	C	518	BCR	C20-C21-C22	-2.26	124.11	127.28
32	Yy	604	CLA	CHB-C4A-NA	2.25	127.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	610	CLA	CHB-C4A-NA	2.25	127.65	124.40
32	N	614	CLA	CHB-C4A-NA	2.25	127.65	124.40
32	a	406	CLA	CHB-C4A-NA	2.25	127.65	124.40
39	22	601	CHL	CMD-C2D-C3D	2.25	129.19	124.68
36	D	410	LHG	C5-O7-C7	-2.25	112.40	117.80
34	KK	103	BCR	C39-C30-C25	-2.25	106.71	110.24
39	y	308	CHL	C4C-CHD-C1D	2.25	124.13	116.07
39	N	608	CHL	C4C-CHD-C1D	2.25	124.13	116.07
46	Ee	101	HEM	C1B-NB-C4B	2.25	107.88	105.21
32	Bb	608	CLA	CHB-C4A-NA	2.25	127.65	124.40
32	s	609	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
39	s	606	CHL	C4D-CHA-CBD	-2.25	106.70	108.97
34	BB	618	BCR	C32-C1-C6	-2.25	106.71	110.24
32	3	610	CLA	CAC-C3C-C4C	2.25	127.72	124.79
32	SS	314	CLA	CHB-C4A-NA	2.25	127.65	124.40
34	c	514	BCR	C15-C16-C17	-2.25	118.91	123.52
34	c	516	BCR	C32-C1-C6	-2.25	106.71	110.24
32	CC	502	CLA	O2D-CGD-CBD	2.25	115.16	111.23
39	11	601	CHL	C3C-C4C-NC	-2.25	109.15	114.65
39	n	608	CHL	C4C-CHD-C1D	2.25	124.12	116.07
32	33	613	CLA	O2D-CGD-CBD	2.25	115.16	111.23
39	S	607	CHL	C3C-C4C-NC	-2.25	109.15	114.65
39	Y	609	CHL	O2A-CGA-O1A	-2.25	118.00	123.63
39	r	605	CHL	C4D-CHA-CBD	-2.25	106.70	108.97
39	G	607	CHL	C3D-C4D-CHA	2.25	111.96	108.54
39	SS	302	CHL	C3C-C4C-NC	-2.25	109.16	114.65
39	S	607	CHL	O1D-CGD-CBD	2.25	128.13	124.72
39	Ss	607	CHL	C4C-CHD-C1D	2.25	124.11	116.07
32	n	602	CLA	C1-C2-C3	-2.25	122.52	126.20
32	b	602	CLA	CHB-C4A-NA	2.25	127.64	124.40
32	d	402	CLA	CHB-C4A-NA	2.25	127.64	124.40
34	B	616	BCR	C12-C13-C14	-2.25	115.48	119.01
36	Ll	102	LHG	O8-C23-C24	2.25	118.68	111.83
39	3	601	CHL	CMD-C2D-C3D	2.24	129.17	124.68
32	Bb	602	CLA	C3B-C4B-NB	-2.24	108.53	110.53
32	Cc	509	CLA	C3B-C4B-NB	-2.24	108.53	110.53
39	33	601	CHL	C3C-C4C-NC	-2.24	109.17	114.65
39	Nn	316	CHL	C4C-CHD-C1D	2.24	124.10	116.07
40	Yy	616	LUT	C20-C13-C12	2.24	121.52	118.09
39	RR	307	CHL	C3D-C4D-CHA	2.24	111.95	108.54
32	n	604	CLA	CHB-C4A-NA	2.24	127.64	124.40
39	n	607	CHL	C3C-C4C-NC	-2.24	109.17	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	y	306	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
32	CC	514	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
32	n	610	CLA	C3B-C4B-NB	-2.24	108.53	110.53
41	RR	316	XAT	C4-C3-C2	-2.24	106.60	110.79
32	G	612	CLA	CAC-C3C-C4C	2.24	127.71	124.79
39	Rr	607	CHL	C3D-C4D-CHA	2.24	111.95	108.54
34	CC	515	BCR	C33-C5-C6	-2.24	122.04	124.48
39	g	606	CHL	C3D-C4D-CHA	2.24	111.94	108.54
32	s	609	CLA	C3B-C4B-NB	-2.24	108.53	110.53
39	r	607	CHL	C3C-C4C-NC	-2.24	109.17	114.65
39	Ss	601	CHL	C3D-C4D-CHA	2.24	111.94	108.54
44	BB	625	DGD	C2G-O2G-C1B	-2.24	112.44	117.80
39	11	605	CHL	C3D-C4D-CHA	2.24	111.94	108.54
32	Rr	608	CLA	CHB-C4A-NA	2.24	127.63	124.40
32	CC	504	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
32	44	609	CLA	CHB-C4A-NA	2.24	127.63	124.40
34	K	102	BCR	C12-C13-C14	-2.24	115.49	119.01
32	CC	504	CLA	C6-C5-C3	2.24	118.92	113.47
32	a	407	CLA	CHB-C4A-NA	2.24	127.63	124.40
32	Nn	314	CLA	CHB-C4A-NA	2.24	127.63	124.40
34	A	409	BCR	C20-C21-C22	-2.24	124.14	127.28
34	b	617	BCR	C29-C30-C25	2.24	113.69	110.44
32	Bb	608	CLA	C3B-C4B-NB	-2.24	108.53	110.53
32	C	515	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
40	NN	616	LUT	C17-C1-C6	-2.24	106.74	110.24
32	D	401	CLA	O2D-CGD-CBD	2.24	115.14	111.23
34	d	403	BCR	C15-C16-C17	-2.24	118.94	123.52
35	d	404	PL9	C7-C3-C2	-2.24	120.75	123.39
32	Bb	608	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
34	D	406	BCR	C16-C15-C14	-2.23	118.95	123.52
32	n	610	CLA	C1D-ND-C4D	-2.23	104.74	106.31
41	y	301	XAT	C15-C35-C34	-2.23	118.95	123.52
41	4	314	XAT	C40-C33-C34	-2.23	119.20	122.82
32	Nn	312	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
40	Ss	614	LUT	C19-C9-C8	2.23	121.50	118.09
42	NN	618	NEX	C40-C33-C34	-2.23	119.20	122.82
39	S	605	CHL	C4D-CHA-CBD	-2.23	106.72	108.97
32	B	605	CLA	C5-C3-C2	2.23	126.18	121.17
32	C	506	CLA	CHB-C4A-NA	2.23	127.62	124.40
39	N	605	CHL	C4D-CHA-CBD	-2.23	106.72	108.97
41	Gg	301	XAT	C12-C13-C14	-2.23	115.50	119.01
32	2	611	CLA	CHB-C4A-NA	2.23	127.62	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Cc	516	BCR	C27-C26-C25	-2.23	119.69	122.70
33	a	409	PHO	CMB-C2B-C3B	2.23	129.14	124.68
32	YY	612	CLA	C1C-C2C-C3C	-2.23	104.63	106.98
39	1	605	CHL	CMD-C2D-C3D	2.23	129.14	124.68
34	BB	618	BCR	C36-C18-C17	-2.23	119.20	122.82
34	T	101	BCR	C40-C30-C25	-2.23	106.74	110.24
39	1	608	CHL	C3C-C4C-NC	-2.23	109.20	114.65
43	R	618	LMU	C1'-O5'-C5'	2.23	118.08	113.72
40	44	612	LUT	C35-C15-C14	-2.23	118.95	123.52
32	YY	612	CLA	O2D-CGD-CBD	2.23	115.13	111.23
39	GG	601	CHL	C3D-C4D-CHA	2.23	111.93	108.54
39	Nn	316	CHL	O2A-CGA-O1A	-2.23	118.05	123.63
32	b	610	CLA	CHB-C4A-NA	2.23	127.62	124.40
32	S	613	CLA	C3B-C4B-NB	-2.23	108.54	110.53
39	RR	306	CHL	C4C-CHD-C1D	2.23	124.05	116.07
40	s	615	LUT	C36-C21-C26	2.23	112.92	109.55
32	Yy	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
39	2	607	CHL	C4C-CHD-C1D	2.23	124.05	116.07
32	RR	310	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
39	y	309	CHL	C3D-C4D-CHA	2.23	111.93	108.54
32	Bb	603	CLA	CHB-C4A-NA	2.23	127.62	124.40
40	YY	616	LUT	C38-C25-C24	-2.23	118.08	123.36
41	R	616	XAT	C4-C3-C2	-2.23	106.62	110.79
40	NN	615	LUT	C12-C13-C14	-2.23	115.50	119.01
38	Aa	412	LMG	O1-C1-C2	2.23	111.66	108.27
39	y	310	CHL	CMD-C2D-C3D	2.23	129.14	124.68
32	Y	614	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
39	S	606	CHL	O2D-CGD-CBD	2.23	113.39	110.95
32	Cc	512	CLA	CHB-C4A-NA	2.23	127.61	124.40
39	g	601	CHL	C1-C2-C3	-2.23	122.55	126.20
33	Aa	409	PHO	O2A-CGA-O1A	-2.23	118.06	123.63
32	C	506	CLA	C3B-C4B-NB	-2.23	108.54	110.53
32	g	611	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
40	4	313	LUT	C35-C15-C14	-2.23	118.96	123.52
42	Y	619	NEX	C11-C10-C9	-2.23	124.16	127.28
32	G	610	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
40	Y	616	LUT	C7-C8-C9	-2.23	122.94	126.23
34	DD	405	BCR	C7-C6-C5	-2.23	116.43	121.56
32	Ss	613	CLA	C3B-C4B-NB	-2.23	108.54	110.53
32	Cc	510	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	AA	406	CLA	O2D-CGD-CBD	2.23	115.12	111.23
34	B	616	BCR	C29-C28-C27	-2.23	106.38	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	s	609	CLA	O2D-CGD-CBD	2.23	115.12	111.23
32	Yy	611	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	n	611	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	Gg	305	CLA	CHB-C4A-NA	2.23	127.61	124.40
39	Yy	608	CHL	O1D-CGD-CBD	2.22	128.10	124.72
39	N	606	CHL	C4C-CHD-C1D	2.22	124.03	116.07
32	c	502	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
32	CC	507	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
39	Nn	318	CHL	C3C-C4C-NC	-2.22	109.22	114.65
32	Ss	609	CLA	C3B-C4B-NB	-2.22	108.55	110.53
32	Nn	312	CLA	CAC-C3C-C4C	2.22	127.68	124.79
39	33	607	CHL	C4C-CHD-C1D	2.22	124.02	116.07
32	B	620	CLA	CHB-C4A-NA	2.22	127.61	124.40
33	A	407	PHO	C1-C2-C3	-2.22	122.56	126.20
32	SS	305	CLA	CAC-C3C-C4C	2.22	127.68	124.79
40	44	612	LUT	C36-C21-C26	2.22	112.91	109.55
39	YY	609	CHL	O2A-CGA-O1A	-2.22	118.07	123.63
40	Yy	616	LUT	C40-C33-C32	2.22	121.48	118.09
39	G	608	CHL	C3D-C4D-CHA	2.22	111.92	108.54
39	y	311	CHL	C3D-C4D-CHA	2.22	111.92	108.54
41	G	619	XAT	C12-C13-C14	-2.22	115.52	119.01
39	33	605	CHL	C4C-CHD-C1D	2.22	124.02	116.07
32	GG	602	CLA	CHC-C4B-NB	2.22	127.38	124.05
39	1	601	CHL	C3C-C4C-NC	-2.22	109.22	114.65
39	22	606	CHL	C3C-C4C-NC	-2.22	109.22	114.65
32	Gg	314	CLA	CHB-C4A-NA	2.22	127.60	124.40
39	y	307	CHL	C3C-C4C-NC	-2.22	109.22	114.65
32	g	613	CLA	CAC-C3C-C4C	2.22	127.68	124.79
39	Gg	308	CHL	CMD-C2D-C3D	2.22	129.12	124.68
34	d	403	BCR	C40-C30-C25	2.22	113.72	110.24
32	CC	506	CLA	C3B-C4B-NB	-2.22	108.55	110.53
40	s	615	LUT	C12-C13-C14	-2.22	115.52	119.01
40	Nn	307	LUT	C38-C25-C24	-2.22	118.11	123.36
33	AA	407	PHO	CMB-C2B-C3B	2.22	129.12	124.68
34	Cc	516	BCR	C15-C16-C17	-2.22	118.98	123.52
39	GG	606	CHL	C4C-CHD-C1D	2.22	124.00	116.07
39	Nn	318	CHL	C3D-C4D-CHA	2.22	111.91	108.54
32	r	602	CLA	C1-C2-C3	-2.22	122.56	126.20
39	s	605	CHL	CMD-C2D-C3D	2.22	129.11	124.68
39	G	606	CHL	C4C-CHD-C1D	2.22	124.00	116.07
32	Y	612	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
39	S	606	CHL	O1D-CGD-CBD	2.22	128.09	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	610	CLA	C3B-C4B-NB	-2.22	108.55	110.53
40	n	616	LUT	C12-C13-C14	-2.22	115.52	119.01
42	Nn	309	NEX	C15-C14-C13	-2.22	124.17	127.28
32	R	614	CLA	CHB-C4A-NA	2.22	127.60	124.40
39	22	606	CHL	CMD-C2D-C3D	2.22	129.11	124.68
39	S	607	CHL	C3D-C4D-CHA	2.22	111.91	108.54
44	B	601	DGD	O6D-C5D-C6D	2.22	111.09	106.69
39	Ss	605	CHL	C3C-C4C-NC	-2.21	109.24	114.65
39	3	601	CHL	C3C-C4C-NC	-2.21	109.24	114.65
32	Rr	610	CLA	CHB-C4A-NA	2.21	127.60	124.40
32	11	610	CLA	CHB-C4A-NA	2.21	127.60	124.40
34	K	102	BCR	C39-C30-C25	-2.21	106.77	110.24
39	YY	609	CHL	C1-C2-C3	-2.21	122.57	126.20
32	Y	604	CLA	O2D-CGD-CBD	2.21	115.10	111.23
39	S	605	CHL	CBC-CAC-C3C	-2.21	109.70	112.87
39	2	606	CHL	C3C-C4C-NC	-2.21	109.24	114.65
34	DD	405	BCR	C16-C15-C14	-2.21	118.99	123.52
32	c	507	CLA	C3B-C4B-NB	-2.21	108.55	110.53
39	SS	307	CHL	C3D-C4D-CHA	2.21	111.90	108.54
39	22	601	CHL	C2A-C1A-CHA	2.21	125.51	121.84
32	N	602	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
32	N	604	CLA	CHB-C4A-NA	2.21	127.59	124.40
32	Bb	607	CLA	CHB-C4A-NA	2.21	127.59	124.40
42	RR	317	NEX	C40-C33-C32	2.21	121.47	118.09
32	c	508	CLA	C1-C2-C3	-2.21	122.57	126.20
32	b	601	CLA	CHB-C4A-NA	2.21	127.59	124.40
32	NN	604	CLA	CHB-C4A-NA	2.21	127.59	124.40
40	GG	616	LUT	C20-C13-C12	2.21	121.47	118.09
32	b	602	CLA	CBC-CAC-C3C	-2.21	106.42	112.42
32	CC	503	CLA	CHB-C4A-NA	2.21	127.59	124.40
32	SS	310	CLA	CHB-C4A-NA	2.21	127.59	124.40
32	YY	611	CLA	CHB-C4A-NA	2.21	127.59	124.40
32	Bb	604	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
39	2	605	CHL	C4C-CHD-C1D	2.21	123.98	116.07
39	11	607	CHL	C3D-C4D-CHA	2.21	111.90	108.54
39	Rr	606	CHL	O2D-CGD-O1D	-2.21	119.55	123.85
39	2	601	CHL	C4C-CHD-C1D	2.21	123.98	116.07
37	C	501	SQD	O48-C23-O10	-2.21	118.10	123.63
39	G	601	CHL	C4C-CHD-C1D	2.21	123.97	116.07
42	Yy	617	NEX	C15-C14-C13	-2.21	124.18	127.28
41	Rr	615	XAT	C35-C15-C14	-2.21	119.00	123.52
32	B	621	CLA	C6-C5-C3	2.21	118.85	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	SS	308	CHL	CMD-C2D-C3D	2.21	129.10	124.68
39	G	607	CHL	C4C-CHD-C1D	2.21	123.97	116.07
39	GG	605	CHL	C4C-CHD-C1D	2.21	123.97	116.07
40	Yy	615	LUT	C1-C2-C3	2.21	118.44	113.59
32	Cc	504	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
39	YY	608	CHL	CMD-C2D-C3D	2.21	129.09	124.68
32	S	602	CLA	CBA-CAA-C2A	2.21	120.36	113.79
32	c	502	CLA	CHB-C4A-NA	2.21	127.59	124.40
32	a	406	CLA	C1C-C2C-C3C	-2.21	104.66	106.98
32	c	506	CLA	C1-C2-C3	-2.21	122.58	126.20
34	BB	620	BCR	C16-C17-C18	-2.21	124.18	127.28
34	d	403	BCR	C1-C6-C7	2.21	121.64	115.65
32	Bb	602	CLA	O1D-CGD-CBD	2.21	128.87	124.52
39	SS	302	CHL	C4C-CHD-C1D	2.21	123.97	116.07
32	RR	310	CLA	C3B-C4B-NB	-2.21	108.56	110.53
39	3	607	CHL	C4C-CHD-C1D	2.21	123.96	116.07
39	GG	608	CHL	C3D-C4D-CHA	2.21	111.89	108.54
32	BB	607	CLA	C1-C2-C3	-2.21	122.58	126.20
39	44	607	CHL	CMD-C2D-C3D	2.21	129.09	124.68
39	22	607	CHL	C4C-CHD-C1D	2.21	123.96	116.07
39	3	605	CHL	C4C-CHD-C1D	2.21	123.96	116.07
34	Dd	403	BCR	C30-C25-C24	2.21	121.63	115.65
39	1	608	CHL	O1D-CGD-CBD	2.21	128.07	124.72
39	Yy	601	CHL	O2A-CGA-O1A	-2.21	118.11	123.63
40	4	313	LUT	C19-C9-C8	2.20	121.46	118.09
32	11	604	CLA	C3B-C4B-NB	-2.20	108.56	110.53
39	N	607	CHL	C4C-CHD-C1D	2.20	123.96	116.07
32	r	611	CLA	CHB-C4A-NA	2.20	127.58	124.40
39	g	601	CHL	C4C-CHD-C1D	2.20	123.95	116.07
32	BB	603	CLA	CHB-C4A-NA	2.20	127.58	124.40
32	Nn	302	CLA	CHB-C4A-NA	2.20	127.58	124.40
39	n	606	CHL	O2A-CGA-O1A	-2.20	118.12	123.63
39	Nn	319	CHL	O2A-CGA-O1A	-2.20	118.12	123.63
34	k	101	BCR	C8-C9-C10	2.20	122.47	119.01
41	44	613	XAT	C8-C9-C10	-2.20	115.54	119.01
32	Yy	604	CLA	C3B-C4B-NB	-2.20	108.56	110.53
32	Gg	314	CLA	C3B-C4B-NB	-2.20	108.56	110.53
39	44	605	CHL	C3C-C4C-NC	-2.20	109.27	114.65
32	Bb	605	CLA	CHB-C4A-NA	2.20	127.58	124.40
39	2	606	CHL	CMD-C2D-C3D	2.20	129.09	124.68
37	L	101	SQD	C45-O47-C7	-2.20	112.52	117.80
34	d	403	BCR	C30-C25-C24	2.20	121.62	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	g	606	CHL	C4C-CHD-C1D	2.20	123.95	116.07
32	SS	312	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
32	Y	610	CLA	C3B-C4B-NB	-2.20	108.56	110.53
32	B	621	CLA	C3B-C4B-NB	-2.20	108.56	110.53
41	R	616	XAT	C12-C13-C14	-2.20	115.55	119.01
39	1	606	CHL	C4C-CHD-C1D	2.20	123.95	116.07
39	NN	606	CHL	C4C-CHD-C1D	2.20	123.95	116.07
37	C	501	SQD	O7-S-C6	2.20	110.04	106.76
39	Rr	607	CHL	C4C-CHD-C1D	2.20	123.95	116.07
39	S	601	CHL	C4C-CHD-C1D	2.20	123.95	116.07
34	BB	618	BCR	C16-C15-C14	-2.20	119.01	123.52
38	Aa	412	LMG	C8-O7-C10	-2.20	112.53	117.80
32	b	609	CLA	CHB-C4A-NA	2.20	127.58	124.40
39	3	606	CHL	CMD-C2D-C3D	2.20	129.08	124.68
38	Mm	101	LMG	O8-C28-C29	2.20	118.55	111.83
32	G	604	CLA	CHB-C4A-NA	2.20	127.58	124.40
40	YY	616	LUT	C20-C13-C12	2.20	121.45	118.09
39	GG	607	CHL	C4C-CHD-C1D	2.20	123.94	116.07
44	c	517	DGD	O1G-C1A-O1A	-2.20	118.13	123.63
32	B	622	CLA	C3B-C4B-NB	-2.20	108.57	110.53
40	NN	616	LUT	C16-C1-C6	2.20	113.69	110.24
34	c	514	BCR	C2-C3-C4	-2.20	106.44	111.28
32	Bb	613	CLA	O1D-CGD-CBD	2.20	128.85	124.52
34	Aa	411	BCR	C36-C18-C17	-2.20	119.25	122.82
39	G	601	CHL	C3D-C4D-CHA	2.20	111.88	108.54
39	Yy	608	CHL	CMD-C2D-C3D	2.20	129.07	124.68
32	Rr	608	CLA	C3B-C4B-NB	-2.20	108.57	110.53
32	b	607	CLA	C3B-C4B-NB	-2.20	108.57	110.53
40	Y	616	LUT	C38-C25-C24	-2.20	118.16	123.36
40	RR	315	LUT	C36-C21-C26	2.20	112.87	109.55
39	Y	606	CHL	C4C-CHD-C1D	2.20	123.93	116.07
34	AA	409	BCR	C40-C30-C25	-2.20	106.80	110.24
32	GG	610	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
39	SS	306	CHL	O1D-CGD-CBD	2.20	128.06	124.72
45	Aa	414	BCT	O3-C-O1	-2.20	114.06	119.68
32	Gg	312	CLA	CHB-C4A-NA	2.20	127.57	124.40
39	YY	609	CHL	C3D-C4D-CHA	2.20	111.88	108.54
46	Ee	101	HEM	C4D-ND-C1D	2.20	107.81	105.21
32	b	606	CLA	O1D-CGD-CBD	2.20	128.85	124.52
42	Y	619	NEX	C15-C14-C13	-2.20	124.20	127.28
39	11	608	CHL	O2D-CGD-CBD	2.20	113.36	110.95
34	a	411	BCR	C4-C5-C6	-2.20	119.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	GG	601	CHL	C4C-CHD-C1D	2.19	123.92	116.07
40	r	614	LUT	C15-C35-C34	-2.19	119.03	123.52
32	Aa	407	CLA	O2D-CGD-CBD	2.19	115.07	111.23
33	AA	407	PHO	C5-C3-C2	2.19	126.09	121.17
32	s	612	CLA	CHB-C4A-NA	2.19	127.57	124.40
32	4	311	CLA	CHB-C4A-NA	2.19	127.57	124.40
39	g	607	CHL	C3D-C4D-CHA	2.19	111.87	108.54
39	4	308	CHL	C3D-C4D-CHA	2.19	111.87	108.54
34	Bb	618	BCR	C33-C5-C6	-2.19	122.09	124.48
34	b	619	BCR	C15-C16-C17	-2.19	119.03	123.52
41	N	617	XAT	C16-C1-C2	-2.19	105.11	108.97
32	S	609	CLA	C3B-C4B-NB	-2.19	108.57	110.53
32	b	608	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
33	Aa	409	PHO	CMB-C2B-C3B	2.19	129.06	124.68
39	11	608	CHL	C3D-C4D-CHA	2.19	111.87	108.54
34	AA	409	BCR	C2-C3-C4	-2.19	106.46	111.28
34	T	101	BCR	C38-C26-C27	2.19	118.27	113.60
39	Gg	307	CHL	C4C-CHD-C1D	2.19	123.91	116.07
34	KK	103	BCR	C12-C13-C14	-2.19	115.56	119.01
32	NN	602	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
39	GG	601	CHL	C4D-CHA-CBD	-2.19	106.76	108.97
39	YY	606	CHL	C4C-CHD-C1D	2.19	123.91	116.07
39	Gg	302	CHL	C4C-CHD-C1D	2.19	123.91	116.07
40	y	318	LUT	C3-C4-C5	-2.19	106.72	112.18
39	Gg	302	CHL	C1-C2-C3	-2.19	122.61	126.20
32	g	604	CLA	CHB-C4A-NA	2.19	127.56	124.40
32	CC	503	CLA	C3B-C4B-NB	-2.19	108.57	110.53
39	NN	607	CHL	C4C-CHD-C1D	2.19	123.91	116.07
42	R	617	NEX	C32-C33-C34	-2.19	115.56	119.01
32	11	612	CLA	C3B-C4B-NB	-2.19	108.58	110.53
39	SS	307	CHL	CMD-C2D-C3D	2.19	129.06	124.68
32	NN	610	CLA	CHB-C4A-NA	2.19	127.56	124.40
34	BB	616	BCR	C34-C9-C8	2.19	121.43	118.09
40	Gg	317	LUT	C40-C33-C32	2.19	121.43	118.09
32	G	611	CLA	CHB-C4A-NA	2.19	127.56	124.40
40	G	615	LUT	C26-C27-C28	-2.19	121.17	124.58
39	N	605	CHL	C3C-C4C-NC	-2.19	109.30	114.65
32	Y	602	CLA	CAC-C3C-C4C	2.19	127.64	124.79
44	BB	624	DGD	O6D-C5D-C6D	2.19	111.03	106.69
39	Gg	308	CHL	C3D-C4D-CHA	2.19	111.86	108.54
40	y	317	LUT	C16-C1-C6	2.19	113.67	110.24
42	YY	617	NEX	C32-C33-C34	-2.19	115.57	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Bb	603	CLA	CBA-CAA-C2A	2.19	120.30	113.79
32	Nn	312	CLA	C1-C2-C3	-2.19	122.61	126.20
39	1	607	CHL	CMD-C2D-C3D	2.19	129.05	124.68
39	Nn	316	CHL	CMD-C2D-C3D	2.19	129.05	124.68
39	g	607	CHL	CMD-C2D-C3D	2.19	129.05	124.68
37	LL	102	SQD	C45-O47-C7	-2.19	112.56	117.80
32	D	401	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
32	Ss	608	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
32	NN	604	CLA	CMA-C3A-C2A	-2.19	111.22	116.23
42	Rr	616	NEX	C11-C10-C9	-2.19	124.21	127.28
39	Y	608	CHL	CMD-C2D-C3D	2.18	129.05	124.68
39	n	601	CHL	C3D-C4D-CHA	2.18	111.86	108.54
34	Hh	101	BCR	C37-C22-C23	2.18	121.42	118.09
42	g	617	NEX	C12-C13-C14	-2.18	115.57	119.01
32	Gg	305	CLA	C3B-C4B-NB	-2.18	108.58	110.53
42	g	617	NEX	C10-C11-C12	-2.18	116.87	123.20
32	4	303	CLA	CHB-C4A-NA	2.18	127.55	124.40
39	Yy	605	CHL	C3D-C4D-CHA	2.18	111.86	108.54
39	S	606	CHL	C3D-C4D-CHA	2.18	111.86	108.54
39	NN	609	CHL	CMD-C2D-C3D	2.18	129.05	124.68
32	CC	505	CLA	C3B-C4B-NB	-2.18	108.58	110.53
33	a	409	PHO	O2A-CGA-O1A	-2.18	118.17	123.63
34	C	518	BCR	C34-C9-C8	2.18	121.42	118.09
32	r	608	CLA	CHB-C4A-NA	2.18	127.55	124.40
39	Nn	311	CHL	C3C-C4C-NC	-2.18	109.32	114.65
34	C	516	BCR	C2-C3-C4	-2.18	106.48	111.28
32	1	609	CLA	O1D-CGD-CBD	2.18	128.82	124.52
34	CC	517	BCR	C27-C26-C25	-2.18	119.76	122.70
32	s	610	CLA	CHB-C4A-NA	2.18	127.55	124.40
32	Y	611	CLA	C3B-C4B-NB	-2.18	108.58	110.53
41	NN	617	XAT	C16-C1-C2	-2.18	105.14	108.97
32	S	611	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
32	n	602	CLA	CAC-C3C-C4C	2.18	127.63	124.79
40	NN	615	LUT	C1-C6-C5	-2.18	119.66	122.64
39	G	605	CHL	C4C-CHD-C1D	2.18	123.87	116.07
39	YY	607	CHL	C3D-C4D-CHA	2.18	111.85	108.54
34	Hh	101	BCR	C38-C26-C27	2.18	118.24	113.60
32	Bb	610	CLA	C3B-C4B-NB	-2.18	108.58	110.53
39	Yy	606	CHL	C3D-C4D-CHA	2.18	111.85	108.54
39	y	308	CHL	C3D-C4D-CHA	2.18	111.85	108.54
32	B	604	CLA	CHB-C4A-NA	2.18	127.55	124.40
40	r	614	LUT	C36-C21-C26	2.18	112.85	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	603	CLA	CBA-CAA-C2A	2.18	120.28	113.79
32	b	604	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
32	BB	610	CLA	C11-C10-C8	-2.18	108.72	115.97
34	Aa	411	BCR	C38-C26-C25	-2.18	122.11	124.48
38	Bb	621	LMG	C8-O7-C10	-2.18	112.58	117.80
34	DD	405	BCR	C38-C26-C27	2.18	118.24	113.60
32	NN	603	CLA	CHB-C4A-NA	2.18	127.54	124.40
32	NN	614	CLA	CHB-C4A-NA	2.18	127.54	124.40
39	S	605	CHL	CMD-C2D-C3D	2.18	129.03	124.68
34	Hh	101	BCR	C7-C6-C5	-2.18	116.54	121.56
32	n	611	CLA	C3B-C4B-NB	-2.18	108.59	110.53
32	Cc	515	CLA	C3B-C4B-NB	-2.18	108.59	110.53
39	22	606	CHL	O1D-CGD-CBD	2.18	128.03	124.72
32	DD	404	CLA	CHB-C4A-NA	2.18	127.54	124.40
32	b	608	CLA	CHB-C4A-NA	2.18	127.54	124.40
33	Aa	408	PHO	C2D-C1D-ND	-2.18	107.86	109.43
39	n	608	CHL	C3D-C4D-CHA	2.18	111.85	108.54
32	Bb	606	CLA	O1D-CGD-CBD	2.18	128.81	124.52
32	BB	603	CLA	O2D-CGD-CBD	2.18	115.03	111.23
39	4	307	CHL	C4D-CHA-CBD	-2.18	106.77	108.97
32	y	314	CLA	C5-C3-C2	2.18	126.05	121.17
36	l	101	LHG	C5-O7-C7	-2.18	112.59	117.80
32	RR	309	CLA	CBA-CAA-C2A	2.18	120.27	113.79
40	RR	315	LUT	C38-C25-C24	-2.18	118.21	123.36
39	3	606	CHL	C3D-C4D-CHA	2.17	111.84	108.54
32	N	604	CLA	CMA-C3A-C2A	-2.17	111.24	116.23
32	b	613	CLA	O1D-CGD-CBD	2.17	128.81	124.52
34	D	406	BCR	C38-C26-C27	2.17	118.23	113.60
39	Y	607	CHL	C3D-C4D-CHA	2.17	111.84	108.54
39	SS	307	CHL	O1D-CGD-CBD	2.17	128.02	124.72
32	n	603	CLA	CHB-C4A-NA	2.17	127.54	124.40
36	Yy	618	LHG	O7-C7-O9	-2.17	118.62	123.70
44	B	603	DGD	C2G-O2G-C1B	-2.17	112.59	117.80
32	Ss	611	CLA	CHB-C4A-NA	2.17	127.54	124.40
32	22	603	CLA	CHB-C4A-NA	2.17	127.54	124.40
41	R	616	XAT	C36-C21-C22	-2.17	105.15	108.97
39	s	606	CHL	CMD-C2D-C3D	2.17	129.03	124.68
32	SS	311	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
32	C	509	CLA	C3B-C4B-NB	-2.17	108.59	110.53
39	33	606	CHL	C4C-CHD-C1D	2.17	123.84	116.07
34	b	619	BCR	C38-C26-C25	-2.17	122.11	124.48
32	c	510	CLA	CHB-C4A-NA	2.17	127.53	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	602	CLA	CHD-C1D-ND	-2.17	121.75	124.80
32	Bb	603	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
32	G	602	CLA	CHB-C4A-NA	2.17	127.53	124.40
32	R	610	CLA	CHB-C4A-NA	2.17	127.53	124.40
39	Rr	607	CHL	C4D-CHA-CBD	-2.17	106.78	108.97
39	Gg	309	CHL	CMD-C2D-C3D	2.17	129.02	124.68
44	CC	522	DGD	O2G-C1B-O1B	-2.17	118.63	123.70
32	C	507	CLA	CHB-C4A-NA	2.17	127.53	124.40
39	N	609	CHL	CMD-C2D-C3D	2.17	129.02	124.68
39	S	607	CHL	CMD-C2D-C3D	2.17	129.02	124.68
32	Gg	303	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
32	Gg	315	CLA	C3B-C4B-NB	-2.17	108.59	110.53
32	N	610	CLA	CBA-CAA-C2A	2.17	120.25	113.79
34	T	101	BCR	C21-C20-C19	-2.17	116.92	123.20
38	j	101	LMG	O1-C1-C2	2.17	111.57	108.27
33	a	409	PHO	C2D-C1D-ND	-2.17	107.86	109.43
40	R	615	LUT	C38-C25-C24	-2.17	118.23	123.36
33	a	408	PHO	CMB-C2B-C3B	2.17	129.01	124.68
32	r	612	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
32	C	505	CLA	CHB-C4A-NA	2.17	127.53	124.40
32	Bb	601	CLA	CHB-C4A-NA	2.17	127.53	124.40
39	Nn	316	CHL	C3C-C4C-NC	-2.17	109.35	114.65
39	g	606	CHL	CMD-C2D-C3D	2.17	129.01	124.68
39	s	601	CHL	C3D-C4D-CHA	2.17	111.83	108.54
36	11	614	LHG	C5-O7-C7	-2.17	112.61	117.80
32	YY	603	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
39	Ss	607	CHL	O2D-CGD-CBD	2.17	113.33	110.95
32	B	619	CLA	C3B-C4B-NB	-2.17	108.60	110.53
34	Cc	516	BCR	C29-C30-C25	2.17	113.59	110.44
39	2	605	CHL	C3D-C4D-CHA	2.17	111.83	108.54
39	1	601	CHL	CMD-C2D-C3D	2.17	129.01	124.68
32	CC	512	CLA	CHB-C4A-NA	2.17	127.53	124.40
32	GG	602	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
34	Cc	516	BCR	C24-C25-C26	-2.17	116.57	121.56
39	Rr	606	CHL	C4D-CHA-CBD	-2.17	106.78	108.97
32	A	408	CLA	O1D-CGD-CBD	2.17	128.79	124.52
39	Gg	310	CHL	C3D-C4D-CHA	2.17	111.83	108.54
39	N	609	CHL	O2A-CGA-O1A	-2.17	118.21	123.63
32	G	614	CLA	CHB-C4A-NA	2.17	127.53	124.40
39	2	601	CHL	CMD-C2D-C3D	2.17	129.01	124.68
39	33	606	CHL	O1D-CGD-CBD	2.16	128.00	124.72
32	R	612	CLA	O2D-CGD-CBD	2.16	115.01	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	514	BCR	C38-C26-C25	-2.16	122.12	124.48
32	b	606	CLA	C1-C2-C3	-2.16	122.65	126.20
36	Ll	102	LHG	C5-O7-C7	-2.16	112.62	117.80
44	Cc	519	DGD	O1G-C1A-O1A	-2.16	118.22	123.63
32	BB	614	CLA	C5-C3-C2	2.16	126.02	121.17
40	G	615	LUT	C40-C33-C32	2.16	121.39	118.09
32	c	503	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
32	r	604	CLA	CHC-C4B-NB	2.16	127.29	124.05
39	Ss	607	CHL	C3D-C4D-CHA	2.16	111.83	108.54
39	Gg	309	CHL	C3D-C4D-CHA	2.16	111.83	108.54
40	44	612	LUT	C19-C9-C8	2.16	121.39	118.09
32	3	610	CLA	CHB-C4A-NA	2.16	127.52	124.40
32	S	612	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
32	Rr	613	CLA	C3B-C4B-NB	-2.16	108.60	110.53
32	c	513	CLA	C3B-C4B-NB	-2.16	108.60	110.53
39	YY	605	CHL	C3D-C4D-CHA	2.16	111.83	108.54
34	h	101	BCR	C37-C22-C23	2.16	121.39	118.09
32	Y	603	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
39	Y	609	CHL	C3D-C4D-CHA	2.16	111.82	108.54
39	YY	601	CHL	C3D-C4D-CHA	2.16	111.82	108.54
34	Bb	619	BCR	C15-C16-C17	-2.16	119.10	123.52
39	y	303	CHL	O2A-CGA-O1A	-2.16	118.22	123.63
39	S	606	CHL	CMD-C2D-C3D	2.16	129.00	124.68
39	G	609	CHL	C3C-C4C-NC	-2.16	109.37	114.65
40	s	614	LUT	C36-C21-C26	2.16	112.82	109.55
32	n	614	CLA	CHB-C4A-NA	2.16	127.52	124.40
40	y	317	LUT	C1-C6-C7	2.16	121.51	115.65
39	YY	608	CHL	C3D-C4D-CHA	2.16	111.82	108.54
40	RR	315	LUT	C20-C13-C12	2.16	121.39	118.09
39	SS	307	CHL	O2D-CGD-CBD	2.16	113.32	110.95
39	SS	306	CHL	CMD-C2D-C3D	2.16	129.00	124.68
32	N	603	CLA	CHB-C4A-NA	2.16	127.52	124.40
32	Y	612	CLA	C4A-NA-C1A	2.16	107.66	106.68
40	YY	616	LUT	C15-C35-C34	-2.16	119.10	123.52
34	H	101	BCR	C4-C5-C6	-2.16	119.79	122.70
32	Bb	616	CLA	C3B-C4B-NB	-2.16	108.60	110.53
39	1	607	CHL	C4C-CHD-C1D	2.16	123.79	116.07
32	s	611	CLA	CHB-C4A-NA	2.16	127.52	124.40
39	33	607	CHL	C3D-C4D-CHA	2.16	111.82	108.54
39	4	302	CHL	C3D-C4D-CHA	2.16	111.82	108.54
39	3	608	CHL	CMD-C2D-C3D	2.16	129.00	124.68
40	G	615	LUT	C35-C15-C14	-2.16	119.10	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H	101	BCR	C38-C26-C27	2.16	118.20	113.60
39	R	605	CHL	CAA-C2A-C3A	2.16	118.83	113.00
32	11	611	CLA	CHB-C4A-NA	2.16	127.51	124.40
32	RR	308	CLA	CHB-C4A-NA	2.16	127.51	124.40
32	Cc	507	CLA	CHB-C4A-NA	2.16	127.51	124.40
39	Y	608	CHL	C3D-C4D-CHA	2.16	111.82	108.54
39	22	606	CHL	C3D-C4D-CHA	2.16	111.82	108.54
32	r	603	CLA	C3B-C4B-NB	-2.16	108.61	110.53
32	R	602	CLA	C1-C2-C3	-2.16	122.66	126.20
41	G	617	XAT	C31-C30-C29	-2.16	124.25	127.28
39	G	601	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
34	Bb	617	BCR	C3-C4-C5	-2.16	110.21	114.06
32	a	407	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
40	22	614	LUT	C39-C29-C30	2.16	126.31	122.82
34	Cc	517	BCR	C39-C30-C25	-2.16	106.86	110.24
32	Bb	612	CLA	C3B-C4B-NB	-2.16	108.61	110.53
39	S	606	CHL	C4C-CHD-C1D	2.16	123.78	116.07
39	r	607	CHL	C3D-C4D-CHA	2.16	111.81	108.54
33	AA	407	PHO	C1-C2-C3	-2.16	122.67	126.20
32	CC	508	CLA	C5-C3-C2	2.16	126.00	121.17
32	1	604	CLA	CHB-C4A-NA	2.16	127.51	124.40
32	B	621	CLA	CHB-C4A-NA	2.16	127.51	124.40
42	N	618	NEX	C40-C33-C34	-2.15	119.33	122.82
32	n	603	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
39	Ss	606	CHL	CMD-C2D-C3D	2.15	128.99	124.68
34	b	618	BCR	C29-C28-C27	-2.15	106.54	111.28
39	4	308	CHL	CMD-C2D-C3D	2.15	128.99	124.68
40	g	616	LUT	C16-C1-C6	2.15	113.62	110.24
39	11	608	CHL	C3C-C4C-NC	-2.15	109.39	114.65
41	RR	316	XAT	C8-C9-C10	-2.15	115.62	119.01
46	e	101	HEM	C4D-ND-C1D	2.15	107.76	105.21
32	GG	612	CLA	CAC-C3C-C4C	2.15	127.59	124.79
39	4	308	CHL	CHA-C1A-C2A	-2.15	128.25	133.31
32	n	610	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
39	n	608	CHL	CMD-C2D-C3D	2.15	128.98	124.68
39	GG	601	CHL	O2A-CGA-O1A	-2.15	118.25	123.63
40	YY	616	LUT	C36-C21-C26	2.15	112.80	109.55
41	4	314	XAT	C12-C13-C14	-2.15	115.62	119.01
39	r	606	CHL	O2D-CGD-CBD	2.15	113.31	110.95
34	Cc	516	BCR	C38-C26-C25	-2.15	122.14	124.48
32	y	306	CLA	C3B-C4B-NB	-2.15	108.61	110.53
39	44	605	CHL	C3D-C4D-CHA	2.15	111.81	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	g	609	CHL	C3D-C4D-CHA	2.15	111.81	108.54
32	RR	312	CLA	CHB-C4A-NA	2.15	127.50	124.40
32	b	603	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
41	GG	619	XAT	C26-C27-C28	-2.15	121.45	125.99
42	Rr	616	NEX	C15-C14-C13	-2.15	124.26	127.28
39	y	307	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
36	AA	411	LHG	O7-C7-O9	-2.15	118.68	123.70
32	11	612	CLA	CHB-C4A-NA	2.15	127.50	124.40
40	Nn	306	LUT	C15-C35-C34	-2.15	119.12	123.52
32	Yy	610	CLA	C4A-NA-C1A	2.15	107.66	106.68
41	y	302	XAT	C19-C9-C10	-2.15	119.34	122.82
39	3	607	CHL	C3D-C4D-CHA	2.15	111.80	108.54
32	R	610	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
32	D	405	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
32	SS	313	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
34	B	614	BCR	C29-C30-C25	2.15	113.56	110.44
39	22	601	CHL	C4C-CHD-C1D	2.15	123.75	116.07
32	1	612	CLA	CHB-C4A-NA	2.15	127.50	124.40
32	G	613	CLA	CHB-C4A-NA	2.15	127.50	124.40
39	Nn	318	CHL	CMD-C2D-C3D	2.15	128.97	124.68
38	BB	619	LMG	O8-C28-C29	2.15	118.38	111.83
39	n	601	CHL	O1D-CGD-CBD	2.15	127.98	124.72
32	22	603	CLA	C3B-C4B-NB	-2.15	108.61	110.53
32	a	407	CLA	C3B-C4B-NB	-2.15	108.61	110.53
33	Aa	408	PHO	O2A-CGA-O1A	-2.15	118.26	123.63
39	y	307	CHL	C3D-C4D-CHA	2.15	111.80	108.54
39	GG	601	CHL	O1D-CGD-CBD	2.15	127.98	124.72
40	R	615	LUT	C28-C29-C30	-2.15	115.63	119.01
32	R	609	CLA	CBA-CAA-C2A	2.15	120.18	113.79
32	BB	604	CLA	CHB-C4A-NA	2.15	127.50	124.40
32	s	611	CLA	C2A-C1A-CHA	2.15	127.59	123.87
32	b	616	CLA	C3B-C4B-NB	-2.15	108.61	110.53
40	Yy	616	LUT	C15-C35-C34	-2.15	119.13	123.52
40	NN	616	LUT	C26-C27-C28	-2.14	121.24	124.58
39	y	309	CHL	CMD-C2D-C3D	2.14	128.97	124.68
32	s	603	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
39	Y	601	CHL	C3D-C4D-CHA	2.14	111.80	108.54
39	SS	307	CHL	C4C-CHD-C1D	2.14	123.74	116.07
32	Nn	314	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
39	33	607	CHL	CMD-C2D-C3D	2.14	128.97	124.68
39	Nn	319	CHL	C3D-C4D-CHA	2.14	111.80	108.54
39	1	601	CHL	O1D-CGD-CBD	2.14	127.97	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Ss	603	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
42	Gg	318	NEX	C37-C21-C36	-2.14	104.26	107.37
40	SS	315	LUT	C7-C8-C9	-2.14	123.06	126.23
39	g	608	CHL	C3D-C4D-CHA	2.14	111.80	108.54
32	R	608	CLA	CHB-C4A-NA	2.14	127.49	124.40
39	Yy	605	CHL	CMD-C2D-C3D	2.14	128.97	124.68
39	33	608	CHL	CMD-C2D-C3D	2.14	128.97	124.68
39	g	606	CHL	C4D-CHA-CBD	-2.14	106.81	108.97
32	C	503	CLA	CBA-CAA-C2A	2.14	120.17	113.79
32	g	614	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
39	Yy	605	CHL	O2A-CGA-O1A	-2.14	118.27	123.63
32	Bb	602	CLA	CHB-C4A-NA	2.14	127.49	124.40
39	Yy	605	CHL	C3C-C4C-NC	-2.14	109.41	114.65
35	Dd	404	PL9	C7-C3-C2	-2.14	120.86	123.39
32	B	610	CLA	C5-C3-C2	2.14	125.98	121.17
39	11	606	CHL	C3D-C4D-CHA	2.14	111.80	108.54
39	1	607	CHL	C3D-C4D-CHA	2.14	111.80	108.54
39	GG	609	CHL	C3D-C4D-CHA	2.14	111.80	108.54
32	Ss	612	CLA	CHB-C4A-NA	2.14	127.49	124.40
42	Yy	617	NEX	C20-C13-C14	-2.14	119.35	122.82
40	S	614	LUT	C7-C8-C9	-2.14	123.07	126.23
38	Dd	408	LMG	C8-O7-C10	-2.14	112.67	117.80
39	2	605	CHL	CMD-C2D-C3D	2.14	128.96	124.68
39	NN	607	CHL	CMD-C2D-C3D	2.14	128.96	124.68
41	RR	316	XAT	C36-C21-C22	-2.14	105.21	108.97
39	YY	605	CHL	CMD-C2D-C3D	2.14	128.96	124.68
32	Cc	511	CLA	C3B-C4B-NB	-2.14	108.62	110.53
34	A	409	BCR	C2-C3-C4	-2.14	106.57	111.28
39	NN	605	CHL	CMD-C2D-C3D	2.14	128.96	124.68
39	3	601	CHL	C4D-CHA-CBD	-2.14	106.81	108.97
40	Yy	615	LUT	C35-C15-C14	-2.14	119.14	123.52
39	NN	608	CHL	C3D-C4D-CHA	2.14	111.79	108.54
32	Rr	601	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
40	RR	315	LUT	C11-C10-C9	-2.14	124.28	127.28
41	GG	617	XAT	C31-C30-C29	-2.14	124.28	127.28
32	Y	610	CLA	C4A-NA-C1A	2.14	107.66	106.68
32	C	505	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
34	AA	409	BCR	C27-C26-C25	-2.14	119.81	122.70
32	r	611	CLA	O1D-CGD-CBD	2.14	128.74	124.52
32	CC	510	CLA	C3B-C4B-NB	-2.14	108.62	110.53
44	c	518	DGD	O1G-C1A-C2A	2.14	118.36	111.83
39	GG	607	CHL	CMD-C2D-C3D	2.14	128.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	r	614	LUT	C20-C13-C12	2.14	121.35	118.09
32	g	611	CLA	C4-C3-C5	2.14	118.94	115.23
40	22	614	LUT	C31-C30-C29	-2.14	124.28	127.28
41	y	302	XAT	O24-C25-C38	2.14	117.44	115.05
32	Aa	410	CLA	CBA-CAA-C2A	2.14	120.15	113.79
32	A	405	CLA	O1D-CGD-CBD	2.14	128.73	124.52
39	44	601	CHL	C3D-C4D-CHA	2.14	111.79	108.54
39	NN	601	CHL	C3D-C4D-CHA	2.14	111.79	108.54
39	g	608	CHL	CMD-C2D-C3D	2.14	128.95	124.68
32	1	602	CLA	CHB-C4A-NA	2.14	127.48	124.40
40	G	616	LUT	C38-C25-C24	-2.14	118.30	123.36
39	G	601	CHL	CMD-C2D-C3D	2.14	128.95	124.68
40	Yy	615	LUT	C38-C25-C24	-2.14	118.30	123.36
32	Bb	609	CLA	CHB-C4A-NA	2.14	127.48	124.40
32	Cc	506	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
39	N	608	CHL	CMD-C2D-C3D	2.14	128.95	124.68
41	G	619	XAT	C31-C30-C29	-2.14	124.28	127.28
34	B	614	BCR	C37-C22-C21	-2.14	119.36	122.82
32	DD	403	CLA	C3B-C4B-NB	-2.14	108.62	110.53
32	RR	304	CLA	C3B-C4B-NB	-2.14	108.62	110.53
39	n	609	CHL	C3D-C4D-CHA	2.14	111.79	108.54
32	Cc	514	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
32	g	613	CLA	CHB-C4A-NA	2.14	127.48	124.40
39	Rr	605	CHL	C4C-CHD-C1D	2.14	123.71	116.07
32	Nn	313	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
32	CC	507	CLA	C3B-C4B-NB	-2.14	108.62	110.53
32	y	313	CLA	CHB-C4A-NA	2.14	127.48	124.40
32	GG	614	CLA	CHB-C4A-NA	2.14	127.48	124.40
39	Y	605	CHL	C3D-C4D-CHA	2.13	111.78	108.54
32	Nn	305	CLA	CHB-C4A-NA	2.13	127.48	124.40
34	c	514	BCR	C27-C26-C25	-2.13	119.82	122.70
39	Gg	307	CHL	C3D-C4D-CHA	2.13	111.78	108.54
34	C	516	BCR	C7-C6-C5	-2.13	116.64	121.56
39	Rr	607	CHL	CMD-C2D-C3D	2.13	128.95	124.68
32	g	610	CLA	CHB-C4A-NA	2.13	127.48	124.40
32	RR	313	CLA	CHB-C4A-NA	2.13	127.48	124.40
34	Cc	518	BCR	C29-C30-C25	2.13	113.54	110.44
32	Ss	613	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
39	Yy	607	CHL	CMD-C2D-C3D	2.13	128.94	124.68
32	B	624	CLA	C1-O2A-CGA	2.13	121.81	116.65
39	r	607	CHL	O1D-CGD-CBD	2.13	127.96	124.72
32	Bb	604	CLA	C3B-C4B-NB	-2.13	108.63	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BB	616	BCR	C33-C5-C6	-2.13	122.16	124.48
33	a	408	PHO	O2A-CGA-O1A	-2.13	118.30	123.63
32	BB	602	CLA	O1D-CGD-CBD	2.13	128.72	124.52
39	n	606	CHL	CMD-C2D-C3D	2.13	128.94	124.68
39	YY	601	CHL	CMD-C2D-C3D	2.13	128.94	124.68
39	S	607	CHL	C4D-CHA-CBD	-2.13	106.82	108.97
32	Ss	609	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
39	Gg	307	CHL	CMD-C2D-C3D	2.13	128.94	124.68
34	K	102	BCR	C2-C1-C6	2.13	113.53	110.44
32	r	610	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
39	N	608	CHL	C3D-C4D-CHA	2.13	111.78	108.54
32	Nn	303	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
41	G	619	XAT	C26-C27-C28	-2.13	121.49	125.99
34	Bb	619	BCR	C39-C30-C25	2.13	113.58	110.24
39	Y	607	CHL	CMD-C2D-C3D	2.13	128.94	124.68
41	G	619	XAT	C20-C13-C14	-2.13	119.37	122.82
32	R	604	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
32	c	504	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
39	11	601	CHL	C3D-C4D-CHA	2.13	111.77	108.54
39	y	307	CHL	CMD-C2D-C3D	2.13	128.93	124.68
40	G	616	LUT	C12-C13-C14	-2.13	115.66	119.01
34	TT	101	BCR	C38-C26-C27	2.13	118.13	113.60
32	A	406	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
32	N	611	CLA	C3B-C4B-NB	-2.13	108.63	110.53
39	Ss	601	CHL	C1-C2-C3	-2.13	122.71	126.20
41	4	314	XAT	C4-C3-C2	-2.13	106.81	110.79
40	y	318	LUT	C26-C27-C28	-2.13	121.27	124.58
39	r	605	CHL	C4C-CHD-C1D	2.13	123.67	116.07
39	y	307	CHL	O2A-CGA-O1A	-2.13	118.31	123.63
40	s	614	LUT	C7-C6-C5	-2.13	116.66	121.56
32	44	610	CLA	CHB-C4A-NA	2.13	127.47	124.40
32	22	604	CLA	CHB-C4A-NA	2.13	127.47	124.40
32	Cc	505	CLA	CHB-C4A-NA	2.13	127.47	124.40
32	Aa	405	CLA	C2A-C1A-CHA	2.13	127.56	123.87
32	44	604	CLA	C3B-C4B-NB	-2.13	108.63	110.53
39	44	607	CHL	C3D-C4D-CHA	2.12	111.77	108.54
32	b	601	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
32	n	604	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
39	g	605	CHL	C3D-C4D-CHA	2.12	111.77	108.54
32	c	505	CLA	C3B-C4B-NB	-2.12	108.63	110.53
40	Y	616	LUT	C20-C13-C12	2.12	121.33	118.09
46	E	101	HEM	CHC-C1C-NC	2.12	126.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	512	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
39	GG	608	CHL	O2D-CGD-CBD	2.12	113.28	110.95
39	2	606	CHL	C3D-C4D-CHA	2.12	111.77	108.54
39	Nn	318	CHL	C4C-CHD-C1D	2.12	123.66	116.07
34	Bb	618	BCR	C29-C28-C27	-2.12	106.61	111.28
39	4	307	CHL	CMD-C2D-C3D	2.12	128.92	124.68
39	Y	605	CHL	O2D-CGD-CBD	2.12	113.28	110.95
34	BB	620	BCR	C19-C18-C17	-2.12	115.67	119.01
32	Y	610	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
39	44	601	CHL	CMD-C2D-C3D	2.12	128.92	124.68
39	n	605	CHL	CMD-C2D-C3D	2.12	128.92	124.68
32	b	616	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
38	c	519	LMG	O8-C28-O10	-2.12	118.32	123.63
39	Yy	608	CHL	O2A-CGA-O1A	-2.12	118.32	123.63
39	g	605	CHL	CMD-C2D-C3D	2.12	128.92	124.68
32	Bb	613	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
34	XX	202	BCR	C35-C13-C12	2.12	121.33	118.09
40	Gg	316	LUT	C38-C25-C24	-2.12	118.34	123.36
32	Bb	616	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
34	KK	103	BCR	C16-C17-C18	-2.12	124.31	127.28
32	1	611	CLA	C2A-C1A-CHA	2.12	126.00	122.71
32	G	612	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
39	NN	609	CHL	CMB-C2B-C3B	2.12	128.92	124.68
32	b	609	CLA	C1-C2-C3	-2.12	122.73	126.20
32	g	612	CLA	CAC-C3C-C4C	2.12	127.55	124.79
34	CC	517	BCR	C20-C21-C22	-2.12	124.31	127.28
32	C	512	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
32	RR	308	CLA	C3B-C4B-NB	-2.12	108.64	110.53
33	Aa	408	PHO	CMB-C2B-C3B	2.12	128.92	124.68
32	3	610	CLA	CHD-C1D-ND	-2.12	121.82	124.80
32	d	401	CLA	CAC-C3C-C4C	2.12	127.55	124.79
40	Y	616	LUT	C19-C9-C8	2.12	121.32	118.09
39	G	609	CHL	O2D-CGD-CBD	2.12	113.27	110.95
39	NN	608	CHL	CMD-C2D-C3D	2.12	128.91	124.68
39	SS	302	CHL	CMD-C2D-C3D	2.12	128.91	124.68
32	11	604	CLA	C2A-C1A-CHA	2.12	125.99	122.71
32	AA	406	CLA	C3B-C4B-NB	-2.12	108.64	110.53
34	k	101	BCR	C7-C8-C9	-2.12	123.10	126.23
37	A	412	SQD	O7-S-C6	2.12	109.92	106.76
32	C	509	CLA	C5-C3-C2	2.12	125.92	121.17
39	1	605	CHL	C2A-C1A-CHA	2.12	125.35	121.84
32	Gg	315	CLA	O2A-CGA-O1A	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Bb	619	BCR	C37-C22-C21	-2.12	119.39	122.82
32	Bb	601	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
32	B	610	CLA	O2D-CGD-CBD	2.12	114.93	111.23
32	AA	406	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
39	22	601	CHL	C3D-C4D-CHA	2.12	111.75	108.54
41	N	617	XAT	C39-C29-C28	2.12	121.32	118.09
39	RR	305	CHL	CMD-C2D-C3D	2.11	128.91	124.68
39	G	601	CHL	O1D-CGD-CBD	2.11	127.93	124.72
32	CC	507	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
34	d	403	BCR	C12-C13-C14	-2.11	115.68	119.01
39	n	607	CHL	C4C-CHD-C1D	2.11	123.63	116.07
32	SS	313	CLA	C3B-C4B-NB	-2.11	108.64	110.53
40	YY	616	LUT	C7-C8-C9	-2.11	123.11	126.23
32	r	612	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
39	33	607	CHL	C2A-C1A-CHA	2.11	125.35	121.84
36	N	619	LHG	O7-C7-O9	-2.11	118.76	123.70
39	44	606	CHL	CMD-C2D-C3D	2.11	128.91	124.68
34	Bb	618	BCR	C2-C1-C6	2.11	113.51	110.44
32	YY	604	CLA	C3B-C4B-NB	-2.11	108.64	110.53
32	BB	614	CLA	O2D-CGD-CBD	2.11	114.92	111.23
32	BB	613	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
40	Yy	615	LUT	C16-C1-C6	2.11	113.56	110.24
39	y	303	CHL	C1-C2-C3	-2.11	122.74	126.20
44	Cc	519	DGD	O2G-C1B-O1B	-2.11	118.77	123.70
32	BB	605	CLA	C3B-C4B-NB	-2.11	108.64	110.53
32	Bb	606	CLA	C3B-C4B-NB	-2.11	108.64	110.53
39	g	601	CHL	O1D-CGD-CBD	2.11	127.92	124.72
42	Y	617	NEX	C15-C14-C13	-2.11	124.32	127.28
41	Rr	615	XAT	C12-C13-C14	-2.11	115.69	119.01
39	33	606	CHL	CMD-C2D-C3D	2.11	128.90	124.68
39	s	607	CHL	O2A-CGA-O1A	-2.11	118.35	123.63
39	Rr	605	CHL	C3D-C4D-CHA	2.11	111.75	108.54
39	3	608	CHL	C4C-CHD-C1D	2.11	123.62	116.07
39	s	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
39	Gg	309	CHL	O1D-CGD-CBD	2.11	127.92	124.72
39	N	605	CHL	C3D-C4D-CHA	2.11	111.75	108.54
34	B	612	BCR	C34-C9-C8	2.11	121.31	118.09
39	G	605	CHL	CMD-C2D-C3D	2.11	128.90	124.68
39	G	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
32	d	401	CLA	O2D-CGD-CBD	2.11	114.92	111.23
34	c	515	BCR	C38-C26-C27	2.11	118.09	113.60
40	Y	615	LUT	C8-C9-C10	-2.11	115.69	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	11	609	CLA	CAC-C3C-C4C	2.11	127.53	124.79
32	Bb	606	CLA	C1-C2-C3	-2.11	122.74	126.20
34	B	613	BCR	C29-C28-C27	-2.11	106.64	111.28
39	Ss	601	CHL	CMD-C2D-C3D	2.11	128.90	124.68
39	n	601	CHL	C4C-CHD-C1D	2.11	123.62	116.07
39	r	606	CHL	CMD-C2D-C3D	2.11	128.90	124.68
32	CC	511	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
39	3	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
40	RR	315	LUT	C16-C1-C6	2.11	113.55	110.24
32	Gg	303	CLA	CHC-C4B-NB	2.11	127.21	124.05
39	YY	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
34	B	616	BCR	C20-C21-C22	-2.11	124.32	127.28
32	D	404	CLA	CAC-C3C-C4C	2.11	127.53	124.79
36	A	413	LHG	O8-C23-O10	-2.11	118.36	123.63
39	1	608	CHL	C3D-C4D-CHA	2.11	111.74	108.54
34	Cc	518	BCR	C7-C8-C9	-2.11	123.12	126.23
39	y	310	CHL	O2A-CGA-O1A	-2.11	118.36	123.63
39	Nn	315	CHL	CMD-C2D-C3D	2.11	128.89	124.68
34	h	101	BCR	C7-C6-C5	-2.11	116.70	121.56
32	r	608	CLA	C3B-C4B-NB	-2.11	108.65	110.53
39	Nn	317	CHL	C4C-CHD-C1D	2.11	123.60	116.07
39	11	607	CHL	CMD-C2D-C3D	2.11	128.89	124.68
32	a	406	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
40	Gg	316	LUT	C35-C15-C14	-2.11	119.21	123.52
34	b	619	BCR	C27-C26-C25	-2.11	119.86	122.70
32	C	513	CLA	C3B-C4B-NB	-2.10	108.65	110.53
32	NN	610	CLA	CBA-CAA-C2A	2.10	120.06	113.79
34	k	101	BCR	C35-C13-C12	2.10	121.30	118.09
39	22	605	CHL	C3D-C4D-CHA	2.10	111.74	108.54
32	2	604	CLA	CHB-C4A-NA	2.10	127.44	124.40
40	GG	615	LUT	C15-C35-C34	-2.10	119.21	123.52
34	B	613	BCR	C33-C5-C4	2.10	118.08	113.60
32	Ss	603	CLA	C3B-C4B-NB	-2.10	108.65	110.53
32	Ss	608	CLA	C3B-C4B-NB	-2.10	108.65	110.53
37	l	102	SQD	O7-S-C6	2.10	109.90	106.76
39	3	601	CHL	O1D-CGD-CBD	2.10	127.91	124.72
42	YY	617	NEX	C15-C14-C13	-2.10	124.33	127.28
32	C	515	CLA	O2D-CGD-CBD	2.10	114.91	111.23
41	GG	619	XAT	C39-C29-C28	2.10	121.30	118.09
38	Cc	501	LMG	O8-C28-O10	-2.10	118.37	123.63
40	GG	615	LUT	C38-C25-C24	-2.10	118.38	123.36
32	B	618	CLA	CHB-C4A-NA	2.10	127.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Yy	619	XAT	C15-C35-C34	-2.10	119.22	123.52
36	KK	101	LHG	C5-O7-C7	-2.10	112.76	117.80
32	Rr	608	CLA	CBA-CAA-C2A	2.10	120.05	113.79
39	2	606	CHL	O1D-CGD-CBD	2.10	127.91	124.72
32	n	612	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
39	Nn	317	CHL	C5-C3-C2	2.10	125.89	121.17
34	XX	202	BCR	C38-C26-C25	-2.10	122.19	124.48
40	YY	615	LUT	C7-C6-C5	-2.10	116.71	121.56
32	y	314	CLA	C4A-NA-C1A	2.10	107.64	106.68
39	SS	307	CHL	C4D-CHA-CBD	-2.10	106.85	108.97
32	b	605	CLA	C5-C3-C2	2.10	125.88	121.17
32	Bb	611	CLA	CHB-C4A-NA	2.10	127.43	124.40
34	h	101	BCR	C34-C9-C8	-2.10	114.88	118.09
32	BB	610	CLA	C4-C3-C5	2.10	118.87	115.23
34	c	516	BCR	C37-C22-C21	-2.10	119.41	122.82
32	Yy	612	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
32	2	612	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	BB	601	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	c	502	CLA	C3B-C4B-NB	-2.10	108.66	110.53
38	B	615	LMG	O8-C28-C29	2.10	118.24	111.83
39	s	607	CHL	C3D-C4D-CHA	2.10	111.73	108.54
39	YY	608	CHL	O2A-CGA-O1A	-2.10	118.38	123.63
39	33	601	CHL	O1D-CGD-CBD	2.10	127.91	124.72
32	c	502	CLA	C5-C3-C2	2.10	125.88	121.17
32	44	603	CLA	C3B-C4B-NB	-2.10	108.66	110.53
32	C	507	CLA	C3B-C4B-NB	-2.10	108.66	110.53
32	r	601	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
33	DD	402	PHO	O2A-CGA-O1A	-2.10	118.38	123.63
32	G	602	CLA	CHC-C4B-NB	2.10	127.20	124.05
38	Bb	621	LMG	O7-C10-O9	-2.10	118.80	123.70
32	y	314	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
39	Ss	601	CHL	C4D-CHA-CBD	-2.10	106.85	108.97
32	33	610	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	GG	604	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	n	610	CLA	CMC-C2C-C1C	2.10	128.31	125.03
37	L	102	SQD	O4-C4-C5	2.10	114.49	109.32
39	G	609	CHL	C3D-C4D-CHA	2.10	111.73	108.54
40	NN	616	LUT	C15-C35-C34	-2.10	119.23	123.52
32	S	602	CLA	C3B-C4B-NB	-2.10	108.66	110.53
32	Nn	304	CLA	O1D-CGD-CBD	2.10	128.65	124.52
32	Bb	613	CLA	CMB-C2B-C3B	2.10	131.48	126.55
39	4	302	CHL	CMD-C2D-C3D	2.10	128.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Cc	501	LMG	O7-C10-O9	-2.10	118.80	123.70
42	Rr	616	NEX	C8-C7-C6	-2.10	175.19	177.66
39	Gg	306	CHL	C3D-C4D-CHA	2.10	111.73	108.54
40	y	317	LUT	C35-C15-C14	-2.10	119.23	123.52
40	44	612	LUT	C38-C25-C24	-2.10	118.40	123.36
32	R	601	CLA	CMB-C2B-C3B	2.10	131.48	126.55
32	s	608	CLA	C3B-C4B-NB	-2.10	108.66	110.53
39	33	605	CHL	CMD-C2D-C3D	2.10	128.87	124.68
39	2	608	CHL	C4C-CHD-C1D	2.10	123.57	116.07
32	Ss	602	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
32	b	613	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
36	CC	523	LHG	O8-C23-O10	-2.10	118.39	123.63
34	h	101	BCR	C12-C13-C14	-2.10	115.71	119.01
32	c	502	CLA	O2D-CGD-CBD	2.10	114.89	111.23
34	b	618	BCR	C33-C5-C6	-2.10	122.20	124.48
34	BB	620	BCR	C8-C9-C10	-2.09	115.71	119.01
40	GG	616	LUT	C12-C13-C14	-2.09	115.71	119.01
32	22	610	CLA	CHB-C4A-NA	2.09	127.42	124.40
32	Yy	612	CLA	C5-C3-C2	2.09	125.87	121.17
32	B	606	CLA	C11-C10-C8	-2.09	109.00	115.97
39	r	607	CHL	C4C-CHD-C1D	2.09	123.56	116.07
40	Ss	614	LUT	C1-C2-C3	2.09	118.19	113.59
39	22	605	CHL	O1D-CGD-CBD	2.09	127.90	124.72
34	CC	517	BCR	C24-C23-C22	-2.09	123.14	126.23
32	b	613	CLA	CMB-C2B-C3B	2.09	131.47	126.55
32	Rr	604	CLA	CAA-C2A-C1A	-2.09	105.11	111.97
33	D	402	PHO	C2D-C1D-ND	-2.09	107.92	109.43
41	y	301	XAT	C39-C29-C30	-2.09	119.42	122.82
39	11	606	CHL	C2A-C1A-CHA	2.09	125.31	121.84
44	D	411	DGD	O1G-C1A-O1A	-2.09	118.39	123.63
39	2	601	CHL	C3D-C4D-CHA	2.09	111.72	108.54
39	s	601	CHL	O2A-CGA-O1A	-2.09	118.39	123.63
32	G	603	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
37	Ll	101	SQD	O7-S-C6	2.09	109.88	106.76
40	R	615	LUT	C12-C13-C14	-2.09	115.72	119.01
34	Dd	403	BCR	C40-C30-C25	2.09	113.52	110.24
32	CC	505	CLA	O2D-CGD-CBD	2.09	114.89	111.23
41	g	619	XAT	O24-C26-C27	2.09	122.87	116.88
41	GG	617	XAT	O24-C25-C26	-2.09	57.27	58.93
32	n	610	CLA	CAC-C3C-C4C	2.09	127.51	124.79
39	Yy	601	CHL	C3D-C4D-CHA	2.09	111.72	108.54
34	Bb	618	BCR	C36-C18-C17	-2.09	119.43	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	GG	616	LUT	C38-C25-C24	-2.09	118.41	123.36
32	B	609	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
32	B	619	CLA	O1D-CGD-CBD	2.09	128.64	124.52
39	N	607	CHL	CMD-C2D-C3D	2.09	128.86	124.68
39	s	601	CHL	CMD-C2D-C3D	2.09	128.86	124.68
42	RR	317	NEX	C30-C31-C32	-2.09	117.15	123.20
39	R	607	CHL	C4C-CHD-C1D	2.09	123.54	116.07
32	Ss	612	CLA	O2D-CGD-CBD	2.09	114.88	111.23
39	y	308	CHL	CMD-C2D-C3D	2.09	128.85	124.68
32	s	608	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	c	510	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
34	KK	103	BCR	C23-C22-C21	-2.09	115.73	119.01
32	BB	607	CLA	C3B-C4B-NB	-2.09	108.67	110.53
40	g	616	LUT	C15-C35-C34	-2.09	119.25	123.52
32	y	316	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	BB	605	CLA	O1D-CGD-CBD	2.09	128.63	124.52
39	33	605	CHL	C3D-C4D-CHA	2.09	111.71	108.54
41	Rr	615	XAT	C16-C1-C6	2.09	115.68	110.05
40	g	615	LUT	C38-C25-C24	-2.09	118.42	123.36
39	Yy	608	CHL	C4D-CHA-CBD	-2.09	106.86	108.97
39	SS	302	CHL	C3D-C4D-CHA	2.09	111.71	108.54
40	GG	615	LUT	C17-C1-C6	-2.09	106.97	110.24
32	YY	614	CLA	C3B-C4B-NB	-2.09	108.67	110.53
39	GG	601	CHL	CMD-C2D-C3D	2.09	128.85	124.68
39	r	605	CHL	C3D-C4D-CHA	2.09	111.71	108.54
32	g	610	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	Ss	604	CLA	CHB-C4A-NA	2.08	127.41	124.40
39	22	607	CHL	C3D-C4D-CHA	2.08	111.71	108.54
32	AA	408	CLA	O1D-CGD-CBD	2.08	128.63	124.52
39	RR	307	CHL	C4C-CHD-C1D	2.08	123.52	116.07
32	CC	505	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
32	NN	611	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
39	S	606	CHL	C4D-CHA-CBD	-2.08	106.87	108.97
32	1	611	CLA	CHC-C4B-NB	2.08	127.17	124.05
39	11	601	CHL	O1D-CGD-CBD	2.08	127.88	124.72
38	F	101	LMG	O8-C28-C29	2.08	118.19	111.83
34	B	613	BCR	C4-C5-C6	-2.08	119.89	122.70
32	G	602	CLA	C3B-C4B-NB	-2.08	108.67	110.53
32	Y	612	CLA	C5-C3-C2	2.08	125.84	121.17
39	Y	608	CHL	O2A-CGA-O1A	-2.08	118.42	123.63
32	Bb	601	CLA	C1-C2-C3	-2.08	122.79	126.20
32	S	608	CLA	CHB-C4A-NA	2.08	127.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Yy	619	XAT	C19-C9-C8	2.08	121.27	118.09
33	AA	407	PHO	O2A-CGA-O1A	-2.08	118.42	123.63
32	Cc	511	CLA	C4-C3-C5	2.08	118.84	115.23
34	B	612	BCR	C19-C18-C17	-2.08	115.73	119.01
40	s	615	LUT	C8-C9-C10	-2.08	115.73	119.01
33	A	407	PHO	O2A-CGA-O1A	-2.08	118.42	123.63
39	g	608	CHL	O1D-CGD-CBD	2.08	127.88	124.72
39	Y	605	CHL	CMD-C2D-C3D	2.08	128.84	124.68
39	Ss	607	CHL	O1D-CGD-CBD	2.08	127.88	124.72
34	c	514	BCR	C24-C25-C26	-2.08	116.76	121.56
32	B	620	CLA	O2D-CGD-CBD	2.08	114.87	111.23
39	Nn	317	CHL	CMD-C2D-C3D	2.08	128.84	124.68
39	G	606	CHL	C3D-C4D-CHA	2.08	111.70	108.54
32	b	606	CLA	C3B-C4B-NB	-2.08	108.67	110.53
39	GG	609	CHL	C4D-CHA-CBD	-2.08	106.87	108.97
34	B	614	BCR	C16-C15-C14	-2.08	119.27	123.52
34	k	101	BCR	C28-C27-C26	-2.08	110.35	114.06
42	y	319	NEX	C24-C23-C22	-2.08	106.90	110.79
39	2	607	CHL	C2A-C1A-CHA	2.08	125.29	121.84
34	H	101	BCR	C16-C17-C18	-2.08	124.36	127.28
32	33	611	CLA	CHB-C4A-NA	2.08	127.40	124.40
34	B	616	BCR	C35-C13-C12	2.08	121.26	118.09
34	B	613	BCR	C37-C22-C21	-2.08	119.45	122.82
39	11	606	CHL	CMD-C2D-C3D	2.08	128.83	124.68
40	y	318	LUT	C15-C35-C34	-2.08	119.27	123.52
34	B	616	BCR	C24-C23-C22	-2.08	123.16	126.23
32	B	624	CLA	C1-C2-C3	-2.08	122.80	126.20
39	1	608	CHL	O2D-CGD-CBD	2.08	113.23	110.95
38	c	519	LMG	O7-C10-O9	-2.08	118.85	123.70
32	BB	610	CLA	O1D-CGD-CBD	2.08	128.61	124.52
39	GG	605	CHL	C3D-C4D-CHA	2.07	111.69	108.54
40	y	318	LUT	C11-C10-C9	-2.07	124.37	127.28
39	Ss	601	CHL	O1D-CGD-CBD	2.07	127.87	124.72
40	y	318	LUT	C16-C1-C6	2.07	113.50	110.24
39	S	605	CHL	CAA-C2A-C3A	-2.07	111.47	116.23
34	Dd	403	BCR	C19-C18-C17	-2.07	115.75	119.01
40	g	616	LUT	C28-C29-C30	-2.07	115.75	119.01
32	B	622	CLA	O1D-CGD-CBD	2.07	128.61	124.52
39	g	609	CHL	O1D-CGD-CBD	2.07	127.87	124.72
39	33	605	CHL	C2A-C1A-CHA	2.07	125.28	121.84
39	Nn	318	CHL	O2D-CGD-CBD	2.07	113.22	110.95
39	33	606	CHL	C3D-C4D-CHA	2.07	111.69	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	BB	615	CLA	CMA-C3A-C2A	-2.07	111.48	116.23
32	Rr	609	CLA	C4-C3-C5	2.07	118.83	115.23
39	3	606	CHL	O1D-CGD-CBD	2.07	127.87	124.72
39	GG	608	CHL	CMD-C2D-C3D	2.07	128.82	124.68
34	Kk	101	BCR	C7-C6-C5	2.07	126.33	121.56
34	b	618	BCR	C2-C1-C6	2.07	113.45	110.44
32	Bb	605	CLA	C5-C3-C2	2.07	125.82	121.17
32	N	612	CLA	CAC-C3C-C4C	2.07	127.48	124.79
39	RR	305	CHL	CBA-CAA-C2A	2.07	119.88	113.78
32	SS	303	CLA	CBA-CAA-C2A	2.07	119.95	113.79
39	S	601	CHL	O1D-CGD-CBD	2.07	127.86	124.72
41	R	616	XAT	C10-C11-C12	-2.07	117.20	123.20
34	BB	617	BCR	C2-C1-C6	2.07	113.45	110.44
34	B	616	BCR	C19-C18-C17	-2.07	115.75	119.01
41	NN	617	XAT	C36-C21-C22	-2.07	105.33	108.97
32	N	611	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
32	Bb	610	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
34	CC	515	BCR	C15-C16-C17	-2.07	119.28	123.52
32	Cc	513	CLA	CHB-C4A-NA	2.07	127.39	124.40
39	GG	606	CHL	C3D-C4D-CHA	2.07	111.68	108.54
32	r	612	CLA	C3B-C4B-NB	-2.07	108.68	110.53
39	y	309	CHL	C4D-CHA-CBD	-2.07	106.88	108.97
32	Cc	504	CLA	C5-C3-C2	2.07	125.81	121.17
32	d	402	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
34	Bb	617	BCR	C4-C5-C6	-2.07	119.91	122.70
39	n	609	CHL	O2A-CGA-O1A	-2.07	118.45	123.63
34	TT	101	BCR	C40-C30-C25	-2.07	107.00	110.24
39	Y	606	CHL	C3D-C4D-CHA	2.07	111.68	108.54
32	c	507	CLA	CHA-C1A-NA	-2.07	121.71	126.39
32	n	614	CLA	O2D-CGD-CBD	2.07	114.84	111.23
39	S	605	CHL	C4C-CHD-C1D	2.07	123.47	116.07
40	Rr	614	LUT	C36-C21-C26	2.07	112.68	109.55
32	Bb	610	CLA	O1D-CGD-CBD	2.07	128.59	124.52
32	b	612	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
39	R	607	CHL	CMD-C2D-C3D	2.07	128.81	124.68
34	k	101	BCR	C12-C13-C14	-2.07	115.76	119.01
40	NN	616	LUT	C37-C21-C22	-2.07	105.55	109.41
32	CC	508	CLA	C3B-C4B-NB	-2.07	108.69	110.53
32	NN	611	CLA	CBA-CAA-C2A	2.07	119.94	113.79
38	c	519	LMG	C8-O7-C10	-2.07	112.85	117.80
40	g	616	LUT	C35-C15-C14	-2.06	119.30	123.52
34	k	101	BCR	C31-C1-C6	-2.06	107.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	YY	617	NEX	C20-C13-C14	-2.06	119.47	122.82
39	Gg	306	CHL	CMD-C2D-C3D	2.06	128.81	124.68
41	Yy	619	XAT	C16-C1-C2	-2.06	105.34	108.97
32	SS	314	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
32	Rr	603	CLA	C3B-C4B-NB	-2.06	108.69	110.53
39	Y	609	CHL	C4D-CHA-CBD	-2.06	106.89	108.97
39	GG	605	CHL	CMD-C2D-C3D	2.06	128.81	124.68
34	TT	101	BCR	C29-C28-C27	-2.06	106.74	111.28
39	Nn	311	CHL	C4C-CHD-C1D	2.06	123.45	116.07
32	b	611	CLA	O2D-CGD-CBD	2.06	114.83	111.23
41	4	314	XAT	C39-C29-C30	-2.06	119.48	122.82
39	22	601	CHL	O1D-CGD-CBD	2.06	127.85	124.72
32	GG	611	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
39	S	601	CHL	C3D-C4D-CHA	2.06	111.67	108.54
32	g	612	CLA	C2A-C1A-CHA	2.06	127.44	123.87
34	BB	616	BCR	C19-C18-C17	-2.06	115.77	119.01
34	b	618	BCR	C36-C18-C17	-2.06	119.48	122.82
39	SS	306	CHL	C4C-CHD-C1D	2.06	123.44	116.07
39	S	601	CHL	CMD-C2D-C3D	2.06	128.80	124.68
39	2	607	CHL	C3D-C4D-CHA	2.06	111.67	108.54
36	A	411	LHG	O7-C7-O9	-2.06	118.89	123.70
38	b	621	LMG	O7-C10-O9	-2.06	118.89	123.70
38	DD	409	LMG	O8-C28-C29	2.06	118.12	111.83
32	s	612	CLA	C3B-C4B-NB	-2.06	108.69	110.53
32	Ss	611	CLA	C2A-C1A-CHA	2.06	127.44	123.87
34	B	616	BCR	C8-C9-C10	-2.06	115.77	119.01
32	c	502	CLA	C4-C3-C2	-2.06	118.34	123.63
40	Ss	615	LUT	C28-C29-C30	-2.06	115.77	119.01
32	Nn	302	CLA	C3B-C4B-NB	-2.06	108.69	110.53
32	g	611	CLA	C2A-C1A-CHA	2.06	127.44	123.87
32	CC	506	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
32	SS	304	CLA	O2A-CGA-O1A	-2.06	118.04	123.33
39	r	607	CHL	CMD-C2D-C3D	2.06	128.80	124.68
32	G	613	CLA	CHC-C4B-NB	2.06	127.14	124.05
39	G	605	CHL	O1D-CGD-CBD	2.06	127.84	124.72
44	C	519	DGD	O6D-C5D-C6D	2.06	110.77	106.69
44	c	517	DGD	O2G-C1B-O1B	-2.06	118.90	123.70
32	Ss	604	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
39	11	607	CHL	C1A-C2A-C3A	-2.06	100.39	103.01
39	n	607	CHL	CMD-C2D-C3D	2.06	128.79	124.68
32	b	611	CLA	CHB-C4A-NA	2.06	127.37	124.40
32	R	602	CLA	CAA-C2A-C3A	2.06	118.56	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Hh	101	BCR	C27-C26-C25	-2.06	119.93	122.70
32	Aa	406	CLA	CMC-C2C-C1C	2.06	128.25	125.03
39	Nn	311	CHL	C3D-C4D-CHA	2.06	111.66	108.54
32	Rr	604	CLA	CHC-C4B-NB	2.06	127.13	124.05
33	a	408	PHO	C2D-C1D-ND	-2.05	107.94	109.43
32	N	611	CLA	CBA-CAA-C2A	2.05	119.91	113.79
34	BB	617	BCR	C4-C5-C6	-2.05	119.93	122.70
34	CC	515	BCR	C7-C6-C5	-2.05	116.82	121.56
39	y	310	CHL	C4D-CHA-CBD	-2.05	106.90	108.97
33	D	402	PHO	O2A-CGA-O1A	-2.05	118.49	123.63
39	3	606	CHL	C4C-CHD-C1D	2.05	123.42	116.07
34	C	516	BCR	C35-C13-C12	2.05	121.22	118.09
40	GG	615	LUT	C19-C9-C8	2.05	121.22	118.09
42	Y	619	NEX	C40-C33-C32	2.05	121.22	118.09
44	Cc	520	DGD	O1G-C1A-C2A	2.05	118.09	111.83
32	Nn	305	CLA	O2D-CGD-CBD	2.05	114.82	111.23
32	CC	503	CLA	C4-C3-C5	2.05	118.79	115.23
32	Yy	603	CLA	CHA-C1A-NA	-2.05	121.74	126.39
32	YY	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
42	g	617	NEX	O24-C25-C38	2.05	117.34	115.05
32	YY	612	CLA	CHA-C1A-NA	-2.05	121.75	126.39
32	GG	612	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
39	SS	302	CHL	O1D-CGD-CBD	2.05	127.83	124.72
34	CC	516	BCR	C4-C5-C6	-2.05	119.93	122.70
32	R	608	CLA	C3B-C4B-NB	-2.05	108.70	110.53
41	44	613	XAT	C10-C11-C12	-2.05	117.26	123.20
39	N	601	CHL	C3D-C4D-CHA	2.05	111.66	108.54
32	3	603	CLA	CHB-C4A-NA	2.05	127.36	124.40
39	3	605	CHL	C3D-C4D-CHA	2.05	111.66	108.54
32	Rr	609	CLA	C3B-C4B-NB	-2.05	108.70	110.53
40	N	615	LUT	C1-C2-C3	2.05	118.09	113.59
39	1	606	CHL	C3D-C4D-CHA	2.05	111.65	108.54
39	y	303	CHL	C3D-C4D-CHA	2.05	111.65	108.54
32	Aa	407	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
32	C	511	CLA	C3B-C4B-NB	-2.05	108.70	110.53
32	Yy	614	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
40	s	614	LUT	C10-C11-C12	-2.05	117.27	123.20
32	NN	611	CLA	C3B-C4B-NB	-2.05	108.70	110.53
42	R	617	NEX	C2-C1-C6	2.05	111.20	109.21
39	RR	305	CHL	CAA-C2A-C3A	2.05	118.53	113.00
32	Gg	313	CLA	CHA-C1A-NA	-2.05	121.75	126.39
40	s	615	LUT	C28-C29-C30	-2.05	115.79	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Y	604	CLA	C3B-C4B-NB	-2.05	108.70	110.53
32	Y	614	CLA	C3B-C4B-NB	-2.05	108.70	110.53
32	Nn	305	CLA	C3B-C4B-NB	-2.05	108.70	110.53
40	Rr	614	LUT	C28-C29-C30	-2.05	115.79	119.01
34	B	614	BCR	C32-C1-C6	-2.05	107.03	110.24
41	NN	617	XAT	C26-C27-C28	-2.05	121.67	125.99
39	SS	306	CHL	C3D-C4D-CHA	2.05	111.65	108.54
32	YY	614	CLA	CAA-C2A-C3A	2.05	118.53	113.00
42	N	618	NEX	C32-C33-C34	-2.05	115.79	119.01
39	r	607	CHL	C4D-CHA-CBD	-2.04	106.91	108.97
34	BB	617	BCR	C33-C5-C4	2.04	117.96	113.60
34	Cc	516	BCR	C38-C26-C27	2.04	117.96	113.60
34	Aa	411	BCR	C29-C28-C27	-2.04	106.78	111.28
34	TT	101	BCR	C21-C20-C19	-2.04	117.28	123.20
39	g	601	CHL	C3D-C4D-CHA	2.04	111.65	108.54
41	Gg	301	XAT	O24-C26-C27	2.04	122.73	116.88
32	33	609	CLA	C3B-C4B-NB	-2.04	108.70	110.53
32	GG	602	CLA	CHB-C4A-NA	2.04	127.35	124.40
39	Nn	319	CHL	C4D-CHA-CBD	-2.04	106.91	108.97
34	BB	617	BCR	C37-C22-C21	-2.04	119.50	122.82
39	S	601	CHL	O2A-CGA-O1A	-2.04	118.52	123.63
39	S	605	CHL	O1D-CGD-CBD	2.04	127.82	124.72
40	Ss	615	LUT	C7-C6-C5	2.04	126.26	121.56
32	B	606	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
39	GG	601	CHL	C1-C2-C3	-2.04	122.85	126.20
32	R	604	CLA	C3B-C4B-NB	-2.04	108.71	110.53
32	BB	614	CLA	C3B-C4B-NB	-2.04	108.71	110.53
41	y	301	XAT	C16-C1-C2	-2.04	105.38	108.97
41	r	615	XAT	O24-C25-C26	-2.04	57.31	58.93
39	G	601	CHL	C1-C2-C3	-2.04	122.85	126.20
32	CC	508	CLA	C2A-C1A-CHA	2.04	127.41	123.87
32	Nn	303	CLA	CHA-C1A-NA	-2.04	121.77	126.39
39	3	605	CHL	CMD-C2D-C3D	2.04	128.76	124.68
32	D	401	CLA	C4-C3-C5	2.04	118.77	115.23
40	n	616	LUT	C15-C35-C34	-2.04	119.34	123.52
34	BB	617	BCR	C29-C28-C27	-2.04	106.79	111.28
32	Cc	515	CLA	O1D-CGD-CBD	2.04	128.54	124.52
32	2	603	CLA	CHB-C4A-NA	2.04	127.34	124.40
39	11	601	CHL	CMD-C2D-C3D	2.04	128.76	124.68
32	G	611	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
32	Cc	504	CLA	CHB-C4A-NA	2.04	127.34	124.40
40	GG	616	LUT	C16-C1-C6	2.04	113.44	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Y	605	CHL	C4D-CHA-CBD	-2.04	106.91	108.97
39	RR	307	CHL	CMD-C2D-C3D	2.04	128.76	124.68
32	YY	612	CLA	C4-C3-C2	-2.04	118.39	123.63
39	2	608	CHL	O1D-CGD-CBD	2.04	127.81	124.72
32	Cc	512	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
32	c	505	CLA	CHB-C4A-NA	2.04	127.34	124.40
34	Cc	516	BCR	C35-C13-C12	2.04	121.20	118.09
32	NN	604	CLA	C3B-C4B-NB	-2.04	108.71	110.53
41	RR	316	XAT	C12-C13-C14	-2.04	115.80	119.01
40	NN	615	LUT	C15-C35-C34	-2.04	119.35	123.52
39	33	608	CHL	C3D-C4D-CHA	2.04	111.64	108.54
36	y	320	LHG	C5-O7-C7	-2.04	112.92	117.80
39	Nn	315	CHL	O2A-CGA-O1A	-2.04	118.53	123.63
39	G	609	CHL	CMD-C2D-C3D	2.04	128.75	124.68
32	Aa	410	CLA	O2D-CGD-CBD	2.04	114.79	111.23
40	RR	315	LUT	C28-C29-C30	-2.04	115.81	119.01
32	Gg	311	CLA	CMC-C2C-C1C	2.04	128.22	125.03
32	n	612	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
32	s	611	CLA	CHA-C1A-NA	-2.04	121.78	126.39
32	3	609	CLA	CHB-C4A-NA	2.04	127.34	124.40
32	S	604	CLA	CAC-C3C-C4C	2.04	127.44	124.79
32	44	602	CLA	CBA-CAA-C2A	2.04	119.85	113.79
39	YY	609	CHL	C4D-CHA-CBD	-2.04	106.91	108.97
32	R	613	CLA	CHB-C4A-NA	2.04	127.34	124.40
32	R	603	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
32	YY	613	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
41	44	613	XAT	C28-C29-C30	-2.04	115.81	119.01
32	Cc	513	CLA	CHD-C1D-ND	-2.04	121.94	124.80
40	Rr	614	LUT	C18-C5-C6	-2.04	122.26	124.48
32	S	612	CLA	C3B-C4B-NB	-2.04	108.71	110.53
40	YY	615	LUT	C38-C25-C24	-2.04	118.54	123.36
34	Cc	518	BCR	C37-C22-C21	-2.04	119.52	122.82
39	G	601	CHL	C4D-CHA-CBD	-2.04	106.92	108.97
39	SS	302	CHL	O2A-CGA-O1A	-2.03	118.54	123.63
32	b	607	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
39	YY	606	CHL	C3D-C4D-CHA	2.03	111.63	108.54
39	G	609	CHL	C4D-CHA-CBD	-2.03	106.92	108.97
39	Y	607	CHL	C4D-CHA-CBD	-2.03	106.92	108.97
42	Yy	617	NEX	C24-C23-C22	-2.03	106.99	110.79
39	Ss	607	CHL	O2A-CGA-O1A	-2.03	118.54	123.63
44	CC	519	DGD	O1G-C1A-O1A	-2.03	118.54	123.63
38	j	101	LMG	C8-O7-C10	-2.03	112.93	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	GG	609	CHL	CMD-C2D-C3D	2.03	128.75	124.68
32	b	608	CLA	C1-C2-C3	-2.03	122.87	126.20
32	CC	503	CLA	C1-C2-C3	-2.03	122.87	126.20
32	BB	602	CLA	CAA-C2A-C3A	2.03	118.49	113.00
39	YY	605	CHL	O2A-CGA-O1A	-2.03	118.55	123.63
32	2	613	CLA	C3B-C4B-NB	-2.03	108.72	110.53
32	NN	614	CLA	C3B-C4B-NB	-2.03	108.72	110.53
39	44	606	CHL	C4D-CHA-CBD	-2.03	106.92	108.97
38	Cc	501	LMG	C8-O7-C10	-2.03	112.93	117.80
40	SS	315	LUT	C26-C27-C28	-2.03	121.42	124.58
32	G	610	CLA	O2D-CGD-CBD	2.03	114.78	111.23
32	Dd	401	CLA	O2D-CGD-CBD	2.03	114.78	111.23
41	N	617	XAT	C26-C27-C28	-2.03	121.70	125.99
32	B	624	CLA	C3B-C4B-NB	-2.03	108.72	110.53
42	NN	618	NEX	C32-C33-C34	-2.03	115.81	119.01
32	Ss	611	CLA	O1D-CGD-CBD	2.03	128.52	124.52
32	11	612	CLA	CMC-C2C-C1C	-2.03	121.86	125.03
41	G	617	XAT	O24-C25-C26	-2.03	57.32	58.93
34	CC	517	BCR	C36-C18-C17	-2.03	119.53	122.82
40	Nn	306	LUT	C7-C8-C9	-2.03	123.23	126.23
32	G	604	CLA	C3B-C4B-NB	-2.03	108.72	110.53
39	2	605	CHL	O1D-CGD-CBD	2.03	127.80	124.72
32	S	609	CLA	O1D-CGD-CBD	2.03	128.52	124.52
32	Ss	611	CLA	CHA-C1A-NA	-2.03	121.80	126.39
32	b	602	CLA	C3B-C4B-NB	-2.03	108.72	110.53
32	r	604	CLA	C3B-C4B-NB	-2.03	108.72	110.53
32	BB	608	CLA	C3B-C4B-NB	-2.03	108.72	110.53
40	Yy	616	LUT	C11-C10-C9	-2.03	124.43	127.28
32	BB	615	CLA	CAC-C3C-C4C	2.03	127.43	124.79
33	Aa	409	PHO	C2D-C1D-ND	-2.03	107.96	109.43
40	NN	615	LUT	C36-C21-C26	2.03	112.62	109.55
40	SS	315	LUT	C11-C10-C9	-2.03	124.43	127.28
39	4	306	CHL	O1D-CGD-CBD	2.03	127.80	124.72
34	a	411	BCR	C36-C18-C17	-2.03	119.53	122.82
41	GG	617	XAT	C12-C13-C14	-2.03	115.82	119.01
39	YY	607	CHL	C4D-CHA-CBD	-2.03	106.92	108.97
42	Yy	617	NEX	C2-C1-C6	2.03	111.18	109.21
32	33	603	CLA	CHB-C4A-NA	2.03	127.33	124.40
32	Nn	301	CLA	CBA-CAA-C2A	2.03	119.82	113.79
39	N	606	CHL	C3D-C4D-CHA	2.03	111.62	108.54
34	Bb	617	BCR	C30-C25-C24	2.03	121.15	115.65
32	Rr	610	CLA	O2A-CGA-O1A	-2.03	118.56	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Ss	608	CLA	CAA-C2A-C3A	2.03	118.47	113.00
32	B	611	CLA	CMA-C3A-C2A	-2.03	111.58	116.23
32	RR	313	CLA	CMA-C3A-C2A	-2.03	111.58	116.23
32	S	603	CLA	O2A-CGA-O1A	-2.03	118.12	123.33
32	s	604	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
32	g	612	CLA	CHA-C1A-NA	-2.03	121.80	126.39
34	d	403	BCR	C19-C18-C17	-2.03	115.82	119.01
40	N	616	LUT	C38-C25-C24	-2.03	118.57	123.36
32	4	311	CLA	C3B-C4B-NB	-2.03	108.72	110.53
32	BB	612	CLA	C3B-C4B-NB	-2.03	108.72	110.53
32	r	613	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
32	Cc	505	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
38	Bb	621	LMG	O8-C28-O10	-2.03	118.56	123.63
39	RR	306	CHL	CMD-C2D-C3D	2.03	128.73	124.68
32	B	608	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
39	3	605	CHL	C2A-C1A-CHA	2.02	125.20	121.84
40	RR	315	LUT	C17-C1-C6	-2.02	107.07	110.24
42	Yy	617	NEX	O24-C25-C26	-2.02	57.33	58.93
34	Kk	101	BCR	C16-C17-C18	-2.02	124.44	127.28
32	a	410	CLA	O2D-CGD-CBD	2.02	114.77	111.23
39	SS	306	CHL	C4D-CHA-CBD	-2.02	106.93	108.97
39	NN	606	CHL	C3D-C4D-CHA	2.02	111.61	108.54
32	SS	304	CLA	O1A-CGA-CBA	2.02	129.51	123.09
40	4	313	LUT	C38-C25-C24	-2.02	118.57	123.36
32	Rr	611	CLA	O1D-CGD-CBD	2.02	128.51	124.52
32	B	606	CLA	O1D-CGD-CBD	2.02	128.51	124.52
32	B	621	CLA	CAC-C3C-C4C	2.02	127.42	124.79
32	b	613	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
32	AA	405	CLA	O1D-CGD-CBD	2.02	128.51	124.52
39	GG	606	CHL	CMD-C2D-C3D	2.02	128.72	124.68
42	NN	618	NEX	C20-C13-C14	-2.02	119.54	122.82
34	c	514	BCR	C35-C13-C12	2.02	121.18	118.09
32	C	506	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
32	Bb	612	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
39	22	605	CHL	CMD-C2D-C3D	2.02	128.72	124.68
40	Yy	615	LUT	C12-C13-C14	-2.02	115.83	119.01
32	Gg	313	CLA	CAC-C3C-C4C	2.02	127.42	124.79
32	22	602	CLA	CHB-C4A-NA	2.02	127.32	124.40
39	G	605	CHL	C3D-C4D-CHA	2.02	111.61	108.54
32	YY	612	CLA	C2A-C3A-C4A	-2.02	98.61	101.87
32	g	602	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
36	44	614	LHG	O8-C23-C24	2.02	120.95	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	n	601	CHL	CMD-C2D-C3D	2.02	128.72	124.68
40	Ss	614	LUT	C26-C27-C28	-2.02	121.44	124.58
32	Cc	509	CLA	CHA-C1A-NA	-2.02	121.82	126.39
32	Rr	612	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
32	33	602	CLA	CHB-C4A-NA	2.02	127.31	124.40
33	A	407	PHO	C2D-C1D-ND	-2.02	107.97	109.43
34	k	101	BCR	C10-C11-C12	-2.02	117.35	123.20
32	G	613	CLA	CAC-C3C-C4C	2.02	127.42	124.79
32	NN	612	CLA	CAC-C3C-C4C	2.02	127.42	124.79
32	r	608	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
39	44	605	CHL	C4C-CHD-C1D	2.02	123.29	116.07
39	N	605	CHL	CMD-C2D-C3D	2.02	128.72	124.68
32	33	604	CLA	CHB-C4A-NA	2.02	127.31	124.40
32	3	602	CLA	CHB-C4A-NA	2.02	127.31	124.40
40	y	318	LUT	C35-C15-C14	-2.02	119.39	123.52
32	d	401	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
34	c	515	BCR	C37-C22-C23	2.02	121.17	118.09
39	Nn	311	CHL	O1D-CGD-CBD	2.02	127.78	124.72
32	44	609	CLA	C3B-C4B-NB	-2.02	108.73	110.53
32	B	610	CLA	C3B-C4B-NB	-2.02	108.73	110.53
32	Bb	601	CLA	CBA-CAA-C2A	2.02	119.79	113.79
32	Rr	609	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
39	Y	605	CHL	O2A-CGA-O1A	-2.02	118.58	123.63
32	3	611	CLA	CHB-C4A-NA	2.02	127.31	124.40
32	b	612	CLA	C1-C2-C3	-2.02	122.89	126.20
39	n	605	CHL	O2A-CGA-O1A	-2.02	118.59	123.63
34	a	411	BCR	C29-C28-C27	-2.01	106.85	111.28
39	RR	306	CHL	C4D-ND-C1D	2.01	106.75	105.22
32	DD	403	CLA	CMB-C2B-C3B	2.01	131.29	126.55
34	Dd	403	BCR	C12-C13-C14	-2.01	115.84	119.01
40	GG	615	LUT	C32-C33-C34	-2.01	115.84	119.01
34	XX	202	BCR	C2-C1-C6	2.01	113.36	110.44
32	Y	614	CLA	CAA-C2A-C3A	2.01	118.44	113.00
39	YY	605	CHL	C4D-CHA-CBD	-2.01	106.94	108.97
32	Ss	610	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
32	S	604	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
32	d	401	CLA	CMB-C2B-C3B	2.01	131.29	126.55
39	22	608	CHL	C3D-C4D-CHA	2.01	111.60	108.54
39	Yy	606	CHL	CMD-C2D-C3D	2.01	128.71	124.68
32	BB	610	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
32	Bb	611	CLA	O2D-CGD-CBD	2.01	114.75	111.23
34	a	411	BCR	C38-C26-C25	-2.01	122.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	514	CLA	C4-C3-C2	-2.01	118.46	123.63
44	C	520	DGD	O1G-C1A-O1A	-2.01	118.59	123.63
39	33	608	CHL	C4C-CHD-C1D	2.01	123.27	116.07
39	Nn	311	CHL	O2A-CGA-O1A	-2.01	118.59	123.63
34	Cc	518	BCR	C30-C25-C24	2.01	121.11	115.65
40	G	616	LUT	C32-C33-C34	-2.01	115.84	119.01
32	N	613	CLA	CHD-C1D-ND	-2.01	121.97	124.80
32	b	615	CLA	CHA-C1A-NA	-2.01	121.83	126.39
40	g	615	LUT	C35-C15-C14	-2.01	119.40	123.52
32	11	602	CLA	CHB-C4A-NA	2.01	127.30	124.40
32	b	601	CLA	CAA-C2A-C3A	2.01	118.44	113.00
34	Bb	619	BCR	C16-C15-C14	-2.01	119.40	123.52
40	Y	615	LUT	C32-C33-C34	-2.01	115.84	119.01
32	4	304	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
32	C	503	CLA	O2D-CGD-CBD	2.01	114.75	111.23
32	Nn	314	CLA	O2D-CGD-CBD	2.01	114.75	111.23
32	NN	611	CLA	O1D-CGD-CBD	2.01	128.48	124.52
32	Dd	402	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
38	c	519	LMG	C4-C3-C2	2.01	114.36	110.83
32	c	508	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
32	44	602	CLA	CAC-C3C-C4C	2.01	127.40	124.79
39	N	601	CHL	O1D-CGD-CBD	2.01	127.77	124.72
34	KK	103	BCR	C34-C9-C10	-2.01	119.56	122.82
41	Nn	308	XAT	C16-C1-C2	-2.01	105.44	108.97
40	RR	315	LUT	C12-C13-C14	-2.01	115.85	119.01
34	CC	517	BCR	C32-C1-C6	-2.01	107.09	110.24
34	T	101	BCR	C29-C28-C27	-2.01	106.86	111.28
32	DD	403	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
38	b	621	LMG	O8-C28-O10	-2.01	118.60	123.63
39	Rr	607	CHL	O2D-CGD-CBD	2.01	113.15	110.95
32	A	406	CLA	O2D-CGD-CBD	2.01	114.74	111.23
32	Bb	613	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
39	Ss	605	CHL	O2A-CGA-O1A	-2.01	118.61	123.63
32	BB	614	CLA	C4-C3-C2	-2.01	118.47	123.63
41	y	302	XAT	C37-C21-C36	-2.01	104.45	107.37
32	Gg	312	CLA	O2D-CGD-CBD	2.01	114.74	111.23
39	YY	609	CHL	CMD-C2D-C3D	2.01	128.69	124.68
32	C	508	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
34	BB	616	BCR	C24-C25-C26	2.01	126.18	121.56
32	11	602	CLA	C3B-C4B-NB	-2.01	108.74	110.53
44	B	603	DGD	O1G-C1A-O1A	-2.01	118.61	123.63
32	c	509	CLA	O1D-CGD-CBD	2.01	128.48	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Y	613	CLA	CAC-C3C-C4C	2.01	127.40	124.79
32	n	602	CLA	CAA-C2A-C3A	2.01	118.42	113.00
39	N	608	CHL	O1D-CGD-CBD	2.01	127.77	124.72
32	BB	604	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
39	Gg	302	CHL	O2A-CGA-O1A	-2.01	118.61	123.63
32	Ss	609	CLA	O2D-CGD-CBD	2.01	114.74	111.23
40	GG	615	LUT	C16-C1-C6	2.01	113.39	110.24
42	y	319	NEX	O24-C25-C26	-2.01	57.34	58.93
39	44	607	CHL	O1D-CGD-CBD	2.01	127.76	124.72
32	BB	609	CLA	C4-C3-C2	-2.01	118.48	123.63
34	k	101	BCR	C1-C6-C7	2.01	121.09	115.65
32	c	511	CLA	CHD-C1D-ND	-2.00	121.98	124.80
39	NN	608	CHL	O1D-CGD-CBD	2.00	127.76	124.72
41	Rr	615	XAT	C28-C29-C30	-2.00	115.86	119.01
32	a	405	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
32	B	607	CLA	O2D-CGD-CBD	2.00	114.73	111.23
39	G	608	CHL	CMD-C2D-C3D	2.00	128.69	124.68
32	Rr	604	CLA	C3B-C4B-NB	-2.00	108.74	110.53
39	2	601	CHL	O1D-CGD-CBD	2.00	127.76	124.72
39	3	608	CHL	C3D-C4D-CHA	2.00	111.58	108.54
39	y	311	CHL	C4C-CHD-C1D	2.00	123.24	116.07
32	1	613	CLA	CHD-C1D-ND	-2.00	121.98	124.80
32	G	602	CLA	CHD-C1D-ND	-2.00	121.98	124.80
34	Dd	403	BCR	C23-C22-C21	-2.00	115.86	119.01
32	RR	313	CLA	CAA-C2A-C3A	-2.00	111.64	116.23
39	1	606	CHL	CMD-C2D-C3D	2.00	128.69	124.68
32	g	611	CLA	CHA-C1A-NA	-2.00	121.86	126.39
32	BB	604	CLA	C4-C3-C5	2.00	118.70	115.23
39	2	606	CHL	C4C-CHD-C1D	2.00	123.23	116.07
42	Gg	318	NEX	C10-C11-C12	-2.00	117.40	123.20
40	G	616	LUT	C15-C35-C34	-2.00	119.42	123.52
40	Ss	615	LUT	C3-C4-C5	-2.00	107.19	112.18
40	Y	615	LUT	C8-C7-C6	-2.00	121.65	127.00
34	D	406	BCR	C12-C13-C14	-2.00	115.86	119.01
32	N	604	CLA	C3B-C4B-NB	-2.00	108.74	110.53
32	n	613	CLA	O1D-CGD-CBD	2.00	128.47	124.52
32	C	511	CLA	O2D-CGD-CBD	2.00	114.73	111.23
32	D	404	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
39	Y	601	CHL	O2A-CGA-O1A	-2.00	118.62	123.63
32	Cc	505	CLA	CAA-CBA-CGA	-2.00	107.53	113.21
32	R	602	CLA	CBA-CAA-C2A	2.00	119.75	113.79
34	KK	103	BCR	C38-C26-C27	2.00	117.86	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Gg	310	CHL	CMD-C2D-C3D	2.00	128.68	124.68
41	GG	619	XAT	O24-C26-C27	2.00	122.61	116.88

All (780) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	405	CLA	ND
32	A	406	CLA	ND
32	A	408	CLA	ND
32	Rr	601	CLA	ND
32	Rr	602	CLA	ND
32	Rr	603	CLA	ND
32	Rr	604	CLA	ND
32	Rr	608	CLA	ND
32	Rr	609	CLA	ND
32	Rr	610	CLA	ND
32	Rr	611	CLA	ND
32	Rr	612	CLA	ND
32	Rr	613	CLA	ND
32	Ss	602	CLA	ND
32	Ss	603	CLA	ND
32	Ss	604	CLA	ND
32	Ss	608	CLA	ND
32	Ss	609	CLA	ND
32	Ss	610	CLA	ND
32	Ss	611	CLA	ND
32	Ss	612	CLA	ND
32	Ss	613	CLA	ND
32	Yy	602	CLA	ND
32	Yy	603	CLA	ND
32	Yy	604	CLA	ND
32	Yy	610	CLA	ND
32	Yy	611	CLA	ND
32	Yy	612	CLA	ND
32	Yy	613	CLA	ND
32	Yy	614	CLA	ND
32	44	602	CLA	ND
32	44	603	CLA	ND
32	44	604	CLA	ND
32	44	609	CLA	ND
32	44	610	CLA	ND
32	44	611	CLA	ND

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Mol	Chain	Res	Type	Atom
32	44	615	CLA	ND
32	11	602	CLA	ND
32	11	603	CLA	ND
32	11	604	CLA	ND
32	11	609	CLA	ND
32	11	610	CLA	ND
32	11	611	CLA	ND
32	11	612	CLA	ND
32	11	613	CLA	ND
32	22	602	CLA	ND
32	22	603	CLA	ND
32	22	604	CLA	ND
32	22	609	CLA	ND
32	22	610	CLA	ND
32	22	611	CLA	ND
32	22	612	CLA	ND
32	22	613	CLA	ND
32	33	602	CLA	ND
32	33	603	CLA	ND
32	33	604	CLA	ND
32	33	609	CLA	ND
32	33	610	CLA	ND
32	33	611	CLA	ND
32	33	612	CLA	ND
32	33	613	CLA	ND
32	1	602	CLA	ND
32	1	603	CLA	ND
32	1	604	CLA	ND
32	1	609	CLA	ND
32	1	610	CLA	ND
32	1	611	CLA	ND
32	1	612	CLA	ND
32	1	613	CLA	ND
32	2	602	CLA	ND
32	2	603	CLA	ND
32	2	604	CLA	ND
32	2	609	CLA	ND
32	2	610	CLA	ND
32	2	611	CLA	ND
32	2	612	CLA	ND
32	2	613	CLA	ND
32	3	602	CLA	ND

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Mol	Chain	Res	Type	Atom
32	3	603	CLA	ND
32	3	604	CLA	ND
32	3	609	CLA	ND
32	3	610	CLA	ND
32	3	611	CLA	ND
32	3	612	CLA	ND
32	3	613	CLA	ND
32	C	503	CLA	ND
32	C	505	CLA	ND
32	C	506	CLA	ND
32	C	507	CLA	ND
32	C	508	CLA	ND
32	C	509	CLA	ND
32	C	510	CLA	ND
32	C	511	CLA	ND
32	C	512	CLA	ND
32	C	513	CLA	ND
32	C	514	CLA	ND
32	C	515	CLA	ND
32	D	401	CLA	ND
32	D	404	CLA	ND
32	D	405	CLA	ND
32	G	602	CLA	ND
32	G	603	CLA	ND
32	G	604	CLA	ND
32	G	610	CLA	ND
32	G	611	CLA	ND
32	G	612	CLA	ND
32	G	613	CLA	ND
32	G	614	CLA	ND
32	N	602	CLA	ND
32	N	603	CLA	ND
32	N	604	CLA	ND
32	N	610	CLA	ND
32	N	611	CLA	ND
32	N	612	CLA	ND
32	N	613	CLA	ND
32	N	614	CLA	ND
32	R	601	CLA	ND
32	R	602	CLA	ND
32	R	603	CLA	ND
32	R	604	CLA	ND

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Mol	Chain	Res	Type	Atom
32	R	608	CLA	ND
32	R	609	CLA	ND
32	R	610	CLA	ND
32	R	611	CLA	ND
32	R	612	CLA	ND
32	R	613	CLA	ND
32	S	602	CLA	ND
32	S	603	CLA	ND
32	S	604	CLA	ND
32	S	608	CLA	ND
32	S	609	CLA	ND
32	S	610	CLA	ND
32	S	611	CLA	ND
32	S	612	CLA	ND
32	S	613	CLA	ND
32	X	201	CLA	ND
32	Y	602	CLA	ND
32	Y	603	CLA	ND
32	Y	610	CLA	ND
32	Y	611	CLA	ND
32	Y	612	CLA	ND
32	Y	613	CLA	ND
32	Y	614	CLA	ND
32	a	405	CLA	ND
32	a	406	CLA	ND
32	a	407	CLA	ND
32	a	410	CLA	ND
32	b	601	CLA	ND
32	b	602	CLA	ND
32	b	603	CLA	ND
32	b	604	CLA	ND
32	b	605	CLA	ND
32	b	606	CLA	ND
32	b	607	CLA	ND
32	b	608	CLA	ND
32	b	609	CLA	ND
32	b	610	CLA	ND
32	b	611	CLA	ND
32	b	612	CLA	ND
32	b	613	CLA	ND
32	b	614	CLA	ND
32	b	615	CLA	ND

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Mol	Chain	Res	Type	Atom
32	b	616	CLA	ND
32	c	501	CLA	ND
32	c	502	CLA	ND
32	c	503	CLA	ND
32	c	504	CLA	ND
32	c	505	CLA	ND
32	c	506	CLA	ND
32	c	507	CLA	ND
32	c	508	CLA	ND
32	c	509	CLA	ND
32	c	510	CLA	ND
32	c	511	CLA	ND
32	c	512	CLA	ND
32	c	513	CLA	ND
32	d	402	CLA	ND
32	g	603	CLA	ND
32	g	604	CLA	ND
32	g	610	CLA	ND
32	g	611	CLA	ND
32	g	612	CLA	ND
32	g	613	CLA	ND
32	g	614	CLA	ND
32	n	602	CLA	ND
32	n	603	CLA	ND
32	n	604	CLA	ND
32	n	610	CLA	ND
32	n	611	CLA	ND
32	n	612	CLA	ND
32	n	613	CLA	ND
32	n	614	CLA	ND
32	r	601	CLA	ND
32	r	602	CLA	ND
32	r	603	CLA	ND
32	r	604	CLA	ND
32	r	608	CLA	ND
32	r	609	CLA	ND
32	r	610	CLA	ND
32	r	611	CLA	ND
32	r	612	CLA	ND
32	r	613	CLA	ND
32	s	602	CLA	ND
32	s	603	CLA	ND

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Mol	Chain	Res	Type	Atom
32	s	604	CLA	ND
32	s	608	CLA	ND
32	s	609	CLA	ND
32	s	610	CLA	ND
32	s	611	CLA	ND
32	s	612	CLA	ND
32	s	613	CLA	ND
32	y	304	CLA	ND
32	y	305	CLA	ND
32	y	306	CLA	ND
32	y	312	CLA	ND
32	y	313	CLA	ND
32	y	314	CLA	ND
32	y	315	CLA	ND
32	y	316	CLA	ND
32	4	303	CLA	ND
32	4	304	CLA	ND
32	4	305	CLA	ND
32	4	310	CLA	ND
32	4	311	CLA	ND
32	4	312	CLA	ND
32	AA	405	CLA	ND
32	AA	406	CLA	ND
32	AA	408	CLA	ND
32	BB	601	CLA	ND
32	BB	602	CLA	ND
32	BB	603	CLA	ND
32	BB	604	CLA	ND
32	BB	605	CLA	ND
32	BB	606	CLA	ND
32	BB	607	CLA	ND
32	BB	608	CLA	ND
32	BB	610	CLA	ND
32	BB	611	CLA	ND
32	BB	612	CLA	ND
32	BB	613	CLA	ND
32	BB	614	CLA	ND
32	BB	615	CLA	ND
32	CC	502	CLA	ND
32	CC	504	CLA	ND
32	CC	505	CLA	ND
32	CC	506	CLA	ND

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Mol	Chain	Res	Type	Atom
32	CC	507	CLA	ND
32	CC	508	CLA	ND
32	CC	509	CLA	ND
32	CC	510	CLA	ND
32	CC	511	CLA	ND
32	CC	512	CLA	ND
32	CC	513	CLA	ND
32	CC	514	CLA	ND
32	DD	401	CLA	ND
32	DD	403	CLA	ND
32	DD	404	CLA	ND
32	B	604	CLA	ND
32	B	606	CLA	ND
32	B	607	CLA	ND
32	B	608	CLA	ND
32	B	609	CLA	ND
32	B	610	CLA	ND
32	B	611	CLA	ND
32	B	618	CLA	ND
32	B	619	CLA	ND
32	B	620	CLA	ND
32	B	621	CLA	ND
32	B	622	CLA	ND
32	B	623	CLA	ND
32	B	624	CLA	ND
32	GG	602	CLA	ND
32	GG	603	CLA	ND
32	GG	604	CLA	ND
32	GG	610	CLA	ND
32	GG	611	CLA	ND
32	GG	612	CLA	ND
32	GG	613	CLA	ND
32	GG	614	CLA	ND
32	NN	602	CLA	ND
32	NN	603	CLA	ND
32	NN	604	CLA	ND
32	NN	610	CLA	ND
32	NN	611	CLA	ND
32	NN	612	CLA	ND
32	NN	613	CLA	ND
32	NN	614	CLA	ND
32	RR	302	CLA	ND

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Mol	Chain	Res	Type	Atom
32	RR	303	CLA	ND
32	RR	304	CLA	ND
32	RR	308	CLA	ND
32	RR	309	CLA	ND
32	RR	310	CLA	ND
32	RR	311	CLA	ND
32	RR	312	CLA	ND
32	RR	313	CLA	ND
32	SS	303	CLA	ND
32	SS	304	CLA	ND
32	SS	305	CLA	ND
32	SS	309	CLA	ND
32	SS	310	CLA	ND
32	SS	311	CLA	ND
32	SS	312	CLA	ND
32	SS	313	CLA	ND
32	SS	314	CLA	ND
32	XX	201	CLA	ND
32	YY	602	CLA	ND
32	YY	603	CLA	ND
32	YY	610	CLA	ND
32	YY	611	CLA	ND
32	YY	612	CLA	ND
32	YY	613	CLA	ND
32	YY	614	CLA	ND
32	Aa	405	CLA	ND
32	Aa	406	CLA	ND
32	Aa	407	CLA	ND
32	Aa	410	CLA	ND
32	Bb	601	CLA	ND
32	Bb	602	CLA	ND
32	Bb	603	CLA	ND
32	Bb	604	CLA	ND
32	Bb	605	CLA	ND
32	Bb	606	CLA	ND
32	Bb	607	CLA	ND
32	Bb	608	CLA	ND
32	Bb	609	CLA	ND
32	Bb	610	CLA	ND
32	Bb	611	CLA	ND
32	Bb	612	CLA	ND
32	Bb	613	CLA	ND

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Mol	Chain	Res	Type	Atom
32	Bb	614	CLA	ND
32	Bb	615	CLA	ND
32	Bb	616	CLA	ND
32	Cc	503	CLA	ND
32	Cc	505	CLA	ND
32	Cc	506	CLA	ND
32	Cc	507	CLA	ND
32	Cc	508	CLA	ND
32	Cc	509	CLA	ND
32	Cc	510	CLA	ND
32	Cc	511	CLA	ND
32	Cc	512	CLA	ND
32	Cc	513	CLA	ND
32	Cc	514	CLA	ND
32	Cc	515	CLA	ND
32	Dd	402	CLA	ND
32	Gg	304	CLA	ND
32	Gg	305	CLA	ND
32	Gg	311	CLA	ND
32	Gg	312	CLA	ND
32	Gg	313	CLA	ND
32	Gg	314	CLA	ND
32	Gg	315	CLA	ND
32	Nn	301	CLA	ND
32	Nn	302	CLA	ND
32	Nn	303	CLA	ND
32	Nn	304	CLA	ND
32	Nn	312	CLA	ND
32	Nn	313	CLA	ND
32	Nn	314	CLA	ND
39	Rr	605	CHL	NA
39	Rr	605	CHL	ND
39	Rr	605	CHL	NC
39	Rr	606	CHL	NA
39	Rr	606	CHL	ND
39	Rr	606	CHL	NC
39	Rr	607	CHL	NA
39	Rr	607	CHL	ND
39	Rr	607	CHL	NC
39	Ss	601	CHL	NA
39	Ss	601	CHL	ND
39	Ss	601	CHL	NC

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Mol	Chain	Res	Type	Atom
39	Ss	605	CHL	NA
39	Ss	605	CHL	ND
39	Ss	605	CHL	NC
39	Ss	606	CHL	NA
39	Ss	606	CHL	ND
39	Ss	606	CHL	NC
39	Ss	607	CHL	NA
39	Ss	607	CHL	ND
39	Ss	607	CHL	NC
39	Yy	601	CHL	NA
39	Yy	601	CHL	ND
39	Yy	601	CHL	NC
39	Yy	605	CHL	NA
39	Yy	605	CHL	ND
39	Yy	605	CHL	NC
39	Yy	606	CHL	NA
39	Yy	606	CHL	ND
39	Yy	606	CHL	NC
39	Yy	607	CHL	NA
39	Yy	607	CHL	ND
39	Yy	607	CHL	NC
39	Yy	608	CHL	NA
39	Yy	608	CHL	ND
39	Yy	608	CHL	NC
39	Yy	609	CHL	NA
39	Yy	609	CHL	ND
39	Yy	609	CHL	NC
39	44	601	CHL	NA
39	44	601	CHL	ND
39	44	601	CHL	NC
39	44	605	CHL	NA
39	44	605	CHL	ND
39	44	605	CHL	NC
39	44	606	CHL	NA
39	44	606	CHL	ND
39	44	606	CHL	NC
39	44	607	CHL	NA
39	44	607	CHL	ND
39	44	607	CHL	NC
39	44	608	CHL	NA
39	44	608	CHL	ND
39	44	608	CHL	NC

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Mol	Chain	Res	Type	Atom
39	11	601	CHL	NA
39	11	601	CHL	ND
39	11	601	CHL	NC
39	11	605	CHL	NA
39	11	605	CHL	ND
39	11	605	CHL	NC
39	11	606	CHL	NA
39	11	606	CHL	ND
39	11	606	CHL	NC
39	11	607	CHL	NA
39	11	607	CHL	ND
39	11	607	CHL	NC
39	11	608	CHL	NA
39	11	608	CHL	ND
39	11	608	CHL	NC
39	22	601	CHL	NA
39	22	601	CHL	ND
39	22	601	CHL	NC
39	22	605	CHL	NA
39	22	605	CHL	ND
39	22	605	CHL	NC
39	22	606	CHL	NA
39	22	606	CHL	ND
39	22	606	CHL	NC
39	22	607	CHL	NA
39	22	607	CHL	ND
39	22	607	CHL	NC
39	22	608	CHL	NA
39	22	608	CHL	ND
39	22	608	CHL	NC
39	33	601	CHL	NA
39	33	601	CHL	ND
39	33	601	CHL	NC
39	33	605	CHL	NA
39	33	605	CHL	ND
39	33	605	CHL	NC
39	33	606	CHL	NA
39	33	606	CHL	ND
39	33	606	CHL	NC
39	33	607	CHL	NA
39	33	607	CHL	ND
39	33	607	CHL	NC

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Mol	Chain	Res	Type	Atom
39	33	608	CHL	NA
39	33	608	CHL	ND
39	33	608	CHL	NC
39	1	601	CHL	NA
39	1	601	CHL	ND
39	1	601	CHL	NC
39	1	605	CHL	NA
39	1	605	CHL	ND
39	1	605	CHL	NC
39	1	606	CHL	NA
39	1	606	CHL	ND
39	1	606	CHL	NC
39	1	607	CHL	NA
39	1	607	CHL	ND
39	1	607	CHL	NC
39	1	608	CHL	NA
39	1	608	CHL	ND
39	1	608	CHL	NC
39	2	601	CHL	NA
39	2	601	CHL	ND
39	2	601	CHL	NC
39	2	605	CHL	NA
39	2	605	CHL	ND
39	2	605	CHL	NC
39	2	606	CHL	NA
39	2	606	CHL	ND
39	2	606	CHL	NC
39	2	607	CHL	NA
39	2	607	CHL	ND
39	2	607	CHL	NC
39	2	608	CHL	NA
39	2	608	CHL	ND
39	2	608	CHL	NC
39	3	601	CHL	NA
39	3	601	CHL	ND
39	3	601	CHL	NC
39	3	605	CHL	NA
39	3	605	CHL	ND
39	3	605	CHL	NC
39	3	606	CHL	NA
39	3	606	CHL	ND
39	3	606	CHL	NC

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Mol	Chain	Res	Type	Atom
39	3	607	CHL	NA
39	3	607	CHL	ND
39	3	607	CHL	NC
39	3	608	CHL	NA
39	3	608	CHL	ND
39	3	608	CHL	NC
39	G	601	CHL	NA
39	G	601	CHL	ND
39	G	601	CHL	NC
39	G	605	CHL	NA
39	G	605	CHL	ND
39	G	605	CHL	NC
39	G	606	CHL	NA
39	G	606	CHL	ND
39	G	606	CHL	NC
39	G	607	CHL	NA
39	G	607	CHL	ND
39	G	607	CHL	NC
39	G	608	CHL	NA
39	G	608	CHL	ND
39	G	608	CHL	NC
39	G	609	CHL	NA
39	G	609	CHL	ND
39	G	609	CHL	NC
39	N	601	CHL	NA
39	N	601	CHL	ND
39	N	601	CHL	NC
39	N	605	CHL	NA
39	N	605	CHL	ND
39	N	605	CHL	NC
39	N	606	CHL	NA
39	N	606	CHL	ND
39	N	606	CHL	NC
39	N	607	CHL	NA
39	N	607	CHL	ND
39	N	607	CHL	NC
39	N	608	CHL	NA
39	N	608	CHL	ND
39	N	608	CHL	NC
39	N	609	CHL	NA
39	N	609	CHL	ND
39	N	609	CHL	NC

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Mol	Chain	Res	Type	Atom
39	R	605	CHL	NA
39	R	605	CHL	ND
39	R	605	CHL	NC
39	R	606	CHL	NA
39	R	606	CHL	ND
39	R	606	CHL	NC
39	R	607	CHL	NA
39	R	607	CHL	ND
39	R	607	CHL	NC
39	S	601	CHL	NA
39	S	601	CHL	ND
39	S	601	CHL	NC
39	S	605	CHL	NA
39	S	605	CHL	ND
39	S	605	CHL	NC
39	S	606	CHL	NA
39	S	606	CHL	ND
39	S	606	CHL	NC
39	S	607	CHL	NA
39	S	607	CHL	ND
39	S	607	CHL	NC
39	Y	601	CHL	NA
39	Y	601	CHL	ND
39	Y	601	CHL	NC
39	Y	605	CHL	NA
39	Y	605	CHL	ND
39	Y	605	CHL	NC
39	Y	606	CHL	NA
39	Y	606	CHL	ND
39	Y	606	CHL	NC
39	Y	607	CHL	NA
39	Y	607	CHL	ND
39	Y	607	CHL	NC
39	Y	608	CHL	NA
39	Y	608	CHL	ND
39	Y	608	CHL	NC
39	Y	609	CHL	NA
39	Y	609	CHL	ND
39	Y	609	CHL	NC
39	g	601	CHL	NA
39	g	601	CHL	ND
39	g	601	CHL	NC

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Mol	Chain	Res	Type	Atom
39	g	605	CHL	NA
39	g	605	CHL	ND
39	g	605	CHL	NC
39	g	606	CHL	NA
39	g	606	CHL	ND
39	g	606	CHL	NC
39	g	607	CHL	NA
39	g	607	CHL	ND
39	g	607	CHL	NC
39	g	608	CHL	NA
39	g	608	CHL	ND
39	g	608	CHL	NC
39	g	609	CHL	NA
39	g	609	CHL	ND
39	g	609	CHL	NC
39	n	601	CHL	NA
39	n	601	CHL	ND
39	n	601	CHL	NC
39	n	605	CHL	NA
39	n	605	CHL	ND
39	n	605	CHL	NC
39	n	606	CHL	NA
39	n	606	CHL	ND
39	n	606	CHL	NC
39	n	607	CHL	NA
39	n	607	CHL	ND
39	n	607	CHL	NC
39	n	608	CHL	NA
39	n	608	CHL	ND
39	n	608	CHL	NC
39	n	609	CHL	NA
39	n	609	CHL	ND
39	n	609	CHL	NC
39	r	605	CHL	NA
39	r	605	CHL	ND
39	r	605	CHL	NC
39	r	606	CHL	NA
39	r	606	CHL	ND
39	r	606	CHL	NC
39	r	607	CHL	NA
39	r	607	CHL	ND
39	r	607	CHL	NC

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Mol	Chain	Res	Type	Atom
39	s	601	CHL	NA
39	s	601	CHL	ND
39	s	601	CHL	NC
39	s	605	CHL	NA
39	s	605	CHL	ND
39	s	605	CHL	NC
39	s	606	CHL	NA
39	s	606	CHL	ND
39	s	606	CHL	NC
39	s	607	CHL	NA
39	s	607	CHL	ND
39	s	607	CHL	NC
39	y	303	CHL	NA
39	y	303	CHL	ND
39	y	303	CHL	NC
39	y	307	CHL	NA
39	y	307	CHL	ND
39	y	307	CHL	NC
39	y	308	CHL	NA
39	y	308	CHL	ND
39	y	308	CHL	NC
39	y	309	CHL	NA
39	y	309	CHL	ND
39	y	309	CHL	NC
39	y	310	CHL	NA
39	y	310	CHL	ND
39	y	310	CHL	NC
39	y	311	CHL	NA
39	y	311	CHL	ND
39	y	311	CHL	NC
39	4	302	CHL	NA
39	4	302	CHL	ND
39	4	302	CHL	NC
39	4	306	CHL	NA
39	4	306	CHL	ND
39	4	306	CHL	NC
39	4	307	CHL	NA
39	4	307	CHL	ND
39	4	307	CHL	NC
39	4	308	CHL	NA
39	4	308	CHL	ND
39	4	308	CHL	NC

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Mol	Chain	Res	Type	Atom
39	4	309	CHL	NA
39	4	309	CHL	ND
39	4	309	CHL	NC
39	GG	601	CHL	NA
39	GG	601	CHL	ND
39	GG	601	CHL	NC
39	GG	605	CHL	NA
39	GG	605	CHL	ND
39	GG	605	CHL	NC
39	GG	606	CHL	NA
39	GG	606	CHL	ND
39	GG	606	CHL	NC
39	GG	607	CHL	NA
39	GG	607	CHL	ND
39	GG	607	CHL	NC
39	GG	608	CHL	NA
39	GG	608	CHL	ND
39	GG	608	CHL	NC
39	GG	609	CHL	NA
39	GG	609	CHL	ND
39	GG	609	CHL	NC
39	NN	601	CHL	NA
39	NN	601	CHL	ND
39	NN	601	CHL	NC
39	NN	605	CHL	NA
39	NN	605	CHL	ND
39	NN	605	CHL	NC
39	NN	606	CHL	NA
39	NN	606	CHL	ND
39	NN	606	CHL	NC
39	NN	607	CHL	NA
39	NN	607	CHL	ND
39	NN	607	CHL	NC
39	NN	608	CHL	NA
39	NN	608	CHL	ND
39	NN	608	CHL	NC
39	NN	609	CHL	NA
39	NN	609	CHL	ND
39	NN	609	CHL	NC
39	RR	305	CHL	NA
39	RR	305	CHL	ND
39	RR	305	CHL	NC

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Mol	Chain	Res	Type	Atom
39	RR	306	CHL	NA
39	RR	306	CHL	ND
39	RR	306	CHL	NC
39	RR	307	CHL	NA
39	RR	307	CHL	ND
39	RR	307	CHL	NC
39	SS	302	CHL	NA
39	SS	302	CHL	ND
39	SS	302	CHL	NC
39	SS	306	CHL	NA
39	SS	306	CHL	ND
39	SS	306	CHL	NC
39	SS	307	CHL	NA
39	SS	307	CHL	ND
39	SS	307	CHL	NC
39	SS	308	CHL	NA
39	SS	308	CHL	ND
39	SS	308	CHL	NC
39	YY	601	CHL	NA
39	YY	601	CHL	ND
39	YY	601	CHL	NC
39	YY	605	CHL	NA
39	YY	605	CHL	ND
39	YY	605	CHL	NC
39	YY	606	CHL	NA
39	YY	606	CHL	ND
39	YY	606	CHL	NC
39	YY	607	CHL	NA
39	YY	607	CHL	ND
39	YY	607	CHL	NC
39	YY	608	CHL	NA
39	YY	608	CHL	ND
39	YY	608	CHL	NC
39	YY	609	CHL	NA
39	YY	609	CHL	ND
39	YY	609	CHL	NC
39	Gg	302	CHL	NA
39	Gg	302	CHL	ND
39	Gg	302	CHL	NC
39	Gg	306	CHL	NA
39	Gg	306	CHL	ND
39	Gg	306	CHL	NC

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Mol	Chain	Res	Type	Atom
39	Gg	307	CHL	NA
39	Gg	307	CHL	ND
39	Gg	307	CHL	NC
39	Gg	308	CHL	NA
39	Gg	308	CHL	ND
39	Gg	308	CHL	NC
39	Gg	309	CHL	NA
39	Gg	309	CHL	ND
39	Gg	309	CHL	NC
39	Gg	310	CHL	NA
39	Gg	310	CHL	ND
39	Gg	310	CHL	NC
39	Nn	311	CHL	NA
39	Nn	311	CHL	ND
39	Nn	311	CHL	NC
39	Nn	315	CHL	NA
39	Nn	315	CHL	ND
39	Nn	315	CHL	NC
39	Nn	316	CHL	NA
39	Nn	316	CHL	ND
39	Nn	316	CHL	NC
39	Nn	317	CHL	NA
39	Nn	317	CHL	ND
39	Nn	317	CHL	NC
39	Nn	318	CHL	NA
39	Nn	318	CHL	ND
39	Nn	318	CHL	NC
39	Nn	319	CHL	NA
39	Nn	319	CHL	ND
39	Nn	319	CHL	NC

All (5624) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	408	CLA	CAD-CBD-CGD-O1D
32	A	408	CLA	CAD-CBD-CGD-O2D
32	Rr	601	CLA	C2B-C3B-CAB-CBB
32	Rr	601	CLA	C4B-C3B-CAB-CBB
32	Rr	601	CLA	CHA-CBD-CGD-O1D
32	Rr	601	CLA	CHA-CBD-CGD-O2D
32	Rr	602	CLA	C1A-C2A-CAA-CBA
32	Rr	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	Rr	603	CLA	CHA-CBD-CGD-O2D
32	Rr	604	CLA	C1A-C2A-CAA-CBA
32	Rr	608	CLA	C1A-C2A-CAA-CBA
32	Rr	608	CLA	CBD-CGD-O2D-CED
32	Rr	609	CLA	C1A-C2A-CAA-CBA
32	Rr	609	CLA	C3A-C2A-CAA-CBA
32	Rr	610	CLA	C1A-C2A-CAA-CBA
32	Rr	610	CLA	C3A-C2A-CAA-CBA
32	Rr	610	CLA	CAD-CBD-CGD-O1D
32	Rr	610	CLA	CAD-CBD-CGD-O2D
32	Rr	611	CLA	CBD-CGD-O2D-CED
32	Rr	612	CLA	C1A-C2A-CAA-CBA
32	Rr	613	CLA	C2B-C3B-CAB-CBB
32	Rr	613	CLA	C4B-C3B-CAB-CBB
32	Ss	602	CLA	C2B-C3B-CAB-CBB
32	Ss	602	CLA	C4B-C3B-CAB-CBB
32	Ss	602	CLA	CHA-CBD-CGD-O1D
32	Ss	602	CLA	CHA-CBD-CGD-O2D
32	Ss	604	CLA	C2B-C3B-CAB-CBB
32	Ss	604	CLA	C4B-C3B-CAB-CBB
32	Ss	604	CLA	CAD-CBD-CGD-O1D
32	Ss	604	CLA	CAD-CBD-CGD-O2D
32	Ss	608	CLA	C3A-C2A-CAA-CBA
32	Ss	609	CLA	C1A-C2A-CAA-CBA
32	Ss	609	CLA	C3A-C2A-CAA-CBA
32	Ss	611	CLA	CAD-CBD-CGD-O1D
32	Ss	611	CLA	CAD-CBD-CGD-O2D
32	Yy	602	CLA	C1A-C2A-CAA-CBA
32	Yy	602	CLA	C3A-C2A-CAA-CBA
32	Yy	602	CLA	CHA-CBD-CGD-O2D
32	Yy	604	CLA	C1A-C2A-CAA-CBA
32	Yy	604	CLA	CHA-CBD-CGD-O1D
32	Yy	604	CLA	CHA-CBD-CGD-O2D
32	Yy	610	CLA	C1A-C2A-CAA-CBA
32	Yy	610	CLA	C3A-C2A-CAA-CBA
32	Yy	610	CLA	C2B-C3B-CAB-CBB
32	Yy	610	CLA	C4B-C3B-CAB-CBB
32	Yy	611	CLA	C1A-C2A-CAA-CBA
32	Yy	612	CLA	C2B-C3B-CAB-CBB
32	Yy	612	CLA	C4B-C3B-CAB-CBB
32	Yy	612	CLA	CBD-CGD-O2D-CED
32	Yy	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Yy	614	CLA	C3A-C2A-CAA-CBA
32	44	602	CLA	CHA-CBD-CGD-O1D
32	44	602	CLA	CHA-CBD-CGD-O2D
32	44	603	CLA	C1A-C2A-CAA-CBA
32	44	603	CLA	CHA-CBD-CGD-O2D
32	44	603	CLA	CBD-CGD-O2D-CED
32	44	604	CLA	CBD-CGD-O2D-CED
32	44	609	CLA	C1A-C2A-CAA-CBA
32	44	609	CLA	C3A-C2A-CAA-CBA
32	44	609	CLA	CHA-CBD-CGD-O2D
32	44	609	CLA	CBD-CGD-O2D-CED
32	44	610	CLA	CHA-CBD-CGD-O1D
32	44	610	CLA	CHA-CBD-CGD-O2D
32	44	610	CLA	CBD-CGD-O2D-CED
32	11	602	CLA	CHA-CBD-CGD-O2D
32	11	603	CLA	CBD-CGD-O2D-CED
32	11	604	CLA	CBD-CGD-O2D-CED
32	11	604	CLA	O1D-CGD-O2D-CED
32	11	609	CLA	CBD-CGD-O2D-CED
32	11	610	CLA	CBD-CGD-O2D-CED
32	11	613	CLA	CBD-CGD-O2D-CED
32	22	602	CLA	CHA-CBD-CGD-O1D
32	22	602	CLA	CHA-CBD-CGD-O2D
32	22	604	CLA	CBD-CGD-O2D-CED
32	22	610	CLA	C1A-C2A-CAA-CBA
32	22	610	CLA	C2B-C3B-CAB-CBB
32	22	610	CLA	C4B-C3B-CAB-CBB
32	22	610	CLA	CBD-CGD-O2D-CED
32	22	611	CLA	CHA-CBD-CGD-O2D
32	22	611	CLA	CBD-CGD-O2D-CED
32	33	602	CLA	C4B-C3B-CAB-CBB
32	33	603	CLA	CHA-CBD-CGD-O1D
32	33	603	CLA	CHA-CBD-CGD-O2D
32	33	610	CLA	CBD-CGD-O2D-CED
32	33	611	CLA	CHA-CBD-CGD-O1D
32	33	611	CLA	CHA-CBD-CGD-O2D
32	33	612	CLA	C2B-C3B-CAB-CBB
32	33	612	CLA	C4B-C3B-CAB-CBB
32	33	612	CLA	CBD-CGD-O2D-CED
32	33	613	CLA	CHA-CBD-CGD-O1D
32	33	613	CLA	CHA-CBD-CGD-O2D
32	1	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	1	603	CLA	C4B-C3B-CAB-CBB
32	1	603	CLA	CAD-CBD-CGD-O2D
32	1	603	CLA	CBD-CGD-O2D-CED
32	1	604	CLA	CBD-CGD-O2D-CED
32	1	609	CLA	CBD-CGD-O2D-CED
32	1	610	CLA	CAD-CBD-CGD-O1D
32	1	610	CLA	CAD-CBD-CGD-O2D
32	1	611	CLA	CBD-CGD-O2D-CED
32	2	602	CLA	CHA-CBD-CGD-O1D
32	2	602	CLA	CHA-CBD-CGD-O2D
32	2	603	CLA	CBD-CGD-O2D-CED
32	2	604	CLA	CBD-CGD-O2D-CED
32	2	610	CLA	CBD-CGD-O2D-CED
32	2	613	CLA	CBD-CGD-O2D-CED
32	3	602	CLA	C4B-C3B-CAB-CBB
32	3	610	CLA	CBD-CGD-O2D-CED
32	3	611	CLA	CHA-CBD-CGD-O1D
32	3	611	CLA	CHA-CBD-CGD-O2D
32	3	612	CLA	CBD-CGD-O2D-CED
32	3	613	CLA	CHA-CBD-CGD-O1D
32	3	613	CLA	CHA-CBD-CGD-O2D
32	C	503	CLA	C1A-C2A-CAA-CBA
32	C	503	CLA	C3A-C2A-CAA-CBA
32	C	504	CLA	C1A-C2A-CAA-CBA
32	C	506	CLA	C2B-C3B-CAB-CBB
32	C	506	CLA	C4B-C3B-CAB-CBB
32	C	507	CLA	CAD-CBD-CGD-O1D
32	C	507	CLA	CAD-CBD-CGD-O2D
32	C	508	CLA	C1A-C2A-CAA-CBA
32	C	508	CLA	C3A-C2A-CAA-CBA
32	C	508	CLA	CAD-CBD-CGD-O1D
32	C	508	CLA	CAD-CBD-CGD-O2D
32	C	508	CLA	CBD-CGD-O2D-CED
32	C	509	CLA	C2B-C3B-CAB-CBB
32	C	509	CLA	C4B-C3B-CAB-CBB
32	C	509	CLA	CHA-CBD-CGD-O1D
32	C	509	CLA	CHA-CBD-CGD-O2D
32	C	511	CLA	C1A-C2A-CAA-CBA
32	C	511	CLA	C3A-C2A-CAA-CBA
32	C	513	CLA	CAD-CBD-CGD-O1D
32	C	513	CLA	CAD-CBD-CGD-O2D
32	C	514	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	C	514	CLA	CHA-CBD-CGD-O2D
32	C	515	CLA	CBD-CGD-O2D-CED
32	D	401	CLA	C2B-C3B-CAB-CBB
32	D	401	CLA	C4B-C3B-CAB-CBB
32	G	602	CLA	CBD-CGD-O2D-CED
32	G	603	CLA	C2B-C3B-CAB-CBB
32	G	603	CLA	C4B-C3B-CAB-CBB
32	G	603	CLA	CBD-CGD-O2D-CED
32	G	610	CLA	C2B-C3B-CAB-CBB
32	G	610	CLA	C4B-C3B-CAB-CBB
32	G	611	CLA	CAD-CBD-CGD-O2D
32	G	611	CLA	CBD-CGD-O2D-CED
32	G	612	CLA	CHA-CBD-CGD-O1D
32	G	612	CLA	CHA-CBD-CGD-O2D
32	G	612	CLA	CBD-CGD-O2D-CED
32	G	613	CLA	CBD-CGD-O2D-CED
32	N	602	CLA	C1A-C2A-CAA-CBA
32	N	602	CLA	C3A-C2A-CAA-CBA
32	N	602	CLA	C2B-C3B-CAB-CBB
32	N	602	CLA	C4B-C3B-CAB-CBB
32	N	603	CLA	CAD-CBD-CGD-O1D
32	N	603	CLA	CAD-CBD-CGD-O2D
32	N	603	CLA	CBD-CGD-O2D-CED
32	N	604	CLA	CBD-CGD-O2D-CED
32	N	610	CLA	C1A-C2A-CAA-CBA
32	N	611	CLA	C1A-C2A-CAA-CBA
32	N	611	CLA	C3A-C2A-CAA-CBA
32	N	612	CLA	CBD-CGD-O2D-CED
32	N	613	CLA	C1A-C2A-CAA-CBA
32	N	613	CLA	CBD-CGD-O2D-CED
32	N	614	CLA	C2B-C3B-CAB-CBB
32	N	614	CLA	C4B-C3B-CAB-CBB
32	N	614	CLA	CBD-CGD-O2D-CED
32	R	601	CLA	CAD-CBD-CGD-O1D
32	R	601	CLA	CAD-CBD-CGD-O2D
32	R	602	CLA	C3A-C2A-CAA-CBA
32	R	602	CLA	C2B-C3B-CAB-CBB
32	R	602	CLA	C4B-C3B-CAB-CBB
32	R	608	CLA	C4B-C3B-CAB-CBB
32	R	608	CLA	CBD-CGD-O2D-CED
32	R	609	CLA	C1A-C2A-CAA-CBA
32	R	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	R	609	CLA	C2B-C3B-CAB-CBB
32	R	609	CLA	C4B-C3B-CAB-CBB
32	R	609	CLA	CBD-CGD-O2D-CED
32	R	610	CLA	C1A-C2A-CAA-CBA
32	R	610	CLA	C3A-C2A-CAA-CBA
32	R	610	CLA	CAD-CBD-CGD-O2D
32	R	611	CLA	CHA-CBD-CGD-O1D
32	R	611	CLA	CHA-CBD-CGD-O2D
32	R	612	CLA	C1A-C2A-CAA-CBA
32	R	613	CLA	C2B-C3B-CAB-CBB
32	R	613	CLA	C4B-C3B-CAB-CBB
32	R	613	CLA	CBD-CGD-O2D-CED
32	S	602	CLA	C1A-C2A-CAA-CBA
32	S	604	CLA	C1A-C2A-CAA-CBA
32	S	604	CLA	CHA-CBD-CGD-O2D
32	S	608	CLA	CAD-CBD-CGD-O1D
32	S	608	CLA	CAD-CBD-CGD-O2D
32	S	609	CLA	CBD-CGD-O2D-CED
32	S	611	CLA	CHA-CBD-CGD-O1D
32	S	611	CLA	CHA-CBD-CGD-O2D
32	S	611	CLA	CBD-CGD-O2D-CED
32	S	612	CLA	CBD-CGD-O2D-CED
32	X	201	CLA	CBD-CGD-O2D-CED
32	Y	602	CLA	C1A-C2A-CAA-CBA
32	Y	602	CLA	C3A-C2A-CAA-CBA
32	Y	603	CLA	CBD-CGD-O2D-CED
32	Y	610	CLA	C1A-C2A-CAA-CBA
32	Y	610	CLA	C3A-C2A-CAA-CBA
32	Y	611	CLA	C2B-C3B-CAB-CBB
32	Y	611	CLA	C4B-C3B-CAB-CBB
32	Y	612	CLA	CBD-CGD-O2D-CED
32	Y	614	CLA	C3A-C2A-CAA-CBA
32	a	406	CLA	C2B-C3B-CAB-CBB
32	a	406	CLA	C4B-C3B-CAB-CBB
32	a	407	CLA	C2B-C3B-CAB-CBB
32	a	407	CLA	C4B-C3B-CAB-CBB
32	a	410	CLA	CAD-CBD-CGD-O1D
32	a	410	CLA	CAD-CBD-CGD-O2D
32	b	601	CLA	C3A-C2A-CAA-CBA
32	b	601	CLA	CAD-CBD-CGD-O1D
32	b	601	CLA	CAD-CBD-CGD-O2D
32	b	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	b	603	CLA	C1A-C2A-CAA-CBA
32	b	603	CLA	C3A-C2A-CAA-CBA
32	b	603	CLA	C4B-C3B-CAB-CBB
32	b	603	CLA	CBD-CGD-O2D-CED
32	b	607	CLA	C2B-C3B-CAB-CBB
32	b	607	CLA	C4B-C3B-CAB-CBB
32	b	608	CLA	C4B-C3B-CAB-CBB
32	b	608	CLA	CBD-CGD-O2D-CED
32	b	609	CLA	C1A-C2A-CAA-CBA
32	b	609	CLA	C3A-C2A-CAA-CBA
32	b	613	CLA	CBD-CGD-O2D-CED
32	b	614	CLA	CBD-CGD-O2D-CED
32	b	615	CLA	C4B-C3B-CAB-CBB
32	c	501	CLA	C2B-C3B-CAB-CBB
32	c	501	CLA	C4B-C3B-CAB-CBB
32	c	501	CLA	CAD-CBD-CGD-O1D
32	c	501	CLA	CAD-CBD-CGD-O2D
32	c	503	CLA	CBD-CGD-O2D-CED
32	c	504	CLA	CBD-CGD-O2D-CED
32	c	506	CLA	C1A-C2A-CAA-CBA
32	c	506	CLA	CAD-CBD-CGD-O1D
32	c	506	CLA	CAD-CBD-CGD-O2D
32	c	506	CLA	CBD-CGD-O2D-CED
32	c	507	CLA	CAD-CBD-CGD-O1D
32	c	507	CLA	CAD-CBD-CGD-O2D
32	c	511	CLA	CBD-CGD-O2D-CED
32	c	512	CLA	CBD-CGD-O2D-CED
32	c	513	CLA	C1A-C2A-CAA-CBA
32	c	513	CLA	CAD-CBD-CGD-O1D
32	c	513	CLA	CAD-CBD-CGD-O2D
32	g	602	CLA	C2B-C3B-CAB-CBB
32	g	602	CLA	C4B-C3B-CAB-CBB
32	g	602	CLA	CHA-CBD-CGD-O2D
32	g	603	CLA	C2B-C3B-CAB-CBB
32	g	603	CLA	C4B-C3B-CAB-CBB
32	g	603	CLA	CBD-CGD-O2D-CED
32	g	604	CLA	C1A-C2A-CAA-CBA
32	g	604	CLA	CAD-CBD-CGD-O1D
32	g	604	CLA	CAD-CBD-CGD-O2D
32	g	604	CLA	CBD-CGD-O2D-CED
32	g	610	CLA	C2B-C3B-CAB-CBB
32	g	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	g	611	CLA	C1A-C2A-CAA-CBA
32	g	612	CLA	C1A-C2A-CAA-CBA
32	g	612	CLA	C3A-C2A-CAA-CBA
32	g	612	CLA	CHA-CBD-CGD-O1D
32	g	612	CLA	CHA-CBD-CGD-O2D
32	g	613	CLA	CBD-CGD-O2D-CED
32	n	602	CLA	C1A-C2A-CAA-CBA
32	n	602	CLA	C3A-C2A-CAA-CBA
32	n	602	CLA	C2B-C3B-CAB-CBB
32	n	602	CLA	C4B-C3B-CAB-CBB
32	n	602	CLA	CHA-CBD-CGD-O1D
32	n	602	CLA	CHA-CBD-CGD-O2D
32	n	603	CLA	CBD-CGD-O2D-CED
32	n	610	CLA	C1A-C2A-CAA-CBA
32	n	610	CLA	C3A-C2A-CAA-CBA
32	n	610	CLA	CBD-CGD-O2D-CED
32	n	612	CLA	CBD-CGD-O2D-CED
32	n	613	CLA	C1A-C2A-CAA-CBA
32	n	614	CLA	CBD-CGD-O2D-CED
32	r	601	CLA	C2B-C3B-CAB-CBB
32	r	601	CLA	C4B-C3B-CAB-CBB
32	r	601	CLA	CHA-CBD-CGD-O2D
32	r	604	CLA	C1A-C2A-CAA-CBA
32	r	604	CLA	CBD-CGD-O2D-CED
32	r	608	CLA	CBD-CGD-O2D-CED
32	r	609	CLA	C1A-C2A-CAA-CBA
32	r	609	CLA	C3A-C2A-CAA-CBA
32	r	610	CLA	C1A-C2A-CAA-CBA
32	r	611	CLA	CBD-CGD-O2D-CED
32	r	613	CLA	C2B-C3B-CAB-CBB
32	r	613	CLA	C4B-C3B-CAB-CBB
32	s	602	CLA	C2B-C3B-CAB-CBB
32	s	602	CLA	C4B-C3B-CAB-CBB
32	s	602	CLA	CAD-CBD-CGD-O2D
32	s	604	CLA	C2B-C3B-CAB-CBB
32	s	604	CLA	C4B-C3B-CAB-CBB
32	s	608	CLA	C1A-C2A-CAA-CBA
32	s	608	CLA	C3A-C2A-CAA-CBA
32	s	609	CLA	C1A-C2A-CAA-CBA
32	s	609	CLA	C3A-C2A-CAA-CBA
32	s	611	CLA	CAD-CBD-CGD-O1D
32	s	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	s	613	CLA	CBD-CGD-O2D-CED
32	y	304	CLA	C1A-C2A-CAA-CBA
32	y	304	CLA	C3A-C2A-CAA-CBA
32	y	306	CLA	CHA-CBD-CGD-O1D
32	y	306	CLA	CHA-CBD-CGD-O2D
32	y	312	CLA	C1A-C2A-CAA-CBA
32	y	312	CLA	C3A-C2A-CAA-CBA
32	y	312	CLA	C4B-C3B-CAB-CBB
32	y	313	CLA	C1A-C2A-CAA-CBA
32	y	314	CLA	C4B-C3B-CAB-CBB
32	y	314	CLA	CBD-CGD-O2D-CED
32	y	314	CLA	O1D-CGD-O2D-CED
32	y	316	CLA	C3A-C2A-CAA-CBA
32	4	303	CLA	C1A-C2A-CAA-CBA
32	4	303	CLA	CHA-CBD-CGD-O1D
32	4	303	CLA	CHA-CBD-CGD-O2D
32	4	304	CLA	C1A-C2A-CAA-CBA
32	4	304	CLA	C3A-C2A-CAA-CBA
32	4	304	CLA	C2B-C3B-CAB-CBB
32	4	304	CLA	C4B-C3B-CAB-CBB
32	4	304	CLA	CBD-CGD-O2D-CED
32	4	305	CLA	CBD-CGD-O2D-CED
32	4	310	CLA	C1A-C2A-CAA-CBA
32	4	310	CLA	C3A-C2A-CAA-CBA
32	4	310	CLA	CHA-CBD-CGD-O1D
32	4	310	CLA	CHA-CBD-CGD-O2D
32	4	310	CLA	CBD-CGD-O2D-CED
32	AA	405	CLA	CBD-CGD-O2D-CED
32	AA	408	CLA	CAD-CBD-CGD-O1D
32	AA	408	CLA	CAD-CBD-CGD-O2D
32	BB	602	CLA	C3A-C2A-CAA-CBA
32	BB	602	CLA	CAD-CBD-CGD-O1D
32	BB	602	CLA	CAD-CBD-CGD-O2D
32	BB	605	CLA	CAD-CBD-CGD-O1D
32	BB	605	CLA	CAD-CBD-CGD-O2D
32	BB	606	CLA	CAD-CBD-CGD-O2D
32	BB	608	CLA	CAD-CBD-CGD-O1D
32	BB	608	CLA	CAD-CBD-CGD-O2D
32	BB	610	CLA	CAD-CBD-CGD-O1D
32	BB	610	CLA	CAD-CBD-CGD-O2D
32	BB	610	CLA	CBD-CGD-O2D-CED
32	BB	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	BB	615	CLA	CHA-CBD-CGD-O1D
32	BB	615	CLA	CHA-CBD-CGD-O2D
32	CC	502	CLA	C1A-C2A-CAA-CBA
32	CC	503	CLA	C1A-C2A-CAA-CBA
32	CC	505	CLA	C2B-C3B-CAB-CBB
32	CC	505	CLA	C4B-C3B-CAB-CBB
32	CC	506	CLA	CAD-CBD-CGD-O1D
32	CC	506	CLA	CAD-CBD-CGD-O2D
32	CC	507	CLA	C1A-C2A-CAA-CBA
32	CC	507	CLA	C3A-C2A-CAA-CBA
32	CC	507	CLA	CAD-CBD-CGD-O1D
32	CC	507	CLA	CAD-CBD-CGD-O2D
32	CC	508	CLA	C2B-C3B-CAB-CBB
32	CC	508	CLA	C4B-C3B-CAB-CBB
32	CC	508	CLA	CHA-CBD-CGD-O1D
32	CC	508	CLA	CHA-CBD-CGD-O2D
32	CC	510	CLA	C1A-C2A-CAA-CBA
32	CC	510	CLA	C3A-C2A-CAA-CBA
32	CC	512	CLA	CAD-CBD-CGD-O1D
32	CC	512	CLA	CAD-CBD-CGD-O2D
32	CC	513	CLA	CHA-CBD-CGD-O1D
32	CC	513	CLA	CHA-CBD-CGD-O2D
32	CC	514	CLA	CBD-CGD-O2D-CED
32	B	604	CLA	C1A-C2A-CAA-CBA
32	B	604	CLA	CAD-CBD-CGD-O2D
32	B	606	CLA	CAD-CBD-CGD-O1D
32	B	606	CLA	CAD-CBD-CGD-O2D
32	B	606	CLA	CBD-CGD-O2D-CED
32	B	608	CLA	CBD-CGD-O2D-CED
32	B	611	CLA	CHA-CBD-CGD-O1D
32	B	611	CLA	CHA-CBD-CGD-O2D
32	B	619	CLA	C3A-C2A-CAA-CBA
32	B	619	CLA	CAD-CBD-CGD-O1D
32	B	619	CLA	CAD-CBD-CGD-O2D
32	B	622	CLA	CAD-CBD-CGD-O1D
32	B	622	CLA	CAD-CBD-CGD-O2D
32	B	622	CLA	CBD-CGD-O2D-CED
32	B	623	CLA	CAD-CBD-CGD-O2D
32	GG	602	CLA	C2B-C3B-CAB-CBB
32	GG	602	CLA	C4B-C3B-CAB-CBB
32	GG	602	CLA	CBD-CGD-O2D-CED
32	GG	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	GG	611	CLA	C2B-C3B-CAB-CBB
32	GG	611	CLA	C4B-C3B-CAB-CBB
32	GG	611	CLA	CBD-CGD-O2D-CED
32	GG	612	CLA	CHA-CBD-CGD-O1D
32	GG	612	CLA	CHA-CBD-CGD-O2D
32	GG	613	CLA	CBD-CGD-O2D-CED
32	NN	602	CLA	C1A-C2A-CAA-CBA
32	NN	602	CLA	C3A-C2A-CAA-CBA
32	NN	602	CLA	C2B-C3B-CAB-CBB
32	NN	602	CLA	C4B-C3B-CAB-CBB
32	NN	603	CLA	CAD-CBD-CGD-O1D
32	NN	603	CLA	CAD-CBD-CGD-O2D
32	NN	603	CLA	CBD-CGD-O2D-CED
32	NN	610	CLA	C1A-C2A-CAA-CBA
32	NN	610	CLA	CBD-CGD-O2D-CED
32	NN	611	CLA	C1A-C2A-CAA-CBA
32	NN	611	CLA	C3A-C2A-CAA-CBA
32	NN	611	CLA	C4B-C3B-CAB-CBB
32	NN	611	CLA	CAD-CBD-CGD-O1D
32	NN	611	CLA	CAD-CBD-CGD-O2D
32	NN	611	CLA	CBD-CGD-O2D-CED
32	NN	613	CLA	C1A-C2A-CAA-CBA
32	NN	613	CLA	CBD-CGD-O2D-CED
32	NN	614	CLA	C2B-C3B-CAB-CBB
32	NN	614	CLA	C4B-C3B-CAB-CBB
32	NN	614	CLA	CBD-CGD-O2D-CED
32	RR	302	CLA	C1A-C2A-CAA-CBA
32	RR	302	CLA	C3A-C2A-CAA-CBA
32	RR	302	CLA	C2B-C3B-CAB-CBB
32	RR	302	CLA	C4B-C3B-CAB-CBB
32	RR	308	CLA	C4B-C3B-CAB-CBB
32	RR	308	CLA	CBD-CGD-O2D-CED
32	RR	309	CLA	C1A-C2A-CAA-CBA
32	RR	309	CLA	C3A-C2A-CAA-CBA
32	RR	309	CLA	C2B-C3B-CAB-CBB
32	RR	309	CLA	C4B-C3B-CAB-CBB
32	RR	309	CLA	CBD-CGD-O2D-CED
32	RR	310	CLA	C1A-C2A-CAA-CBA
32	RR	310	CLA	C3A-C2A-CAA-CBA
32	RR	310	CLA	CAD-CBD-CGD-O2D
32	RR	311	CLA	CHA-CBD-CGD-O1D
32	RR	311	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	RR	312	CLA	C1A-C2A-CAA-CBA
32	RR	313	CLA	C2B-C3B-CAB-CBB
32	RR	313	CLA	C4B-C3B-CAB-CBB
32	RR	313	CLA	CBD-CGD-O2D-CED
32	SS	304	CLA	CBD-CGD-O2D-CED
32	SS	305	CLA	C1A-C2A-CAA-CBA
32	SS	305	CLA	CHA-CBD-CGD-O1D
32	SS	305	CLA	CHA-CBD-CGD-O2D
32	SS	309	CLA	C2B-C3B-CAB-CBB
32	SS	309	CLA	C4B-C3B-CAB-CBB
32	SS	310	CLA	CBD-CGD-O2D-CED
32	SS	312	CLA	CHA-CBD-CGD-O2D
32	SS	312	CLA	CBD-CGD-O2D-CED
32	SS	313	CLA	CBD-CGD-O2D-CED
32	XX	201	CLA	CHA-CBD-CGD-O2D
32	XX	201	CLA	CBD-CGD-O2D-CED
32	YY	602	CLA	C1A-C2A-CAA-CBA
32	YY	602	CLA	C3A-C2A-CAA-CBA
32	YY	603	CLA	CBD-CGD-O2D-CED
32	YY	610	CLA	C1A-C2A-CAA-CBA
32	YY	610	CLA	C3A-C2A-CAA-CBA
32	YY	610	CLA	CBD-CGD-O2D-CED
32	YY	611	CLA	C2B-C3B-CAB-CBB
32	YY	611	CLA	C4B-C3B-CAB-CBB
32	YY	611	CLA	CBD-CGD-O2D-CED
32	YY	612	CLA	CBD-CGD-O2D-CED
32	YY	614	CLA	C3A-C2A-CAA-CBA
32	Aa	405	CLA	C1A-C2A-CAA-CBA
32	Aa	405	CLA	CBD-CGD-O2D-CED
32	Aa	407	CLA	C2B-C3B-CAB-CBB
32	Aa	407	CLA	C4B-C3B-CAB-CBB
32	Aa	410	CLA	CAD-CBD-CGD-O1D
32	Aa	410	CLA	CAD-CBD-CGD-O2D
32	Bb	601	CLA	C3A-C2A-CAA-CBA
32	Bb	601	CLA	CAD-CBD-CGD-O2D
32	Bb	601	CLA	CBD-CGD-O2D-CED
32	Bb	603	CLA	C1A-C2A-CAA-CBA
32	Bb	603	CLA	C3A-C2A-CAA-CBA
32	Bb	603	CLA	CAD-CBD-CGD-O2D
32	Bb	603	CLA	CBD-CGD-O2D-CED
32	Bb	607	CLA	C4B-C3B-CAB-CBB
32	Bb	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	Bb	608	CLA	C4B-C3B-CAB-CBB
32	Bb	609	CLA	C1A-C2A-CAA-CBA
32	Bb	609	CLA	C3A-C2A-CAA-CBA
32	Bb	612	CLA	CHA-CBD-CGD-O1D
32	Bb	612	CLA	CHA-CBD-CGD-O2D
32	Bb	613	CLA	CBD-CGD-O2D-CED
32	Cc	503	CLA	CAD-CBD-CGD-O2D
32	Cc	504	CLA	CAD-CBD-CGD-O1D
32	Cc	504	CLA	CAD-CBD-CGD-O2D
32	Cc	506	CLA	CBD-CGD-O2D-CED
32	Cc	508	CLA	C1A-C2A-CAA-CBA
32	Cc	508	CLA	C3A-C2A-CAA-CBA
32	Cc	508	CLA	CAD-CBD-CGD-O1D
32	Cc	508	CLA	CAD-CBD-CGD-O2D
32	Cc	509	CLA	CAD-CBD-CGD-O1D
32	Cc	509	CLA	CAD-CBD-CGD-O2D
32	Cc	511	CLA	CAD-CBD-CGD-O1D
32	Cc	511	CLA	CAD-CBD-CGD-O2D
32	Cc	511	CLA	CBD-CGD-O2D-CED
32	Cc	513	CLA	CBD-CGD-O2D-CED
32	Cc	514	CLA	CBD-CGD-O2D-CED
32	Cc	515	CLA	C1A-C2A-CAA-CBA
32	Cc	515	CLA	CAD-CBD-CGD-O1D
32	Cc	515	CLA	CAD-CBD-CGD-O2D
32	Cc	515	CLA	CBD-CGD-O2D-CED
32	Gg	303	CLA	CAD-CBD-CGD-O1D
32	Gg	303	CLA	CAD-CBD-CGD-O2D
32	Gg	305	CLA	C1A-C2A-CAA-CBA
32	Gg	305	CLA	CAD-CBD-CGD-O2D
32	Gg	305	CLA	CBD-CGD-O2D-CED
32	Gg	311	CLA	CBD-CGD-O2D-CED
32	Gg	312	CLA	C1A-C2A-CAA-CBA
32	Gg	313	CLA	C2B-C3B-CAB-CBB
32	Gg	313	CLA	C4B-C3B-CAB-CBB
32	Gg	313	CLA	CHA-CBD-CGD-O1D
32	Gg	313	CLA	CHA-CBD-CGD-O2D
32	Gg	313	CLA	CBD-CGD-O2D-CED
32	Gg	314	CLA	CBD-CGD-O2D-CED
32	Gg	315	CLA	C2B-C3B-CAB-CBB
32	Gg	315	CLA	C4B-C3B-CAB-CBB
32	Nn	301	CLA	C1A-C2A-CAA-CBA
32	Nn	301	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	Nn	301	CLA	CBD-CGD-O2D-CED
32	Nn	303	CLA	CBD-CGD-O2D-CED
32	Nn	304	CLA	C1A-C2A-CAA-CBA
32	Nn	305	CLA	CBD-CGD-O2D-CED
32	Nn	312	CLA	C1A-C2A-CAA-CBA
32	Nn	312	CLA	C3A-C2A-CAA-CBA
32	Nn	312	CLA	C2B-C3B-CAB-CBB
32	Nn	312	CLA	C4B-C3B-CAB-CBB
32	Nn	312	CLA	CHA-CBD-CGD-O1D
32	Nn	312	CLA	CHA-CBD-CGD-O2D
32	Nn	312	CLA	CBD-CGD-O2D-CED
32	Nn	313	CLA	CBD-CGD-O2D-CED
34	C	516	BCR	C23-C24-C25-C26
34	C	517	BCR	C23-C24-C25-C26
34	K	102	BCR	C23-C24-C25-C26
34	K	102	BCR	C23-C24-C25-C30
34	T	101	BCR	C1-C6-C7-C8
34	T	101	BCR	C5-C6-C7-C8
34	a	411	BCR	C5-C6-C7-C8
34	b	617	BCR	C5-C6-C7-C8
34	b	617	BCR	C23-C24-C25-C26
34	b	617	BCR	C23-C24-C25-C30
34	c	515	BCR	C5-C6-C7-C8
34	c	515	BCR	C23-C24-C25-C26
34	d	403	BCR	C5-C6-C7-C8
34	d	403	BCR	C23-C24-C25-C26
34	BB	616	BCR	C23-C24-C25-C26
34	BB	616	BCR	C23-C24-C25-C30
34	BB	620	BCR	C23-C24-C25-C26
34	CC	515	BCR	C23-C24-C25-C26
34	CC	516	BCR	C23-C24-C25-C26
34	B	612	BCR	C23-C24-C25-C26
34	B	612	BCR	C23-C24-C25-C30
34	B	616	BCR	C23-C24-C25-C26
34	B	616	BCR	C23-C24-C25-C30
34	KK	103	BCR	C23-C24-C25-C26
34	KK	103	BCR	C23-C24-C25-C30
34	TT	101	BCR	C1-C6-C7-C8
34	TT	101	BCR	C5-C6-C7-C8
34	XX	202	BCR	C1-C6-C7-C8
34	XX	202	BCR	C5-C6-C7-C8
34	Aa	411	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	Bb	617	BCR	C23-C24-C25-C26
34	Bb	617	BCR	C23-C24-C25-C30
34	Cc	517	BCR	C5-C6-C7-C8
34	Cc	517	BCR	C23-C24-C25-C26
34	Dd	403	BCR	C5-C6-C7-C8
34	Dd	403	BCR	C23-C24-C25-C26
34	Hh	101	BCR	C11-C12-C13-C14
34	Kk	101	BCR	C5-C6-C7-C8
34	Kk	101	BCR	C23-C24-C25-C26
34	Kk	101	BCR	C23-C24-C25-C30
35	A	410	PL9	C11-C12-C13-C14
35	A	410	PL9	C12-C13-C14-C15
35	A	410	PL9	C17-C18-C19-C21
35	A	410	PL9	C23-C24-C26-C27
35	A	410	PL9	C27-C28-C29-C31
35	A	410	PL9	C32-C33-C34-C35
35	A	410	PL9	C32-C33-C34-C36
35	A	410	PL9	C37-C38-C39-C40
35	A	410	PL9	C42-C43-C44-C45
35	A	410	PL9	C47-C48-C49-C51
35	D	407	PL9	C12-C13-C14-C15
35	D	407	PL9	C17-C18-C19-C20
35	D	407	PL9	C17-C18-C19-C21
35	D	407	PL9	C20-C19-C21-C22
35	D	407	PL9	C25-C24-C26-C27
35	D	407	PL9	C27-C28-C29-C31
35	D	407	PL9	C32-C33-C34-C36
35	D	407	PL9	C40-C39-C41-C42
35	D	407	PL9	C42-C43-C44-C46
35	d	404	PL9	C7-C8-C9-C10
35	d	404	PL9	C12-C13-C14-C15
35	d	404	PL9	C22-C23-C24-C25
35	d	404	PL9	C22-C23-C24-C26
35	d	404	PL9	C27-C28-C29-C30
35	d	404	PL9	C27-C28-C29-C31
35	d	404	PL9	C37-C38-C39-C41
35	d	404	PL9	C38-C39-C41-C42
35	d	404	PL9	C42-C43-C44-C46
35	d	404	PL9	C45-C44-C46-C47
35	d	404	PL9	C47-C48-C49-C51
35	AA	410	PL9	C17-C18-C19-C20
35	AA	410	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
35	AA	410	PL9	C22-C23-C24-C26
35	AA	410	PL9	C27-C28-C29-C31
35	AA	410	PL9	C37-C38-C39-C40
35	AA	410	PL9	C47-C48-C49-C51
35	DD	406	PL9	C7-C8-C9-C10
35	DD	406	PL9	C17-C18-C19-C20
35	DD	406	PL9	C22-C23-C24-C25
35	DD	406	PL9	C27-C28-C29-C31
35	DD	406	PL9	C32-C33-C34-C35
35	DD	406	PL9	C37-C38-C39-C41
35	DD	406	PL9	C40-C39-C41-C42
35	DD	406	PL9	C42-C43-C44-C46
35	Dd	404	PL9	C7-C8-C9-C11
35	Dd	404	PL9	C12-C13-C14-C16
35	Dd	404	PL9	C15-C14-C16-C17
35	Dd	404	PL9	C22-C23-C24-C25
35	Dd	404	PL9	C22-C23-C24-C26
35	Dd	404	PL9	C27-C28-C29-C30
35	Dd	404	PL9	C27-C28-C29-C31
35	Dd	404	PL9	C37-C38-C39-C41
35	Dd	404	PL9	C42-C43-C44-C46
35	Dd	404	PL9	C47-C48-C49-C51
36	A	411	LHG	C3-O3-P-O5
36	A	411	LHG	C4-O6-P-O3
36	A	411	LHG	C4-O6-P-O4
36	A	413	LHG	C3-O3-P-O4
36	A	413	LHG	C3-O3-P-O6
36	A	413	LHG	C4-O6-P-O3
36	A	413	LHG	C4-O6-P-O5
36	A	414	LHG	C3-O3-P-O6
36	Rr	617	LHG	C3-O3-P-O4
36	Rr	617	LHG	C3-O3-P-O6
36	Rr	617	LHG	C4-O6-P-O3
36	Rr	617	LHG	C4-O6-P-O4
36	Ss	616	LHG	C4-O6-P-O3
36	Ss	616	LHG	C4-O6-P-O4
36	Yy	618	LHG	O2-C2-C3-O3
36	Yy	618	LHG	C3-O3-P-O4
36	Yy	618	LHG	C3-O3-P-O6
36	Yy	618	LHG	C4-O6-P-O3
36	Yy	618	LHG	C4-O6-P-O4
36	44	614	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
36	44	614	LHG	C3-O3-P-O5
36	44	614	LHG	C3-O3-P-O6
36	44	616	LHG	C3-O3-P-O4
36	44	616	LHG	C3-O3-P-O6
36	44	616	LHG	C4-O6-P-O5
36	44	616	LHG	O9-C7-O7-C5
36	11	614	LHG	C3-O3-P-O4
36	11	614	LHG	C3-O3-P-O5
36	11	614	LHG	C3-O3-P-O6
36	11	614	LHG	C4-O6-P-O3
36	11	614	LHG	C4-O6-P-O4
36	22	615	LHG	C3-O3-P-O5
36	22	615	LHG	C4-O6-P-O3
36	22	615	LHG	C4-O6-P-O4
36	22	615	LHG	C4-O6-P-O5
36	33	614	LHG	C3-O3-P-O4
36	33	614	LHG	C3-O3-P-O5
36	33	614	LHG	C3-O3-P-O6
36	33	614	LHG	C4-O6-P-O4
36	1	614	LHG	C3-O3-P-O5
36	1	614	LHG	C4-O6-P-O4
36	3	614	LHG	C3-O3-P-O4
36	3	614	LHG	C3-O3-P-O5
36	3	614	LHG	C3-O3-P-O6
36	C	522	LHG	C3-O3-P-O6
36	C	522	LHG	C4-O6-P-O3
36	D	408	LHG	C3-O3-P-O5
36	D	408	LHG	C3-O3-P-O6
36	D	408	LHG	C4-O6-P-O3
36	D	408	LHG	C4-O6-P-O5
36	D	410	LHG	C3-O3-P-O6
36	D	410	LHG	C4-O6-P-O3
36	G	618	LHG	C8-C7-O7-C5
36	J	101	LHG	C3-O3-P-O4
36	J	101	LHG	C3-O3-P-O6
36	J	101	LHG	C4-O6-P-O3
36	J	101	LHG	C4-O6-P-O4
36	K	101	LHG	C3-O3-P-O4
36	K	101	LHG	C3-O3-P-O6
36	K	101	LHG	C4-O6-P-O3
36	K	101	LHG	C4-O6-P-O4
36	N	619	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
36	Y	618	LHG	C3-O3-P-O4
36	Y	618	LHG	C3-O3-P-O6
36	Y	618	LHG	C4-O6-P-O3
36	Y	618	LHG	C4-O6-P-O4
36	d	405	LHG	C4-O6-P-O3
36	d	405	LHG	C4-O6-P-O4
36	d	406	LHG	C3-O3-P-O4
36	d	406	LHG	C3-O3-P-O6
36	d	406	LHG	C4-O6-P-O3
36	d	406	LHG	C4-O6-P-O4
36	g	618	LHG	C1-C2-C3-O3
36	g	618	LHG	C3-O3-P-O5
36	l	101	LHG	C3-O3-P-O4
36	l	101	LHG	C3-O3-P-O5
36	l	101	LHG	C3-O3-P-O6
36	l	101	LHG	C4-O6-P-O5
36	n	618	LHG	C8-C7-O7-C5
36	r	616	LHG	C3-O3-P-O4
36	r	616	LHG	C3-O3-P-O6
36	r	616	LHG	C4-O6-P-O3
36	r	616	LHG	C4-O6-P-O4
36	s	616	LHG	C4-O6-P-O3
36	s	616	LHG	C4-O6-P-O4
36	y	320	LHG	C3-O3-P-O4
36	y	320	LHG	C3-O3-P-O6
36	y	320	LHG	C4-O6-P-O3
36	y	320	LHG	C4-O6-P-O4
36	4	301	LHG	O1-C1-C2-C3
36	4	301	LHG	C4-O6-P-O5
36	4	301	LHG	O9-C7-O7-C5
36	4	315	LHG	C3-O3-P-O4
36	4	315	LHG	C3-O3-P-O5
36	4	315	LHG	C3-O3-P-O6
36	AA	411	LHG	C3-O3-P-O5
36	AA	411	LHG	C3-O3-P-O6
36	AA	411	LHG	C4-O6-P-O3
36	AA	411	LHG	C4-O6-P-O4
36	AA	414	LHG	C3-O3-P-O6
36	BB	622	LHG	C3-O3-P-O6
36	BB	622	LHG	C4-O6-P-O5
36	CC	521	LHG	C3-O3-P-O5
36	CC	521	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
36	CC	521	LHG	C4-O6-P-O3
36	CC	523	LHG	C3-O3-P-O4
36	CC	523	LHG	C3-O3-P-O6
36	CC	523	LHG	C4-O6-P-O3
36	CC	523	LHG	C4-O6-P-O5
36	DD	407	LHG	C3-O3-P-O6
36	DD	407	LHG	C4-O6-P-O3
36	DD	407	LHG	C4-O6-P-O5
36	GG	618	LHG	C8-C7-O7-C5
36	II	101	LHG	C4-O6-P-O5
36	JJ	101	LHG	C3-O3-P-O4
36	JJ	101	LHG	C3-O3-P-O6
36	KK	101	LHG	C4-O6-P-O3
36	NN	619	LHG	C8-C7-O7-C5
36	SS	301	LHG	C3-O3-P-O4
36	SS	301	LHG	C3-O3-P-O6
36	SS	301	LHG	C4-O6-P-O3
36	SS	301	LHG	C4-O6-P-O4
36	YY	618	LHG	C3-O3-P-O4
36	YY	618	LHG	C4-O6-P-O3
36	YY	618	LHG	C4-O6-P-O4
36	Dd	405	LHG	C4-O6-P-O3
36	Dd	405	LHG	C4-O6-P-O4
36	Dd	406	LHG	C3-O3-P-O4
36	Dd	406	LHG	C3-O3-P-O6
36	Dd	406	LHG	C4-O6-P-O3
36	Dd	406	LHG	C4-O6-P-O4
36	Gg	319	LHG	C3-O3-P-O4
36	Gg	319	LHG	C3-O3-P-O6
36	Ll	102	LHG	C3-O3-P-O4
36	Ll	102	LHG	C3-O3-P-O5
36	Ll	102	LHG	C3-O3-P-O6
36	Nn	310	LHG	C8-C7-O7-C5
37	A	412	SQD	O5-C5-C6-S
37	C	501	SQD	C2-C1-O6-C44
37	C	501	SQD	O5-C1-O6-C44
37	l	102	SQD	O5-C1-O6-C44
37	BB	621	SQD	C5-C6-S-O8
37	B	617	SQD	C5-C6-S-O8
37	Ll	101	SQD	O5-C1-O6-C44
38	b	621	LMG	O9-C10-O7-C8
38	Aa	412	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
38	Bb	621	LMG	O9-C10-O7-C8
38	Bb	621	LMG	C11-C10-O7-C8
39	Rr	605	CHL	CHA-CBD-CGD-O2D
39	Rr	606	CHL	CBD-CGD-O2D-CED
39	Ss	601	CHL	CBD-CGD-O2D-CED
39	Ss	606	CHL	CAD-CBD-CGD-O1D
39	Ss	606	CHL	CAD-CBD-CGD-O2D
39	Yy	601	CHL	CBD-CGD-O2D-CED
39	Yy	605	CHL	CAD-CBD-CGD-O1D
39	Yy	605	CHL	CAD-CBD-CGD-O2D
39	Yy	607	CHL	CBD-CGD-O2D-CED
39	44	605	CHL	CBD-CGD-O2D-CED
39	44	606	CHL	CBD-CGD-O2D-CED
39	44	607	CHL	CBD-CGD-O2D-CED
39	11	601	CHL	CBD-CGD-O2D-CED
39	11	607	CHL	CBD-CGD-O2D-CED
39	22	606	CHL	CHA-CBD-CGD-O1D
39	22	606	CHL	CHA-CBD-CGD-O2D
39	22	606	CHL	CBD-CGD-O2D-CED
39	22	608	CHL	CBD-CGD-O2D-CED
39	33	601	CHL	CBD-CGD-O2D-CED
39	33	605	CHL	CBD-CGD-O2D-CED
39	33	606	CHL	CBD-CGD-O2D-CED
39	33	607	CHL	CBD-CGD-O2D-CED
39	33	608	CHL	CBD-CGD-O2D-CED
39	1	601	CHL	CBD-CGD-O2D-CED
39	1	607	CHL	CBD-CGD-O2D-CED
39	2	608	CHL	CBD-CGD-O2D-CED
39	3	601	CHL	CBD-CGD-O2D-CED
39	3	606	CHL	CBD-CGD-O2D-CED
39	G	606	CHL	C1A-C2A-CAA-CBA
39	G	606	CHL	C3A-C2A-CAA-CBA
39	G	606	CHL	CBD-CGD-O2D-CED
39	G	607	CHL	CBD-CGD-O2D-CED
39	G	608	CHL	CAD-CBD-CGD-O1D
39	G	608	CHL	CAD-CBD-CGD-O2D
39	N	608	CHL	CBD-CGD-O2D-CED
39	R	605	CHL	C1A-C2A-CAA-CBA
39	R	605	CHL	C3A-C2A-CAA-CBA
39	R	606	CHL	C1A-C2A-CAA-CBA
39	R	606	CHL	C3A-C2A-CAA-CBA
39	R	606	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	S	601	CHL	CBD-CGD-O2D-CED
39	S	605	CHL	CBD-CGD-O2D-CED
39	Y	601	CHL	CBD-CGD-O2D-CED
39	Y	606	CHL	C1A-C2A-CAA-CBA
39	g	605	CHL	C1A-C2A-CAA-CBA
39	g	605	CHL	CBD-CGD-O2D-CED
39	g	606	CHL	C1A-C2A-CAA-CBA
39	g	606	CHL	C3A-C2A-CAA-CBA
39	g	606	CHL	CBD-CGD-O2D-CED
39	g	607	CHL	CHA-CBD-CGD-O1D
39	g	607	CHL	CBD-CGD-O2D-CED
39	n	601	CHL	CBD-CGD-O2D-CED
39	n	605	CHL	C1A-C2A-CAA-CBA
39	n	607	CHL	CBD-CGD-O2D-CED
39	n	608	CHL	CBD-CGD-O2D-CED
39	r	606	CHL	CBD-CGD-O2D-CED
39	s	601	CHL	CBD-CGD-O2D-CED
39	s	606	CHL	CAD-CBD-CGD-O1D
39	s	606	CHL	CAD-CBD-CGD-O2D
39	y	303	CHL	CBD-CGD-O2D-CED
39	y	307	CHL	CAD-CBD-CGD-O1D
39	y	307	CHL	CAD-CBD-CGD-O2D
39	y	311	CHL	CHA-CBD-CGD-O1D
39	y	311	CHL	CHA-CBD-CGD-O2D
39	4	306	CHL	CBD-CGD-O2D-CED
39	4	307	CHL	CBD-CGD-O2D-CED
39	4	308	CHL	CBD-CGD-O2D-CED
39	4	309	CHL	C1A-C2A-CAA-CBA
39	GG	606	CHL	CBD-CGD-O2D-CED
39	GG	607	CHL	CBD-CGD-O2D-CED
39	GG	608	CHL	CAD-CBD-CGD-O1D
39	GG	608	CHL	CAD-CBD-CGD-O2D
39	GG	608	CHL	CBD-CGD-O2D-CED
39	GG	609	CHL	CBD-CGD-O2D-CED
39	NN	608	CHL	CBD-CGD-O2D-CED
39	RR	305	CHL	C1A-C2A-CAA-CBA
39	RR	305	CHL	C3A-C2A-CAA-CBA
39	RR	306	CHL	C1A-C2A-CAA-CBA
39	RR	306	CHL	C3A-C2A-CAA-CBA
39	RR	306	CHL	CBD-CGD-O2D-CED
39	SS	302	CHL	CBD-CGD-O2D-CED
39	SS	308	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	YY	606	CHL	C1A-C2A-CAA-CBA
39	YY	608	CHL	CBD-CGD-O2D-CED
39	Gg	302	CHL	CBD-CGD-O2D-CED
39	Gg	306	CHL	C1A-C2A-CAA-CBA
39	Gg	306	CHL	CBD-CGD-O2D-CED
39	Gg	307	CHL	C1A-C2A-CAA-CBA
39	Gg	307	CHL	C3A-C2A-CAA-CBA
39	Gg	308	CHL	CHA-CBD-CGD-O1D
39	Gg	308	CHL	CHA-CBD-CGD-O2D
39	Gg	308	CHL	CBD-CGD-O2D-CED
39	Gg	310	CHL	CAD-CBD-CGD-O2D
39	Gg	310	CHL	CBD-CGD-O2D-CED
39	Nn	311	CHL	CBD-CGD-O2D-CED
39	Nn	315	CHL	C1A-C2A-CAA-CBA
39	Nn	318	CHL	CBD-CGD-O2D-CED
40	Y	615	LUT	C21-C26-C27-C28
40	Y	615	LUT	C25-C26-C27-C28
40	YY	615	LUT	C25-C26-C27-C28
41	Rr	615	XAT	C5-C6-C7-C8
41	Rr	615	XAT	O4-C6-C7-C8
41	Yy	619	XAT	C21-C26-C27-C28
41	Yy	619	XAT	C25-C26-C27-C28
41	Yy	619	XAT	O24-C26-C27-C28
41	G	619	XAT	O24-C26-C27-C28
41	g	619	XAT	O24-C26-C27-C28
41	r	615	XAT	O4-C6-C7-C8
41	y	301	XAT	C21-C26-C27-C28
41	y	301	XAT	C25-C26-C27-C28
41	y	301	XAT	O24-C26-C27-C28
41	y	302	XAT	O24-C26-C27-C28
41	GG	619	XAT	O24-C26-C27-C28
41	Gg	301	XAT	O24-C26-C27-C28
41	Nn	308	XAT	O24-C26-C27-C28
43	C	502	LMU	C2'-C1'-O1'-C1
43	C	502	LMU	O5'-C1'-O1'-C1
43	R	618	LMU	O5'-C1'-O1'-C1
44	a	415	DGD	O6D-C1D-O3G-C3G
44	CC	522	DGD	C2B-C1B-O2G-C2G
44	CC	522	DGD	O2G-C2G-C3G-O3G
44	CC	522	DGD	C4D-C5D-C6D-O5D
44	Aa	401	DGD	O6D-C1D-O3G-C3G
32	Rr	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Yy	603	CLA	O1D-CGD-O2D-CED
32	44	615	CLA	O1D-CGD-O2D-CED
32	11	611	CLA	O1D-CGD-O2D-CED
32	22	612	CLA	O1D-CGD-O2D-CED
32	1	609	CLA	O1D-CGD-O2D-CED
32	1	613	CLA	O1D-CGD-O2D-CED
32	2	612	CLA	O1D-CGD-O2D-CED
32	3	602	CLA	O1D-CGD-O2D-CED
32	C	508	CLA	O1D-CGD-O2D-CED
32	C	515	CLA	O1D-CGD-O2D-CED
32	G	604	CLA	O1D-CGD-O2D-CED
32	G	612	CLA	O1D-CGD-O2D-CED
32	N	610	CLA	O1D-CGD-O2D-CED
32	R	601	CLA	O1D-CGD-O2D-CED
32	R	610	CLA	O1D-CGD-O2D-CED
32	S	603	CLA	O1D-CGD-O2D-CED
32	X	201	CLA	O1D-CGD-O2D-CED
32	Y	603	CLA	O1D-CGD-O2D-CED
32	Y	612	CLA	O1D-CGD-O2D-CED
32	b	607	CLA	O1D-CGD-O2D-CED
32	c	506	CLA	O1D-CGD-O2D-CED
32	n	603	CLA	O1D-CGD-O2D-CED
32	s	604	CLA	O1D-CGD-O2D-CED
32	s	611	CLA	O1D-CGD-O2D-CED
32	CC	507	CLA	O1D-CGD-O2D-CED
32	GG	613	CLA	O1D-CGD-O2D-CED
32	RR	310	CLA	O1D-CGD-O2D-CED
32	SS	304	CLA	O1D-CGD-O2D-CED
32	YY	612	CLA	O1D-CGD-O2D-CED
32	Bb	609	CLA	O1D-CGD-O2D-CED
32	Bb	614	CLA	O1D-CGD-O2D-CED
32	Gg	303	CLA	O1D-CGD-O2D-CED
32	Gg	314	CLA	O1D-CGD-O2D-CED
32	Nn	301	CLA	O1D-CGD-O2D-CED
32	Nn	303	CLA	O1D-CGD-O2D-CED
32	Nn	313	CLA	O1D-CGD-O2D-CED
39	2	606	CHL	O1D-CGD-O2D-CED
39	G	605	CHL	O1D-CGD-O2D-CED
39	4	307	CHL	O1D-CGD-O2D-CED
39	GG	605	CHL	O1D-CGD-O2D-CED
39	Nn	311	CHL	O1D-CGD-O2D-CED
39	Nn	317	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Rr	608	CLA	O1D-CGD-O2D-CED
32	Ss	604	CLA	O1D-CGD-O2D-CED
32	Ss	611	CLA	O1D-CGD-O2D-CED
32	44	603	CLA	O1D-CGD-O2D-CED
32	44	604	CLA	O1D-CGD-O2D-CED
32	44	609	CLA	O1D-CGD-O2D-CED
32	44	610	CLA	O1D-CGD-O2D-CED
32	11	609	CLA	O1D-CGD-O2D-CED
32	11	613	CLA	O1D-CGD-O2D-CED
32	22	611	CLA	O1D-CGD-O2D-CED
32	33	604	CLA	O1D-CGD-O2D-CED
32	33	610	CLA	O1D-CGD-O2D-CED
32	1	610	CLA	O1D-CGD-O2D-CED
32	1	611	CLA	O1D-CGD-O2D-CED
32	2	611	CLA	O1D-CGD-O2D-CED
32	3	610	CLA	O1D-CGD-O2D-CED
32	G	602	CLA	O1D-CGD-O2D-CED
32	G	611	CLA	O1D-CGD-O2D-CED
32	G	613	CLA	O1D-CGD-O2D-CED
32	R	608	CLA	O1D-CGD-O2D-CED
32	R	613	CLA	O1D-CGD-O2D-CED
32	S	609	CLA	O1D-CGD-O2D-CED
32	S	611	CLA	O1D-CGD-O2D-CED
32	b	614	CLA	O1D-CGD-O2D-CED
32	g	604	CLA	O1D-CGD-O2D-CED
32	g	611	CLA	O1D-CGD-O2D-CED
32	g	612	CLA	O1D-CGD-O2D-CED
32	g	613	CLA	O1D-CGD-O2D-CED
32	n	612	CLA	O1D-CGD-O2D-CED
32	n	614	CLA	O1D-CGD-O2D-CED
32	r	608	CLA	O1D-CGD-O2D-CED
32	s	610	CLA	O1D-CGD-O2D-CED
32	y	305	CLA	O1D-CGD-O2D-CED
32	4	304	CLA	O1D-CGD-O2D-CED
32	4	305	CLA	O1D-CGD-O2D-CED
32	4	310	CLA	O1D-CGD-O2D-CED
32	CC	514	CLA	O1D-CGD-O2D-CED
32	GG	602	CLA	O1D-CGD-O2D-CED
32	GG	603	CLA	O1D-CGD-O2D-CED
32	GG	604	CLA	O1D-CGD-O2D-CED
32	GG	612	CLA	O1D-CGD-O2D-CED
32	RR	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	RR	309	CLA	O1D-CGD-O2D-CED
32	RR	313	CLA	O1D-CGD-O2D-CED
32	SS	311	CLA	O1D-CGD-O2D-CED
32	SS	312	CLA	O1D-CGD-O2D-CED
32	XX	201	CLA	O1D-CGD-O2D-CED
32	YY	603	CLA	O1D-CGD-O2D-CED
32	Bb	607	CLA	O1D-CGD-O2D-CED
32	Cc	508	CLA	O1D-CGD-O2D-CED
32	Cc	514	CLA	O1D-CGD-O2D-CED
32	Gg	313	CLA	O1D-CGD-O2D-CED
39	Ss	601	CHL	O1D-CGD-O2D-CED
39	Yy	601	CHL	O1D-CGD-O2D-CED
39	44	605	CHL	O1D-CGD-O2D-CED
39	44	607	CHL	O1D-CGD-O2D-CED
39	11	607	CHL	O1D-CGD-O2D-CED
39	22	601	CHL	O1D-CGD-O2D-CED
39	22	605	CHL	O1D-CGD-O2D-CED
39	22	606	CHL	O1D-CGD-O2D-CED
39	33	601	CHL	O1D-CGD-O2D-CED
39	33	606	CHL	O1D-CGD-O2D-CED
39	1	607	CHL	O1D-CGD-O2D-CED
39	3	606	CHL	O1D-CGD-O2D-CED
39	G	606	CHL	O1D-CGD-O2D-CED
39	G	607	CHL	O1D-CGD-O2D-CED
39	G	609	CHL	O1D-CGD-O2D-CED
39	R	606	CHL	O1D-CGD-O2D-CED
39	g	601	CHL	O1D-CGD-O2D-CED
39	g	605	CHL	O1D-CGD-O2D-CED
39	n	601	CHL	O1D-CGD-O2D-CED
39	n	607	CHL	O1D-CGD-O2D-CED
39	y	303	CHL	O1D-CGD-O2D-CED
39	4	306	CHL	O1D-CGD-O2D-CED
39	4	308	CHL	O1D-CGD-O2D-CED
39	GG	606	CHL	O1D-CGD-O2D-CED
39	GG	607	CHL	O1D-CGD-O2D-CED
39	GG	609	CHL	O1D-CGD-O2D-CED
39	Gg	302	CHL	O1D-CGD-O2D-CED
39	Gg	306	CHL	O1D-CGD-O2D-CED
39	Gg	307	CHL	O1D-CGD-O2D-CED
36	44	614	LHG	C8-C7-O7-C5
32	A	405	CLA	CBD-CGD-O2D-CED
32	Rr	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Rr	609	CLA	CBD-CGD-O2D-CED
32	Rr	610	CLA	CBD-CGD-O2D-CED
32	Ss	603	CLA	CBD-CGD-O2D-CED
32	Ss	604	CLA	CBD-CGD-O2D-CED
32	Ss	609	CLA	CBD-CGD-O2D-CED
32	Ss	610	CLA	CBD-CGD-O2D-CED
32	Ss	611	CLA	CBD-CGD-O2D-CED
32	Ss	613	CLA	CBD-CGD-O2D-CED
32	Yy	603	CLA	CBD-CGD-O2D-CED
32	Yy	614	CLA	CBD-CGD-O2D-CED
32	44	615	CLA	CBD-CGD-O2D-CED
32	11	602	CLA	CBD-CGD-O2D-CED
32	11	611	CLA	CBD-CGD-O2D-CED
32	22	603	CLA	CBD-CGD-O2D-CED
32	22	612	CLA	CBD-CGD-O2D-CED
32	33	602	CLA	CBD-CGD-O2D-CED
32	33	604	CLA	CBD-CGD-O2D-CED
32	1	602	CLA	CBD-CGD-O2D-CED
32	1	610	CLA	CBD-CGD-O2D-CED
32	1	613	CLA	CBD-CGD-O2D-CED
32	2	611	CLA	CBD-CGD-O2D-CED
32	2	612	CLA	CBD-CGD-O2D-CED
32	3	602	CLA	CBD-CGD-O2D-CED
32	3	604	CLA	CBD-CGD-O2D-CED
32	C	505	CLA	CBD-CGD-O2D-CED
32	C	513	CLA	CBD-CGD-O2D-CED
32	D	401	CLA	CBD-CGD-O2D-CED
32	G	604	CLA	CBD-CGD-O2D-CED
32	G	614	CLA	CBD-CGD-O2D-CED
32	N	610	CLA	CBD-CGD-O2D-CED
32	R	601	CLA	CBD-CGD-O2D-CED
32	R	610	CLA	CBD-CGD-O2D-CED
32	S	603	CLA	CBD-CGD-O2D-CED
32	S	608	CLA	CBD-CGD-O2D-CED
32	Y	610	CLA	CBD-CGD-O2D-CED
32	a	405	CLA	CBD-CGD-O2D-CED
32	b	602	CLA	CBD-CGD-O2D-CED
32	b	605	CLA	CBD-CGD-O2D-CED
32	b	607	CLA	CBD-CGD-O2D-CED
32	b	609	CLA	CBD-CGD-O2D-CED
32	b	615	CLA	CBD-CGD-O2D-CED
32	c	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	g	602	CLA	CBD-CGD-O2D-CED
32	g	611	CLA	CBD-CGD-O2D-CED
32	g	612	CLA	CBD-CGD-O2D-CED
32	g	614	CLA	CBD-CGD-O2D-CED
32	n	602	CLA	CBD-CGD-O2D-CED
32	n	611	CLA	CBD-CGD-O2D-CED
32	r	601	CLA	CBD-CGD-O2D-CED
32	r	609	CLA	CBD-CGD-O2D-CED
32	r	610	CLA	CBD-CGD-O2D-CED
32	r	612	CLA	CBD-CGD-O2D-CED
32	s	603	CLA	CBD-CGD-O2D-CED
32	s	604	CLA	CBD-CGD-O2D-CED
32	s	608	CLA	CBD-CGD-O2D-CED
32	s	610	CLA	CBD-CGD-O2D-CED
32	s	611	CLA	CBD-CGD-O2D-CED
32	y	305	CLA	CBD-CGD-O2D-CED
32	y	312	CLA	CBD-CGD-O2D-CED
32	y	313	CLA	CBD-CGD-O2D-CED
32	y	316	CLA	CBD-CGD-O2D-CED
32	BB	604	CLA	CBD-CGD-O2D-CED
32	BB	605	CLA	CBD-CGD-O2D-CED
32	BB	608	CLA	CBD-CGD-O2D-CED
32	CC	507	CLA	CBD-CGD-O2D-CED
32	CC	512	CLA	CBD-CGD-O2D-CED
32	B	604	CLA	CBD-CGD-O2D-CED
32	B	621	CLA	CBD-CGD-O2D-CED
32	GG	603	CLA	CBD-CGD-O2D-CED
32	GG	610	CLA	CBD-CGD-O2D-CED
32	GG	612	CLA	CBD-CGD-O2D-CED
32	GG	614	CLA	CBD-CGD-O2D-CED
32	NN	604	CLA	CBD-CGD-O2D-CED
32	NN	612	CLA	CBD-CGD-O2D-CED
32	RR	310	CLA	CBD-CGD-O2D-CED
32	SS	311	CLA	CBD-CGD-O2D-CED
32	Bb	605	CLA	CBD-CGD-O2D-CED
32	Bb	607	CLA	CBD-CGD-O2D-CED
32	Bb	609	CLA	CBD-CGD-O2D-CED
32	Bb	614	CLA	CBD-CGD-O2D-CED
32	Cc	504	CLA	CBD-CGD-O2D-CED
32	Cc	508	CLA	CBD-CGD-O2D-CED
32	Gg	303	CLA	CBD-CGD-O2D-CED
32	Gg	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Gg	312	CLA	CBD-CGD-O2D-CED
33	A	407	PHO	CBD-CGD-O2D-CED
39	Ss	606	CHL	CBD-CGD-O2D-CED
39	Ss	607	CHL	CBD-CGD-O2D-CED
39	11	605	CHL	CBD-CGD-O2D-CED
39	11	608	CHL	CBD-CGD-O2D-CED
39	22	601	CHL	CBD-CGD-O2D-CED
39	22	605	CHL	CBD-CGD-O2D-CED
39	22	607	CHL	CBD-CGD-O2D-CED
39	2	601	CHL	CBD-CGD-O2D-CED
39	2	605	CHL	CBD-CGD-O2D-CED
39	2	606	CHL	CBD-CGD-O2D-CED
39	2	607	CHL	CBD-CGD-O2D-CED
39	3	608	CHL	CBD-CGD-O2D-CED
39	G	601	CHL	CBD-CGD-O2D-CED
39	G	605	CHL	CBD-CGD-O2D-CED
39	G	608	CHL	CBD-CGD-O2D-CED
39	G	609	CHL	CBD-CGD-O2D-CED
39	Y	607	CHL	CBD-CGD-O2D-CED
39	Y	608	CHL	CBD-CGD-O2D-CED
39	g	601	CHL	CBD-CGD-O2D-CED
39	g	608	CHL	CBD-CGD-O2D-CED
39	g	609	CHL	CBD-CGD-O2D-CED
39	s	606	CHL	CBD-CGD-O2D-CED
39	y	307	CHL	CBD-CGD-O2D-CED
39	GG	601	CHL	CBD-CGD-O2D-CED
39	GG	605	CHL	CBD-CGD-O2D-CED
39	SS	306	CHL	CBD-CGD-O2D-CED
39	YY	601	CHL	CBD-CGD-O2D-CED
39	YY	607	CHL	CBD-CGD-O2D-CED
39	Gg	307	CHL	CBD-CGD-O2D-CED
39	Gg	309	CHL	CBD-CGD-O2D-CED
39	Nn	315	CHL	CBD-CGD-O2D-CED
39	Nn	317	CHL	CBD-CGD-O2D-CED
32	Ss	608	CLA	O1A-CGA-O2A-C1
32	C	512	CLA	O1A-CGA-O2A-C1
32	G	603	CLA	O1A-CGA-O2A-C1
32	N	610	CLA	O1A-CGA-O2A-C1
32	Y	602	CLA	O1A-CGA-O2A-C1
32	Y	610	CLA	O1A-CGA-O2A-C1
32	g	611	CLA	O1A-CGA-O2A-C1
32	n	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	r	613	CLA	O1A-CGA-O2A-C1
32	CC	511	CLA	O1A-CGA-O2A-C1
32	B	624	CLA	O1A-CGA-O2A-C1
32	NN	610	CLA	O1A-CGA-O2A-C1
32	SS	312	CLA	O1A-CGA-O2A-C1
32	YY	602	CLA	O1A-CGA-O2A-C1
32	Gg	312	CLA	O1A-CGA-O2A-C1
32	Nn	301	CLA	O1A-CGA-O2A-C1
39	Y	605	CHL	O1A-CGA-O2A-C1
39	g	607	CHL	O1A-CGA-O2A-C1
39	Gg	308	CHL	O1A-CGA-O2A-C1
32	22	610	CLA	O1D-CGD-O2D-CED
32	33	612	CLA	O1D-CGD-O2D-CED
32	3	612	CLA	O1D-CGD-O2D-CED
32	R	609	CLA	O1D-CGD-O2D-CED
32	c	512	CLA	O1D-CGD-O2D-CED
32	n	610	CLA	O1D-CGD-O2D-CED
32	NN	610	CLA	O1D-CGD-O2D-CED
32	Gg	305	CLA	O1D-CGD-O2D-CED
32	Nn	305	CLA	O1D-CGD-O2D-CED
39	Rr	606	CHL	O1D-CGD-O2D-CED
39	44	606	CHL	O1D-CGD-O2D-CED
39	3	601	CHL	O1D-CGD-O2D-CED
39	r	606	CHL	O1D-CGD-O2D-CED
39	s	601	CHL	O1D-CGD-O2D-CED
39	RR	306	CHL	O1D-CGD-O2D-CED
39	SS	308	CHL	O1D-CGD-O2D-CED
35	A	410	PL9	C47-C48-C49-C50
35	D	407	PL9	C47-C48-C49-C50
35	D	407	PL9	C47-C48-C49-C51
35	AA	410	PL9	C47-C48-C49-C50
35	DD	406	PL9	C47-C48-C49-C50
35	DD	406	PL9	C47-C48-C49-C51
32	Rr	609	CLA	O1D-CGD-O2D-CED
32	G	614	CLA	O1D-CGD-O2D-CED
32	a	405	CLA	O1D-CGD-O2D-CED
32	b	609	CLA	O1D-CGD-O2D-CED
32	g	614	CLA	O1D-CGD-O2D-CED
32	n	602	CLA	O1D-CGD-O2D-CED
32	r	609	CLA	O1D-CGD-O2D-CED
32	GG	614	CLA	O1D-CGD-O2D-CED
32	Cc	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Gg	312	CLA	O1D-CGD-O2D-CED
39	Ss	606	CHL	O1D-CGD-O2D-CED
39	2	601	CHL	O1D-CGD-O2D-CED
39	2	605	CHL	O1D-CGD-O2D-CED
39	2	607	CHL	O1D-CGD-O2D-CED
39	G	608	CHL	O1D-CGD-O2D-CED
39	Y	607	CHL	O1D-CGD-O2D-CED
39	Y	608	CHL	O1D-CGD-O2D-CED
39	g	608	CHL	O1D-CGD-O2D-CED
39	g	609	CHL	O1D-CGD-O2D-CED
39	s	606	CHL	O1D-CGD-O2D-CED
39	GG	601	CHL	O1D-CGD-O2D-CED
39	YY	607	CHL	O1D-CGD-O2D-CED
32	S	611	CLA	CBA-CGA-O2A-C1
32	r	613	CLA	CBA-CGA-O2A-C1
32	Gg	312	CLA	CBA-CGA-O2A-C1
32	Yy	611	CLA	CBD-CGD-O2D-CED
32	33	613	CLA	CBD-CGD-O2D-CED
32	B	607	CLA	CBD-CGD-O2D-CED
32	Cc	510	CLA	CBD-CGD-O2D-CED
39	Ss	605	CHL	CBD-CGD-O2D-CED
32	Rr	608	CLA	O1A-CGA-O2A-C1
32	Rr	611	CLA	O1A-CGA-O2A-C1
32	Rr	613	CLA	O1A-CGA-O2A-C1
32	Ss	602	CLA	O1A-CGA-O2A-C1
32	Ss	609	CLA	O1A-CGA-O2A-C1
32	Ss	611	CLA	O1A-CGA-O2A-C1
32	Ss	613	CLA	O1A-CGA-O2A-C1
32	Yy	610	CLA	O1A-CGA-O2A-C1
32	C	504	CLA	O1A-CGA-O2A-C1
32	C	511	CLA	O1A-CGA-O2A-C1
32	N	611	CLA	O1A-CGA-O2A-C1
32	S	611	CLA	O1A-CGA-O2A-C1
32	b	603	CLA	O1A-CGA-O2A-C1
32	b	612	CLA	O1A-CGA-O2A-C1
32	b	613	CLA	O1A-CGA-O2A-C1
32	c	503	CLA	O1A-CGA-O2A-C1
32	s	608	CLA	O1A-CGA-O2A-C1
32	s	611	CLA	O1A-CGA-O2A-C1
32	y	312	CLA	O1A-CGA-O2A-C1
32	BB	607	CLA	O1A-CGA-O2A-C1
32	CC	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	CC	510	CLA	O1A-CGA-O2A-C1
32	GG	603	CLA	O1A-CGA-O2A-C1
32	NN	611	CLA	O1A-CGA-O2A-C1
32	YY	610	CLA	O1A-CGA-O2A-C1
32	Bb	603	CLA	O1A-CGA-O2A-C1
32	Bb	612	CLA	O1A-CGA-O2A-C1
32	Bb	613	CLA	O1A-CGA-O2A-C1
32	Cc	503	CLA	O1A-CGA-O2A-C1
39	Ss	601	CHL	O1A-CGA-O2A-C1
39	R	606	CHL	O1A-CGA-O2A-C1
39	n	601	CHL	O1A-CGA-O2A-C1
39	n	609	CHL	O1A-CGA-O2A-C1
39	YY	605	CHL	O1A-CGA-O2A-C1
39	Nn	311	CHL	O1A-CGA-O2A-C1
39	Nn	319	CHL	O1A-CGA-O2A-C1
32	11	602	CLA	O1D-CGD-O2D-CED
32	11	603	CLA	O1D-CGD-O2D-CED
32	22	603	CLA	O1D-CGD-O2D-CED
32	2	603	CLA	O1D-CGD-O2D-CED
32	2	610	CLA	O1D-CGD-O2D-CED
32	3	604	CLA	O1D-CGD-O2D-CED
32	G	603	CLA	O1D-CGD-O2D-CED
32	N	612	CLA	O1D-CGD-O2D-CED
32	N	613	CLA	O1D-CGD-O2D-CED
32	b	603	CLA	O1D-CGD-O2D-CED
32	b	605	CLA	O1D-CGD-O2D-CED
32	b	613	CLA	O1D-CGD-O2D-CED
32	r	610	CLA	O1D-CGD-O2D-CED
32	BB	610	CLA	O1D-CGD-O2D-CED
32	B	606	CLA	O1D-CGD-O2D-CED
32	B	608	CLA	O1D-CGD-O2D-CED
32	NN	612	CLA	O1D-CGD-O2D-CED
32	NN	614	CLA	O1D-CGD-O2D-CED
32	YY	610	CLA	O1D-CGD-O2D-CED
32	YY	611	CLA	O1D-CGD-O2D-CED
32	Bb	601	CLA	O1D-CGD-O2D-CED
32	Bb	605	CLA	O1D-CGD-O2D-CED
32	Bb	613	CLA	O1D-CGD-O2D-CED
32	Cc	511	CLA	O1D-CGD-O2D-CED
32	Cc	513	CLA	O1D-CGD-O2D-CED
32	Gg	311	CLA	O1D-CGD-O2D-CED
39	2	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	S	605	CHL	O1D-CGD-O2D-CED
39	g	607	CHL	O1D-CGD-O2D-CED
39	GG	608	CHL	O1D-CGD-O2D-CED
39	Gg	308	CHL	O1D-CGD-O2D-CED
39	Gg	309	CHL	O1D-CGD-O2D-CED
39	Gg	310	CHL	O1D-CGD-O2D-CED
32	Rr	611	CLA	O1D-CGD-O2D-CED
32	22	604	CLA	O1D-CGD-O2D-CED
32	1	603	CLA	O1D-CGD-O2D-CED
32	1	604	CLA	O1D-CGD-O2D-CED
32	2	604	CLA	O1D-CGD-O2D-CED
32	N	614	CLA	O1D-CGD-O2D-CED
32	S	612	CLA	O1D-CGD-O2D-CED
32	b	601	CLA	O1D-CGD-O2D-CED
32	b	608	CLA	O1D-CGD-O2D-CED
32	c	503	CLA	O1D-CGD-O2D-CED
32	r	604	CLA	O1D-CGD-O2D-CED
32	r	611	CLA	O1D-CGD-O2D-CED
32	s	613	CLA	O1D-CGD-O2D-CED
32	AA	405	CLA	O1D-CGD-O2D-CED
32	BB	612	CLA	O1D-CGD-O2D-CED
32	GG	611	CLA	O1D-CGD-O2D-CED
32	NN	613	CLA	O1D-CGD-O2D-CED
32	SS	310	CLA	O1D-CGD-O2D-CED
32	SS	313	CLA	O1D-CGD-O2D-CED
32	Bb	603	CLA	O1D-CGD-O2D-CED
32	Cc	506	CLA	O1D-CGD-O2D-CED
32	Nn	312	CLA	O1D-CGD-O2D-CED
39	22	608	CHL	O1D-CGD-O2D-CED
39	33	605	CHL	O1D-CGD-O2D-CED
39	33	607	CHL	O1D-CGD-O2D-CED
39	1	601	CHL	O1D-CGD-O2D-CED
39	N	608	CHL	O1D-CGD-O2D-CED
39	NN	608	CHL	O1D-CGD-O2D-CED
39	SS	302	CHL	O1D-CGD-O2D-CED
39	YY	608	CHL	O1D-CGD-O2D-CED
32	Ss	608	CLA	CBD-CGD-O2D-CED
32	3	603	CLA	CBD-CGD-O2D-CED
32	BB	613	CLA	CBD-CGD-O2D-CED
32	Bb	602	CLA	CBD-CGD-O2D-CED
32	Bb	615	CLA	CBD-CGD-O2D-CED
32	A	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	r	611	CLA	O1A-CGA-O2A-C1
32	AA	405	CLA	O1A-CGA-O2A-C1
39	RR	306	CHL	O1A-CGA-O2A-C1
36	G	618	LHG	O9-C7-O7-C5
36	N	619	LHG	O9-C7-O7-C5
36	n	618	LHG	O9-C7-O7-C5
36	GG	618	LHG	O9-C7-O7-C5
36	NN	619	LHG	O9-C7-O7-C5
36	Nn	310	LHG	O9-C7-O7-C5
44	CC	522	DGD	O1B-C1B-O2G-C2G
32	11	610	CLA	O1D-CGD-O2D-CED
32	c	511	CLA	O1D-CGD-O2D-CED
39	Y	601	CHL	O1D-CGD-O2D-CED
32	C	508	CLA	C3-C5-C6-C7
32	C	514	CLA	C3-C5-C6-C7
32	R	609	CLA	C3-C5-C6-C7
32	Y	610	CLA	C3-C5-C6-C7
32	Y	613	CLA	C3-C5-C6-C7
32	b	604	CLA	C3-C5-C6-C7
32	b	605	CLA	C3-C5-C6-C7
32	b	614	CLA	C3-C5-C6-C7
32	b	615	CLA	C3-C5-C6-C7
32	d	401	CLA	C3-C5-C6-C7
32	r	602	CLA	C3-C5-C6-C7
32	y	314	CLA	C3-C5-C6-C7
32	BB	603	CLA	C3-C5-C6-C7
32	CC	507	CLA	C3-C5-C6-C7
32	CC	513	CLA	C3-C5-C6-C7
32	B	620	CLA	C3-C5-C6-C7
32	RR	309	CLA	C3-C5-C6-C7
32	YY	613	CLA	C3-C5-C6-C7
32	Bb	604	CLA	C3-C5-C6-C7
32	Bb	605	CLA	C3-C5-C6-C7
32	Bb	614	CLA	C3-C5-C6-C7
32	Nn	301	CLA	C3-C5-C6-C7
33	D	402	PHO	C3-C5-C6-C7
33	a	409	PHO	C3-C5-C6-C7
33	Aa	409	PHO	C3-C5-C6-C7
32	B	622	CLA	O1D-CGD-O2D-CED
32	Aa	405	CLA	O1D-CGD-O2D-CED
32	Ss	608	CLA	CBA-CGA-O2A-C1
32	Ss	609	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	C	504	CLA	CBA-CGA-O2A-C1
32	C	511	CLA	CBA-CGA-O2A-C1
32	C	512	CLA	CBA-CGA-O2A-C1
32	G	603	CLA	CBA-CGA-O2A-C1
32	G	611	CLA	CBA-CGA-O2A-C1
32	N	610	CLA	CBA-CGA-O2A-C1
32	Y	602	CLA	CBA-CGA-O2A-C1
32	Y	610	CLA	CBA-CGA-O2A-C1
32	c	501	CLA	CBA-CGA-O2A-C1
32	c	503	CLA	CBA-CGA-O2A-C1
32	g	611	CLA	CBA-CGA-O2A-C1
32	n	603	CLA	CBA-CGA-O2A-C1
32	n	610	CLA	CBA-CGA-O2A-C1
32	CC	503	CLA	CBA-CGA-O2A-C1
32	CC	504	CLA	CBA-CGA-O2A-C1
32	CC	510	CLA	CBA-CGA-O2A-C1
32	CC	511	CLA	CBA-CGA-O2A-C1
32	B	608	CLA	CBA-CGA-O2A-C1
32	B	624	CLA	CBA-CGA-O2A-C1
32	NN	610	CLA	CBA-CGA-O2A-C1
32	SS	312	CLA	CBA-CGA-O2A-C1
32	YY	602	CLA	CBA-CGA-O2A-C1
32	YY	610	CLA	CBA-CGA-O2A-C1
32	Nn	301	CLA	CBA-CGA-O2A-C1
37	L	101	SQD	C24-C23-O48-C46
37	LL	102	SQD	C24-C23-O48-C46
39	Y	605	CHL	CBA-CGA-O2A-C1
39	g	607	CHL	CBA-CGA-O2A-C1
39	n	601	CHL	CBA-CGA-O2A-C1
39	YY	605	CHL	CBA-CGA-O2A-C1
39	Gg	308	CHL	CBA-CGA-O2A-C1
39	Nn	311	CHL	CBA-CGA-O2A-C1
36	4	315	LHG	C8-C7-O7-C5
32	Rr	601	CLA	CBD-CGD-O2D-CED
32	22	613	CLA	CBD-CGD-O2D-CED
32	33	603	CLA	CBD-CGD-O2D-CED
32	33	611	CLA	CBD-CGD-O2D-CED
32	2	602	CLA	CBD-CGD-O2D-CED
32	3	609	CLA	CBD-CGD-O2D-CED
32	3	611	CLA	CBD-CGD-O2D-CED
32	3	613	CLA	CBD-CGD-O2D-CED
32	C	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	C	512	CLA	CBD-CGD-O2D-CED
32	N	602	CLA	CBD-CGD-O2D-CED
32	S	602	CLA	CBD-CGD-O2D-CED
32	S	610	CLA	CBD-CGD-O2D-CED
32	Y	604	CLA	CBD-CGD-O2D-CED
32	Y	611	CLA	CBD-CGD-O2D-CED
32	c	501	CLA	CBD-CGD-O2D-CED
32	c	508	CLA	CBD-CGD-O2D-CED
32	r	603	CLA	CBD-CGD-O2D-CED
32	s	602	CLA	CBD-CGD-O2D-CED
32	BB	602	CLA	CBD-CGD-O2D-CED
32	BB	603	CLA	CBD-CGD-O2D-CED
32	BB	614	CLA	CBD-CGD-O2D-CED
32	CC	504	CLA	CBD-CGD-O2D-CED
32	CC	511	CLA	CBD-CGD-O2D-CED
32	DD	401	CLA	CBD-CGD-O2D-CED
32	B	609	CLA	CBD-CGD-O2D-CED
32	B	610	CLA	CBD-CGD-O2D-CED
32	B	619	CLA	CBD-CGD-O2D-CED
32	B	620	CLA	CBD-CGD-O2D-CED
32	NN	602	CLA	CBD-CGD-O2D-CED
32	SS	309	CLA	CBD-CGD-O2D-CED
32	YY	602	CLA	CBD-CGD-O2D-CED
32	Cc	505	CLA	CBD-CGD-O2D-CED
32	Gg	315	CLA	CBD-CGD-O2D-CED
32	Nn	302	CLA	CBD-CGD-O2D-CED
33	AA	407	PHO	CBD-CGD-O2D-CED
39	Yy	605	CHL	CBD-CGD-O2D-CED
39	r	605	CHL	CBD-CGD-O2D-CED
39	s	605	CHL	CBD-CGD-O2D-CED
39	y	308	CHL	CBD-CGD-O2D-CED
39	NN	601	CHL	CBD-CGD-O2D-CED
39	NN	605	CHL	CBD-CGD-O2D-CED
39	YY	606	CHL	CBD-CGD-O2D-CED
38	b	621	LMG	C11-C10-O7-C8
32	A	405	CLA	O1D-CGD-O2D-CED
32	2	613	CLA	O1D-CGD-O2D-CED
32	N	603	CLA	O1D-CGD-O2D-CED
32	N	604	CLA	O1D-CGD-O2D-CED
32	c	504	CLA	O1D-CGD-O2D-CED
32	g	603	CLA	O1D-CGD-O2D-CED
32	NN	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	NN	611	CLA	O1D-CGD-O2D-CED
32	Cc	515	CLA	O1D-CGD-O2D-CED
39	Yy	607	CHL	O1D-CGD-O2D-CED
39	11	601	CHL	O1D-CGD-O2D-CED
39	33	608	CHL	O1D-CGD-O2D-CED
39	S	601	CHL	O1D-CGD-O2D-CED
39	n	608	CHL	O1D-CGD-O2D-CED
39	SS	306	CHL	O1D-CGD-O2D-CED
39	YY	601	CHL	O1D-CGD-O2D-CED
39	Nn	318	CHL	O1D-CGD-O2D-CED
32	YY	612	CLA	O1A-CGA-O2A-C1
39	Ss	607	CHL	O1A-CGA-O2A-C1
32	c	509	CLA	O1D-CGD-O2D-CED
39	g	606	CHL	O1D-CGD-O2D-CED
35	A	410	PL9	C15-C14-C16-C17
35	A	410	PL9	C35-C34-C36-C37
35	AA	410	PL9	C20-C19-C21-C22
35	AA	410	PL9	C30-C29-C31-C32
35	AA	410	PL9	C45-C44-C46-C47
35	DD	406	PL9	C12-C11-C9-C10
35	DD	406	PL9	C20-C19-C21-C22
35	DD	406	PL9	C25-C24-C26-C27
35	Dd	404	PL9	C45-C44-C46-C47
35	A	410	PL9	C12-C11-C9-C8
35	D	407	PL9	C38-C39-C41-C42
35	d	404	PL9	C18-C19-C21-C22
35	AA	410	PL9	C23-C24-C26-C27
35	AA	410	PL9	C38-C39-C41-C42
35	DD	406	PL9	C33-C34-C36-C37
35	DD	406	PL9	C38-C39-C41-C42
35	Dd	404	PL9	C18-C19-C21-C22
35	Dd	404	PL9	C38-C39-C41-C42
32	b	612	CLA	CBD-CGD-O2D-CED
32	Ss	610	CLA	O1D-CGD-O2D-CED
32	C	505	CLA	O1D-CGD-O2D-CED
32	S	608	CLA	O1D-CGD-O2D-CED
32	r	601	CLA	O1D-CGD-O2D-CED
32	y	312	CLA	O1D-CGD-O2D-CED
32	y	316	CLA	O1D-CGD-O2D-CED
39	Nn	315	CHL	O1D-CGD-O2D-CED
36	J	101	LHG	C8-C7-O7-C5
38	Dd	408	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
32	Yy	604	CLA	C2A-CAA-CBA-CGA
32	Y	604	CLA	C2A-CAA-CBA-CGA
32	r	602	CLA	C2A-CAA-CBA-CGA
32	Gg	312	CLA	C2A-CAA-CBA-CGA
33	a	409	PHO	C2A-CAA-CBA-CGA
33	Aa	409	PHO	C2A-CAA-CBA-CGA
35	Dd	404	PL9	C47-C48-C49-C50
32	y	304	CLA	O1A-CGA-O2A-C1
37	L	101	SQD	O10-C23-O48-C46
32	Rr	602	CLA	C3-C5-C6-C7
32	C	504	CLA	C3-C5-C6-C7
32	D	404	CLA	C3-C5-C6-C7
32	c	501	CLA	C3-C5-C6-C7
32	BB	604	CLA	C3-C5-C6-C7
32	CC	509	CLA	C3-C5-C6-C7
32	DD	403	CLA	C3-C5-C6-C7
32	B	621	CLA	C3-C5-C6-C7
32	Dd	401	CLA	C3-C5-C6-C7
39	Yy	609	CHL	C3-C5-C6-C7
39	N	607	CHL	C3-C5-C6-C7
32	Yy	614	CLA	O1D-CGD-O2D-CED
32	A	405	CLA	CBA-CGA-O2A-C1
32	Rr	608	CLA	CBA-CGA-O2A-C1
32	Rr	611	CLA	CBA-CGA-O2A-C1
32	Rr	613	CLA	CBA-CGA-O2A-C1
32	Ss	602	CLA	CBA-CGA-O2A-C1
32	Ss	611	CLA	CBA-CGA-O2A-C1
32	Ss	613	CLA	CBA-CGA-O2A-C1
32	Yy	610	CLA	CBA-CGA-O2A-C1
32	N	611	CLA	CBA-CGA-O2A-C1
32	Y	603	CLA	CBA-CGA-O2A-C1
32	Y	612	CLA	CBA-CGA-O2A-C1
32	a	405	CLA	CBA-CGA-O2A-C1
32	b	603	CLA	CBA-CGA-O2A-C1
32	b	612	CLA	CBA-CGA-O2A-C1
32	b	613	CLA	CBA-CGA-O2A-C1
32	c	512	CLA	CBA-CGA-O2A-C1
32	r	611	CLA	CBA-CGA-O2A-C1
32	s	608	CLA	CBA-CGA-O2A-C1
32	s	611	CLA	CBA-CGA-O2A-C1
32	y	312	CLA	CBA-CGA-O2A-C1
32	AA	405	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	AA	406	CLA	CBA-CGA-O2A-C1
32	BB	603	CLA	CBA-CGA-O2A-C1
32	BB	607	CLA	CBA-CGA-O2A-C1
32	BB	609	CLA	CBA-CGA-O2A-C1
32	BB	612	CLA	CBA-CGA-O2A-C1
32	B	605	CLA	CBA-CGA-O2A-C1
32	B	620	CLA	CBA-CGA-O2A-C1
32	GG	603	CLA	CBA-CGA-O2A-C1
32	GG	611	CLA	CBA-CGA-O2A-C1
32	NN	611	CLA	CBA-CGA-O2A-C1
32	RR	310	CLA	CBA-CGA-O2A-C1
32	YY	603	CLA	CBA-CGA-O2A-C1
32	Bb	603	CLA	CBA-CGA-O2A-C1
32	Bb	609	CLA	CBA-CGA-O2A-C1
32	Bb	612	CLA	CBA-CGA-O2A-C1
32	Bb	613	CLA	CBA-CGA-O2A-C1
32	Cc	503	CLA	CBA-CGA-O2A-C1
32	Cc	514	CLA	CBA-CGA-O2A-C1
32	Gg	304	CLA	CBA-CGA-O2A-C1
32	Nn	305	CLA	CBA-CGA-O2A-C1
32	Nn	313	CLA	CBA-CGA-O2A-C1
33	A	407	PHO	CBA-CGA-O2A-C1
33	AA	407	PHO	CBA-CGA-O2A-C1
39	Ss	601	CHL	CBA-CGA-O2A-C1
39	R	606	CHL	CBA-CGA-O2A-C1
39	n	607	CHL	CBA-CGA-O2A-C1
39	n	609	CHL	CBA-CGA-O2A-C1
39	RR	306	CHL	CBA-CGA-O2A-C1
39	Nn	319	CHL	CBA-CGA-O2A-C1
36	44	614	LHG	O9-C7-O7-C5
35	A	410	PL9	C7-C8-C9-C10
35	D	407	PL9	C7-C8-C9-C10
35	D	407	PL9	C22-C23-C24-C25
35	d	404	PL9	C32-C33-C34-C35
35	AA	410	PL9	C7-C8-C9-C10
35	AA	410	PL9	C12-C13-C14-C15
35	AA	410	PL9	C42-C43-C44-C45
35	DD	406	PL9	C12-C13-C14-C15
35	Dd	404	PL9	C32-C33-C34-C35
35	A	410	PL9	C22-C23-C24-C26
35	A	410	PL9	C37-C38-C39-C41
35	D	407	PL9	C37-C38-C39-C41

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Mol	Chain	Res	Type	Atoms
35	d	404	PL9	C12-C13-C14-C16
35	d	404	PL9	C17-C18-C19-C21
35	AA	410	PL9	C17-C18-C19-C21
35	AA	410	PL9	C32-C33-C34-C36
35	AA	410	PL9	C37-C38-C39-C41
35	DD	406	PL9	C17-C18-C19-C21
35	Dd	404	PL9	C17-C18-C19-C21
32	A	406	CLA	O1A-CGA-O2A-C1
32	Ss	604	CLA	O1A-CGA-O2A-C1
32	G	610	CLA	O1A-CGA-O2A-C1
32	R	610	CLA	O1A-CGA-O2A-C1
32	Y	603	CLA	O1A-CGA-O2A-C1
32	a	410	CLA	O1A-CGA-O2A-C1
32	b	616	CLA	O1A-CGA-O2A-C1
32	n	603	CLA	O1A-CGA-O2A-C1
32	n	604	CLA	O1A-CGA-O2A-C1
32	r	608	CLA	O1A-CGA-O2A-C1
32	s	604	CLA	O1A-CGA-O2A-C1
32	s	609	CLA	O1A-CGA-O2A-C1
32	CC	504	CLA	O1A-CGA-O2A-C1
32	RR	310	CLA	O1A-CGA-O2A-C1
32	Aa	410	CLA	O1A-CGA-O2A-C1
32	Bb	608	CLA	O1A-CGA-O2A-C1
32	Bb	616	CLA	O1A-CGA-O2A-C1
32	Nn	305	CLA	O1A-CGA-O2A-C1
32	Nn	313	CLA	O1A-CGA-O2A-C1
32	Nn	314	CLA	O1A-CGA-O2A-C1
33	a	408	PHO	O1A-CGA-O2A-C1
33	Aa	408	PHO	O1A-CGA-O2A-C1
37	LL	102	SQD	O10-C23-O48-C46
39	G	601	CHL	O1A-CGA-O2A-C1
39	n	608	CHL	O1A-CGA-O2A-C1
32	Rr	604	CLA	O1D-CGD-O2D-CED
32	Ss	603	CLA	O1D-CGD-O2D-CED
32	1	602	CLA	O1D-CGD-O2D-CED
32	y	313	CLA	O1D-CGD-O2D-CED
32	Ss	609	CLA	O1D-CGD-O2D-CED
32	BB	604	CLA	O1D-CGD-O2D-CED
32	BB	605	CLA	O1D-CGD-O2D-CED
39	G	601	CHL	O1D-CGD-O2D-CED
35	d	404	PL9	C47-C48-C49-C50
32	C	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	n	610	CLA	C3-C5-C6-C7
32	CC	503	CLA	C3-C5-C6-C7
32	Bb	603	CLA	C3-C5-C6-C7
33	DD	402	PHO	C3-C5-C6-C7
39	NN	607	CHL	C3-C5-C6-C7
32	Ss	602	CLA	CBD-CGD-O2D-CED
32	11	612	CLA	CBD-CGD-O2D-CED
32	y	304	CLA	CBD-CGD-O2D-CED
32	Cc	503	CLA	CBD-CGD-O2D-CED
32	Nn	304	CLA	CBD-CGD-O2D-CED
39	N	609	CHL	CBD-CGD-O2D-CED
39	Y	605	CHL	CBD-CGD-O2D-CED
39	NN	609	CHL	CBD-CGD-O2D-CED
36	K	101	LHG	O2-C2-C3-O3
36	g	618	LHG	O2-C2-C3-O3
36	y	320	LHG	O2-C2-C3-O3
36	KK	101	LHG	O2-C2-C3-O3
32	Ss	613	CLA	O1D-CGD-O2D-CED
32	b	615	CLA	O1D-CGD-O2D-CED
32	s	603	CLA	O1D-CGD-O2D-CED
32	B	604	CLA	O1D-CGD-O2D-CED
32	GG	610	CLA	O1D-CGD-O2D-CED
32	NN	604	CLA	O1D-CGD-O2D-CED
33	A	407	PHO	O1D-CGD-O2D-CED
39	Ss	607	CHL	O1D-CGD-O2D-CED
39	3	608	CHL	O1D-CGD-O2D-CED
39	y	307	CHL	O1D-CGD-O2D-CED
32	A	406	CLA	CBA-CGA-O2A-C1
32	Ss	604	CLA	CBA-CGA-O2A-C1
32	Yy	602	CLA	CBA-CGA-O2A-C1
32	C	508	CLA	CBA-CGA-O2A-C1
32	G	610	CLA	CBA-CGA-O2A-C1
32	R	608	CLA	CBA-CGA-O2A-C1
32	Y	614	CLA	CBA-CGA-O2A-C1
32	a	410	CLA	CBA-CGA-O2A-C1
32	b	608	CLA	CBA-CGA-O2A-C1
32	b	609	CLA	CBA-CGA-O2A-C1
32	b	616	CLA	CBA-CGA-O2A-C1
32	c	506	CLA	CBA-CGA-O2A-C1
32	c	510	CLA	CBA-CGA-O2A-C1
32	n	604	CLA	CBA-CGA-O2A-C1
32	n	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	r	602	CLA	CBA-CGA-O2A-C1
32	s	602	CLA	CBA-CGA-O2A-C1
32	CC	506	CLA	CBA-CGA-O2A-C1
32	CC	507	CLA	CBA-CGA-O2A-C1
32	RR	308	CLA	CBA-CGA-O2A-C1
32	YY	612	CLA	CBA-CGA-O2A-C1
32	YY	614	CLA	CBA-CGA-O2A-C1
32	Aa	410	CLA	CBA-CGA-O2A-C1
32	Cc	508	CLA	CBA-CGA-O2A-C1
32	Nn	314	CLA	CBA-CGA-O2A-C1
39	Ss	607	CHL	CBA-CGA-O2A-C1
39	Yy	605	CHL	CBA-CGA-O2A-C1
39	G	601	CHL	CBA-CGA-O2A-C1
39	n	608	CHL	CBA-CGA-O2A-C1
39	s	607	CHL	CBA-CGA-O2A-C1
39	y	307	CHL	CBA-CGA-O2A-C1
39	GG	601	CHL	CBA-CGA-O2A-C1
32	Yy	602	CLA	O1A-CGA-O2A-C1
32	C	508	CLA	O1A-CGA-O2A-C1
32	G	611	CLA	O1A-CGA-O2A-C1
32	a	405	CLA	O1A-CGA-O2A-C1
32	b	608	CLA	O1A-CGA-O2A-C1
32	c	501	CLA	O1A-CGA-O2A-C1
32	c	512	CLA	O1A-CGA-O2A-C1
32	CC	507	CLA	O1A-CGA-O2A-C1
32	B	608	CLA	O1A-CGA-O2A-C1
33	A	407	PHO	O1A-CGA-O2A-C1
33	AA	407	PHO	O1A-CGA-O2A-C1
39	GG	601	CHL	O1A-CGA-O2A-C1
38	Dd	408	LMG	C4-C5-C6-O5
44	C	523	DGD	C4E-C5E-C6E-O5E
32	n	611	CLA	O1D-CGD-O2D-CED
32	r	613	CLA	CBD-CGD-O2D-CED
32	s	609	CLA	CBD-CGD-O2D-CED
32	B	624	CLA	CBD-CGD-O2D-CED
33	DD	402	PHO	CBD-CGD-O2D-CED
39	Yy	606	CHL	CBD-CGD-O2D-CED
39	R	607	CHL	CBD-CGD-O2D-CED
36	g	618	LHG	C8-C7-O7-C5
36	KK	101	LHG	C8-C7-O7-C5
38	a	412	LMG	C11-C10-O7-C8
38	Aa	412	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
44	BB	624	DGD	C2B-C1B-O2G-C2G
32	Gg	304	CLA	O1D-CGD-O2D-CED
32	BB	609	CLA	O1A-CGA-O2A-C1
32	GG	611	CLA	O1A-CGA-O2A-C1
43	RR	301	LMU	O5'-C5'-C6'-O6'
32	Y	610	CLA	O1D-CGD-O2D-CED
32	b	602	CLA	O1D-CGD-O2D-CED
32	BB	608	CLA	O1D-CGD-O2D-CED
39	11	608	CHL	O1D-CGD-O2D-CED
39	22	607	CHL	O1D-CGD-O2D-CED
32	Y	612	CLA	C3-C5-C6-C7
32	b	603	CLA	C3-C5-C6-C7
32	Bb	615	CLA	C3-C5-C6-C7
32	Yy	613	CLA	CBD-CGD-O2D-CED
32	Y	614	CLA	CBD-CGD-O2D-CED
32	d	401	CLA	CBD-CGD-O2D-CED
32	4	311	CLA	CBD-CGD-O2D-CED
39	Rr	605	CHL	CBD-CGD-O2D-CED
39	N	601	CHL	CBD-CGD-O2D-CED
39	4	309	CHL	CBD-CGD-O2D-CED
39	YY	609	CHL	CBD-CGD-O2D-CED
32	33	602	CLA	O1D-CGD-O2D-CED
32	D	401	CLA	O1D-CGD-O2D-CED
32	r	612	CLA	O1D-CGD-O2D-CED
32	s	608	CLA	O1D-CGD-O2D-CED
32	CC	512	CLA	O1D-CGD-O2D-CED
32	B	621	CLA	O1D-CGD-O2D-CED
39	11	605	CHL	O1D-CGD-O2D-CED
32	R	610	CLA	CBA-CGA-O2A-C1
32	c	509	CLA	CBA-CGA-O2A-C1
32	r	608	CLA	CBA-CGA-O2A-C1
32	s	604	CLA	CBA-CGA-O2A-C1
32	s	609	CLA	CBA-CGA-O2A-C1
32	y	304	CLA	CBA-CGA-O2A-C1
32	Bb	608	CLA	CBA-CGA-O2A-C1
32	Bb	616	CLA	CBA-CGA-O2A-C1
33	a	408	PHO	CBA-CGA-O2A-C1
33	Aa	408	PHO	CBA-CGA-O2A-C1
35	D	407	PL9	C13-C14-C16-C17
35	DD	406	PL9	C13-C14-C16-C17
32	Y	612	CLA	O1A-CGA-O2A-C1
32	b	609	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	c	506	CLA	O1A-CGA-O2A-C1
32	c	510	CLA	O1A-CGA-O2A-C1
32	r	602	CLA	O1A-CGA-O2A-C1
32	AA	406	CLA	O1A-CGA-O2A-C1
32	BB	603	CLA	O1A-CGA-O2A-C1
32	BB	612	CLA	O1A-CGA-O2A-C1
32	B	605	CLA	O1A-CGA-O2A-C1
32	YY	603	CLA	O1A-CGA-O2A-C1
32	Cc	514	CLA	O1A-CGA-O2A-C1
39	s	607	CHL	O1A-CGA-O2A-C1
36	KK	101	LHG	O9-C7-O7-C5
35	A	410	PL9	C14-C16-C17-C18
35	A	410	PL9	C34-C36-C37-C38
35	A	410	PL9	C39-C41-C42-C43
35	D	407	PL9	C14-C16-C17-C18
35	AA	410	PL9	C9-C11-C12-C13
35	DD	406	PL9	C14-C16-C17-C18
35	DD	406	PL9	C44-C46-C47-C48
35	Dd	404	PL9	C19-C21-C22-C23
43	RR	301	LMU	C4'-C5'-C6'-O6'
32	22	609	CLA	CBD-CGD-O2D-CED
32	Y	602	CLA	CBD-CGD-O2D-CED
32	n	604	CLA	CBD-CGD-O2D-CED
39	1	608	CHL	CBD-CGD-O2D-CED
44	CC	522	DGD	O6D-C5D-C6D-O5D
46	Ee	101	HEM	C3D-CAD-CBD-CGD
32	B	605	CLA	C2A-CAA-CBA-CGA
32	Cc	503	CLA	C2A-CAA-CBA-CGA
32	B	607	CLA	O1D-CGD-O2D-CED
32	R	608	CLA	O1A-CGA-O2A-C1
32	Y	614	CLA	O1A-CGA-O2A-C1
32	c	509	CLA	O1A-CGA-O2A-C1
32	n	612	CLA	O1A-CGA-O2A-C1
32	CC	506	CLA	O1A-CGA-O2A-C1
32	B	620	CLA	O1A-CGA-O2A-C1
32	YY	614	CLA	O1A-CGA-O2A-C1
32	Bb	609	CLA	O1A-CGA-O2A-C1
32	Cc	508	CLA	O1A-CGA-O2A-C1
32	Gg	304	CLA	O1A-CGA-O2A-C1
39	n	607	CHL	O1A-CGA-O2A-C1
39	y	307	CHL	O1A-CGA-O2A-C1
37	L	102	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
37	LL	101	SQD	O5-C1-O6-C44
32	Yy	611	CLA	O1D-CGD-O2D-CED
32	C	513	CLA	O1D-CGD-O2D-CED
32	C	503	CLA	CBA-CGA-O2A-C1
32	g	603	CLA	CBA-CGA-O2A-C1
32	g	614	CLA	CBA-CGA-O2A-C1
32	Cc	505	CLA	CBA-CGA-O2A-C1
32	Cc	511	CLA	CBA-CGA-O2A-C1
32	Gg	311	CLA	CBA-CGA-O2A-C1
32	Gg	315	CLA	CBA-CGA-O2A-C1
39	g	601	CHL	CBA-CGA-O2A-C1
32	Rr	613	CLA	CBD-CGD-O2D-CED
32	2	609	CLA	CBD-CGD-O2D-CED
32	R	614	CLA	CBD-CGD-O2D-CED
32	c	507	CLA	CBD-CGD-O2D-CED
32	n	613	CLA	CBD-CGD-O2D-CED
32	BB	607	CLA	CBD-CGD-O2D-CED
32	CC	505	CLA	CBD-CGD-O2D-CED
32	B	623	CLA	CBD-CGD-O2D-CED
32	YY	604	CLA	CBD-CGD-O2D-CED
32	YY	614	CLA	CBD-CGD-O2D-CED
32	Bb	612	CLA	CBD-CGD-O2D-CED
32	Dd	402	CLA	CBD-CGD-O2D-CED
33	a	409	PHO	CBD-CGD-O2D-CED
33	Aa	409	PHO	CBD-CGD-O2D-CED
39	1	606	CHL	CBD-CGD-O2D-CED
39	N	605	CHL	CBD-CGD-O2D-CED
39	s	607	CHL	CBD-CGD-O2D-CED
39	y	309	CHL	CBD-CGD-O2D-CED
32	s	602	CLA	O1A-CGA-O2A-C1
32	RR	308	CLA	O1A-CGA-O2A-C1
39	Yy	605	CHL	O1A-CGA-O2A-C1
32	Ss	608	CLA	O1D-CGD-O2D-CED
32	33	613	CLA	O1D-CGD-O2D-CED
32	3	603	CLA	O1D-CGD-O2D-CED
39	Ss	605	CHL	O1D-CGD-O2D-CED
32	b	604	CLA	CBD-CGD-O2D-CED
32	b	606	CLA	CBD-CGD-O2D-CED
39	11	606	CHL	CBD-CGD-O2D-CED
32	Bb	615	CLA	O1D-CGD-O2D-CED
32	g	603	CLA	O1A-CGA-O2A-C1
32	g	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	n	602	CLA	O1A-CGA-O2A-C1
32	Cc	505	CLA	O1A-CGA-O2A-C1
32	Cc	511	CLA	O1A-CGA-O2A-C1
32	Gg	315	CLA	O1A-CGA-O2A-C1
39	g	601	CHL	O1A-CGA-O2A-C1
36	g	618	LHG	O9-C7-O7-C5
36	K	101	LHG	C1-C2-C3-O3
36	KK	101	LHG	C1-C2-C3-O3
32	Rr	610	CLA	CBA-CGA-O2A-C1
32	Yy	603	CLA	CBA-CGA-O2A-C1
32	Yy	612	CLA	CBA-CGA-O2A-C1
32	Yy	614	CLA	CBA-CGA-O2A-C1
32	C	505	CLA	CBA-CGA-O2A-C1
32	C	506	CLA	CBA-CGA-O2A-C1
32	C	507	CLA	CBA-CGA-O2A-C1
32	D	405	CLA	CBA-CGA-O2A-C1
32	N	613	CLA	CBA-CGA-O2A-C1
32	R	602	CLA	CBA-CGA-O2A-C1
32	S	604	CLA	CBA-CGA-O2A-C1
32	S	610	CLA	CBA-CGA-O2A-C1
32	a	406	CLA	CBA-CGA-O2A-C1
32	b	610	CLA	CBA-CGA-O2A-C1
32	c	502	CLA	CBA-CGA-O2A-C1
32	c	505	CLA	CBA-CGA-O2A-C1
32	g	612	CLA	CBA-CGA-O2A-C1
32	n	602	CLA	CBA-CGA-O2A-C1
32	n	613	CLA	CBA-CGA-O2A-C1
32	r	610	CLA	CBA-CGA-O2A-C1
32	y	314	CLA	CBA-CGA-O2A-C1
32	y	316	CLA	CBA-CGA-O2A-C1
32	BB	602	CLA	CBA-CGA-O2A-C1
32	BB	605	CLA	CBA-CGA-O2A-C1
32	BB	614	CLA	CBA-CGA-O2A-C1
32	CC	502	CLA	CBA-CGA-O2A-C1
32	CC	505	CLA	CBA-CGA-O2A-C1
32	B	610	CLA	CBA-CGA-O2A-C1
32	B	619	CLA	CBA-CGA-O2A-C1
32	B	622	CLA	CBA-CGA-O2A-C1
32	GG	610	CLA	CBA-CGA-O2A-C1
32	NN	613	CLA	CBA-CGA-O2A-C1
32	RR	302	CLA	CBA-CGA-O2A-C1
32	SS	305	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	SS	311	CLA	CBA-CGA-O2A-C1
32	Aa	405	CLA	CBA-CGA-O2A-C1
32	Aa	406	CLA	CBA-CGA-O2A-C1
32	Bb	610	CLA	CBA-CGA-O2A-C1
32	Cc	507	CLA	CBA-CGA-O2A-C1
32	Cc	512	CLA	CBA-CGA-O2A-C1
32	Dd	402	CLA	CBA-CGA-O2A-C1
32	Nn	303	CLA	CBA-CGA-O2A-C1
32	Nn	304	CLA	CBA-CGA-O2A-C1
32	Nn	312	CLA	CBA-CGA-O2A-C1
39	Rr	606	CHL	CBA-CGA-O2A-C1
39	Rr	607	CHL	CBA-CGA-O2A-C1
39	Yy	609	CHL	CBA-CGA-O2A-C1
39	R	605	CHL	CBA-CGA-O2A-C1
39	S	601	CHL	CBA-CGA-O2A-C1
39	Y	608	CHL	CBA-CGA-O2A-C1
39	Y	609	CHL	CBA-CGA-O2A-C1
39	r	607	CHL	CBA-CGA-O2A-C1
39	s	601	CHL	CBA-CGA-O2A-C1
39	y	311	CHL	CBA-CGA-O2A-C1
39	RR	305	CHL	CBA-CGA-O2A-C1
39	YY	608	CHL	CBA-CGA-O2A-C1
39	YY	609	CHL	CBA-CGA-O2A-C1
39	Gg	302	CHL	CBA-CGA-O2A-C1
39	1	605	CHL	CBD-CGD-O2D-CED
39	Y	609	CHL	CBD-CGD-O2D-CED
39	YY	605	CHL	CBD-CGD-O2D-CED
32	33	611	CLA	O1D-CGD-O2D-CED
32	BB	613	CLA	O1D-CGD-O2D-CED
32	CC	504	CLA	O1D-CGD-O2D-CED
32	B	609	CLA	O1D-CGD-O2D-CED
32	Bb	602	CLA	O1D-CGD-O2D-CED
32	Cc	510	CLA	O1D-CGD-O2D-CED
32	Nn	302	CLA	O1D-CGD-O2D-CED
39	Yy	605	CHL	O1D-CGD-O2D-CED
32	S	604	CLA	O1A-CGA-O2A-C1
32	DD	401	CLA	O1D-CGD-O2D-CED
35	D	407	PL9	C12-C11-C9-C10
35	D	407	PL9	C33-C34-C36-C37
35	d	404	PL9	C12-C11-C9-C8
35	d	404	PL9	C13-C14-C16-C17
35	Dd	404	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
39	NN	606	CHL	CBD-CGD-O2D-CED
32	C	511	CLA	C11-C12-C13-C14
32	Y	612	CLA	C6-C7-C8-C9
32	b	610	CLA	C6-C7-C8-C9
32	y	314	CLA	C11-C10-C8-C9
32	CC	510	CLA	C11-C12-C13-C14
32	Bb	610	CLA	C6-C7-C8-C9
32	Cc	503	CLA	C6-C7-C8-C9
32	2	602	CLA	O1D-CGD-O2D-CED
32	Y	611	CLA	O1D-CGD-O2D-CED
32	BB	603	CLA	O1D-CGD-O2D-CED
32	SS	309	CLA	O1D-CGD-O2D-CED
39	r	605	CHL	O1D-CGD-O2D-CED
36	BB	622	LHG	O2-C2-C3-O3
32	Rr	601	CLA	O1D-CGD-O2D-CED
32	3	609	CLA	O1D-CGD-O2D-CED
32	S	602	CLA	O1D-CGD-O2D-CED
32	c	501	CLA	O1D-CGD-O2D-CED
32	c	508	CLA	O1D-CGD-O2D-CED
39	YY	606	CHL	O1D-CGD-O2D-CED
32	Yy	603	CLA	O1A-CGA-O2A-C1
32	Yy	612	CLA	O1A-CGA-O2A-C1
32	B	619	CLA	O1A-CGA-O2A-C1
32	Aa	406	CLA	O1A-CGA-O2A-C1
32	Cc	507	CLA	O1A-CGA-O2A-C1
32	Nn	312	CLA	O1A-CGA-O2A-C1
32	BB	606	CLA	CBD-CGD-O2D-CED
32	RR	314	CLA	CBD-CGD-O2D-CED
32	N	602	CLA	O1D-CGD-O2D-CED
32	S	610	CLA	O1D-CGD-O2D-CED
32	g	602	CLA	O1D-CGD-O2D-CED
32	B	619	CLA	O1D-CGD-O2D-CED
32	NN	602	CLA	O1D-CGD-O2D-CED
34	c	514	BCR	C7-C8-C9-C34
34	Cc	516	BCR	C7-C8-C9-C34
34	Hh	101	BCR	C7-C8-C9-C34
41	G	617	XAT	C27-C28-C29-C39
41	GG	617	XAT	C27-C28-C29-C39
44	C	523	DGD	O6E-C5E-C6E-O5E
34	A	409	BCR	C21-C22-C23-C24
34	k	101	BCR	C7-C8-C9-C10
34	AA	409	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
41	G	617	XAT	C27-C28-C29-C30
41	GG	617	XAT	C27-C28-C29-C30
32	s	602	CLA	C2A-CAA-CBA-CGA
32	BB	609	CLA	C2A-CAA-CBA-CGA
39	Ss	605	CHL	C2A-CAA-CBA-CGA
36	l	101	LHG	C23-C24-C25-C26
32	C	505	CLA	O1A-CGA-O2A-C1
32	C	507	CLA	O1A-CGA-O2A-C1
32	R	602	CLA	O1A-CGA-O2A-C1
32	c	505	CLA	O1A-CGA-O2A-C1
32	BB	602	CLA	O1A-CGA-O2A-C1
32	CC	505	CLA	O1A-CGA-O2A-C1
32	GG	610	CLA	O1A-CGA-O2A-C1
32	SS	305	CLA	O1A-CGA-O2A-C1
32	Cc	512	CLA	O1A-CGA-O2A-C1
39	Rr	606	CHL	O1A-CGA-O2A-C1
39	R	605	CHL	O1A-CGA-O2A-C1
39	Y	608	CHL	O1A-CGA-O2A-C1
39	r	607	CHL	O1A-CGA-O2A-C1
39	RR	305	CHL	O1A-CGA-O2A-C1
39	Gg	302	CHL	O1A-CGA-O2A-C1
39	YY	601	CHL	C5-C6-C7-C8
32	D	404	CLA	C4C-C3C-CAC-CBC
32	Bb	608	CLA	CBD-CGD-O2D-CED
36	3	614	LHG	C8-C7-O7-C5
36	Gg	319	LHG	C8-C7-O7-C5
37	BB	621	SQD	C8-C7-O47-C45
44	B	601	DGD	C2B-C1B-O2G-C2G
32	Rr	612	CLA	CBA-CGA-O2A-C1
32	N	602	CLA	CBA-CGA-O2A-C1
32	NN	602	CLA	CBA-CGA-O2A-C1
36	N	619	LHG	C24-C23-O8-C6
32	Ss	611	CLA	C2-C1-O2A-CGA
32	s	611	CLA	C2-C1-O2A-CGA
32	CC	502	CLA	O1A-CGA-O2A-C1
32	s	602	CLA	O1D-CGD-O2D-CED
32	B	610	CLA	O1D-CGD-O2D-CED
32	B	620	CLA	O1D-CGD-O2D-CED
32	YY	602	CLA	O1D-CGD-O2D-CED
33	AA	407	PHO	O1D-CGD-O2D-CED
39	s	605	CHL	O1D-CGD-O2D-CED
39	y	308	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	NN	605	CHL	O1D-CGD-O2D-CED
32	Y	602	CLA	C8-C10-C11-C12
32	b	612	CLA	C13-C15-C16-C17
32	g	603	CLA	C10-C11-C12-C13
32	r	609	CLA	C8-C10-C11-C12
32	BB	605	CLA	C5-C6-C7-C8
32	BB	614	CLA	C10-C11-C12-C13
32	B	610	CLA	C10-C11-C12-C13
32	NN	610	CLA	C5-C6-C7-C8
32	Gg	304	CLA	C10-C11-C12-C13
39	YY	601	CHL	C8-C10-C11-C12
32	DD	403	CLA	C4C-C3C-CAC-CBC
44	D	411	DGD	C1A-C2A-C3A-C4A
44	BB	623	DGD	C1A-C2A-C3A-C4A
32	33	603	CLA	O1D-CGD-O2D-CED
32	3	611	CLA	O1D-CGD-O2D-CED
32	Y	604	CLA	O1D-CGD-O2D-CED
32	Gg	315	CLA	O1D-CGD-O2D-CED
32	N	613	CLA	O1A-CGA-O2A-C1
32	a	406	CLA	O1A-CGA-O2A-C1
32	BB	614	CLA	O1A-CGA-O2A-C1
32	Bb	610	CLA	O1A-CGA-O2A-C1
32	44	602	CLA	CBD-CGD-O2D-CED
32	N	611	CLA	CBD-CGD-O2D-CED
32	Cc	509	CLA	CBD-CGD-O2D-CED
39	3	605	CHL	CBD-CGD-O2D-CED
36	NN	619	LHG	C24-C23-O8-C6
39	SS	302	CHL	CBA-CGA-O2A-C1
36	AA	414	LHG	C7-C8-C9-C10
36	II	101	LHG	C7-C8-C9-C10
36	Ll	102	LHG	C7-C8-C9-C10
38	a	412	LMG	O9-C10-O7-C8
38	Aa	412	LMG	O9-C10-O7-C8
44	BB	624	DGD	O1B-C1B-O2G-C2G
35	A	410	PL9	C29-C31-C32-C33
35	D	407	PL9	C29-C31-C32-C33
32	Cc	504	CLA	C15-C16-C17-C18
36	C	522	LHG	C7-C8-C9-C10
36	CC	521	LHG	C7-C8-C9-C10
38	b	621	LMG	C10-C11-C12-C13
32	Yy	614	CLA	O1A-CGA-O2A-C1
32	g	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	r	610	CLA	O1A-CGA-O2A-C1
32	BB	605	CLA	O1A-CGA-O2A-C1
32	B	622	CLA	O1A-CGA-O2A-C1
32	RR	302	CLA	O1A-CGA-O2A-C1
32	Aa	405	CLA	O1A-CGA-O2A-C1
32	Dd	402	CLA	O1A-CGA-O2A-C1
32	Gg	311	CLA	O1A-CGA-O2A-C1
39	S	601	CHL	O1A-CGA-O2A-C1
39	Y	609	CHL	O1A-CGA-O2A-C1
39	YY	608	CHL	O1A-CGA-O2A-C1
39	YY	609	CHL	O1A-CGA-O2A-C1
37	B	617	SQD	C8-C7-O47-C45
38	C	521	LMG	C11-C10-O7-C8
32	22	613	CLA	O1D-CGD-O2D-CED
32	3	613	CLA	O1D-CGD-O2D-CED
32	C	512	CLA	O1D-CGD-O2D-CED
32	N	610	CLA	C5-C6-C7-C8
32	b	615	CLA	C10-C11-C12-C13
32	c	503	CLA	C10-C11-C12-C13
32	y	312	CLA	C15-C16-C17-C18
32	y	315	CLA	C8-C10-C11-C12
32	BB	606	CLA	C5-C6-C7-C8
32	BB	610	CLA	C10-C11-C12-C13
32	CC	502	CLA	C5-C6-C7-C8
32	B	604	CLA	C5-C6-C7-C8
32	B	606	CLA	C10-C11-C12-C13
32	YY	602	CLA	C8-C10-C11-C12
32	Bb	603	CLA	C5-C6-C7-C8
32	Bb	615	CLA	C10-C11-C12-C13
32	Cc	512	CLA	C5-C6-C7-C8
39	G	601	CHL	C5-C6-C7-C8
39	n	607	CHL	C15-C16-C17-C18
32	Rr	601	CLA	C2A-CAA-CBA-CGA
32	Rr	608	CLA	C2A-CAA-CBA-CGA
32	Ss	610	CLA	C2A-CAA-CBA-CGA
32	44	611	CLA	C2A-CAA-CBA-CGA
32	D	404	CLA	C2A-CAA-CBA-CGA
32	R	604	CLA	C2A-CAA-CBA-CGA
32	b	606	CLA	C2A-CAA-CBA-CGA
32	b	616	CLA	C2A-CAA-CBA-CGA
32	g	611	CLA	C2A-CAA-CBA-CGA
32	r	601	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	r	604	CLA	C2A-CAA-CBA-CGA
32	s	610	CLA	C2A-CAA-CBA-CGA
32	y	306	CLA	C2A-CAA-CBA-CGA
32	4	312	CLA	C2A-CAA-CBA-CGA
32	BB	605	CLA	C2A-CAA-CBA-CGA
32	DD	403	CLA	C2A-CAA-CBA-CGA
32	B	622	CLA	C2A-CAA-CBA-CGA
32	RR	304	CLA	C2A-CAA-CBA-CGA
32	YY	604	CLA	C2A-CAA-CBA-CGA
32	Bb	606	CLA	C2A-CAA-CBA-CGA
32	Bb	616	CLA	C2A-CAA-CBA-CGA
39	N	607	CHL	C2A-CAA-CBA-CGA
39	S	601	CHL	C2A-CAA-CBA-CGA
39	n	607	CHL	C2A-CAA-CBA-CGA
39	n	608	CHL	C2A-CAA-CBA-CGA
39	NN	607	CHL	C2A-CAA-CBA-CGA
39	SS	302	CHL	C2A-CAA-CBA-CGA
32	11	612	CLA	O1D-CGD-O2D-CED
32	C	506	CLA	O1D-CGD-O2D-CED
32	r	603	CLA	O1D-CGD-O2D-CED
32	Rr	609	CLA	C8-C10-C11-C12
32	Y	612	CLA	C8-C10-C11-C12
32	b	611	CLA	C15-C16-C17-C18
32	Bb	612	CLA	C13-C15-C16-C17
32	Cc	503	CLA	C5-C6-C7-C8
32	Cc	505	CLA	C10-C11-C12-C13
39	Yy	609	CHL	C5-C6-C7-C8
39	y	303	CHL	C10-C11-C12-C13
39	y	303	CHL	C13-C15-C16-C17
39	Nn	317	CHL	C15-C16-C17-C18
38	Bb	621	LMG	C10-C11-C12-C13
44	C	523	DGD	C1A-C2A-C3A-C4A
32	BB	614	CLA	O1D-CGD-O2D-CED
32	Rr	610	CLA	O1A-CGA-O2A-C1
32	D	405	CLA	O1A-CGA-O2A-C1
32	S	610	CLA	O1A-CGA-O2A-C1
32	c	502	CLA	O1A-CGA-O2A-C1
32	n	613	CLA	O1A-CGA-O2A-C1
32	y	314	CLA	O1A-CGA-O2A-C1
32	y	316	CLA	O1A-CGA-O2A-C1
32	B	610	CLA	O1A-CGA-O2A-C1
32	NN	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	SS	311	CLA	O1A-CGA-O2A-C1
32	Nn	303	CLA	O1A-CGA-O2A-C1
39	Rr	607	CHL	O1A-CGA-O2A-C1
39	Yy	609	CHL	O1A-CGA-O2A-C1
39	s	601	CHL	O1A-CGA-O2A-C1
39	y	311	CHL	O1A-CGA-O2A-C1
32	b	613	CLA	C3-C5-C6-C7
38	Aa	412	LMG	O6-C1-O1-C7
43	KK	102	LMU	O5'-C1'-O1'-C1
32	Yy	610	CLA	C15-C16-C17-C18
32	Yy	613	CLA	C8-C10-C11-C12
32	BB	608	CLA	C5-C6-C7-C8
32	B	623	CLA	C5-C6-C7-C8
32	Aa	406	CLA	C13-C15-C16-C17
32	Bb	611	CLA	C15-C16-C17-C18
39	Yy	601	CHL	C13-C15-C16-C17
39	N	607	CHL	C10-C11-C12-C13
39	Y	601	CHL	C5-C6-C7-C8
39	Y	601	CHL	C8-C10-C11-C12
39	n	607	CHL	C10-C11-C12-C13
36	1	614	LHG	O2-C2-C3-O3
32	Cc	505	CLA	O1D-CGD-O2D-CED
32	Bb	614	CLA	CBA-CGA-O2A-C1
39	r	606	CHL	CBA-CGA-O2A-C1
44	Cc	520	DGD	C4D-C5D-C6D-O5D
32	C	503	CLA	O1A-CGA-O2A-C1
32	C	506	CLA	O1A-CGA-O2A-C1
32	b	610	CLA	O1A-CGA-O2A-C1
32	Nn	304	CLA	O1A-CGA-O2A-C1
38	c	519	LMG	C4-C5-C6-O5
36	A	414	LHG	C7-C8-C9-C10
37	L	102	SQD	C7-C8-C9-C10
32	Yy	610	CLA	C5-C6-C7-C8
32	BB	614	CLA	C5-C6-C7-C8
36	Gg	319	LHG	O9-C7-O7-C5
32	Nn	304	CLA	O1D-CGD-O2D-CED
39	N	609	CHL	O1D-CGD-O2D-CED
32	b	612	CLA	O1D-CGD-O2D-CED
32	y	304	CLA	O1D-CGD-O2D-CED
32	BB	602	CLA	O1D-CGD-O2D-CED
39	NN	609	CHL	O1D-CGD-O2D-CED
32	B	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	Y	601	CHL	C13-C15-C16-C17
39	Nn	317	CHL	C10-C11-C12-C13
32	y	315	CLA	CBD-CGD-O2D-CED
32	CC	511	CLA	O1D-CGD-O2D-CED
39	Y	605	CHL	O1D-CGD-O2D-CED
39	NN	601	CHL	O1D-CGD-O2D-CED
36	4	315	LHG	O9-C7-O7-C5
32	C	512	CLA	C10-C11-C12-C13
32	b	603	CLA	C5-C6-C7-C8
32	c	510	CLA	C5-C6-C7-C8
32	c	511	CLA	C10-C11-C12-C13
32	BB	608	CLA	C15-C16-C17-C18
39	Yy	601	CHL	C10-C11-C12-C13
39	GG	601	CHL	C5-C6-C7-C8
32	S	612	CLA	CBA-CGA-O2A-C1
32	b	605	CLA	CBA-CGA-O2A-C1
32	b	614	CLA	CBA-CGA-O2A-C1
32	Bb	605	CLA	CBA-CGA-O2A-C1
39	Y	601	CHL	CBA-CGA-O2A-C1
39	s	607	CHL	O2A-C1-C2-C3
32	Aa	407	CLA	CBD-CGD-O2D-CED
32	Dd	401	CLA	CBD-CGD-O2D-CED
39	Y	606	CHL	CBD-CGD-O2D-CED
39	n	605	CHL	CBD-CGD-O2D-CED
36	l	101	LHG	C8-C7-O7-C5
32	N	602	CLA	O1A-CGA-O2A-C1
32	NN	602	CLA	O1A-CGA-O2A-C1
32	Cc	503	CLA	O1D-CGD-O2D-CED
33	DD	402	PHO	O1D-CGD-O2D-CED
39	y	311	CHL	C3-C5-C6-C7
32	Ss	602	CLA	O1D-CGD-O2D-CED
32	B	624	CLA	O1D-CGD-O2D-CED
32	C	503	CLA	C15-C16-C17-C18
32	CC	505	CLA	C15-C16-C17-C18
32	Cc	509	CLA	C10-C11-C12-C13
39	SS	302	CHL	O1A-CGA-O2A-C1
36	3	614	LHG	O9-C7-O7-C5
36	l	101	LHG	O9-C7-O7-C5
37	BB	621	SQD	O49-C7-O47-C45
37	B	617	SQD	O49-C7-O47-C45
38	C	521	LMG	O9-C10-O7-C8
44	B	601	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
36	Yy	618	LHG	C1-C2-C3-O3
36	1	614	LHG	C1-C2-C3-O3
36	y	320	LHG	C1-C2-C3-O3
32	Ss	602	CLA	C2A-CAA-CBA-CGA
39	s	605	CHL	C2A-CAA-CBA-CGA
39	YY	601	CHL	C2A-CAA-CBA-CGA
32	C	509	CLA	CBA-CGA-O2A-C1
32	C	514	CLA	CBA-CGA-O2A-C1
32	c	504	CLA	CBA-CGA-O2A-C1
32	g	610	CLA	CBA-CGA-O2A-C1
32	CC	508	CLA	CBA-CGA-O2A-C1
32	SS	303	CLA	CBA-CGA-O2A-C1
32	SS	313	CLA	CBA-CGA-O2A-C1
32	Cc	506	CLA	CBA-CGA-O2A-C1
32	Cc	510	CLA	CBA-CGA-O2A-C1
39	Ss	605	CHL	CBA-CGA-O2A-C1
39	n	605	CHL	CBA-CGA-O2A-C1
39	YY	601	CHL	CBA-CGA-O2A-C1
44	B	601	DGD	C2A-C1A-O1G-C1G
32	C	513	CLA	C15-C16-C17-C18
32	a	406	CLA	C13-C15-C16-C17
32	b	615	CLA	C5-C6-C7-C8
32	c	509	CLA	C10-C11-C12-C13
32	c	512	CLA	C15-C16-C17-C18
32	g	603	CLA	C13-C15-C16-C17
32	y	312	CLA	C5-C6-C7-C8
32	y	314	CLA	C13-C15-C16-C17
32	BB	607	CLA	C5-C6-C7-C8
32	CC	502	CLA	C15-C16-C17-C18
32	CC	506	CLA	C5-C6-C7-C8
32	B	618	CLA	C10-C11-C12-C13
32	B	624	CLA	C5-C6-C7-C8
32	Bb	609	CLA	C5-C6-C7-C8
32	Gg	304	CLA	C13-C15-C16-C17
33	a	409	PHO	C10-C11-C12-C13
39	Yy	606	CHL	O1D-CGD-O2D-CED
32	Bb	606	CLA	CBD-CGD-O2D-CED
44	c	518	DGD	C4D-C5D-C6D-O5D
32	d	401	CLA	O1D-CGD-O2D-CED
32	Yy	612	CLA	C10-C11-C12-C13
32	c	507	CLA	C10-C11-C12-C13
32	Bb	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	Cc	511	CLA	C8-C10-C11-C12
32	Nn	312	CLA	C13-C15-C16-C17
33	Aa	409	PHO	C10-C11-C12-C13
39	G	601	CHL	C15-C16-C17-C18
39	y	311	CHL	C5-C6-C7-C8
32	C	506	CLA	C15-C16-C17-C18
32	C	507	CLA	C8-C10-C11-C12
32	R	602	CLA	C15-C16-C17-C18
32	b	609	CLA	C5-C6-C7-C8
32	c	505	CLA	C13-C15-C16-C17
32	B	605	CLA	C10-C11-C12-C13
32	RR	302	CLA	C15-C16-C17-C18
32	Gg	313	CLA	CBA-CGA-O2A-C1
44	BB	624	DGD	C2A-C1A-O1G-C1G
36	J	101	LHG	O9-C7-O7-C5
32	Cc	515	CLA	C2A-CAA-CBA-CGA
36	Ll	102	LHG	C23-C24-C25-C26
35	AA	410	PL9	C25-C24-C26-C27
32	4	311	CLA	O1D-CGD-O2D-CED
32	c	502	CLA	C15-C16-C17-C18
32	Bb	615	CLA	C13-C15-C16-C17
32	Cc	507	CLA	C13-C15-C16-C17
39	YY	601	CHL	C13-C15-C16-C17
32	CC	506	CLA	C3-C5-C6-C7
36	AA	411	LHG	C8-C7-O7-C5
37	L	102	SQD	C8-C7-O47-C45
44	c	517	DGD	C2B-C1B-O2G-C2G
32	r	613	CLA	O1D-CGD-O2D-CED
32	s	609	CLA	O1D-CGD-O2D-CED
39	Rr	605	CHL	O1D-CGD-O2D-CED
39	R	607	CHL	O1D-CGD-O2D-CED
37	L	102	SQD	O49-C7-O47-C45
43	R	618	LMU	C2'-C1'-O1'-C1
43	KK	102	LMU	C2'-C1'-O1'-C1
32	Cc	508	CLA	C10-C11-C12-C13
38	m	101	LMG	C10-C11-C12-C13
44	C	519	DGD	C1B-C2B-C3B-C4B
35	d	404	PL9	C24-C26-C27-C28
35	Dd	404	PL9	C24-C26-C27-C28
32	Bb	605	CLA	C10-C11-C12-C13
32	Bb	613	CLA	C13-C15-C16-C17
32	Bb	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	Cc	505	CLA	C3-C5-C6-C7
44	Cc	519	DGD	C1B-C2B-C3B-C4B
39	N	601	CHL	O1D-CGD-O2D-CED
34	A	409	BCR	C37-C22-C23-C24
34	C	516	BCR	C7-C8-C9-C34
34	h	101	BCR	C7-C8-C9-C34
34	k	101	BCR	C7-C8-C9-C34
34	AA	409	BCR	C37-C22-C23-C24
34	CC	515	BCR	C7-C8-C9-C34
32	c	513	CLA	C2A-CAA-CBA-CGA
34	C	516	BCR	C7-C8-C9-C10
34	H	101	BCR	C21-C22-C23-C24
34	c	514	BCR	C7-C8-C9-C10
34	h	101	BCR	C7-C8-C9-C10
34	CC	515	BCR	C7-C8-C9-C10
34	Cc	516	BCR	C7-C8-C9-C10
34	Hh	101	BCR	C7-C8-C9-C10
44	c	518	DGD	O6D-C5D-C6D-O5D
44	Cc	520	DGD	O6D-C5D-C6D-O5D
32	SS	313	CLA	O1A-CGA-O2A-C1
36	N	619	LHG	O10-C23-O8-C6
32	a	405	CLA	C2A-CAA-CBA-CGA
32	CC	511	CLA	C2A-CAA-CBA-CGA
39	Yy	601	CHL	C2A-CAA-CBA-CGA
39	Y	601	CHL	C2A-CAA-CBA-CGA
39	y	303	CHL	C2A-CAA-CBA-CGA
32	AA	405	CLA	C5-C6-C7-C8
36	G	618	LHG	O1-C1-C2-C3
36	GG	618	LHG	O1-C1-C2-C3
32	Y	614	CLA	O1D-CGD-O2D-CED
32	b	607	CLA	C16-C17-C18-C20
32	B	605	CLA	C16-C17-C18-C19
32	Bb	607	CLA	C16-C17-C18-C20
39	Nn	317	CHL	C16-C17-C18-C20
32	Yy	613	CLA	O1D-CGD-O2D-CED
39	YY	609	CHL	O1D-CGD-O2D-CED
32	Rr	612	CLA	O1A-CGA-O2A-C1
36	NN	619	LHG	O10-C23-O8-C6
39	Ss	605	CHL	O1A-CGA-O2A-C1
39	r	606	CHL	O1A-CGA-O2A-C1
32	C	511	CLA	C3-C5-C6-C7
32	CC	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	b	605	CLA	C10-C11-C12-C13
39	GG	601	CHL	C15-C16-C17-C18
36	AA	411	LHG	O9-C7-O7-C5
36	Dd	407	LHG	O6-C4-C5-O7
39	4	309	CHL	O1D-CGD-O2D-CED
36	A	411	LHG	C8-C7-O7-C5
36	BB	622	LHG	C8-C7-O7-C5
36	CC	521	LHG	C8-C7-O7-C5
37	CC	501	SQD	C8-C7-O47-C45
37	LL	101	SQD	C8-C7-O47-C45
38	A	415	LMG	C11-C10-O7-C8
38	AA	415	LMG	C11-C10-O7-C8
38	CC	520	LMG	C11-C10-O7-C8
32	Cc	503	CLA	C13-C15-C16-C17
32	22	609	CLA	O1D-CGD-O2D-CED
32	n	604	CLA	O1D-CGD-O2D-CED
39	1	608	CHL	O1D-CGD-O2D-CED
36	Yy	618	LHG	C24-C23-O8-C6
32	b	615	CLA	C13-C15-C16-C17
32	Bb	610	CLA	C13-C15-C16-C17
32	CC	509	CLA	CBD-CGD-O2D-CED
32	Y	602	CLA	O1D-CGD-O2D-CED
32	BB	607	CLA	O1D-CGD-O2D-CED
39	N	605	CHL	O1D-CGD-O2D-CED
32	b	607	CLA	C16-C17-C18-C19
32	Bb	607	CLA	C16-C17-C18-C19
32	C	514	CLA	O1A-CGA-O2A-C1
32	b	605	CLA	O1A-CGA-O2A-C1
32	b	614	CLA	O1A-CGA-O2A-C1
32	Bb	614	CLA	O1A-CGA-O2A-C1
32	Cc	506	CLA	O1A-CGA-O2A-C1
39	n	605	CHL	O1A-CGA-O2A-C1
39	YY	601	CHL	O1A-CGA-O2A-C1
32	b	601	CLA	C5-C6-C7-C8
32	Dd	402	CLA	C8-C10-C11-C12
32	RR	314	CLA	C4C-C3C-CAC-CBC
36	d	405	LHG	C28-C29-C30-C31
37	B	602	SQD	C25-C26-C27-C28
39	RR	307	CHL	CBD-CGD-O2D-CED
36	Dd	405	LHG	C28-C29-C30-C31
36	Dd	407	LHG	C25-C26-C27-C28
38	Mm	101	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
33	Aa	409	PHO	O1D-CGD-O2D-CED
39	s	607	CHL	O1D-CGD-O2D-CED
37	LL	101	SQD	C7-C8-C9-C10
36	d	406	LHG	C11-C10-C9-C8
36	d	406	LHG	C31-C32-C33-C34
32	S	612	CLA	O1A-CGA-O2A-C1
32	SS	303	CLA	O1A-CGA-O2A-C1
32	a	407	CLA	CBA-CGA-O2A-C1
36	Y	618	LHG	C10-C11-C12-C13
36	a	414	LHG	C25-C26-C27-C28
36	NN	619	LHG	C10-C11-C12-C13
37	CC	501	SQD	C17-C18-C19-C20
44	BB	624	DGD	C7B-C8B-C9B-CAB
36	BB	622	LHG	O9-C7-O7-C5
36	CC	521	LHG	O9-C7-O7-C5
38	AA	415	LMG	O9-C10-O7-C8
38	CC	520	LMG	O9-C10-O7-C8
44	c	517	DGD	O1B-C1B-O2G-C2G
32	n	613	CLA	O1D-CGD-O2D-CED
32	Bb	612	CLA	O1D-CGD-O2D-CED
32	Rr	602	CLA	C4B-C3B-CAB-CBB
32	Rr	608	CLA	C4B-C3B-CAB-CBB
32	44	603	CLA	C4B-C3B-CAB-CBB
32	22	602	CLA	C4B-C3B-CAB-CBB
32	1	609	CLA	C4B-C3B-CAB-CBB
32	2	609	CLA	C4B-C3B-CAB-CBB
32	3	603	CLA	C4B-C3B-CAB-CBB
32	C	505	CLA	C4B-C3B-CAB-CBB
32	C	511	CLA	C4B-C3B-CAB-CBB
32	D	405	CLA	C4B-C3B-CAB-CBB
32	G	612	CLA	C4B-C3B-CAB-CBB
32	G	613	CLA	C4B-C3B-CAB-CBB
32	N	610	CLA	C4B-C3B-CAB-CBB
32	N	611	CLA	C4B-C3B-CAB-CBB
32	R	612	CLA	C4B-C3B-CAB-CBB
32	S	608	CLA	C4B-C3B-CAB-CBB
32	Y	610	CLA	C4B-C3B-CAB-CBB
32	c	511	CLA	C4B-C3B-CAB-CBB
32	BB	602	CLA	C4B-C3B-CAB-CBB
32	DD	404	CLA	C4B-C3B-CAB-CBB
32	B	619	CLA	C4B-C3B-CAB-CBB
32	NN	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	Bb	603	CLA	C4B-C3B-CAB-CBB
32	Bb	615	CLA	C4B-C3B-CAB-CBB
32	Cc	503	CLA	C4B-C3B-CAB-CBB
32	Cc	513	CLA	C4B-C3B-CAB-CBB
32	Gg	303	CLA	C4B-C3B-CAB-CBB
36	N	619	LHG	C10-C11-C12-C13
32	g	611	CLA	C16-C17-C18-C20
32	BB	605	CLA	C16-C17-C18-C20
32	B	605	CLA	C16-C17-C18-C20
33	a	409	PHO	O1D-CGD-O2D-CED
32	G	610	CLA	C2A-CAA-CBA-CGA
39	NN	607	CHL	C10-C11-C12-C13
32	C	510	CLA	CBD-CGD-O2D-CED
36	11	614	LHG	C8-C7-O7-C5
36	D	410	LHG	C8-C7-O7-C5
37	L	101	SQD	C8-C7-O47-C45
37	AA	412	SQD	C8-C7-O47-C45
37	LL	102	SQD	C8-C7-O47-C45
38	c	519	LMG	C11-C10-O7-C8
38	Cc	501	LMG	C11-C10-O7-C8
38	Dd	408	LMG	C11-C10-O7-C8
44	Cc	519	DGD	C2B-C1B-O2G-C2G
36	Yy	618	LHG	C9-C10-C11-C12
32	D	404	CLA	C2C-C3C-CAC-CBC
32	b	612	CLA	C6-C7-C8-C10
32	Bb	608	CLA	C11-C12-C13-C15
32	Bb	610	CLA	C12-C13-C15-C16
32	Bb	612	CLA	C6-C7-C8-C10
38	m	101	LMG	C39-C40-C41-C42
32	B	621	CLA	CBA-CGA-O2A-C1
32	c	506	CLA	C10-C11-C12-C13
44	h	102	DGD	C8B-C9B-CAB-CBB
44	B	601	DGD	C7B-C8B-C9B-CAB
32	c	504	CLA	O1A-CGA-O2A-C1
32	Gg	313	CLA	O1A-CGA-O2A-C1
39	Y	601	CHL	O1A-CGA-O2A-C1
44	B	601	DGD	O1A-C1A-O1G-C1G
32	Bb	613	CLA	C3-C5-C6-C7
32	A	405	CLA	C3A-C2A-CAA-CBA
32	Rr	601	CLA	C3A-C2A-CAA-CBA
32	Rr	604	CLA	C3A-C2A-CAA-CBA
32	Rr	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	Rr	612	CLA	C3A-C2A-CAA-CBA
32	Ss	603	CLA	C3A-C2A-CAA-CBA
32	44	603	CLA	C3A-C2A-CAA-CBA
32	44	611	CLA	C3A-C2A-CAA-CBA
32	C	504	CLA	C3A-C2A-CAA-CBA
32	C	505	CLA	C3A-C2A-CAA-CBA
32	G	602	CLA	C3A-C2A-CAA-CBA
32	R	604	CLA	C3A-C2A-CAA-CBA
32	R	611	CLA	C3A-C2A-CAA-CBA
32	a	405	CLA	C3A-C2A-CAA-CBA
32	b	616	CLA	C3A-C2A-CAA-CBA
32	c	510	CLA	C3A-C2A-CAA-CBA
32	d	401	CLA	C3A-C2A-CAA-CBA
32	n	603	CLA	C3A-C2A-CAA-CBA
32	n	613	CLA	C3A-C2A-CAA-CBA
32	r	601	CLA	C3A-C2A-CAA-CBA
32	r	610	CLA	C3A-C2A-CAA-CBA
32	r	611	CLA	C3A-C2A-CAA-CBA
32	s	603	CLA	C3A-C2A-CAA-CBA
32	4	312	CLA	C3A-C2A-CAA-CBA
32	AA	405	CLA	C3A-C2A-CAA-CBA
32	CC	503	CLA	C3A-C2A-CAA-CBA
32	CC	504	CLA	C3A-C2A-CAA-CBA
32	RR	304	CLA	C3A-C2A-CAA-CBA
32	RR	311	CLA	C3A-C2A-CAA-CBA
32	SS	305	CLA	C3A-C2A-CAA-CBA
32	Aa	405	CLA	C3A-C2A-CAA-CBA
32	Bb	616	CLA	C3A-C2A-CAA-CBA
32	Cc	512	CLA	C3A-C2A-CAA-CBA
32	Cc	515	CLA	C3A-C2A-CAA-CBA
32	Dd	401	CLA	C3A-C2A-CAA-CBA
32	Gg	312	CLA	C3A-C2A-CAA-CBA
32	Nn	304	CLA	C3A-C2A-CAA-CBA
32	Nn	313	CLA	C3A-C2A-CAA-CBA
39	Rr	605	CHL	C3A-C2A-CAA-CBA
39	Ss	605	CHL	C3A-C2A-CAA-CBA
39	Ss	606	CHL	C3A-C2A-CAA-CBA
39	44	607	CHL	C3A-C2A-CAA-CBA
39	44	608	CHL	C3A-C2A-CAA-CBA
39	Y	606	CHL	C3A-C2A-CAA-CBA
39	n	605	CHL	C3A-C2A-CAA-CBA
39	r	605	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	s	606	CHL	C3A-C2A-CAA-CBA
39	4	308	CHL	C3A-C2A-CAA-CBA
39	4	309	CHL	C3A-C2A-CAA-CBA
39	YY	606	CHL	C3A-C2A-CAA-CBA
39	Nn	315	CHL	C3A-C2A-CAA-CBA
39	Nn	317	CHL	C3A-C2A-CAA-CBA
32	YY	604	CLA	O1D-CGD-O2D-CED
32	YY	614	CLA	O1D-CGD-O2D-CED
39	1	606	CHL	O1D-CGD-O2D-CED
36	y	320	LHG	C9-C10-C11-C12
32	SS	303	CLA	CBD-CGD-O2D-CED
32	B	622	CLA	C5-C6-C7-C8
38	Cc	501	LMG	C4-C5-C6-O5
38	Mm	101	LMG	C10-C11-C12-C13
32	B	622	CLA	C16-C17-C18-C20
39	n	607	CHL	C16-C17-C18-C20
32	C	509	CLA	O1A-CGA-O2A-C1
32	g	610	CLA	O1A-CGA-O2A-C1
32	CC	508	CLA	O1A-CGA-O2A-C1
32	Cc	510	CLA	O1A-CGA-O2A-C1
43	RR	301	LMU	O1'-C1-C2-C3
38	A	415	LMG	O9-C10-O7-C8
39	Ss	607	CHL	O2A-C1-C2-C3
32	c	507	CLA	O1D-CGD-O2D-CED
32	Rr	602	CLA	CBA-CGA-O2A-C1
32	Ss	603	CLA	CBA-CGA-O2A-C1
32	d	402	CLA	CBA-CGA-O2A-C1
32	s	603	CLA	CBA-CGA-O2A-C1
32	CC	513	CLA	CBA-CGA-O2A-C1
32	YY	613	CLA	CBA-CGA-O2A-C1
32	Aa	407	CLA	CBA-CGA-O2A-C1
39	Yy	601	CHL	CBA-CGA-O2A-C1
35	Dd	404	PL9	C44-C46-C47-C48
36	YY	618	LHG	C25-C26-C27-C28
37	C	501	SQD	C18-C19-C20-C21
44	Aa	401	DGD	C2B-C3B-C4B-C5B
32	Nn	312	CLA	C8-C10-C11-C12
32	R	614	CLA	O1D-CGD-O2D-CED
36	Y	618	LHG	C25-C26-C27-C28
36	DD	408	LHG	C13-C14-C15-C16
36	YY	618	LHG	C13-C14-C15-C16
44	a	415	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
44	BB	624	DGD	O1A-C1A-O1G-C1G
32	2	609	CLA	O1D-CGD-O2D-CED
38	c	519	LMG	O6-C5-C6-O5
32	CC	511	CLA	C10-C11-C12-C13
32	Rr	613	CLA	O1D-CGD-O2D-CED
36	D	409	LHG	C13-C14-C15-C16
32	Cc	503	CLA	C16-C17-C18-C20
32	Rr	602	CLA	C2B-C3B-CAB-CBB
32	44	603	CLA	C2B-C3B-CAB-CBB
32	33	602	CLA	C2B-C3B-CAB-CBB
32	3	602	CLA	C2B-C3B-CAB-CBB
32	3	603	CLA	C2B-C3B-CAB-CBB
32	G	612	CLA	C2B-C3B-CAB-CBB
32	N	611	CLA	C2B-C3B-CAB-CBB
32	R	608	CLA	C2B-C3B-CAB-CBB
32	S	608	CLA	C2B-C3B-CAB-CBB
32	b	603	CLA	C2B-C3B-CAB-CBB
32	b	608	CLA	C2B-C3B-CAB-CBB
32	n	611	CLA	C2B-C3B-CAB-CBB
32	y	312	CLA	C2B-C3B-CAB-CBB
32	y	314	CLA	C2B-C3B-CAB-CBB
32	GG	612	CLA	C2B-C3B-CAB-CBB
32	NN	611	CLA	C2B-C3B-CAB-CBB
32	RR	308	CLA	C2B-C3B-CAB-CBB
32	Bb	607	CLA	C2B-C3B-CAB-CBB
32	Cc	503	CLA	C2B-C3B-CAB-CBB
32	Gg	303	CLA	C2B-C3B-CAB-CBB
32	Nn	302	CLA	C2B-C3B-CAB-CBB
34	A	409	BCR	C1-C6-C7-C8
34	A	409	BCR	C5-C6-C7-C8
34	C	516	BCR	C5-C6-C7-C8
34	C	516	BCR	C23-C24-C25-C30
34	C	517	BCR	C1-C6-C7-C8
34	C	517	BCR	C5-C6-C7-C8
34	C	517	BCR	C23-C24-C25-C30
34	C	518	BCR	C23-C24-C25-C26
34	C	518	BCR	C23-C24-C25-C30
34	D	406	BCR	C23-C24-C25-C26
34	D	406	BCR	C23-C24-C25-C30
34	K	102	BCR	C5-C6-C7-C8
34	a	411	BCR	C1-C6-C7-C8
34	a	411	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
34	a	411	BCR	C23-C24-C25-C30
34	b	617	BCR	C1-C6-C7-C8
34	b	618	BCR	C1-C6-C7-C8
34	b	618	BCR	C5-C6-C7-C8
34	b	618	BCR	C23-C24-C25-C26
34	b	618	BCR	C23-C24-C25-C30
34	b	619	BCR	C1-C6-C7-C8
34	b	619	BCR	C5-C6-C7-C8
34	b	619	BCR	C23-C24-C25-C26
34	c	514	BCR	C5-C6-C7-C8
34	c	515	BCR	C1-C6-C7-C8
34	c	515	BCR	C23-C24-C25-C30
34	c	516	BCR	C23-C24-C25-C26
34	d	403	BCR	C1-C6-C7-C8
34	d	403	BCR	C23-C24-C25-C30
34	h	101	BCR	C23-C24-C25-C26
34	h	101	BCR	C23-C24-C25-C30
34	k	101	BCR	C1-C6-C7-C8
34	k	101	BCR	C5-C6-C7-C8
34	k	101	BCR	C23-C24-C25-C26
34	k	101	BCR	C23-C24-C25-C30
34	AA	409	BCR	C1-C6-C7-C8
34	AA	409	BCR	C5-C6-C7-C8
34	BB	616	BCR	C1-C6-C7-C8
34	BB	616	BCR	C5-C6-C7-C8
34	BB	617	BCR	C1-C6-C7-C8
34	BB	617	BCR	C5-C6-C7-C8
34	BB	617	BCR	C23-C24-C25-C26
34	BB	617	BCR	C23-C24-C25-C30
34	BB	618	BCR	C1-C6-C7-C8
34	BB	618	BCR	C5-C6-C7-C8
34	BB	618	BCR	C23-C24-C25-C26
34	BB	620	BCR	C1-C6-C7-C8
34	BB	620	BCR	C5-C6-C7-C8
34	BB	620	BCR	C23-C24-C25-C30
34	CC	515	BCR	C5-C6-C7-C8
34	CC	515	BCR	C23-C24-C25-C30
34	CC	516	BCR	C1-C6-C7-C8
34	CC	516	BCR	C5-C6-C7-C8
34	CC	516	BCR	C23-C24-C25-C30
34	CC	517	BCR	C23-C24-C25-C26
34	CC	517	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
34	DD	405	BCR	C23-C24-C25-C26
34	DD	405	BCR	C23-C24-C25-C30
34	B	612	BCR	C1-C6-C7-C8
34	B	612	BCR	C5-C6-C7-C8
34	B	613	BCR	C1-C6-C7-C8
34	B	613	BCR	C5-C6-C7-C8
34	B	613	BCR	C23-C24-C25-C26
34	B	613	BCR	C23-C24-C25-C30
34	B	614	BCR	C1-C6-C7-C8
34	B	614	BCR	C5-C6-C7-C8
34	B	614	BCR	C23-C24-C25-C26
34	B	616	BCR	C1-C6-C7-C8
34	B	616	BCR	C5-C6-C7-C8
34	KK	103	BCR	C5-C6-C7-C8
34	XX	202	BCR	C23-C24-C25-C26
34	XX	202	BCR	C23-C24-C25-C30
34	Aa	411	BCR	C1-C6-C7-C8
34	Aa	411	BCR	C23-C24-C25-C26
34	Aa	411	BCR	C23-C24-C25-C30
34	Bb	617	BCR	C1-C6-C7-C8
34	Bb	617	BCR	C5-C6-C7-C8
34	Bb	618	BCR	C1-C6-C7-C8
34	Bb	618	BCR	C5-C6-C7-C8
34	Bb	618	BCR	C23-C24-C25-C26
34	Bb	618	BCR	C23-C24-C25-C30
34	Bb	619	BCR	C5-C6-C7-C8
34	Cc	516	BCR	C5-C6-C7-C8
34	Cc	517	BCR	C1-C6-C7-C8
34	Cc	517	BCR	C23-C24-C25-C30
34	Cc	518	BCR	C23-C24-C25-C26
34	Dd	403	BCR	C1-C6-C7-C8
34	Dd	403	BCR	C23-C24-C25-C30
34	Hh	101	BCR	C23-C24-C25-C26
34	Hh	101	BCR	C23-C24-C25-C30
34	Kk	101	BCR	C1-C6-C7-C8
40	Rr	614	LUT	C5-C6-C7-C8
40	Ss	614	LUT	C5-C6-C7-C8
40	Yy	615	LUT	C5-C6-C7-C8
40	Yy	616	LUT	C5-C6-C7-C8
40	44	612	LUT	C5-C6-C7-C8
40	22	614	LUT	C5-C6-C7-C8
40	2	614	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
40	G	615	LUT	C5-C6-C7-C8
40	G	616	LUT	C1-C6-C7-C8
40	G	616	LUT	C5-C6-C7-C8
40	N	616	LUT	C5-C6-C7-C8
40	Y	615	LUT	C5-C6-C7-C8
40	Y	616	LUT	C1-C6-C7-C8
40	Y	616	LUT	C5-C6-C7-C8
40	g	616	LUT	C5-C6-C7-C8
40	n	616	LUT	C5-C6-C7-C8
40	r	614	LUT	C5-C6-C7-C8
40	s	614	LUT	C5-C6-C7-C8
40	s	615	LUT	C5-C6-C7-C8
40	y	318	LUT	C5-C6-C7-C8
40	4	313	LUT	C1-C6-C7-C8
40	4	313	LUT	C5-C6-C7-C8
40	GG	615	LUT	C5-C6-C7-C8
40	GG	616	LUT	C5-C6-C7-C8
40	NN	615	LUT	C5-C6-C7-C8
40	NN	616	LUT	C5-C6-C7-C8
40	SS	315	LUT	C5-C6-C7-C8
40	YY	615	LUT	C5-C6-C7-C8
40	YY	616	LUT	C5-C6-C7-C8
40	Gg	316	LUT	C5-C6-C7-C8
40	Gg	317	LUT	C5-C6-C7-C8
40	Nn	307	LUT	C1-C6-C7-C8
40	Nn	307	LUT	C5-C6-C7-C8
37	Aa	413	SQD	C25-C26-C27-C28
37	Ll	101	SQD	C11-C10-C9-C8
36	II	101	LHG	C8-C7-O7-C5
36	JJ	101	LHG	C8-C7-O7-C5
36	Dd	405	LHG	C8-C7-O7-C5
44	BB	625	DGD	C2B-C1B-O2G-C2G
44	B	603	DGD	C2B-C1B-O2G-C2G
36	YY	618	LHG	C24-C23-O8-C6
32	c	511	CLA	C5-C6-C7-C8
32	BB	609	CLA	C10-C11-C12-C13
32	Bb	611	CLA	C10-C11-C12-C13
36	Yy	618	LHG	C25-C26-C27-C28
37	l	102	SQD	C11-C10-C9-C8
32	CC	505	CLA	O1D-CGD-O2D-CED
32	Dd	402	CLA	O1D-CGD-O2D-CED
37	B	602	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	CC	503	CLA	C2A-CAA-CBA-CGA
36	Nn	310	LHG	C23-C24-C25-C26
44	c	517	DGD	C1B-C2B-C3B-C4B
39	Yy	601	CHL	C8-C10-C11-C12
32	a	407	CLA	O1A-CGA-O2A-C1
36	A	411	LHG	O9-C7-O7-C5
36	11	614	LHG	O9-C7-O7-C5
36	D	410	LHG	O9-C7-O7-C5
36	JJ	101	LHG	O9-C7-O7-C5
37	CC	501	SQD	O49-C7-O47-C45
37	LL	101	SQD	O49-C7-O47-C45
37	LL	102	SQD	O49-C7-O47-C45
38	c	519	LMG	O9-C10-O7-C8
38	j	101	LMG	O9-C10-O7-C8
38	Cc	501	LMG	O9-C10-O7-C8
38	Dd	408	LMG	O9-C10-O7-C8
44	Cc	519	DGD	O1B-C1B-O2G-C2G
32	Cc	514	CLA	C15-C16-C17-C18
32	Bb	613	CLA	C2-C3-C5-C6
36	y	320	LHG	C25-C26-C27-C28
43	C	502	LMU	O1'-C1-C2-C3
32	b	606	CLA	O1D-CGD-O2D-CED
32	C	510	CLA	CBA-CGA-O2A-C1
32	BB	604	CLA	CBA-CGA-O2A-C1
32	CC	509	CLA	CBA-CGA-O2A-C1
39	Yy	608	CHL	CBA-CGA-O2A-C1
39	y	303	CHL	CBA-CGA-O2A-C1
39	y	310	CHL	CBA-CGA-O2A-C1
36	11	614	LHG	C26-C27-C28-C29
36	YY	618	LHG	C10-C11-C12-C13
37	CC	501	SQD	O5-C1-O6-C44
38	b	620	LMG	C30-C31-C32-C33
39	3	607	CHL	CBD-CGD-O2D-CED
32	BB	611	CLA	C5-C6-C7-C8
32	B	623	CLA	C10-C11-C12-C13
32	CC	513	CLA	O1A-CGA-O2A-C1
32	Aa	407	CLA	O1A-CGA-O2A-C1
38	Bb	620	LMG	C30-C31-C32-C33
36	Rr	617	LHG	C9-C10-C11-C12
33	D	402	PHO	CBA-CGA-O2A-C1
36	33	614	LHG	C8-C7-O7-C5
36	K	101	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
36	d	405	LHG	C8-C7-O7-C5
36	Ll	102	LHG	C8-C7-O7-C5
37	A	412	SQD	C8-C7-O47-C45
38	j	101	LMG	C11-C10-O7-C8
38	BB	619	LMG	C11-C10-O7-C8
38	B	615	LMG	C11-C10-O7-C8
36	y	320	LHG	C7-C8-C9-C10
43	KK	102	LMU	C3'-C4'-O1B-C1B
32	CC	512	CLA	C5-C6-C7-C8
32	Cc	511	CLA	C10-C11-C12-C13
36	Ll	102	LHG	O9-C7-O7-C5
37	L	101	SQD	O49-C7-O47-C45
38	B	615	LMG	O9-C10-O7-C8
32	c	510	CLA	CBD-CGD-O2D-CED
32	d	402	CLA	O1A-CGA-O2A-C1
32	YY	613	CLA	O1A-CGA-O2A-C1
32	YY	610	CLA	C5-C6-C7-C8
34	H	101	BCR	C37-C22-C23-C24
36	Ss	616	LHG	C15-C16-C17-C18
32	b	612	CLA	C2A-CAA-CBA-CGA
39	Nn	318	CHL	C2A-CAA-CBA-CGA
32	Gg	312	CLA	C16-C17-C18-C19
32	Gg	312	CLA	C16-C17-C18-C20
32	DD	403	CLA	C2C-C3C-CAC-CBC
32	RR	314	CLA	C2C-C3C-CAC-CBC
32	Bb	613	CLA	C4-C3-C5-C6
39	n	607	CHL	C4-C3-C5-C6
32	Rr	602	CLA	O1A-CGA-O2A-C1
35	A	410	PL9	C38-C39-C41-C42
39	y	303	CHL	C8-C10-C11-C12
43	KK	102	LMU	C5'-C4'-O1B-C1B
39	y	309	CHL	O1D-CGD-O2D-CED
32	B	621	CLA	O1A-CGA-O2A-C1
36	Yy	618	LHG	O10-C23-O8-C6
39	Yy	601	CHL	O1A-CGA-O2A-C1
32	NN	602	CLA	C3-C5-C6-C7
33	a	408	PHO	C3-C5-C6-C7
44	CC	519	DGD	O6E-C5E-C6E-O5E
33	DD	402	PHO	CBA-CGA-O2A-C1
36	Dd	406	LHG	C24-C23-O8-C6
37	AA	412	SQD	O49-C7-O47-C45
36	44	616	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
36	a	414	LHG	O6-C4-C5-O7
36	Dd	406	LHG	C9-C10-C11-C12
35	DD	406	PL9	C39-C41-C42-C43
32	b	613	CLA	C13-C15-C16-C17
32	c	501	CLA	C13-C15-C16-C17
32	Cc	509	CLA	C13-C15-C16-C17
32	g	611	CLA	C16-C17-C18-C19
32	BB	605	CLA	C16-C17-C18-C19
32	B	622	CLA	C16-C17-C18-C19
32	Ss	603	CLA	O1A-CGA-O2A-C1
32	s	603	CLA	O1A-CGA-O2A-C1
32	B	623	CLA	O1D-CGD-O2D-CED
44	D	411	DGD	C1B-C2B-C3B-C4B
32	A	405	CLA	C5-C6-C7-C8
39	YY	605	CHL	O1D-CGD-O2D-CED
44	C	520	DGD	O6E-C5E-C6E-O5E
37	C	501	SQD	O47-C45-C46-O48
39	1	605	CHL	O1D-CGD-O2D-CED
39	Y	609	CHL	O1D-CGD-O2D-CED
32	n	614	CLA	CBA-CGA-O2A-C1
36	Y	618	LHG	C24-C23-O8-C6
32	Rr	602	CLA	C15-C16-C17-C18
32	NN	602	CLA	C8-C10-C11-C12
38	F	101	LMG	O6-C5-C6-O5
38	DD	409	LMG	O6-C5-C6-O5
39	N	601	CHL	C2A-CAA-CBA-CGA
39	11	606	CHL	O1D-CGD-O2D-CED
36	Y	618	LHG	C13-C14-C15-C16
32	CC	510	CLA	C2-C1-O2A-CGA
39	g	605	CHL	C3A-C2A-CAA-CBA
39	GG	606	CHL	C3A-C2A-CAA-CBA
39	Gg	306	CHL	C3A-C2A-CAA-CBA
32	Bb	601	CLA	C16-C17-C18-C20
32	Cc	503	CLA	C16-C17-C18-C19
32	n	602	CLA	C13-C15-C16-C17
33	Aa	408	PHO	C3-C5-C6-C7
39	n	607	CHL	C2-C3-C5-C6
38	BB	619	LMG	O9-C10-O7-C8
32	Rr	602	CLA	C8-C10-C11-C12
32	Bb	612	CLA	C8-C10-C11-C12
37	Aa	413	SQD	C27-C28-C29-C30
32	Rr	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	c	501	CLA	C2A-CAA-CBA-CGA
32	c	505	CLA	C2A-CAA-CBA-CGA
32	c	510	CLA	C2A-CAA-CBA-CGA
32	r	610	CLA	C2A-CAA-CBA-CGA
32	4	305	CLA	C2A-CAA-CBA-CGA
32	CC	506	CLA	C2A-CAA-CBA-CGA
32	SS	313	CLA	C2A-CAA-CBA-CGA
32	YY	613	CLA	C2A-CAA-CBA-CGA
32	b	604	CLA	O1D-CGD-O2D-CED
32	b	607	CLA	CBA-CGA-O2A-C1
38	Mm	101	LMG	C12-C13-C14-C15
32	44	602	CLA	O1D-CGD-O2D-CED
32	Yy	602	CLA	C15-C16-C17-C18
32	b	612	CLA	C8-C10-C11-C12
32	BB	606	CLA	C10-C11-C12-C13
32	YY	602	CLA	C5-C6-C7-C8
39	NN	606	CHL	O1D-CGD-O2D-CED
32	B	606	CLA	C16-C17-C18-C19
38	BB	619	LMG	O6-C5-C6-O5
38	B	615	LMG	O6-C5-C6-O5
44	h	102	DGD	O6E-C5E-C6E-O5E
32	Bb	608	CLA	O1D-CGD-O2D-CED
39	n	605	CHL	O1D-CGD-O2D-CED
36	4	301	LHG	O1-C1-C2-O2
32	C	510	CLA	O1A-CGA-O2A-C1
33	D	402	PHO	O1A-CGA-O2A-C1
32	A	405	CLA	C1A-C2A-CAA-CBA
32	Rr	601	CLA	C1A-C2A-CAA-CBA
32	Rr	611	CLA	C1A-C2A-CAA-CBA
32	Rr	613	CLA	C1A-C2A-CAA-CBA
32	Ss	603	CLA	C1A-C2A-CAA-CBA
32	Ss	608	CLA	C1A-C2A-CAA-CBA
32	Yy	614	CLA	C1A-C2A-CAA-CBA
32	44	611	CLA	C1A-C2A-CAA-CBA
32	C	505	CLA	C1A-C2A-CAA-CBA
32	C	510	CLA	C1A-C2A-CAA-CBA
32	G	602	CLA	C1A-C2A-CAA-CBA
32	G	611	CLA	C1A-C2A-CAA-CBA
32	R	602	CLA	C1A-C2A-CAA-CBA
32	R	604	CLA	C1A-C2A-CAA-CBA
32	R	611	CLA	C1A-C2A-CAA-CBA
32	Y	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	Y	614	CLA	C1A-C2A-CAA-CBA
32	a	405	CLA	C1A-C2A-CAA-CBA
32	b	601	CLA	C1A-C2A-CAA-CBA
32	b	616	CLA	C1A-C2A-CAA-CBA
32	c	503	CLA	C1A-C2A-CAA-CBA
32	c	510	CLA	C1A-C2A-CAA-CBA
32	d	401	CLA	C1A-C2A-CAA-CBA
32	d	402	CLA	C1A-C2A-CAA-CBA
32	n	603	CLA	C1A-C2A-CAA-CBA
32	r	601	CLA	C1A-C2A-CAA-CBA
32	r	608	CLA	C1A-C2A-CAA-CBA
32	r	611	CLA	C1A-C2A-CAA-CBA
32	s	603	CLA	C1A-C2A-CAA-CBA
32	y	316	CLA	C1A-C2A-CAA-CBA
32	4	312	CLA	C1A-C2A-CAA-CBA
32	AA	405	CLA	C1A-C2A-CAA-CBA
32	BB	602	CLA	C1A-C2A-CAA-CBA
32	BB	604	CLA	C1A-C2A-CAA-CBA
32	BB	608	CLA	C1A-C2A-CAA-CBA
32	CC	504	CLA	C1A-C2A-CAA-CBA
32	CC	509	CLA	C1A-C2A-CAA-CBA
32	B	619	CLA	C1A-C2A-CAA-CBA
32	B	621	CLA	C1A-C2A-CAA-CBA
32	GG	611	CLA	C1A-C2A-CAA-CBA
32	RR	304	CLA	C1A-C2A-CAA-CBA
32	RR	311	CLA	C1A-C2A-CAA-CBA
32	SS	303	CLA	C1A-C2A-CAA-CBA
32	YY	614	CLA	C1A-C2A-CAA-CBA
32	Bb	601	CLA	C1A-C2A-CAA-CBA
32	Bb	616	CLA	C1A-C2A-CAA-CBA
32	Cc	504	CLA	C1A-C2A-CAA-CBA
32	Cc	512	CLA	C1A-C2A-CAA-CBA
32	Dd	401	CLA	C1A-C2A-CAA-CBA
32	Nn	313	CLA	C1A-C2A-CAA-CBA
32	c	513	CLA	CBD-CGD-O2D-CED
32	Yy	602	CLA	C10-C11-C12-C13
32	n	602	CLA	C8-C10-C11-C12
32	r	609	CLA	C15-C16-C17-C18
32	Bb	607	CLA	C5-C6-C7-C8
32	Cc	503	CLA	C8-C10-C11-C12
44	BB	623	DGD	O6E-C5E-C6E-O5E
32	CC	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	Yy	618	LHG	O6-C4-C5-C6
36	Y	618	LHG	O6-C4-C5-C6
36	a	414	LHG	O6-C4-C5-C6
36	y	320	LHG	O6-C4-C5-C6
36	YY	618	LHG	O6-C4-C5-C6
36	Dd	407	LHG	O6-C4-C5-C6
36	33	614	LHG	O9-C7-O7-C5
36	K	101	LHG	O9-C7-O7-C5
36	d	405	LHG	O9-C7-O7-C5
36	Dd	405	LHG	O9-C7-O7-C5
32	Yy	610	CLA	C11-C12-C13-C15
32	Yy	612	CLA	C11-C12-C13-C15
32	C	505	CLA	C6-C7-C8-C10
32	R	609	CLA	C11-C12-C13-C15
32	Y	612	CLA	C6-C7-C8-C10
32	a	405	CLA	C12-C13-C15-C16
32	b	608	CLA	C11-C12-C13-C15
32	b	613	CLA	C6-C7-C8-C10
32	c	503	CLA	C11-C10-C8-C7
32	d	401	CLA	C11-C12-C13-C15
32	BB	608	CLA	C11-C12-C13-C15
32	BB	610	CLA	C6-C7-C8-C10
32	BB	611	CLA	C12-C13-C15-C16
32	BB	612	CLA	C6-C7-C8-C10
32	CC	503	CLA	C6-C7-C8-C10
32	DD	403	CLA	C6-C7-C8-C10
32	B	604	CLA	C11-C12-C13-C15
32	B	606	CLA	C6-C7-C8-C10
32	B	608	CLA	C6-C7-C8-C10
32	B	608	CLA	C12-C13-C15-C16
32	B	618	CLA	C12-C13-C15-C16
32	RR	302	CLA	C11-C12-C13-C15
32	RR	309	CLA	C11-C12-C13-C15
32	YY	610	CLA	C11-C12-C13-C15
32	YY	612	CLA	C11-C10-C8-C7
32	Aa	405	CLA	C12-C13-C15-C16
32	Bb	613	CLA	C6-C7-C8-C10
32	Cc	505	CLA	C11-C10-C8-C7
32	Dd	401	CLA	C11-C12-C13-C15
39	Yy	601	CHL	C11-C12-C13-C15
39	g	601	CHL	C6-C7-C8-C10
39	g	601	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
39	y	303	CHL	C11-C12-C13-C15
39	Nn	317	CHL	C6-C7-C8-C10
39	Nn	317	CHL	C12-C13-C15-C16
32	BB	610	CLA	C16-C17-C18-C19
33	DD	402	PHO	O1A-CGA-O2A-C1
36	YY	618	LHG	O10-C23-O8-C6
39	Yy	608	CHL	O1A-CGA-O2A-C1
39	y	303	CHL	O1A-CGA-O2A-C1
39	y	310	CHL	O1A-CGA-O2A-C1
44	D	411	DGD	O6E-C5E-C6E-O5E
32	CC	505	CLA	C8-C10-C11-C12
32	B	622	CLA	C8-C10-C11-C12
32	Bb	604	CLA	C10-C11-C12-C13
32	Bb	611	CLA	C5-C6-C7-C8
36	Yy	618	LHG	C7-C8-C9-C10
44	CC	522	DGD	C3B-C4B-C5B-C6B
32	GG	611	CLA	C2-C3-C5-C6
32	n	614	CLA	O1A-CGA-O2A-C1
32	RR	314	CLA	O1D-CGD-O2D-CED
38	b	621	LMG	O6-C5-C6-O5
32	c	507	CLA	C13-C15-C16-C17
32	C	512	CLA	C2A-CAA-CBA-CGA
32	S	612	CLA	C2A-CAA-CBA-CGA
32	n	614	CLA	C2A-CAA-CBA-CGA
32	Cc	507	CLA	C2A-CAA-CBA-CGA
32	Yy	610	CLA	C11-C12-C13-C14
32	Yy	612	CLA	C11-C12-C13-C14
32	C	505	CLA	C6-C7-C8-C9
32	D	405	CLA	C14-C13-C15-C16
32	R	602	CLA	C11-C12-C13-C14
32	a	405	CLA	C14-C13-C15-C16
32	b	612	CLA	C11-C12-C13-C14
32	b	613	CLA	C6-C7-C8-C9
32	b	615	CLA	C11-C10-C8-C9
32	c	503	CLA	C11-C10-C8-C9
32	d	401	CLA	C11-C12-C13-C14
32	y	304	CLA	C11-C10-C8-C9
32	BB	612	CLA	C14-C13-C15-C16
32	B	604	CLA	C11-C12-C13-C14
32	B	607	CLA	C14-C13-C15-C16
32	RR	302	CLA	C11-C12-C13-C14
32	Aa	405	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	Bb	610	CLA	C14-C13-C15-C16
32	Bb	612	CLA	C11-C12-C13-C14
32	Cc	511	CLA	C11-C10-C8-C9
32	Dd	401	CLA	C11-C12-C13-C14
33	DD	402	PHO	C6-C7-C8-C9
33	Aa	409	PHO	C6-C7-C8-C9
39	y	303	CHL	C11-C12-C13-C14
39	Nn	317	CHL	C6-C7-C8-C9
38	b	620	LMG	O6-C5-C6-O5
32	B	606	CLA	C16-C17-C18-C20
32	Ss	612	CLA	CBA-CGA-O2A-C1
32	C	513	CLA	CBA-CGA-O2A-C1
32	G	602	CLA	CBA-CGA-O2A-C1
32	Y	613	CLA	CBA-CGA-O2A-C1
32	BB	613	CLA	CBA-CGA-O2A-C1
32	Dd	401	CLA	CBA-CGA-O2A-C1
33	a	409	PHO	CBA-CGA-O2A-C1
33	Aa	409	PHO	CBA-CGA-O2A-C1
36	22	615	LHG	C24-C23-O8-C6
36	n	618	LHG	C24-C23-O8-C6
32	b	611	CLA	C5-C6-C7-C8
32	g	611	CLA	C5-C6-C7-C8
35	d	404	PL9	C42-C43-C44-C45
35	Dd	404	PL9	C12-C13-C14-C15
36	II	101	LHG	O9-C7-O7-C5
37	CC	501	SQD	C2-C1-O6-C44
44	CC	522	DGD	C2D-C1D-O3G-C3G
32	Yy	610	CLA	C13-C15-C16-C17
32	B	608	CLA	C10-C11-C12-C13
38	Bb	621	LMG	O6-C5-C6-O5
38	Cc	501	LMG	C28-C29-C30-C31
35	D	407	PL9	C44-C46-C47-C48
35	d	404	PL9	C19-C21-C22-C23
36	D	410	LHG	C4-C5-C6-O8
37	C	501	SQD	C44-C45-C46-O48
37	L	101	SQD	C44-C45-C46-O48
37	L	102	SQD	O6-C44-C45-C46
37	B	602	SQD	O6-C44-C45-C46
37	LL	102	SQD	C44-C45-C46-O48
38	C	521	LMG	O1-C7-C8-C9
44	a	415	DGD	C1G-C2G-C3G-O3G
44	CC	522	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
36	J	101	LHG	C24-C25-C26-C27
38	A	415	LMG	O6-C5-C6-O5
44	Hh	102	DGD	C5A-C6A-C7A-C8A
32	b	611	CLA	C10-C11-C12-C13
32	y	304	CLA	C15-C16-C17-C18
38	C	521	LMG	C32-C33-C34-C35
32	N	611	CLA	O1D-CGD-O2D-CED
32	BB	606	CLA	O1D-CGD-O2D-CED
32	n	611	CLA	CBA-CGA-O2A-C1
32	CC	512	CLA	CBA-CGA-O2A-C1
32	B	609	CLA	CBA-CGA-O2A-C1
32	Bb	607	CLA	CBA-CGA-O2A-C1
32	Bb	615	CLA	CBA-CGA-O2A-C1
32	Gg	303	CLA	CBA-CGA-O2A-C1
36	d	406	LHG	C24-C23-O8-C6
38	Bb	620	LMG	O6-C5-C6-O5
32	BB	610	CLA	C16-C17-C18-C20
36	AA	411	LHG	C10-C11-C12-C13
38	AA	415	LMG	O6-C5-C6-O5
33	a	408	PHO	CHA-CBD-CGD-O1D
33	a	408	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O2D
39	Rr	605	CHL	CHA-CBD-CGD-O1D
39	Yy	609	CHL	CHA-CBD-CGD-O1D
39	Yy	609	CHL	CHA-CBD-CGD-O2D
39	1	607	CHL	CHA-CBD-CGD-O1D
39	1	607	CHL	CHA-CBD-CGD-O2D
39	2	606	CHL	CHA-CBD-CGD-O1D
39	2	606	CHL	CHA-CBD-CGD-O2D
39	N	605	CHL	CHA-CBD-CGD-O1D
39	N	605	CHL	CHA-CBD-CGD-O2D
39	R	605	CHL	CHA-CBD-CGD-O1D
39	R	605	CHL	CHA-CBD-CGD-O2D
39	g	607	CHL	CHA-CBD-CGD-O2D
39	NN	605	CHL	CHA-CBD-CGD-O1D
39	NN	605	CHL	CHA-CBD-CGD-O2D
39	RR	305	CHL	CHA-CBD-CGD-O1D
39	RR	305	CHL	CHA-CBD-CGD-O2D
32	CC	512	CLA	C15-C16-C17-C18
37	B	602	SQD	C7-C8-C9-C10
38	C	521	LMG	O6-C5-C6-O5
43	R	618	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
32	BB	604	CLA	O1A-CGA-O2A-C1
38	C	521	LMG	C35-C36-C37-C38
32	GG	611	CLA	C4-C3-C5-C6
32	Y	602	CLA	C5-C6-C7-C8
32	CC	509	CLA	C10-C11-C12-C13
32	B	619	CLA	C10-C11-C12-C13
44	BB	625	DGD	O1B-C1B-O2G-C2G
32	Bb	601	CLA	C16-C17-C18-C19
32	Cc	509	CLA	O1D-CGD-O2D-CED
44	Hh	102	DGD	O6E-C5E-C6E-O5E
34	XX	202	BCR	C7-C8-C9-C10
32	Y	613	CLA	O1A-CGA-O2A-C1
32	C	513	CLA	C5-C6-C7-C8
32	44	604	CLA	C2A-CAA-CBA-CGA
32	Y	613	CLA	C2A-CAA-CBA-CGA
32	SS	314	CLA	C2A-CAA-CBA-CGA
38	m	101	LMG	C12-C13-C14-C15
37	Aa	413	SQD	C7-C8-C9-C10
32	b	607	CLA	O1A-CGA-O2A-C1
39	3	605	CHL	O1D-CGD-O2D-CED
32	CC	514	CLA	CBA-CGA-O2A-C1
32	c	501	CLA	O2A-C1-C2-C3
32	C	503	CLA	C8-C10-C11-C12
32	BB	601	CLA	C13-C15-C16-C17
32	Bb	615	CLA	C15-C16-C17-C18
36	Y	618	LHG	C11-C12-C13-C14
44	C	519	DGD	C5A-C6A-C7A-C8A
38	c	519	LMG	C28-C29-C30-C31
32	BB	613	CLA	O1A-CGA-O2A-C1
36	44	614	LHG	O6-C4-C5-O7
36	4	315	LHG	O6-C4-C5-O7
38	a	412	LMG	O6-C1-O1-C7
37	C	501	SQD	C17-C18-C19-C20
32	R	609	CLA	CBA-CGA-O2A-C1
32	b	615	CLA	CBA-CGA-O2A-C1
32	RR	309	CLA	CBA-CGA-O2A-C1
32	RR	314	CLA	CBA-CGA-O2A-C1
36	r	616	LHG	C9-C10-C11-C12
32	b	604	CLA	C4-C3-C5-C6
32	B	622	CLA	C2-C3-C5-C6
44	BB	623	DGD	C3B-C4B-C5B-C6B
39	G	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	D	410	LHG	O7-C5-C6-O8
36	y	320	LHG	O7-C5-C6-O8
38	C	521	LMG	O1-C7-C8-O7
38	a	412	LMG	O1-C7-C8-O7
44	a	415	DGD	O2G-C2G-C3G-O3G
44	Aa	401	DGD	O2G-C2G-C3G-O3G
38	BB	619	LMG	C17-C18-C19-C20
44	Hh	102	DGD	C4B-C5B-C6B-C7B
32	d	401	CLA	CBA-CGA-O2A-C1
32	DD	403	CLA	CBA-CGA-O2A-C1
32	Cc	504	CLA	CBA-CGA-O2A-C1
32	Ss	612	CLA	C2A-CAA-CBA-CGA
32	Cc	513	CLA	C3-C5-C6-C7
32	Dd	401	CLA	O1D-CGD-O2D-CED
32	Bb	610	CLA	C5-C6-C7-C8
43	R	618	LMU	C5'-C4'-O1B-C1B
32	Dd	401	CLA	O1A-CGA-O2A-C1
36	Dd	406	LHG	O10-C23-O8-C6
36	K	101	LHG	C23-C24-C25-C26
36	Yy	618	LHG	C13-C14-C15-C16
44	CC	518	DGD	CCB-CDB-CEB-CFB
32	D	404	CLA	CBA-CGA-O2A-C1
32	BB	606	CLA	CBA-CGA-O2A-C1
32	B	618	CLA	CBA-CGA-O2A-C1
36	r	616	LHG	C24-C23-O8-C6
37	Aa	413	SQD	C24-C23-O48-C46
39	s	605	CHL	CBA-CGA-O2A-C1
44	CC	518	DGD	C2B-C1B-O2G-C2G
38	m	101	LMG	C31-C32-C33-C34
32	C	510	CLA	C10-C11-C12-C13
32	y	315	CLA	O1D-CGD-O2D-CED
32	Bb	606	CLA	O1D-CGD-O2D-CED
32	r	602	CLA	C15-C16-C17-C18
32	BB	612	CLA	C10-C11-C12-C13
32	Aa	407	CLA	O1D-CGD-O2D-CED
32	C	513	CLA	C4-C3-C5-C6
32	g	611	CLA	C4-C3-C5-C6
32	CC	512	CLA	C4-C3-C5-C6
32	B	622	CLA	C4-C3-C5-C6
35	d	404	PL9	C30-C29-C31-C32
32	r	609	CLA	CBA-CGA-O2A-C1
32	s	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	NN	602	CLA	C5-C6-C7-C8
36	d	406	LHG	C9-C10-C11-C12
44	B	603	DGD	O1B-C1B-O2G-C2G
36	G	618	LHG	O1-C1-C2-O2
43	KK	102	LMU	C2-C1-O1'-C1'
32	b	610	CLA	C3-C5-C6-C7
32	C	507	CLA	C14-C13-C15-C16
32	R	609	CLA	C11-C12-C13-C14
32	b	608	CLA	C11-C12-C13-C14
32	BB	605	CLA	C14-C13-C15-C16
32	BB	608	CLA	C11-C12-C13-C14
32	BB	610	CLA	C6-C7-C8-C9
32	BB	611	CLA	C14-C13-C15-C16
32	BB	612	CLA	C6-C7-C8-C9
32	CC	502	CLA	C11-C10-C8-C9
32	CC	504	CLA	C6-C7-C8-C9
32	CC	511	CLA	C6-C7-C8-C9
32	DD	403	CLA	C6-C7-C8-C9
32	DD	404	CLA	C14-C13-C15-C16
32	B	606	CLA	C6-C7-C8-C9
32	B	608	CLA	C6-C7-C8-C9
32	B	608	CLA	C14-C13-C15-C16
32	B	618	CLA	C14-C13-C15-C16
32	RR	309	CLA	C11-C12-C13-C14
32	YY	610	CLA	C11-C12-C13-C14
32	YY	610	CLA	C14-C13-C15-C16
32	YY	612	CLA	C11-C10-C8-C9
32	Bb	608	CLA	C11-C12-C13-C14
32	Cc	505	CLA	C11-C10-C8-C9
32	Nn	301	CLA	C11-C12-C13-C14
33	D	402	PHO	C6-C7-C8-C9
33	a	409	PHO	C6-C7-C8-C9
33	Aa	409	PHO	C11-C12-C13-C14
39	Yy	601	CHL	C11-C12-C13-C14
39	G	601	CHL	C11-C12-C13-C14
39	Y	601	CHL	C11-C12-C13-C14
39	g	601	CHL	C6-C7-C8-C9
39	g	601	CHL	C11-C12-C13-C14
39	n	607	CHL	C14-C13-C15-C16
39	NN	607	CHL	C14-C13-C15-C16
39	YY	601	CHL	C11-C12-C13-C14
39	Gg	302	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
39	Nn	317	CHL	C14-C13-C15-C16
36	NN	619	LHG	C5-C4-O6-P
32	Gg	303	CLA	O1A-CGA-O2A-C1
32	A	406	CLA	C4B-C3B-CAB-CBB
32	Rr	604	CLA	C4B-C3B-CAB-CBB
32	Yy	611	CLA	C4B-C3B-CAB-CBB
32	44	604	CLA	C4B-C3B-CAB-CBB
32	44	610	CLA	C4B-C3B-CAB-CBB
32	44	611	CLA	C4B-C3B-CAB-CBB
32	11	612	CLA	C4B-C3B-CAB-CBB
32	11	613	CLA	C4B-C3B-CAB-CBB
32	22	609	CLA	C4B-C3B-CAB-CBB
32	22	611	CLA	C4B-C3B-CAB-CBB
32	1	604	CLA	C4B-C3B-CAB-CBB
32	2	602	CLA	C4B-C3B-CAB-CBB
32	2	604	CLA	C4B-C3B-CAB-CBB
32	2	611	CLA	C4B-C3B-CAB-CBB
32	3	611	CLA	C4B-C3B-CAB-CBB
32	3	612	CLA	C4B-C3B-CAB-CBB
32	N	613	CLA	C4B-C3B-CAB-CBB
32	R	611	CLA	C4B-C3B-CAB-CBB
32	Y	603	CLA	C4B-C3B-CAB-CBB
32	Y	614	CLA	C4B-C3B-CAB-CBB
32	c	512	CLA	C4B-C3B-CAB-CBB
32	r	602	CLA	C4B-C3B-CAB-CBB
32	4	311	CLA	C4B-C3B-CAB-CBB
32	4	312	CLA	C4B-C3B-CAB-CBB
32	AA	406	CLA	C4B-C3B-CAB-CBB
32	CC	504	CLA	C4B-C3B-CAB-CBB
32	CC	510	CLA	C4B-C3B-CAB-CBB
32	DD	401	CLA	C4B-C3B-CAB-CBB
32	B	621	CLA	C4B-C3B-CAB-CBB
32	GG	603	CLA	C4B-C3B-CAB-CBB
32	GG	614	CLA	C4B-C3B-CAB-CBB
32	NN	613	CLA	C4B-C3B-CAB-CBB
32	YY	614	CLA	C4B-C3B-CAB-CBB
32	Aa	406	CLA	C4B-C3B-CAB-CBB
32	Aa	410	CLA	C4B-C3B-CAB-CBB
32	Cc	514	CLA	C4B-C3B-CAB-CBB
32	Nn	302	CLA	C4B-C3B-CAB-CBB
32	r	604	CLA	CAA-CBA-CGA-O2A
36	Dd	406	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	a	409	PHO	C15-C16-C17-C18
32	c	501	CLA	C16-C17-C18-C20
32	C	515	CLA	C2A-CAA-CBA-CGA
32	BB	607	CLA	C2A-CAA-CBA-CGA
36	A	414	LHG	C11-C12-C13-C14
32	Cc	508	CLA	C15-C16-C17-C18
36	DD	408	LHG	C33-C34-C35-C36
38	m	101	LMG	C17-C18-C19-C20
36	44	614	LHG	O6-C4-C5-C6
36	D	408	LHG	O6-C4-C5-C6
36	DD	407	LHG	O6-C4-C5-C6
32	C	507	CLA	C12-C13-C15-C16
32	C	512	CLA	C6-C7-C8-C10
32	R	602	CLA	C11-C12-C13-C15
32	Y	602	CLA	C6-C7-C8-C10
32	b	602	CLA	C12-C13-C15-C16
32	b	612	CLA	C11-C12-C13-C15
32	b	615	CLA	C11-C10-C8-C7
32	c	506	CLA	C11-C10-C8-C7
32	n	610	CLA	C11-C12-C13-C15
32	r	602	CLA	C6-C7-C8-C10
32	y	304	CLA	C11-C10-C8-C7
32	y	314	CLA	C11-C10-C8-C7
32	y	314	CLA	C11-C12-C13-C15
32	BB	609	CLA	C6-C7-C8-C10
32	BB	612	CLA	C12-C13-C15-C16
32	CC	502	CLA	C11-C10-C8-C7
32	CC	504	CLA	C6-C7-C8-C10
32	CC	508	CLA	C11-C10-C8-C7
32	CC	511	CLA	C6-C7-C8-C10
32	DD	404	CLA	C12-C13-C15-C16
32	B	605	CLA	C6-C7-C8-C10
32	B	607	CLA	C12-C13-C15-C16
32	B	620	CLA	C11-C12-C13-C15
32	YY	602	CLA	C6-C7-C8-C10
32	YY	610	CLA	C6-C7-C8-C10
32	YY	610	CLA	C12-C13-C15-C16
32	Bb	612	CLA	C11-C12-C13-C15
32	Cc	508	CLA	C11-C10-C8-C7
32	Cc	511	CLA	C11-C10-C8-C7
32	Cc	513	CLA	C11-C10-C8-C7
32	Gg	312	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	Nn	301	CLA	C11-C12-C13-C15
33	D	402	PHO	C6-C7-C8-C10
33	a	409	PHO	C6-C7-C8-C10
33	a	409	PHO	C11-C12-C13-C15
33	DD	402	PHO	C6-C7-C8-C10
33	Aa	409	PHO	C6-C7-C8-C10
39	Yy	609	CHL	C12-C13-C15-C16
39	G	601	CHL	C11-C12-C13-C15
39	Y	601	CHL	C11-C12-C13-C15
39	n	607	CHL	C12-C13-C15-C16
39	y	311	CHL	C12-C13-C15-C16
39	NN	607	CHL	C12-C13-C15-C16
39	YY	601	CHL	C11-C12-C13-C15
39	Gg	302	CHL	C11-C12-C13-C15
32	n	611	CLA	O1A-CGA-O2A-C1
32	Bb	607	CLA	O1A-CGA-O2A-C1
33	a	409	PHO	O1A-CGA-O2A-C1
33	Aa	409	PHO	O1A-CGA-O2A-C1
36	Y	618	LHG	O10-C23-O8-C6
32	B	623	CLA	CBA-CGA-O2A-C1
37	L	101	SQD	C25-C26-C27-C28
39	Y	606	CHL	O1D-CGD-O2D-CED
32	G	602	CLA	O1A-CGA-O2A-C1
32	B	609	CLA	O1A-CGA-O2A-C1
36	n	618	LHG	O10-C23-O8-C6
44	CC	522	DGD	C7B-C8B-C9B-CAB
32	Rr	602	CLA	C3A-C2A-CAA-CBA
32	Rr	608	CLA	C3A-C2A-CAA-CBA
32	Yy	604	CLA	C3A-C2A-CAA-CBA
32	N	610	CLA	C3A-C2A-CAA-CBA
32	S	602	CLA	C3A-C2A-CAA-CBA
32	S	604	CLA	C3A-C2A-CAA-CBA
32	Y	604	CLA	C3A-C2A-CAA-CBA
32	c	506	CLA	C3A-C2A-CAA-CBA
32	c	513	CLA	C3A-C2A-CAA-CBA
32	y	305	CLA	C3A-C2A-CAA-CBA
32	4	303	CLA	C3A-C2A-CAA-CBA
32	AA	406	CLA	C3A-C2A-CAA-CBA
32	BB	608	CLA	C3A-C2A-CAA-CBA
32	CC	502	CLA	C3A-C2A-CAA-CBA
32	B	604	CLA	C3A-C2A-CAA-CBA
32	NN	610	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	NN	613	CLA	C3A-C2A-CAA-CBA
32	SS	303	CLA	C3A-C2A-CAA-CBA
32	Bb	611	CLA	C4-C3-C5-C6
32	Gg	312	CLA	C4-C3-C5-C6
35	d	404	PL9	C25-C24-C26-C27
35	Dd	404	PL9	C25-C24-C26-C27
35	Dd	404	PL9	C30-C29-C31-C32
32	BB	609	CLA	C8-C10-C11-C12
32	CC	506	CLA	C8-C10-C11-C12
32	Bb	616	CLA	C15-C16-C17-C18
44	Hh	102	DGD	C5B-C6B-C7B-C8B
37	B	602	SQD	O5-C1-O6-C44
37	Aa	413	SQD	O5-C1-O6-C44
32	Ss	612	CLA	O1A-CGA-O2A-C1
32	C	513	CLA	O1A-CGA-O2A-C1
32	CC	512	CLA	O1A-CGA-O2A-C1
32	b	603	CLA	C13-C15-C16-C17
43	R	618	LMU	C3'-C4'-O1B-C1B
32	C	515	CLA	CBA-CGA-O2A-C1
32	c	501	CLA	C16-C17-C18-C19
32	b	610	CLA	C13-C15-C16-C17
36	n	618	LHG	C11-C10-C9-C8
32	Bb	615	CLA	O1A-CGA-O2A-C1
32	CC	509	CLA	O1D-CGD-O2D-CED
36	y	320	LHG	C15-C16-C17-C18
44	D	411	DGD	CCB-CDB-CEB-CFB
32	CC	513	CLA	C8-C10-C11-C12
39	N	607	CHL	CBD-CGD-O2D-CED
34	TT	101	BCR	C21-C22-C23-C24
44	CC	522	DGD	C1B-C2B-C3B-C4B
36	DD	407	LHG	C28-C29-C30-C31
32	Ss	603	CLA	O2A-C1-C2-C3
32	r	608	CLA	O2A-C1-C2-C3
32	r	610	CLA	O2A-C1-C2-C3
32	s	603	CLA	O2A-C1-C2-C3
32	s	613	CLA	O2A-C1-C2-C3
32	RR	310	CLA	O2A-C1-C2-C3
32	Nn	314	CLA	O2A-C1-C2-C3
39	NN	609	CHL	O2A-C1-C2-C3
39	Nn	311	CHL	O2A-C1-C2-C3
36	Nn	310	LHG	C11-C10-C9-C8
44	CC	518	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
32	c	506	CLA	C15-C16-C17-C18
36	A	413	LHG	C4-C5-C6-O8
37	LL	101	SQD	O6-C44-C45-C46
37	Aa	413	SQD	O6-C44-C45-C46
38	a	412	LMG	O1-C7-C8-C9
38	BB	619	LMG	C7-C8-C9-O8
38	Aa	412	LMG	O1-C7-C8-C9
44	Aa	401	DGD	C1G-C2G-C3G-O3G
32	Bb	603	CLA	C13-C15-C16-C17
39	Rr	605	CHL	C1A-C2A-CAA-CBA
39	Ss	605	CHL	C1A-C2A-CAA-CBA
39	Ss	606	CHL	C1A-C2A-CAA-CBA
39	44	607	CHL	C1A-C2A-CAA-CBA
39	44	608	CHL	C1A-C2A-CAA-CBA
39	r	605	CHL	C1A-C2A-CAA-CBA
39	s	606	CHL	C1A-C2A-CAA-CBA
39	4	308	CHL	C1A-C2A-CAA-CBA
39	Nn	317	CHL	C1A-C2A-CAA-CBA
37	LL	102	SQD	C25-C26-C27-C28
44	CC	519	DGD	CAA-CBA-CCA-CDA
32	a	405	CLA	C4-C3-C5-C6
32	b	611	CLA	C4-C3-C5-C6
32	c	501	CLA	C4-C3-C5-C6
36	0	201	LHG	C23-C24-C25-C26
44	D	411	DGD	C3B-C4B-C5B-C6B
32	C	513	CLA	C2-C3-C5-C6
32	g	611	CLA	C2-C3-C5-C6
32	CC	512	CLA	C2-C3-C5-C6
32	d	401	CLA	O1A-CGA-O2A-C1
36	d	406	LHG	O10-C23-O8-C6
32	N	602	CLA	C3-C5-C6-C7
32	AA	408	CLA	C3-C5-C6-C7
32	Dd	402	CLA	C3-C5-C6-C7
36	AA	414	LHG	C11-C12-C13-C14
32	b	615	CLA	C15-C16-C17-C18
32	C	510	CLA	O1D-CGD-O2D-CED
38	Mm	101	LMG	C31-C32-C33-C34
32	b	601	CLA	C16-C17-C18-C20
32	Bb	606	CLA	C16-C17-C18-C20
36	11	614	LHG	O6-C4-C5-O7
36	3	614	LHG	O6-C4-C5-O7
36	4	301	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
36	CC	523	LHG	O6-C4-C5-O7
36	II	101	LHG	O6-C4-C5-O7
36	22	615	LHG	O10-C23-O8-C6
32	Yy	611	CLA	C2B-C3B-CAB-CBB
32	2	609	CLA	C2B-C3B-CAB-CBB
32	C	511	CLA	C2B-C3B-CAB-CBB
32	Y	610	CLA	C2B-C3B-CAB-CBB
32	y	313	CLA	C2B-C3B-CAB-CBB
32	DD	401	CLA	C2B-C3B-CAB-CBB
34	A	409	BCR	C23-C24-C25-C26
34	T	101	BCR	C23-C24-C25-C26
34	KK	103	BCR	C1-C6-C7-C8
34	TT	101	BCR	C23-C24-C25-C26
40	Rr	614	LUT	C1-C6-C7-C8
40	44	612	LUT	C1-C6-C7-C8
40	22	614	LUT	C1-C6-C7-C8
40	N	615	LUT	C5-C6-C7-C8
40	S	614	LUT	C5-C6-C7-C8
40	g	615	LUT	C5-C6-C7-C8
40	n	616	LUT	C1-C6-C7-C8
40	r	614	LUT	C1-C6-C7-C8
40	y	317	LUT	C5-C6-C7-C8
40	RR	315	LUT	C5-C6-C7-C8
36	Ll	102	LHG	C14-C15-C16-C17
32	SS	303	CLA	O1D-CGD-O2D-CED
32	y	315	CLA	CBA-CGA-O2A-C1
32	C	507	CLA	C5-C6-C7-C8
32	D	405	CLA	C5-C6-C7-C8
32	c	508	CLA	C5-C6-C7-C8
32	B	605	CLA	C8-C10-C11-C12
36	D	408	LHG	C28-C29-C30-C31
36	N	619	LHG	C5-C4-O6-P
32	CC	514	CLA	O1A-CGA-O2A-C1
32	Gg	312	CLA	C5-C6-C7-C8
32	4	303	CLA	CBD-CGD-O2D-CED
36	A	414	LHG	C13-C14-C15-C16
38	Mm	101	LMG	C17-C18-C19-C20
32	Ss	613	CLA	C2A-CAA-CBA-CGA
44	B	603	DGD	C1A-C2A-C3A-C4A
37	L	101	SQD	O6-C44-C45-O47
37	L	101	SQD	O47-C45-C46-O48
37	LL	102	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
37	LL	102	SQD	O47-C45-C46-O48
35	D	407	PL9	C4-C3-C7-C8
35	DD	406	PL9	C4-C3-C7-C8
37	A	412	SQD	O49-C7-O47-C45
32	RR	309	CLA	O1A-CGA-O2A-C1
32	RR	314	CLA	O1A-CGA-O2A-C1
36	D	409	LHG	C10-C11-C12-C13
37	l	102	SQD	C30-C31-C32-C33
32	A	405	CLA	C8-C10-C11-C12
32	b	603	CLA	C8-C10-C11-C12
32	BB	602	CLA	C10-C11-C12-C13
32	Gg	304	CLA	C8-C10-C11-C12
32	a	405	CLA	C2-C3-C5-C6
32	Bb	611	CLA	C2-C3-C5-C6
32	Gg	312	CLA	C2-C3-C5-C6
36	YY	618	LHG	C11-C12-C13-C14
39	n	607	CHL	C16-C17-C18-C19
38	a	412	LMG	C10-C11-C12-C13
32	C	512	CLA	C6-C7-C8-C9
32	C	513	CLA	C6-C7-C8-C9
32	b	601	CLA	C11-C12-C13-C14
32	n	610	CLA	C11-C12-C13-C14
32	BB	601	CLA	C14-C13-C15-C16
32	CC	506	CLA	C14-C13-C15-C16
32	Bb	613	CLA	C6-C7-C8-C9
32	Bb	615	CLA	C11-C10-C8-C9
33	a	409	PHO	C11-C12-C13-C14
39	Yy	609	CHL	C14-C13-C15-C16
39	N	607	CHL	C14-C13-C15-C16
39	y	311	CHL	C14-C13-C15-C16
32	D	404	CLA	C8-C10-C11-C12
38	Cc	501	LMG	O6-C5-C6-O5
32	b	602	CLA	C16-C17-C18-C19
39	y	303	CHL	C16-C17-C18-C20
39	RR	307	CHL	O1D-CGD-O2D-CED
32	Rr	601	CLA	O2A-C1-C2-C3
32	Ss	604	CLA	O2A-C1-C2-C3
32	R	601	CLA	O2A-C1-C2-C3
32	R	610	CLA	O2A-C1-C2-C3
32	R	611	CLA	O2A-C1-C2-C3
32	S	602	CLA	O2A-C1-C2-C3
32	Y	603	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	r	601	CLA	O2A-C1-C2-C3
32	r	612	CLA	O2A-C1-C2-C3
32	s	604	CLA	O2A-C1-C2-C3
32	RR	311	CLA	O2A-C1-C2-C3
32	Gg	311	CLA	O2A-C1-C2-C3
32	Nn	302	CLA	O2A-C1-C2-C3
39	N	609	CHL	O2A-C1-C2-C3
32	r	609	CLA	O1A-CGA-O2A-C1
36	AA	414	LHG	C13-C14-C15-C16
37	Ll	101	SQD	C7-C8-C9-C10
32	N	612	CLA	C1A-C2A-CAA-CBA
32	NN	612	CLA	C1A-C2A-CAA-CBA
32	b	616	CLA	C15-C16-C17-C18
32	BB	602	CLA	C15-C16-C17-C18
32	S	602	CLA	CBA-CGA-O2A-C1
32	g	602	CLA	CBA-CGA-O2A-C1
36	Nn	310	LHG	C24-C23-O8-C6
39	Nn	315	CHL	CBA-CGA-O2A-C1
36	D	409	LHG	C27-C28-C29-C30
37	A	412	SQD	O47-C7-C8-C9
32	b	611	CLA	C2-C3-C5-C6
32	b	601	CLA	C16-C17-C18-C19
32	b	602	CLA	C16-C17-C18-C20
32	Bb	606	CLA	C16-C17-C18-C19
38	c	519	LMG	C12-C13-C14-C15
36	C	522	LHG	C8-C7-O7-C5
32	Bb	609	CLA	C10-C11-C12-C13
32	c	510	CLA	O1D-CGD-O2D-CED
32	c	502	CLA	C13-C15-C16-C17
36	l	101	LHG	C14-C15-C16-C17
36	y	320	LHG	C13-C14-C15-C16
32	R	609	CLA	O1A-CGA-O2A-C1
32	BB	609	CLA	C13-C15-C16-C17
36	44	616	LHG	O6-C4-C5-C6
39	YY	601	CHL	C16-C17-C18-C20
39	Nn	317	CHL	C16-C17-C18-C19
32	C	506	CLA	C8-C10-C11-C12
32	N	602	CLA	C8-C10-C11-C12
34	XX	202	BCR	C7-C8-C9-C34
32	C	503	CLA	C6-C7-C8-C10
32	D	405	CLA	C12-C13-C15-C16
32	N	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	b	601	CLA	C11-C12-C13-C15
32	b	603	CLA	C11-C10-C8-C7
32	b	610	CLA	C6-C7-C8-C10
32	r	609	CLA	C11-C12-C13-C15
32	BB	601	CLA	C12-C13-C15-C16
32	BB	603	CLA	C11-C12-C13-C15
32	BB	605	CLA	C11-C10-C8-C7
32	BB	605	CLA	C12-C13-C15-C16
32	BB	611	CLA	C6-C7-C8-C10
32	CC	506	CLA	C12-C13-C15-C16
32	Bb	601	CLA	C11-C12-C13-C15
32	Bb	603	CLA	C11-C10-C8-C7
32	Bb	605	CLA	C12-C13-C15-C16
32	Bb	608	CLA	C11-C10-C8-C7
32	Bb	615	CLA	C11-C10-C8-C7
32	Cc	504	CLA	C11-C12-C13-C15
33	Aa	409	PHO	C11-C12-C13-C15
39	N	607	CHL	C12-C13-C15-C16
39	GG	601	CHL	C11-C12-C13-C15
32	BB	603	CLA	C8-C10-C11-C12
32	Bb	603	CLA	C8-C10-C11-C12
34	K	102	BCR	C7-C8-C9-C10
40	y	317	LUT	C7-C8-C9-C10
44	Aa	401	DGD	C2A-C1A-O1G-C1G
38	DD	409	LMG	C31-C32-C33-C34
32	D	404	CLA	O1A-CGA-O2A-C1
32	b	615	CLA	O1A-CGA-O2A-C1
32	s	612	CLA	O1A-CGA-O2A-C1
32	DD	403	CLA	O1A-CGA-O2A-C1
32	Cc	504	CLA	O1A-CGA-O2A-C1
32	A	405	CLA	C13-C15-C16-C17
32	b	610	CLA	C5-C6-C7-C8
32	Bb	602	CLA	C15-C16-C17-C18
32	CC	514	CLA	C2A-CAA-CBA-CGA
32	RR	302	CLA	C2A-CAA-CBA-CGA
39	s	606	CHL	C2A-CAA-CBA-CGA
39	3	607	CHL	O1D-CGD-O2D-CED
32	c	510	CLA	C4-C3-C5-C6
32	DD	401	CLA	C4-C3-C5-C6
35	d	404	PL9	C35-C34-C36-C37
32	BB	606	CLA	O1A-CGA-O2A-C1
36	r	616	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
39	s	605	CHL	O1A-CGA-O2A-C1
38	BB	619	LMG	C33-C34-C35-C36
36	0	201	LHG	C14-C15-C16-C17
32	CC	513	CLA	O2A-C1-C2-C3
32	Bb	612	CLA	O2A-C1-C2-C3
44	BB	623	DGD	CDB-CEB-CFB-CGB
32	y	315	CLA	O1A-CGA-O2A-C1
32	B	618	CLA	O1A-CGA-O2A-C1
32	B	623	CLA	O1A-CGA-O2A-C1
37	Aa	413	SQD	O10-C23-O48-C46
33	Aa	409	PHO	C15-C16-C17-C18
39	Yy	601	CHL	C16-C17-C18-C20
32	Bb	610	CLA	C3-C5-C6-C7
32	Bb	610	CLA	C8-C10-C11-C12
36	A	411	LHG	C10-C11-C12-C13
36	DD	408	LHG	C10-C11-C12-C13
32	DD	404	CLA	C5-C6-C7-C8
36	C	522	LHG	O9-C7-O7-C5
44	CC	518	DGD	O1B-C1B-O2G-C2G
32	Rr	604	CLA	CAA-CBA-CGA-O2A
36	A	413	LHG	O6-C4-C5-O7
36	33	614	LHG	O6-C4-C5-O7
36	D	408	LHG	O6-C4-C5-O7
36	AA	411	LHG	O6-C4-C5-O7
36	DD	407	LHG	O6-C4-C5-O7
32	Ss	608	CLA	O2A-C1-C2-C3
32	G	610	CLA	O2A-C1-C2-C3
32	g	614	CLA	O2A-C1-C2-C3
32	r	611	CLA	O2A-C1-C2-C3
32	s	608	CLA	O2A-C1-C2-C3
32	Gg	315	CLA	O2A-C1-C2-C3
39	RR	306	CHL	O2A-C1-C2-C3
39	SS	308	CHL	O2A-C1-C2-C3
35	d	404	PL9	C44-C46-C47-C48
36	CC	523	LHG	C4-C5-C6-O8
44	C	523	DGD	C2B-C1B-O2G-C2G
37	l	102	SQD	C7-C8-C9-C10
32	b	607	CLA	C5-C6-C7-C8
32	Aa	406	CLA	C8-C10-C11-C12
32	Bb	610	CLA	C15-C16-C17-C18
46	e	101	HEM	C4B-C3B-CAB-CBB
46	EE	102	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
46	Ee	101	HEM	C4B-C3B-CAB-CBB
39	YY	601	CHL	C16-C17-C18-C19
36	Rr	617	LHG	C25-C26-C27-C28
38	F	101	LMG	C31-C32-C33-C34
32	g	602	CLA	O1A-CGA-O2A-C1
32	BB	601	CLA	CBA-CGA-O2A-C1
32	b	609	CLA	C13-C15-C16-C17
32	B	604	CLA	C15-C16-C17-C18
32	D	401	CLA	C4-C3-C5-C6
35	AA	410	PL9	C15-C14-C16-C17
32	Bb	612	CLA	C2A-CAA-CBA-CGA
32	Bb	601	CLA	C5-C6-C7-C8
38	B	615	LMG	C17-C18-C19-C20
36	YY	618	LHG	O7-C5-C6-O8
37	L	102	SQD	O6-C44-C45-O47
37	B	602	SQD	O6-C44-C45-O47
37	Aa	413	SQD	O6-C44-C45-O47
38	b	621	LMG	O7-C8-C9-O8
38	Bb	621	LMG	O7-C8-C9-O8
38	Mm	101	LMG	O1-C7-C8-O7
44	C	523	DGD	O2G-C2G-C3G-O3G
32	Yy	602	CLA	C11-C10-C8-C9
32	N	610	CLA	C11-C12-C13-C14
32	Y	602	CLA	C6-C7-C8-C9
32	b	603	CLA	C11-C10-C8-C9
32	BB	603	CLA	C11-C12-C13-C14
32	BB	605	CLA	C11-C10-C8-C9
32	B	622	CLA	C14-C13-C15-C16
32	Bb	603	CLA	C11-C10-C8-C9
32	Cc	504	CLA	C11-C12-C13-C14
32	C	515	CLA	O1A-CGA-O2A-C1
39	Nn	315	CHL	O1A-CGA-O2A-C1
44	Aa	401	DGD	O1A-C1A-O1G-C1G
36	Yy	618	LHG	C15-C16-C17-C18
36	s	616	LHG	C17-C18-C19-C20
32	g	603	CLA	C8-C10-C11-C12
32	Bb	607	CLA	C10-C11-C12-C13
44	Aa	401	DGD	C5B-C6B-C7B-C8B
36	r	616	LHG	C25-C26-C27-C28
32	C	511	CLA	C2-C1-O2A-CGA
39	Gg	308	CHL	C2-C1-O2A-CGA
32	c	508	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
44	a	415	DGD	C2A-C1A-O1G-C1G
32	c	505	CLA	C16-C17-C18-C20
32	CC	503	CLA	C16-C17-C18-C20
32	CC	504	CLA	C16-C17-C18-C19
32	RR	302	CLA	C16-C17-C18-C20
32	YY	602	CLA	C16-C17-C18-C20
39	Y	609	CHL	C16-C17-C18-C20
32	CC	510	CLA	C10-C11-C12-C13
36	CC	523	LHG	C24-C25-C26-C27
38	j	101	LMG	C29-C30-C31-C32
37	L	101	SQD	C28-C29-C30-C31
37	LL	102	SQD	C12-C13-C14-C15
32	CC	506	CLA	C4-C3-C5-C6
32	b	604	CLA	C2-C3-C5-C6
35	D	407	PL9	C43-C44-C46-C47
32	c	510	CLA	C15-C16-C17-C18
36	J	101	LHG	O2-C2-C3-O3
38	B	615	LMG	C30-C31-C32-C33
32	C	507	CLA	C2A-CAA-CBA-CGA
32	Nn	312	CLA	C2A-CAA-CBA-CGA
44	C	520	DGD	C2A-C3A-C4A-C5A
32	Y	602	CLA	C16-C17-C18-C20
32	b	606	CLA	C16-C17-C18-C20
32	Cc	507	CLA	C16-C17-C18-C20
39	YY	609	CHL	C16-C17-C18-C20
37	LL	102	SQD	C28-C29-C30-C31
44	CC	522	DGD	C1A-C2A-C3A-C4A
44	a	415	DGD	O1A-C1A-O1G-C1G
32	Cc	512	CLA	C15-C16-C17-C18
32	d	402	CLA	C3-C5-C6-C7
32	c	513	CLA	O1D-CGD-O2D-CED
37	CC	501	SQD	C11-C10-C9-C8
38	Mm	101	LMG	O9-C10-O7-C8
32	c	508	CLA	O1A-CGA-O2A-C1
32	A	408	CLA	C3-C5-C6-C7
32	y	315	CLA	C3-C5-C6-C7
36	BB	622	LHG	C11-C10-C9-C8
34	Hh	101	BCR	C11-C12-C13-C35
40	y	317	LUT	C7-C8-C9-C19
35	D	407	PL9	C39-C41-C42-C43
32	Rr	603	CLA	C4B-C3B-CAB-CBB
32	Rr	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	Rr	611	CLA	C4B-C3B-CAB-CBB
32	Ss	603	CLA	C4B-C3B-CAB-CBB
32	Ss	610	CLA	C4B-C3B-CAB-CBB
32	44	602	CLA	C1A-C2A-CAA-CBA
32	11	610	CLA	C4B-C3B-CAB-CBB
32	33	604	CLA	C4B-C3B-CAB-CBB
32	33	609	CLA	C4B-C3B-CAB-CBB
32	1	613	CLA	C4B-C3B-CAB-CBB
32	S	610	CLA	C4B-C3B-CAB-CBB
32	Y	612	CLA	C4B-C3B-CAB-CBB
32	a	410	CLA	C4B-C3B-CAB-CBB
32	b	601	CLA	C4B-C3B-CAB-CBB
32	b	610	CLA	C4B-C3B-CAB-CBB
32	c	509	CLA	C4B-C3B-CAB-CBB
32	d	402	CLA	C4B-C3B-CAB-CBB
32	n	611	CLA	C4B-C3B-CAB-CBB
32	r	603	CLA	C4B-C3B-CAB-CBB
32	r	611	CLA	C4B-C3B-CAB-CBB
32	s	603	CLA	C4B-C3B-CAB-CBB
32	s	610	CLA	C4B-C3B-CAB-CBB
32	y	313	CLA	C4B-C3B-CAB-CBB
32	BB	603	CLA	C1A-C2A-CAA-CBA
32	B	605	CLA	C4B-C3B-CAB-CBB
32	GG	602	CLA	C1A-C2A-CAA-CBA
32	GG	612	CLA	C4B-C3B-CAB-CBB
32	RR	311	CLA	C4B-C3B-CAB-CBB
32	SS	311	CLA	C4B-C3B-CAB-CBB
32	Bb	601	CLA	C4B-C3B-CAB-CBB
32	Bb	610	CLA	C4B-C3B-CAB-CBB
32	Cc	505	CLA	C1A-C2A-CAA-CBA
32	Dd	402	CLA	C1A-C2A-CAA-CBA
32	Dd	402	CLA	C4B-C3B-CAB-CBB
39	N	607	CHL	O1D-CGD-O2D-CED
37	L	101	SQD	C12-C13-C14-C15
32	b	613	CLA	C4-C3-C5-C6
32	CC	503	CLA	C4-C3-C5-C6
35	DD	406	PL9	C35-C34-C36-C37
32	AA	405	CLA	C13-C15-C16-C17
32	DD	401	CLA	C2-C3-C5-C6
34	CC	516	BCR	C21-C22-C23-C24
40	Yy	616	LUT	C7-C8-C9-C10
32	R	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
44	h	102	DGD	C5A-C6A-C7A-C8A
32	b	609	CLA	C2A-CAA-CBA-CGA
32	n	602	CLA	C2A-CAA-CBA-CGA
32	Cc	512	CLA	C2A-CAA-CBA-CGA
39	Gg	302	CHL	C2A-CAA-CBA-CGA
38	a	412	LMG	C13-C14-C15-C16
44	CC	518	DGD	C2B-C3B-C4B-C5B
32	4	303	CLA	O1D-CGD-O2D-CED
36	11	614	LHG	O6-C4-C5-C6
36	3	614	LHG	O6-C4-C5-C6
36	4	315	LHG	O6-C4-C5-C6
36	AA	411	LHG	O6-C4-C5-C6
36	II	101	LHG	O6-C4-C5-C6
38	b	620	LMG	C11-C10-O7-C8
38	b	620	LMG	O9-C10-O7-C8
38	m	101	LMG	O9-C10-O7-C8
32	Rr	602	CLA	C6-C7-C8-C10
32	Rr	609	CLA	C11-C12-C13-C15
32	Yy	602	CLA	C11-C10-C8-C7
32	C	509	CLA	C11-C10-C8-C7
32	R	602	CLA	C12-C13-C15-C16
32	Y	610	CLA	C6-C7-C8-C10
32	b	608	CLA	C11-C10-C8-C7
32	b	609	CLA	C11-C10-C8-C7
32	c	502	CLA	C6-C7-C8-C10
32	g	611	CLA	C11-C12-C13-C15
32	n	610	CLA	C6-C7-C8-C10
32	BB	602	CLA	C6-C7-C8-C10
32	BB	607	CLA	C11-C10-C8-C7
32	BB	610	CLA	C11-C10-C8-C7
32	CC	502	CLA	C6-C7-C8-C10
32	B	606	CLA	C11-C10-C8-C7
32	B	607	CLA	C6-C7-C8-C10
32	B	619	CLA	C6-C7-C8-C10
32	B	622	CLA	C12-C13-C15-C16
32	B	624	CLA	C11-C10-C8-C7
32	NN	610	CLA	C12-C13-C15-C16
32	RR	302	CLA	C12-C13-C15-C16
32	Cc	503	CLA	C6-C7-C8-C10
32	Cc	505	CLA	C12-C13-C15-C16
39	N	607	CHL	C11-C10-C8-C7
39	Y	609	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	c	506	CLA	C16-C17-C18-C20
36	r	616	LHG	C10-C11-C12-C13
39	y	311	CHL	CBD-CGD-O2D-CED
32	S	602	CLA	O1A-CGA-O2A-C1
36	A	413	LHG	C24-C25-C26-C27
36	AA	411	LHG	C11-C10-C9-C8
32	C	509	CLA	C13-C15-C16-C17
32	B	605	CLA	C13-C15-C16-C17
32	A	406	CLA	C3A-C2A-CAA-CBA
32	G	603	CLA	C16-C17-C18-C20
32	GG	603	CLA	C16-C17-C18-C20
32	Dd	402	CLA	C16-C17-C18-C19
39	y	303	CHL	C16-C17-C18-C19
35	D	407	PL9	C2-C3-C7-C8
35	DD	406	PL9	C2-C3-C7-C8
36	A	411	LHG	O6-C4-C5-O7
36	Y	618	LHG	O6-C4-C5-O7
36	g	618	LHG	C7-C8-C9-C10
38	DD	409	LMG	C32-C33-C34-C35
37	C	501	SQD	C8-C7-O47-C45
32	s	612	CLA	C2A-CAA-CBA-CGA
32	c	506	CLA	C11-C10-C8-C9
32	r	602	CLA	C6-C7-C8-C9
32	r	609	CLA	C11-C12-C13-C14
32	y	312	CLA	C11-C12-C13-C14
32	y	314	CLA	C11-C12-C13-C14
32	CC	508	CLA	C11-C10-C8-C9
32	Bb	608	CLA	C11-C10-C8-C9
39	GG	601	CHL	C11-C12-C13-C14
36	Nn	310	LHG	O10-C23-O8-C6
37	Aa	413	SQD	C24-C25-C26-C27
37	Ll	101	SQD	C30-C31-C32-C33
38	WW	201	LMG	C38-C39-C40-C41
44	D	411	DGD	C7A-C8A-C9A-CAA
44	a	415	DGD	C5B-C6B-C7B-C8B
32	Bb	602	CLA	C5-C6-C7-C8
32	A	406	CLA	C1-C2-C3-C4
32	Rr	601	CLA	C1-C2-C3-C4
32	Rr	603	CLA	C1-C2-C3-C4
32	Rr	604	CLA	C1-C2-C3-C4
32	Rr	608	CLA	C1-C2-C3-C4
32	Rr	610	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	Rr	611	CLA	C1-C2-C3-C4
32	Rr	612	CLA	C1-C2-C3-C4
32	Rr	613	CLA	C1-C2-C3-C4
32	Ss	602	CLA	C1-C2-C3-C4
32	Ss	603	CLA	C1-C2-C3-C4
32	Ss	604	CLA	C1-C2-C3-C4
32	Ss	608	CLA	C1-C2-C3-C4
32	Ss	609	CLA	C1-C2-C3-C4
32	Ss	610	CLA	C1-C2-C3-C4
32	Ss	611	CLA	C1-C2-C3-C4
32	Ss	612	CLA	C1-C2-C3-C4
32	Ss	613	CLA	C1-C2-C3-C4
32	Yy	603	CLA	C1-C2-C3-C4
32	Yy	604	CLA	C1-C2-C3-C4
32	Yy	614	CLA	C1-C2-C3-C4
32	44	615	CLA	C1-C2-C3-C4
32	G	610	CLA	C1-C2-C3-C4
32	G	612	CLA	C1-C2-C3-C4
32	N	611	CLA	C1-C2-C3-C4
32	N	613	CLA	C1-C2-C3-C4
32	R	601	CLA	C1-C2-C3-C4
32	R	603	CLA	C1-C2-C3-C4
32	R	604	CLA	C1-C2-C3-C4
32	R	608	CLA	C1-C2-C3-C4
32	R	610	CLA	C1-C2-C3-C4
32	R	614	CLA	C1-C2-C3-C4
32	S	602	CLA	C1-C2-C3-C4
32	S	604	CLA	C1-C2-C3-C4
32	S	610	CLA	C1-C2-C3-C4
32	S	611	CLA	C1-C2-C3-C4
32	Y	603	CLA	C1-C2-C3-C4
32	Y	604	CLA	C1-C2-C3-C4
32	Y	614	CLA	C1-C2-C3-C4
32	a	407	CLA	C1-C2-C3-C4
32	g	610	CLA	C1-C2-C3-C4
32	g	612	CLA	C1-C2-C3-C4
32	g	614	CLA	C1-C2-C3-C4
32	n	603	CLA	C1-C2-C3-C4
32	n	604	CLA	C1-C2-C3-C4
32	n	612	CLA	C1-C2-C3-C4
32	n	613	CLA	C1-C2-C3-C4
32	n	614	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	r	601	CLA	C1-C2-C3-C4
32	r	603	CLA	C1-C2-C3-C4
32	r	604	CLA	C1-C2-C3-C4
32	r	608	CLA	C1-C2-C3-C4
32	r	610	CLA	C1-C2-C3-C4
32	r	611	CLA	C1-C2-C3-C4
32	r	612	CLA	C1-C2-C3-C4
32	r	613	CLA	C1-C2-C3-C4
32	s	602	CLA	C1-C2-C3-C4
32	s	603	CLA	C1-C2-C3-C4
32	s	604	CLA	C1-C2-C3-C4
32	s	608	CLA	C1-C2-C3-C4
32	s	609	CLA	C1-C2-C3-C4
32	s	610	CLA	C1-C2-C3-C4
32	s	611	CLA	C1-C2-C3-C4
32	s	612	CLA	C1-C2-C3-C4
32	s	613	CLA	C1-C2-C3-C4
32	y	305	CLA	C1-C2-C3-C4
32	y	306	CLA	C1-C2-C3-C4
32	y	316	CLA	C1-C2-C3-C4
32	AA	406	CLA	C1-C2-C3-C4
32	GG	610	CLA	C1-C2-C3-C4
32	GG	612	CLA	C1-C2-C3-C4
32	NN	611	CLA	C1-C2-C3-C4
32	NN	613	CLA	C1-C2-C3-C4
32	RR	303	CLA	C1-C2-C3-C4
32	RR	304	CLA	C1-C2-C3-C4
32	RR	308	CLA	C1-C2-C3-C4
32	RR	310	CLA	C1-C2-C3-C4
32	RR	314	CLA	C1-C2-C3-C4
32	SS	303	CLA	C1-C2-C3-C4
32	SS	305	CLA	C1-C2-C3-C4
32	SS	311	CLA	C1-C2-C3-C4
32	SS	312	CLA	C1-C2-C3-C4
32	SS	314	CLA	C1-C2-C3-C4
32	YY	603	CLA	C1-C2-C3-C4
32	YY	604	CLA	C1-C2-C3-C4
32	YY	614	CLA	C1-C2-C3-C4
32	Aa	407	CLA	C1-C2-C3-C4
32	Gg	311	CLA	C1-C2-C3-C4
32	Gg	313	CLA	C1-C2-C3-C4
32	Gg	315	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	Nn	303	CLA	C1-C2-C3-C4
32	Nn	304	CLA	C1-C2-C3-C4
32	Nn	305	CLA	C1-C2-C3-C4
32	Nn	313	CLA	C1-C2-C3-C4
32	Nn	314	CLA	C1-C2-C3-C4
37	AA	412	SQD	O5-C5-C6-S
39	Rr	607	CHL	C1-C2-C3-C4
39	Ss	605	CHL	C1-C2-C3-C4
39	Ss	606	CHL	C1-C2-C3-C4
39	Yy	608	CHL	C1-C2-C3-C4
39	R	606	CHL	C1-C2-C3-C4
39	R	607	CHL	C1-C2-C3-C4
39	Y	608	CHL	C1-C2-C3-C4
39	n	608	CHL	C1-C2-C3-C4
39	n	609	CHL	C1-C2-C3-C4
39	r	607	CHL	C1-C2-C3-C4
39	s	605	CHL	C1-C2-C3-C4
39	s	606	CHL	C1-C2-C3-C4
39	y	310	CHL	C1-C2-C3-C4
39	RR	306	CHL	C1-C2-C3-C4
39	RR	307	CHL	C1-C2-C3-C4
39	YY	608	CHL	C1-C2-C3-C4
39	Nn	318	CHL	C1-C2-C3-C4
39	Nn	319	CHL	C1-C2-C3-C4
40	YY	615	LUT	C21-C26-C27-C28
44	BB	623	DGD	C1B-C2B-C3B-C4B
32	Gg	304	CLA	C3-C5-C6-C7
36	A	413	LHG	O7-C5-C6-O8
37	LL	101	SQD	O6-C44-C45-O47
38	m	101	LMG	O1-C7-C8-O7
36	Dd	405	LHG	C25-C26-C27-C28
44	C	519	DGD	C2B-C3B-C4B-C5B
32	G	602	CLA	O2A-C1-C2-C3
32	n	604	CLA	O2A-C1-C2-C3
39	n	601	CHL	O2A-C1-C2-C3
32	DD	404	CLA	CBD-CGD-O2D-CED
36	r	616	LHG	C4-C5-C6-O8
38	b	621	LMG	O1-C7-C8-C9
38	m	101	LMG	O1-C7-C8-C9
38	Bb	621	LMG	O1-C7-C8-C9
38	Mm	101	LMG	O1-C7-C8-C9
32	Rr	609	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	GG	603	CLA	C5-C6-C7-C8
32	RR	302	CLA	C13-C15-C16-C17
32	Bb	602	CLA	C13-C15-C16-C17
32	Rr	604	CLA	CAD-CBD-CGD-O2D
32	Ss	603	CLA	CAD-CBD-CGD-O2D
32	Ss	610	CLA	CAD-CBD-CGD-O2D
32	44	615	CLA	CAD-CBD-CGD-O2D
32	11	603	CLA	CAD-CBD-CGD-O2D
32	22	609	CLA	CAD-CBD-CGD-O2D
32	22	610	CLA	CAD-CBD-CGD-O2D
32	33	610	CLA	CAD-CBD-CGD-O2D
32	3	610	CLA	CAD-CBD-CGD-O2D
32	C	505	CLA	CAD-CBD-CGD-O2D
32	C	506	CLA	CAD-CBD-CGD-O2D
32	G	604	CLA	CAD-CBD-CGD-O2D
32	N	604	CLA	CAD-CBD-CGD-O2D
32	Y	614	CLA	CAD-CBD-CGD-O2D
32	b	602	CLA	CAD-CBD-CGD-O2D
32	b	603	CLA	CAD-CBD-CGD-O2D
32	b	613	CLA	CAD-CBD-CGD-O2D
32	c	502	CLA	CAD-CBD-CGD-O2D
32	c	505	CLA	CAD-CBD-CGD-O2D
32	c	509	CLA	CAD-CBD-CGD-O2D
32	g	614	CLA	CAD-CBD-CGD-O2D
32	n	612	CLA	CAD-CBD-CGD-O2D
32	r	604	CLA	CAD-CBD-CGD-O2D
32	s	603	CLA	CAD-CBD-CGD-O2D
32	s	604	CLA	CAD-CBD-CGD-O2D
32	s	610	CLA	CAD-CBD-CGD-O2D
32	BB	604	CLA	CAD-CBD-CGD-O2D
32	CC	504	CLA	CAD-CBD-CGD-O2D
32	B	621	CLA	CAD-CBD-CGD-O2D
32	GG	604	CLA	CAD-CBD-CGD-O2D
32	NN	604	CLA	CAD-CBD-CGD-O2D
32	SS	309	CLA	CAD-CBD-CGD-O2D
32	YY	614	CLA	CAD-CBD-CGD-O2D
32	Bb	602	CLA	CAD-CBD-CGD-O2D
32	Bb	613	CLA	CAD-CBD-CGD-O2D
32	Cc	507	CLA	CAD-CBD-CGD-O2D
32	Gg	315	CLA	CAD-CBD-CGD-O2D
38	Mm	101	LMG	C11-C10-O7-C8
39	Rr	607	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
39	Yy	607	CHL	CAD-CBD-CGD-O2D
39	33	601	CHL	CAD-CBD-CGD-O2D
39	3	601	CHL	CAD-CBD-CGD-O2D
39	3	605	CHL	CAD-CBD-CGD-O2D
39	S	601	CHL	CAD-CBD-CGD-O2D
39	g	609	CHL	CAD-CBD-CGD-O2D
39	r	607	CHL	CAD-CBD-CGD-O2D
39	GG	606	CHL	C1A-C2A-CAA-CBA
39	SS	302	CHL	CAD-CBD-CGD-O2D
32	G	603	CLA	C13-C15-C16-C17
36	EE	101	LHG	C15-C16-C17-C18
32	GG	603	CLA	C13-C15-C16-C17
36	A	411	LHG	C23-C24-C25-C26
39	Yy	601	CHL	C16-C17-C18-C19
32	R	611	CLA	C2A-CAA-CBA-CGA
32	y	315	CLA	C2A-CAA-CBA-CGA
38	F	101	LMG	C32-C33-C34-C35
32	C	503	CLA	C5-C6-C7-C8
32	b	601	CLA	C15-C16-C17-C18
32	AA	405	CLA	C8-C10-C11-C12
36	d	405	LHG	C25-C26-C27-C28
32	BB	601	CLA	O1A-CGA-O2A-C1
32	Rr	604	CLA	CAD-CBD-CGD-O1D
32	Ss	603	CLA	CAD-CBD-CGD-O1D
32	Ss	610	CLA	CAD-CBD-CGD-O1D
32	Yy	602	CLA	CHA-CBD-CGD-O1D
32	44	603	CLA	CHA-CBD-CGD-O1D
32	44	609	CLA	CHA-CBD-CGD-O1D
32	44	611	CLA	CHA-CBD-CGD-O1D
32	44	611	CLA	CHA-CBD-CGD-O2D
32	44	615	CLA	CAD-CBD-CGD-O1D
32	11	602	CLA	CHA-CBD-CGD-O1D
32	11	603	CLA	CAD-CBD-CGD-O1D
32	11	612	CLA	CHA-CBD-CGD-O1D
32	11	612	CLA	CHA-CBD-CGD-O2D
32	22	609	CLA	CAD-CBD-CGD-O1D
32	22	610	CLA	CAD-CBD-CGD-O1D
32	22	611	CLA	CHA-CBD-CGD-O1D
32	33	610	CLA	CAD-CBD-CGD-O1D
32	1	603	CLA	CAD-CBD-CGD-O1D
32	1	613	CLA	CHA-CBD-CGD-O1D
32	1	613	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	2	609	CLA	CHA-CBD-CGD-O1D
32	2	609	CLA	CHA-CBD-CGD-O2D
32	2	612	CLA	CHA-CBD-CGD-O1D
32	2	612	CLA	CHA-CBD-CGD-O2D
32	3	603	CLA	CHA-CBD-CGD-O1D
32	3	603	CLA	CHA-CBD-CGD-O2D
32	3	610	CLA	CAD-CBD-CGD-O1D
32	C	505	CLA	CAD-CBD-CGD-O1D
32	C	506	CLA	CAD-CBD-CGD-O1D
32	C	511	CLA	CHA-CBD-CGD-O1D
32	C	511	CLA	CHA-CBD-CGD-O2D
32	G	604	CLA	CAD-CBD-CGD-O1D
32	G	611	CLA	CAD-CBD-CGD-O1D
32	N	604	CLA	CAD-CBD-CGD-O1D
32	R	604	CLA	CHA-CBD-CGD-O1D
32	R	604	CLA	CHA-CBD-CGD-O2D
32	R	610	CLA	CAD-CBD-CGD-O1D
32	S	602	CLA	CHA-CBD-CGD-O1D
32	S	602	CLA	CHA-CBD-CGD-O2D
32	S	603	CLA	CHA-CBD-CGD-O1D
32	S	603	CLA	CHA-CBD-CGD-O2D
32	S	604	CLA	CHA-CBD-CGD-O1D
32	X	201	CLA	CHA-CBD-CGD-O1D
32	X	201	CLA	CHA-CBD-CGD-O2D
32	Y	614	CLA	CAD-CBD-CGD-O1D
32	b	602	CLA	CAD-CBD-CGD-O1D
32	b	603	CLA	CAD-CBD-CGD-O1D
32	b	605	CLA	CHA-CBD-CGD-O1D
32	b	605	CLA	CHA-CBD-CGD-O2D
32	b	612	CLA	CHA-CBD-CGD-O1D
32	b	612	CLA	CHA-CBD-CGD-O2D
32	b	613	CLA	CAD-CBD-CGD-O1D
32	c	502	CLA	CAD-CBD-CGD-O1D
32	c	505	CLA	CAD-CBD-CGD-O1D
32	c	509	CLA	CAD-CBD-CGD-O1D
32	g	602	CLA	CHA-CBD-CGD-O1D
32	g	614	CLA	CAD-CBD-CGD-O1D
32	n	612	CLA	CAD-CBD-CGD-O1D
32	r	601	CLA	CHA-CBD-CGD-O1D
32	r	604	CLA	CAD-CBD-CGD-O1D
32	s	602	CLA	CAD-CBD-CGD-O1D
32	s	603	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	s	604	CLA	CAD-CBD-CGD-O1D
32	s	610	CLA	CAD-CBD-CGD-O1D
32	y	316	CLA	CHA-CBD-CGD-O1D
32	4	304	CLA	CHA-CBD-CGD-O1D
32	4	304	CLA	CHA-CBD-CGD-O2D
32	4	312	CLA	CHA-CBD-CGD-O1D
32	4	312	CLA	CHA-CBD-CGD-O2D
32	BB	604	CLA	CAD-CBD-CGD-O1D
32	BB	606	CLA	CAD-CBD-CGD-O1D
32	BB	614	CLA	CHA-CBD-CGD-O1D
32	CC	504	CLA	CAD-CBD-CGD-O1D
32	CC	505	CLA	CAD-CBD-CGD-O1D
32	CC	510	CLA	CHA-CBD-CGD-O1D
32	CC	510	CLA	CHA-CBD-CGD-O2D
32	B	604	CLA	CAD-CBD-CGD-O1D
32	B	621	CLA	CAD-CBD-CGD-O1D
32	B	623	CLA	CAD-CBD-CGD-O1D
32	GG	602	CLA	CHA-CBD-CGD-O1D
32	GG	602	CLA	CHA-CBD-CGD-O2D
32	GG	604	CLA	CAD-CBD-CGD-O1D
32	NN	604	CLA	CAD-CBD-CGD-O1D
32	RR	304	CLA	CHA-CBD-CGD-O1D
32	RR	304	CLA	CHA-CBD-CGD-O2D
32	RR	310	CLA	CAD-CBD-CGD-O1D
32	SS	303	CLA	CHA-CBD-CGD-O1D
32	SS	303	CLA	CHA-CBD-CGD-O2D
32	SS	304	CLA	CHA-CBD-CGD-O1D
32	SS	304	CLA	CHA-CBD-CGD-O2D
32	SS	309	CLA	CAD-CBD-CGD-O1D
32	SS	312	CLA	CHA-CBD-CGD-O1D
32	XX	201	CLA	CHA-CBD-CGD-O1D
32	YY	614	CLA	CAD-CBD-CGD-O1D
32	Bb	601	CLA	CAD-CBD-CGD-O1D
32	Bb	602	CLA	CAD-CBD-CGD-O1D
32	Bb	603	CLA	CAD-CBD-CGD-O1D
32	Bb	605	CLA	CHA-CBD-CGD-O1D
32	Bb	605	CLA	CHA-CBD-CGD-O2D
32	Bb	608	CLA	CHA-CBD-CGD-O1D
32	Bb	613	CLA	CAD-CBD-CGD-O1D
32	Cc	503	CLA	CAD-CBD-CGD-O1D
32	Cc	507	CLA	CAD-CBD-CGD-O1D
32	Dd	401	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	Gg	305	CLA	CAD-CBD-CGD-O1D
32	Gg	315	CLA	CAD-CBD-CGD-O1D
33	D	402	PHO	CHA-CBD-CGD-O1D
33	D	402	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O1D
33	DD	402	PHO	CHA-CBD-CGD-O1D
33	DD	402	PHO	CHA-CBD-CGD-O2D
33	Aa	408	PHO	CHA-CBD-CGD-O2D
33	Aa	409	PHO	CHA-CBD-CGD-O1D
33	Aa	409	PHO	CHA-CBD-CGD-O2D
36	A	414	LHG	C3-O3-P-O5
36	44	614	LHG	C4-O6-P-O5
36	3	614	LHG	C4-O6-P-O4
36	0	201	LHG	C3-O3-P-O5
36	C	522	LHG	C3-O3-P-O5
36	C	522	LHG	C4-O6-P-O5
36	D	410	LHG	C3-O3-P-O5
36	D	410	LHG	C4-O6-P-O5
36	K	101	LHG	C4-O6-P-O5
36	d	405	LHG	C3-O3-P-O5
36	g	618	LHG	C4-O6-P-O5
36	4	315	LHG	C4-O6-P-O5
36	AA	414	LHG	C3-O3-P-O5
36	BB	622	LHG	C3-O3-P-O5
36	CC	521	LHG	C4-O6-P-O5
36	DD	407	LHG	C3-O3-P-O5
36	EE	101	LHG	C3-O3-P-O5
36	EE	101	LHG	C4-O6-P-O5
36	II	101	LHG	C4-O6-P-O3
36	KK	101	LHG	C4-O6-P-O5
36	NN	619	LHG	C3-O3-P-O4
36	NN	619	LHG	C3-O3-P-O6
36	YY	618	LHG	C3-O3-P-O6
36	Dd	405	LHG	C3-O3-P-O5
36	Gg	319	LHG	C4-O6-P-O5
36	Ll	102	LHG	C4-O6-P-O5
39	Rr	607	CHL	CAD-CBD-CGD-O1D
39	Yy	607	CHL	CAD-CBD-CGD-O1D
39	11	605	CHL	CHA-CBD-CGD-O1D
39	11	605	CHL	CHA-CBD-CGD-O2D
39	11	607	CHL	CHA-CBD-CGD-O2D
39	33	601	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	3	601	CHL	CAD-CBD-CGD-O1D
39	3	605	CHL	CAD-CBD-CGD-O1D
39	R	606	CHL	CHA-CBD-CGD-O1D
39	R	606	CHL	CHA-CBD-CGD-O2D
39	S	601	CHL	CAD-CBD-CGD-O1D
39	g	609	CHL	CAD-CBD-CGD-O1D
39	n	606	CHL	CHA-CBD-CGD-O2D
39	r	605	CHL	CHA-CBD-CGD-O1D
39	r	605	CHL	CHA-CBD-CGD-O2D
39	r	607	CHL	CAD-CBD-CGD-O1D
39	SS	302	CHL	CAD-CBD-CGD-O1D
39	Gg	310	CHL	CAD-CBD-CGD-O1D
39	Nn	316	CHL	CHA-CBD-CGD-O1D
39	Nn	316	CHL	CHA-CBD-CGD-O2D
39	Nn	318	CHL	CAD-CBD-CGD-O1D
32	b	606	CLA	C16-C17-C18-C19
32	AA	408	CLA	C11-C12-C13-C15
32	CC	504	CLA	C16-C17-C18-C20
38	Mm	101	LMG	C33-C34-C35-C36
32	BB	610	CLA	C4-C3-C5-C6
32	Bb	604	CLA	C4-C3-C5-C6
32	Rr	603	CLA	C2B-C3B-CAB-CBB
32	Rr	608	CLA	C2B-C3B-CAB-CBB
32	11	612	CLA	C2B-C3B-CAB-CBB
32	11	613	CLA	C2B-C3B-CAB-CBB
32	22	602	CLA	C2B-C3B-CAB-CBB
32	33	604	CLA	C2B-C3B-CAB-CBB
32	1	609	CLA	C2B-C3B-CAB-CBB
32	3	612	CLA	C2B-C3B-CAB-CBB
32	C	505	CLA	C2B-C3B-CAB-CBB
32	D	405	CLA	C2B-C3B-CAB-CBB
32	G	613	CLA	C2B-C3B-CAB-CBB
32	N	610	CLA	C2B-C3B-CAB-CBB
32	R	612	CLA	C2B-C3B-CAB-CBB
32	Y	612	CLA	C2B-C3B-CAB-CBB
32	b	615	CLA	C2B-C3B-CAB-CBB
32	c	511	CLA	C2B-C3B-CAB-CBB
32	r	603	CLA	C2B-C3B-CAB-CBB
32	s	610	CLA	C2B-C3B-CAB-CBB
32	BB	602	CLA	C2B-C3B-CAB-CBB
32	CC	510	CLA	C2B-C3B-CAB-CBB
32	DD	404	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	B	619	CLA	C2B-C3B-CAB-CBB
32	B	621	CLA	C2B-C3B-CAB-CBB
32	NN	610	CLA	C2B-C3B-CAB-CBB
32	Aa	406	CLA	C2B-C3B-CAB-CBB
32	Aa	410	CLA	C2B-C3B-CAB-CBB
32	Bb	603	CLA	C2B-C3B-CAB-CBB
32	Cc	513	CLA	C2B-C3B-CAB-CBB
34	H	101	BCR	C23-C24-C25-C26
34	b	619	BCR	C23-C24-C25-C30
34	AA	409	BCR	C23-C24-C25-C26
34	BB	618	BCR	C23-C24-C25-C30
34	B	614	BCR	C23-C24-C25-C30
34	Bb	619	BCR	C1-C6-C7-C8
34	Cc	516	BCR	C1-C6-C7-C8
34	Cc	518	BCR	C23-C24-C25-C30
40	2	614	LUT	C1-C6-C7-C8
40	G	615	LUT	C1-C6-C7-C8
40	GG	616	LUT	C1-C6-C7-C8
40	SS	315	LUT	C1-C6-C7-C8
38	Aa	412	LMG	C13-C14-C15-C16
32	c	510	CLA	C2-C3-C5-C6
38	W	201	LMG	C29-C30-C31-C32
34	TT	101	BCR	C37-C22-C23-C24
36	22	615	LHG	C5-C4-O6-P
36	K	101	LHG	C5-C4-O6-P
36	n	618	LHG	C5-C4-O6-P
36	Nn	310	LHG	C5-C4-O6-P
38	Dd	408	LMG	C29-C30-C31-C32
32	RR	302	CLA	C16-C17-C18-C19
32	CC	508	CLA	C13-C15-C16-C17
44	BB	623	DGD	C7A-C8A-C9A-CAA
36	AA	411	LHG	C23-C24-C25-C26
32	R	614	CLA	O1A-CGA-O2A-C1
36	Yy	618	LHG	C31-C32-C33-C34
35	A	410	PL9	C4-C3-C7-C8
32	B	619	CLA	C15-C16-C17-C18
32	Aa	406	CLA	C2C-C3C-CAC-CBC
36	D	410	LHG	C23-C24-C25-C26
36	s	616	LHG	C11-C10-C9-C8
44	C	523	DGD	O1B-C1B-O2G-C2G
32	NN	602	CLA	C13-C15-C16-C17
32	Yy	603	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	r	604	CLA	O2A-C1-C2-C3
32	s	609	CLA	O2A-C1-C2-C3
32	NN	611	CLA	O2A-C1-C2-C3
32	SS	303	CLA	O2A-C1-C2-C3
32	YY	603	CLA	O2A-C1-C2-C3
39	Rr	605	CHL	O2A-C1-C2-C3
39	R	606	CHL	O2A-C1-C2-C3
32	G	603	CLA	C5-C6-C7-C8
32	R	602	CLA	C13-C15-C16-C17
39	Yy	609	CHL	C8-C10-C11-C12
32	D	401	CLA	C2-C3-C5-C6
32	G	613	CLA	C4C-C3C-CAC-CBC
32	Y	613	CLA	C11-C12-C13-C14
44	Hh	102	DGD	CDB-CEB-CFB-CGB
32	A	408	CLA	C11-C12-C13-C15
32	Y	602	CLA	C16-C17-C18-C19
32	d	402	CLA	C16-C17-C18-C19
32	Cc	508	CLA	C16-C17-C18-C20
36	A	411	LHG	O6-C4-C5-C6
36	A	414	LHG	C16-C17-C18-C19
36	AA	414	LHG	C16-C17-C18-C19
32	Rr	602	CLA	C6-C7-C8-C9
32	b	616	CLA	C14-C13-C15-C16
32	BB	602	CLA	C6-C7-C8-C9
32	BB	609	CLA	C6-C7-C8-C9
32	BB	611	CLA	C6-C7-C8-C9
32	CC	502	CLA	C6-C7-C8-C9
32	B	607	CLA	C6-C7-C8-C9
32	B	619	CLA	C6-C7-C8-C9
32	B	620	CLA	C11-C12-C13-C14
32	NN	610	CLA	C11-C12-C13-C14
32	YY	602	CLA	C6-C7-C8-C9
32	YY	610	CLA	C6-C7-C8-C9
32	Bb	601	CLA	C11-C12-C13-C14
32	Bb	607	CLA	C11-C10-C8-C9
32	Cc	505	CLA	C14-C13-C15-C16
32	Cc	508	CLA	C11-C10-C8-C9
32	Cc	513	CLA	C11-C10-C8-C9
32	N	610	CLA	C11-C12-C13-C15
32	c	501	CLA	C11-C12-C13-C15
32	y	312	CLA	C11-C12-C13-C15
32	NN	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	Bb	607	CLA	C11-C10-C8-C7
32	Dd	401	CLA	C11-C10-C8-C7
32	Nn	301	CLA	C6-C7-C8-C10
38	C	521	LMG	C12-C13-C14-C15
32	c	511	CLA	O1A-CGA-O2A-C1
32	a	406	CLA	C2C-C3C-CAC-CBC
36	Yy	618	LHG	O6-C4-C5-O7
36	y	320	LHG	O6-C4-C5-O7
36	YY	618	LHG	O6-C4-C5-O7
36	Nn	310	LHG	O6-C4-C5-O7
38	A	415	LMG	O6-C1-O1-C7
32	A	405	CLA	C16-C17-C18-C20
32	C	505	CLA	C16-C17-C18-C19
32	R	602	CLA	C16-C17-C18-C19
32	c	505	CLA	C16-C17-C18-C19
32	CC	503	CLA	C16-C17-C18-C19
32	YY	602	CLA	C16-C17-C18-C19
32	Dd	402	CLA	C16-C17-C18-C20
39	YY	609	CHL	C16-C17-C18-C19
39	y	311	CHL	O1D-CGD-O2D-CED
32	R	614	CLA	CBA-CGA-O2A-C1
32	DD	404	CLA	O1A-CGA-O2A-C1
32	B	605	CLA	C5-C6-C7-C8
38	m	101	LMG	C33-C34-C35-C36
32	Y	613	CLA	CBD-CGD-O2D-CED
32	Bb	601	CLA	C15-C16-C17-C18
35	AA	410	PL9	C40-C39-C41-C42
44	BB	623	DGD	C5B-C6B-C7B-C8B
44	Hh	102	DGD	C4A-C5A-C6A-C7A
32	b	613	CLA	C2-C3-C5-C6
32	c	501	CLA	C2-C3-C5-C6
36	11	614	LHG	C24-C25-C26-C27
32	c	506	CLA	C16-C17-C18-C19
32	Cc	507	CLA	C16-C17-C18-C19
39	Y	609	CHL	C16-C17-C18-C19
36	l	101	LHG	C24-C25-C26-C27
44	Cc	520	DGD	C9B-CAB-CBB-CCB
36	Rr	617	LHG	O9-C7-O7-C5
37	C	501	SQD	O49-C7-O47-C45
38	Bb	620	LMG	O9-C10-O7-C8
44	CC	519	DGD	CBA-CCA-CDA-CEA
36	CC	523	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
38	BB	619	LMG	O7-C8-C9-O8
38	Bb	621	LMG	O1-C7-C8-O7
32	Gg	304	CLA	CAA-CBA-CGA-O2A
36	11	614	LHG	O10-C23-O8-C6
32	G	603	CLA	C16-C17-C18-C19
32	GG	603	CLA	C16-C17-C18-C19
32	Dd	402	CLA	C5-C6-C7-C8
44	CC	518	DGD	C1B-C2B-C3B-C4B
36	Nn	310	LHG	C11-C12-C13-C14
32	44	603	CLA	C2A-CAA-CBA-CGA
32	RR	311	CLA	C2A-CAA-CBA-CGA
32	b	616	CLA	C8-C10-C11-C12
36	Ll	102	LHG	C35-C36-C37-C38
32	B	624	CLA	C2-C1-O2A-CGA
39	s	605	CHL	C2-C1-O2A-CGA
32	C	505	CLA	C4-C3-C5-C6
32	Ss	609	CLA	O2A-C1-C2-C3
32	n	611	CLA	O2A-C1-C2-C3
32	n	614	CLA	O2A-C1-C2-C3
32	Nn	305	CLA	O2A-C1-C2-C3
39	Y	608	CHL	O2A-C1-C2-C3
39	n	606	CHL	O2A-C1-C2-C3
39	r	605	CHL	O2A-C1-C2-C3
37	AA	412	SQD	O47-C7-C8-C9
38	WW	201	LMG	C12-C13-C14-C15
35	d	404	PL9	C34-C36-C37-C38
36	y	320	LHG	C4-C5-C6-O8
37	LL	102	SQD	O6-C44-C45-C46
37	L	102	SQD	C9-C10-C11-C12
32	Cc	506	CLA	C5-C6-C7-C8
38	c	519	LMG	O7-C10-C11-C12
32	C	509	CLA	C16-C17-C18-C19
44	C	519	DGD	C2B-C1B-O2G-C2G
36	0	201	LHG	C32-C33-C34-C35
34	c	515	BCR	C21-C22-C23-C24
34	c	516	BCR	C7-C8-C9-C10
36	11	614	LHG	C24-C23-O8-C6
37	C	501	SQD	C45-C44-O6-C1
38	a	412	LMG	C11-C12-C13-C14
32	YY	602	CLA	C15-C16-C17-C18
38	WW	201	LMG	C29-C30-C31-C32
32	Aa	405	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	Bb	609	CLA	C2A-CAA-CBA-CGA
39	Yy	609	CHL	C16-C17-C18-C20
36	0	201	LHG	C15-C16-C17-C18
44	c	518	DGD	C9B-CAB-CBB-CCB
44	Cc	520	DGD	C3B-C4B-C5B-C6B
38	W	201	LMG	C12-C13-C14-C15
32	Cc	512	CLA	C4-C3-C5-C6
35	D	407	PL9	C30-C29-C31-C32
32	CC	506	CLA	C2-C3-C5-C6
35	AA	410	PL9	C12-C11-C9-C8
32	Cc	506	CLA	C2C-C3C-CAC-CBC
32	CC	508	CLA	C16-C17-C18-C19
44	c	517	DGD	C2B-C3B-C4B-C5B
32	C	503	CLA	C6-C7-C8-C9
32	C	509	CLA	C11-C10-C8-C9
32	D	404	CLA	C6-C7-C8-C9
32	Y	610	CLA	C6-C7-C8-C9
32	Y	610	CLA	C14-C13-C15-C16
32	b	607	CLA	C11-C10-C8-C9
32	b	608	CLA	C11-C10-C8-C9
32	b	609	CLA	C11-C10-C8-C9
32	b	612	CLA	C6-C7-C8-C9
32	n	610	CLA	C6-C7-C8-C9
32	B	605	CLA	C6-C7-C8-C9
32	Bb	612	CLA	C6-C7-C8-C9
39	n	607	CHL	C6-C7-C8-C9
32	Rr	609	CLA	CBA-CGA-O2A-C1
32	c	511	CLA	CBA-CGA-O2A-C1
36	Rr	617	LHG	C24-C23-O8-C6
32	BB	609	CLA	C5-C6-C7-C8
37	C	501	SQD	C11-C10-C9-C8
32	22	604	CLA	C4B-C3B-CAB-CBB
32	33	603	CLA	C4B-C3B-CAB-CBB
32	33	611	CLA	C4B-C3B-CAB-CBB
32	1	610	CLA	C4B-C3B-CAB-CBB
32	G	602	CLA	C4B-C3B-CAB-CBB
32	G	614	CLA	C4B-C3B-CAB-CBB
32	S	603	CLA	C4B-C3B-CAB-CBB
32	c	507	CLA	C4B-C3B-CAB-CBB
32	g	611	CLA	C4B-C3B-CAB-CBB
32	g	614	CLA	C4B-C3B-CAB-CBB
32	r	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	s	613	CLA	C4B-C3B-CAB-CBB
32	GG	613	CLA	C4B-C3B-CAB-CBB
32	SS	304	CLA	C4B-C3B-CAB-CBB
32	SS	313	CLA	C4B-C3B-CAB-CBB
32	YY	603	CLA	C4B-C3B-CAB-CBB
32	Cc	509	CLA	C4B-C3B-CAB-CBB
32	Gg	311	CLA	C4B-C3B-CAB-CBB
43	C	502	LMU	O5B-C5B-C6B-O6B
32	Rr	609	CLA	O1A-CGA-O2A-C1
35	D	407	PL9	C32-C33-C34-C35
32	DD	404	CLA	CBA-CGA-O2A-C1
32	b	604	CLA	C10-C11-C12-C13
32	Bb	616	CLA	C8-C10-C11-C12
36	l	101	LHG	C35-C36-C37-C38
36	A	411	LHG	C9-C10-C11-C12
32	C	504	CLA	C4-C3-C5-C6
32	Rr	609	CLA	C2-C3-C5-C6
32	BB	610	CLA	C2-C3-C5-C6
36	n	618	LHG	O6-C4-C5-O7
36	KK	101	LHG	O6-C4-C5-O7
32	Rr	604	CLA	O2A-C1-C2-C3
32	Rr	611	CLA	O2A-C1-C2-C3
32	Ss	612	CLA	O2A-C1-C2-C3
32	s	612	CLA	O2A-C1-C2-C3
39	g	607	CHL	O2A-C1-C2-C3
39	Gg	308	CHL	O2A-C1-C2-C3
36	0	201	LHG	C29-C30-C31-C32
32	R	613	CLA	C2C-C3C-CAC-CBC
32	Cc	510	CLA	C5-C6-C7-C8
32	d	402	CLA	C16-C17-C18-C20
32	Cc	508	CLA	C16-C17-C18-C19
37	Ll	101	SQD	C10-C11-C12-C13
44	Hh	102	DGD	O2G-C1B-C2B-C3B
36	DD	408	LHG	C27-C28-C29-C30
32	C	504	CLA	C6-C7-C8-C10
32	Y	610	CLA	C12-C13-C15-C16
32	b	607	CLA	C11-C10-C8-C7
32	AA	405	CLA	C11-C10-C8-C7
32	CC	510	CLA	C11-C12-C13-C15
32	B	623	CLA	C11-C10-C8-C7
32	b	609	CLA	C10-C11-C12-C13
38	C	521	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
36	D	410	LHG	O2-C2-C3-O3
37	B	602	SQD	C24-C23-O48-C46
36	Dd	406	LHG	O7-C7-C8-C9
36	NN	619	LHG	C13-C14-C15-C16
32	c	509	CLA	C16-C17-C18-C19
32	AA	408	CLA	C11-C12-C13-C14
32	b	601	CLA	O1A-CGA-O2A-C1
37	B	602	SQD	O10-C23-O48-C46
32	44	602	CLA	C3A-C2A-CAA-CBA
32	N	613	CLA	C3A-C2A-CAA-CBA
32	g	611	CLA	C3A-C2A-CAA-CBA
32	r	604	CLA	C3A-C2A-CAA-CBA
32	r	608	CLA	C3A-C2A-CAA-CBA
32	BB	604	CLA	C4-C3-C5-C6
35	Dd	404	PL9	C12-C11-C9-C10
37	Ll	101	SQD	C11-C12-C13-C14
32	Bb	601	CLA	CAA-CBA-CGA-O2A
35	d	404	PL9	C28-C29-C31-C32
36	YY	618	LHG	C9-C10-C11-C12
38	W	201	LMG	C38-C39-C40-C41
38	Cc	501	LMG	C12-C13-C14-C15
32	C	514	CLA	C13-C15-C16-C17
38	AA	415	LMG	O6-C1-O1-C7
40	22	614	LUT	C20-C13-C14-C15
40	2	614	LUT	C20-C13-C14-C15
42	Rr	616	NEX	C39-C29-C30-C31
42	Yy	617	NEX	C39-C29-C30-C31
42	N	618	NEX	C39-C29-C30-C31
42	R	617	NEX	C39-C29-C30-C31
42	Y	617	NEX	C39-C29-C30-C31
42	Y	619	NEX	C39-C29-C30-C31
42	g	617	NEX	C39-C29-C30-C31
42	n	617	NEX	C39-C29-C30-C31
42	y	319	NEX	C39-C29-C30-C31
42	NN	618	NEX	C39-C29-C30-C31
42	RR	317	NEX	C39-C29-C30-C31
42	YY	617	NEX	C39-C29-C30-C31
42	Gg	318	NEX	C39-C29-C30-C31
42	Nn	309	NEX	C39-C29-C30-C31
32	C	511	CLA	C10-C11-C12-C13
32	Y	602	CLA	C15-C16-C17-C18
33	a	409	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	Y	618	LHG	C18-C19-C20-C21
44	Hh	102	DGD	C9B-CAB-CBB-CCB
36	Ss	616	LHG	O9-C7-O7-C5
36	1	614	LHG	C25-C26-C27-C28
37	l	102	SQD	C10-C11-C12-C13
36	y	320	LHG	C10-C11-C12-C13
36	Dd	406	LHG	C24-C25-C26-C27
36	Ll	102	LHG	C24-C25-C26-C27
32	R	608	CLA	C2-C1-O2A-CGA
32	r	613	CLA	C2-C1-O2A-CGA
32	GG	610	CLA	C2-C1-O2A-CGA
32	RR	308	CLA	C2-C1-O2A-CGA
32	SS	312	CLA	C2-C1-O2A-CGA
32	YY	612	CLA	C2-C1-O2A-CGA
32	C	511	CLA	C8-C10-C11-C12
32	c	503	CLA	C13-C15-C16-C17
37	Aa	413	SQD	C32-C33-C34-C35
36	DD	408	LHG	C19-C20-C21-C22
32	Y	613	CLA	O1D-CGD-O2D-CED
32	CC	512	CLA	C8-C10-C11-C12
32	G	611	CLA	C4-C3-C5-C6
32	Y	613	CLA	C4-C3-C5-C6
32	Cc	511	CLA	C4-C3-C5-C6
32	g	613	CLA	C4C-C3C-CAC-CBC
32	CC	503	CLA	C2-C3-C5-C6
44	C	519	DGD	O1B-C1B-O2G-C2G
32	C	504	CLA	C16-C17-C18-C20
32	a	405	CLA	C16-C17-C18-C20
32	Aa	410	CLA	C11-C12-C13-C15
39	Y	601	CHL	C16-C17-C18-C20
36	Ss	616	LHG	C11-C10-C9-C8
32	Bb	605	CLA	C15-C16-C17-C18
32	N	611	CLA	O2A-C1-C2-C3
39	R	607	CHL	O2A-C1-C2-C3
39	RR	307	CHL	O2A-C1-C2-C3
32	44	611	CLA	CAA-CBA-CGA-O1A
36	Ll	102	LHG	C31-C32-C33-C34
35	D	407	PL9	C9-C11-C12-C13
38	B	615	LMG	C7-C8-C9-O8
37	C	501	SQD	C15-C16-C17-C18
39	NN	607	CHL	O1D-CGD-O2D-CED
32	C	508	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	AA	405	CLA	C11-C10-C8-C9
32	BB	606	CLA	C11-C10-C8-C9
32	CC	507	CLA	C6-C7-C8-C9
32	CC	512	CLA	C6-C7-C8-C9
32	DD	401	CLA	C11-C12-C13-C14
32	B	618	CLA	C6-C7-C8-C9
32	B	623	CLA	C11-C10-C8-C9
32	Bb	616	CLA	C14-C13-C15-C16
33	A	407	PHO	C14-C13-C15-C16
33	AA	407	PHO	C14-C13-C15-C16
36	DD	408	LHG	C17-C18-C19-C20
32	r	604	CLA	CAA-CBA-CGA-O1A
37	LL	101	SQD	C9-C10-C11-C12
38	Cc	501	LMG	O7-C10-C11-C12
32	C	514	CLA	O2A-C1-C2-C3
32	b	607	CLA	C10-C11-C12-C13
32	CC	510	CLA	C8-C10-C11-C12
33	Aa	409	PHO	C8-C10-C11-C12
39	Yy	605	CHL	C1A-C2A-CAA-CBA
39	Y	605	CHL	C1A-C2A-CAA-CBA
39	YY	605	CHL	C1A-C2A-CAA-CBA
38	B	615	LMG	C16-C17-C18-C19
32	44	611	CLA	CAA-CBA-CGA-O2A
39	y	311	CHL	C16-C17-C18-C20
32	Cc	511	CLA	C2-C3-C5-C6
39	NN	601	CHL	C2A-CAA-CBA-CGA
32	CC	502	CLA	C3-C5-C6-C7
44	BB	624	DGD	C2D-C1D-O3G-C3G
36	Y	618	LHG	C7-C8-C9-C10
39	NN	607	CHL	CBD-CGD-O2D-CED
32	Yy	613	CLA	C2A-CAA-CBA-CGA
39	Y	609	CHL	C2A-CAA-CBA-CGA
32	N	602	CLA	C5-C6-C7-C8
32	A	406	CLA	C1A-C2A-CAA-CBA
32	y	305	CLA	C1A-C2A-CAA-CBA
32	AA	406	CLA	C1A-C2A-CAA-CBA
32	DD	404	CLA	C1A-C2A-CAA-CBA
32	YY	604	CLA	C1A-C2A-CAA-CBA
32	Gg	313	CLA	C1A-C2A-CAA-CBA
40	22	614	LUT	C12-C13-C14-C15
40	2	614	LUT	C12-C13-C14-C15
42	Rr	616	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
42	Yy	617	NEX	C28-C29-C30-C31
42	N	618	NEX	C28-C29-C30-C31
42	R	617	NEX	C28-C29-C30-C31
42	Y	617	NEX	C28-C29-C30-C31
42	Y	619	NEX	C28-C29-C30-C31
42	g	617	NEX	C28-C29-C30-C31
42	n	617	NEX	C28-C29-C30-C31
42	y	319	NEX	C28-C29-C30-C31
42	NN	618	NEX	C28-C29-C30-C31
42	RR	317	NEX	C28-C29-C30-C31
42	YY	617	NEX	C28-C29-C30-C31
42	Gg	318	NEX	C28-C29-C30-C31
42	Nn	309	NEX	C28-C29-C30-C31
36	A	411	LHG	C11-C10-C9-C8
44	BB	625	DGD	O6D-C5D-C6D-O5D
36	D	408	LHG	C27-C28-C29-C30
36	CC	523	LHG	C30-C31-C32-C33
37	C	501	SQD	C16-C17-C18-C19
32	Rr	610	CLA	C2B-C3B-CAB-CBB
32	Rr	611	CLA	C2B-C3B-CAB-CBB
32	Ss	603	CLA	C2B-C3B-CAB-CBB
32	Ss	608	CLA	C2B-C3B-CAB-CBB
32	Ss	610	CLA	C2B-C3B-CAB-CBB
32	Yy	614	CLA	C2B-C3B-CAB-CBB
32	44	604	CLA	C2B-C3B-CAB-CBB
32	11	610	CLA	C2B-C3B-CAB-CBB
32	22	609	CLA	C2B-C3B-CAB-CBB
32	22	613	CLA	C2B-C3B-CAB-CBB
32	33	603	CLA	C2B-C3B-CAB-CBB
32	33	609	CLA	C2B-C3B-CAB-CBB
32	33	611	CLA	C2B-C3B-CAB-CBB
32	33	613	CLA	C2B-C3B-CAB-CBB
32	1	613	CLA	C2B-C3B-CAB-CBB
32	2	603	CLA	C2B-C3B-CAB-CBB
32	2	610	CLA	C2B-C3B-CAB-CBB
32	2	613	CLA	C2B-C3B-CAB-CBB
32	3	611	CLA	C2B-C3B-CAB-CBB
32	3	613	CLA	C2B-C3B-CAB-CBB
32	C	504	CLA	C2B-C3B-CAB-CBB
32	G	604	CLA	C2B-C3B-CAB-CBB
32	G	611	CLA	C2B-C3B-CAB-CBB
32	S	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	S	612	CLA	C2B-C3B-CAB-CBB
32	Y	604	CLA	C2B-C3B-CAB-CBB
32	a	410	CLA	C2B-C3B-CAB-CBB
32	b	601	CLA	C2B-C3B-CAB-CBB
32	b	610	CLA	C2B-C3B-CAB-CBB
32	c	504	CLA	C2B-C3B-CAB-CBB
32	c	512	CLA	C2B-C3B-CAB-CBB
32	d	402	CLA	C2B-C3B-CAB-CBB
32	g	613	CLA	C2B-C3B-CAB-CBB
32	r	602	CLA	C2B-C3B-CAB-CBB
32	r	604	CLA	C2B-C3B-CAB-CBB
32	r	611	CLA	C2B-C3B-CAB-CBB
32	s	603	CLA	C2B-C3B-CAB-CBB
32	y	316	CLA	C2B-C3B-CAB-CBB
32	4	311	CLA	C2B-C3B-CAB-CBB
32	4	312	CLA	C2B-C3B-CAB-CBB
32	B	605	CLA	C2B-C3B-CAB-CBB
32	GG	613	CLA	C2B-C3B-CAB-CBB
32	RR	311	CLA	C2B-C3B-CAB-CBB
32	SS	313	CLA	C2B-C3B-CAB-CBB
32	YY	604	CLA	C2B-C3B-CAB-CBB
32	YY	614	CLA	C2B-C3B-CAB-CBB
32	Bb	601	CLA	C2B-C3B-CAB-CBB
32	Bb	610	CLA	C2B-C3B-CAB-CBB
32	Bb	615	CLA	C2B-C3B-CAB-CBB
32	Cc	506	CLA	C2B-C3B-CAB-CBB
32	Cc	514	CLA	C2B-C3B-CAB-CBB
32	Dd	402	CLA	C2B-C3B-CAB-CBB
32	Gg	311	CLA	C2B-C3B-CAB-CBB
34	c	516	BCR	C23-C24-C25-C30
40	Ss	614	LUT	C1-C6-C7-C8
40	YY	616	LUT	C1-C6-C7-C8
38	m	101	LMG	C11-C10-O7-C8
32	4	303	CLA	CAA-CBA-CGA-O1A
32	A	408	CLA	C11-C12-C13-C14
32	C	509	CLA	C16-C17-C18-C20
44	Cc	520	DGD	C1A-C2A-C3A-C4A
36	n	618	LHG	C11-C12-C13-C14
32	4	312	CLA	CAA-CBA-CGA-O1A
32	C	507	CLA	C4-C3-C5-C6
37	B	602	SQD	C24-C25-C26-C27
32	G	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	Y	613	CLA	C2-C3-C5-C6
36	AA	411	LHG	C9-C10-C11-C12
36	Dd	405	LHG	C33-C34-C35-C36
44	c	518	DGD	C3B-C4B-C5B-C6B
32	Rr	603	CLA	O2A-C1-C2-C3
32	Ss	611	CLA	O2A-C1-C2-C3
32	44	615	CLA	O2A-C1-C2-C3
32	R	603	CLA	O2A-C1-C2-C3
32	R	608	CLA	O2A-C1-C2-C3
32	S	611	CLA	O2A-C1-C2-C3
32	g	602	CLA	O2A-C1-C2-C3
32	r	603	CLA	O2A-C1-C2-C3
32	r	613	CLA	O2A-C1-C2-C3
32	GG	602	CLA	O2A-C1-C2-C3
32	SS	312	CLA	O2A-C1-C2-C3
32	Gg	303	CLA	O2A-C1-C2-C3
32	Gg	313	CLA	O2A-C1-C2-C3
39	Rr	607	CHL	O2A-C1-C2-C3
39	Yy	608	CHL	O2A-C1-C2-C3
32	44	610	CLA	CAA-CBA-CGA-O2A
39	44	607	CHL	CAA-CBA-CGA-O2A
36	A	413	LHG	C30-C31-C32-C33
36	r	616	LHG	C31-C32-C33-C34
32	A	405	CLA	C12-C13-C15-C16
32	D	404	CLA	C6-C7-C8-C10
32	b	604	CLA	C12-C13-C15-C16
32	b	605	CLA	C12-C13-C15-C16
32	b	606	CLA	C11-C10-C8-C7
32	b	609	CLA	C11-C12-C13-C15
32	c	510	CLA	C12-C13-C15-C16
32	c	512	CLA	C11-C10-C8-C7
32	r	602	CLA	C11-C10-C8-C7
32	AA	405	CLA	C12-C13-C15-C16
32	BB	602	CLA	C12-C13-C15-C16
32	BB	604	CLA	C11-C10-C8-C7
32	BB	606	CLA	C11-C10-C8-C7
32	B	618	CLA	C6-C7-C8-C10
32	B	619	CLA	C12-C13-C15-C16
32	Bb	604	CLA	C12-C13-C15-C16
32	Bb	609	CLA	C11-C10-C8-C7
32	Cc	514	CLA	C11-C10-C8-C7
32	Dd	402	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
33	A	407	PHO	C6-C7-C8-C10
39	n	607	CHL	C6-C7-C8-C10
39	YY	609	CHL	C12-C13-C15-C16
38	a	412	LMG	C31-C32-C33-C34
39	Y	601	CHL	C16-C17-C18-C19
39	Ss	606	CHL	C2A-CAA-CBA-CGA
36	d	406	LHG	C24-C25-C26-C27
32	B	606	CLA	C5-C6-C7-C8
36	A	414	LHG	O7-C5-C6-O8
36	l	101	LHG	O7-C5-C6-O8
36	EE	101	LHG	O7-C5-C6-O8
36	Ll	102	LHG	O7-C5-C6-O8
38	CC	520	LMG	O1-C7-C8-O7
39	44	608	CHL	CAA-CBA-CGA-O2A
35	AA	410	PL9	C4-C3-C7-C8
35	Dd	404	PL9	C4-C3-C7-C8
36	0	201	LHG	C28-C29-C30-C31
36	s	616	LHG	C9-C10-C11-C12
36	DD	407	LHG	C27-C28-C29-C30
38	C	521	LMG	C18-C19-C20-C21
32	g	603	CLA	C3-C5-C6-C7
36	d	405	LHG	C33-C34-C35-C36
32	4	303	CLA	CAA-CBA-CGA-O2A
36	Yy	618	LHG	C10-C11-C12-C13
44	CC	518	DGD	CAB-CBB-CCB-CDB
32	C	513	CLA	C8-C10-C11-C12
33	DD	402	PHO	C8-C10-C11-C12
32	AA	405	CLA	C16-C17-C18-C20
37	L	101	SQD	C45-C46-O48-C23
36	Y	618	LHG	C16-C17-C18-C19
36	Y	618	LHG	C31-C32-C33-C34
39	44	608	CHL	CAA-CBA-CGA-O1A
39	4	308	CHL	CAA-CBA-CGA-O2A
32	B	621	CLA	C4-C3-C5-C6
32	YY	613	CLA	C4-C3-C5-C6
35	AA	410	PL9	C35-C34-C36-C37
35	Dd	404	PL9	C35-C34-C36-C37
39	Rr	607	CHL	CAA-CBA-CGA-O2A
32	C	504	CLA	C2-C3-C5-C6
32	C	505	CLA	C2-C3-C5-C6
32	Bb	604	CLA	C2-C3-C5-C6
32	Cc	512	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
35	DD	406	PL9	C28-C29-C31-C32
32	S	611	CLA	C2-C1-O2A-CGA
32	NN	610	CLA	C2-C1-O2A-CGA
32	CC	508	CLA	C10-C11-C12-C13
39	44	605	CHL	CAA-CBA-CGA-O2A
34	Cc	517	BCR	C21-C22-C23-C24
32	B	618	CLA	C13-C15-C16-C17
32	b	601	CLA	CBA-CGA-O2A-C1
39	44	605	CHL	CAA-CBA-CGA-O1A
32	b	609	CLA	C11-C12-C13-C14
32	B	622	CLA	C11-C10-C8-C9
32	CC	513	CLA	C13-C15-C16-C17
36	II	101	LHG	C24-C25-C26-C27
36	Ll	102	LHG	C9-C10-C11-C12
32	A	408	CLA	C8-C10-C11-C12
32	G	603	CLA	C10-C11-C12-C13
32	c	509	CLA	C16-C17-C18-C20
32	CC	508	CLA	C16-C17-C18-C20
32	c	509	CLA	C4-C3-C5-C6
38	Aa	412	LMG	C29-C30-C31-C32
44	CC	518	DGD	C7B-C8B-C9B-CAB
32	YY	613	CLA	C2-C3-C5-C6
32	Cc	509	CLA	O1A-CGA-O2A-C1
36	YY	618	LHG	C31-C32-C33-C34
32	b	606	CLA	C5-C6-C7-C8
32	C	505	CLA	C16-C17-C18-C20
44	B	603	DGD	CCA-CDA-CEA-CFA
32	S	603	CLA	CAA-CBA-CGA-O2A
39	4	308	CHL	CAA-CBA-CGA-O1A
46	Ee	101	HEM	CAA-CBA-CGA-O2A
46	Ee	101	HEM	CAD-CBD-CGD-O2D
32	Ss	602	CLA	O2A-C1-C2-C3
32	G	612	CLA	O2A-C1-C2-C3
32	Y	614	CLA	O2A-C1-C2-C3
32	s	602	CLA	O2A-C1-C2-C3
32	s	611	CLA	O2A-C1-C2-C3
32	y	316	CLA	O2A-C1-C2-C3
32	RR	308	CLA	O2A-C1-C2-C3
32	RR	314	CLA	O2A-C1-C2-C3
32	Aa	407	CLA	O2A-C1-C2-C3
39	R	605	CHL	O2A-C1-C2-C3
39	n	608	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
39	r	607	CHL	O2A-C1-C2-C3
39	s	605	CHL	O2A-C1-C2-C3
39	y	310	CHL	O2A-C1-C2-C3
39	YY	608	CHL	O2A-C1-C2-C3
39	Nn	316	CHL	O2A-C1-C2-C3
32	C	512	CLA	C13-C15-C16-C17
38	Bb	620	LMG	C11-C10-O7-C8
36	Rr	617	LHG	O10-C23-O8-C6
36	1	614	LHG	O8-C23-C24-C25
36	YY	618	LHG	C16-C17-C18-C19
38	W	201	LMG	C33-C34-C35-C36
38	b	621	LMG	C7-C8-C9-O8
38	Bb	621	LMG	C7-C8-C9-O8
39	44	607	CHL	CAA-CBA-CGA-O1A
39	4	302	CHL	CAA-CBA-CGA-O2A
32	G	604	CLA	C1A-C2A-CAA-CBA
32	Y	611	CLA	C1A-C2A-CAA-CBA
36	0	201	LHG	C27-C28-C29-C30
32	b	614	CLA	C2A-CAA-CBA-CGA
32	YY	612	CLA	C2A-CAA-CBA-CGA
32	Bb	614	CLA	C2A-CAA-CBA-CGA
38	a	412	LMG	C29-C30-C31-C32
32	Bb	607	CLA	C15-C16-C17-C18
44	B	603	DGD	O6D-C5D-C6D-O5D
32	44	610	CLA	CAA-CBA-CGA-O1A
36	Yy	618	LHG	O9-C7-O7-C5
32	C	514	CLA	C8-C10-C11-C12
36	AA	414	LHG	C15-C16-C17-C18
32	B	606	CLA	C4-C3-C5-C6
32	44	603	CLA	CAA-CBA-CGA-O2A
36	11	614	LHG	O7-C7-C8-C9
35	DD	406	PL9	C43-C44-C46-C47
44	C	519	DGD	CAB-CBB-CCB-CDB
32	Yy	602	CLA	C16-C17-C18-C20
32	C	510	CLA	C13-C15-C16-C17
38	BB	619	LMG	C12-C13-C14-C15
32	Ss	608	CLA	C4B-C3B-CAB-CBB
32	Yy	614	CLA	C4B-C3B-CAB-CBB
32	22	613	CLA	C4B-C3B-CAB-CBB
32	33	613	CLA	C4B-C3B-CAB-CBB
32	2	603	CLA	C4B-C3B-CAB-CBB
32	2	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	2	613	CLA	C4B-C3B-CAB-CBB
32	3	613	CLA	C4B-C3B-CAB-CBB
32	G	611	CLA	C4B-C3B-CAB-CBB
32	S	612	CLA	C4B-C3B-CAB-CBB
32	Y	604	CLA	C4B-C3B-CAB-CBB
32	b	606	CLA	C4B-C3B-CAB-CBB
32	c	506	CLA	C4B-C3B-CAB-CBB
32	c	513	CLA	C4B-C3B-CAB-CBB
32	n	610	CLA	C4B-C3B-CAB-CBB
32	y	305	CLA	C4B-C3B-CAB-CBB
32	y	316	CLA	C4B-C3B-CAB-CBB
32	YY	604	CLA	C4B-C3B-CAB-CBB
32	Gg	304	CLA	C4B-C3B-CAB-CBB
32	Gg	312	CLA	C4B-C3B-CAB-CBB
32	Nn	305	CLA	C4B-C3B-CAB-CBB
44	Cc	519	DGD	C2B-C3B-C4B-C5B
32	g	603	CLA	CAA-CBA-CGA-O2A
32	C	504	CLA	C16-C17-C18-C19
32	a	405	CLA	C16-C17-C18-C19
36	N	619	LHG	C1-C2-C3-O3
33	Aa	408	PHO	CHA-CBD-CGD-O1D
39	11	607	CHL	CHA-CBD-CGD-O1D
39	G	608	CHL	CHA-CBD-CGD-O2D
39	N	601	CHL	CHA-CBD-CGD-O1D
39	N	601	CHL	CHA-CBD-CGD-O2D
39	g	605	CHL	CHA-CBD-CGD-O1D
39	g	605	CHL	CHA-CBD-CGD-O2D
39	s	605	CHL	CHA-CBD-CGD-O1D
39	YY	608	CHL	CHA-CBD-CGD-O2D
39	Gg	306	CHL	CHA-CBD-CGD-O1D
39	Gg	306	CHL	CHA-CBD-CGD-O2D
32	Dd	401	CLA	C5-C6-C7-C8
33	D	402	PHO	C8-C10-C11-C12
32	4	312	CLA	CAA-CBA-CGA-O2A
44	h	102	DGD	C4A-C5A-C6A-C7A
32	Yy	613	CLA	O1A-CGA-O2A-C1
36	33	614	LHG	O6-C4-C5-C6
36	4	301	LHG	O6-C4-C5-C6
36	Nn	310	LHG	O6-C4-C5-C6
32	g	603	CLA	C16-C17-C18-C20
32	r	609	CLA	C4-C3-C5-C6
32	y	315	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
38	b	621	LMG	O1-C7-C8-O7
32	GG	603	CLA	C10-C11-C12-C13
36	AA	414	LHG	C23-C24-C25-C26
32	c	509	CLA	C2-C3-C5-C6
32	B	606	CLA	C2-C3-C5-C6
35	A	410	PL9	C36-C37-C38-C39
32	N	610	CLA	C15-C16-C17-C18
32	g	603	CLA	C5-C6-C7-C8
34	c	516	BCR	C7-C8-C9-C34
36	y	320	LHG	C5-C4-O6-P
44	C	520	DGD	O6D-C5D-C6D-O5D
32	S	613	CLA	CAA-CBA-CGA-O2A
37	Ll	101	SQD	C18-C19-C20-C21
32	n	602	CLA	C5-C6-C7-C8
32	Yy	614	CLA	O2A-C1-C2-C3
32	S	604	CLA	O2A-C1-C2-C3
32	a	407	CLA	O2A-C1-C2-C3
32	GG	612	CLA	O2A-C1-C2-C3
32	RR	303	CLA	O2A-C1-C2-C3
32	SS	305	CLA	O2A-C1-C2-C3
32	SS	311	CLA	O2A-C1-C2-C3
32	YY	614	CLA	O2A-C1-C2-C3
39	Ss	605	CHL	O2A-C1-C2-C3
39	Ss	606	CHL	O2A-C1-C2-C3
32	Bb	610	CLA	C16-C17-C18-C20
32	b	607	CLA	C15-C16-C17-C18
32	44	603	CLA	CAA-CBA-CGA-O1A
39	4	306	CHL	CAA-CBA-CGA-O2A
39	4	307	CHL	CAA-CBA-CGA-O2A
39	4	309	CHL	CAA-CBA-CGA-O2A
46	Ee	101	HEM	CAA-CBA-CGA-O1A
32	C	503	CLA	C11-C10-C8-C9
32	D	401	CLA	C11-C12-C13-C14
32	D	404	CLA	C14-C13-C15-C16
32	b	602	CLA	C11-C10-C8-C9
32	c	502	CLA	C6-C7-C8-C9
32	c	510	CLA	C11-C12-C13-C14
32	c	511	CLA	C6-C7-C8-C9
32	BB	610	CLA	C11-C10-C8-C9
32	B	606	CLA	C11-C10-C8-C9
32	B	620	CLA	C14-C13-C15-C16
32	Bb	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
33	Aa	408	PHO	C11-C10-C8-C9
39	N	607	CHL	C11-C10-C8-C9
36	EE	101	LHG	C16-C17-C18-C19
37	AA	412	SQD	C5-C6-S-O8
38	m	101	LMG	C8-C7-O1-C1
38	Mm	101	LMG	C8-C7-O1-C1
44	c	518	DGD	C2G-C3G-O3G-C1D
44	Cc	520	DGD	C2G-C3G-O3G-C1D
36	N	619	LHG	C13-C14-C15-C16
32	Aa	406	CLA	C2A-CAA-CBA-CGA
32	Yy	602	CLA	C2-C1-O2A-CGA
32	N	610	CLA	C2-C1-O2A-CGA
32	Y	602	CLA	C2-C1-O2A-CGA
32	Y	610	CLA	C2-C1-O2A-CGA
32	y	304	CLA	C2-C1-O2A-CGA
32	RR	302	CLA	C2-C1-O2A-CGA
32	RR	314	CLA	C2-C1-O2A-CGA
32	r	604	CLA	O1A-CGA-O2A-C1
37	l	102	SQD	C18-C19-C20-C21
32	Cc	511	CLA	C16-C17-C18-C19
39	Yy	609	CHL	C16-C17-C18-C19
36	Rr	617	LHG	C8-C7-O7-C5
32	Cc	509	CLA	CBA-CGA-O2A-C1
32	y	306	CLA	C3A-C2A-CAA-CBA
32	YY	604	CLA	C3A-C2A-CAA-CBA
39	s	601	CHL	C3A-C2A-CAA-CBA
39	r	607	CHL	CAA-CBA-CGA-O2A
32	BB	604	CLA	C2-C3-C5-C6
33	a	408	PHO	O1D-CGD-O2D-CED
44	BB	623	DGD	C9B-CAB-CBB-CCB
39	44	606	CHL	CAA-CBA-CGA-O2A
32	a	410	CLA	C11-C12-C13-C15
32	GG	613	CLA	C4C-C3C-CAC-CBC
32	b	612	CLA	O2A-C1-C2-C3
32	Cc	503	CLA	O2A-C1-C2-C3
32	S	603	CLA	CAA-CBA-CGA-O1A
36	y	320	LHG	C31-C32-C33-C34
44	h	102	DGD	C5B-C6B-C7B-C8B
32	BB	601	CLA	CAA-CBA-CGA-O2A
32	d	402	CLA	C5-C6-C7-C8
32	c	510	CLA	C16-C17-C18-C19
32	Bb	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	4	302	CHL	CAA-CBA-CGA-O1A
39	GG	607	CHL	CAA-CBA-CGA-O2A
46	Ee	101	HEM	CAD-CBD-CGD-O1D
32	y	315	CLA	C11-C12-C13-C14
35	Dd	404	PL9	C28-C29-C31-C32
32	DD	404	CLA	O1D-CGD-O2D-CED
36	JJ	101	LHG	C11-C10-C9-C8
32	C	509	CLA	C10-C11-C12-C13
32	BB	601	CLA	C10-C11-C12-C13
32	CC	502	CLA	C8-C10-C11-C12
37	l	102	SQD	C11-C12-C13-C14
42	Rr	616	NEX	O24-C26-C27-C28
42	Yy	617	NEX	O24-C26-C27-C28
42	Y	619	NEX	O24-C26-C27-C28
42	n	617	NEX	O24-C26-C27-C28
42	y	319	NEX	O24-C26-C27-C28
42	RR	317	NEX	O24-C26-C27-C28
32	4	305	CLA	CAA-CBA-CGA-O2A
36	N	619	LHG	O6-C4-C5-O7
32	Rr	612	CLA	O2A-C1-C2-C3
32	Yy	604	CLA	O2A-C1-C2-C3
32	R	614	CLA	O2A-C1-C2-C3
32	S	610	CLA	O2A-C1-C2-C3
32	S	612	CLA	O2A-C1-C2-C3
32	g	610	CLA	O2A-C1-C2-C3
32	n	612	CLA	O2A-C1-C2-C3
32	NN	613	CLA	O2A-C1-C2-C3
39	n	609	CHL	O2A-C1-C2-C3
39	s	606	CHL	O2A-C1-C2-C3
39	RR	305	CHL	O2A-C1-C2-C3
39	Nn	319	CHL	O2A-C1-C2-C3
44	BB	624	DGD	O6D-C1D-O3G-C3G
32	44	602	CLA	CAA-CBA-CGA-O2A
32	S	613	CLA	CAA-CBA-CGA-O1A
39	44	601	CHL	CAA-CBA-CGA-O2A
39	G	607	CHL	CAA-CBA-CGA-O2A
39	4	306	CHL	CAA-CBA-CGA-O1A
39	4	309	CHL	CAA-CBA-CGA-O1A
35	AA	410	PL9	C14-C16-C17-C18
33	a	408	PHO	CBD-CGD-O2D-CED
32	CC	509	CLA	C5-C6-C7-C8
46	E	101	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
36	GG	618	LHG	O1-C1-C2-O2
32	4	305	CLA	CAA-CBA-CGA-O1A
36	Rr	617	LHG	C31-C32-C33-C34
36	DD	407	LHG	C31-C32-C33-C34
32	Yy	613	CLA	CBA-CGA-O2A-C1
32	r	604	CLA	CBA-CGA-O2A-C1
36	EE	101	LHG	C14-C15-C16-C17
38	m	101	LMG	C32-C33-C34-C35
39	g	601	CHL	C2A-CAA-CBA-CGA
39	44	606	CHL	CAA-CBA-CGA-O1A
39	4	307	CHL	CAA-CBA-CGA-O1A
44	Hh	102	DGD	C2A-C3A-C4A-C5A
37	B	602	SQD	C32-C33-C34-C35
32	44	604	CLA	CAA-CBA-CGA-O1A
32	44	615	CLA	CAA-CBA-CGA-O2A
32	B	618	CLA	CAA-CBA-CGA-O2A
37	LL	101	SQD	O47-C7-C8-C9
36	Y	618	LHG	O7-C5-C6-O8
36	AA	414	LHG	O7-C5-C6-O8
37	A	412	SQD	O47-C45-C46-O48
32	44	602	CLA	CAA-CBA-CGA-O1A
32	AA	408	CLA	C8-C10-C11-C12
32	Gg	304	CLA	C5-C6-C7-C8
32	R	602	CLA	C14-C13-C15-C16
32	g	611	CLA	C14-C13-C15-C16
32	BB	603	CLA	C14-C13-C15-C16
32	NN	610	CLA	C14-C13-C15-C16
32	Gg	312	CLA	C11-C12-C13-C14
32	Gg	312	CLA	C14-C13-C15-C16
39	G	601	CHL	C11-C10-C8-C9
32	c	510	CLA	C16-C17-C18-C20
32	y	304	CLA	C16-C17-C18-C20
32	Aa	410	CLA	C11-C12-C13-C14
32	Cc	511	CLA	C16-C17-C18-C20
32	Cc	512	CLA	C16-C17-C18-C19
32	Gg	304	CLA	C16-C17-C18-C20
44	Cc	519	DGD	C3A-C4A-C5A-C6A
44	Cc	520	DGD	C2A-C3A-C4A-C5A
32	a	410	CLA	CAA-CBA-CGA-O2A
36	JJ	101	LHG	O8-C23-C24-C25
36	Nn	310	LHG	O8-C23-C24-C25
37	L	101	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	L	102	SQD	O47-C7-C8-C9
37	B	617	SQD	O47-C7-C8-C9
36	CC	523	LHG	O6-C4-C5-C6
36	DD	408	LHG	O6-C4-C5-C6
39	G	607	CHL	CAA-CBA-CGA-O1A
36	Nn	310	LHG	C18-C19-C20-C21
32	B	607	CLA	C5-C6-C7-C8
32	Ss	602	CLA	CAA-CBA-CGA-O2A
32	DD	403	CLA	CAA-CBA-CGA-O2A
32	Gg	313	CLA	CAA-CBA-CGA-O2A
37	BB	621	SQD	O47-C7-C8-C9
37	LL	102	SQD	C45-C46-O48-C23
32	C	503	CLA	C11-C10-C8-C7
32	C	511	CLA	C11-C12-C13-C15
32	D	401	CLA	C11-C12-C13-C15
32	D	404	CLA	C11-C12-C13-C15
32	D	404	CLA	C12-C13-C15-C16
32	R	602	CLA	C6-C7-C8-C10
32	Y	613	CLA	C6-C7-C8-C10
32	b	602	CLA	C11-C10-C8-C7
32	c	501	CLA	C11-C10-C8-C7
32	c	510	CLA	C11-C12-C13-C15
32	d	401	CLA	C11-C10-C8-C7
32	DD	401	CLA	C11-C12-C13-C15
32	B	620	CLA	C12-C13-C15-C16
32	B	621	CLA	C11-C10-C8-C7
32	B	622	CLA	C11-C10-C8-C7
32	Bb	602	CLA	C11-C10-C8-C7
32	Bb	603	CLA	C12-C13-C15-C16
32	Cc	504	CLA	C6-C7-C8-C10
32	Cc	512	CLA	C12-C13-C15-C16
33	AA	407	PHO	C6-C7-C8-C10
32	BB	609	CLA	C4C-C3C-CAC-CBC
44	C	519	DGD	C7B-C8B-C9B-CAB
32	44	604	CLA	CAA-CBA-CGA-O2A
32	A	406	CLA	C2B-C3B-CAB-CBB
32	Rr	604	CLA	C2B-C3B-CAB-CBB
32	44	610	CLA	C2B-C3B-CAB-CBB
32	44	611	CLA	C2B-C3B-CAB-CBB
32	44	615	CLA	C2B-C3B-CAB-CBB
32	11	609	CLA	C2B-C3B-CAB-CBB
32	22	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	22	611	CLA	C2B-C3B-CAB-CBB
32	1	604	CLA	C2B-C3B-CAB-CBB
32	2	602	CLA	C2B-C3B-CAB-CBB
32	2	604	CLA	C2B-C3B-CAB-CBB
32	2	611	CLA	C2B-C3B-CAB-CBB
32	G	602	CLA	C2B-C3B-CAB-CBB
32	G	614	CLA	C2B-C3B-CAB-CBB
32	N	613	CLA	C2B-C3B-CAB-CBB
32	R	611	CLA	C2B-C3B-CAB-CBB
32	S	603	CLA	C2B-C3B-CAB-CBB
32	Y	603	CLA	C2B-C3B-CAB-CBB
32	Y	614	CLA	C2B-C3B-CAB-CBB
32	c	506	CLA	C2B-C3B-CAB-CBB
32	c	507	CLA	C2B-C3B-CAB-CBB
32	c	513	CLA	C2B-C3B-CAB-CBB
32	g	611	CLA	C2B-C3B-CAB-CBB
32	g	614	CLA	C2B-C3B-CAB-CBB
32	s	609	CLA	C2B-C3B-CAB-CBB
32	s	613	CLA	C2B-C3B-CAB-CBB
32	AA	406	CLA	C2B-C3B-CAB-CBB
32	CC	503	CLA	C2B-C3B-CAB-CBB
32	CC	504	CLA	C2B-C3B-CAB-CBB
32	B	610	CLA	C2B-C3B-CAB-CBB
32	GG	603	CLA	C2B-C3B-CAB-CBB
32	GG	614	CLA	C2B-C3B-CAB-CBB
32	NN	613	CLA	C2B-C3B-CAB-CBB
32	SS	304	CLA	C2B-C3B-CAB-CBB
32	Cc	508	CLA	C2B-C3B-CAB-CBB
32	Cc	509	CLA	C2B-C3B-CAB-CBB
32	Nn	305	CLA	C2B-C3B-CAB-CBB
34	C	516	BCR	C1-C6-C7-C8
34	K	102	BCR	C1-C6-C7-C8
34	c	514	BCR	C1-C6-C7-C8
34	h	101	BCR	C1-C6-C7-C8
34	h	101	BCR	C5-C6-C7-C8
34	CC	515	BCR	C1-C6-C7-C8
34	Hh	101	BCR	C1-C6-C7-C8
34	Hh	101	BCR	C5-C6-C7-C8
40	Yy	616	LUT	C1-C6-C7-C8
40	Y	615	LUT	C1-C6-C7-C8
40	g	616	LUT	C1-C6-C7-C8
40	s	614	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
40	s	615	LUT	C1-C6-C7-C8
40	GG	615	LUT	C1-C6-C7-C8
40	NN	616	LUT	C1-C6-C7-C8
40	YY	615	LUT	C1-C6-C7-C8
40	Nn	306	LUT	C5-C6-C7-C8
36	Ss	616	LHG	C8-C7-O7-C5
32	Y	603	CLA	CAA-CBA-CGA-O2A
32	BB	607	CLA	CAA-CBA-CGA-O2A
32	Bb	609	CLA	CAA-CBA-CGA-O2A
36	GG	618	LHG	O7-C7-C8-C9
37	LL	102	SQD	O47-C7-C8-C9
32	C	510	CLA	C2-C1-O2A-CGA
32	D	405	CLA	C2-C1-O2A-CGA
32	n	603	CLA	C2-C1-O2A-CGA
32	n	614	CLA	C2-C1-O2A-CGA
32	B	619	CLA	C2-C1-O2A-CGA
32	Cc	507	CLA	C2-C1-O2A-CGA
32	Nn	313	CLA	C2-C1-O2A-CGA
39	Y	609	CHL	C2-C1-O2A-CGA
32	Ss	610	CLA	O2A-C1-C2-C3
32	g	612	CLA	O2A-C1-C2-C3
32	n	603	CLA	O2A-C1-C2-C3
32	s	610	CLA	O2A-C1-C2-C3
32	SS	313	CLA	O2A-C1-C2-C3
32	SS	314	CLA	O2A-C1-C2-C3
39	Rr	606	CHL	O2A-C1-C2-C3
36	D	408	LHG	C29-C30-C31-C32
44	D	411	DGD	C9B-CAB-CBB-CCB
39	GG	607	CHL	CAA-CBA-CGA-O1A
42	g	617	NEX	C26-C27-C28-C29
42	Gg	318	NEX	C26-C27-C28-C29
32	YY	612	CLA	C8-C10-C11-C12
35	d	404	PL9	C9-C11-C12-C13
44	c	518	DGD	C5B-C6B-C7B-C8B
32	Rr	601	CLA	CAA-CBA-CGA-O2A
36	n	618	LHG	O8-C23-C24-C25
36	s	616	LHG	C13-C14-C15-C16
36	D	409	LHG	C19-C20-C21-C22
32	Yy	602	CLA	C16-C17-C18-C19
44	B	601	DGD	CCB-CDB-CEB-CFB
36	Gg	319	LHG	C7-C8-C9-C10
32	GG	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	Aa	410	CLA	CAA-CBA-CGA-O2A
36	JJ	101	LHG	O7-C7-C8-C9
37	l	102	SQD	O47-C7-C8-C9
37	LL	102	SQD	O48-C23-C24-C25
39	Yy	609	CHL	CAA-CBA-CGA-O2A
44	a	415	DGD	O2G-C1B-C2B-C3B
36	BB	622	LHG	C1-C2-C3-O3
36	C	522	LHG	O2-C2-C3-O3
32	BB	613	CLA	C2A-CAA-CBA-CGA
32	B	624	CLA	C2A-CAA-CBA-CGA
36	Yy	618	LHG	C8-C7-O7-C5
35	Dd	404	PL9	C42-C43-C44-C45
38	BB	619	LMG	C16-C17-C18-C19
44	Hh	102	DGD	C7B-C8B-C9B-CAB
46	e	101	HEM	CAA-CBA-CGA-O2A
32	GG	602	CLA	CAA-CBA-CGA-O2A
36	II	101	LHG	O7-C7-C8-C9
37	L	101	SQD	O48-C23-C24-C25
36	J	101	LHG	C26-C27-C28-C29
44	B	603	DGD	C2A-C3A-C4A-C5A
32	Cc	512	CLA	C16-C17-C18-C20
35	d	404	PL9	C4-C3-C7-C8
32	Y	612	CLA	C15-C16-C17-C18
39	NN	607	CHL	C13-C15-C16-C17
32	G	610	CLA	CAA-CBA-CGA-O2A
32	b	613	CLA	CAA-CBA-CGA-O2A
32	r	601	CLA	CAA-CBA-CGA-O2A
37	CC	501	SQD	O47-C7-C8-C9
37	Ll	101	SQD	O47-C7-C8-C9
39	GG	601	CHL	CAA-CBA-CGA-O2A
44	Aa	401	DGD	O2G-C1B-C2B-C3B
32	Cc	508	CLA	C8-C10-C11-C12
44	c	517	DGD	C3A-C4A-C5A-C6A
37	C	501	SQD	C4-C5-C6-S
37	CC	501	SQD	C4-C5-C6-S
39	y	311	CHL	C16-C17-C18-C19
32	Yy	613	CLA	C4-C3-C5-C6
44	h	102	DGD	C1B-C2B-C3B-C4B
44	C	523	DGD	C6B-C7B-C8B-C9B
32	R	602	CLA	CAA-CBA-CGA-O2A
32	Bb	613	CLA	CAA-CBA-CGA-O2A
36	G	618	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
39	y	311	CHL	CAA-CBA-CGA-O2A
32	c	506	CLA	C8-C10-C11-C12
32	B	621	CLA	C2-C3-C5-C6
35	AA	410	PL9	C18-C19-C21-C22
36	DD	407	LHG	C29-C30-C31-C32
36	A	414	LHG	C15-C16-C17-C18
44	Cc	520	DGD	C5B-C6B-C7B-C8B
44	C	520	DGD	CDA-CEA-CFA-CGA
36	l	101	LHG	C31-C32-C33-C34
39	YY	609	CHL	C2A-CAA-CBA-CGA
38	B	615	LMG	C12-C13-C14-C15
39	44	601	CHL	CAA-CBA-CGA-O1A
32	g	612	CLA	CAA-CBA-CGA-O2A
36	EE	101	LHG	C9-C10-C11-C12
44	c	518	DGD	C1A-C2A-C3A-C4A
36	y	320	LHG	O9-C7-O7-C5
32	Rr	608	CLA	O2A-C1-C2-C3
32	Y	604	CLA	O2A-C1-C2-C3
32	Nn	313	CLA	O2A-C1-C2-C3
36	D	409	LHG	C17-C18-C19-C20
32	A	405	CLA	C14-C13-C15-C16
32	b	602	CLA	C14-C13-C15-C16
32	g	611	CLA	C11-C12-C13-C14
32	r	602	CLA	C11-C10-C8-C9
32	BB	607	CLA	C6-C7-C8-C9
32	BB	607	CLA	C11-C10-C8-C9
32	Bb	611	CLA	C6-C7-C8-C9
39	Y	609	CHL	C14-C13-C15-C16
36	22	615	LHG	C24-C25-C26-C27
32	A	406	CLA	CAA-CBA-CGA-O2A
32	Ss	609	CLA	CAA-CBA-CGA-O2A
32	Ss	612	CLA	CAA-CBA-CGA-O2A
32	B	624	CLA	CAA-CBA-CGA-O2A
36	3	614	LHG	O7-C7-C8-C9
36	YY	618	LHG	C4-C5-C6-O8
37	L	101	SQD	O6-C44-C45-C46
44	C	523	DGD	C1G-C2G-C3G-O3G
44	Cc	519	DGD	C1G-C2G-C3G-O3G
36	11	614	LHG	C25-C26-C27-C28
32	A	408	CLA	C4B-C3B-CAB-CBB
32	44	615	CLA	C4B-C3B-CAB-CBB
32	11	609	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	3	604	CLA	C4B-C3B-CAB-CBB
32	C	515	CLA	C1A-C2A-CAA-CBA
32	G	603	CLA	C1A-C2A-CAA-CBA
32	G	604	CLA	C4B-C3B-CAB-CBB
32	R	601	CLA	C4B-C3B-CAB-CBB
32	R	604	CLA	C4B-C3B-CAB-CBB
32	c	504	CLA	C4B-C3B-CAB-CBB
32	g	613	CLA	C4B-C3B-CAB-CBB
32	n	613	CLA	C4B-C3B-CAB-CBB
32	s	609	CLA	C4B-C3B-CAB-CBB
32	BB	604	CLA	C4B-C3B-CAB-CBB
32	BB	609	CLA	C4B-C3B-CAB-CBB
32	CC	513	CLA	C4B-C3B-CAB-CBB
32	CC	514	CLA	C1A-C2A-CAA-CBA
32	B	620	CLA	C1A-C2A-CAA-CBA
32	RR	304	CLA	C4B-C3B-CAB-CBB
32	RR	310	CLA	C4B-C3B-CAB-CBB
32	YY	612	CLA	C1A-C2A-CAA-CBA
32	Bb	606	CLA	C4B-C3B-CAB-CBB
32	Cc	506	CLA	C4B-C3B-CAB-CBB
32	Cc	508	CLA	C4B-C3B-CAB-CBB
32	Cc	511	CLA	C4B-C3B-CAB-CBB
32	Gg	303	CLA	C1A-C2A-CAA-CBA
32	Gg	314	CLA	C4B-C3B-CAB-CBB
44	CC	519	DGD	O6D-C5D-C6D-O5D
32	Yy	604	CLA	O1D-CGD-O2D-CED
32	BB	608	CLA	C4-C3-C5-C6
38	WW	201	LMG	O6-C1-O1-C7
44	Cc	519	DGD	O6D-C1D-O3G-C3G
32	Rr	608	CLA	CAA-CBA-CGA-O2A
32	G	612	CLA	CAA-CBA-CGA-O2A
32	Y	610	CLA	CAA-CBA-CGA-O2A
32	b	616	CLA	CAA-CBA-CGA-O2A
32	c	508	CLA	CAA-CBA-CGA-O2A
32	B	608	CLA	CAA-CBA-CGA-O2A
32	GG	612	CLA	CAA-CBA-CGA-O2A
32	SS	314	CLA	CAA-CBA-CGA-O2A
32	YY	604	CLA	CAA-CBA-CGA-O2A
39	G	601	CHL	CAA-CBA-CGA-O2A
35	A	410	PL9	C43-C44-C46-C47
36	44	616	LHG	O7-C5-C6-O8
36	0	201	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
37	L	102	SQD	C13-C14-C15-C16
34	C	517	BCR	C21-C22-C23-C24
34	h	101	BCR	C11-C12-C13-C14
34	BB	620	BCR	C21-C22-C23-C24
34	Bb	617	BCR	C21-C22-C23-C24
34	Cc	518	BCR	C7-C8-C9-C10
40	Yy	615	LUT	C7-C8-C9-C10
40	N	616	LUT	C7-C8-C9-C10
40	n	616	LUT	C7-C8-C9-C10
40	y	318	LUT	C7-C8-C9-C10
40	RR	315	LUT	C7-C8-C9-C10
32	g	603	CLA	C16-C17-C18-C19
37	A	412	SQD	O49-C7-C8-C9
38	WW	201	LMG	C29-C28-O8-C9
32	Yy	604	CLA	CAA-CBA-CGA-O2A
32	b	605	CLA	CAA-CBA-CGA-O2A
32	r	603	CLA	CAA-CBA-CGA-O2A
32	r	608	CLA	CAA-CBA-CGA-O2A
32	r	611	CLA	CAA-CBA-CGA-O2A
32	s	612	CLA	CAA-CBA-CGA-O2A
32	BB	612	CLA	CAA-CBA-CGA-O2A
32	Bb	616	CLA	CAA-CBA-CGA-O2A
32	Cc	509	CLA	CAA-CBA-CGA-O2A
39	Ss	605	CHL	CAA-CBA-CGA-O2A
39	R	607	CHL	CAA-CBA-CGA-O2A
39	g	601	CHL	CAA-CBA-CGA-O2A
39	s	601	CHL	CAA-CBA-CGA-O2A
39	RR	307	CHL	CAA-CBA-CGA-O2A
39	Gg	302	CHL	CAA-CBA-CGA-O2A
44	CC	518	DGD	O2G-C1B-C2B-C3B
32	B	609	CLA	C2A-CAA-CBA-CGA
38	m	101	LMG	C35-C36-C37-C38
44	h	102	DGD	C2A-C3A-C4A-C5A
32	Yy	612	CLA	C3-C5-C6-C7
44	Hh	102	DGD	C1B-C2B-C3B-C4B
36	A	413	LHG	O6-C4-C5-C6
32	b	609	CLA	CAA-CBA-CGA-O2A
32	c	507	CLA	CAA-CBA-CGA-O2A
36	D	408	LHG	O8-C23-C24-C25
36	s	616	LHG	O8-C23-C24-C25
36	DD	407	LHG	O8-C23-C24-C25
36	A	413	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
37	AA	412	SQD	C5-C6-S-O7
37	AA	412	SQD	C5-C6-S-O9
32	a	406	CLA	C8-C10-C11-C12
32	Rr	604	CLA	CAA-CBA-CGA-O1A
32	c	505	CLA	C2-C1-O2A-CGA
32	r	602	CLA	C2-C1-O2A-CGA
32	BB	602	CLA	C2-C1-O2A-CGA
32	YY	602	CLA	C2-C1-O2A-CGA
39	YY	609	CHL	C2-C1-O2A-CGA
32	Yy	602	CLA	C12-C13-C15-C16
32	Yy	610	CLA	C6-C7-C8-C10
32	C	510	CLA	C11-C12-C13-C15
32	C	513	CLA	C6-C7-C8-C10
32	C	513	CLA	C11-C10-C8-C7
32	Y	610	CLA	C11-C12-C13-C15
32	b	602	CLA	C6-C7-C8-C10
32	b	604	CLA	C6-C7-C8-C10
32	b	611	CLA	C6-C7-C8-C10
32	b	616	CLA	C11-C12-C13-C15
32	c	506	CLA	C12-C13-C15-C16
32	c	511	CLA	C6-C7-C8-C10
32	y	312	CLA	C6-C7-C8-C10
32	CC	512	CLA	C11-C10-C8-C7
32	B	605	CLA	C12-C13-C15-C16
32	RR	302	CLA	C6-C7-C8-C10
32	Bb	604	CLA	C6-C7-C8-C10
32	Bb	606	CLA	C11-C10-C8-C7
32	Bb	610	CLA	C6-C7-C8-C10
32	Bb	611	CLA	C6-C7-C8-C10
32	Bb	616	CLA	C11-C12-C13-C15
32	Cc	508	CLA	C12-C13-C15-C16
32	Cc	513	CLA	C12-C13-C15-C16
38	W	201	LMG	C29-C28-O8-C9
32	C	507	CLA	C2-C3-C5-C6
32	Bb	606	CLA	C5-C6-C7-C8
32	Aa	405	CLA	O2A-C1-C2-C3
39	N	607	CHL	C13-C15-C16-C17
38	BB	619	LMG	C30-C31-C32-C33
44	BB	624	DGD	CCB-CDB-CEB-CFB
32	D	404	CLA	CAA-CBA-CGA-O2A
36	r	616	LHG	O8-C23-C24-C25
37	C	501	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	CC	506	CLA	C4C-C3C-CAC-CBC
32	d	402	CLA	C13-C15-C16-C17
32	BB	613	CLA	C5-C6-C7-C8
37	BB	621	SQD	O49-C7-C8-C9
32	A	405	CLA	C2A-CAA-CBA-CGA
32	Bb	608	CLA	C2A-CAA-CBA-CGA
32	C	512	CLA	C16-C17-C18-C20
32	R	604	CLA	O2A-C1-C2-C3
32	y	306	CLA	O2A-C1-C2-C3
32	RR	304	CLA	O2A-C1-C2-C3
37	AA	412	SQD	O48-C23-C24-C25
36	D	408	LHG	C25-C26-C27-C28
36	DD	407	LHG	C25-C26-C27-C28
32	a	406	CLA	CAA-CBA-CGA-O2A
32	SS	303	CLA	CAA-CBA-CGA-O2A
32	Gg	312	CLA	CAA-CBA-CGA-O2A
36	Ss	616	LHG	O8-C23-C24-C25
32	Gg	313	CLA	CAA-CBA-CGA-O1A
44	a	415	DGD	O1B-C1B-C2B-C3B
36	YY	618	LHG	C11-C10-C9-C8
36	AA	411	LHG	C5-C4-O6-P
32	Gg	303	CLA	C3A-C2A-CAA-CBA
32	Gg	313	CLA	C3A-C2A-CAA-CBA
33	D	402	PHO	C4-C3-C5-C6
39	N	609	CHL	C3A-C2A-CAA-CBA
39	NN	609	CHL	C3A-C2A-CAA-CBA
39	YY	601	CHL	C4-C3-C5-C6
36	n	618	LHG	O10-C23-C24-C25
32	N	602	CLA	C13-C15-C16-C17
39	Gg	302	CHL	C10-C11-C12-C13
35	AA	410	PL9	C28-C29-C31-C32
36	DD	407	LHG	C24-C25-C26-C27
46	e	101	HEM	CAA-CBA-CGA-O1A
32	D	404	CLA	CAA-CBA-CGA-O1A
32	BB	607	CLA	CAA-CBA-CGA-O1A
37	LL	102	SQD	O10-C23-C24-C25
37	Ll	101	SQD	O49-C7-C8-C9
44	C	519	DGD	C6B-C7B-C8B-C9B
32	Rr	603	CLA	CAA-CBA-CGA-O2A
32	g	611	CLA	CAA-CBA-CGA-O2A
32	y	306	CLA	CAA-CBA-CGA-O2A
32	AA	406	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	Bb	605	CLA	CAA-CBA-CGA-O2A
37	l	102	SQD	O10-C23-O48-C46
32	Ss	602	CLA	CAA-CBA-CGA-O1A
32	G	610	CLA	CAA-CBA-CGA-O1A
36	JJ	101	LHG	O9-C7-C8-C9
37	l	102	SQD	O49-C7-C8-C9
36	y	320	LHG	C8-C7-O7-C5
36	DD	408	LHG	C7-C8-C9-C10
32	Bb	609	CLA	C15-C16-C17-C18
36	y	320	LHG	C24-C23-O8-C6
32	3	610	CLA	C2C-C3C-CAC-CBC
32	Rr	609	CLA	C11-C12-C13-C14
32	D	404	CLA	C11-C12-C13-C14
32	N	610	CLA	C14-C13-C15-C16
32	R	602	CLA	C6-C7-C8-C9
32	b	604	CLA	C14-C13-C15-C16
32	b	606	CLA	C11-C10-C8-C9
32	b	611	CLA	C6-C7-C8-C9
32	AA	405	CLA	C14-C13-C15-C16
32	BB	604	CLA	C11-C10-C8-C9
32	B	619	CLA	C14-C13-C15-C16
32	B	624	CLA	C11-C10-C8-C9
32	RR	302	CLA	C14-C13-C15-C16
32	Bb	604	CLA	C14-C13-C15-C16
32	Bb	605	CLA	C14-C13-C15-C16
32	Bb	609	CLA	C11-C10-C8-C9
32	Cc	504	CLA	C6-C7-C8-C9
32	Cc	514	CLA	C11-C10-C8-C9
32	Dd	401	CLA	C11-C10-C8-C9
32	Nn	301	CLA	C6-C7-C8-C9
33	A	407	PHO	C6-C7-C8-C9
39	NN	607	CHL	C6-C7-C8-C9
32	Rr	601	CLA	CAA-CBA-CGA-O1A
32	Yy	604	CLA	CAA-CBA-CGA-O1A
37	L	101	SQD	O10-C23-C24-C25
37	B	617	SQD	O49-C7-C8-C9
36	33	614	LHG	C24-C25-C26-C27
38	b	621	LMG	C11-C12-C13-C14
34	Hh	101	BCR	C9-C10-C11-C12
32	CC	509	CLA	C16-C17-C18-C20
32	CC	504	CLA	C8-C10-C11-C12
32	Y	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
37	LL	102	SQD	O49-C7-C8-C9
39	R	607	CHL	CAA-CBA-CGA-O1A
39	y	311	CHL	CAA-CBA-CGA-O1A
33	A	407	PHO	C2-C3-C5-C6
35	A	410	PL9	C28-C29-C31-C32
37	C	501	SQD	O5-C5-C6-S
37	CC	501	SQD	O5-C5-C6-S
41	Rr	615	XAT	C1-C6-C7-C8
32	B	605	CLA	C4C-C3C-CAC-CBC
32	a	410	CLA	CAA-CBA-CGA-O1A
32	DD	403	CLA	CAA-CBA-CGA-O1A
32	Bb	609	CLA	CAA-CBA-CGA-O1A
36	3	614	LHG	O9-C7-C8-C9
36	II	101	LHG	O9-C7-C8-C9
37	L	101	SQD	O49-C7-C8-C9
32	C	505	CLA	C8-C10-C11-C12
32	CC	509	CLA	C13-C15-C16-C17
32	NN	602	CLA	CAA-CBA-CGA-O2A
32	Aa	406	CLA	CAA-CBA-CGA-O2A
32	Nn	305	CLA	CAA-CBA-CGA-O2A
36	A	414	LHG	O8-C23-C24-C25
36	C	522	LHG	O7-C7-C8-C9
32	Bb	612	CLA	C16-C17-C18-C20
40	n	615	LUT	C11-C12-C13-C14
32	R	613	CLA	C4C-C3C-CAC-CBC
44	Hh	102	DGD	C3B-C4B-C5B-C6B
32	c	507	CLA	CAA-CBA-CGA-O1A
32	g	612	CLA	CAA-CBA-CGA-O1A
32	s	612	CLA	CAA-CBA-CGA-O1A
32	B	624	CLA	CAA-CBA-CGA-O1A
37	CC	501	SQD	O49-C7-C8-C9
37	LL	101	SQD	O49-C7-C8-C9
32	YY	613	CLA	C8-C10-C11-C12
37	CC	501	SQD	C45-C44-O6-C1
44	c	518	DGD	C5D-C6D-O5D-C1E
44	BB	624	DGD	C5D-C6D-O5D-C1E
44	CC	522	DGD	C2G-C3G-O3G-C1D
44	B	601	DGD	C5D-C6D-O5D-C1E
44	Cc	520	DGD	C5D-C6D-O5D-C1E
36	y	320	LHG	O10-C23-O8-C6
44	Cc	519	DGD	O2G-C2G-C3G-O3G
32	4	311	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	Ss	609	CLA	CAA-CBA-CGA-O1A
32	44	615	CLA	CAA-CBA-CGA-O1A
32	b	616	CLA	CAA-CBA-CGA-O1A
32	r	601	CLA	CAA-CBA-CGA-O1A
32	YY	604	CLA	CAA-CBA-CGA-O1A
32	Bb	613	CLA	CAA-CBA-CGA-O1A
32	Cc	509	CLA	CAA-CBA-CGA-O1A
36	GG	618	LHG	O9-C7-C8-C9
36	Nn	310	LHG	O10-C23-C24-C25
37	L	102	SQD	O49-C7-C8-C9
39	G	601	CHL	CAA-CBA-CGA-O1A
39	s	601	CHL	CAA-CBA-CGA-O1A
39	GG	601	CHL	CAA-CBA-CGA-O1A
32	N	602	CLA	CAA-CBA-CGA-O2A
32	Y	604	CLA	CAA-CBA-CGA-O2A
32	YY	603	CLA	CAA-CBA-CGA-O2A
36	Y	618	LHG	O7-C7-C8-C9
38	W	201	LMG	O7-C10-C11-C12
38	WW	201	LMG	O7-C10-C11-C12
32	y	304	CLA	C16-C17-C18-C19
36	1	614	LHG	C4-C5-C6-O8
32	Rr	608	CLA	CAA-CBA-CGA-O1A
32	Ss	612	CLA	CAA-CBA-CGA-O1A
32	Y	610	CLA	CAA-CBA-CGA-O1A
32	b	613	CLA	CAA-CBA-CGA-O1A
32	B	608	CLA	CAA-CBA-CGA-O1A
32	GG	602	CLA	CAA-CBA-CGA-O1A
32	SS	303	CLA	CAA-CBA-CGA-O1A
36	G	618	LHG	O9-C7-C8-C9
39	Gg	302	CHL	CAA-CBA-CGA-O1A
44	Aa	401	DGD	O1B-C1B-C2B-C3B
36	D	408	LHG	C23-C24-C25-C26
32	BB	602	CLA	C5-C6-C7-C8
32	BB	609	CLA	C15-C16-C17-C18
32	Bb	614	CLA	C15-C16-C17-C18
36	11	614	LHG	O8-C23-C24-C25
44	h	102	DGD	O2G-C1B-C2B-C3B
35	D	407	PL9	C28-C29-C31-C32
32	c	502	CLA	C3-C5-C6-C7
32	Y	613	CLA	C8-C10-C11-C12
32	G	612	CLA	CAA-CBA-CGA-O1A
32	R	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	b	609	CLA	CAA-CBA-CGA-O1A
32	r	603	CLA	CAA-CBA-CGA-O1A
32	r	608	CLA	CAA-CBA-CGA-O1A
37	C	501	SQD	O49-C7-C8-C9
39	g	601	CHL	CAA-CBA-CGA-O1A
36	Nn	310	LHG	C19-C20-C21-C22
44	C	523	DGD	CAB-CBB-CCB-CDB
32	Rr	611	CLA	CAD-CBD-CGD-O2D
32	Ss	613	CLA	CAD-CBD-CGD-O2D
32	2	611	CLA	CAD-CBD-CGD-O2D
32	3	609	CLA	CAD-CBD-CGD-O2D
32	S	610	CLA	CAD-CBD-CGD-O2D
32	b	609	CLA	CAD-CBD-CGD-O2D
32	b	610	CLA	CAD-CBD-CGD-O2D
32	r	611	CLA	CAD-CBD-CGD-O2D
32	BB	603	CLA	CAD-CBD-CGD-O2D
32	Bb	610	CLA	CAD-CBD-CGD-O2D
32	Bb	616	CLA	CAD-CBD-CGD-O2D
32	Nn	313	CLA	CAD-CBD-CGD-O2D
39	g	609	CHL	C1A-C2A-CAA-CBA
39	Gg	310	CHL	C1A-C2A-CAA-CBA
39	Nn	318	CHL	CAD-CBD-CGD-O2D
32	CC	506	CLA	CAA-CBA-CGA-O2A
32	B	619	CLA	CAA-CBA-CGA-O2A
32	Cc	507	CLA	CAA-CBA-CGA-O2A
32	A	406	CLA	CAA-CBA-CGA-O1A
32	r	611	CLA	CAA-CBA-CGA-O1A
32	GG	612	CLA	CAA-CBA-CGA-O1A
32	SS	314	CLA	CAA-CBA-CGA-O1A
32	Aa	410	CLA	CAA-CBA-CGA-O1A
32	Bb	616	CLA	CAA-CBA-CGA-O1A
39	RR	307	CHL	CAA-CBA-CGA-O1A
36	KK	101	LHG	O6-C4-C5-C6
37	CC	501	SQD	C19-C20-C21-C22
32	s	602	CLA	C2-C1-O2A-CGA
32	CC	509	CLA	C2-C1-O2A-CGA
32	c	508	CLA	CAA-CBA-CGA-O1A
32	y	306	CLA	CAA-CBA-CGA-O1A
36	r	616	LHG	O10-C23-C24-C25
39	Yy	609	CHL	CAA-CBA-CGA-O1A
38	m	101	LMG	O8-C28-C29-C30
32	a	410	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	Gg	304	CLA	C16-C17-C18-C19
38	DD	409	LMG	C11-C12-C13-C14
32	c	504	CLA	C5-C6-C7-C8
44	CC	519	DGD	C2A-C3A-C4A-C5A
36	33	614	LHG	C11-C10-C9-C8
36	J	101	LHG	C25-C26-C27-C28
32	Y	604	CLA	CAA-CBA-CGA-O1A
39	Ss	605	CHL	CAA-CBA-CGA-O1A
44	CC	518	DGD	O1B-C1B-C2B-C3B
38	WW	201	LMG	O10-C28-O8-C9
32	G	603	CLA	CAA-CBA-CGA-O2A
32	c	505	CLA	CAA-CBA-CGA-O2A
32	r	602	CLA	CAA-CBA-CGA-O2A
39	r	605	CHL	CAA-CBA-CGA-O2A
44	C	519	DGD	CDB-CEB-CFB-CGB
32	b	610	CLA	C15-C16-C17-C18
32	AA	406	CLA	CAA-CBA-CGA-O1A
44	Cc	519	DGD	C8B-C9B-CAB-CBB
32	Yy	602	CLA	CAA-CBA-CGA-O2A
32	Y	602	CLA	CAA-CBA-CGA-O2A
32	Cc	510	CLA	CAA-CBA-CGA-O2A
36	d	406	LHG	O7-C7-C8-C9
36	YY	618	LHG	O7-C7-C8-C9
39	RR	306	CHL	CAA-CBA-CGA-O2A
33	Aa	408	PHO	O1D-CGD-O2D-CED
36	n	618	LHG	C10-C11-C12-C13
37	CC	501	SQD	C15-C16-C17-C18
32	b	605	CLA	CAA-CBA-CGA-O1A
36	DD	407	LHG	O10-C23-C24-C25
44	BB	623	DGD	CAB-CBB-CCB-CDB

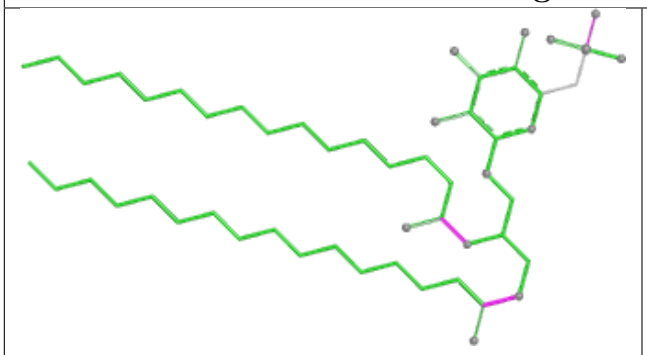
There are no ring outliers.

No monomer is involved in short contacts.

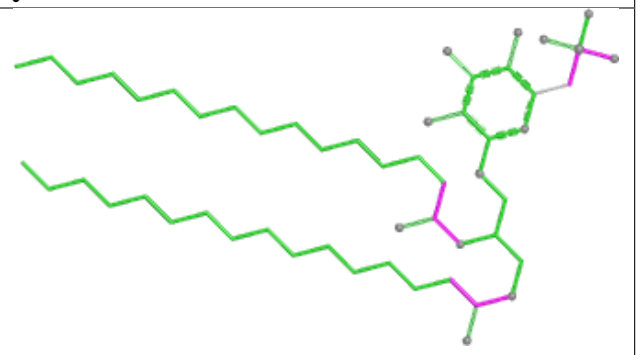
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

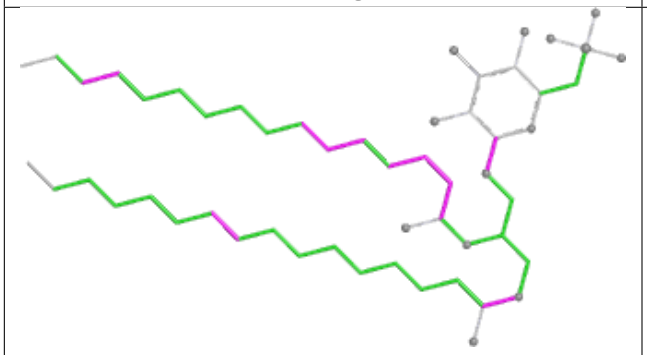
Ligand SQD l 102



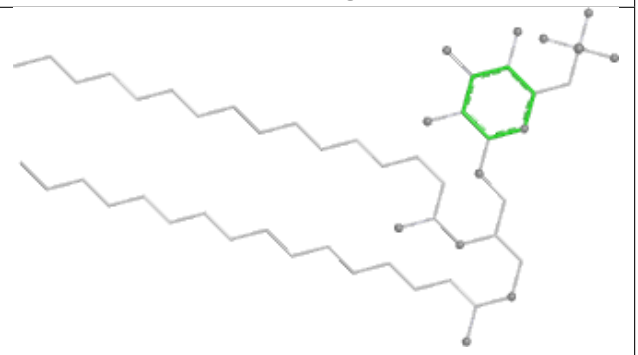
Bond lengths



Bond angles

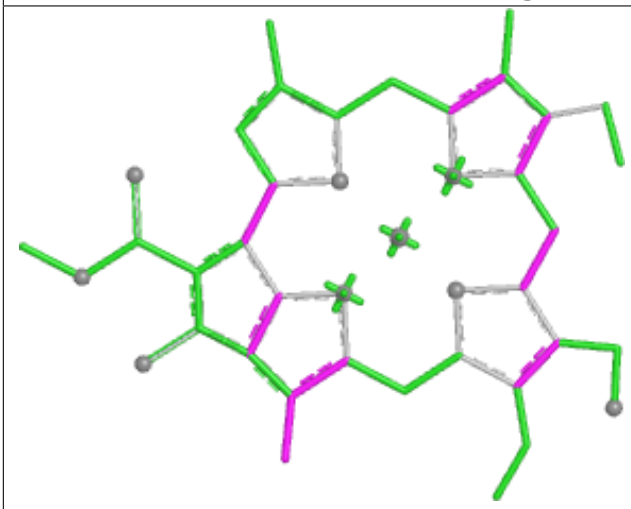


Torsions

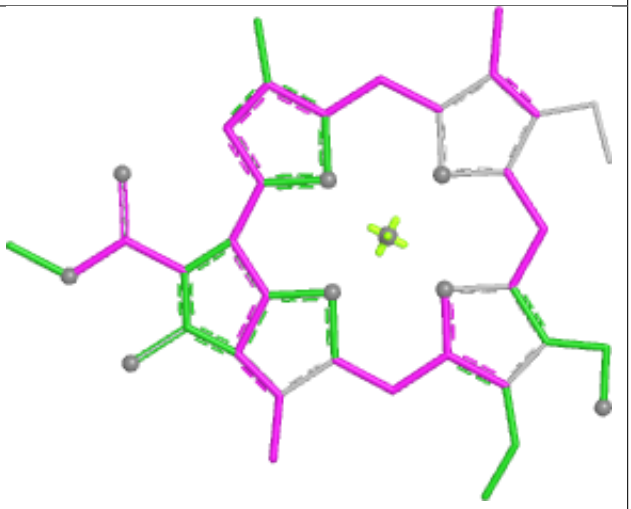


Rings

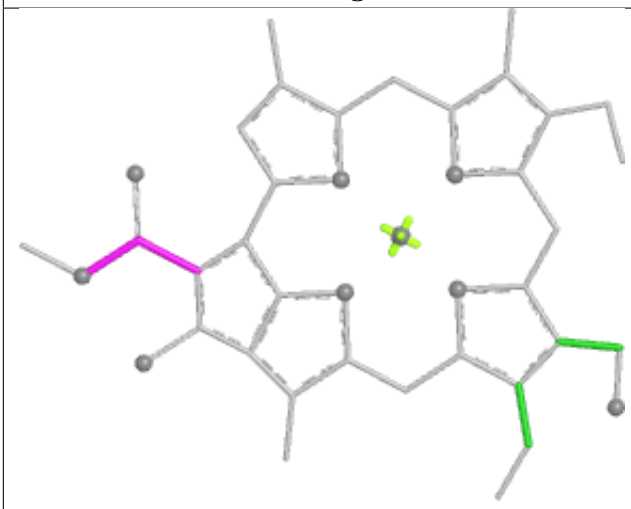
Ligand CHL 11 607



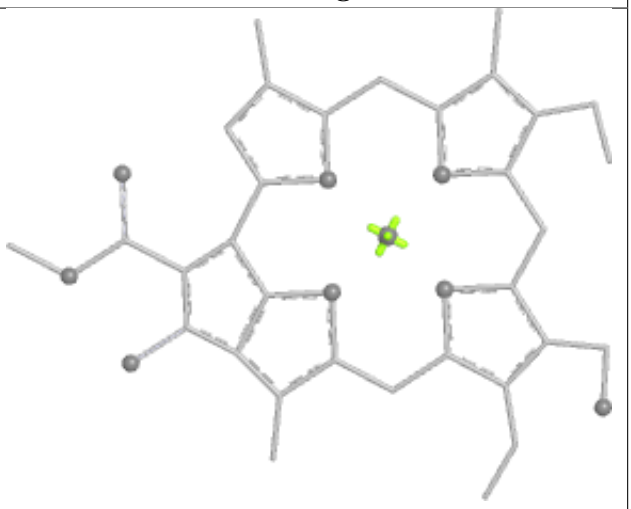
Bond lengths



Bond angles

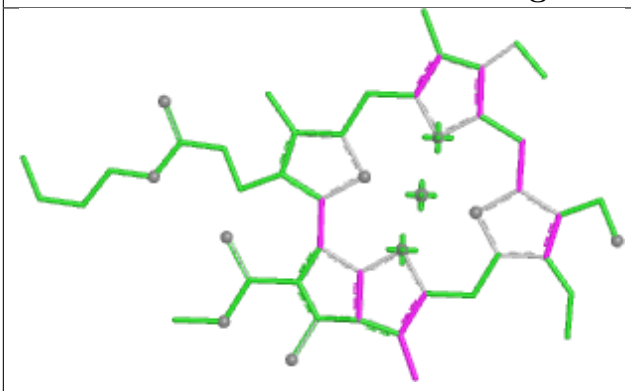


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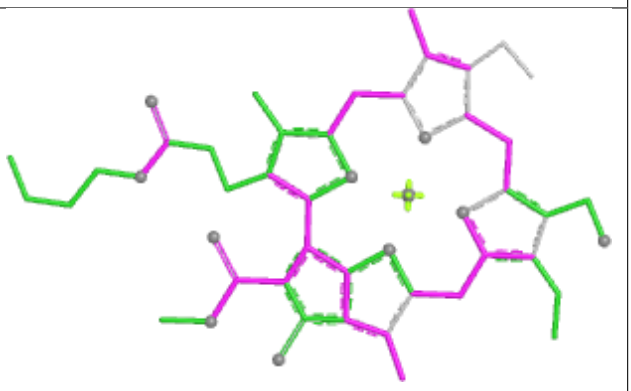


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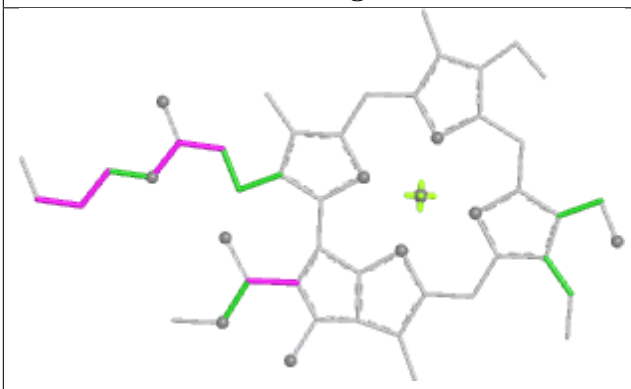
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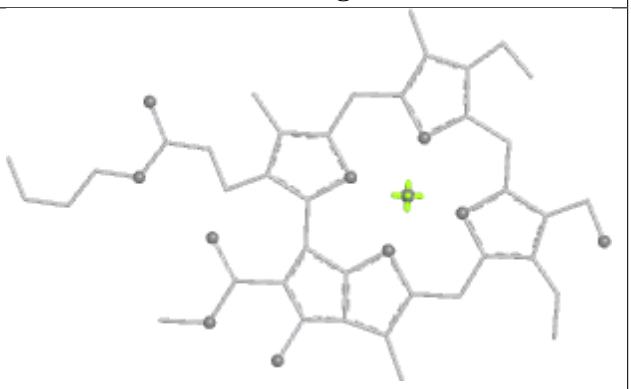
Bond lengths



Bond angles

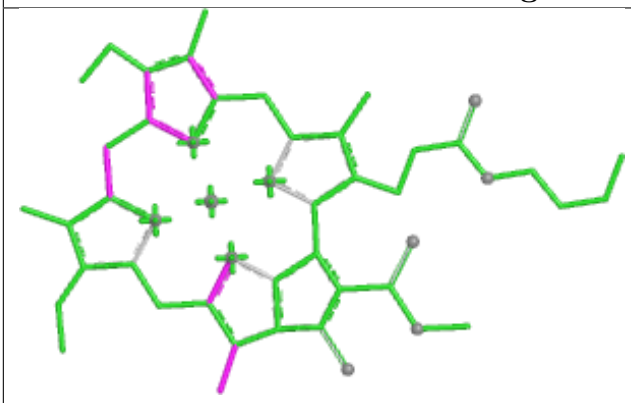


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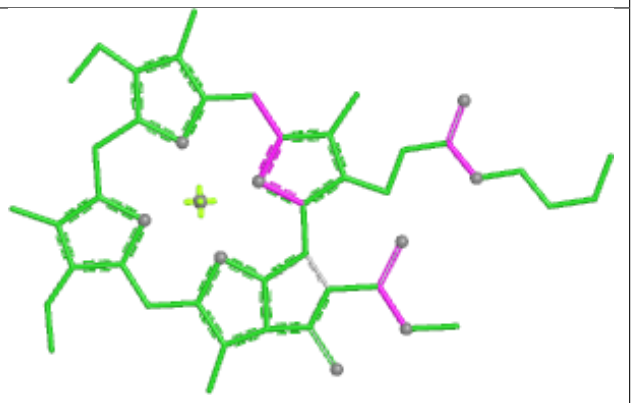


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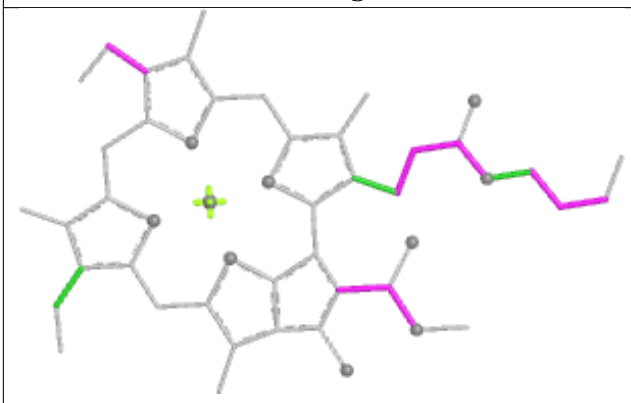
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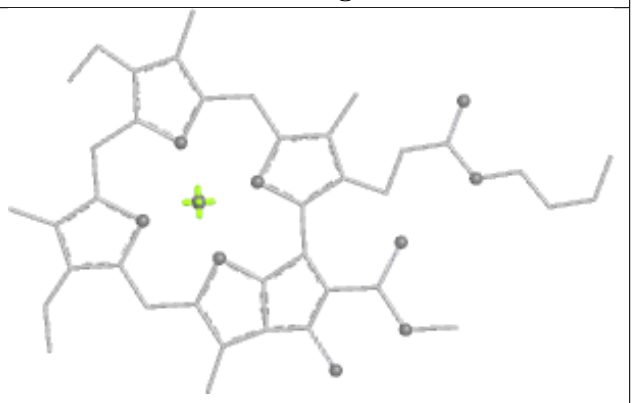
Bond lengths



Bond angles

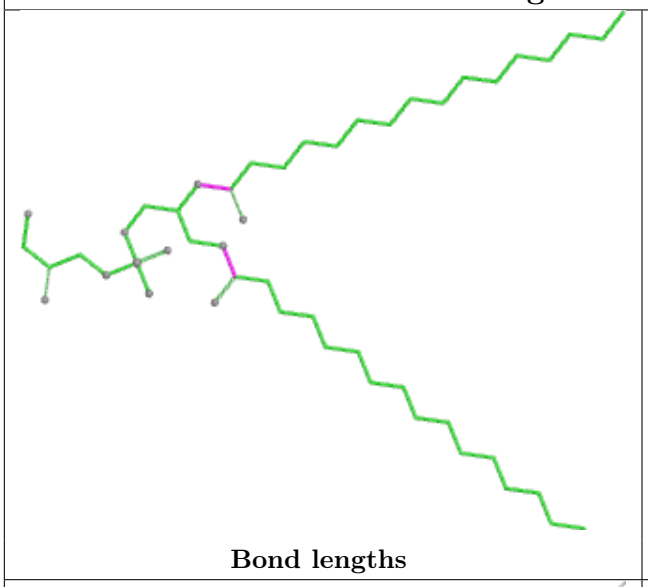


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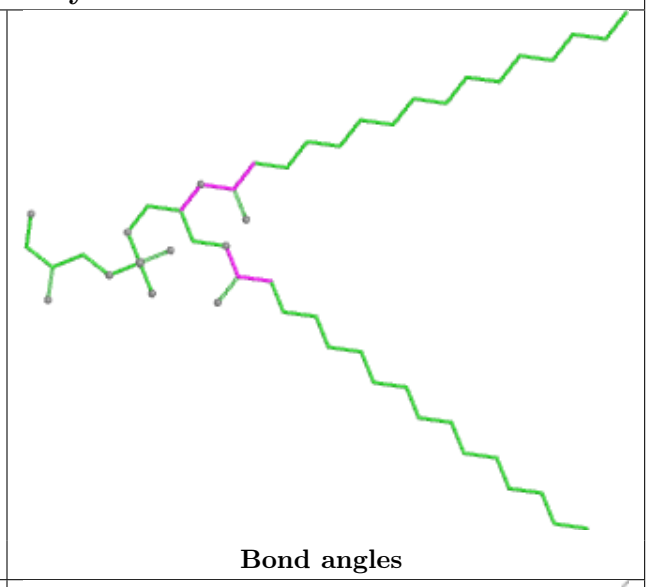


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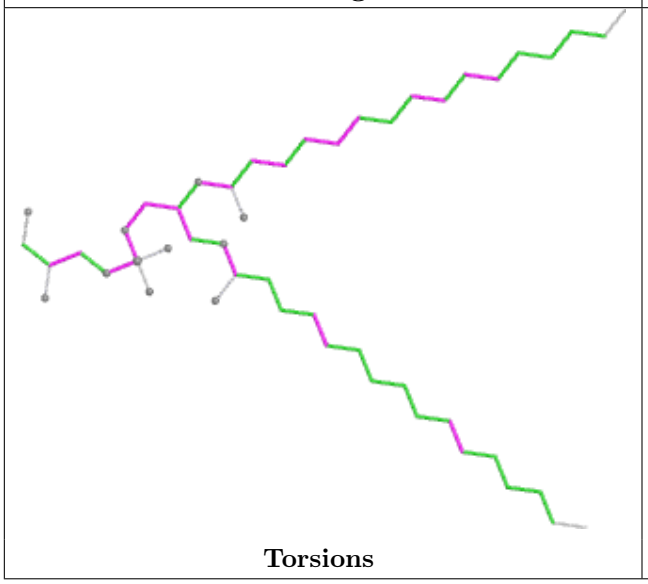
Ligand LHG y 320



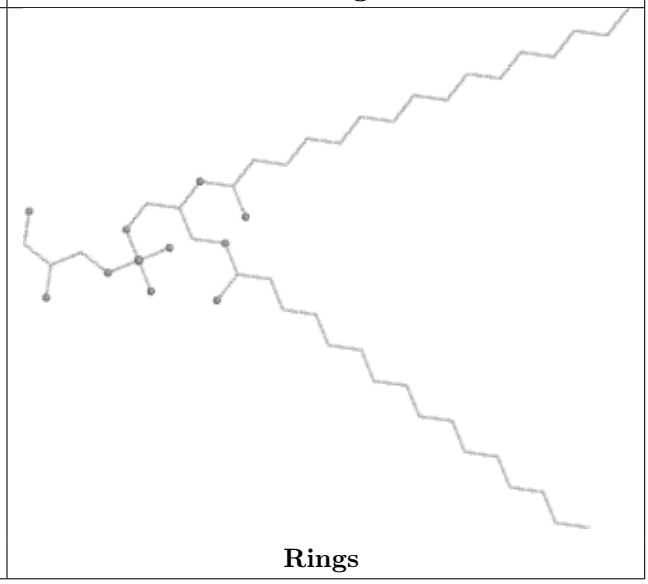
Bond lengths



Bond angles

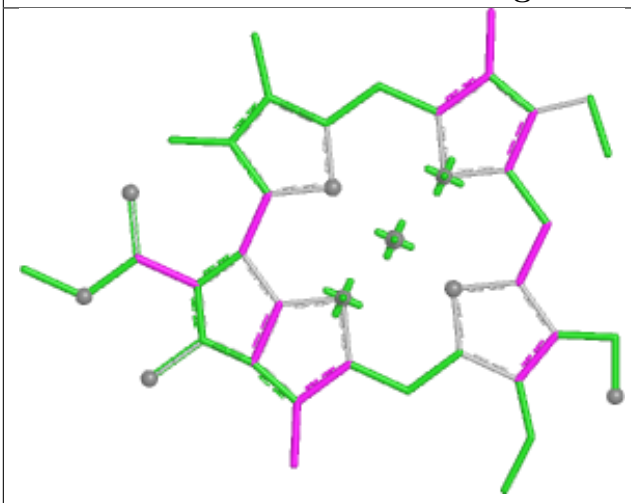


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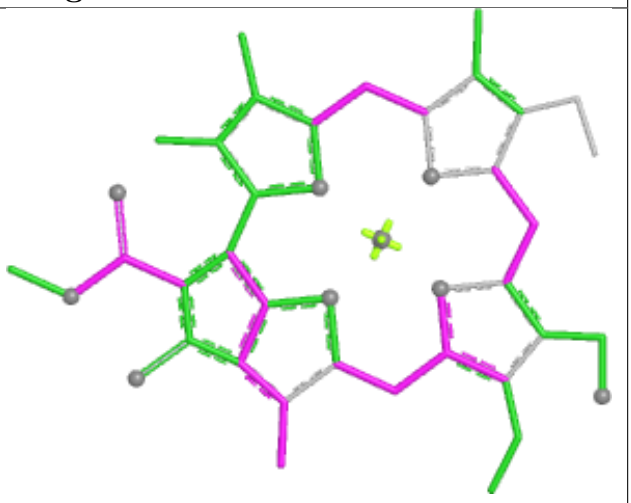


Rings

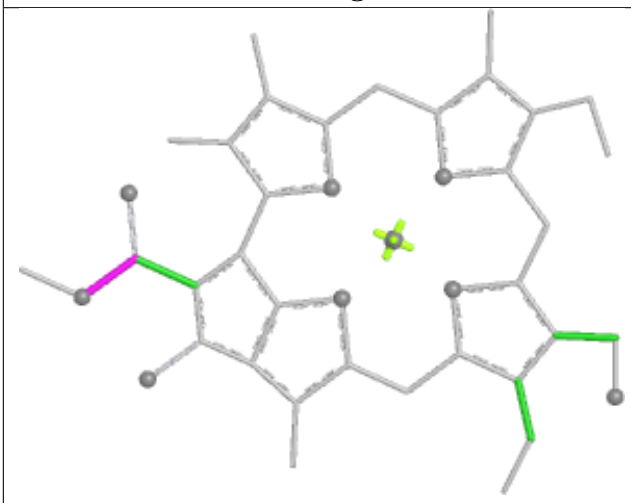
Ligand CHL Gg 309



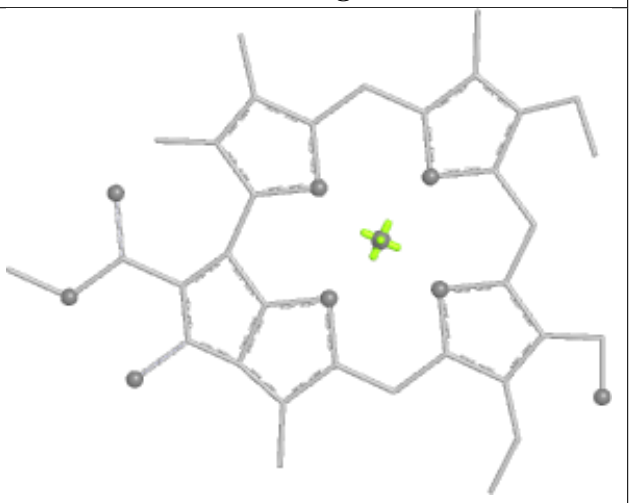
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Bond angles

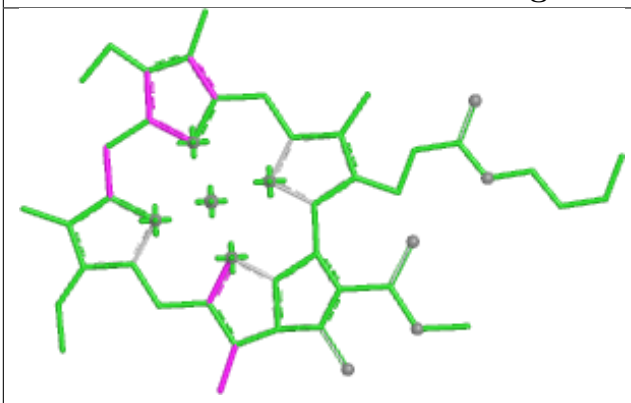


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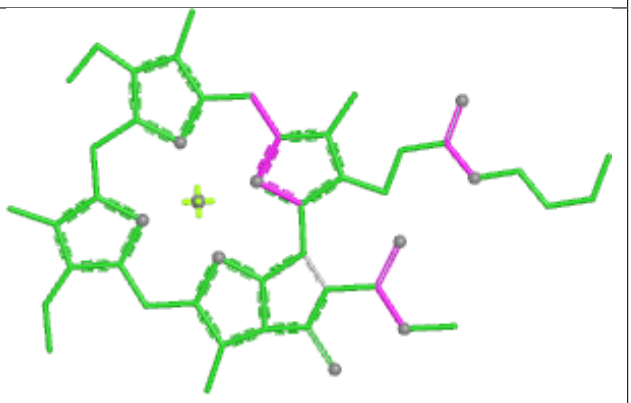


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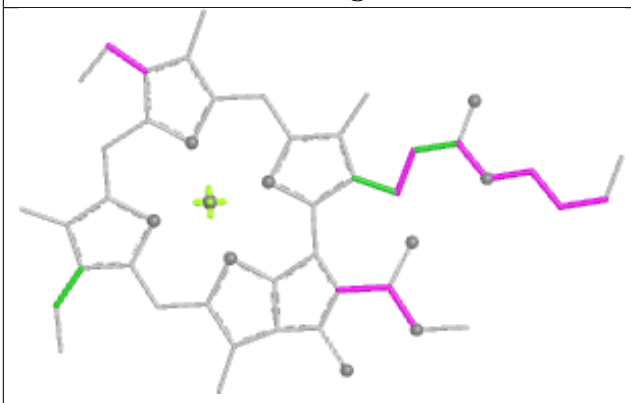
Ligand CLA s 602



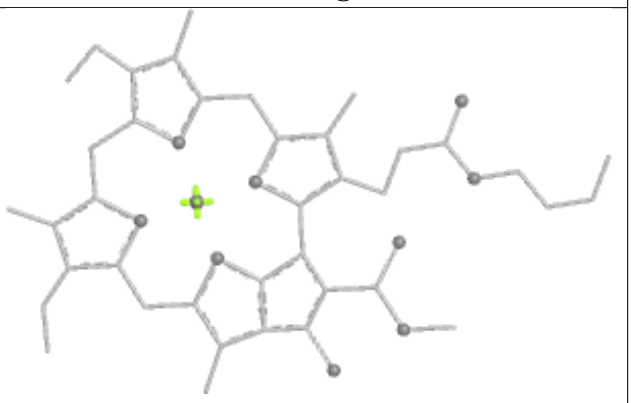
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Bond angles

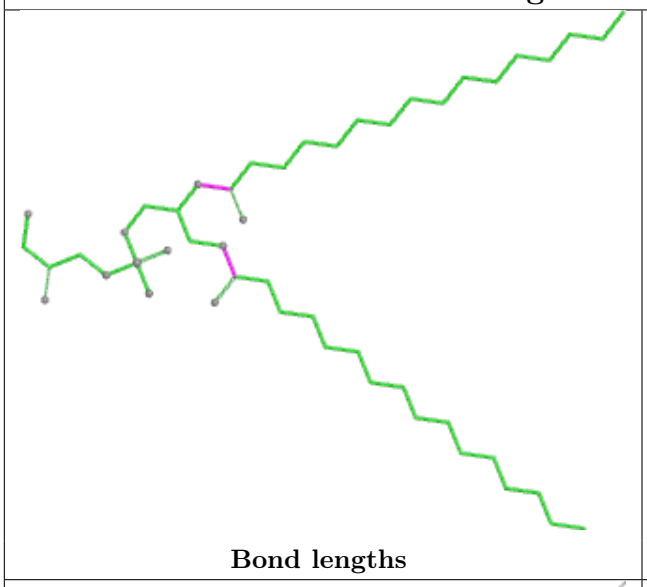


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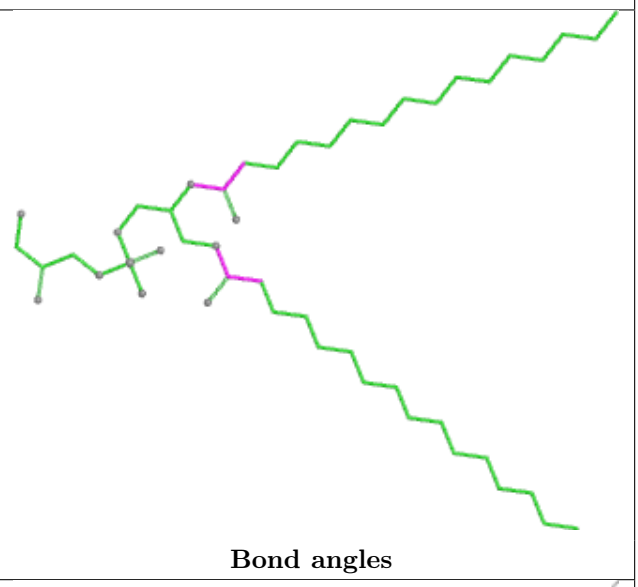


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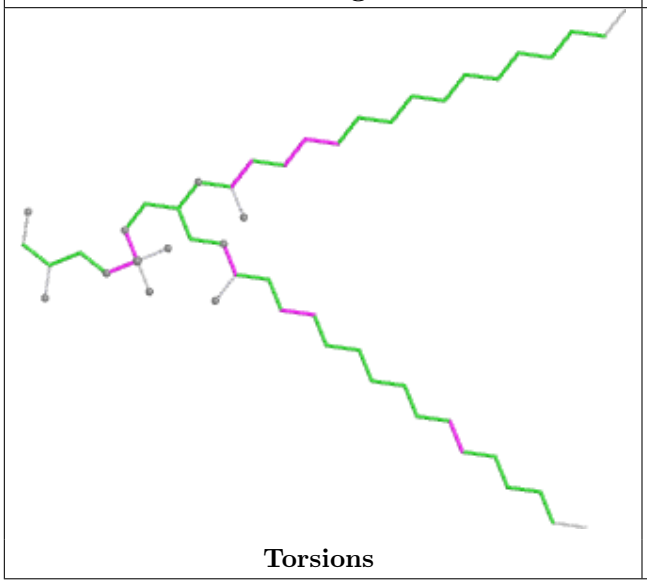
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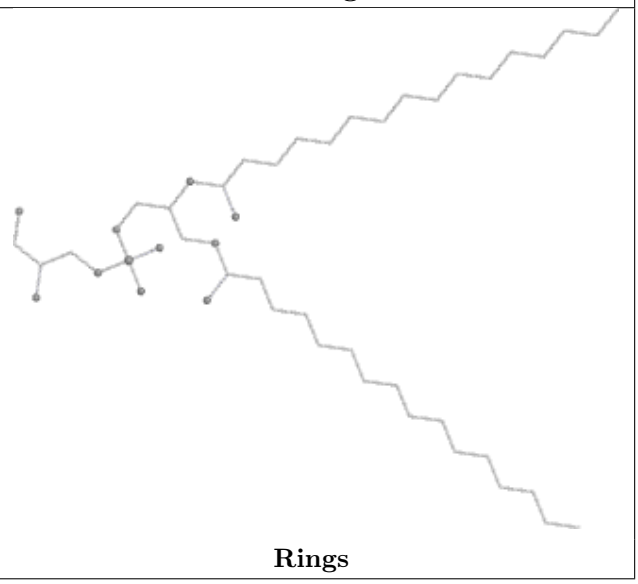
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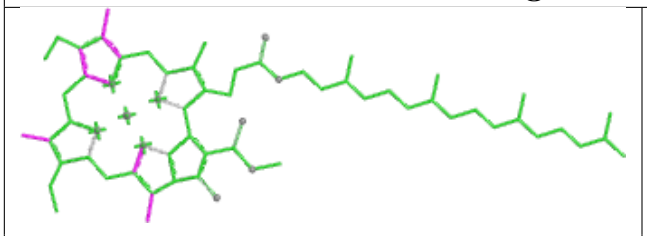


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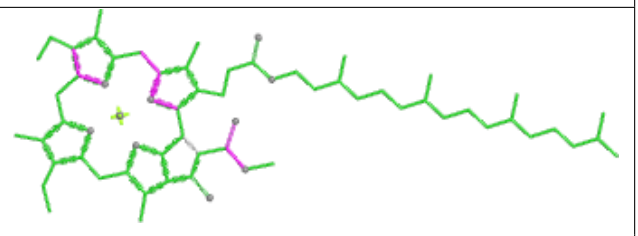


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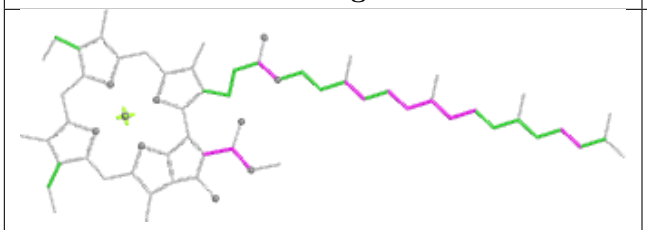
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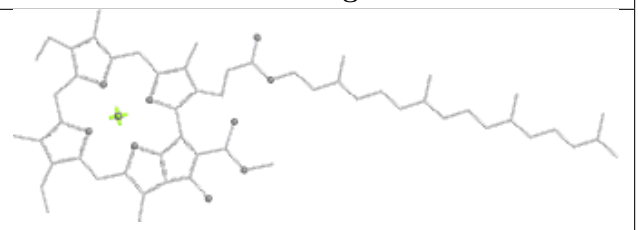
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Bond angles

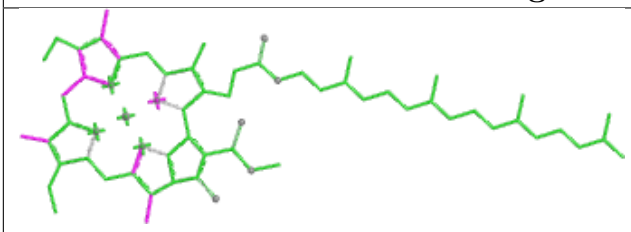


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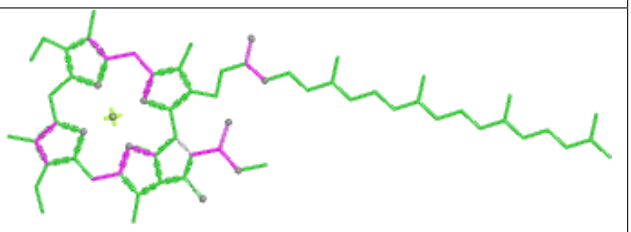


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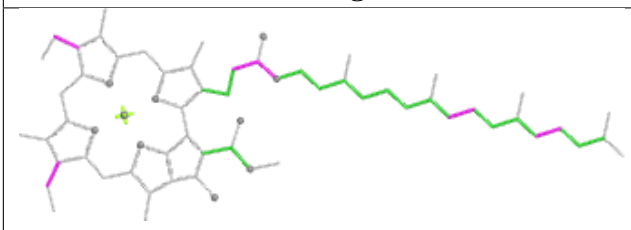
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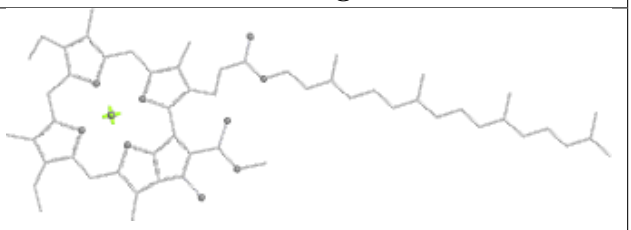
Bond lengths



Bond angles

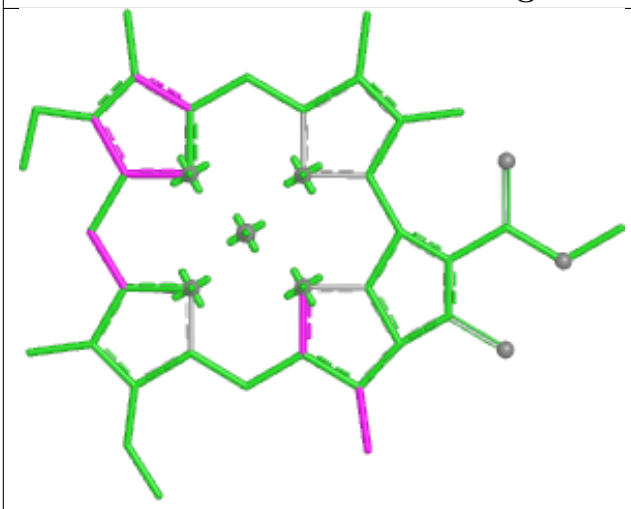


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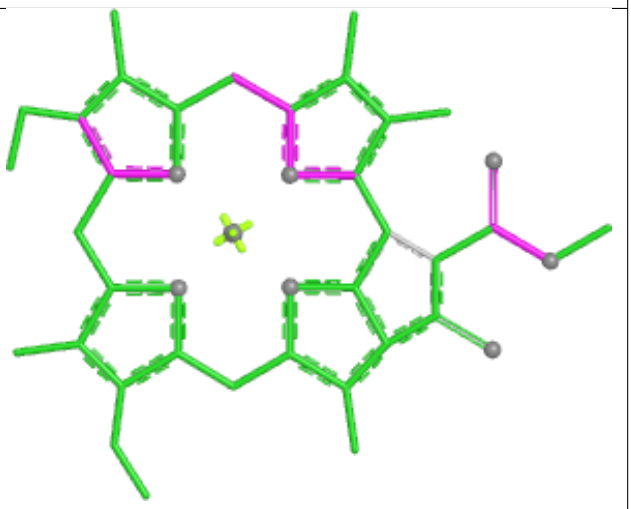


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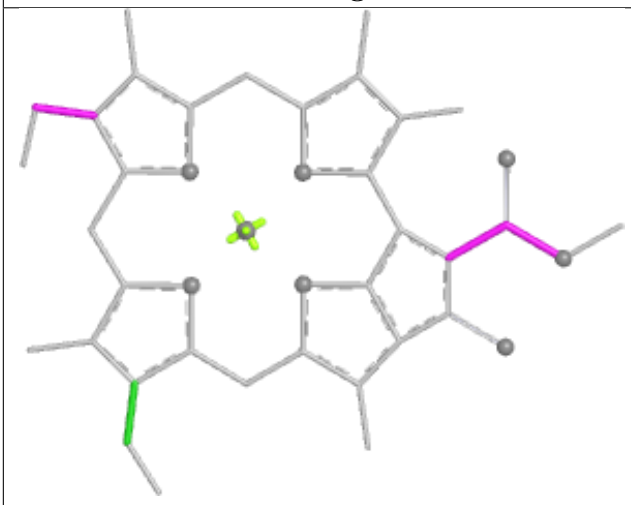
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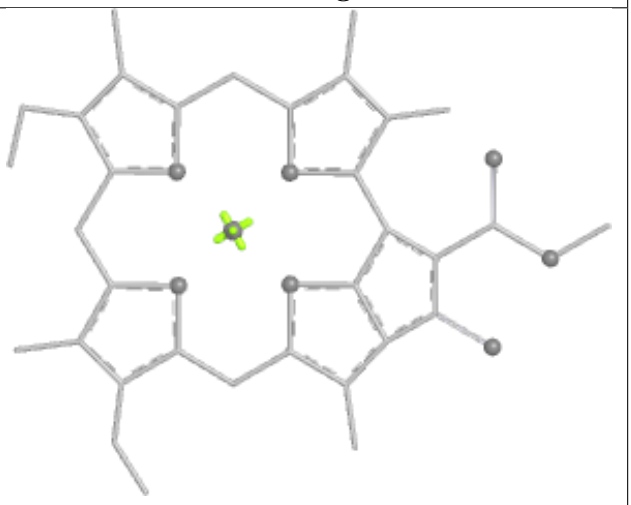
Bond lengths



Bond angles

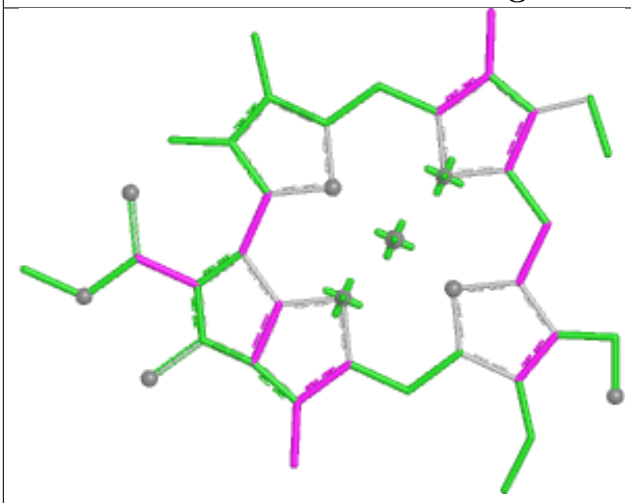


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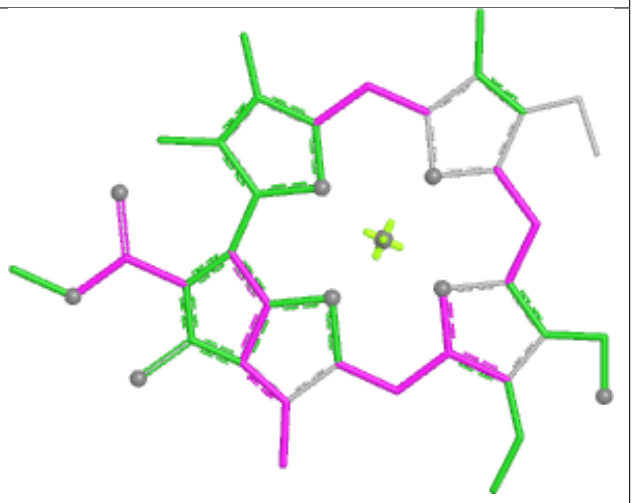


Rings

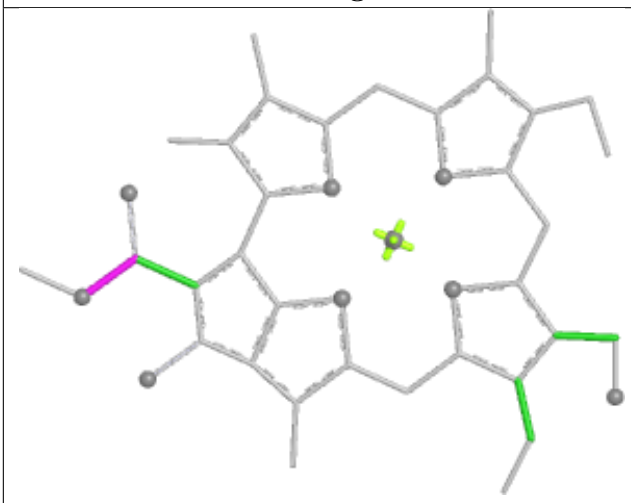
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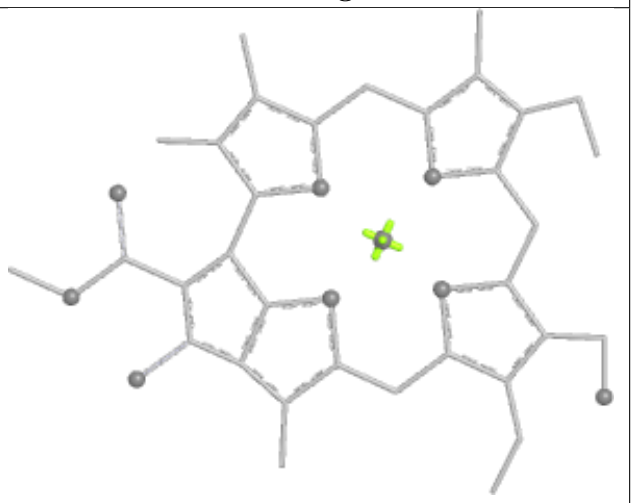
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Bond angles

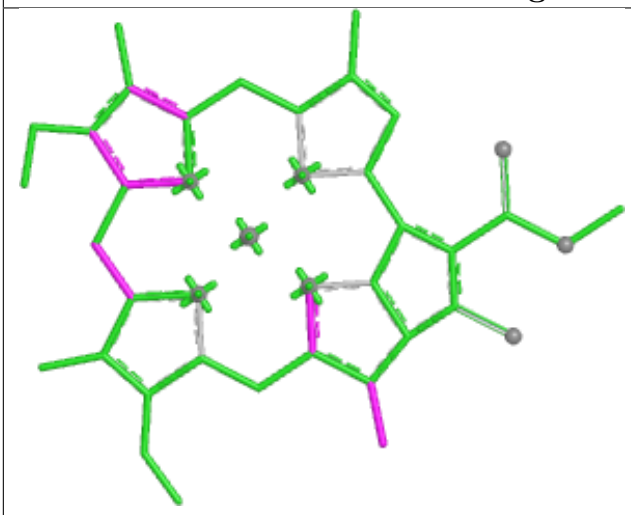


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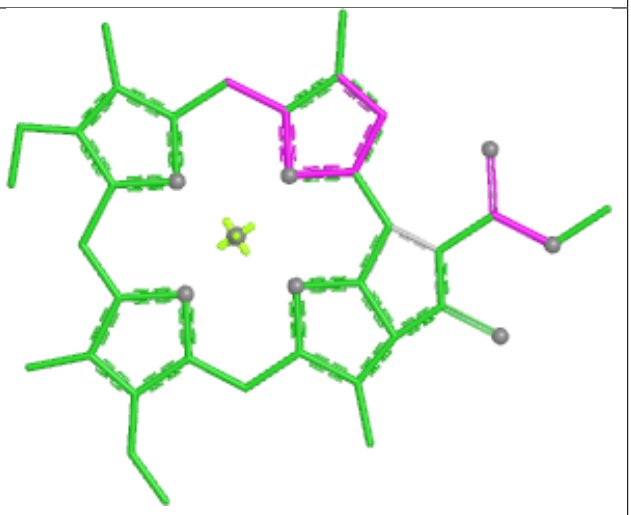


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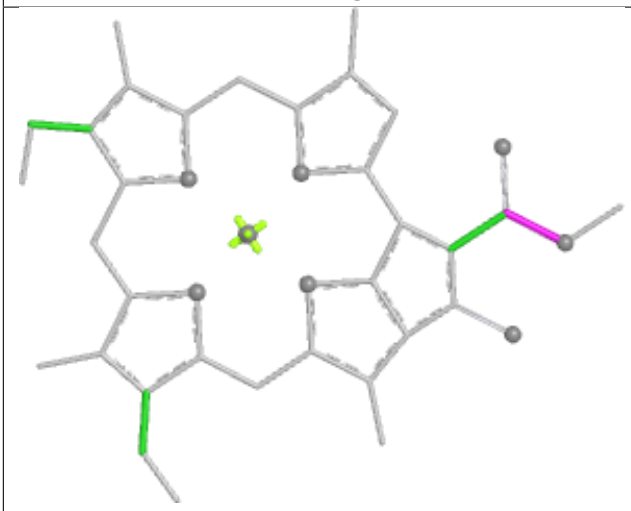
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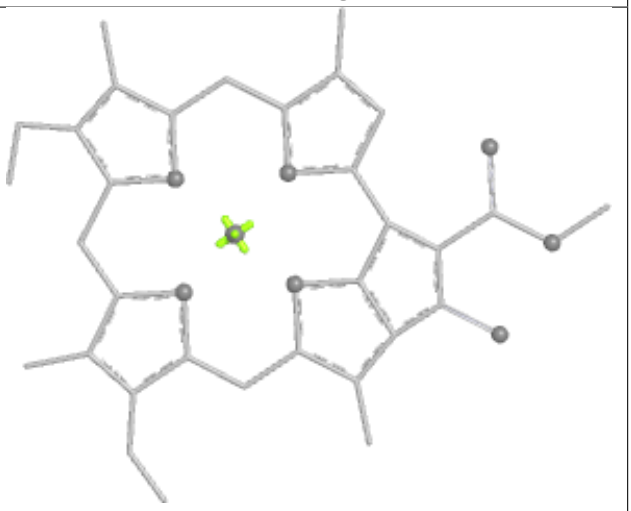
Bond lengths



Bond angles

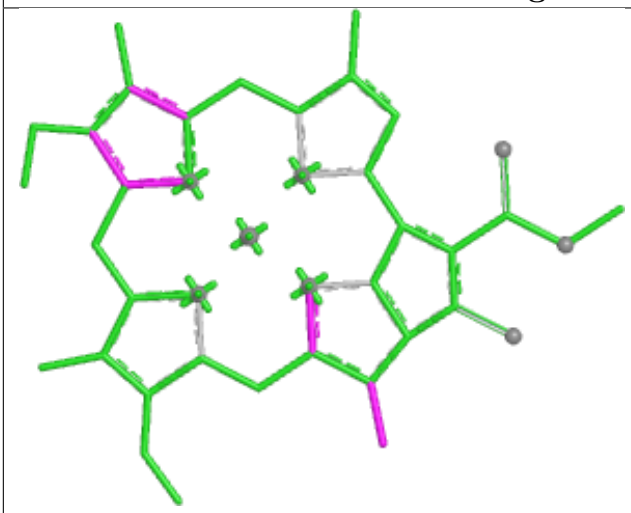


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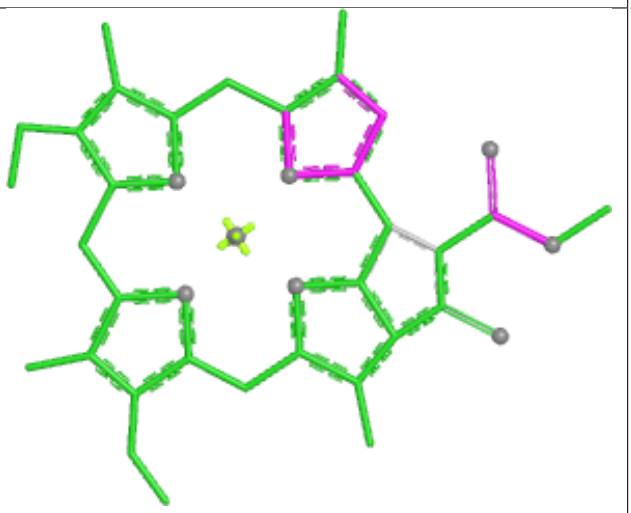


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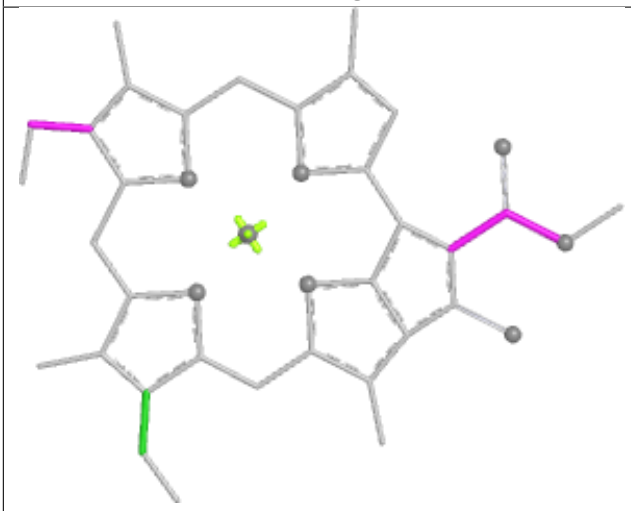
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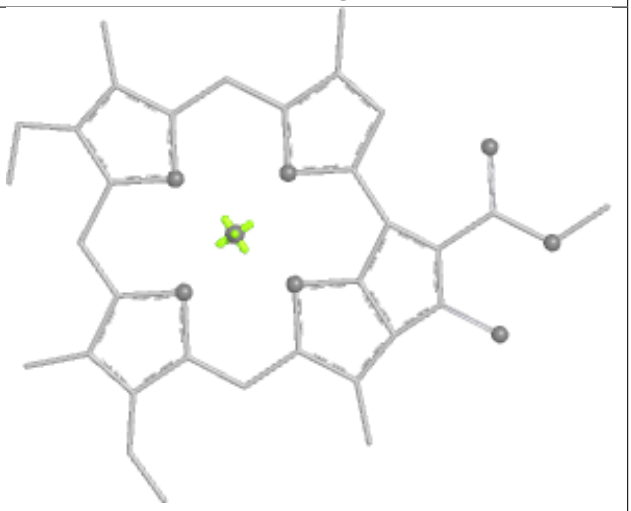
Bond lengths



Bond angles

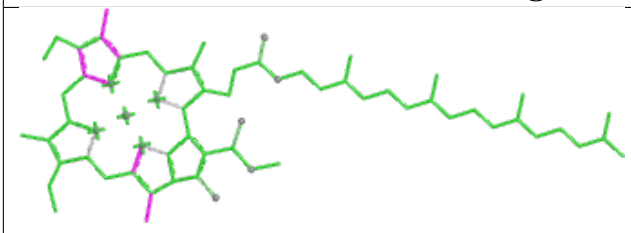


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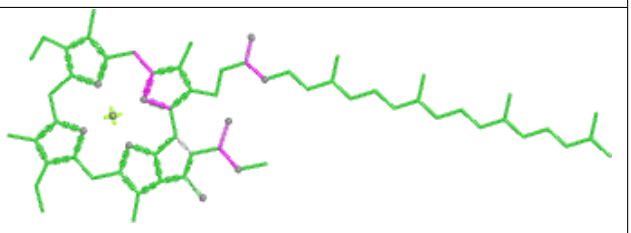


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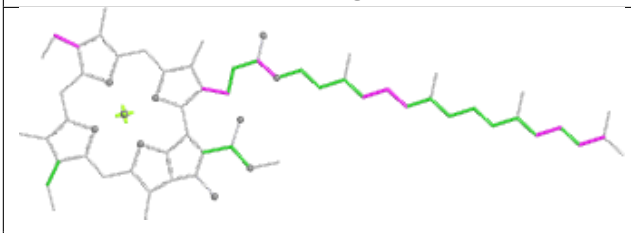
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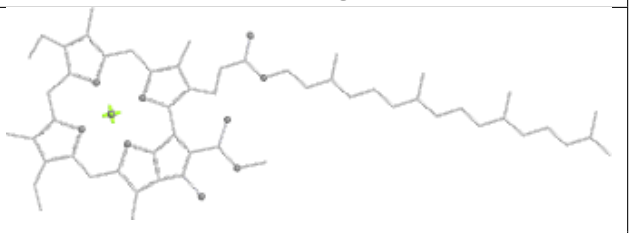
Bond lengths



Bond angles

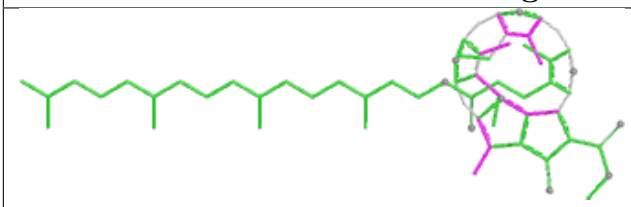


Torsions

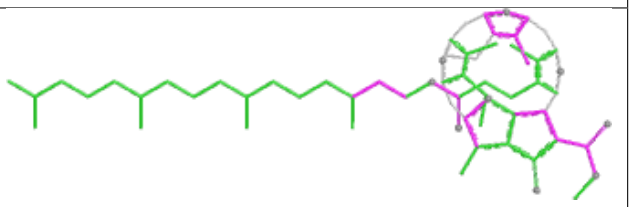


Rings

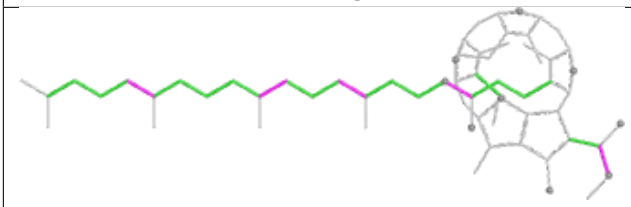
Ligand PHO A 407



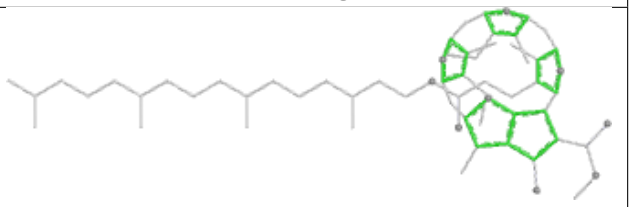
Bond lengths



Bond angles

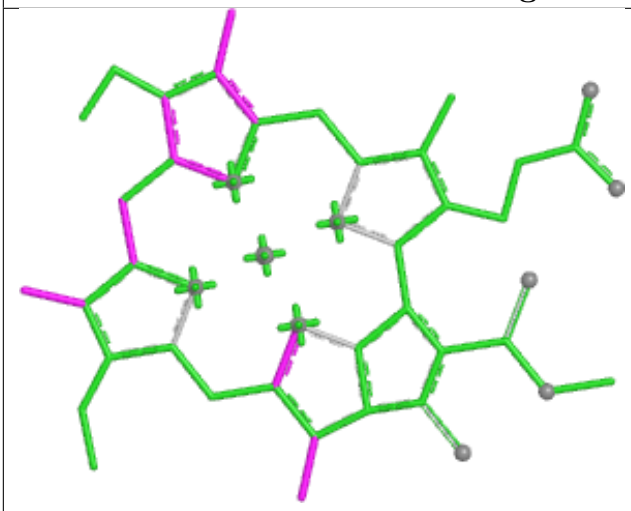


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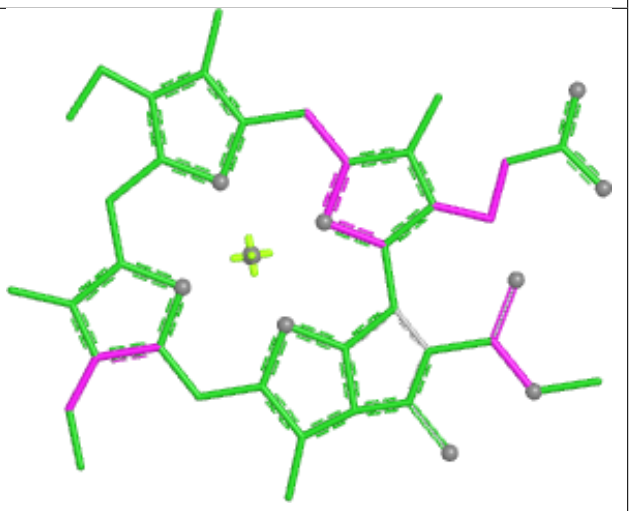


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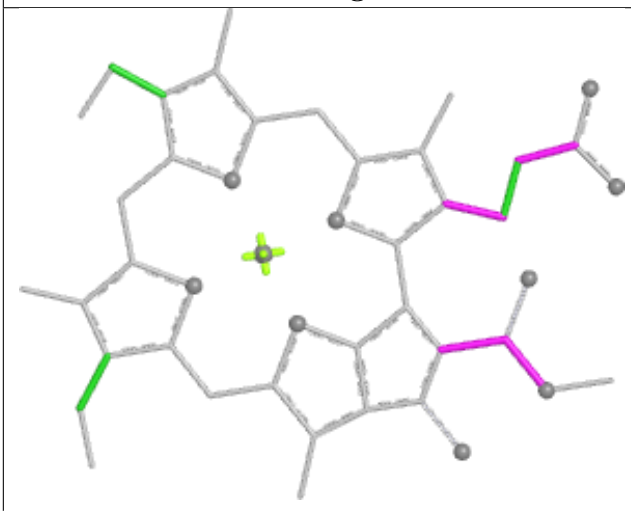
Ligand CLA 44 602



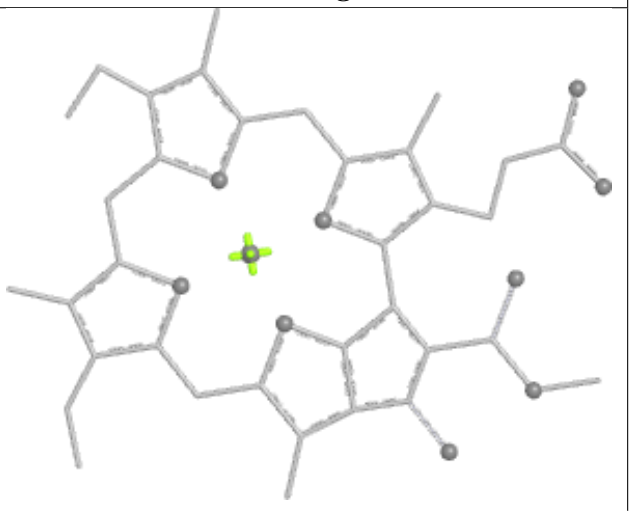
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Bond angles

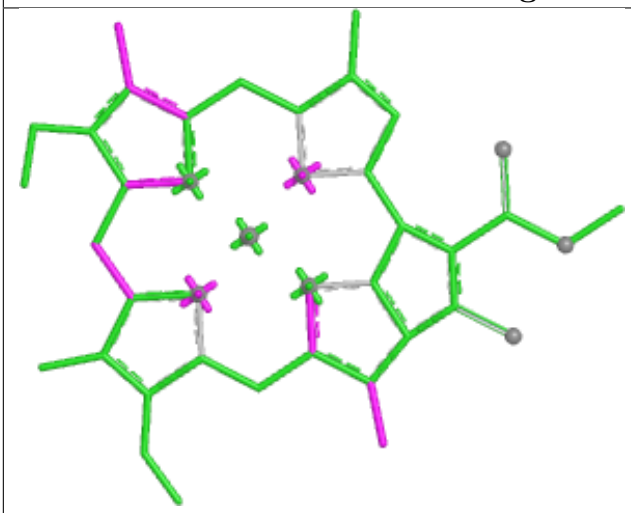


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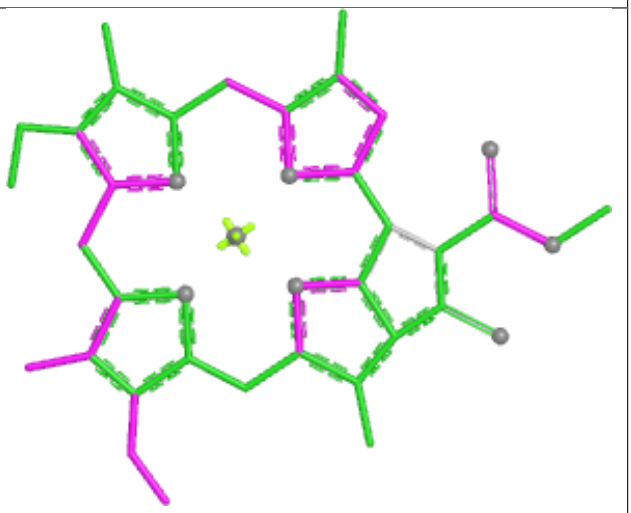


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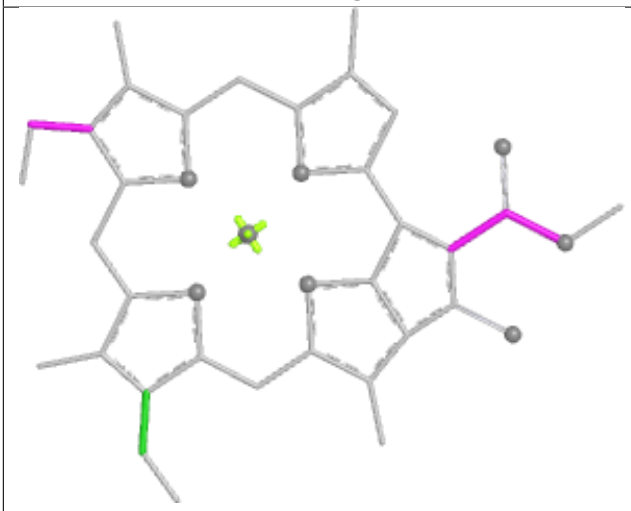
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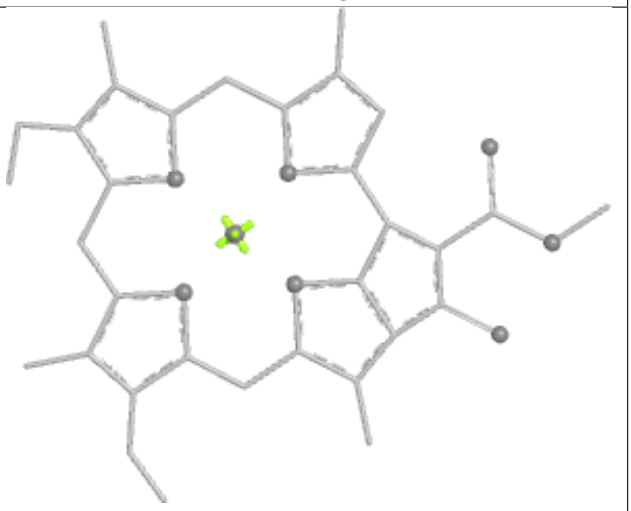
Bond lengths



Bond angles

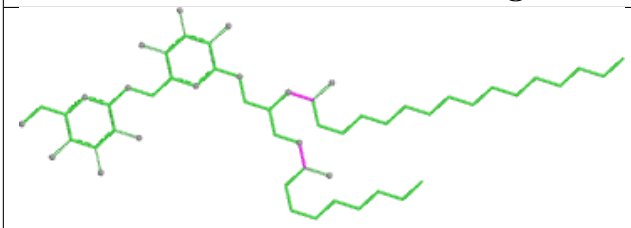


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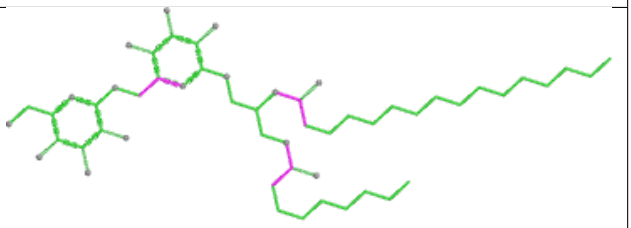


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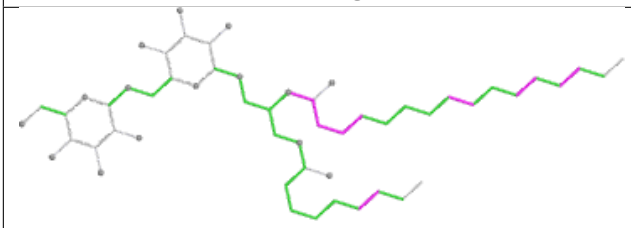
Ligand DGD CC 518



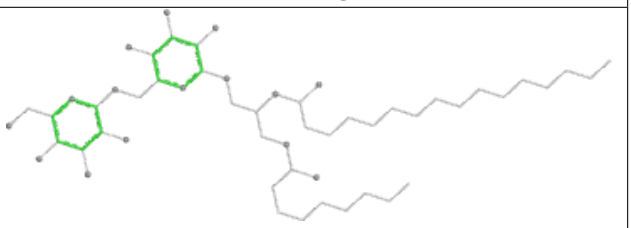
Bond lengths



Bond angles

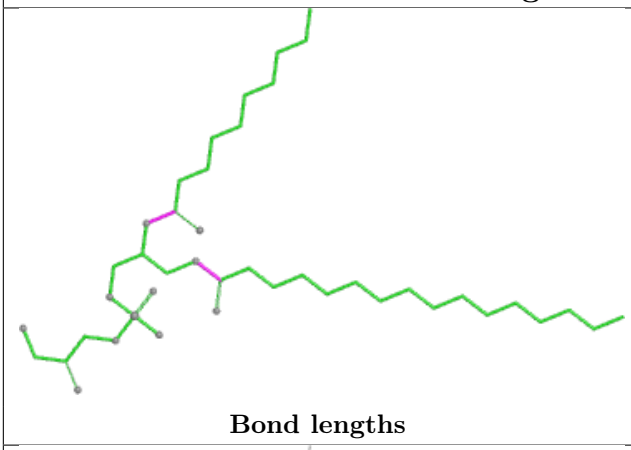


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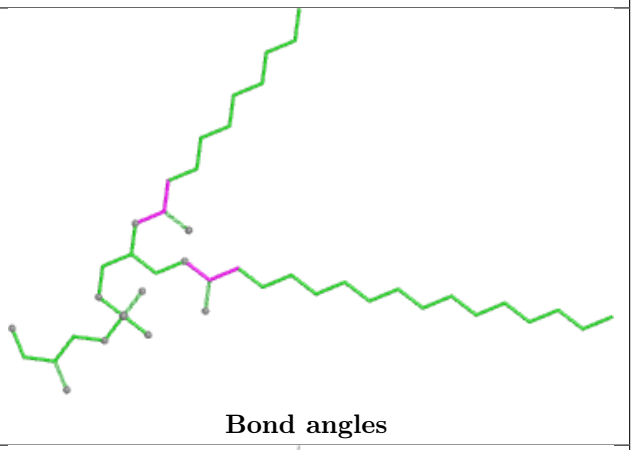


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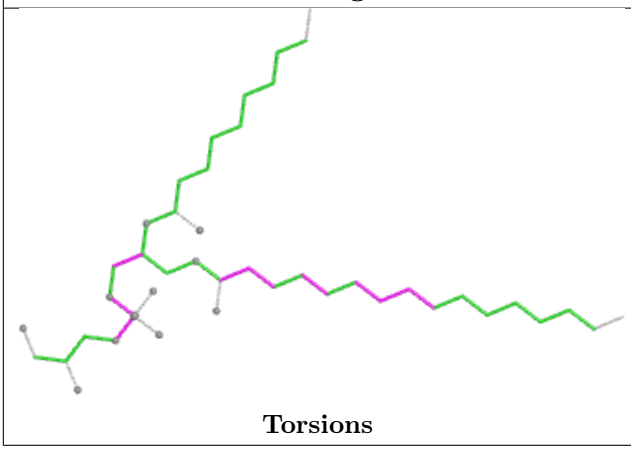
Ligand LHG D 408



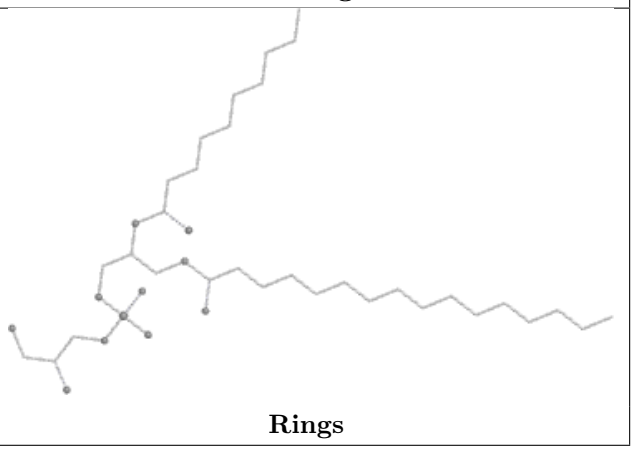
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Bond angles

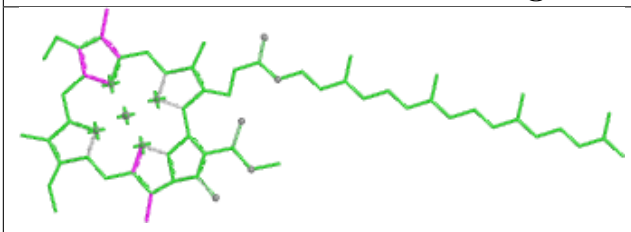


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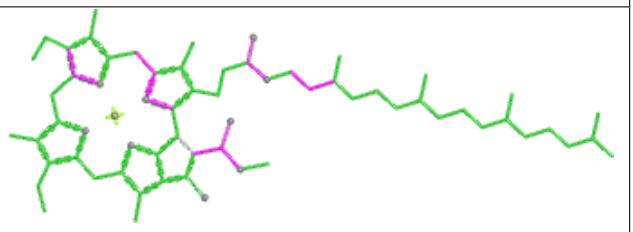


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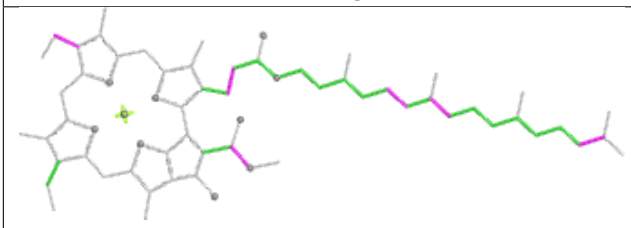
Ligand CLA b 606



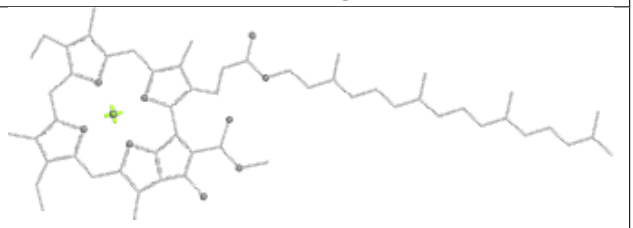
Bond lengths



Bond angles

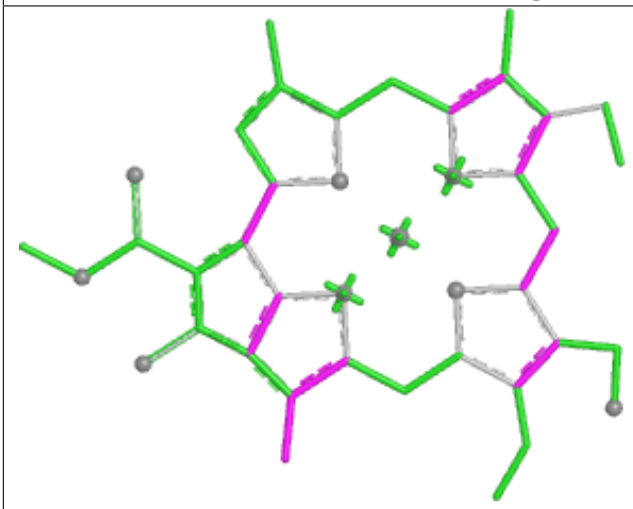


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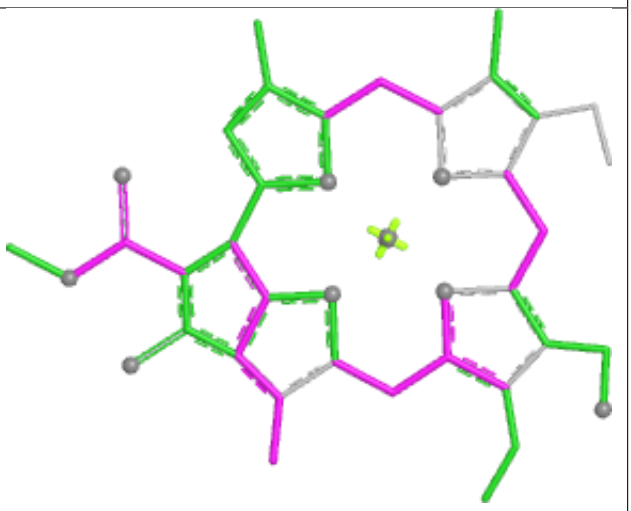


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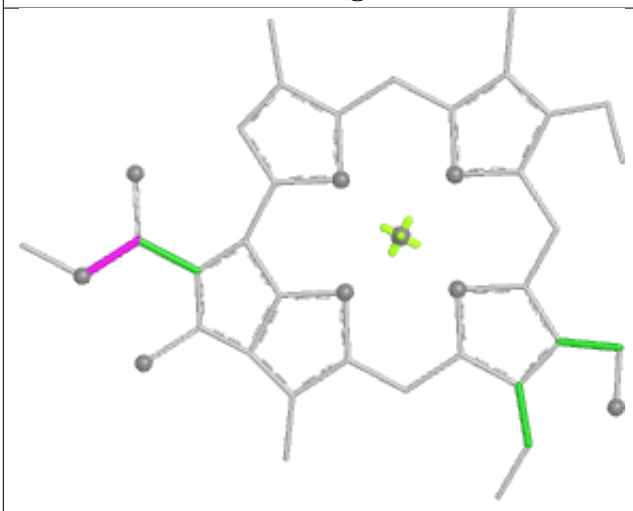
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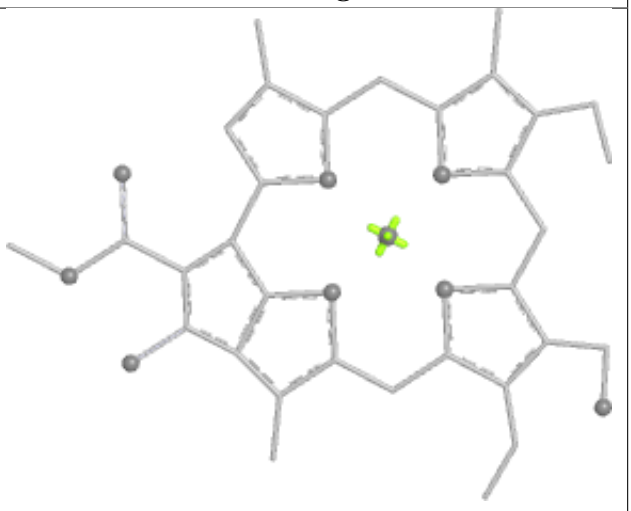
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Bond angles

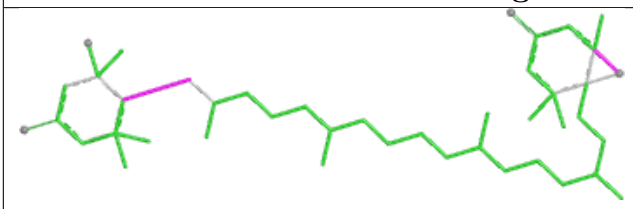


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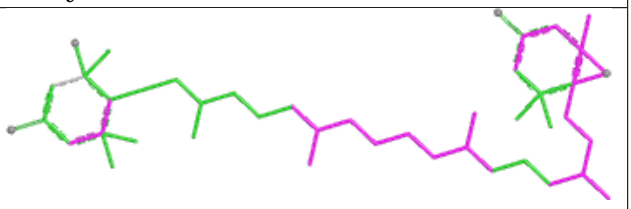


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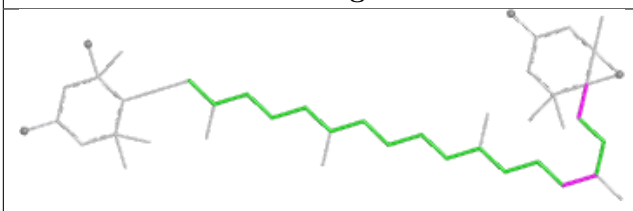
Ligand NEX Yy 617



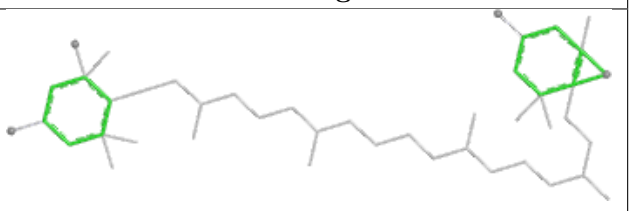
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Bond angles

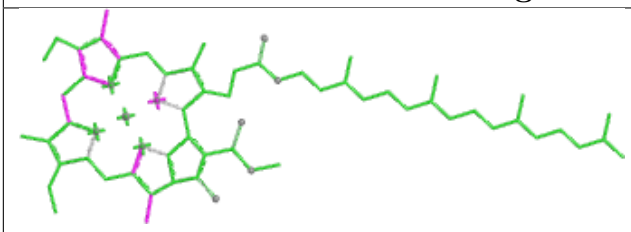


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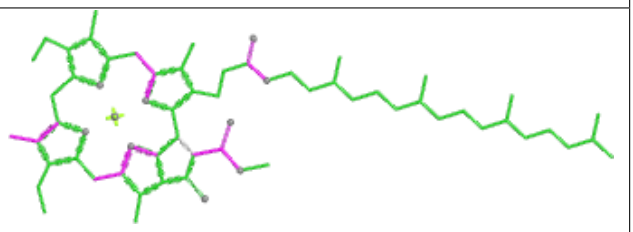


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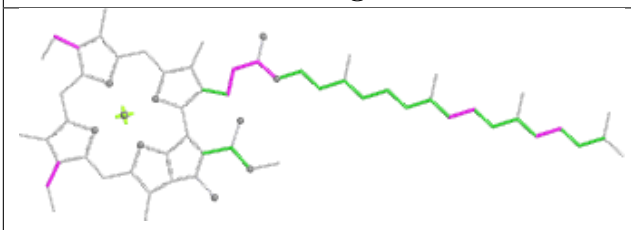
Ligand CLA Aa 406



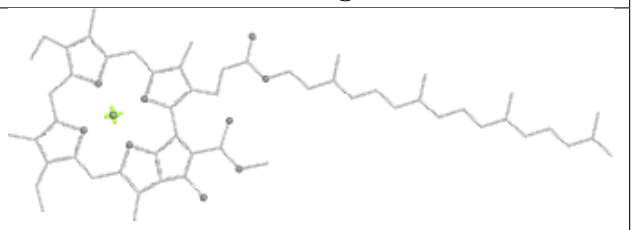
Bond lengths



Bond angles

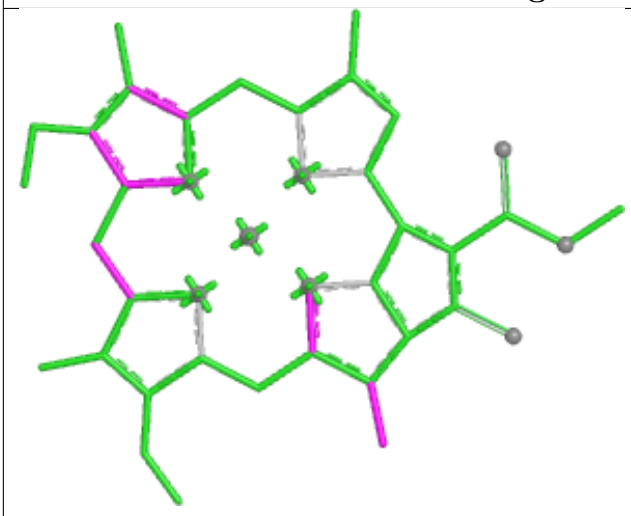


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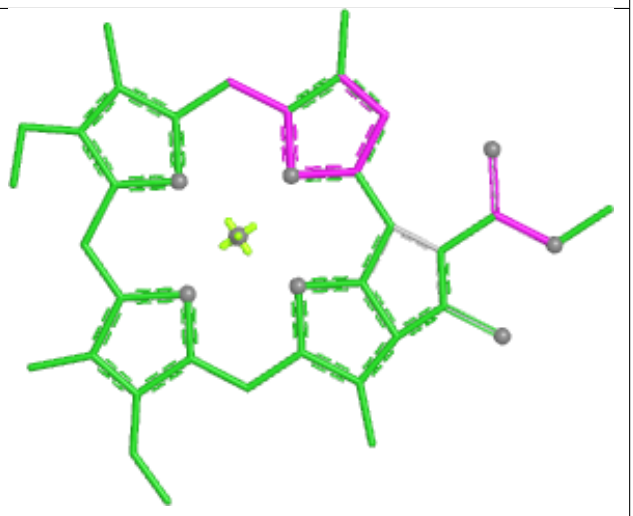


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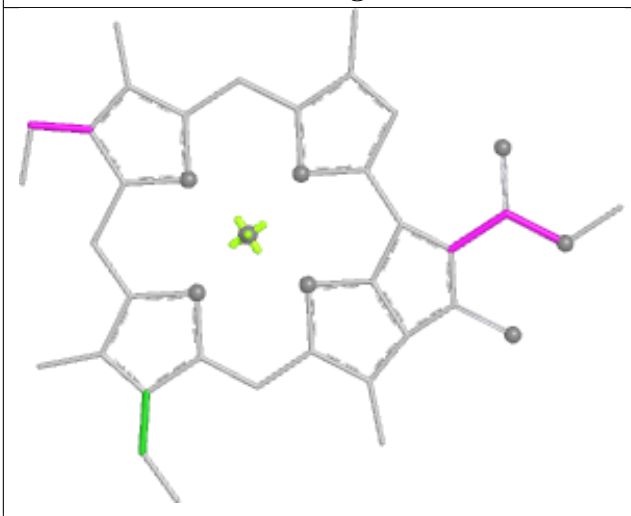
Ligand CLA 3 613



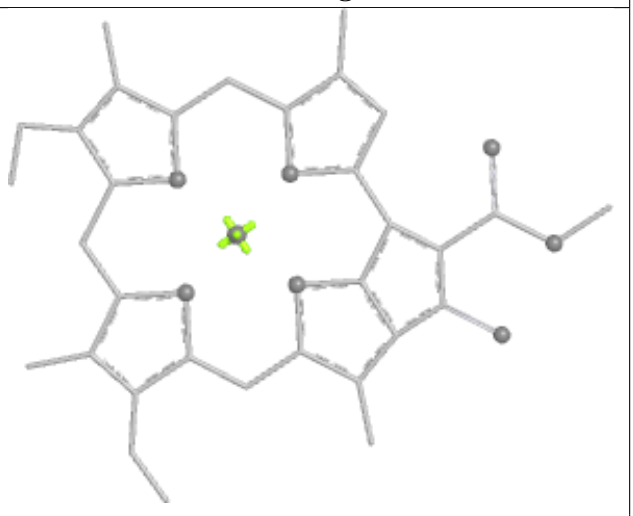
Bond lengths



Bond angles

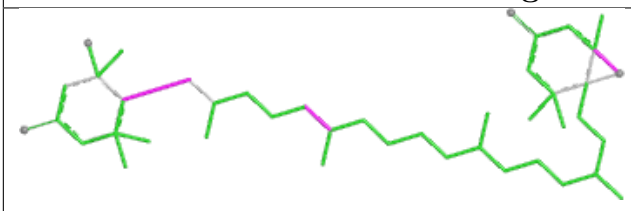


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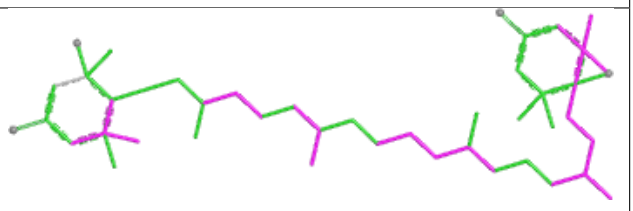


Rings

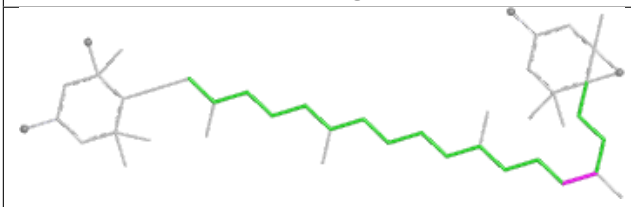
Ligand NEX R 617



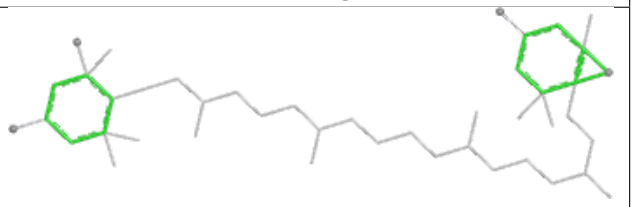
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Bond angles

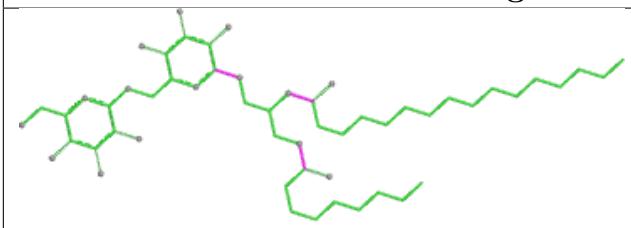


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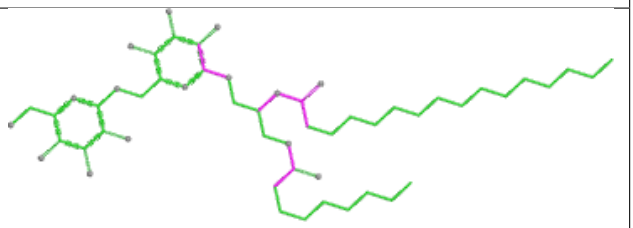


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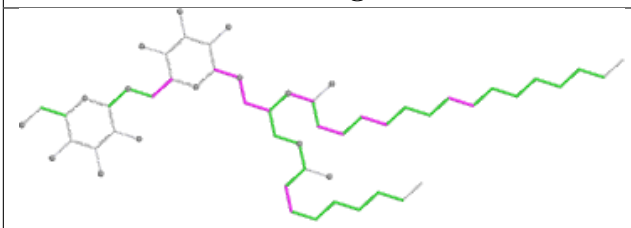
Ligand DGD CC 522



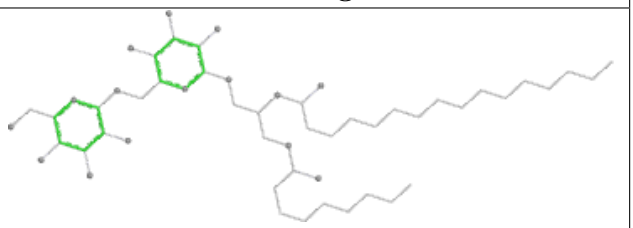
Bond lengths



Bond angles

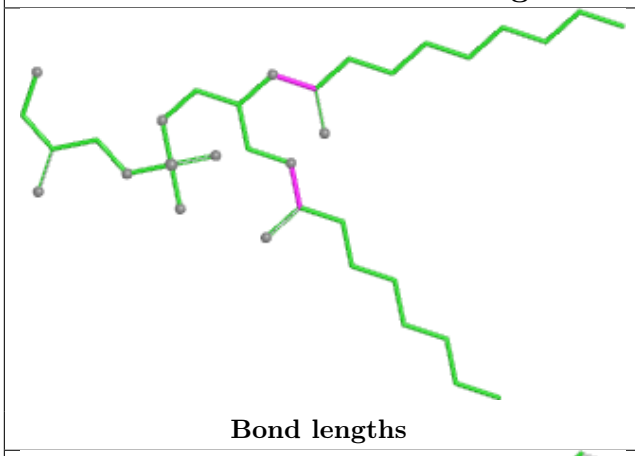


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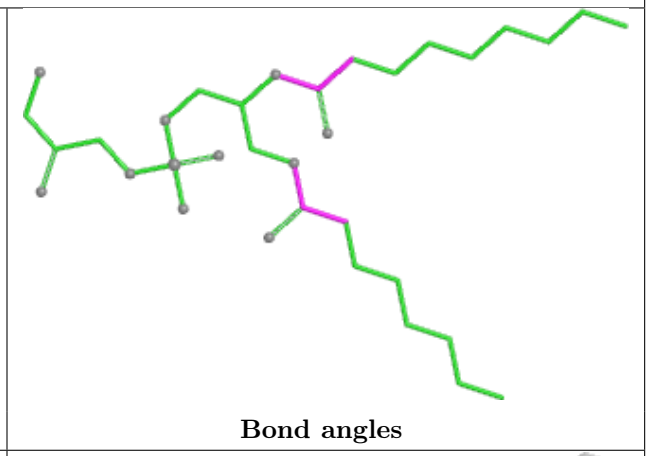


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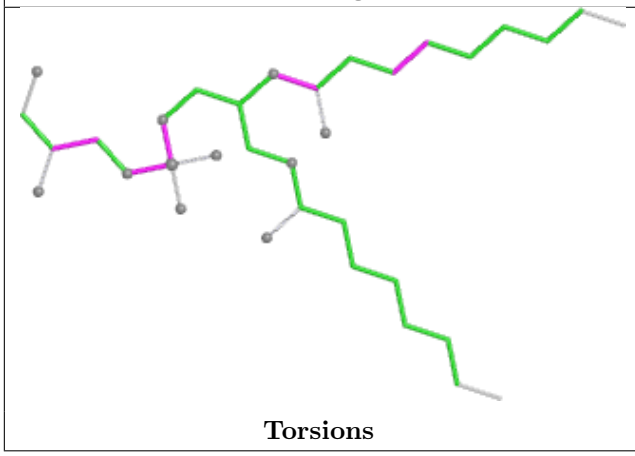
Ligand LHG BB 622



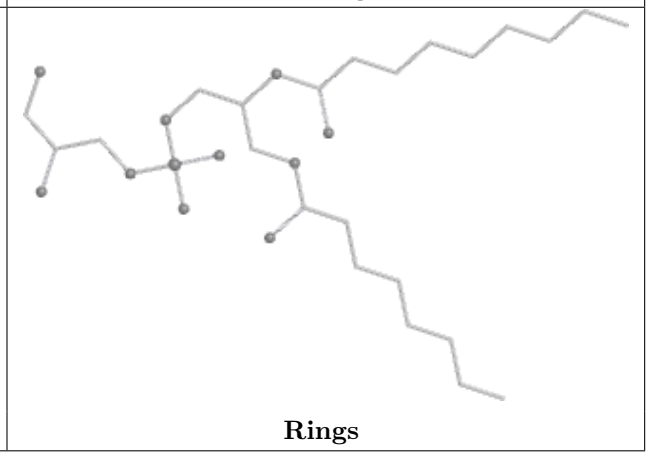
Bond lengths



Bond angles

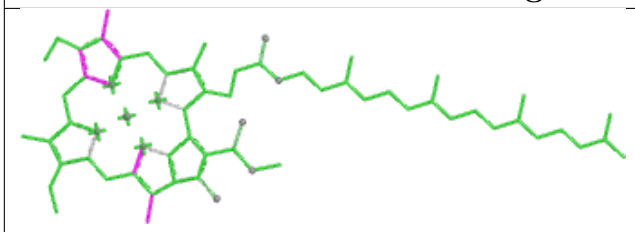


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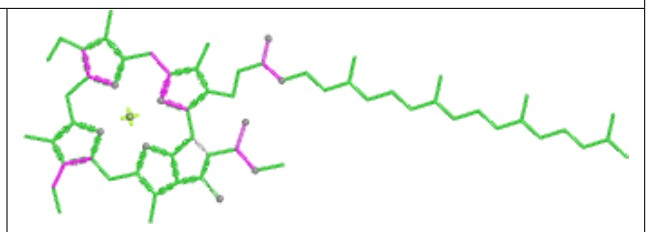


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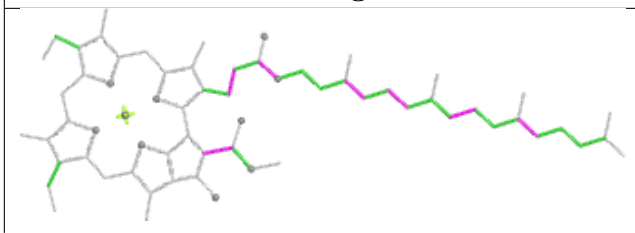
Ligand CLA C 507



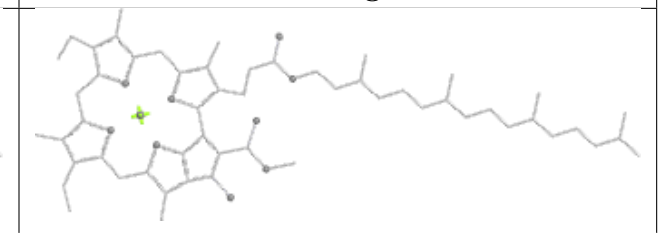
Bond lengths



Bond angles

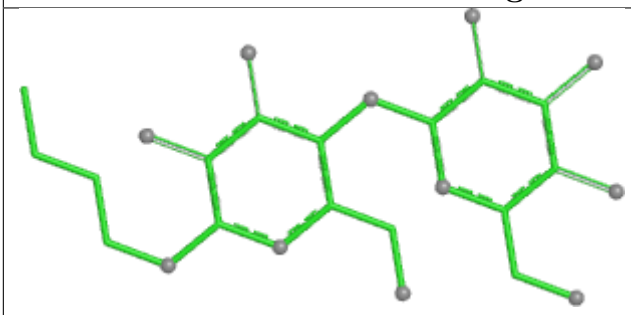


Torsions

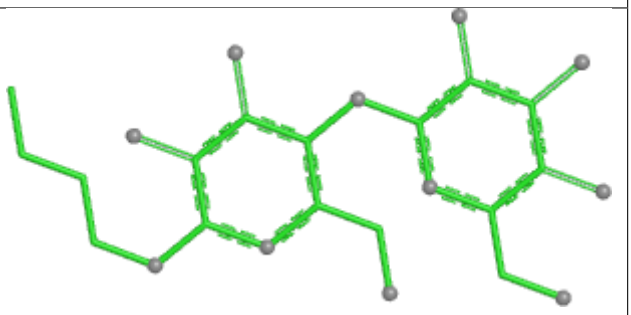


Rings

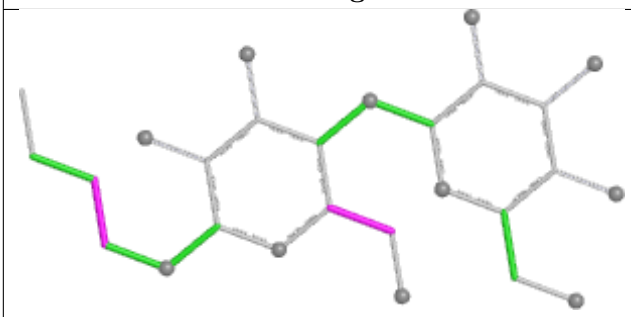
Ligand LMU RR 301



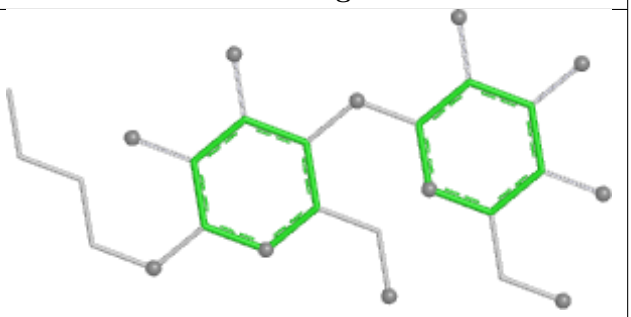
Bond lengths



Bond angles

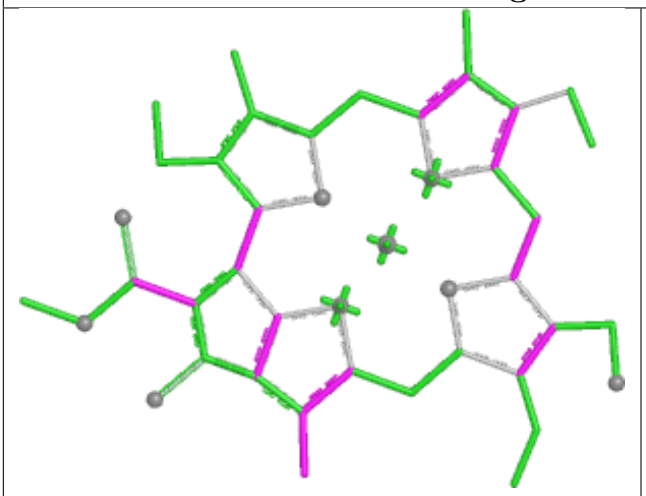


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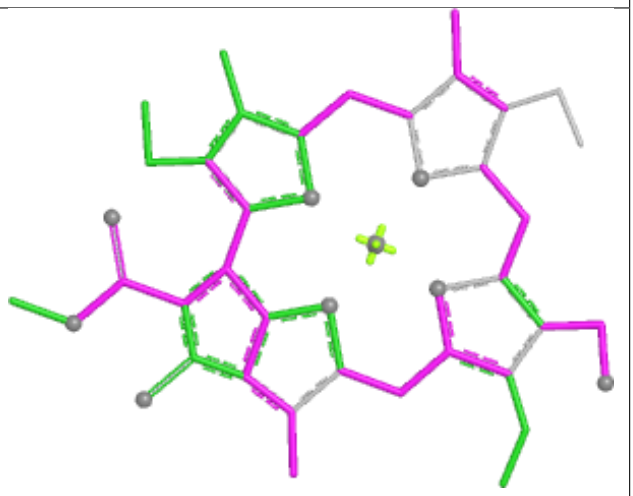


Rings

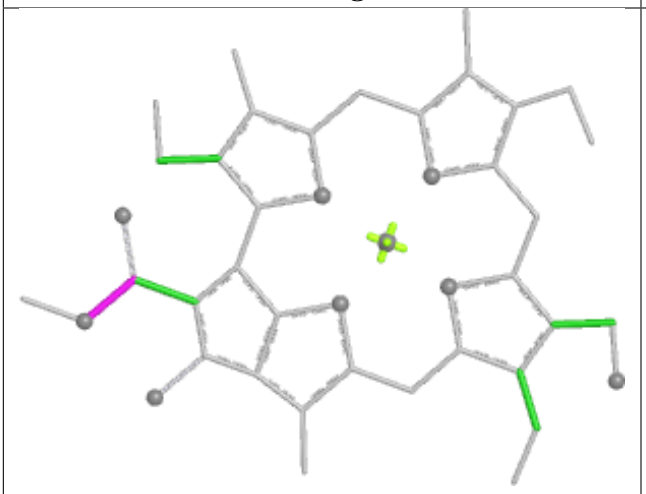
Ligand CHL YY 607



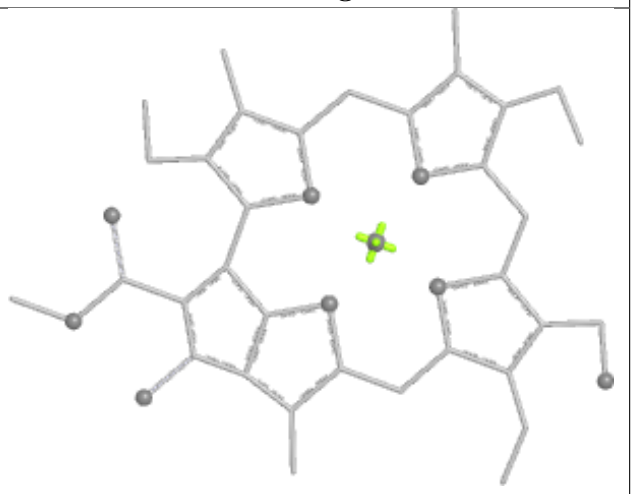
Bond lengths



Bond angles

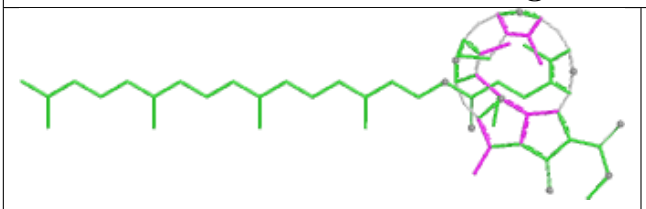


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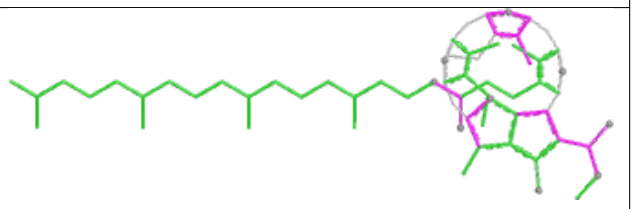


Rings

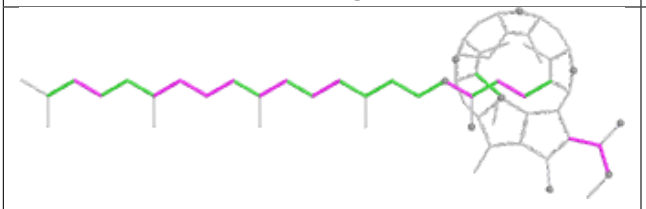
Ligand PHO a 409



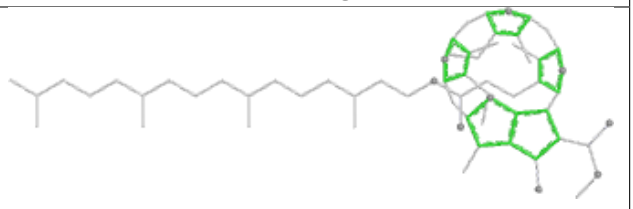
Bond lengths



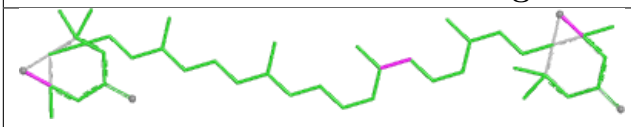
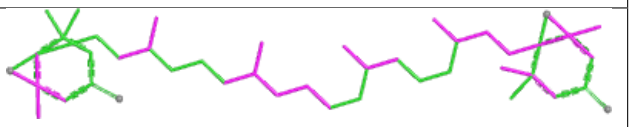
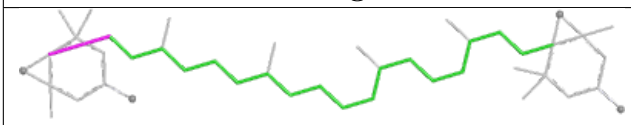
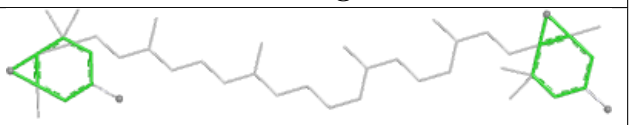
Bond angles

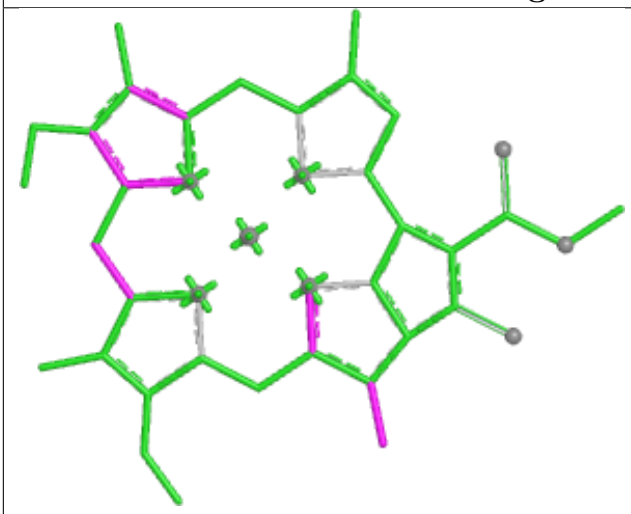
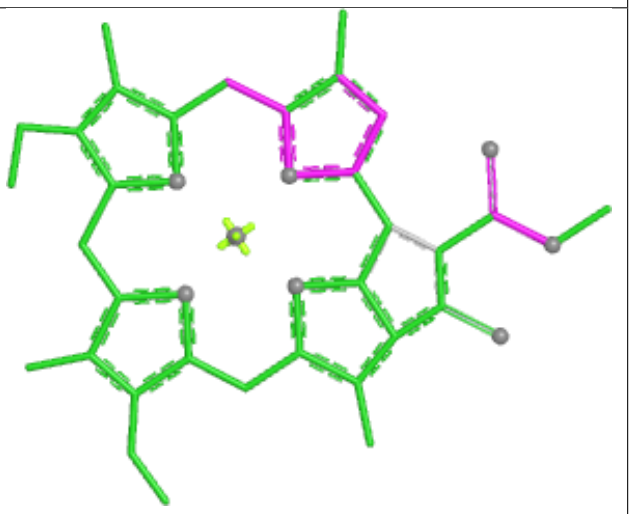
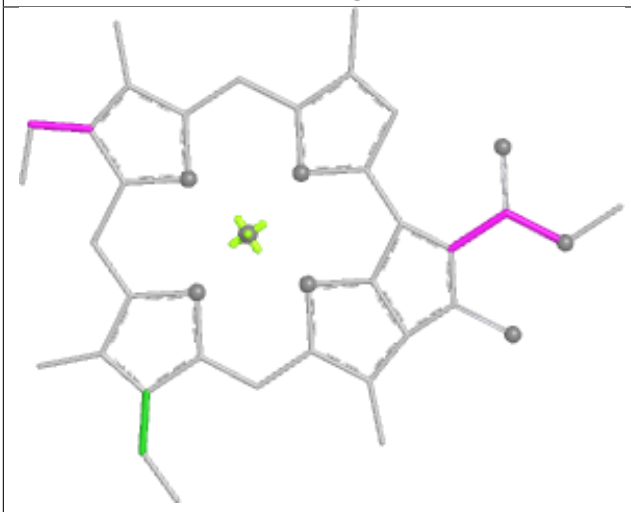
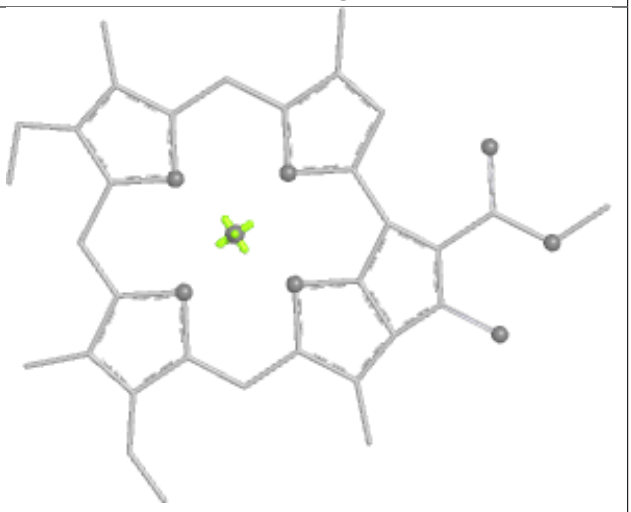


Torsions

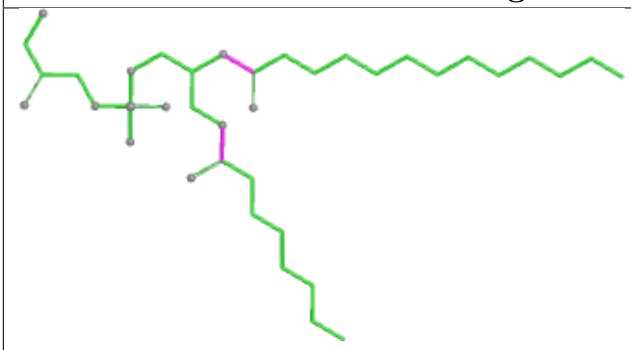


Rings

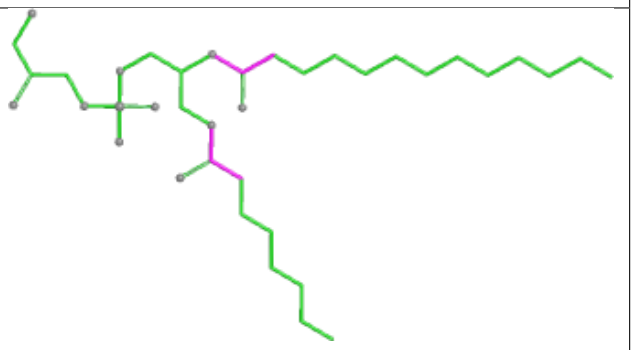
Ligand XAT Nn 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

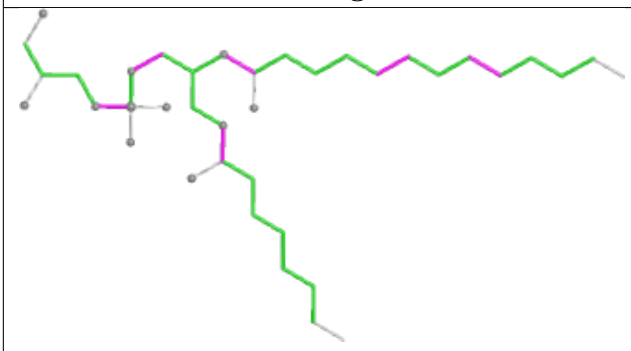
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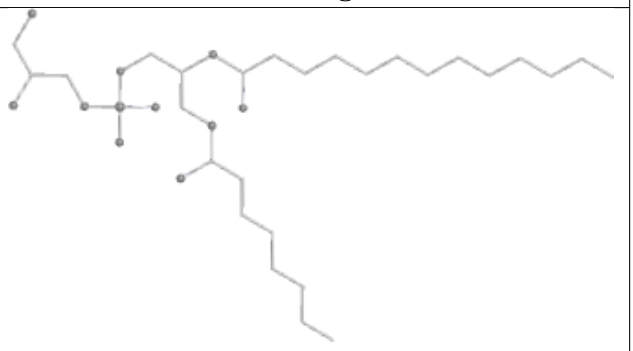
Bond lengths



Bond angles

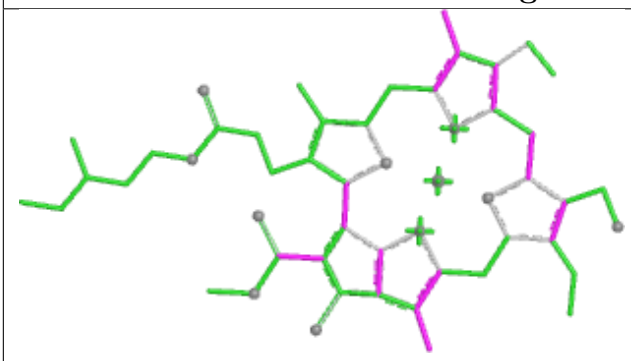


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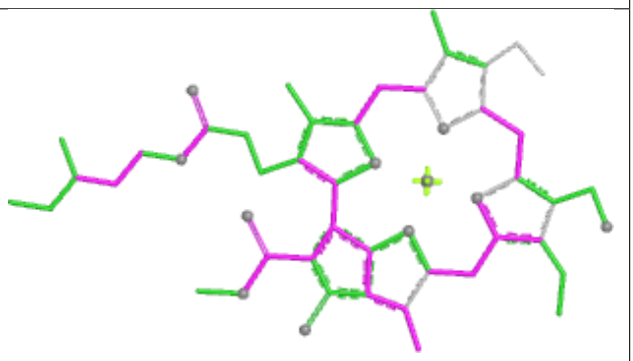


Rings

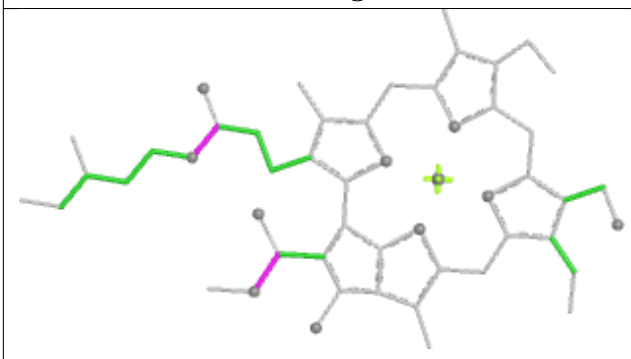
Ligand CHL Ss 601



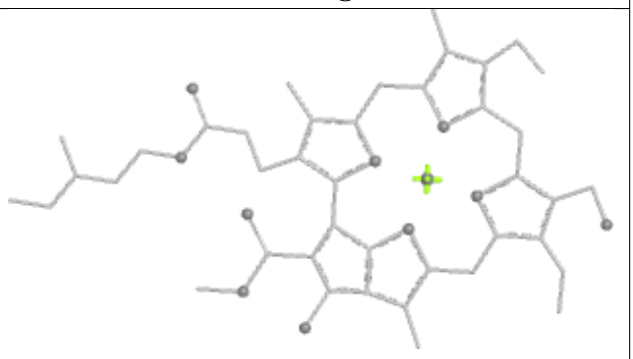
Bond lengths



Bond angles

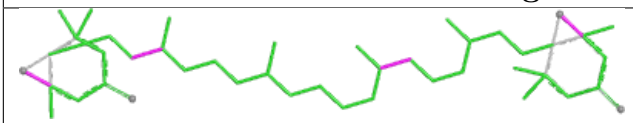


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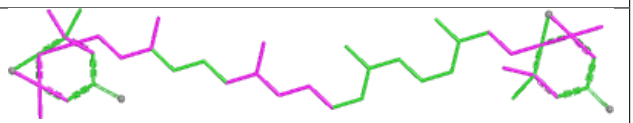


Rings

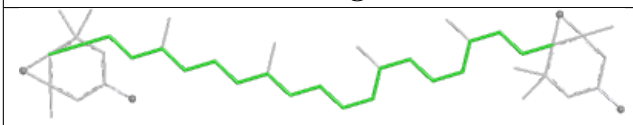
Ligand XAT N 617



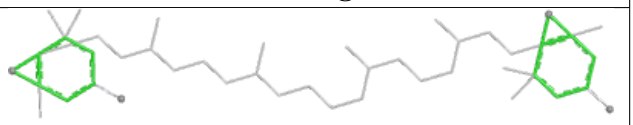
Bond lengths



Bond angles

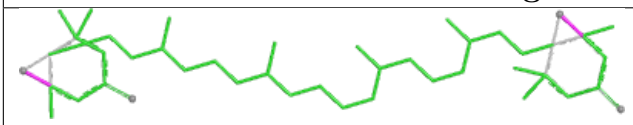


Torsions

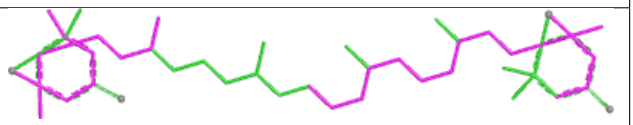


Rings

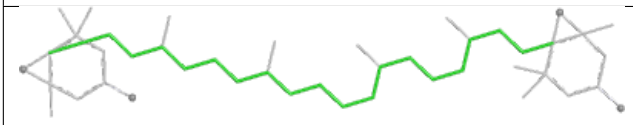
Ligand XAT R 616



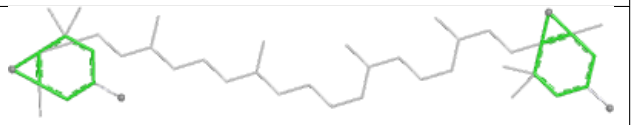
Bond lengths



Bond angles

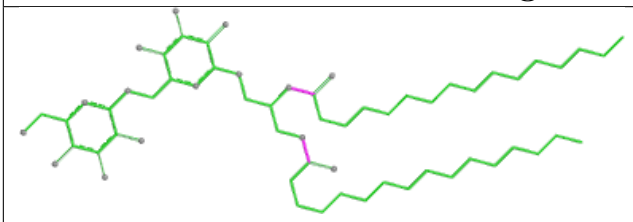


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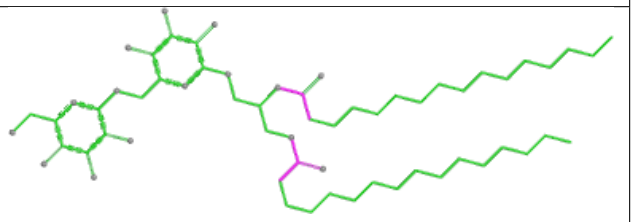


Rings

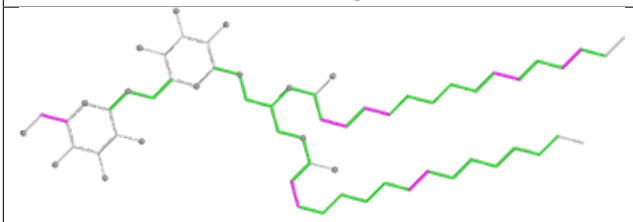
Ligand DGD D 411



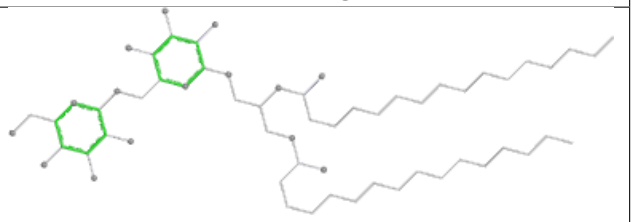
Bond lengths



Bond angles

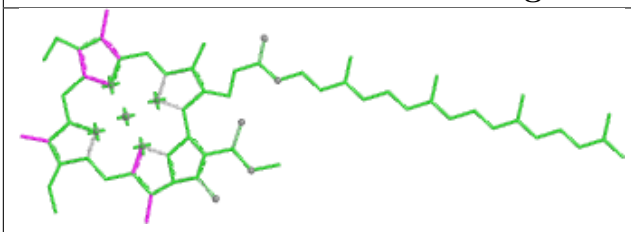


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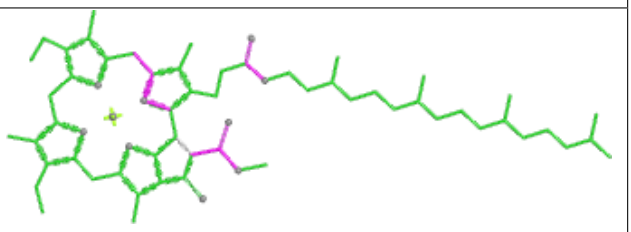


Rings

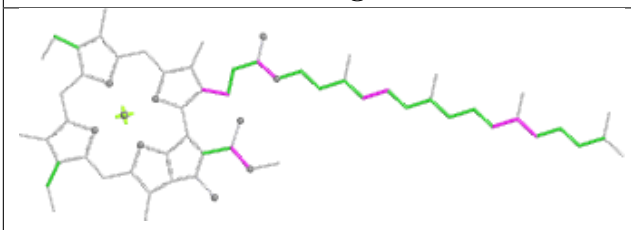
Ligand CLA B 620



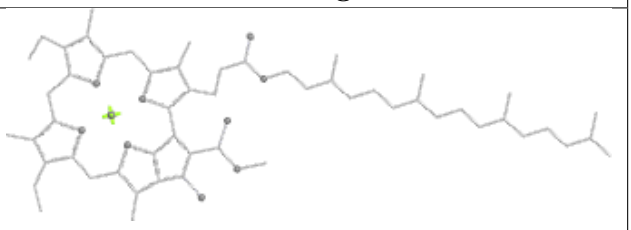
Bond lengths



Bond angles

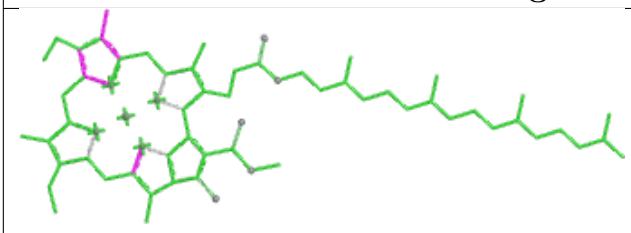


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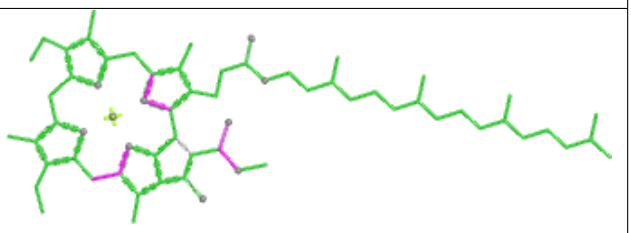


Rings

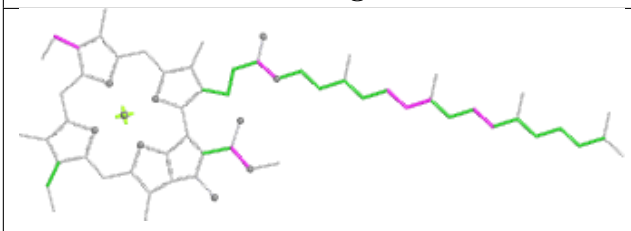
Ligand CLA c 511



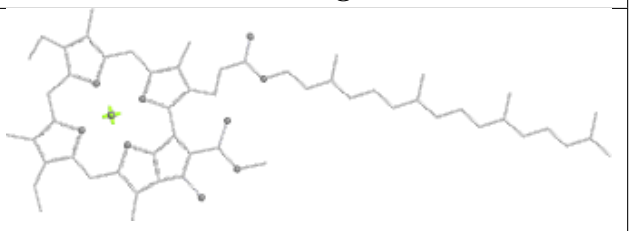
Bond lengths



Bond angles

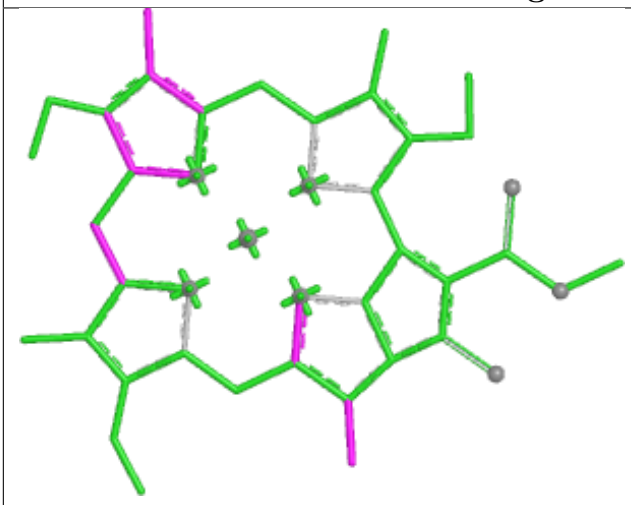


Torsions

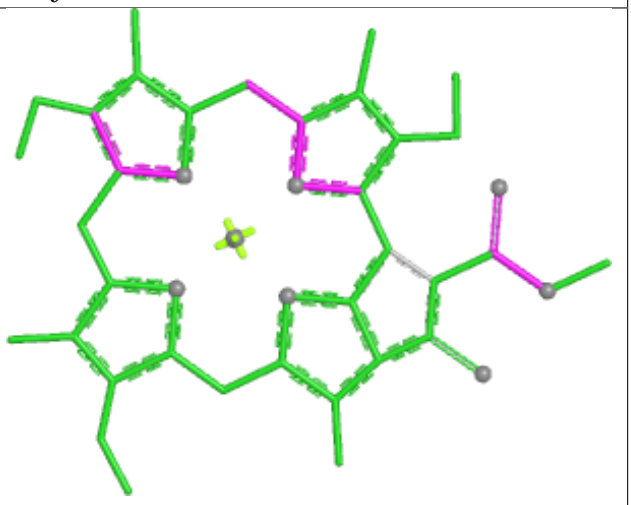


Rings

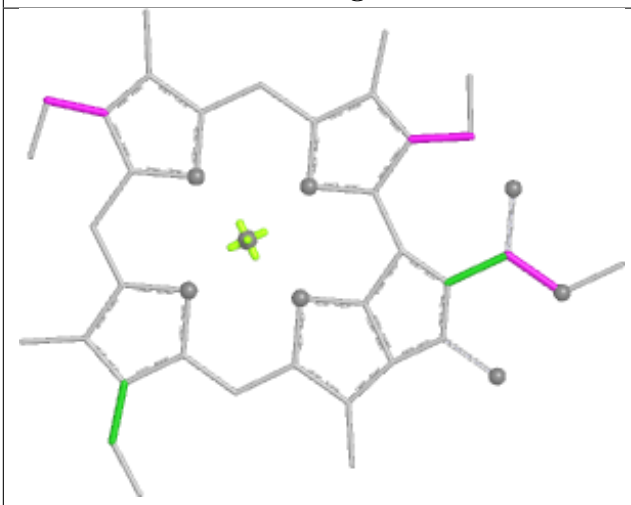
Ligand CLA y 313



Bond lengths



Bond angles

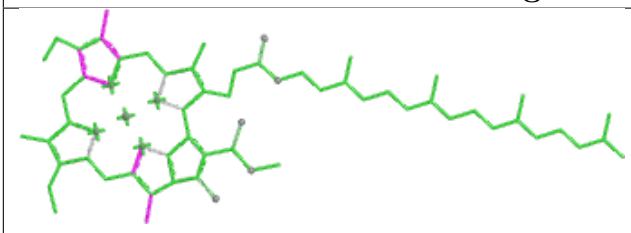


Torsions

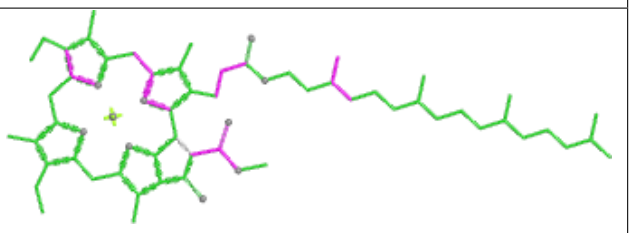


Rings

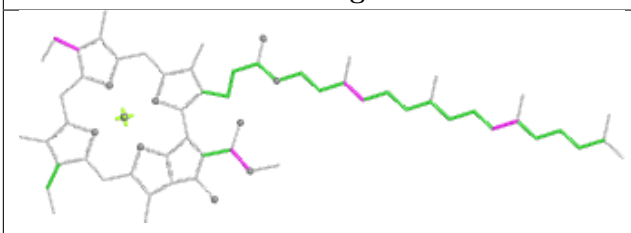
Ligand CLA D 401



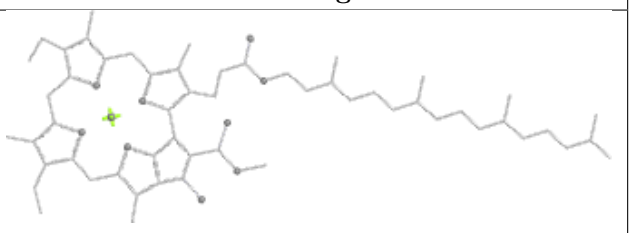
Bond lengths



Bond angles

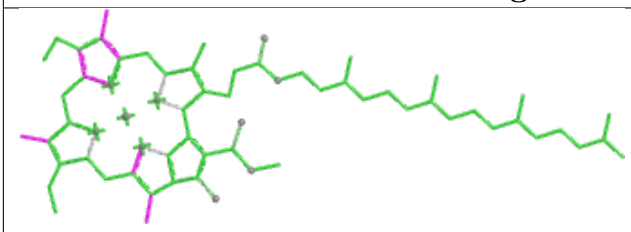


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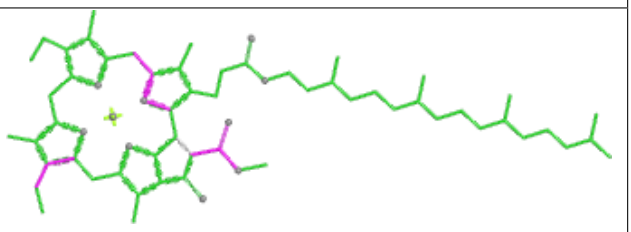


Rings

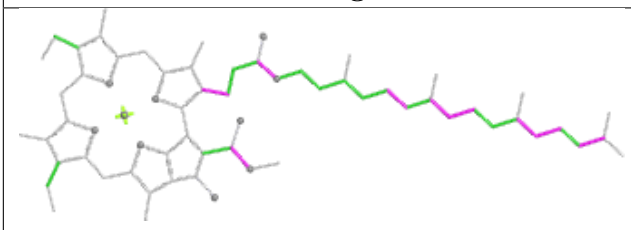
Ligand CLA AA 405



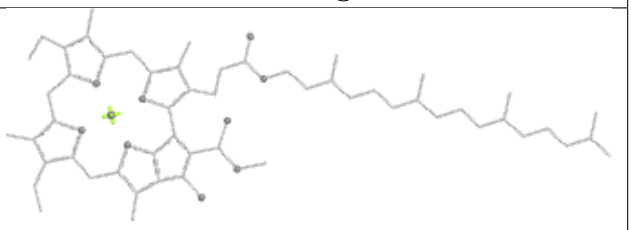
Bond lengths



Bond angles

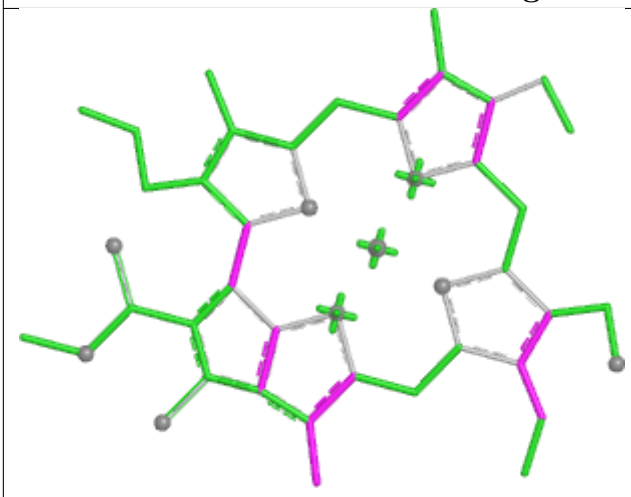


Torsions

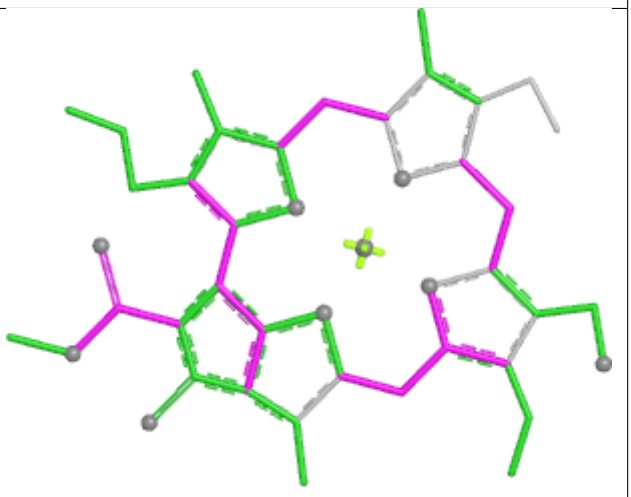


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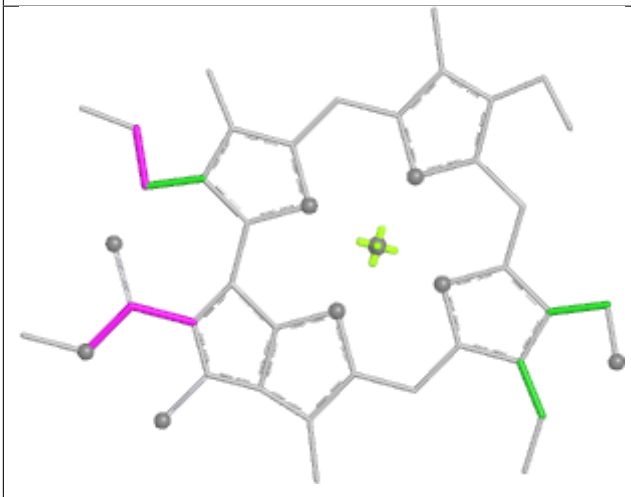
Ligand CHL N 601



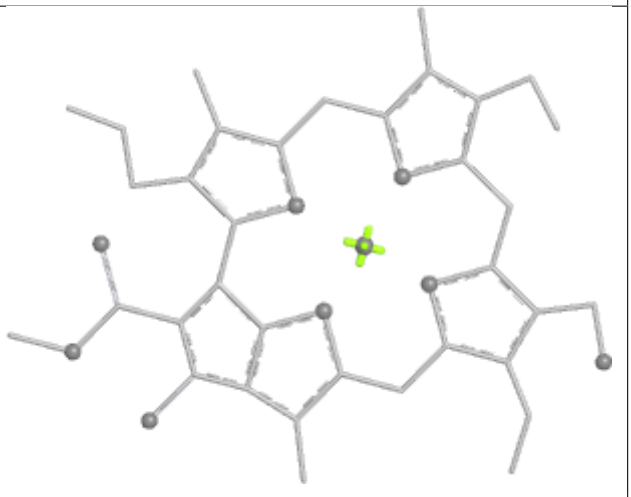
Bond lengths



Bond angles

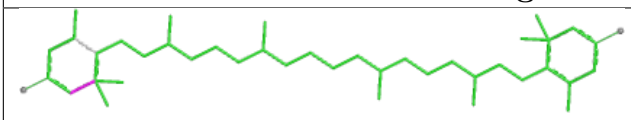


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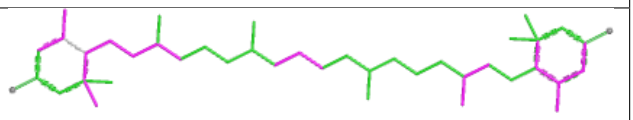


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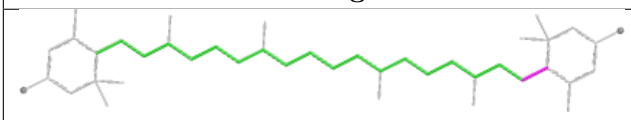
Ligand LUT Rr 614



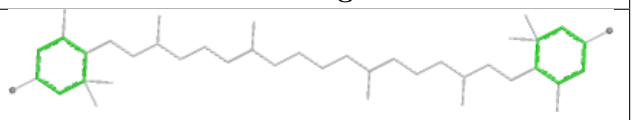
Bond lengths



Bond angles

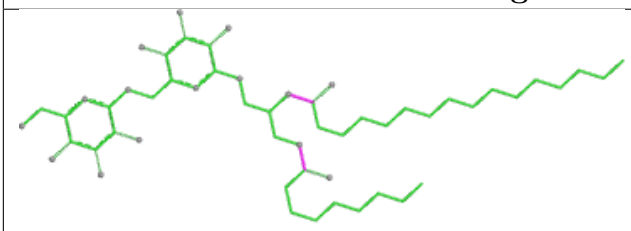


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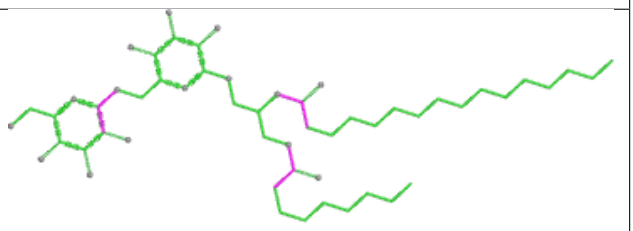


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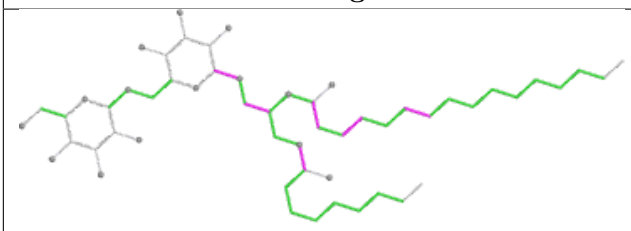
Ligand DGD Aa 401



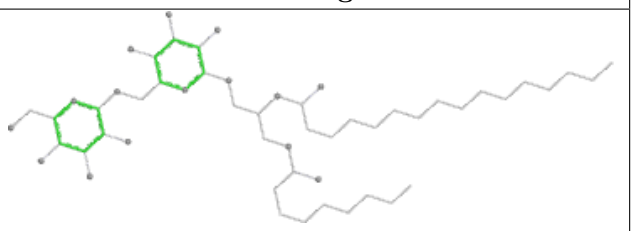
Bond lengths



Bond angles

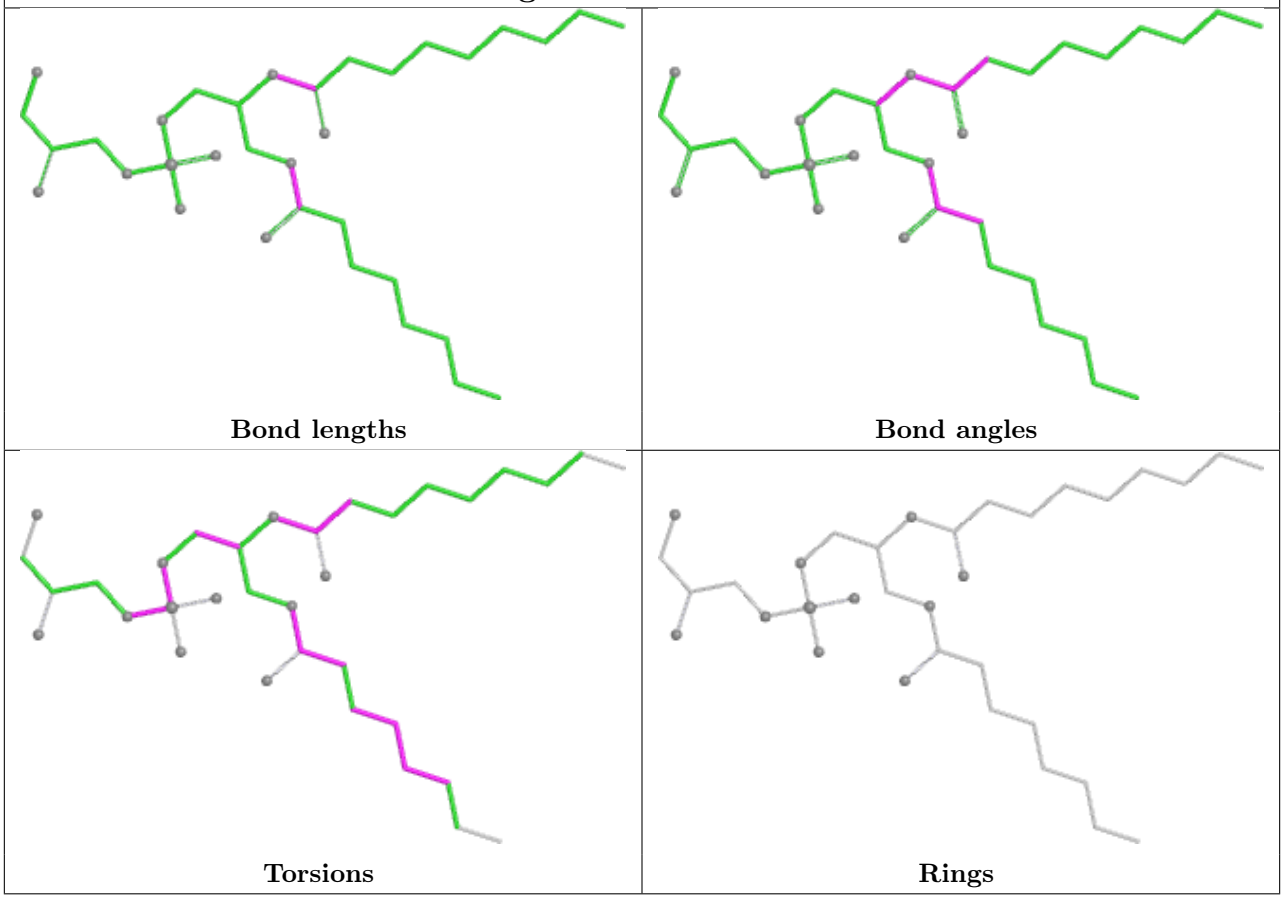


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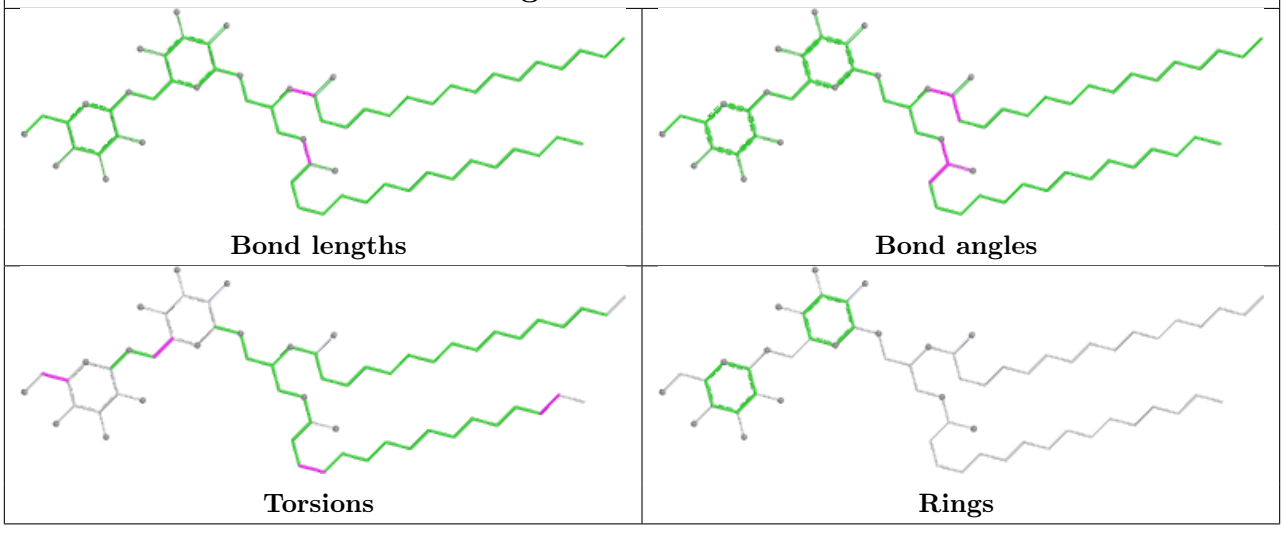


Rings

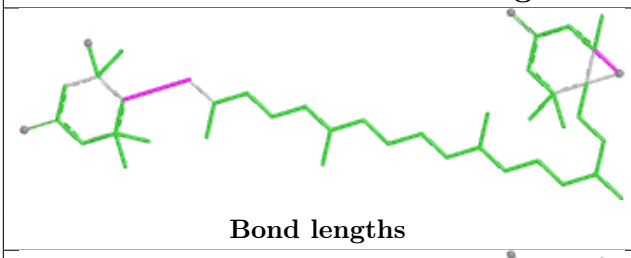
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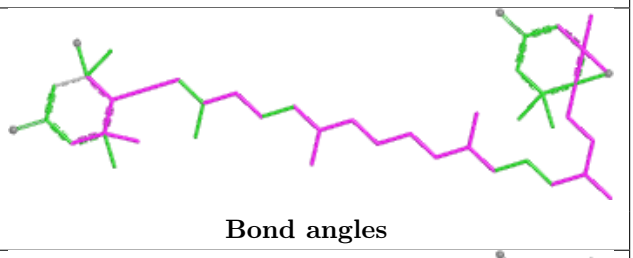
Ligand DGD C 520



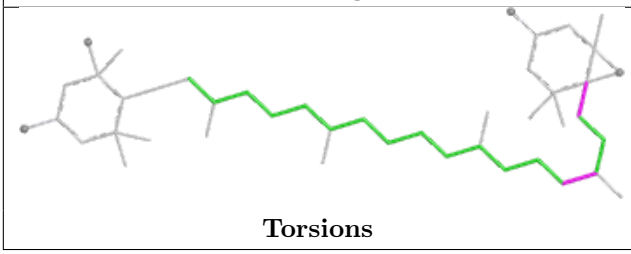
Ligand NEX Rr 616



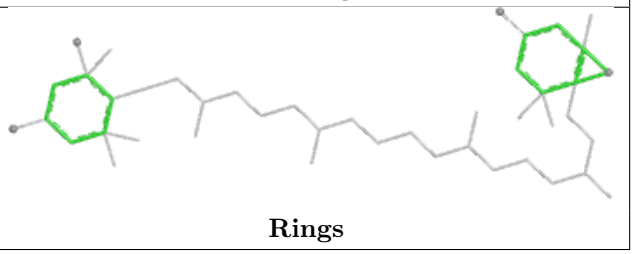
Bond lengths



Bond angles

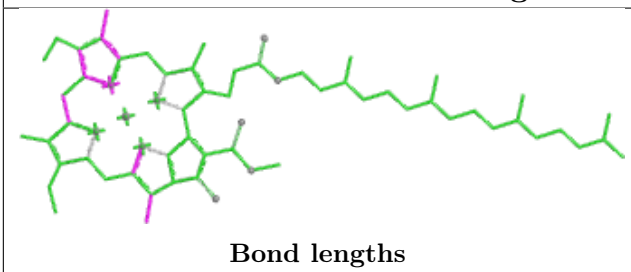


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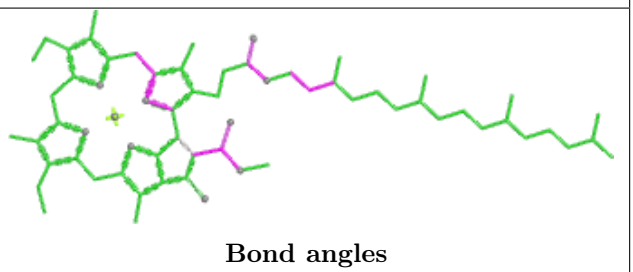


Rings

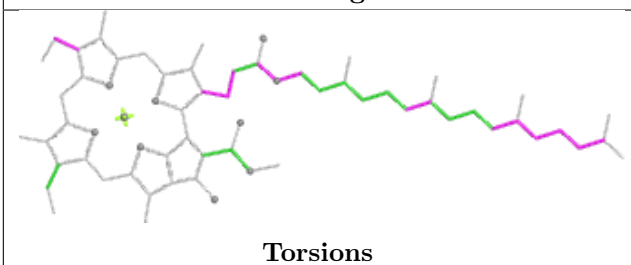
Ligand CLA RR 302



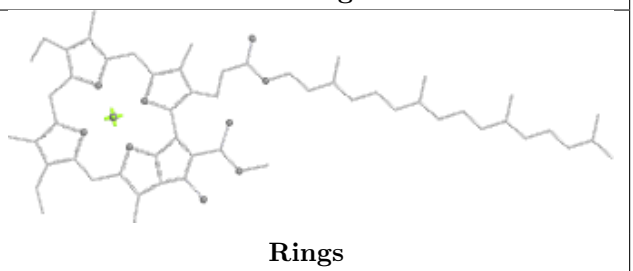
Bond lengths



Bond angles

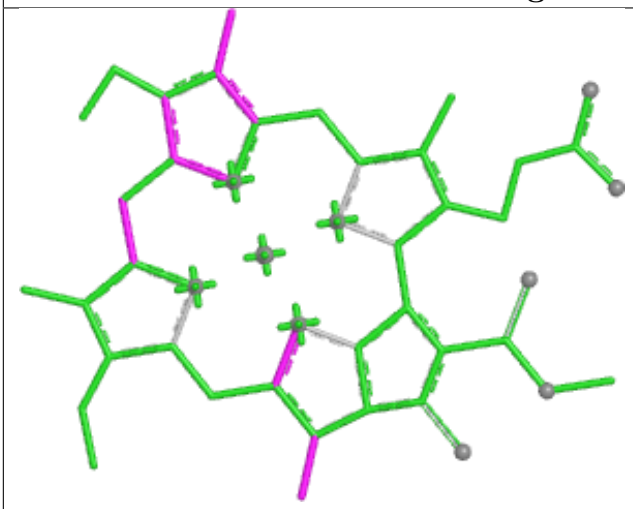


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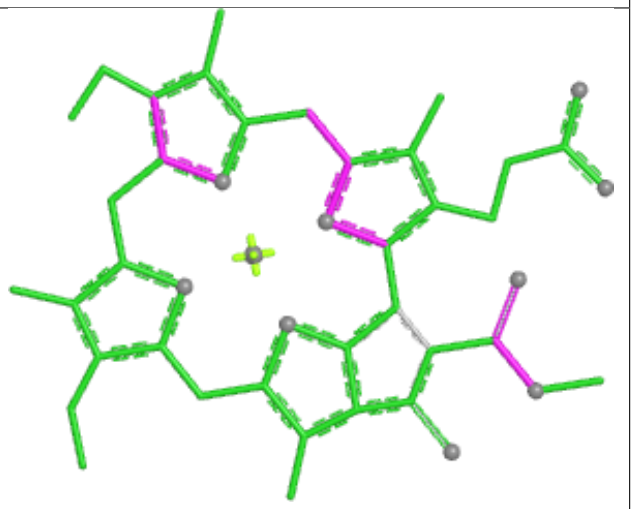


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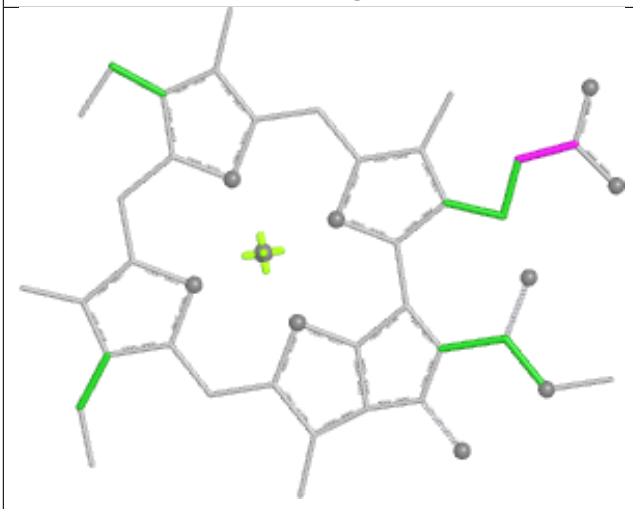
Ligand CLA S 613



Bond lengths



Bond angles

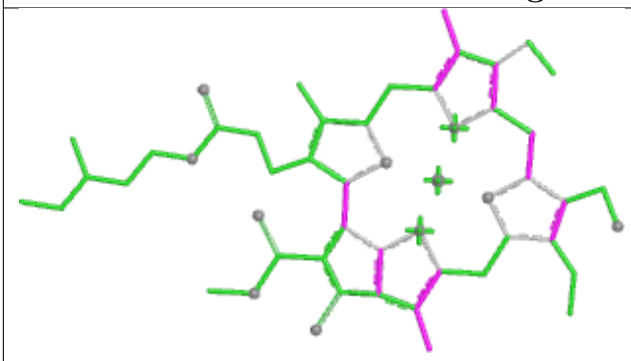


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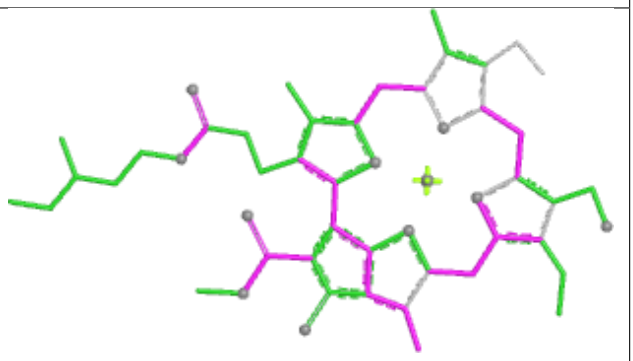


Rings

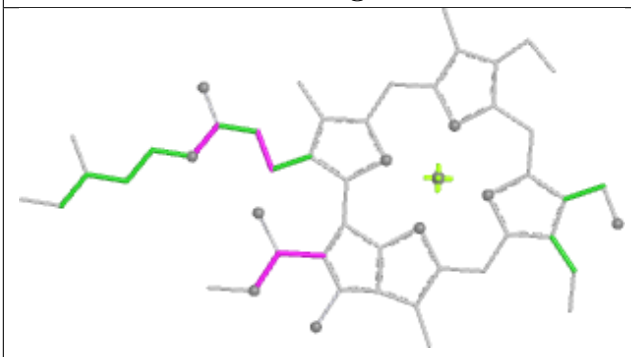
Ligand CHL S 601



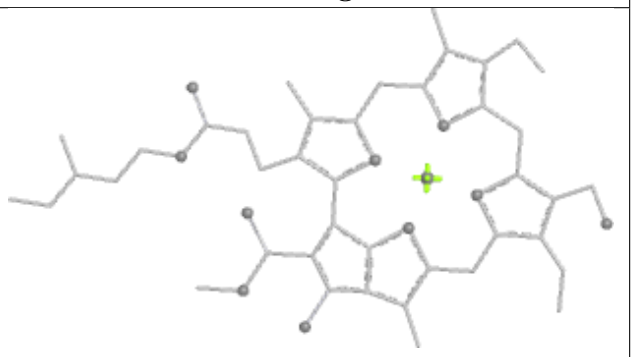
Bond lengths



Bond angles

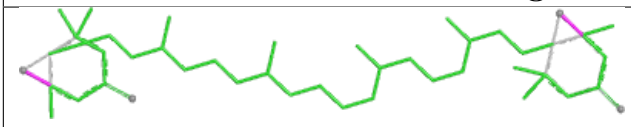


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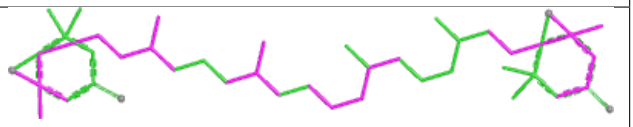


Rings

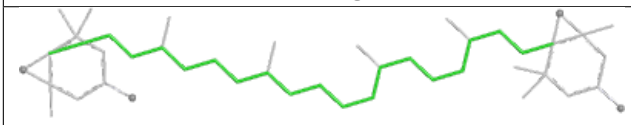
Ligand XAT 4 314



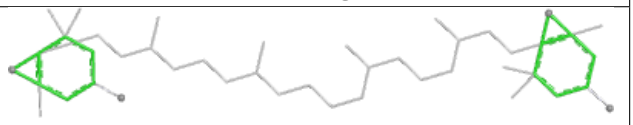
Bond lengths



Bond angles

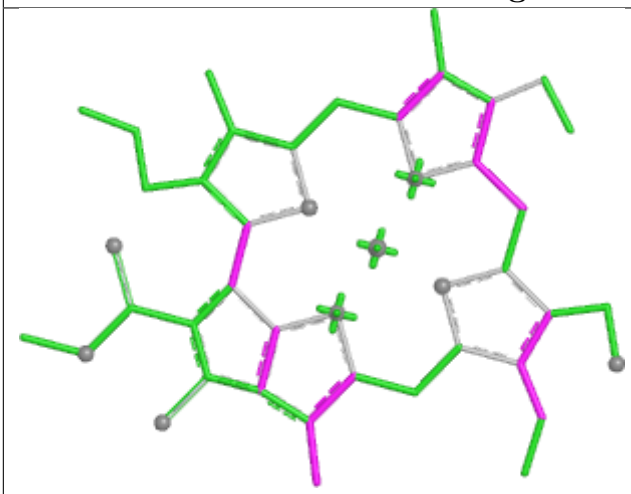


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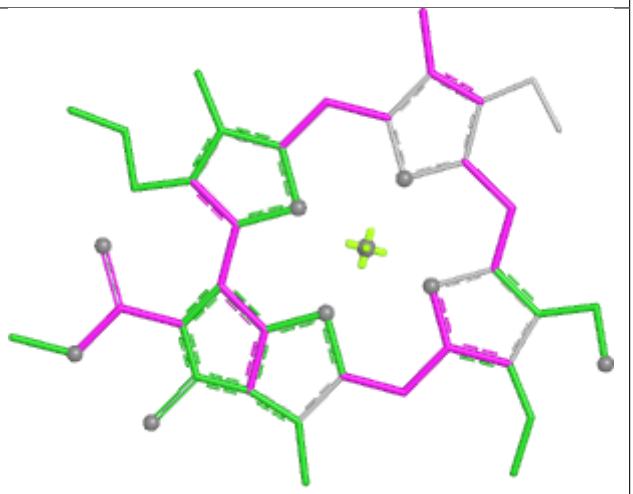


Rings

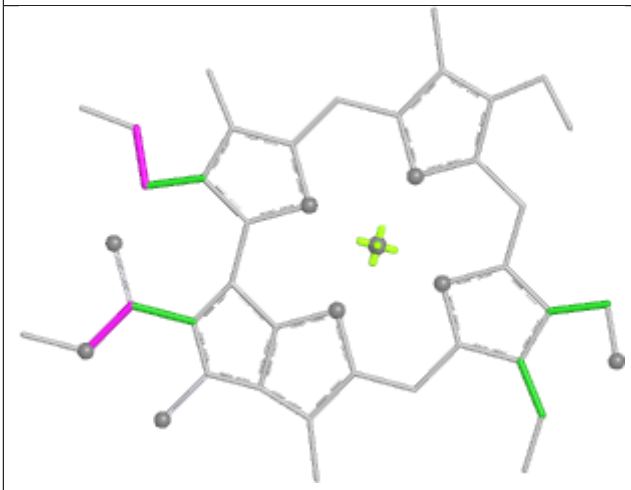
Ligand CHL NN 601



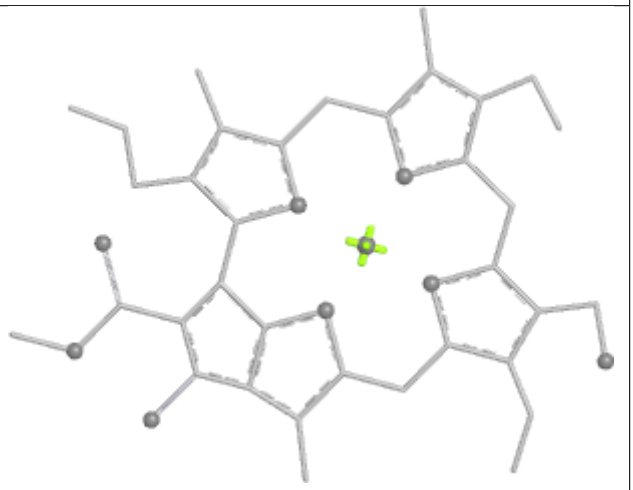
Bond lengths



Bond angles

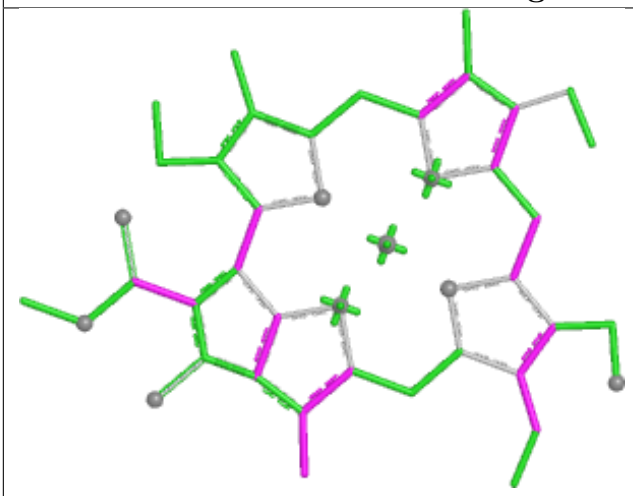


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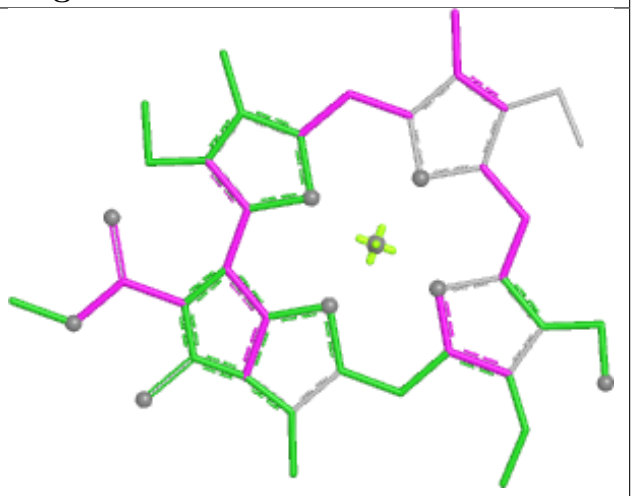


Rings

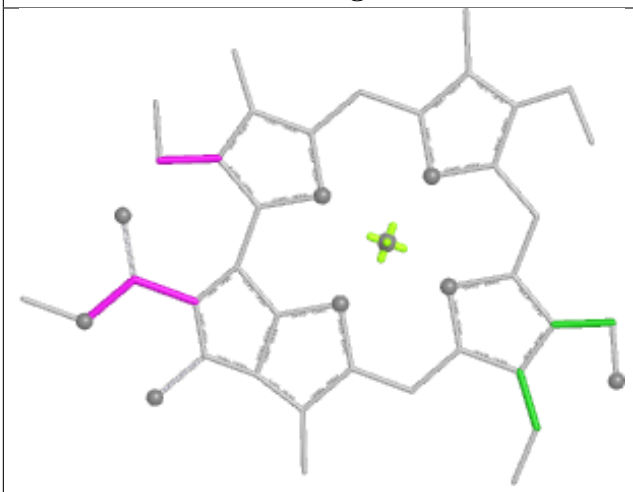
Ligand CHL g 609



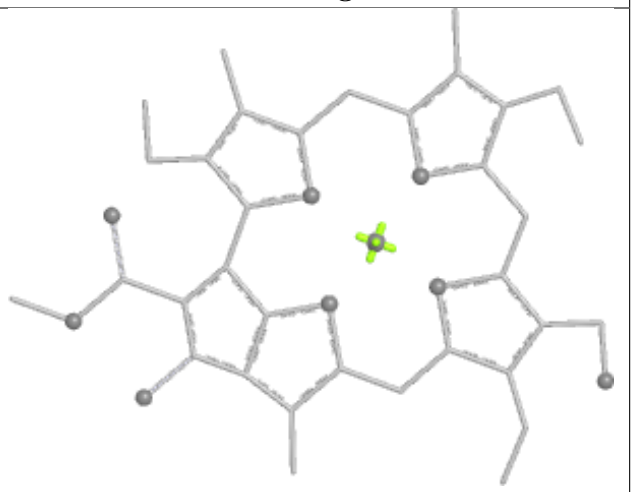
Bond lengths



Bond angles

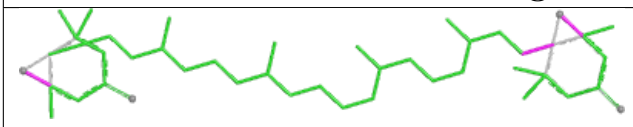


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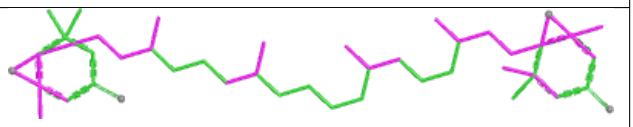


Rings

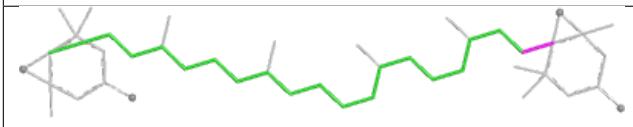
Ligand XAT r 615



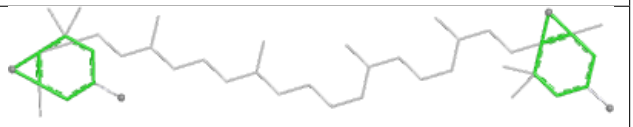
Bond lengths



Bond angles

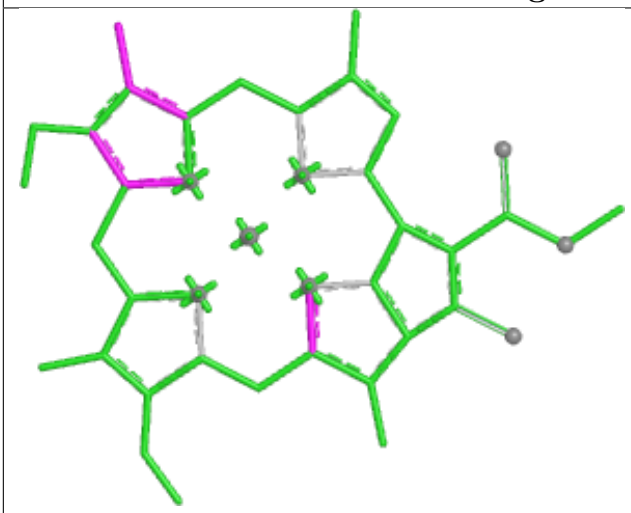


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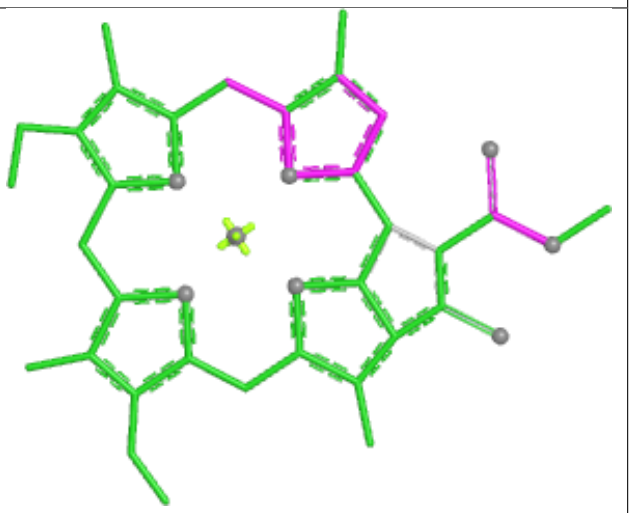


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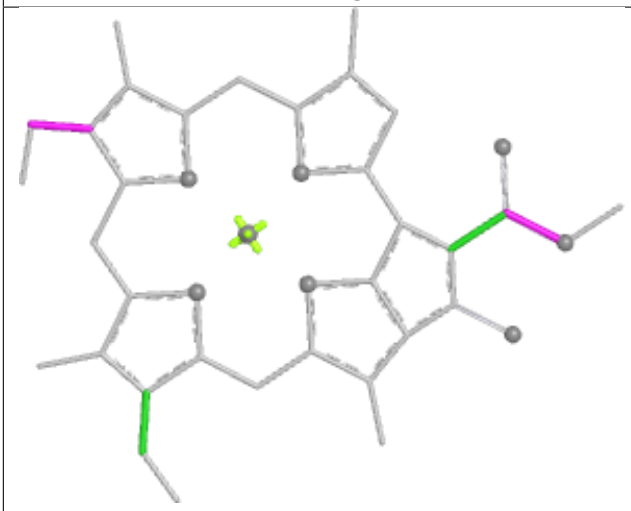
Ligand CLA 3 602



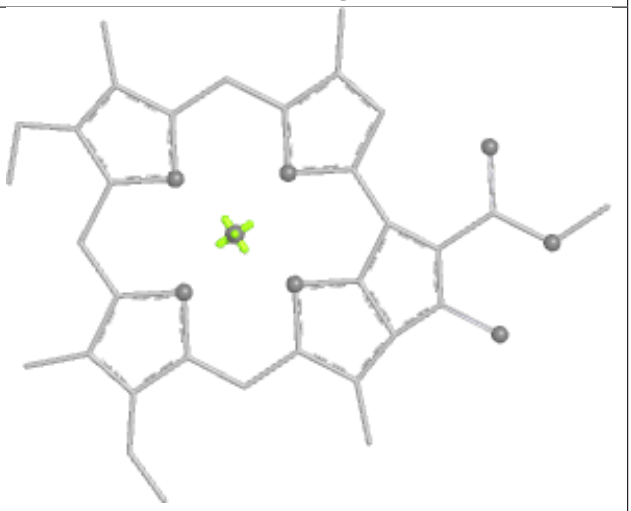
Bond lengths



Bond angles

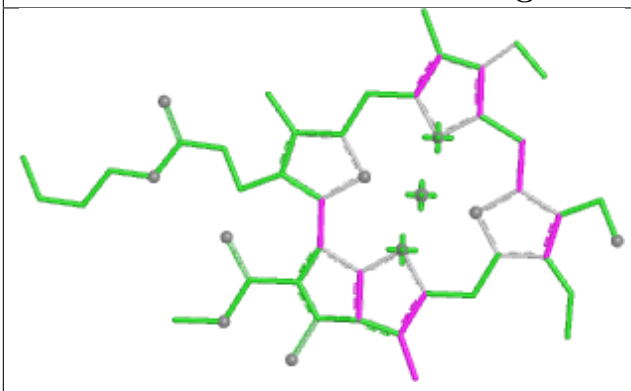


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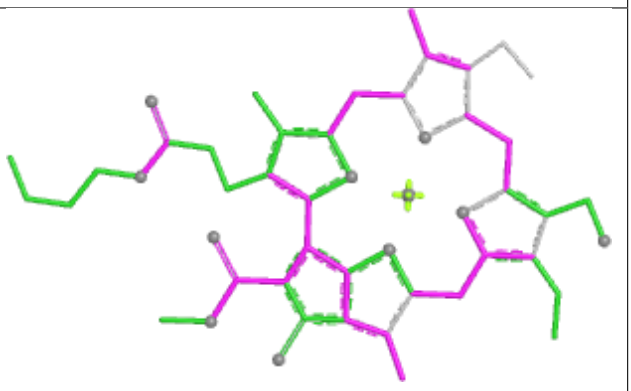


Rings

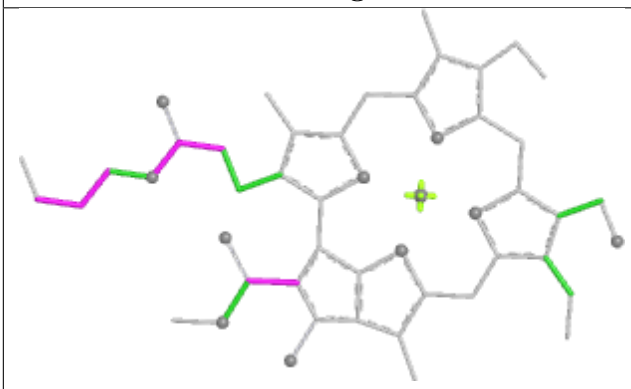
Ligand CHL Rr 607



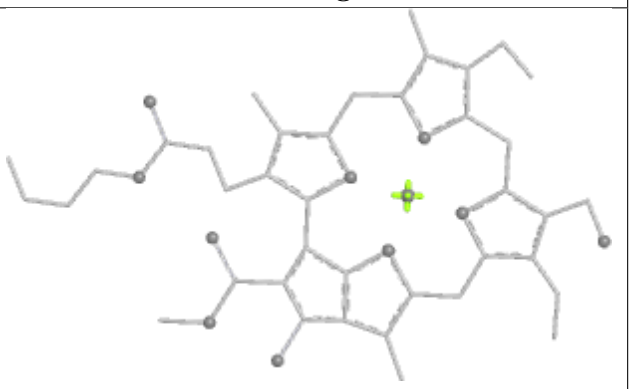
Bond lengths



Bond angles

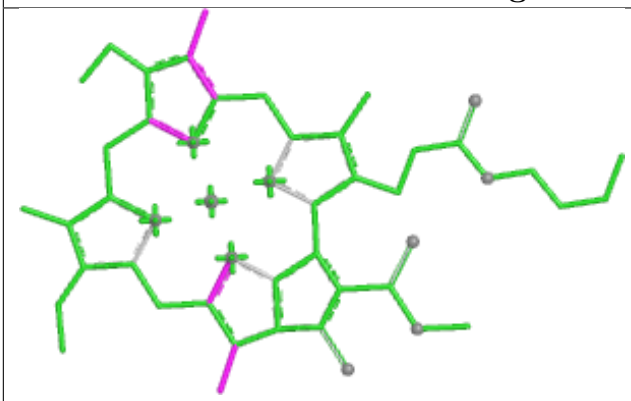


Torsions

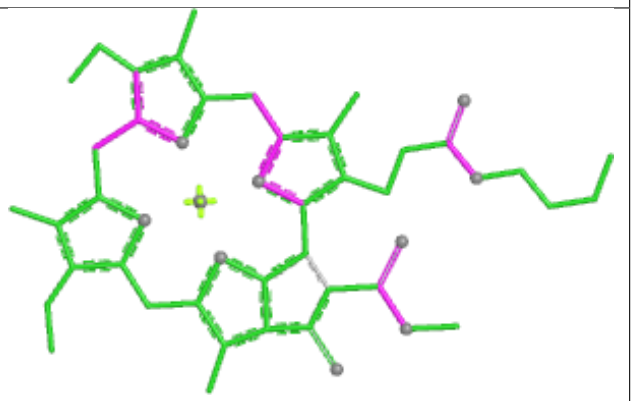


Rings

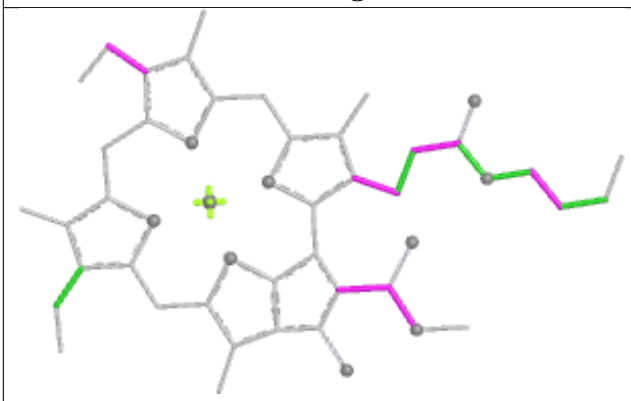
Ligand CLA GG 602



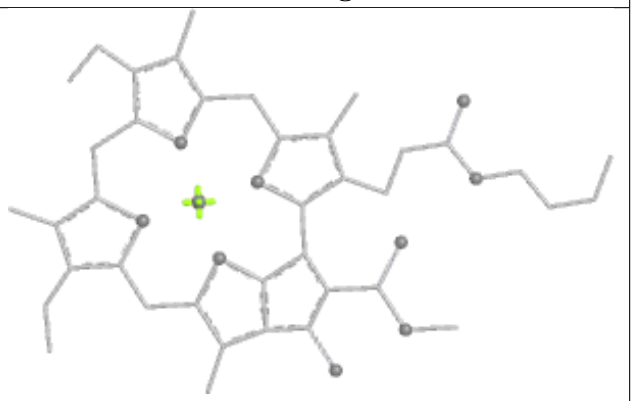
Bond lengths



Bond angles

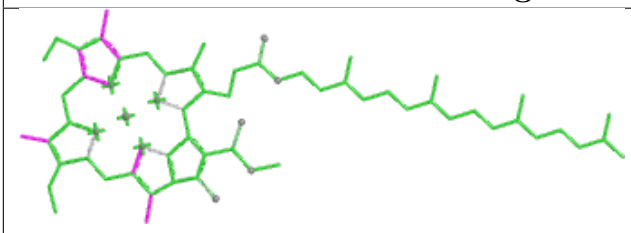


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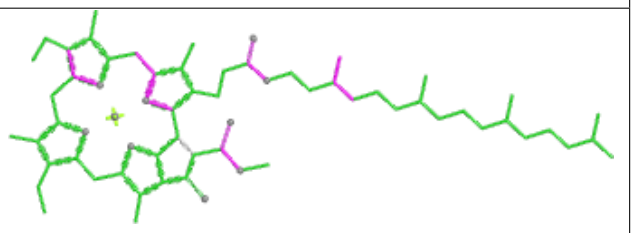


Rings

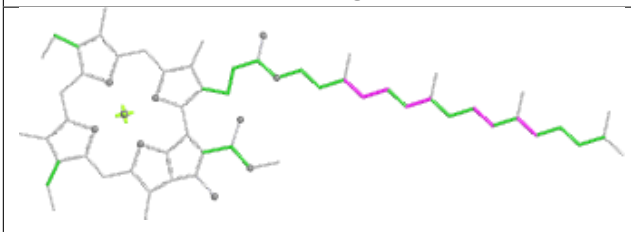
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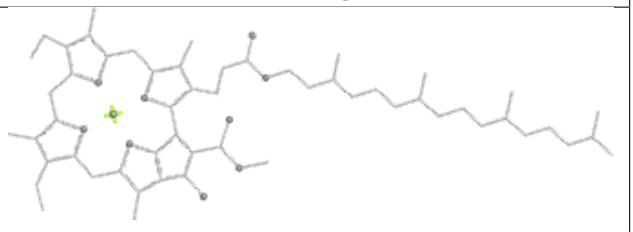
Bond lengths



Bond angles

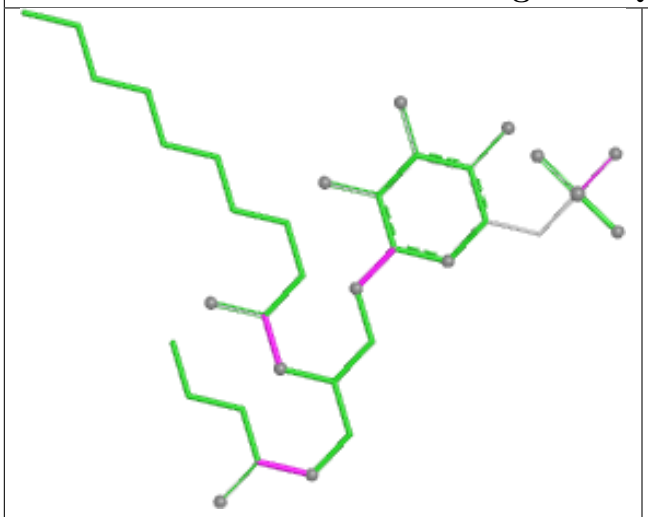


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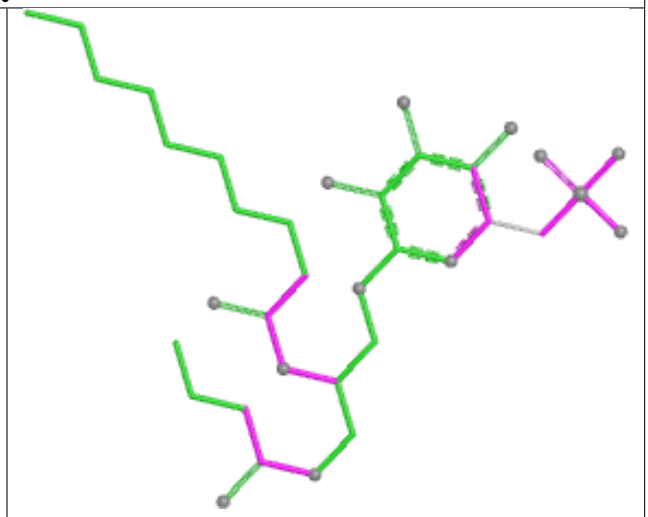


Rings

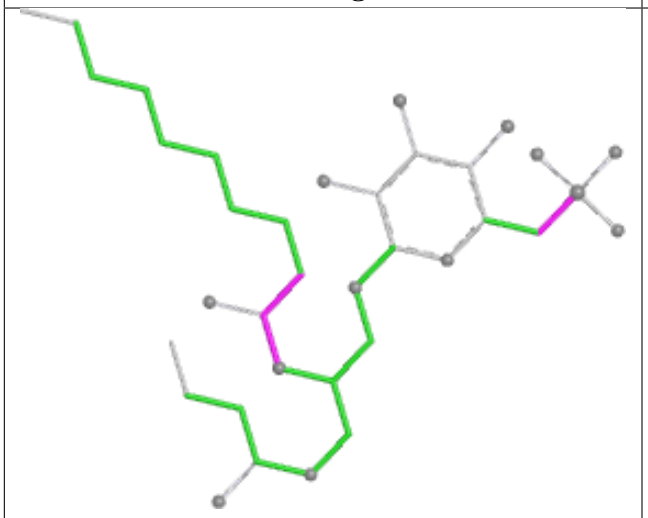
Ligand SQD BB 621



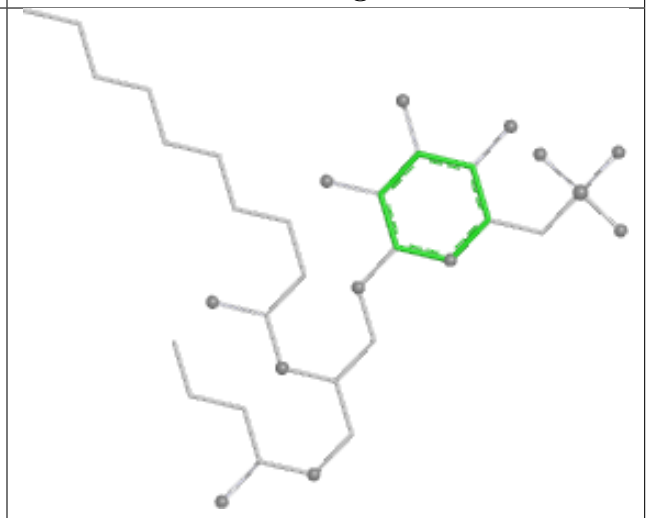
Bond lengths



Bond angles

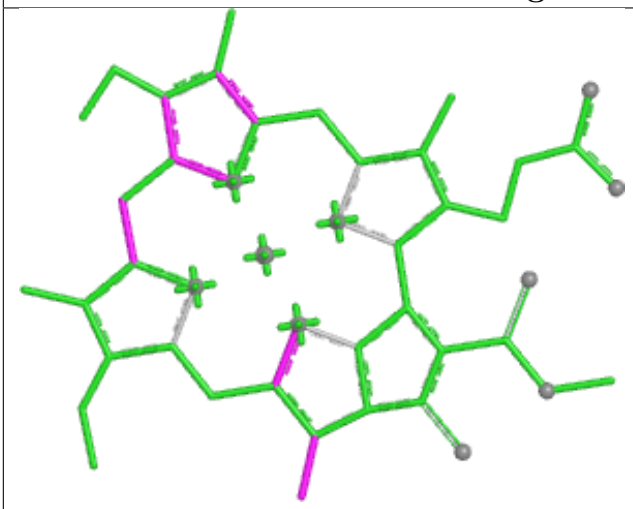


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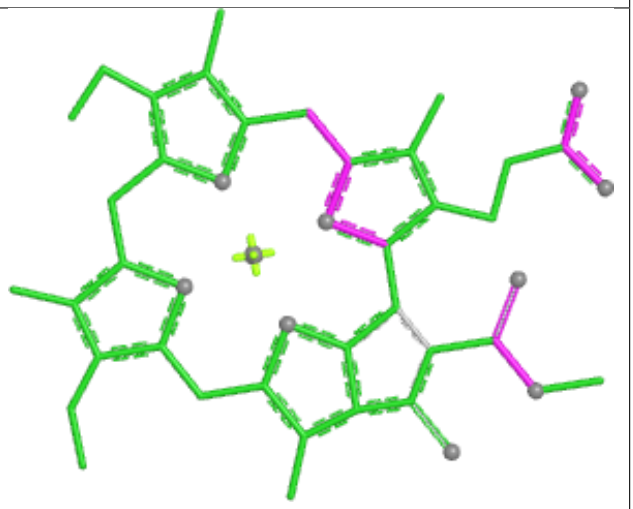


Rings

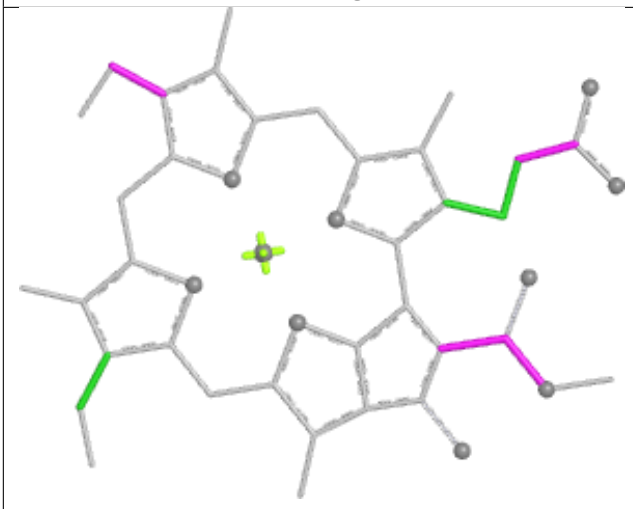
Ligand CLA S 603



Bond lengths



Bond angles

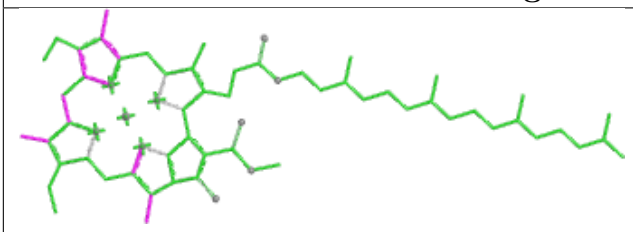


Torsions

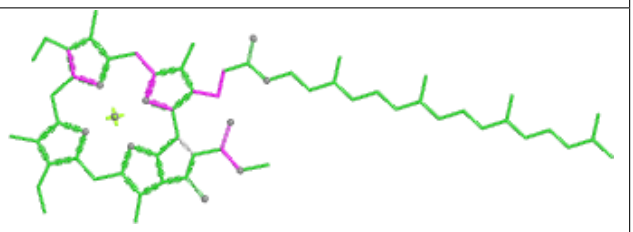


Rings

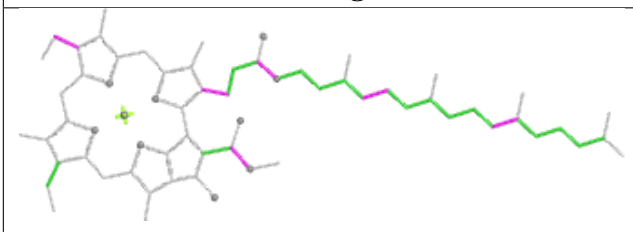
Ligand CLA R 609



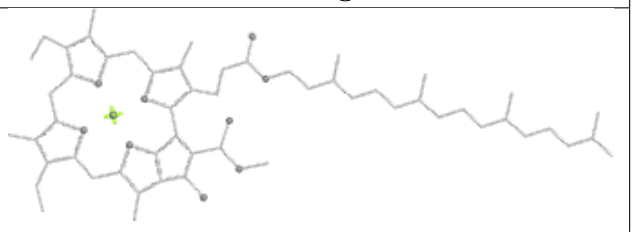
Bond lengths



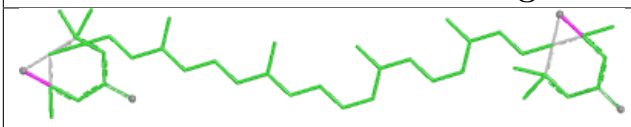
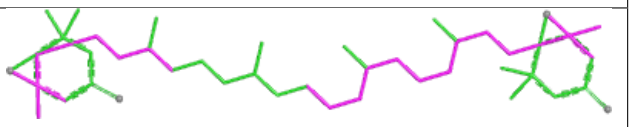
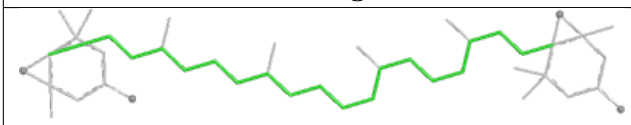
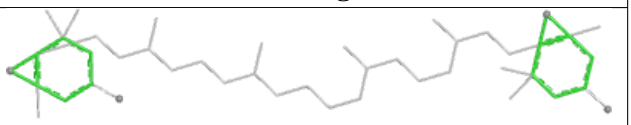
Bond angles

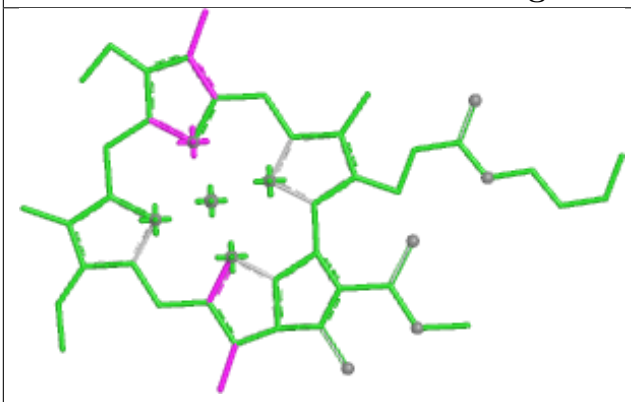
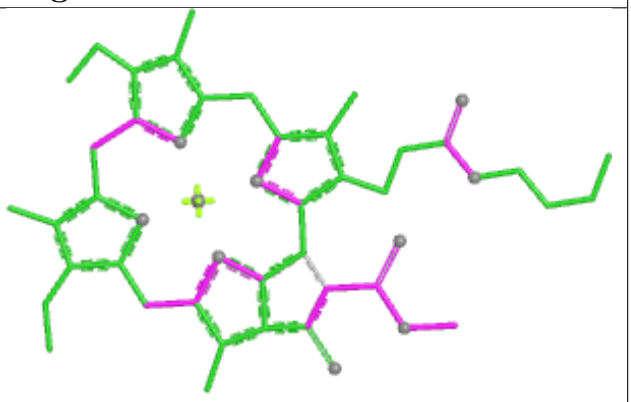
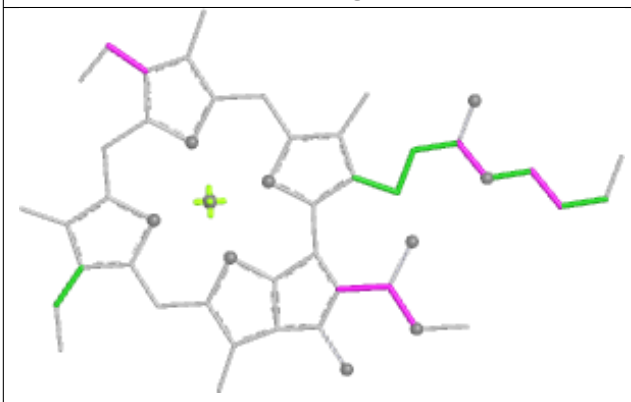
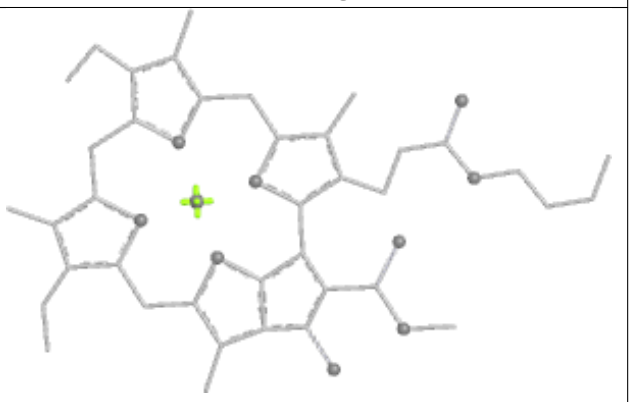


Torsions

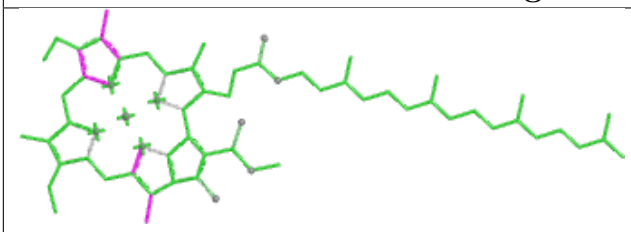


Rings

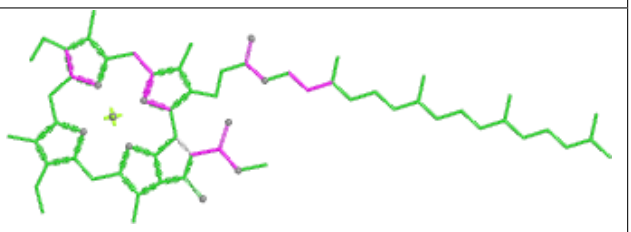
Ligand XAT 44 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

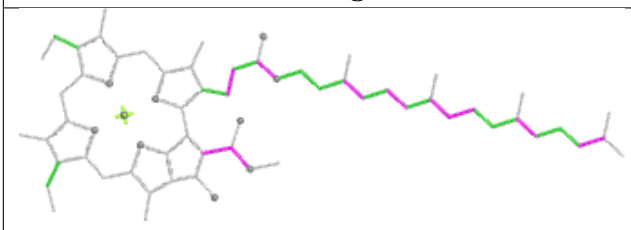
Ligand CLA B 622



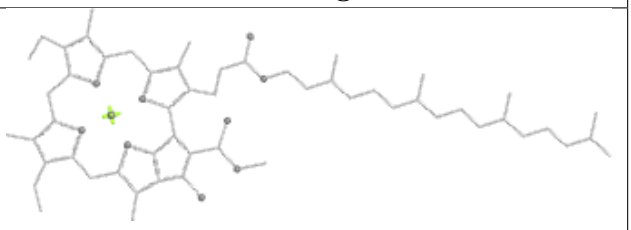
Bond lengths



Bond angles



Torsions

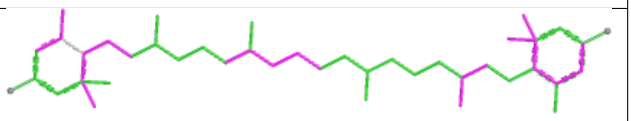


Rings

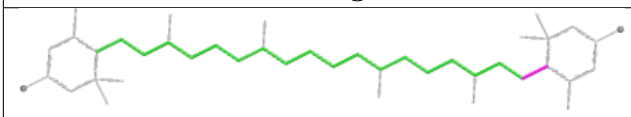
Ligand LUT GG 615



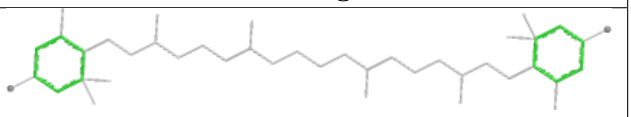
Bond lengths



Bond angles

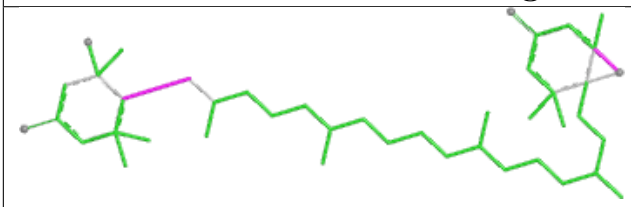


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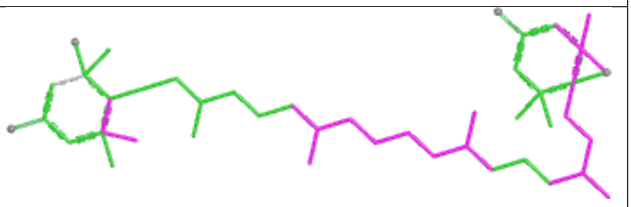


Rings

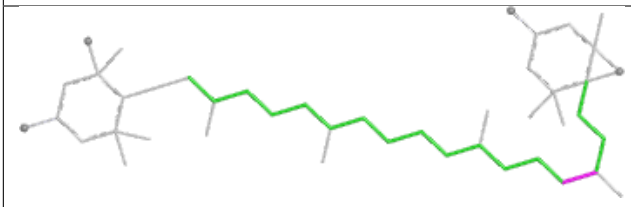
Ligand NEX Y 617



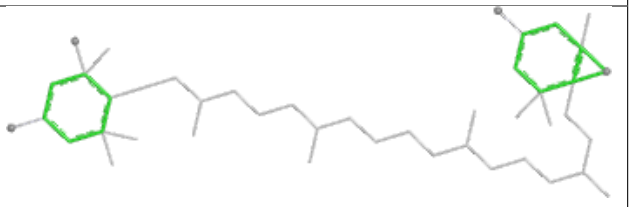
Bond lengths



Bond angles

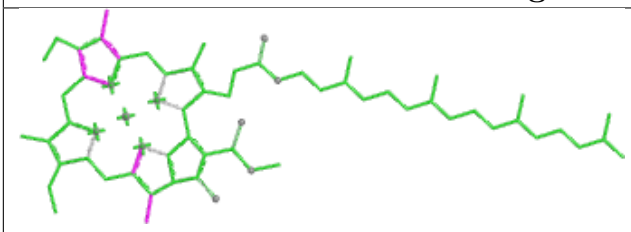


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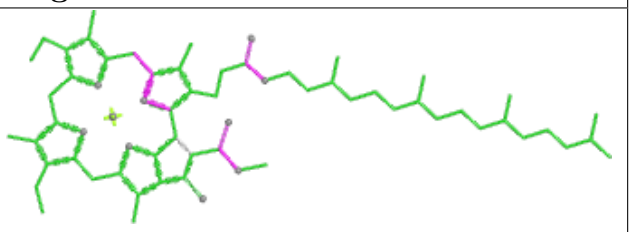


Rings

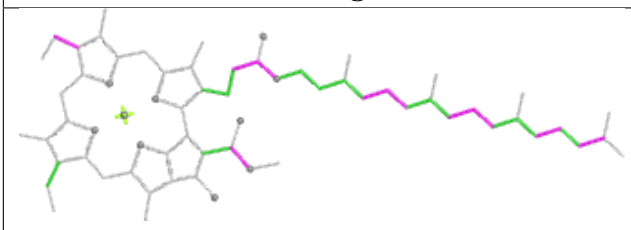
Ligand CLA g 603



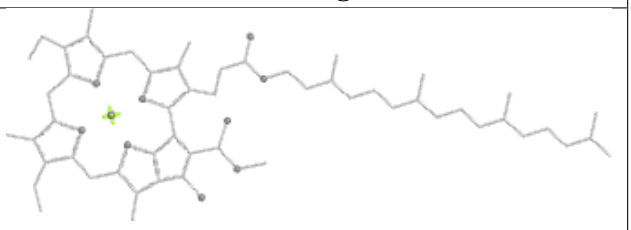
Bond lengths



Bond angles

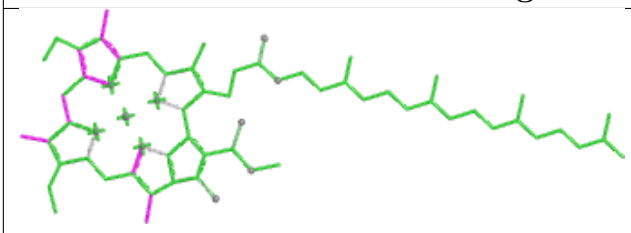


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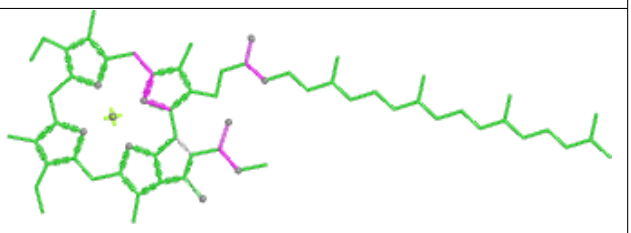


Rings

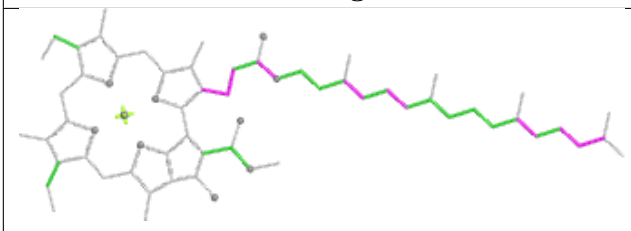
Ligand CLA Cc 512



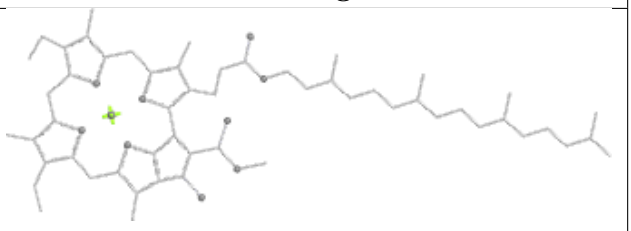
Bond lengths



Bond angles

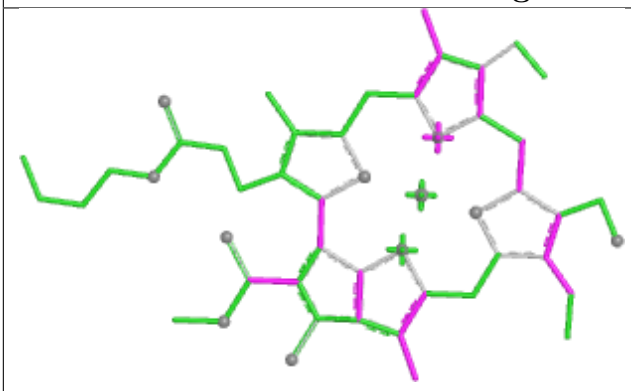


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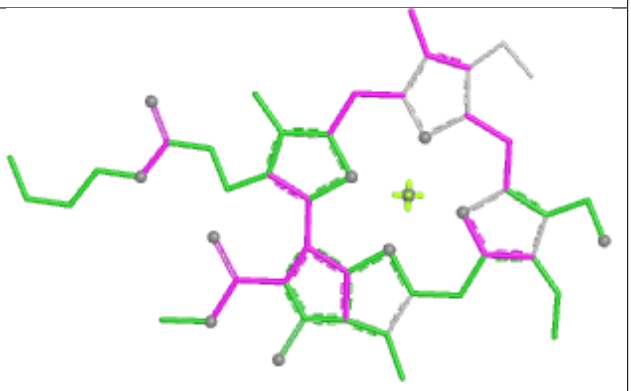


Rings

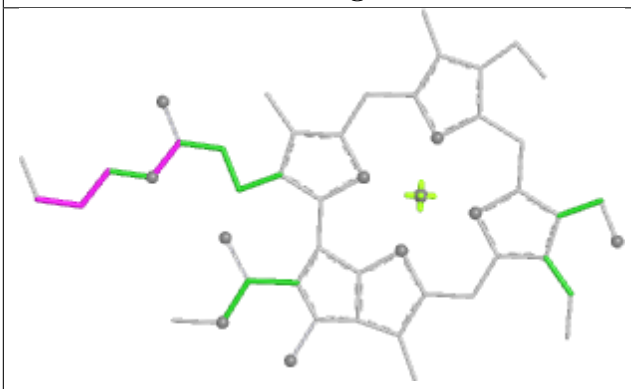
Ligand CHL Nn 319



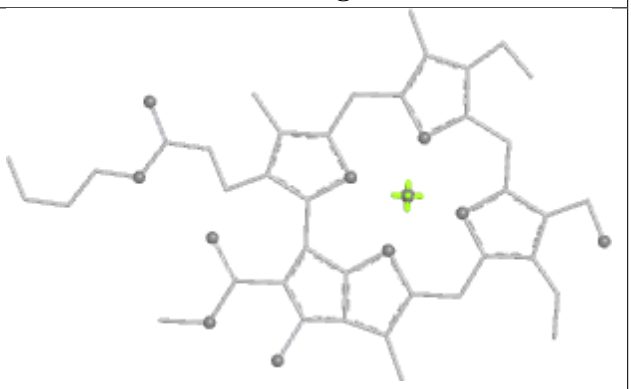
Bond lengths



Bond angles

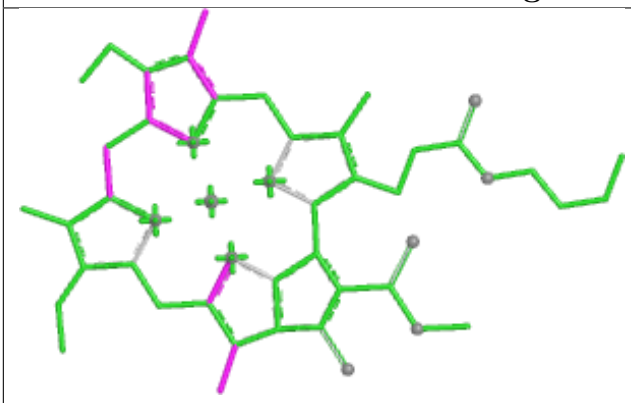


Torsions

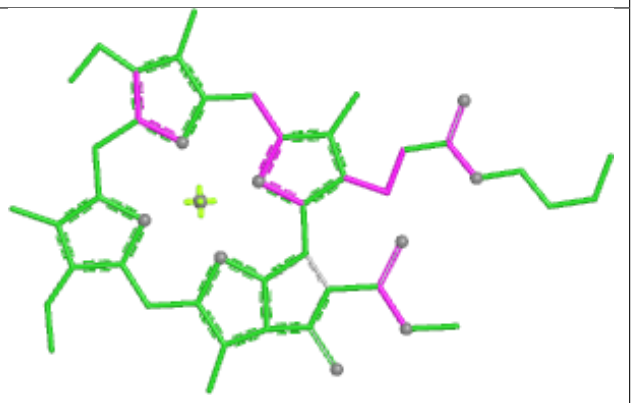


Rings

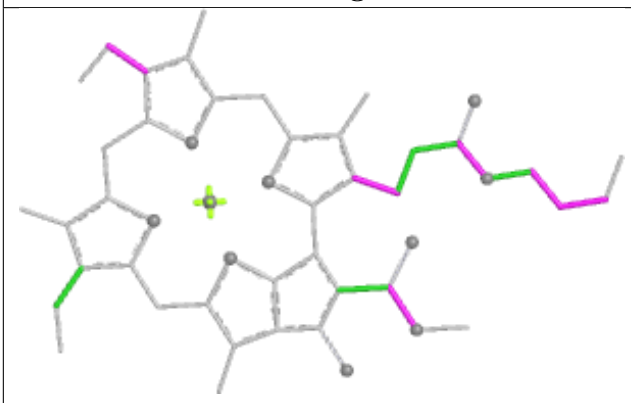
Ligand CLA N 611



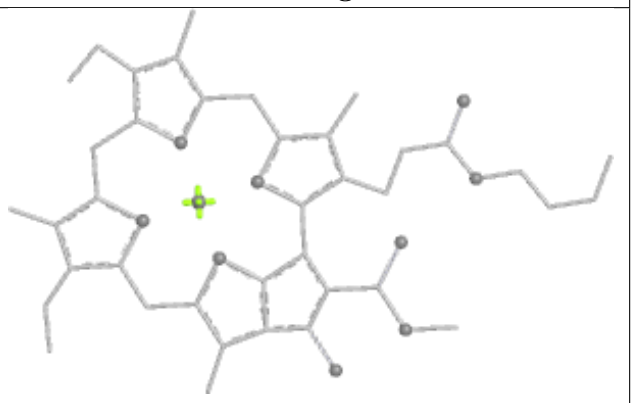
Bond lengths



Bond angles

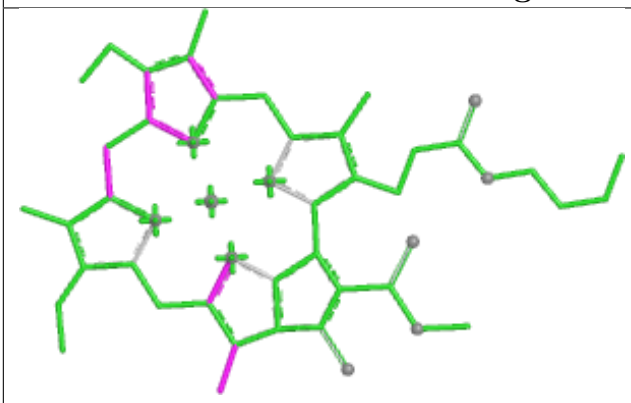


Torsions

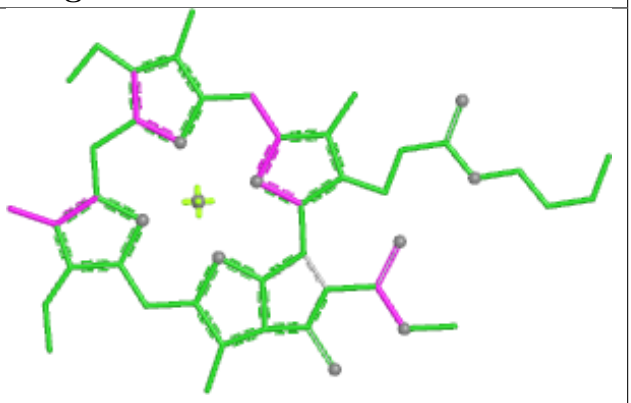


Rings

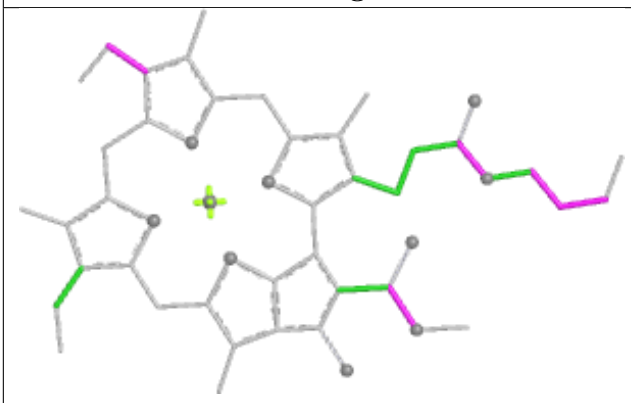
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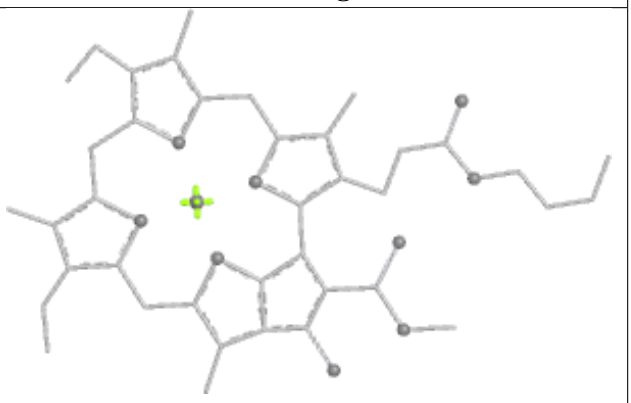
Bond lengths



Bond angles

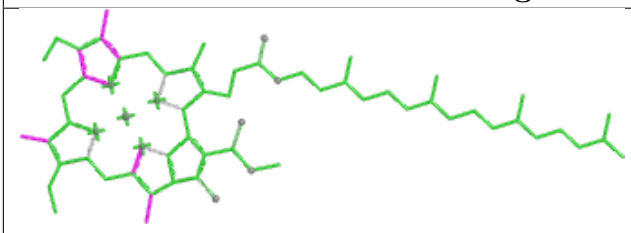


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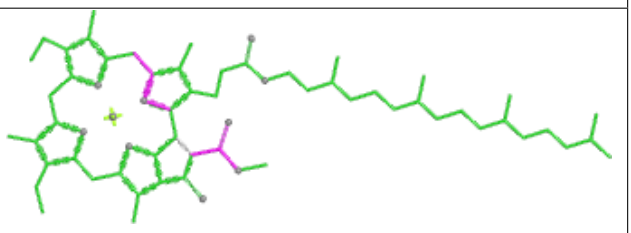


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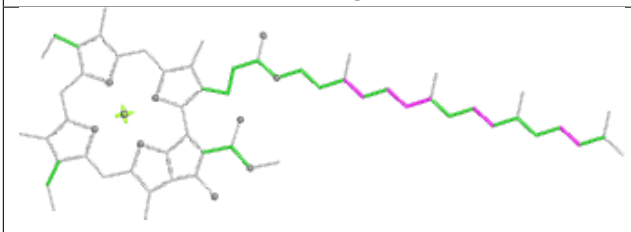
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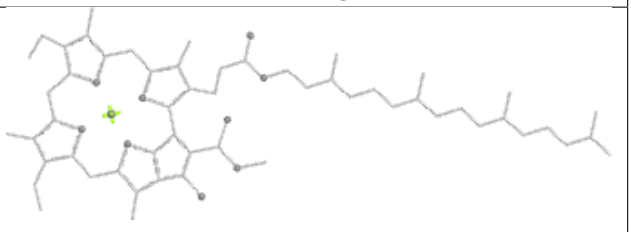
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Bond angles

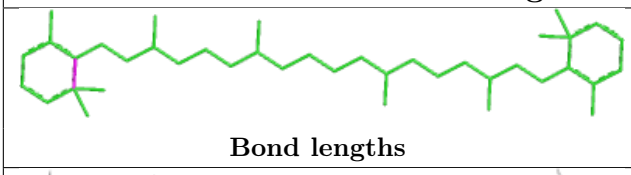


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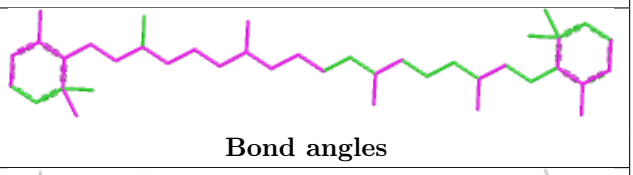


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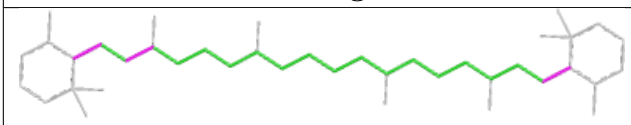
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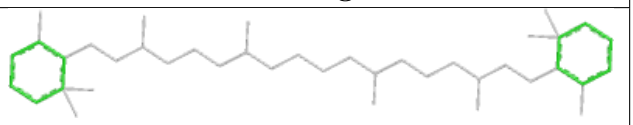
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Bond angles

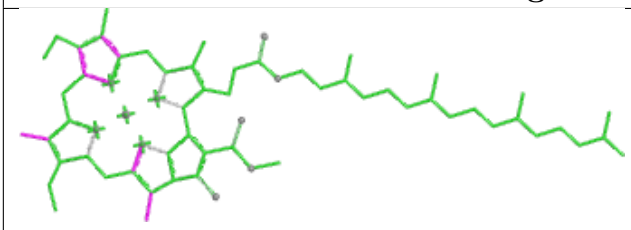


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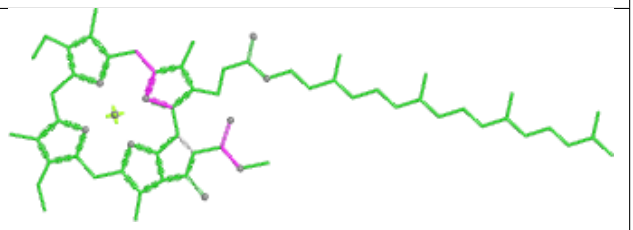


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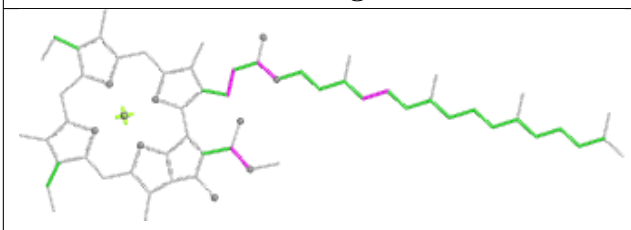
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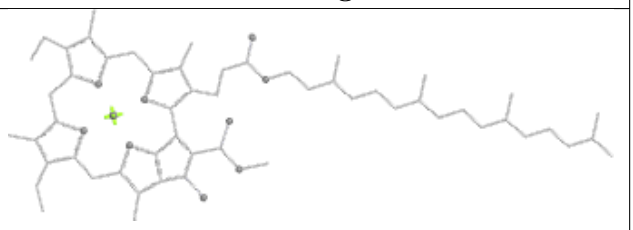
Bond lengths



Bond angles

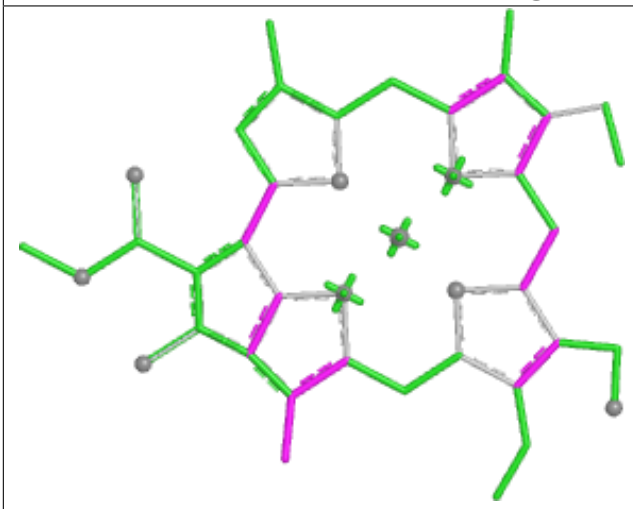


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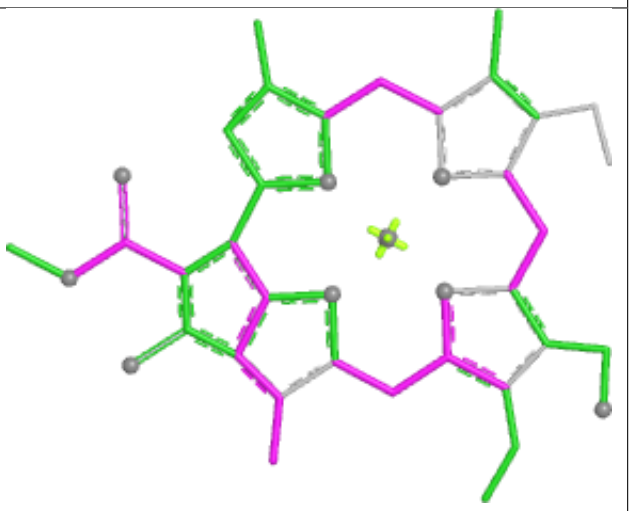


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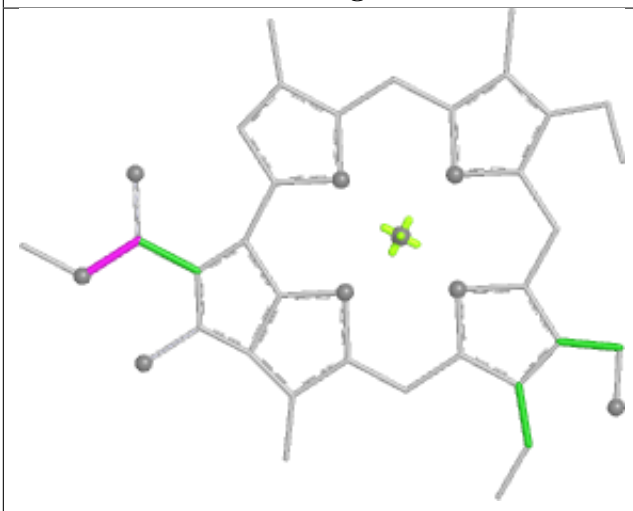
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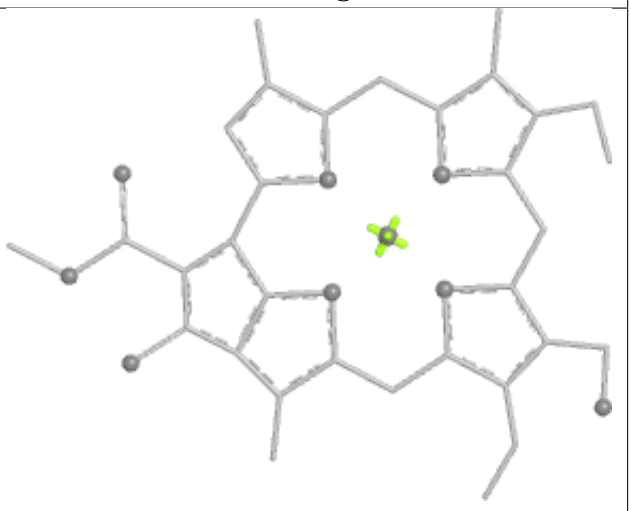
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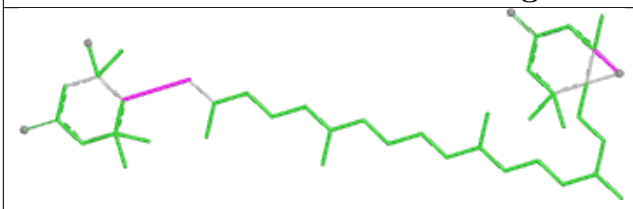


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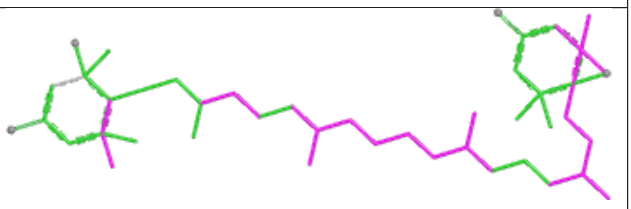


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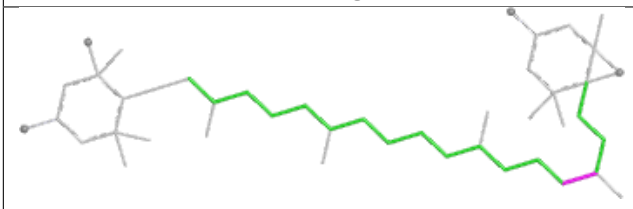
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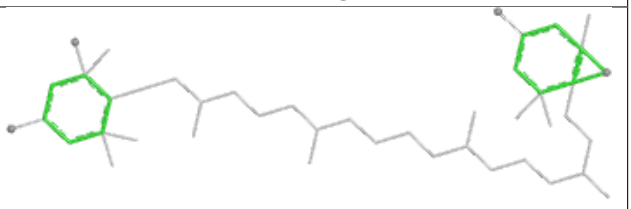
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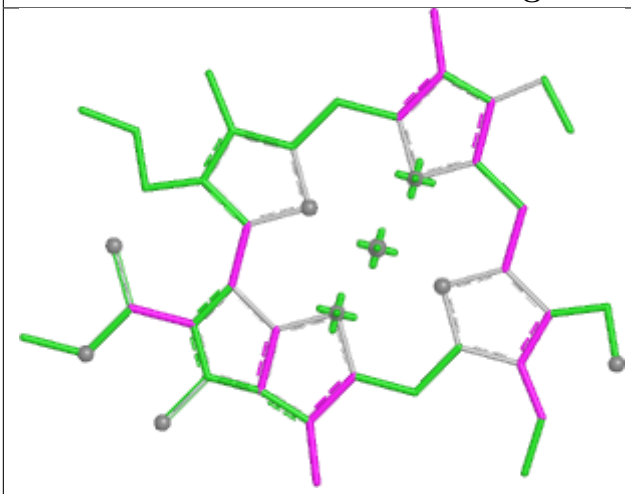


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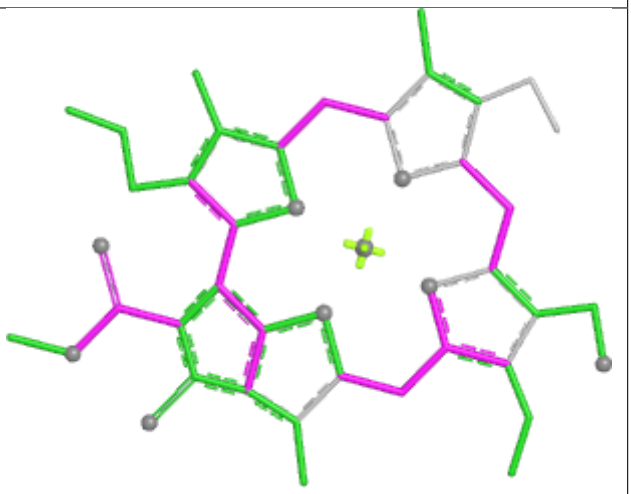


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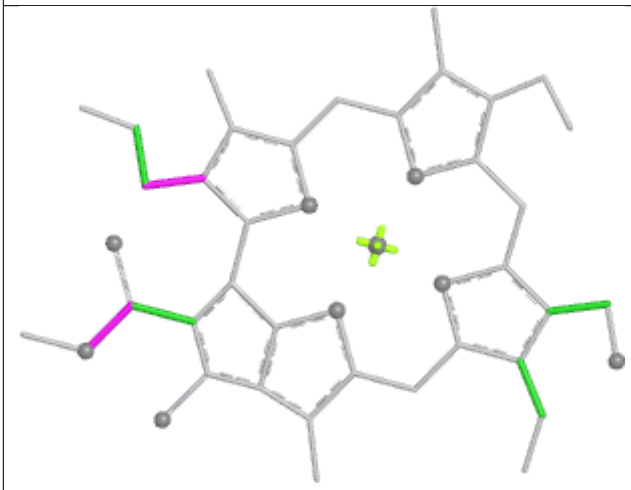
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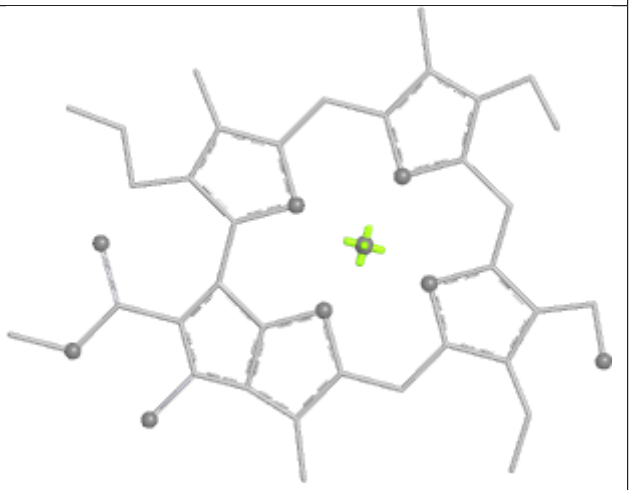
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Bond angles

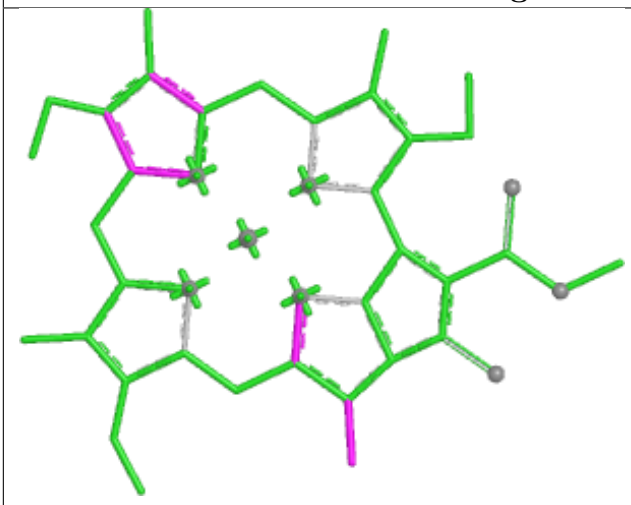


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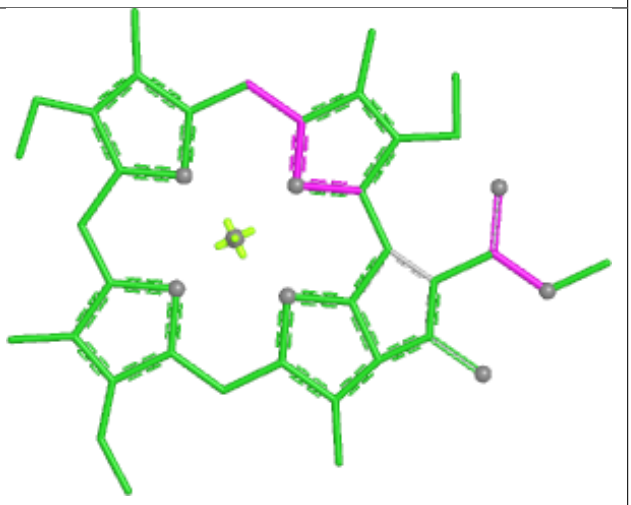


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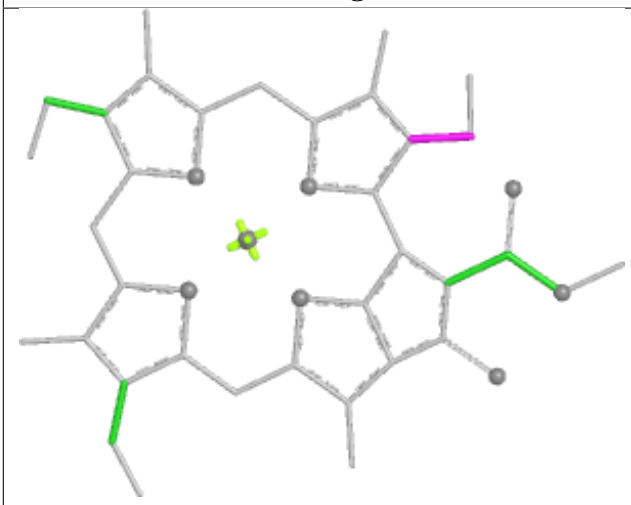
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Bond lengths



Bond angles

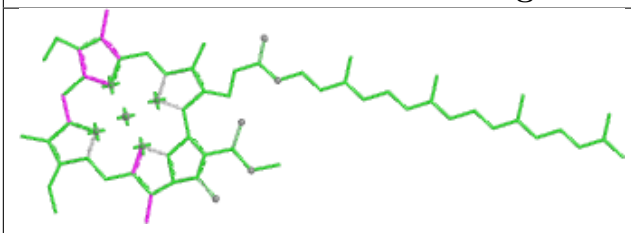


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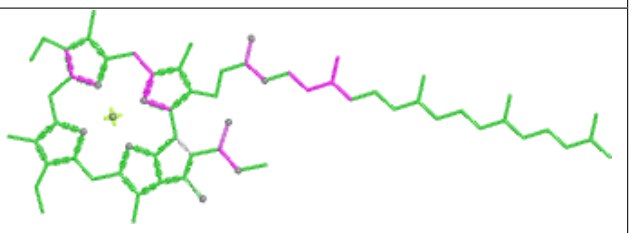


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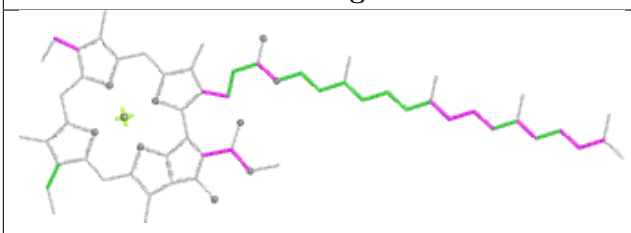
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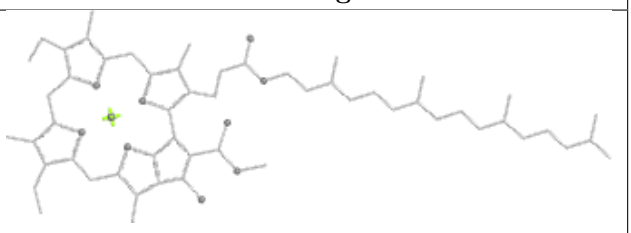
Bond lengths



Bond angles

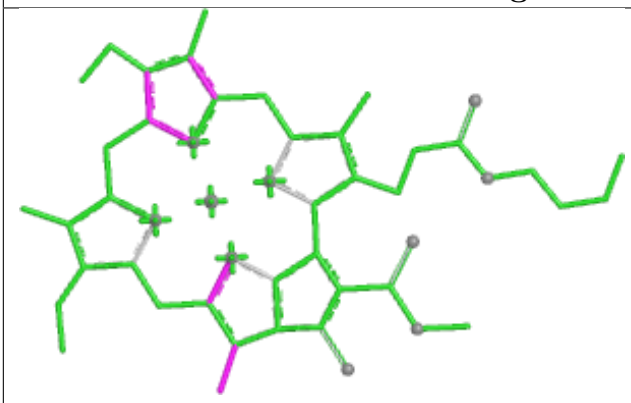


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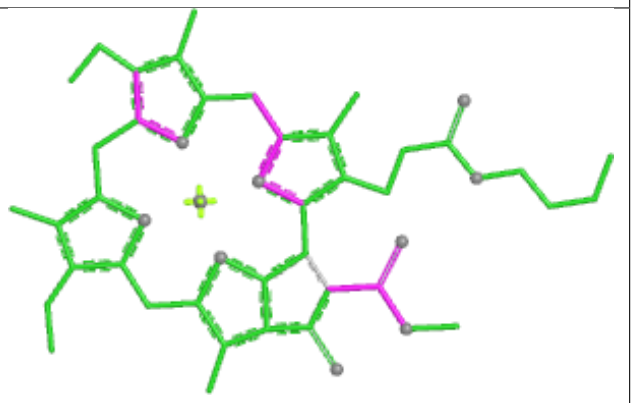


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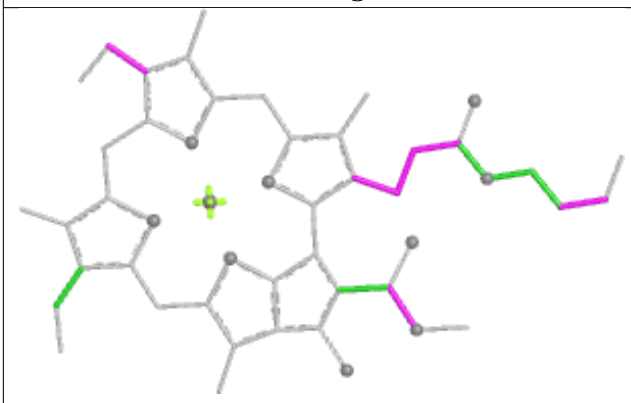
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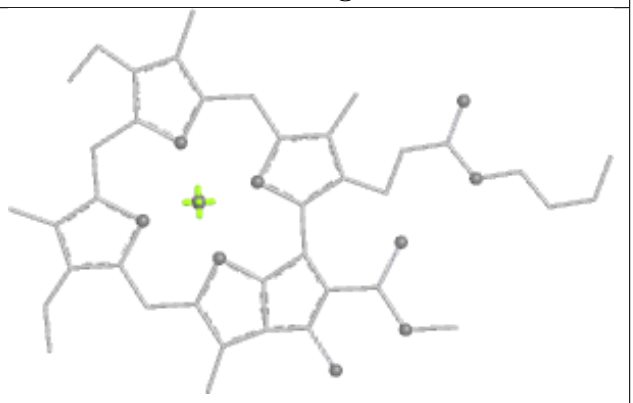
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Bond angles

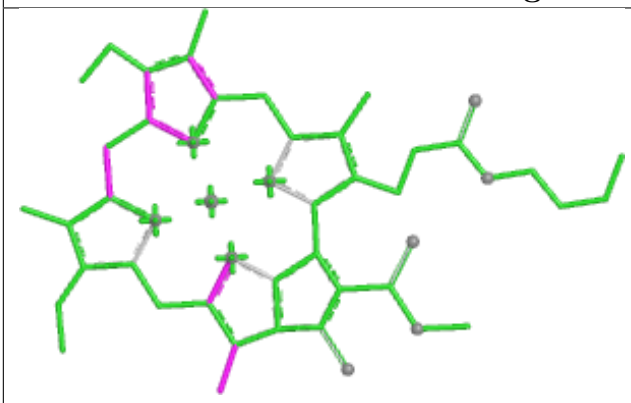


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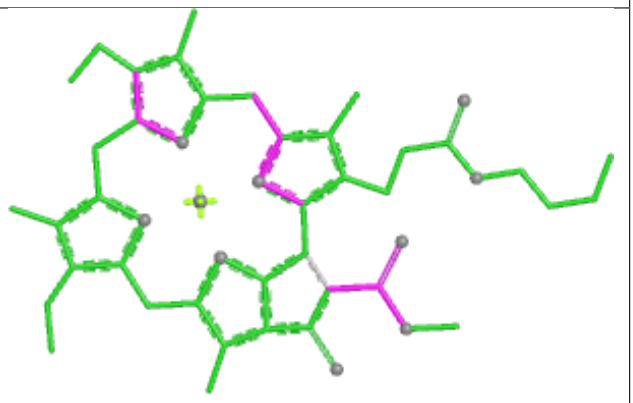


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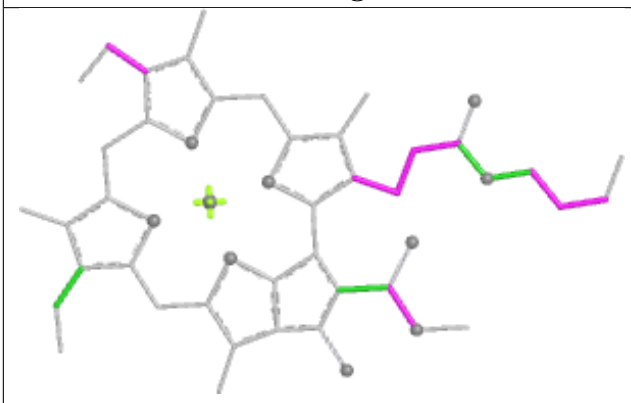
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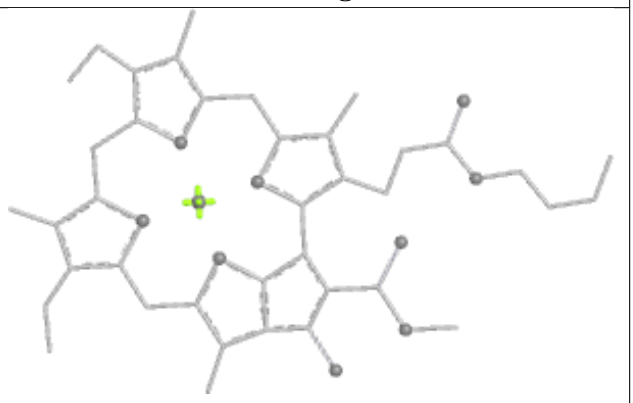
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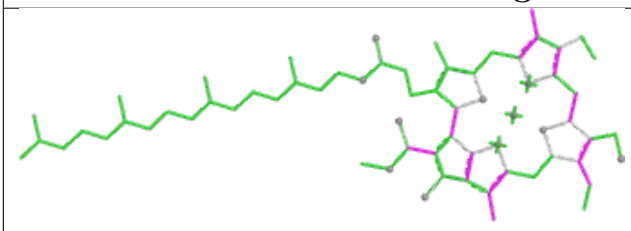


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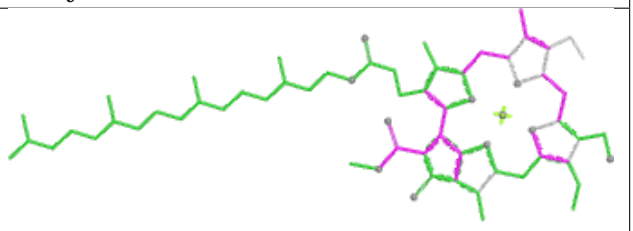


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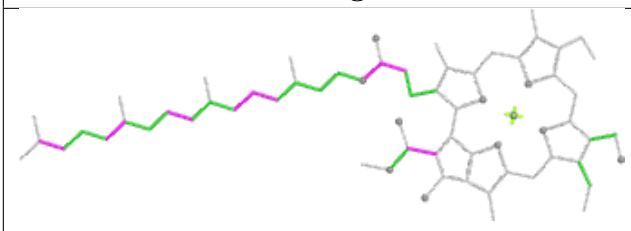
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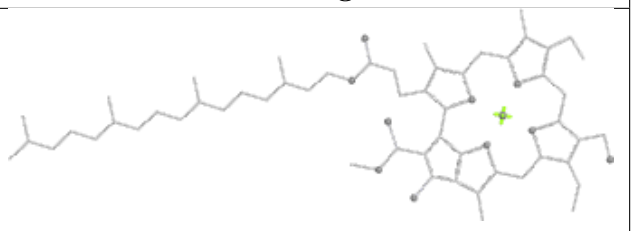
Bond lengths



Bond angles

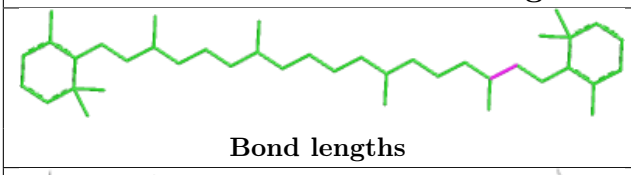


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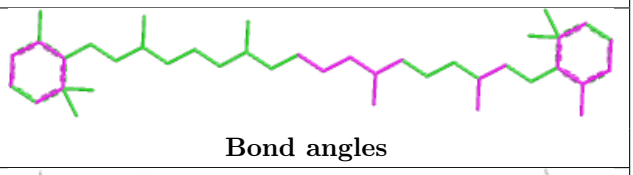


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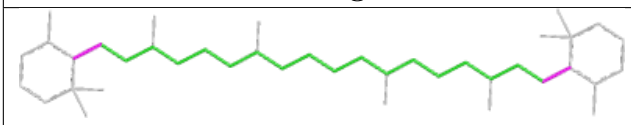
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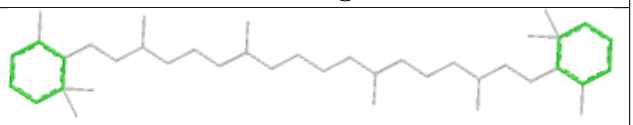
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Bond angles

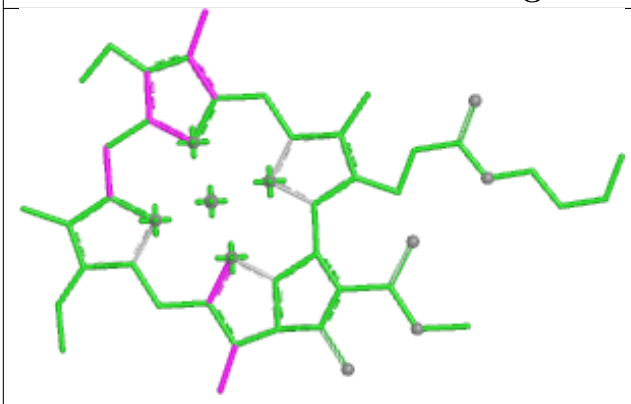


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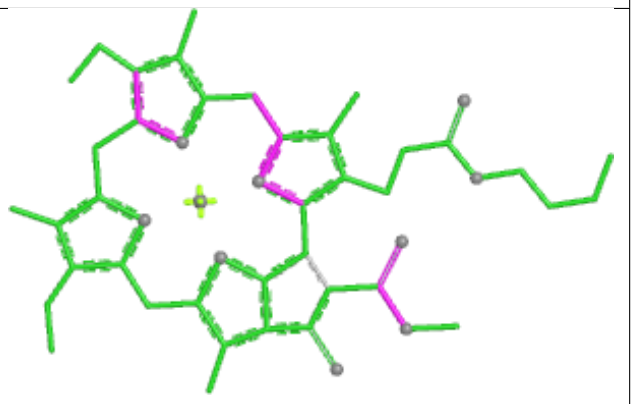


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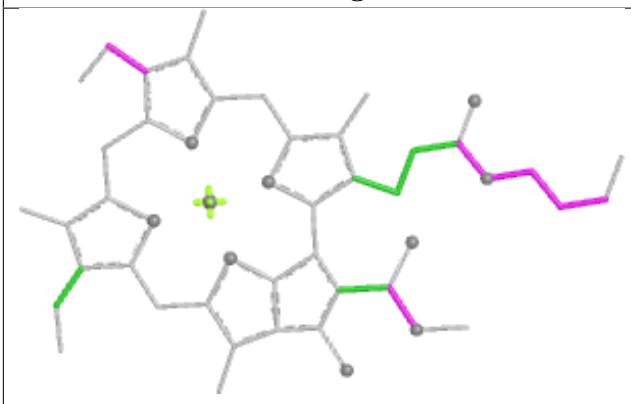
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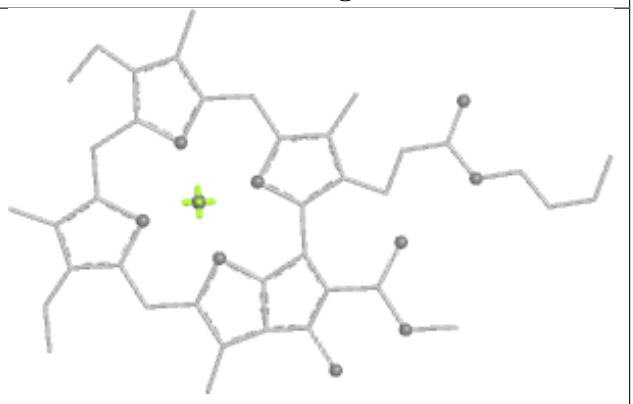
Bond lengths



Bond angles

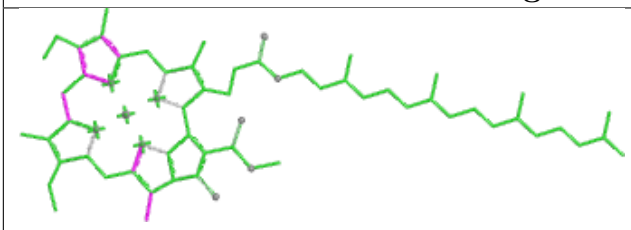


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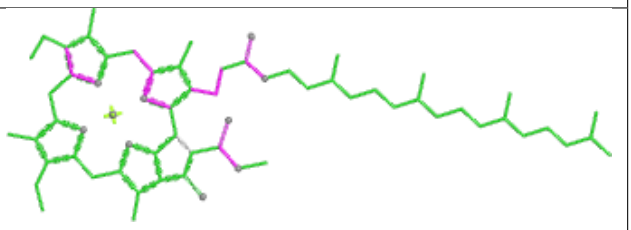


Rings

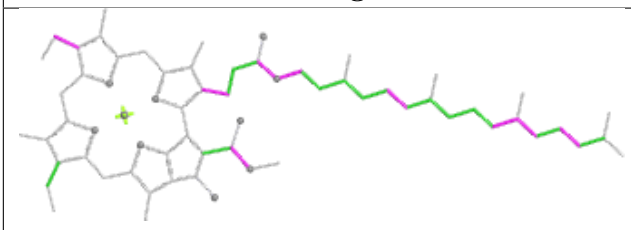
Ligand CLA N 610



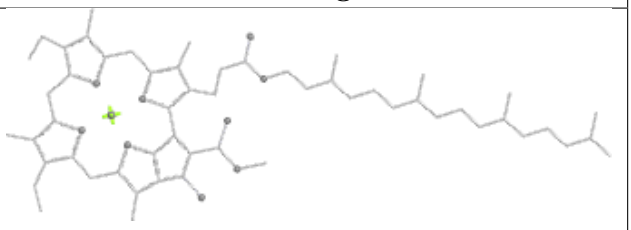
Bond lengths



Bond angles

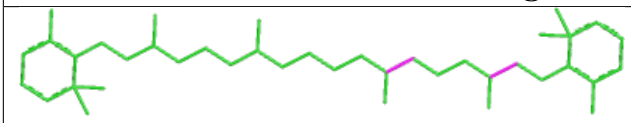


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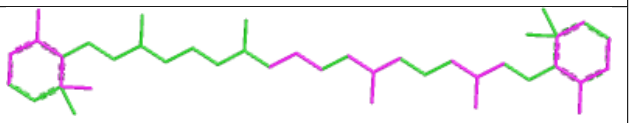


Rings

Ligand BCR B 614



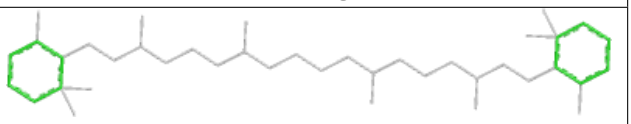
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Bond angles

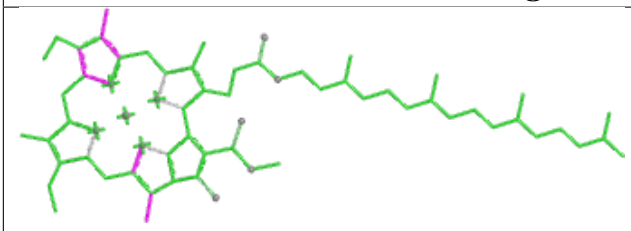


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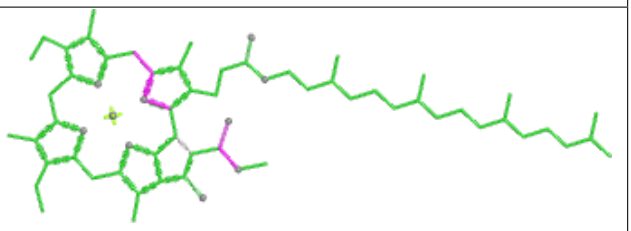


Rings

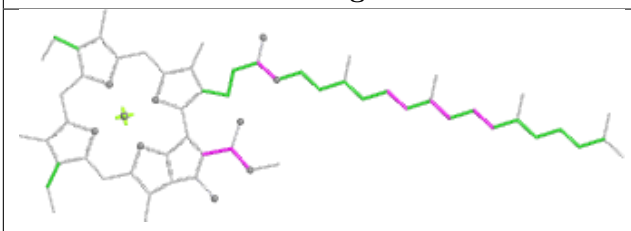
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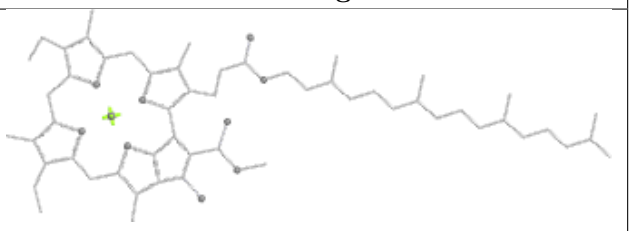
Bond lengths



Bond angles

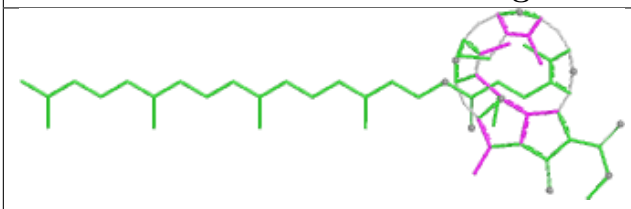


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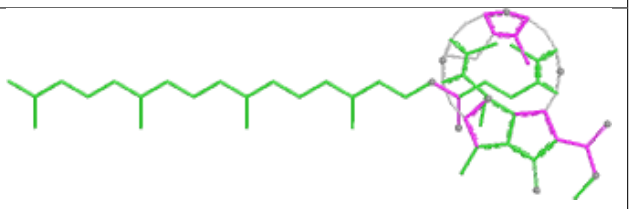


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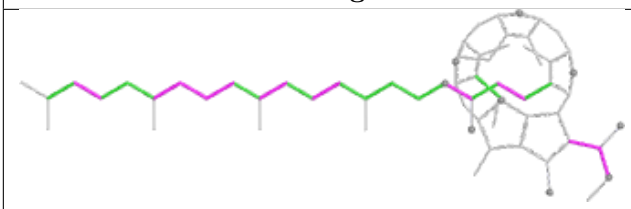
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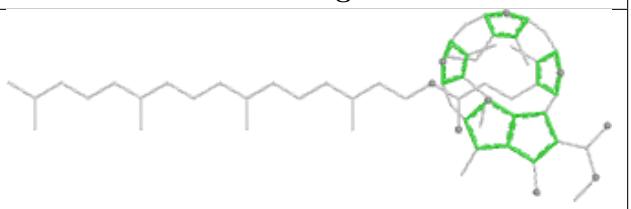
Bond lengths



Bond angles



Torsions

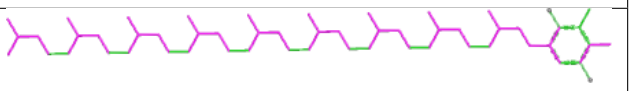


Rings

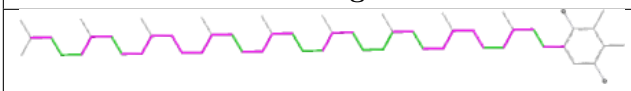
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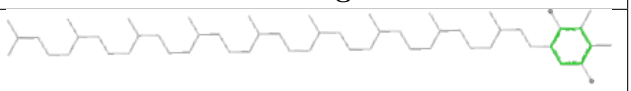
Bond lengths



Bond angles

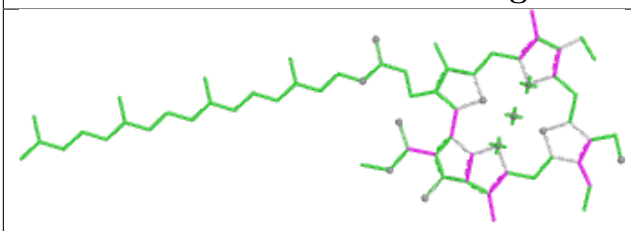


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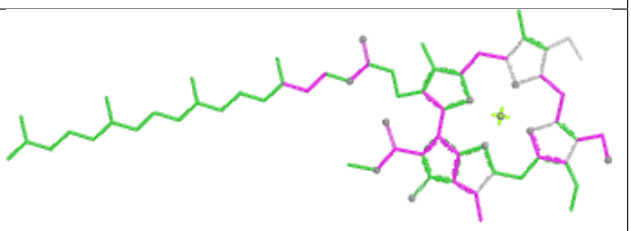


Rings

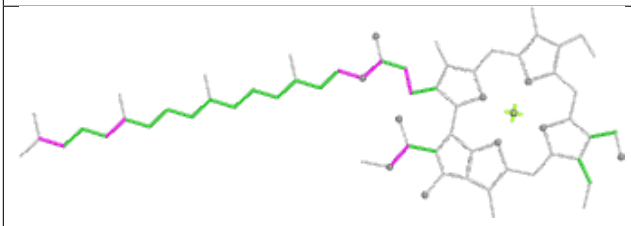
Ligand CHL YY 609



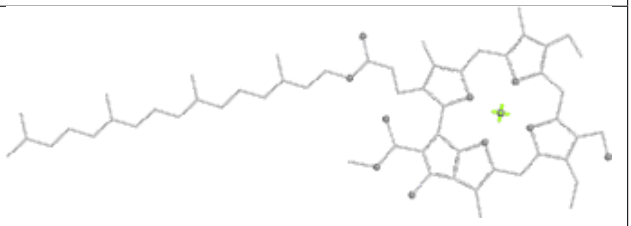
Bond lengths



Bond angles

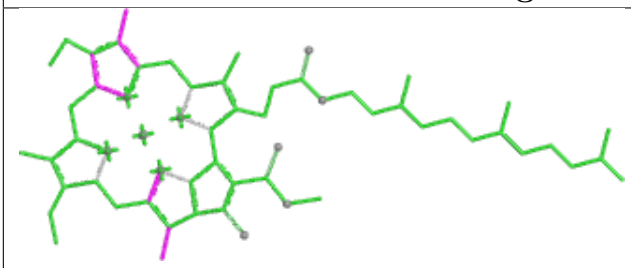


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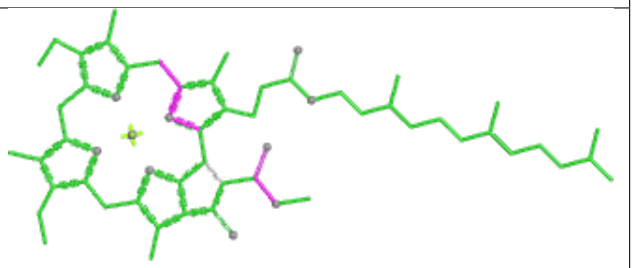


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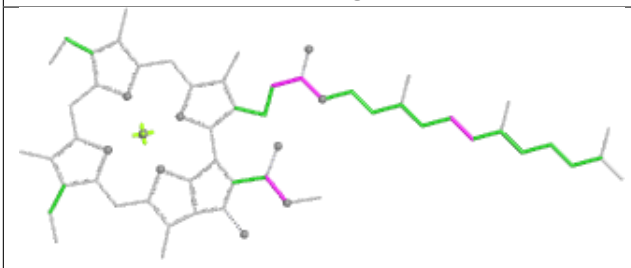
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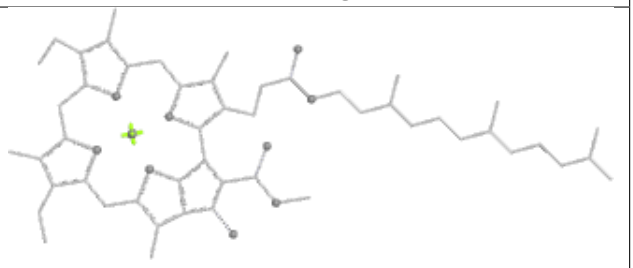
Bond lengths



Bond angles

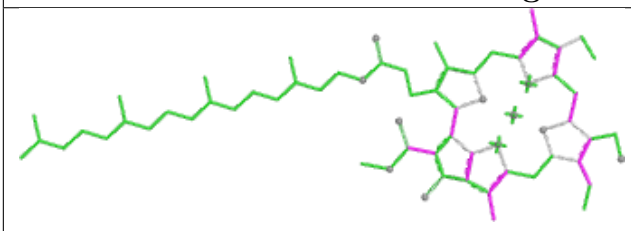


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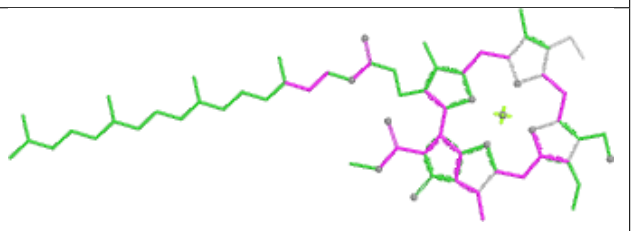


Rings

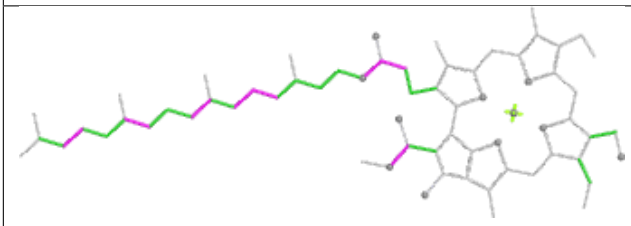
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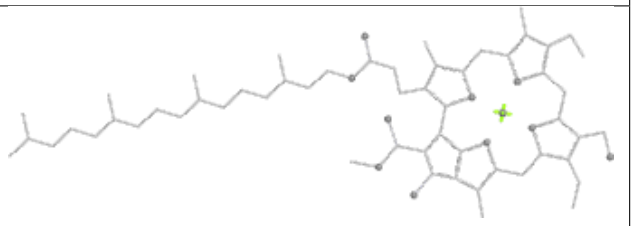
Bond lengths



Bond angles

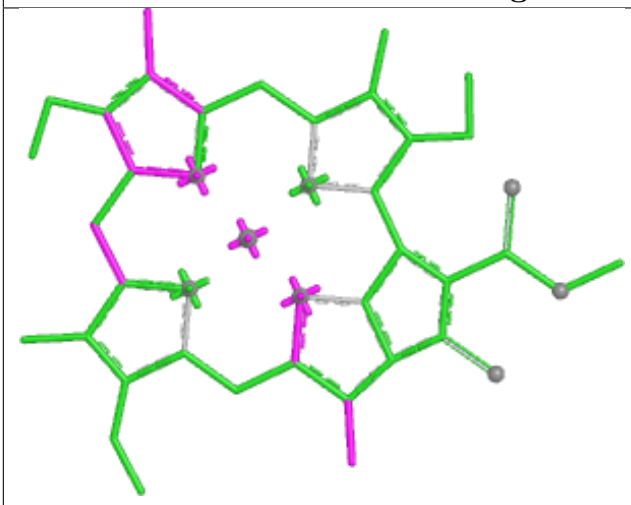


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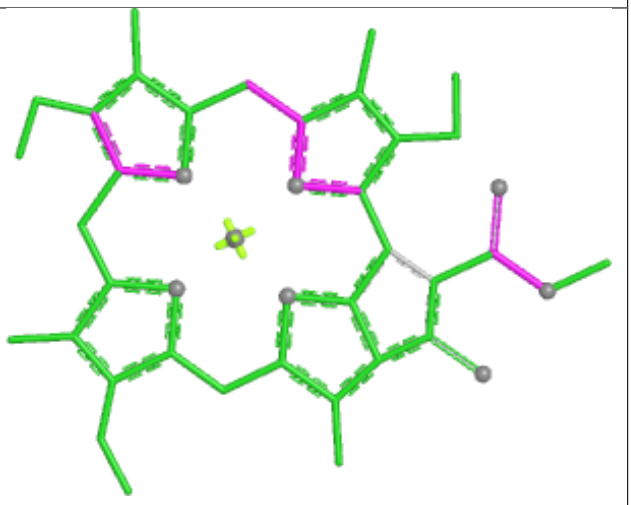


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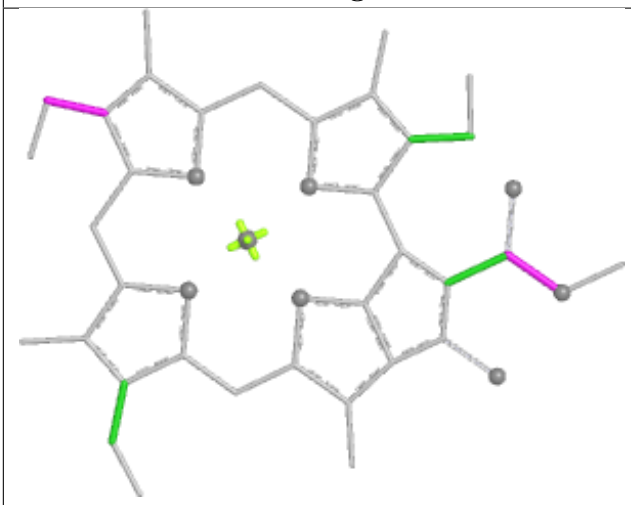
Ligand CLA YY 611



Bond lengths



Bond angles

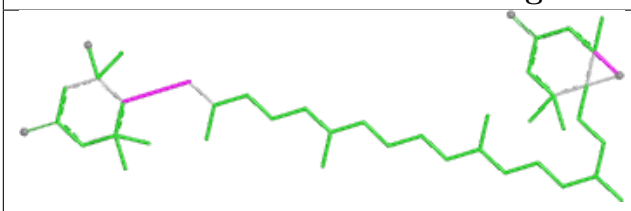


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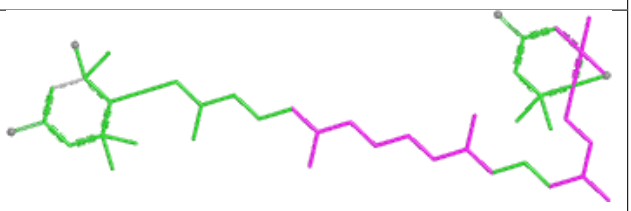


Rings

Ligand NEX n 617



Bond lengths



Bond angles

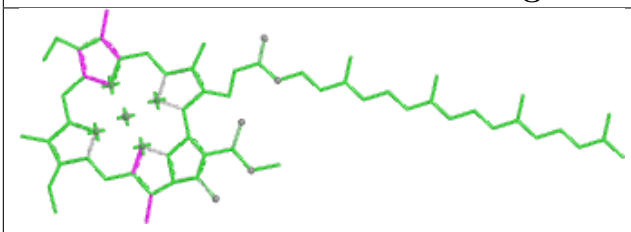


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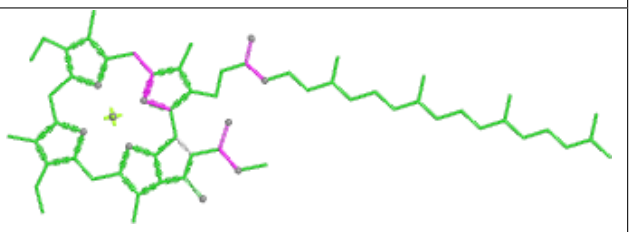


Rings

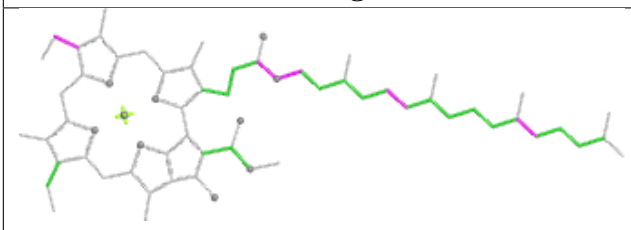
Ligand CLA D 405



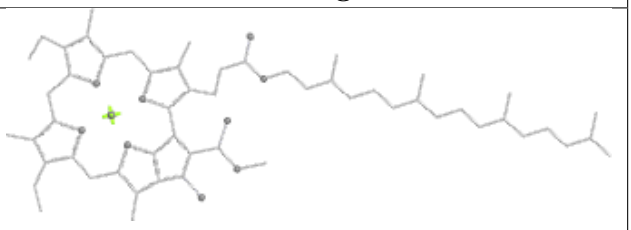
Bond lengths



Bond angles



Torsions

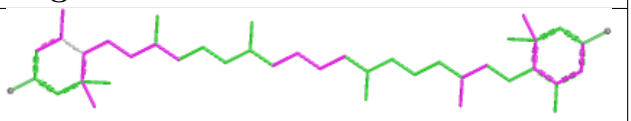


Rings

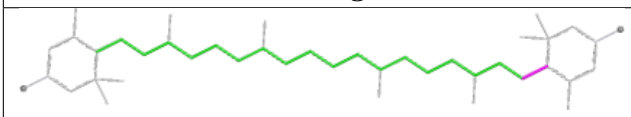
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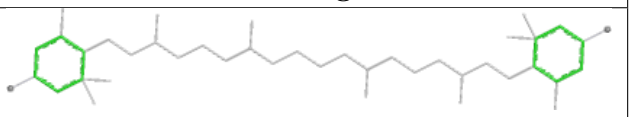
Bond lengths



Bond angles

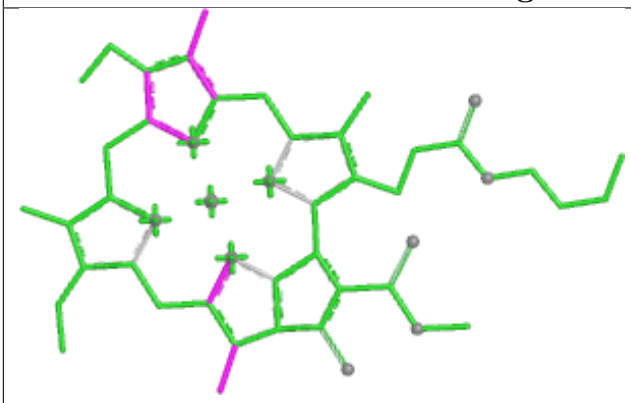


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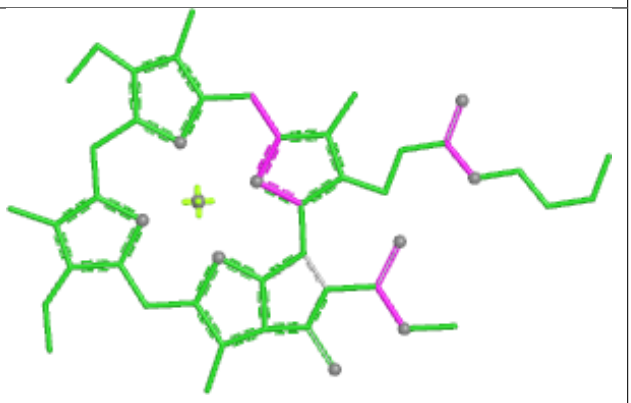


Rings

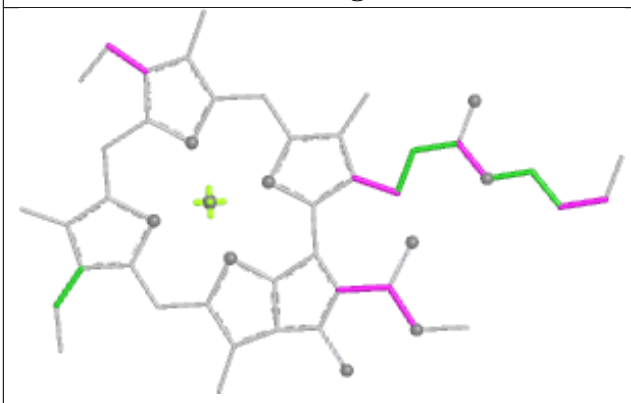
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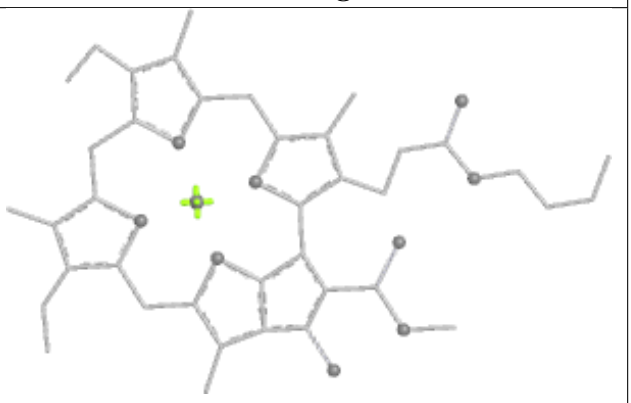
Bond lengths



Bond angles



Torsions

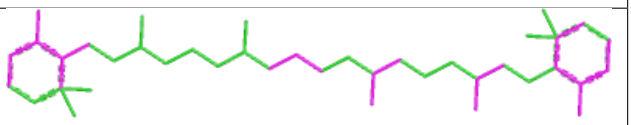


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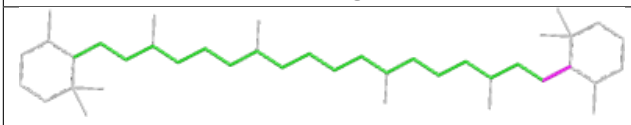
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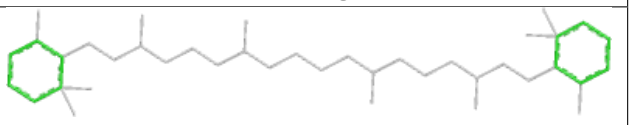
Bond lengths



Bond angles

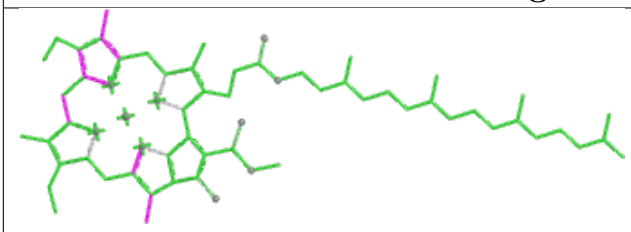


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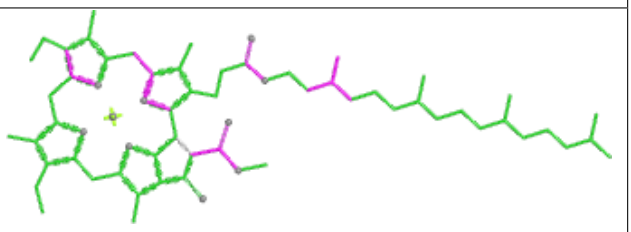


Rings

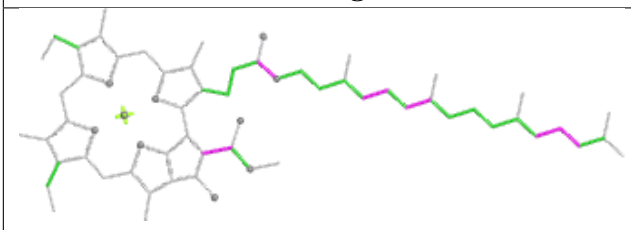
Ligand CLA c 502



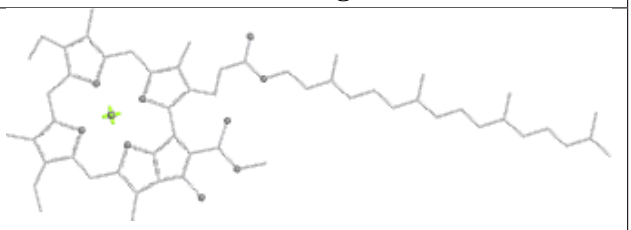
Bond lengths



Bond angles

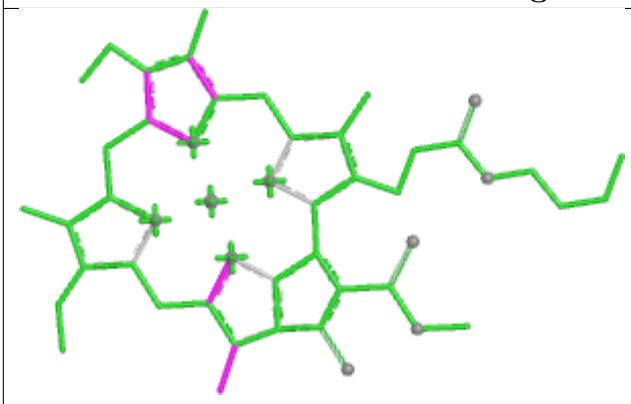


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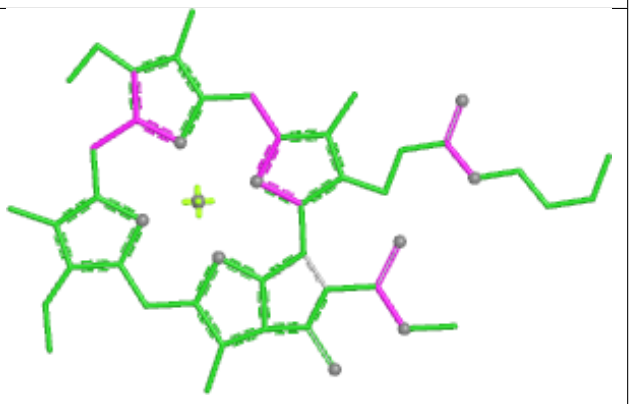


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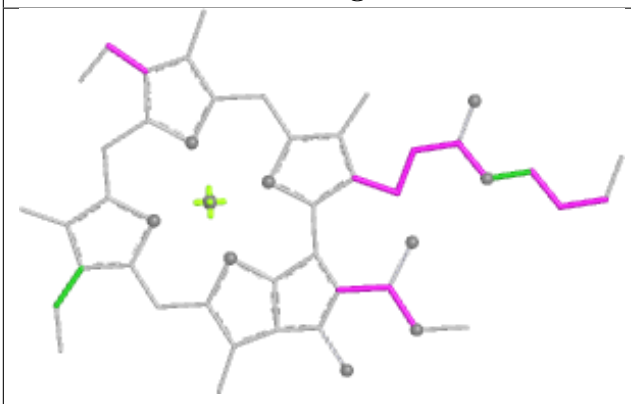
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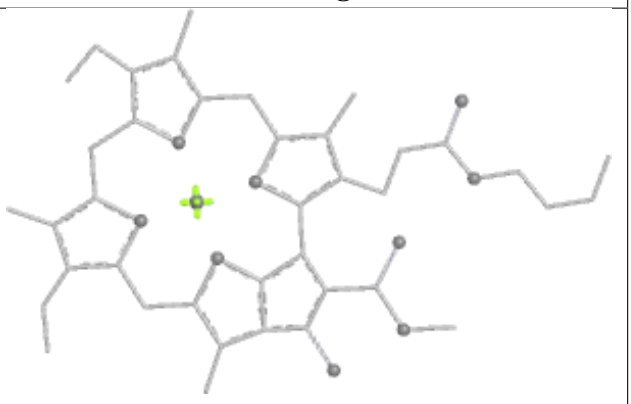
Bond lengths



Bond angles

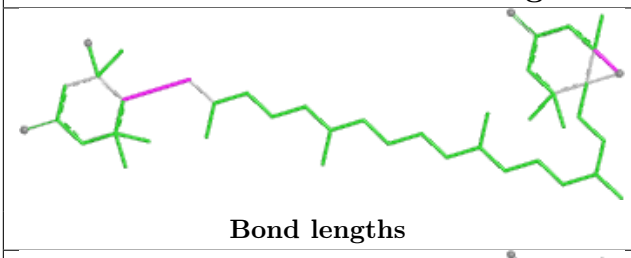


Torsions

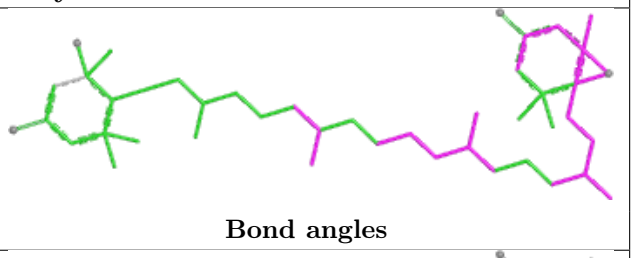


Rings

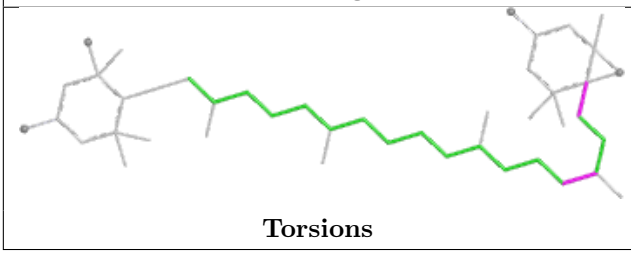
Ligand NEX y 319



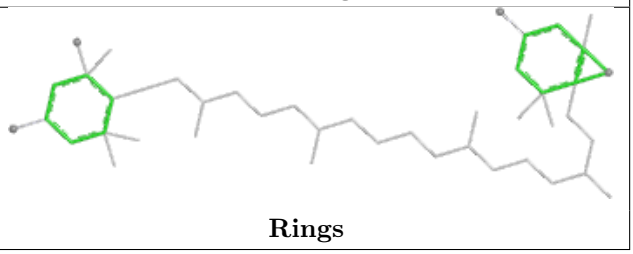
Bond lengths



Bond angles

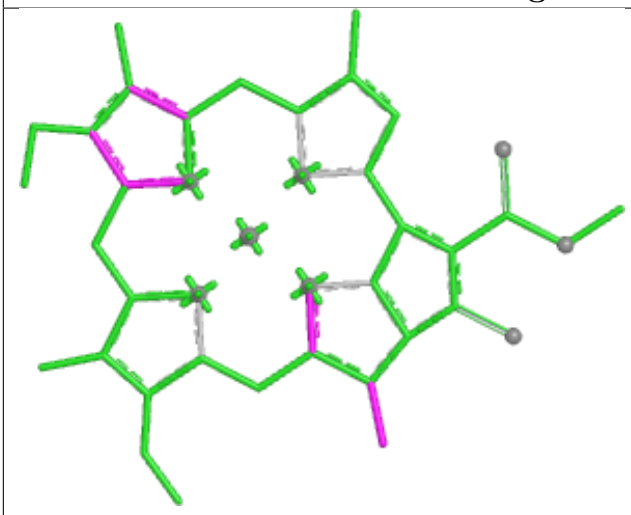


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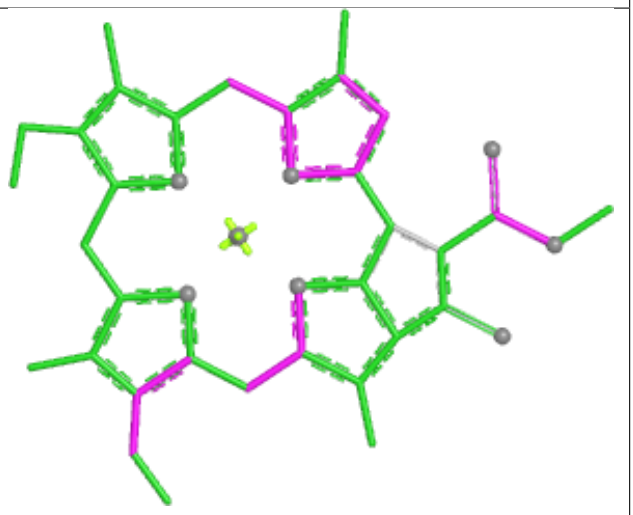


Rings

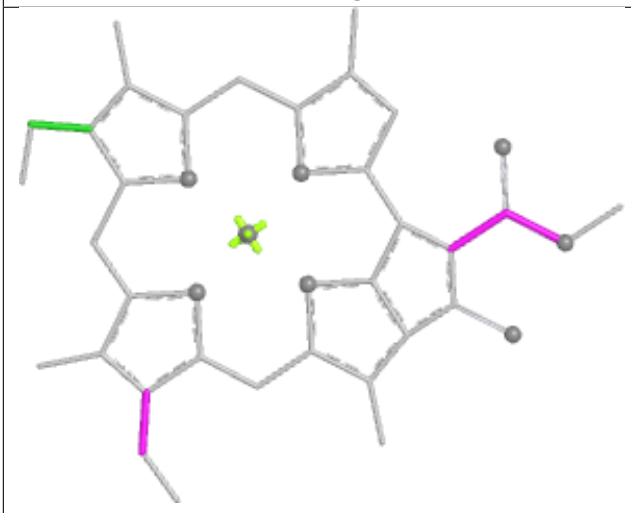
Ligand CLA 3 610



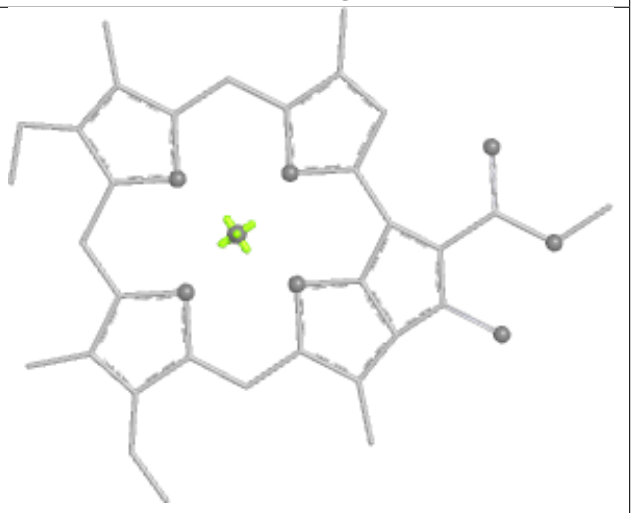
Bond lengths



Bond angles

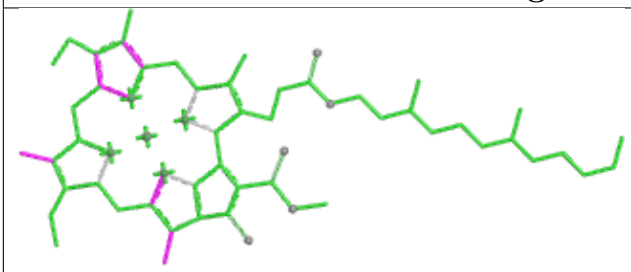


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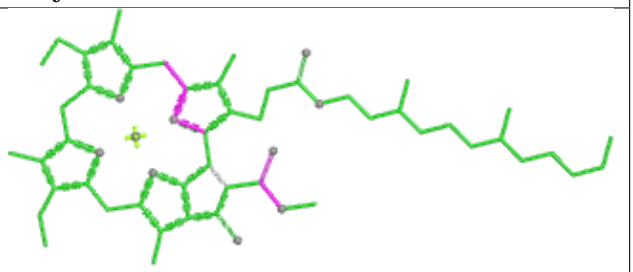


Rings

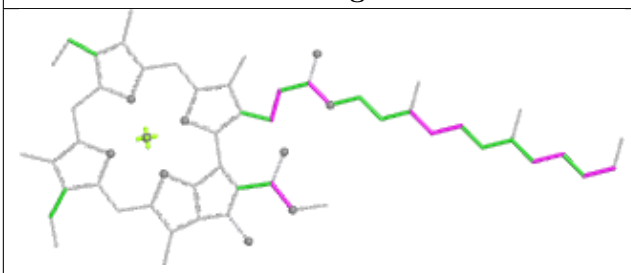
Ligand CLA y 315



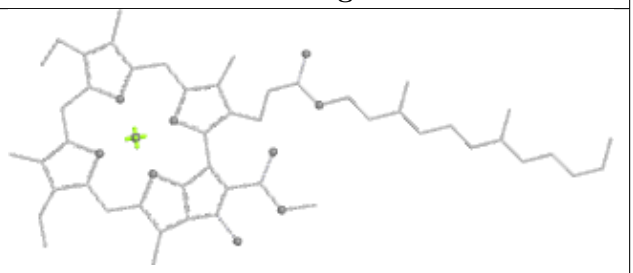
Bond lengths



Bond angles

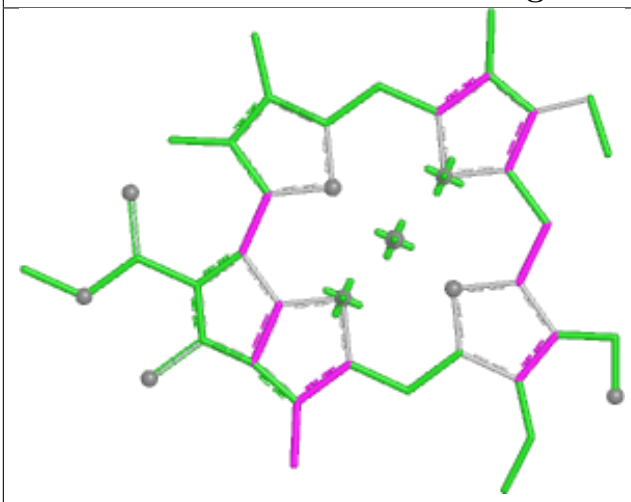


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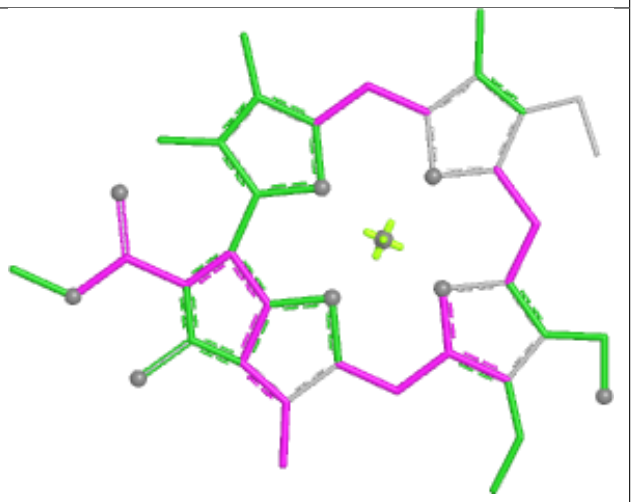


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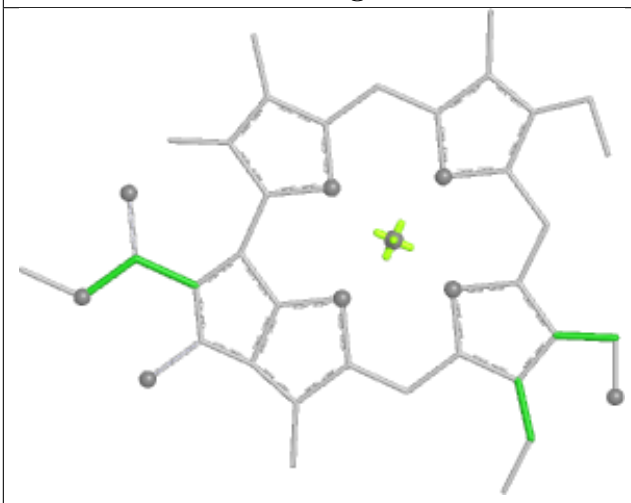
Ligand CHL S 606



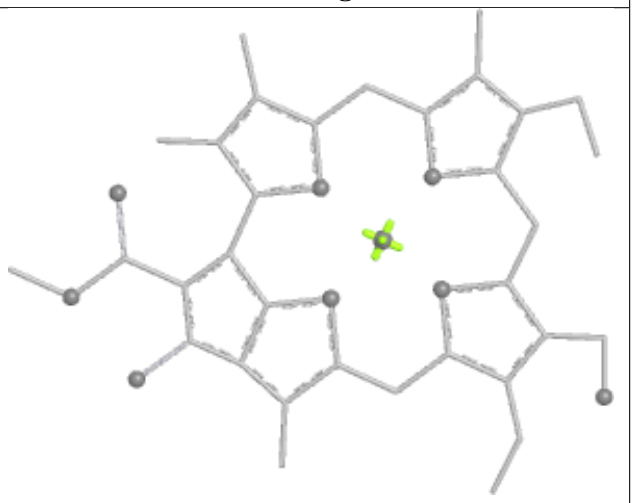
Bond lengths



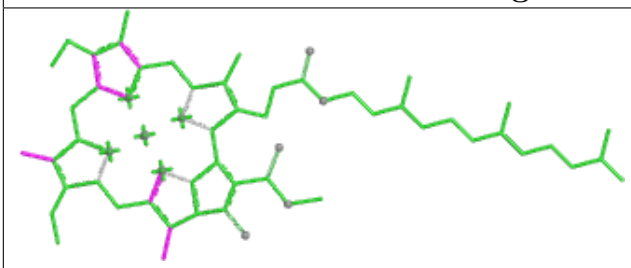
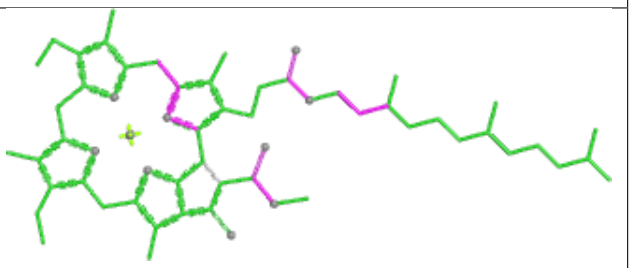
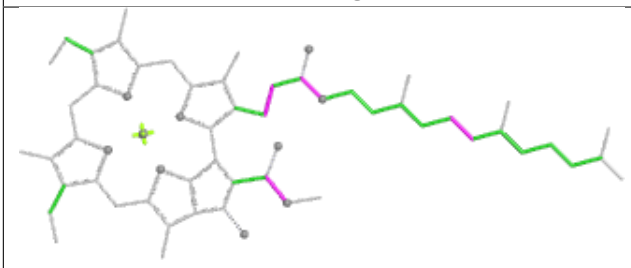
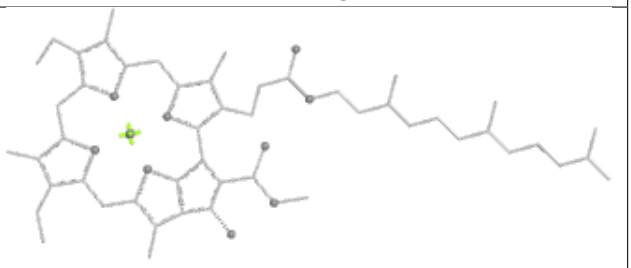
Bond angles

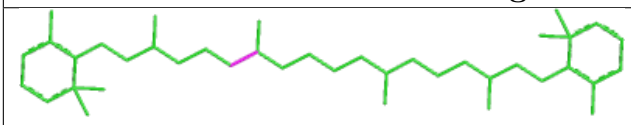
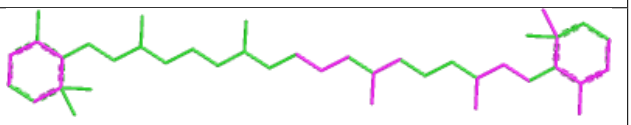
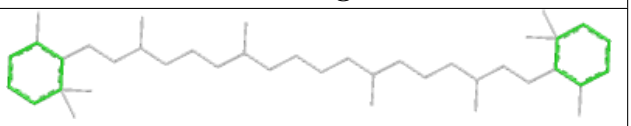


Torsions

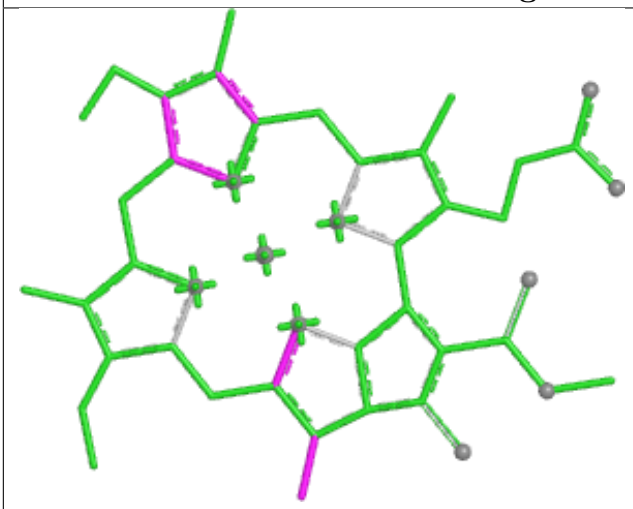


Rings

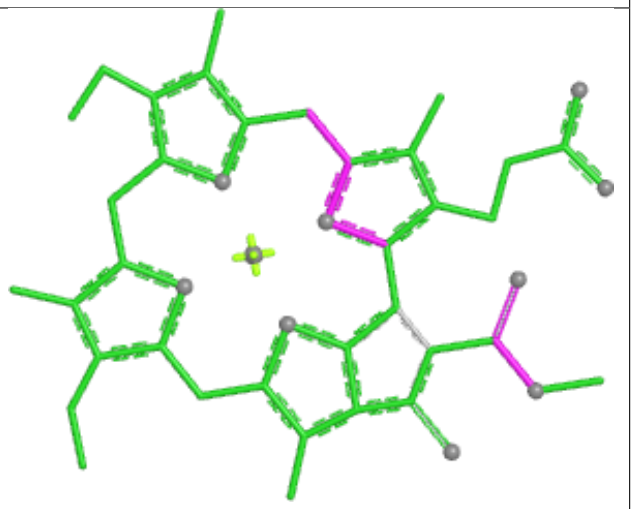
Ligand CLA BB 613	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR CC 516	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

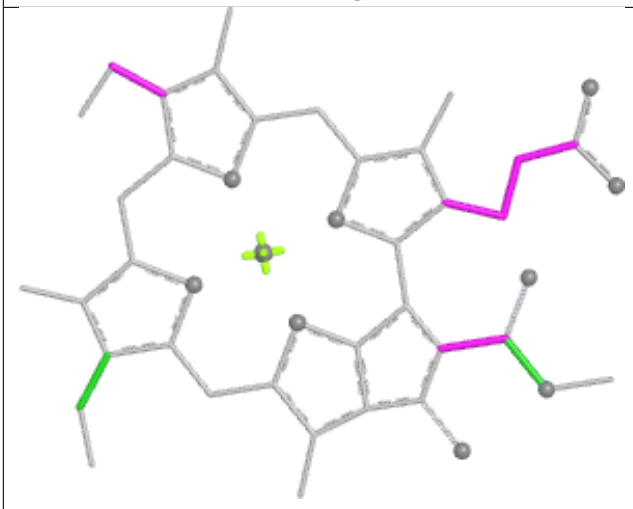
Ligand CLA 44 611



Bond lengths



Bond angles

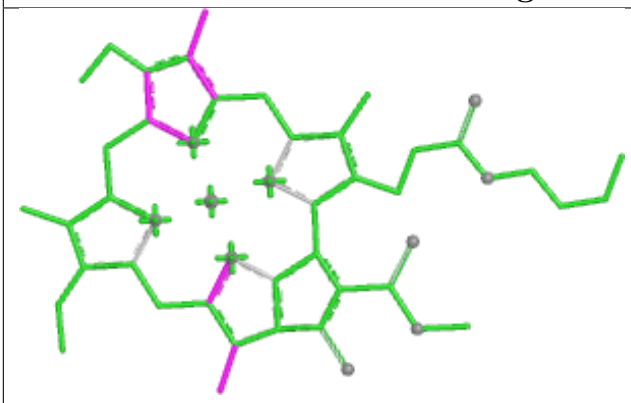


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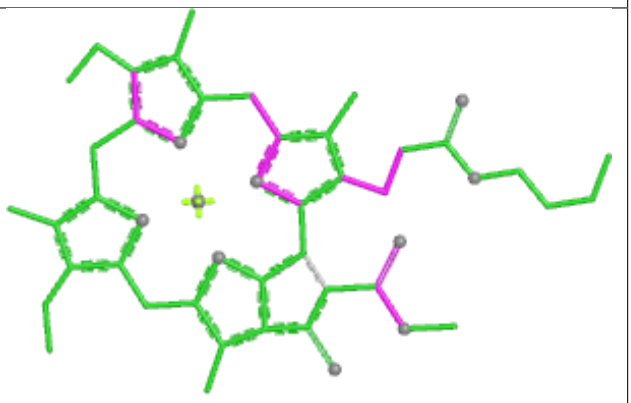


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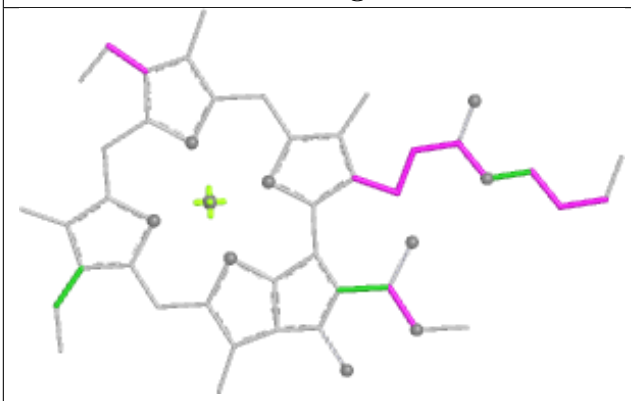
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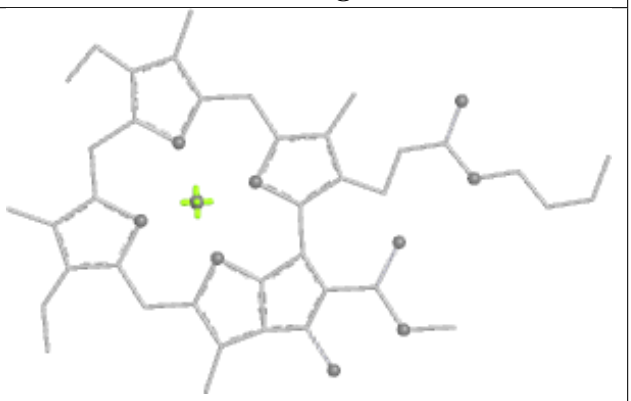
Bond lengths



Bond angles



Torsions

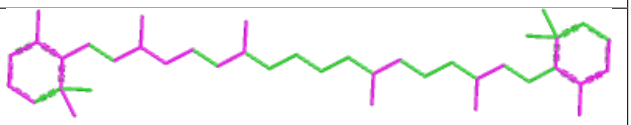


Rings

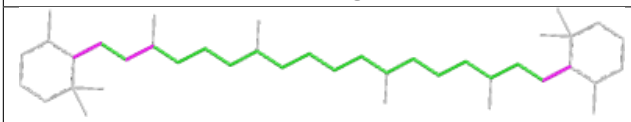
Ligand BCR C 516



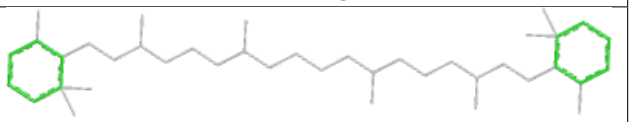
Bond lengths



Bond angles

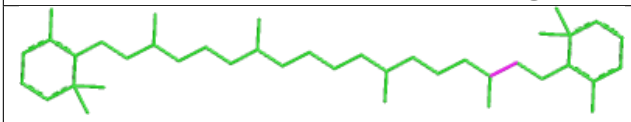


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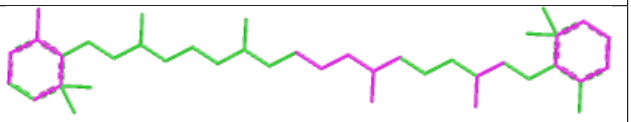


Rings

Ligand BCR b 618



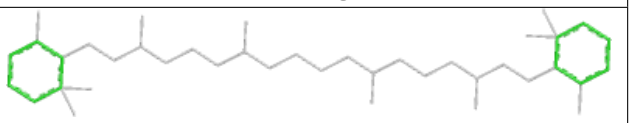
Bond lengths



Bond angles

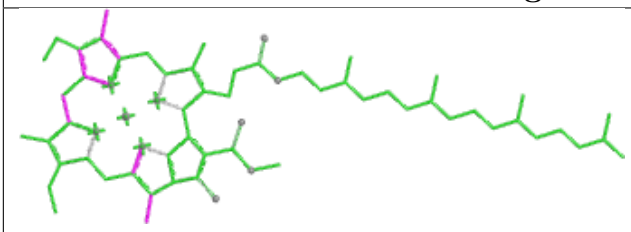


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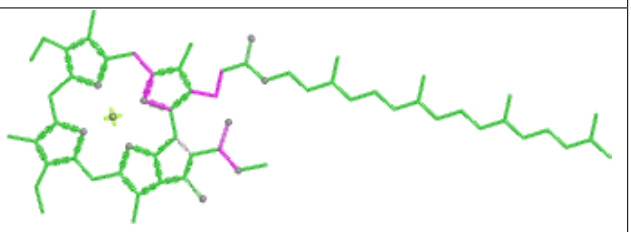


Rings

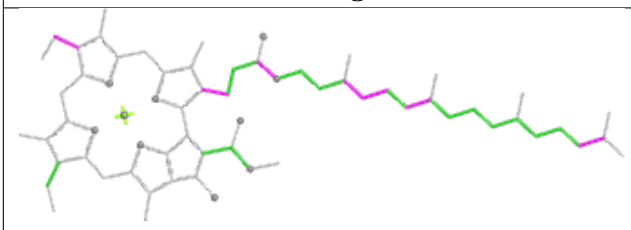
Ligand CLA C 504



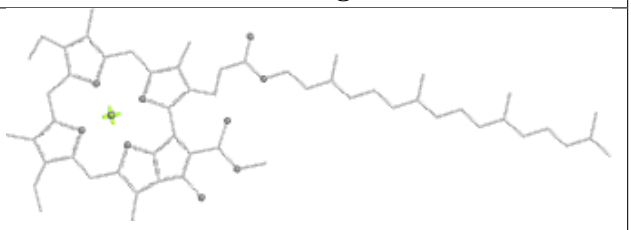
Bond lengths



Bond angles

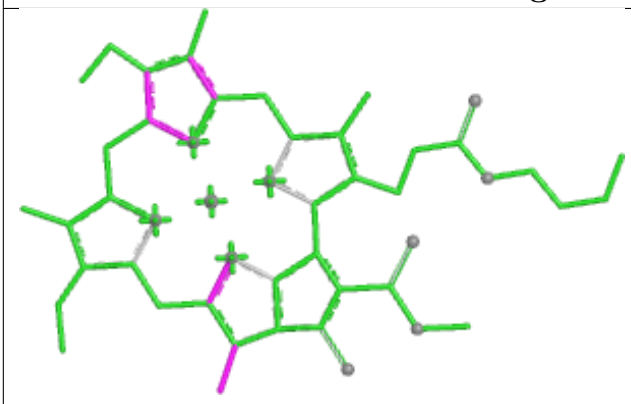


Torsions

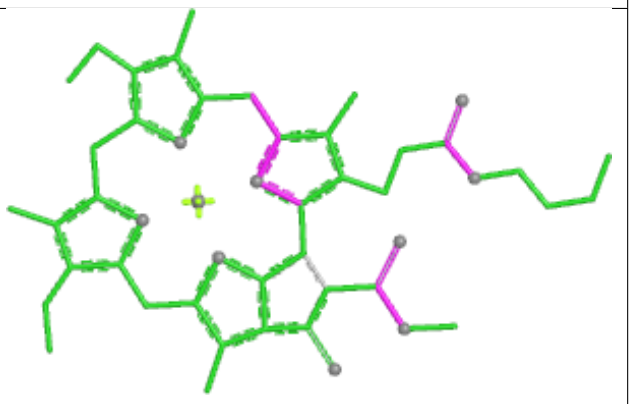


Rings

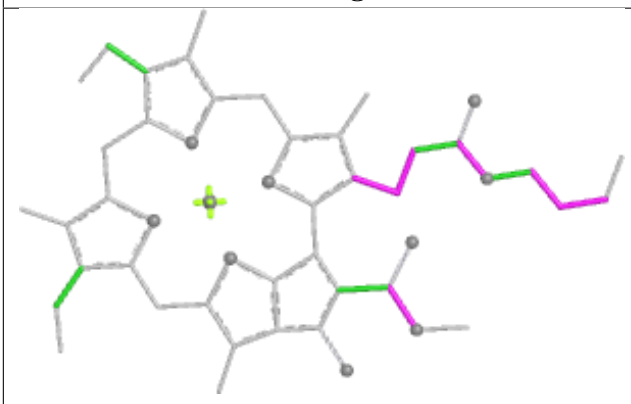
Ligand CLA r 610



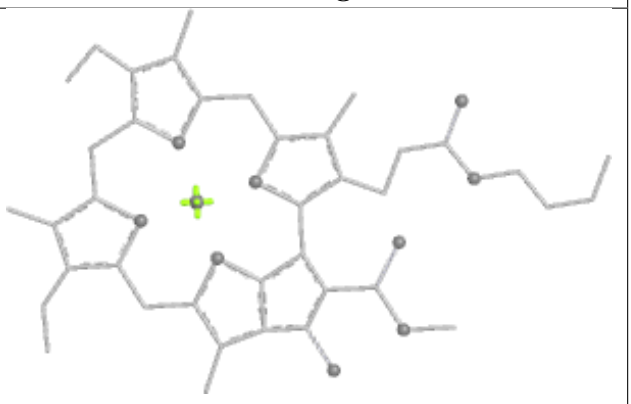
Bond lengths



Bond angles

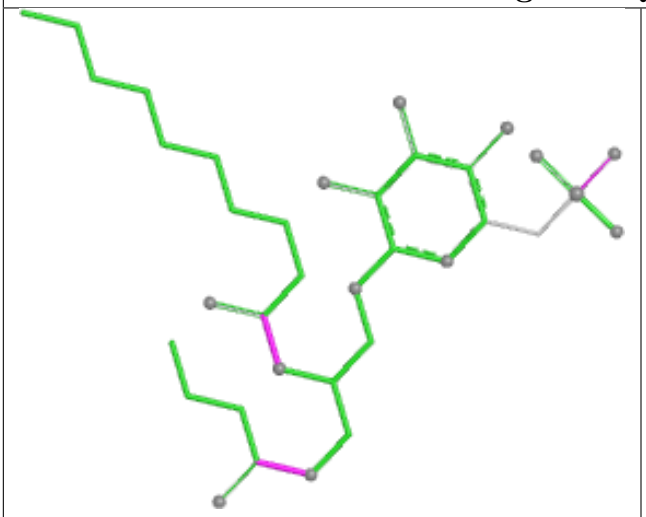


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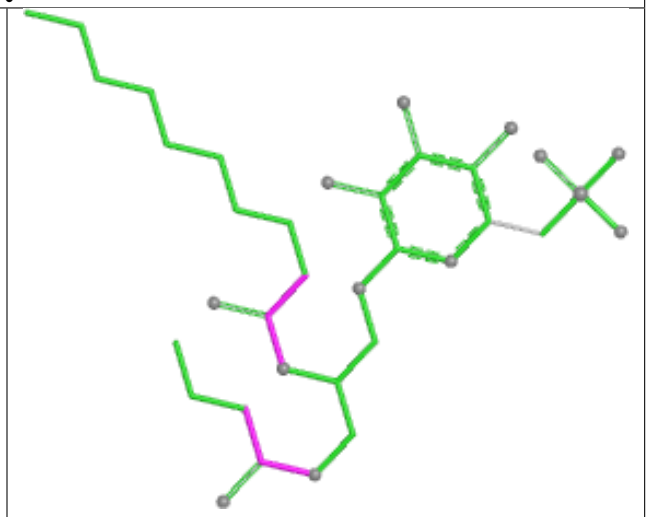


Rings

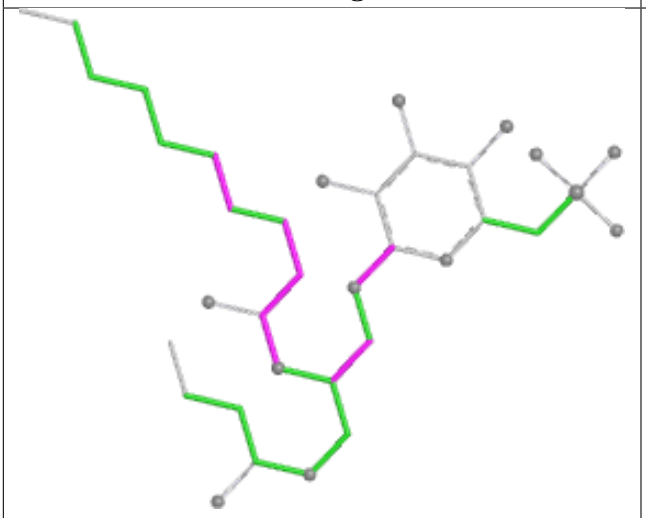
Ligand SQD LL 101



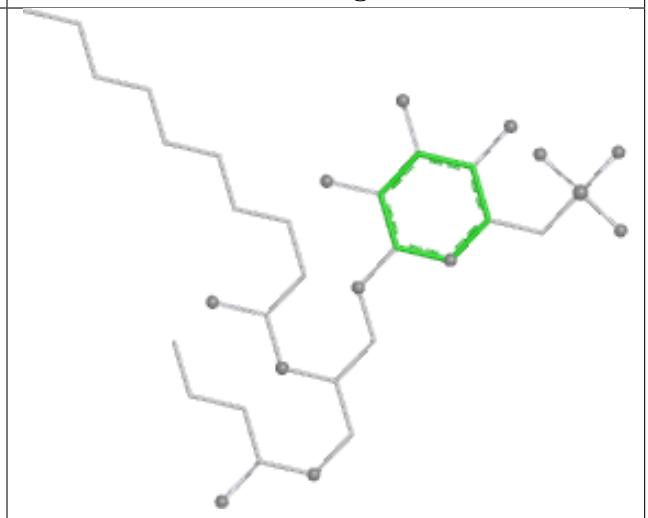
Bond lengths



Bond angles

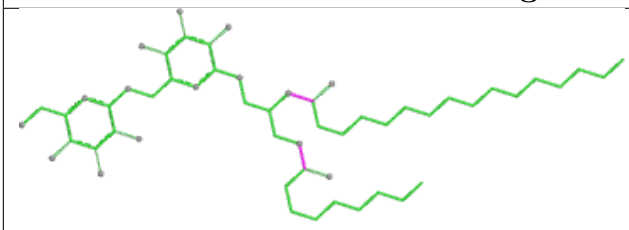


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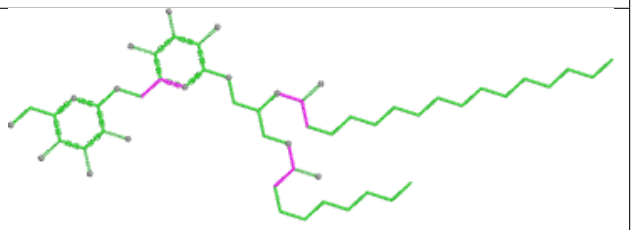


Rings

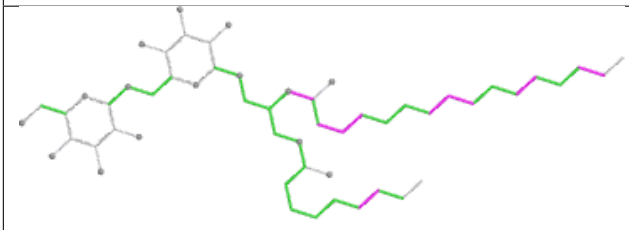
Ligand DGD C 519



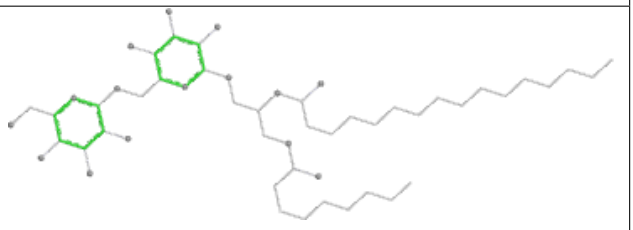
Bond lengths



Bond angles

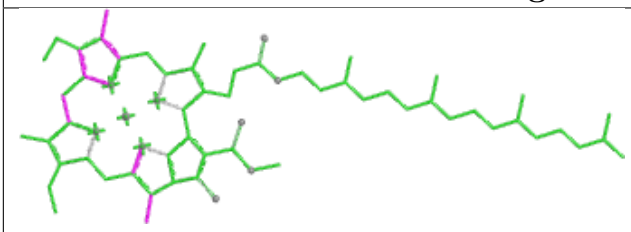


Torsions

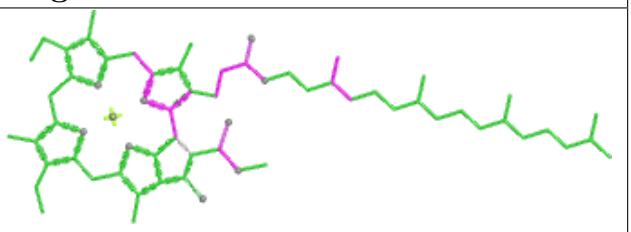


Rings

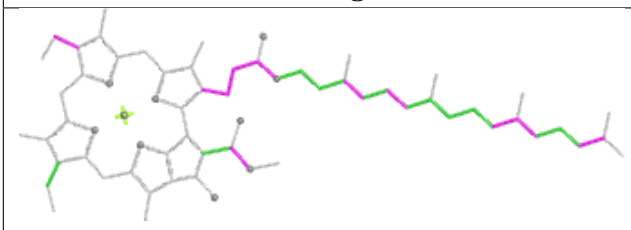
Ligand CLA g 611



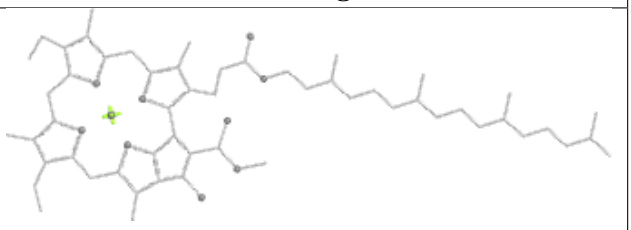
Bond lengths



Bond angles

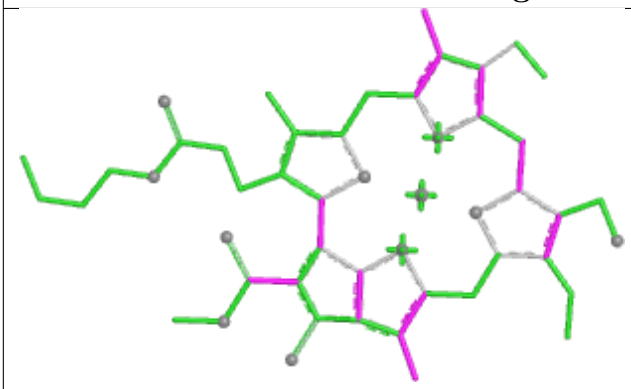


Torsions

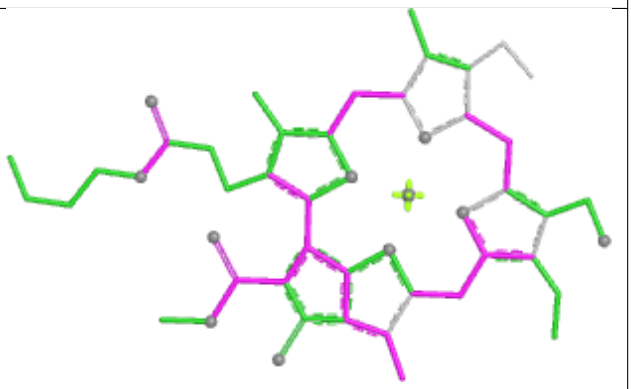


Rings

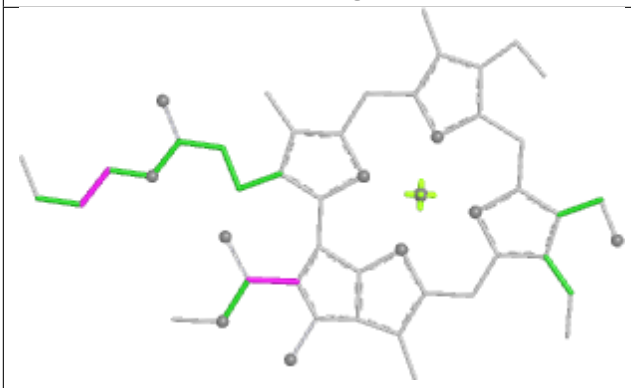
Ligand CHL Nn 316



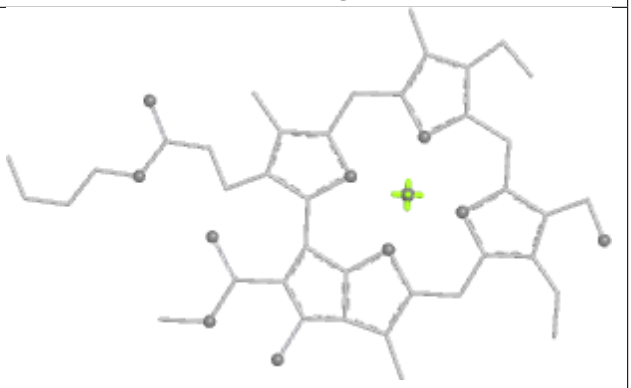
Bond lengths



Bond angles

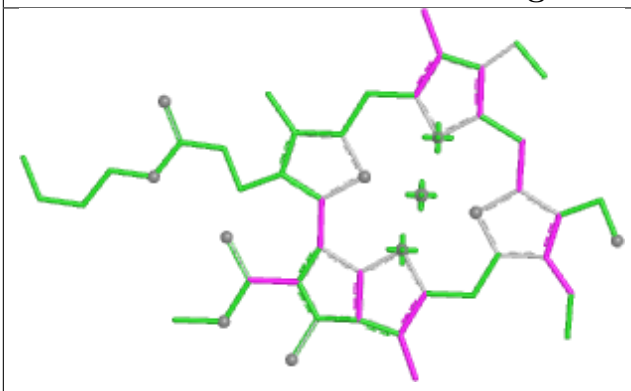


Torsions

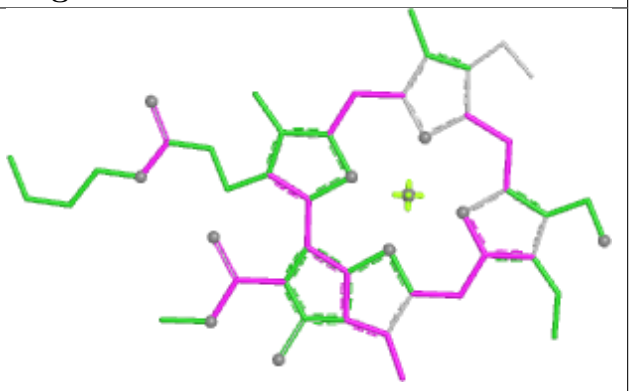


Rings

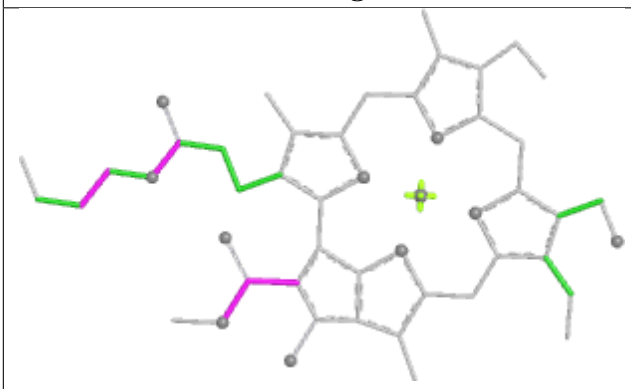
Ligand CHL g 607



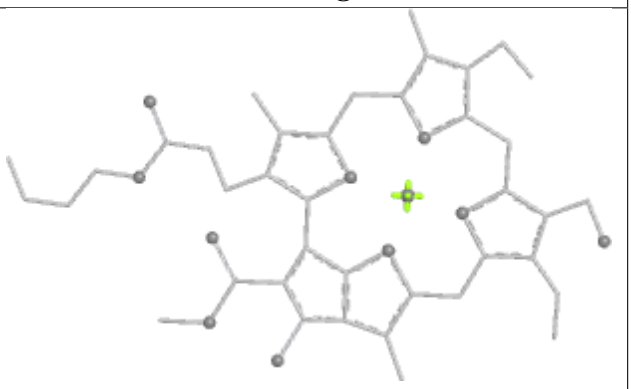
Bond lengths



Bond angles

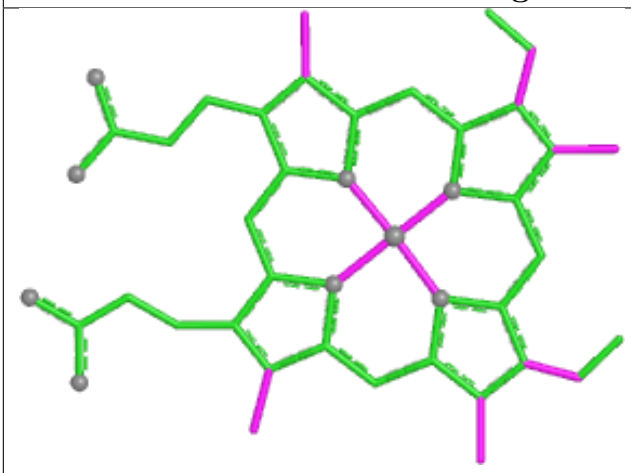


Torsions

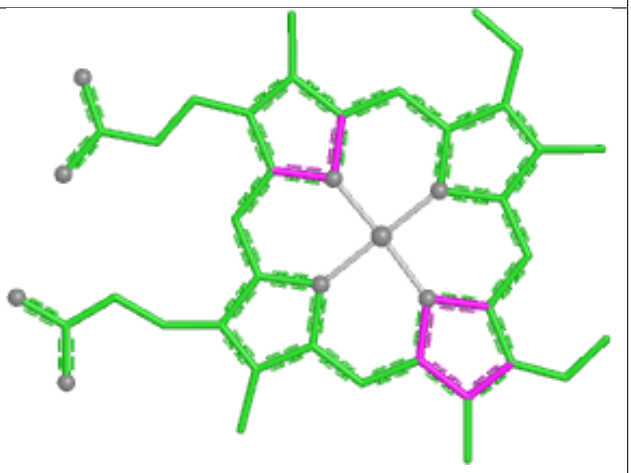


Rings

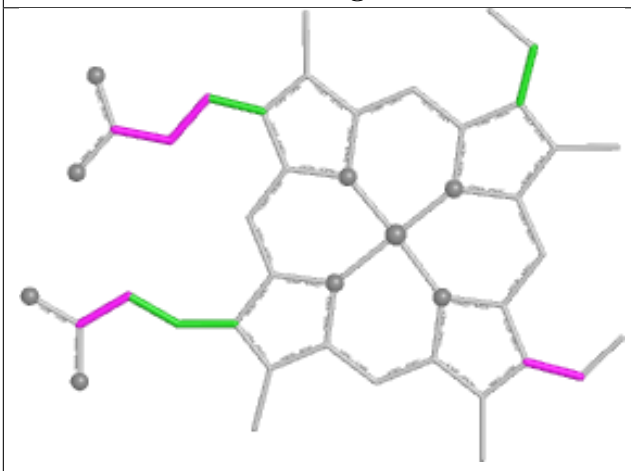
Ligand HEM Ee 101



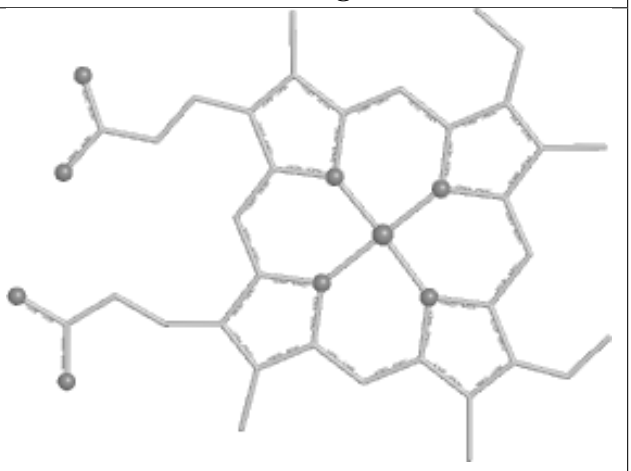
Bond lengths



Bond angles

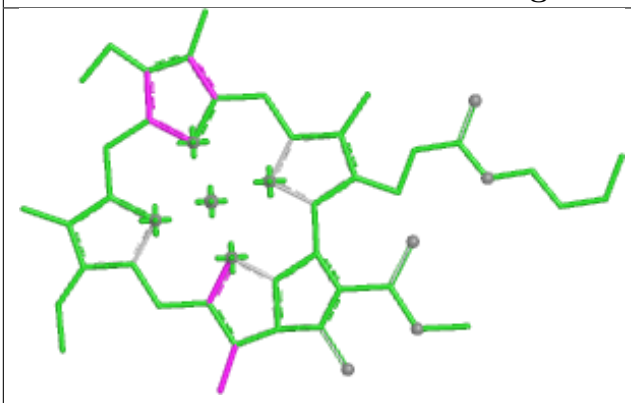


Torsions

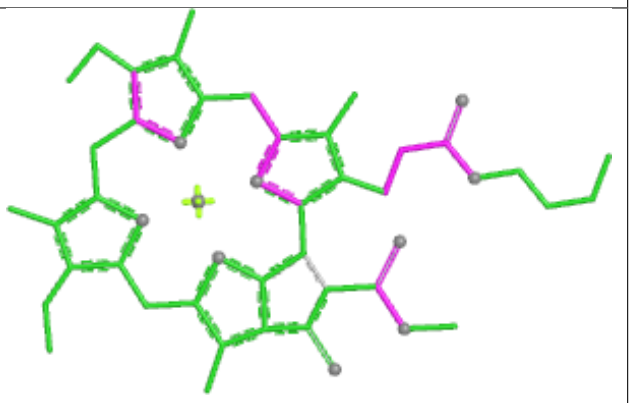


Rings

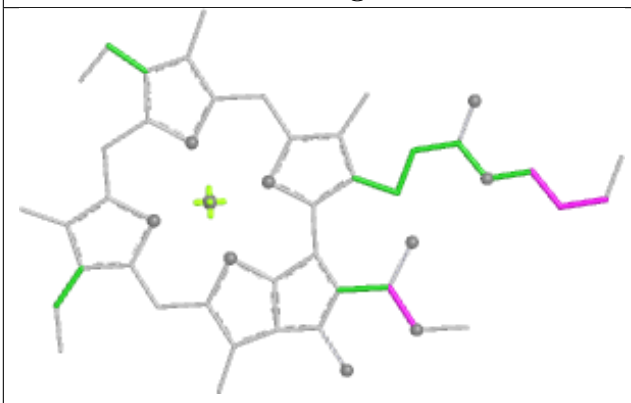
Ligand CLA r 612



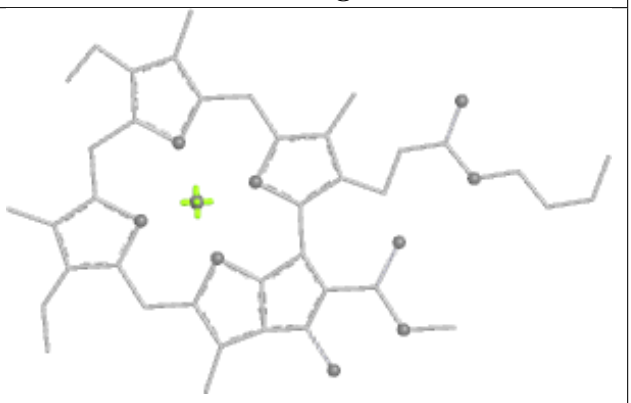
Bond lengths



Bond angles

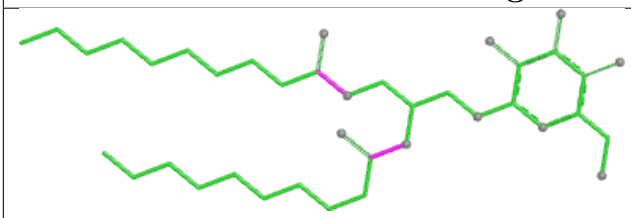


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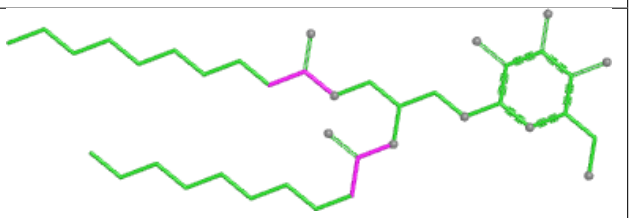


Rings

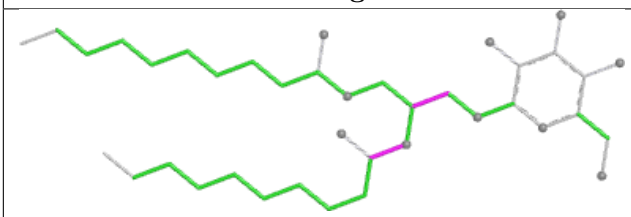
Ligand LMG CC 520



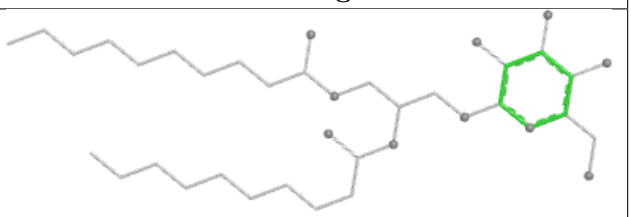
Bond lengths



Bond angles

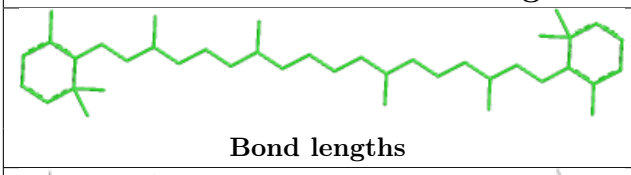


Torsions

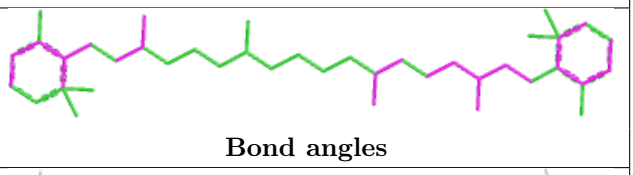


Rings

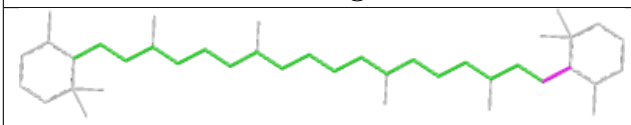
Ligand BCR C 518



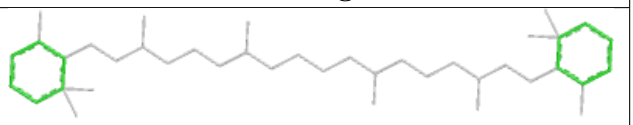
Bond lengths



Bond angles

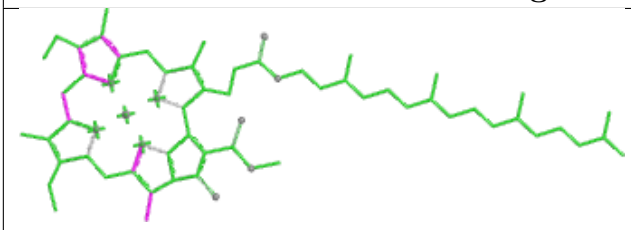


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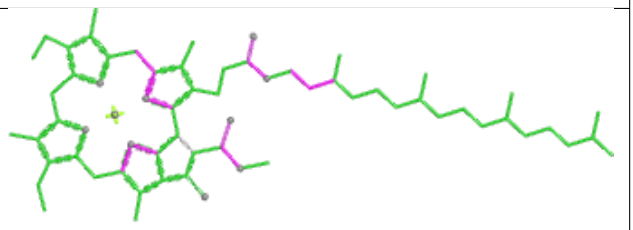


Rings

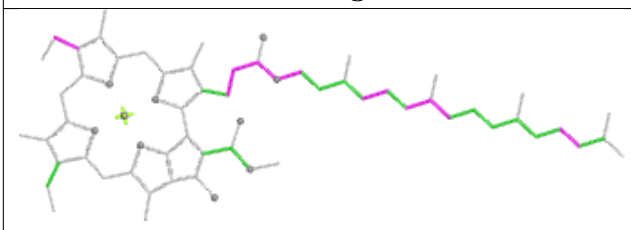
Ligand CLA r 602



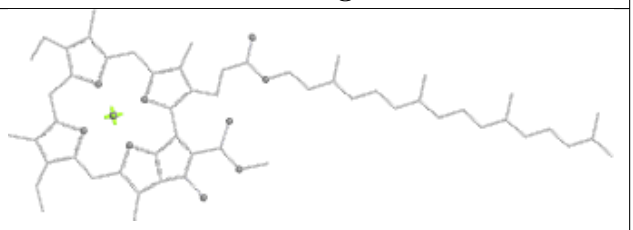
Bond lengths



Bond angles

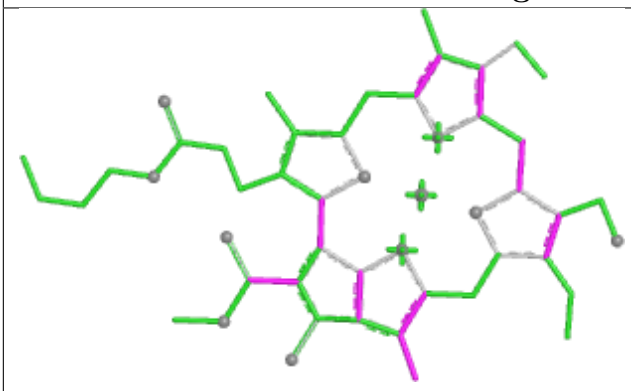


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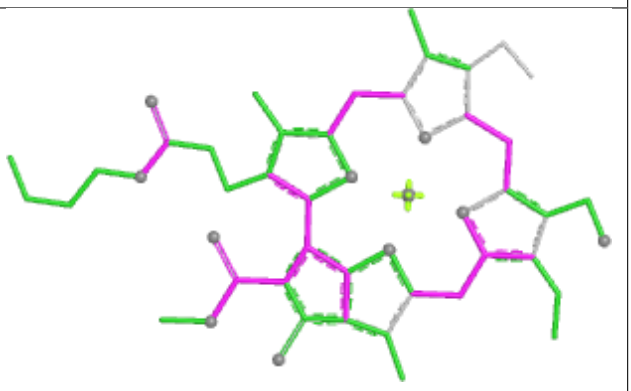


Rings

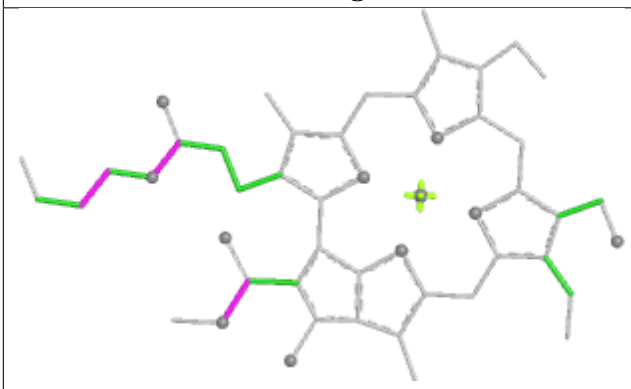
Ligand CHL Nn 311



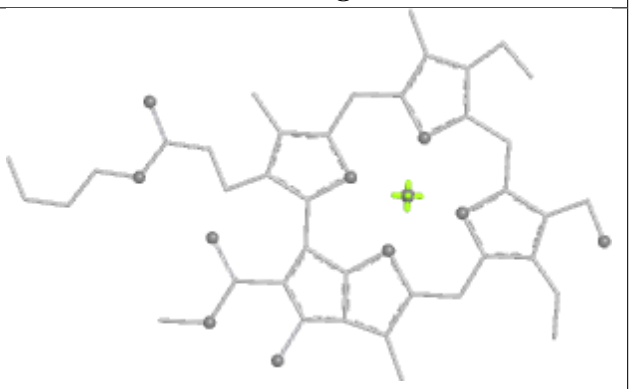
Bond lengths



Bond angles

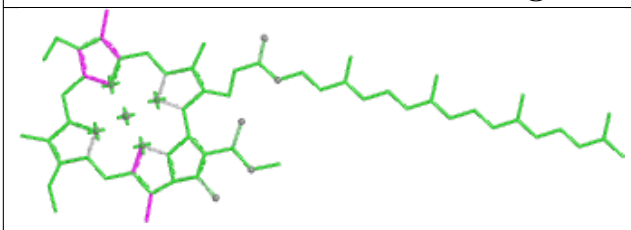


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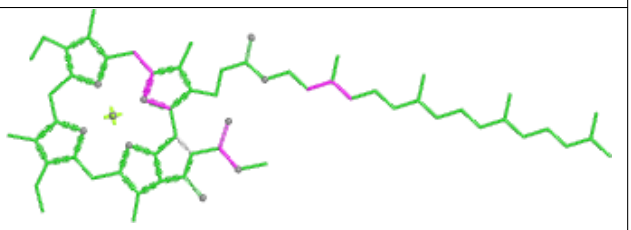


Rings

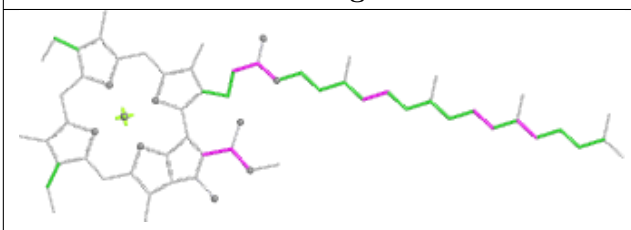
Ligand CLA b 605



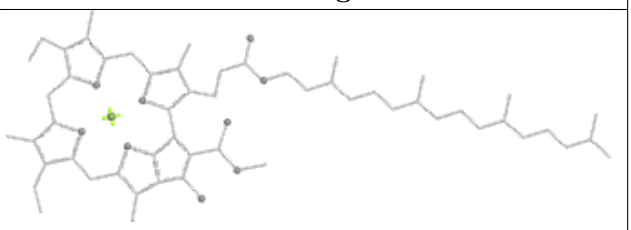
Bond lengths



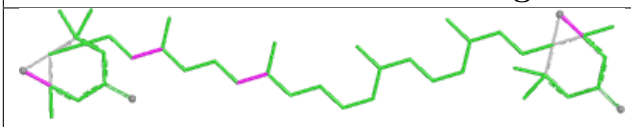
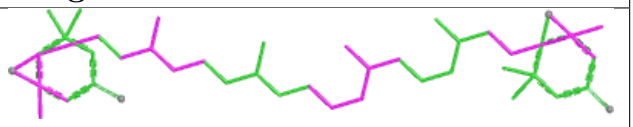
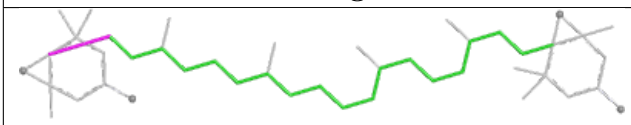
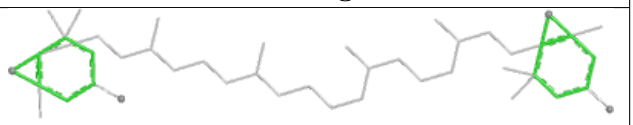
Bond angles

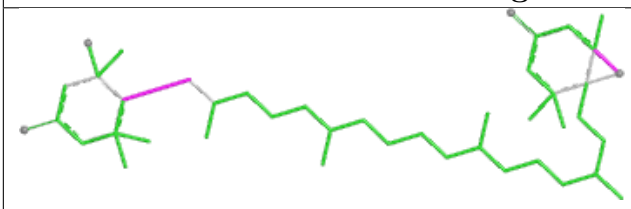
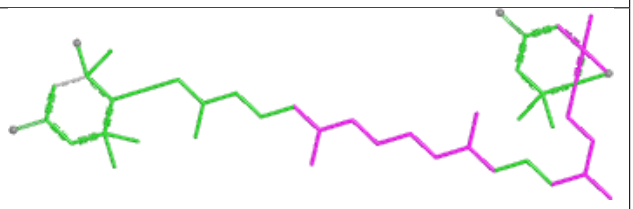
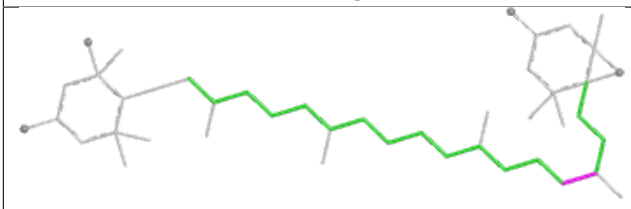
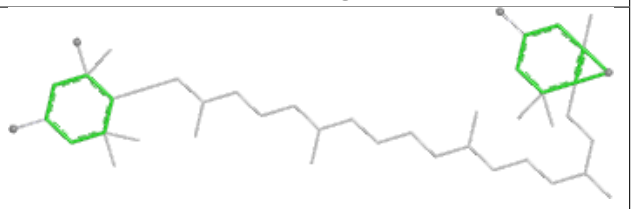


Torsions

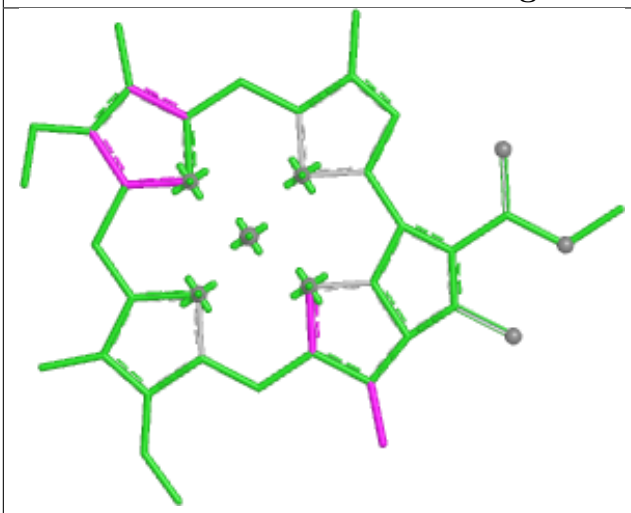


Rings

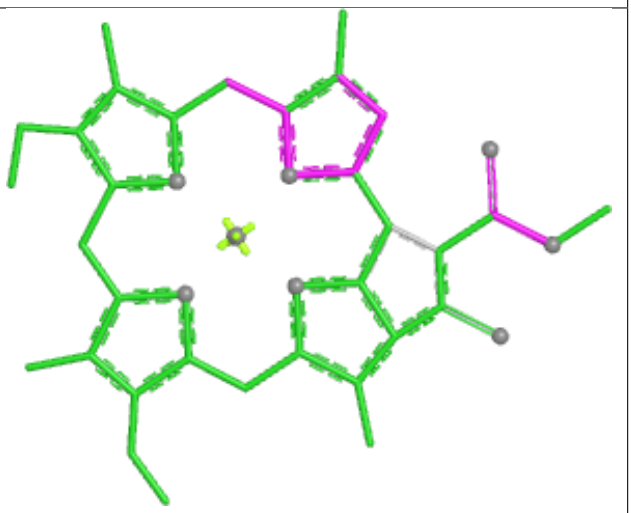
Ligand XAT Gg 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX Nn 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

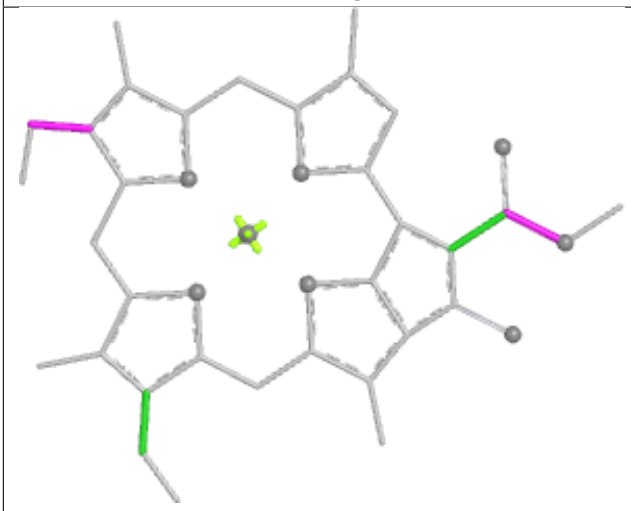
Ligand CLA 22 604



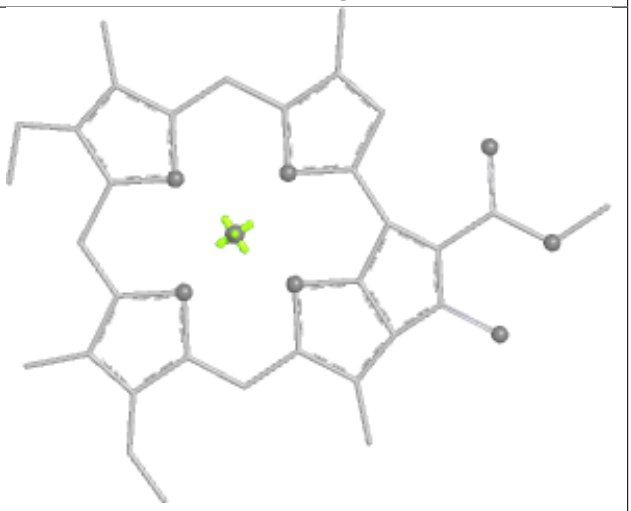
Bond lengths



Bond angles

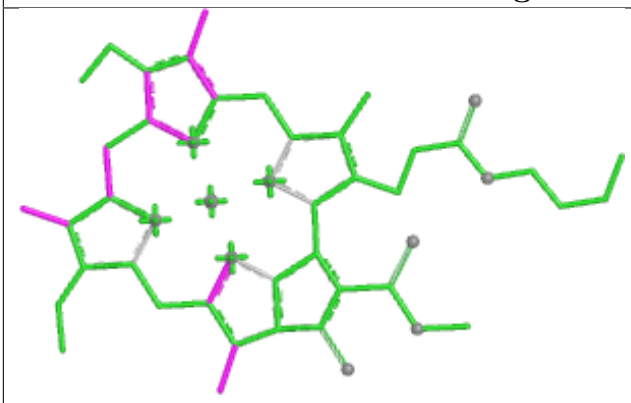


Torsions

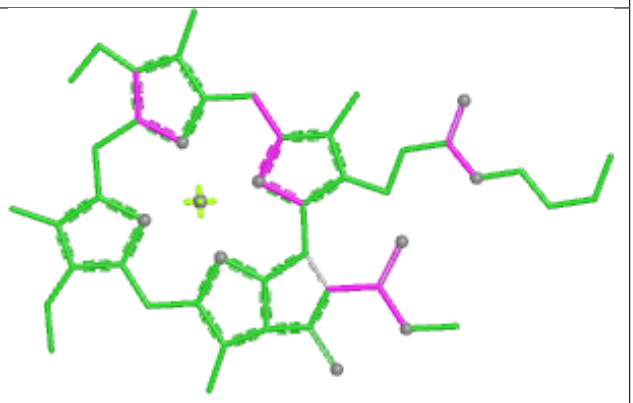


Rings

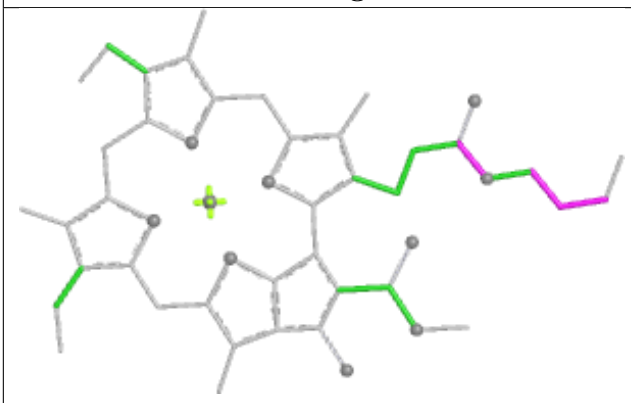
Ligand CLA Nn 314



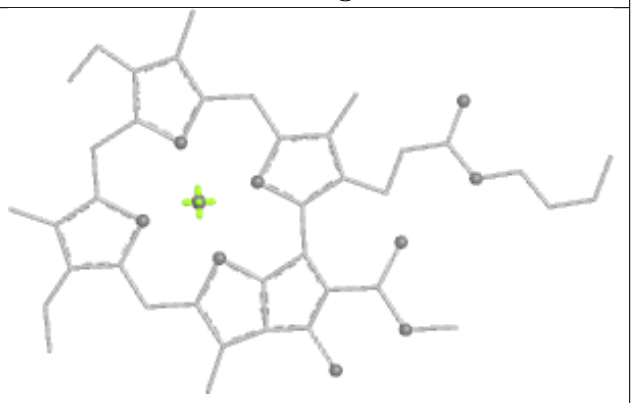
Bond lengths



Bond angles

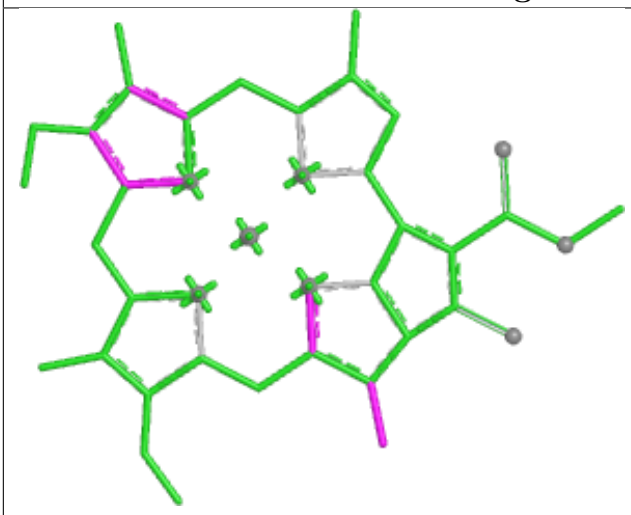


Torsions

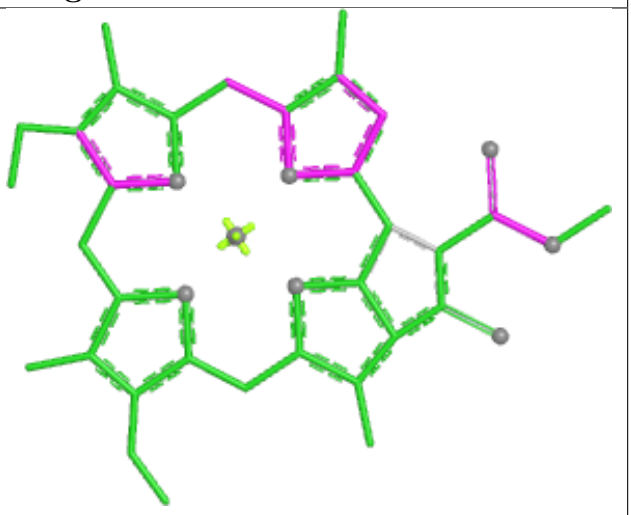


Rings

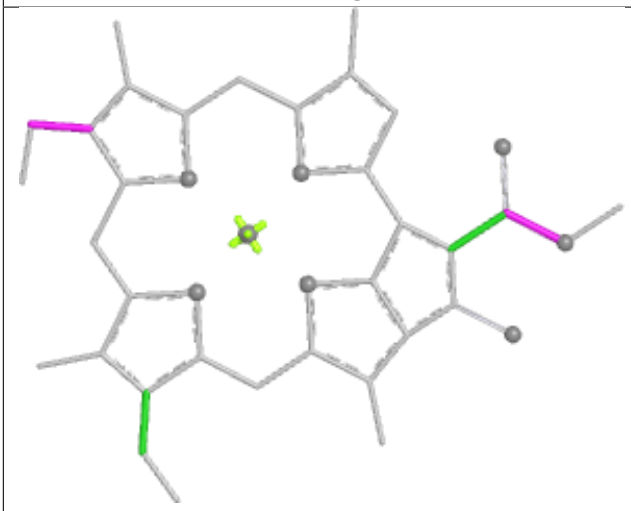
Ligand CLA Gg 314



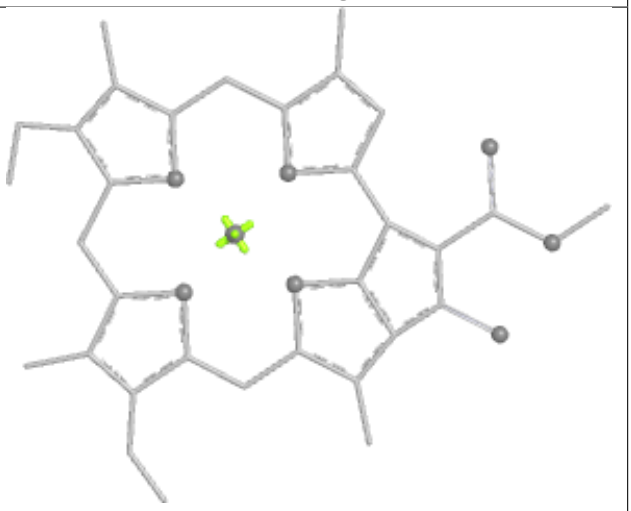
Bond lengths



Bond angles

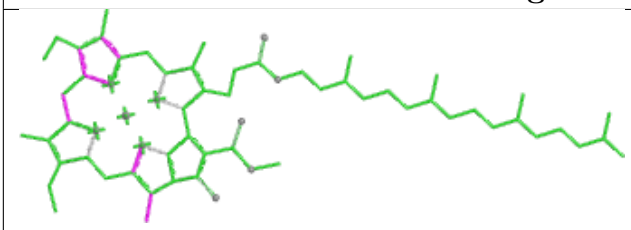


Torsions

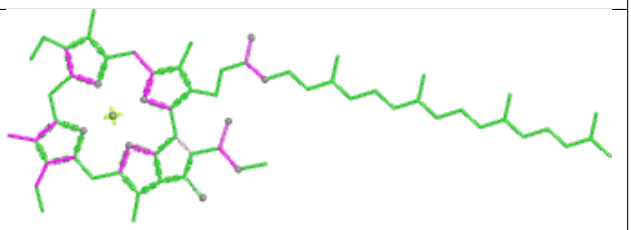


Rings

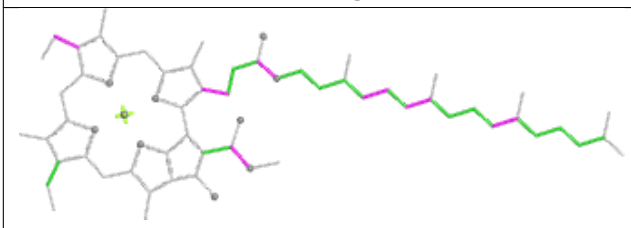
Ligand CLA n 610



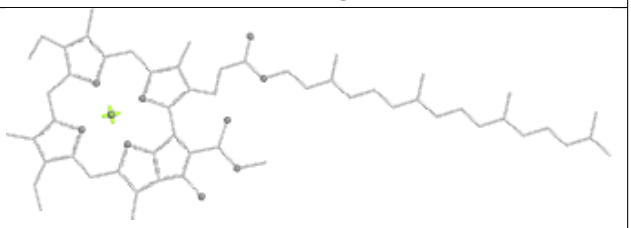
Bond lengths



Bond angles

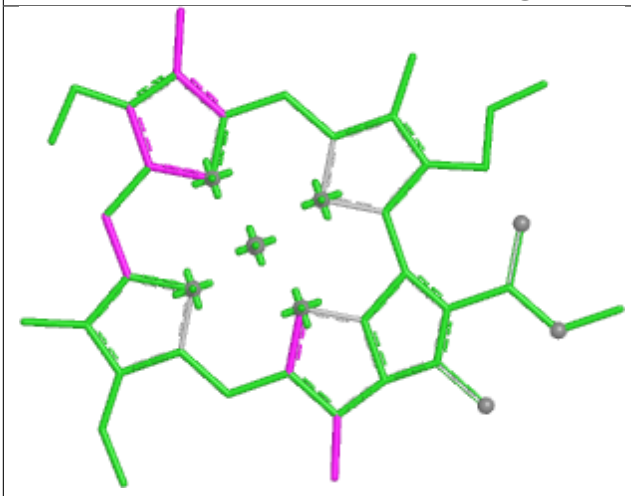


Torsions

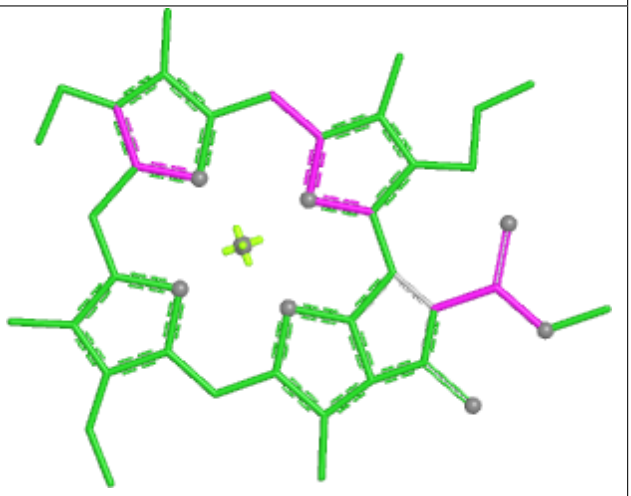


Rings

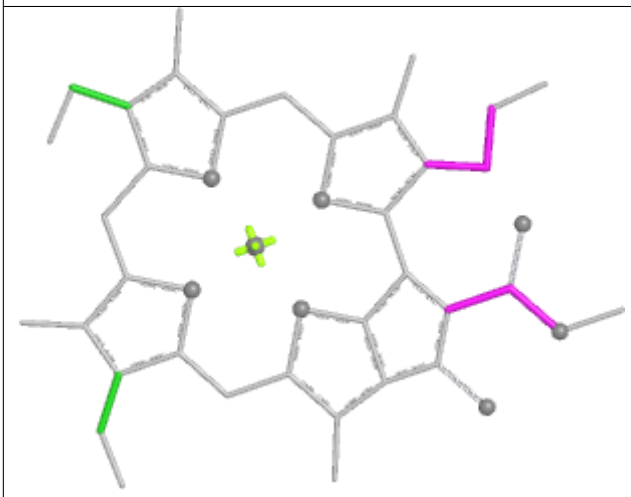
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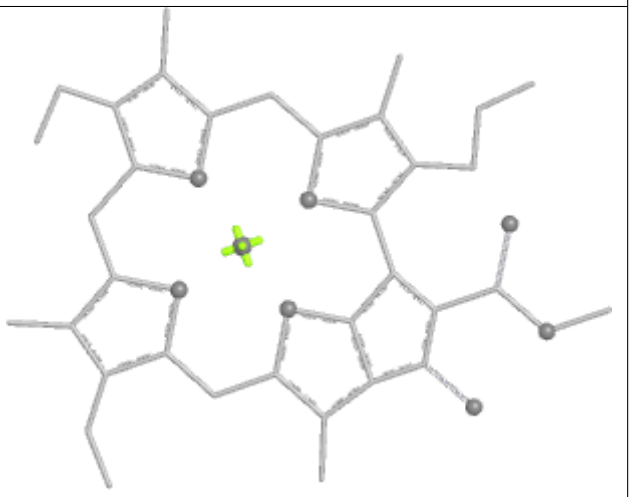
Bond lengths



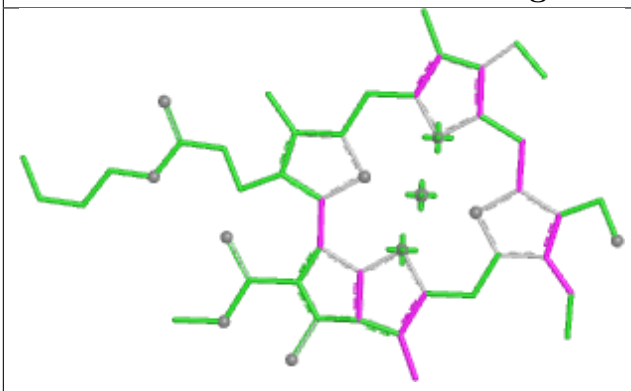
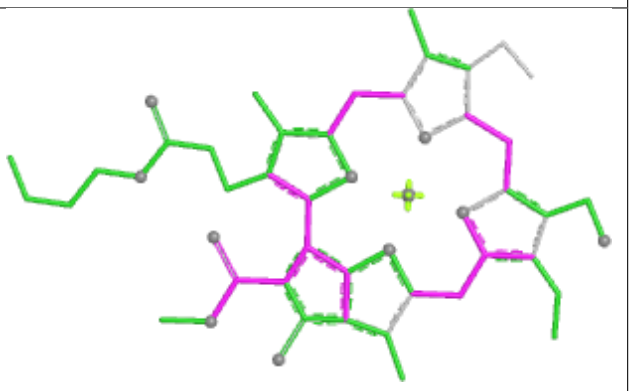
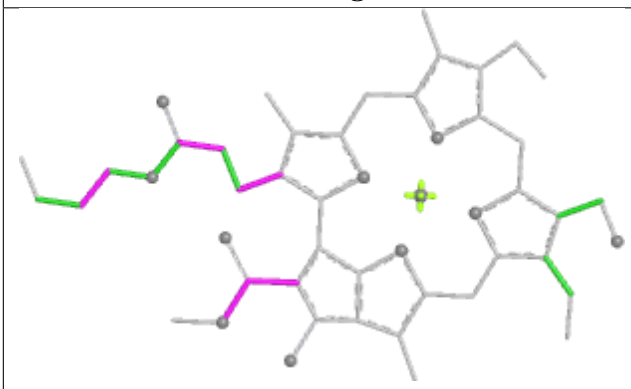
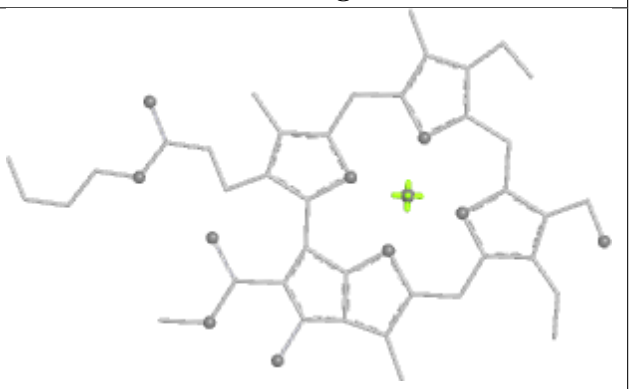
Bond angles

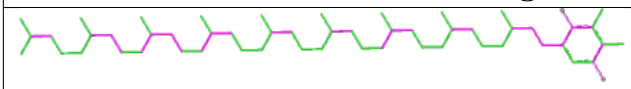
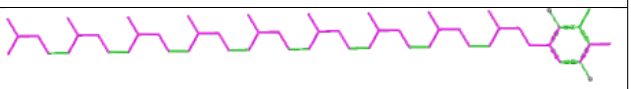
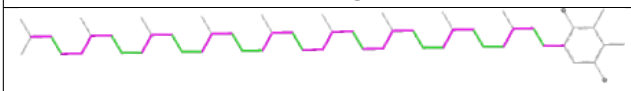
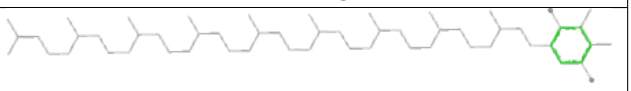


Torsions

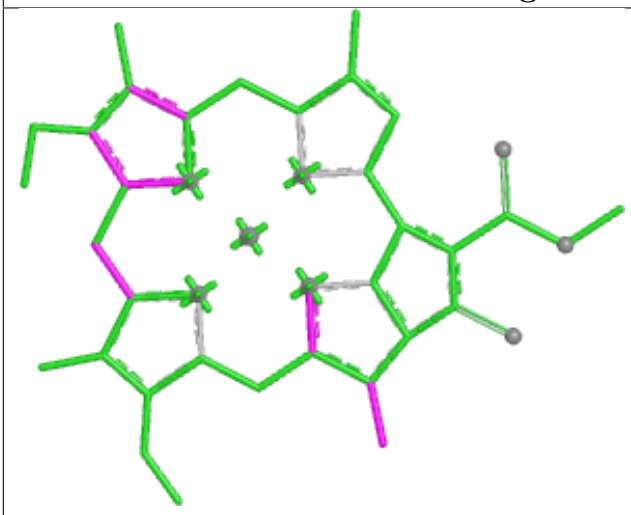


Rings

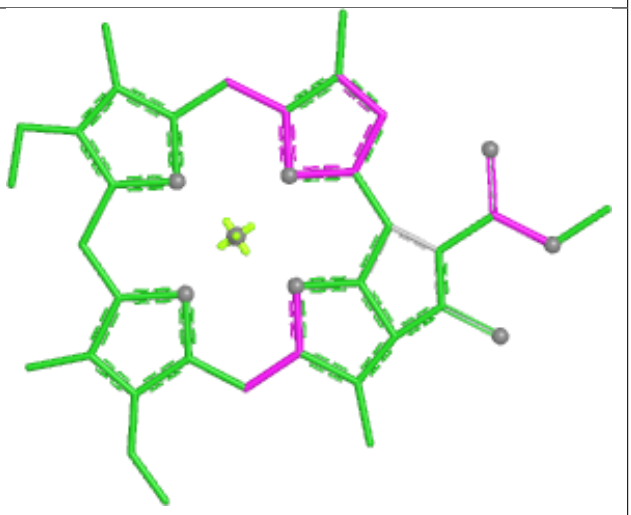
Ligand CHL r 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 Dd 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

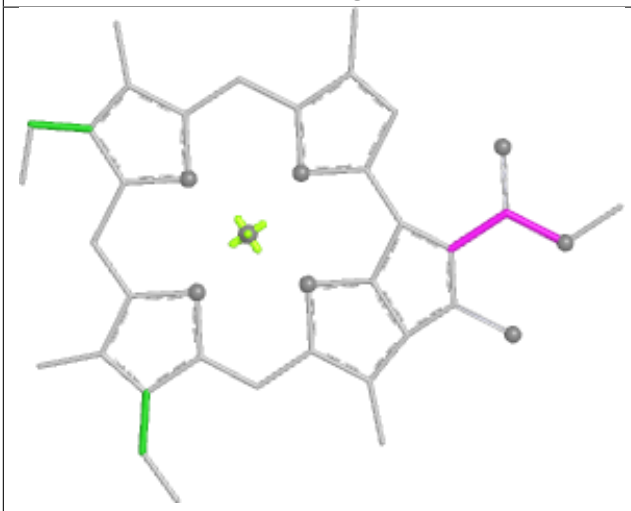
Ligand CLA 33 610



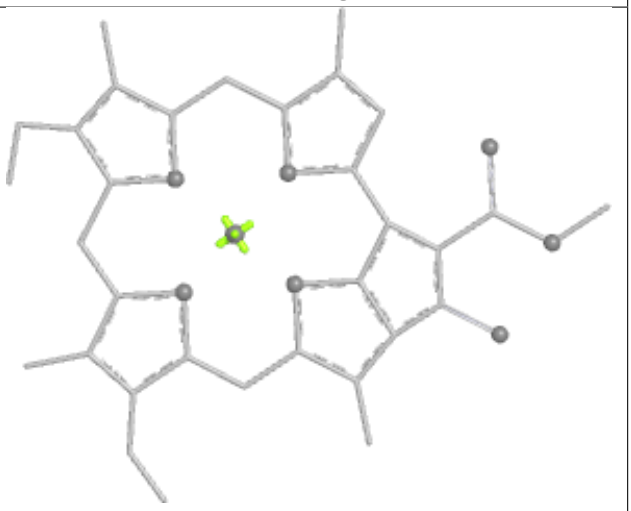
Bond lengths



Bond angles

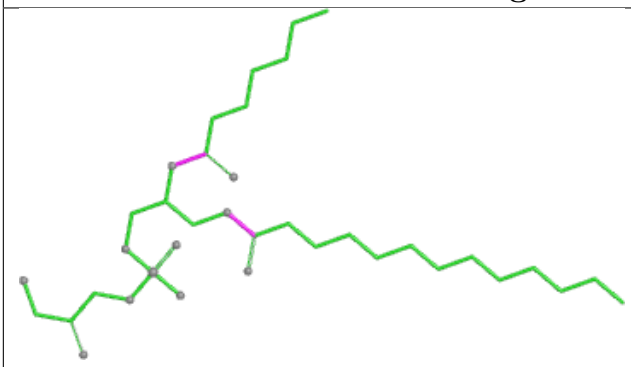


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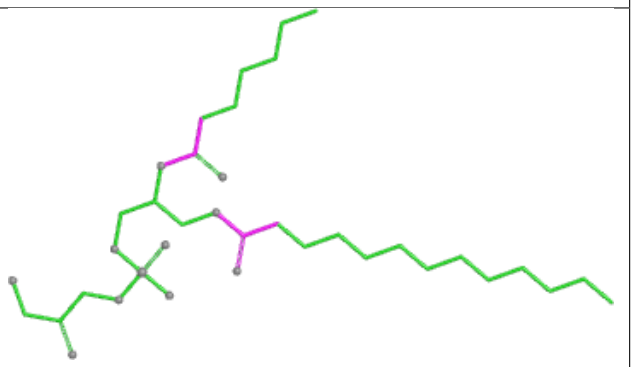


Rings

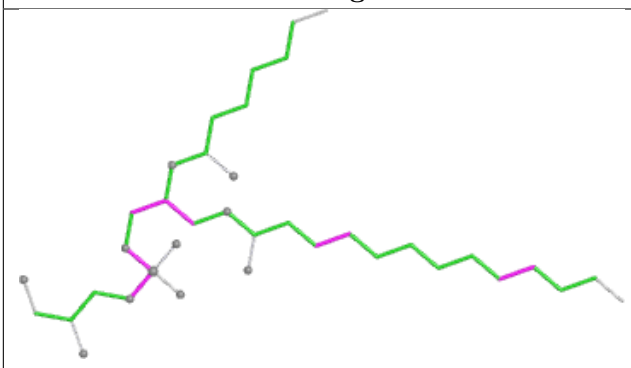
Ligand LHG CC 523



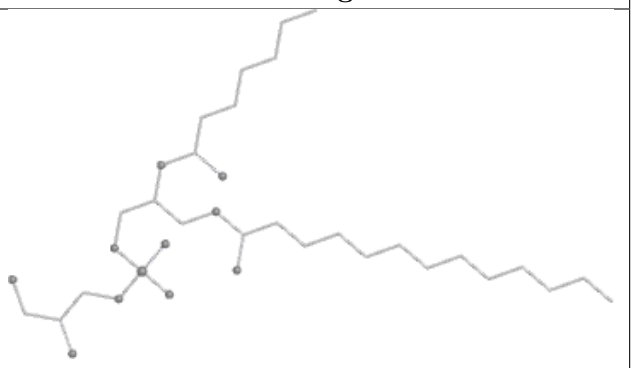
Bond lengths



Bond angles

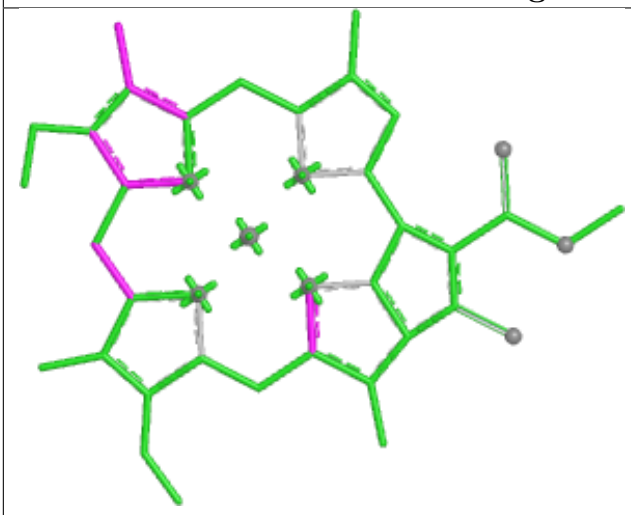


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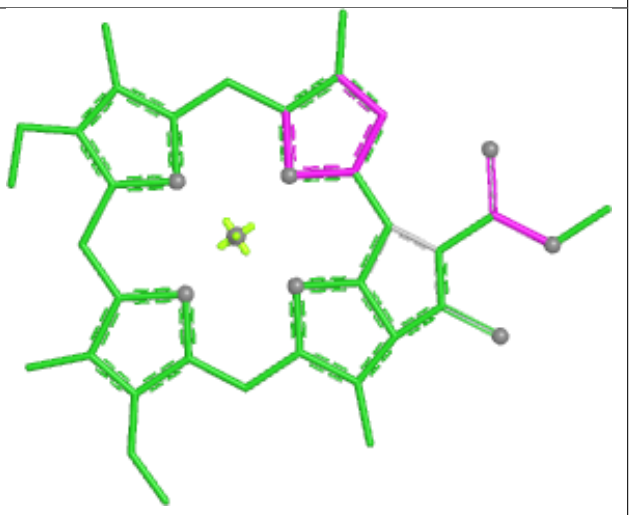


Rings

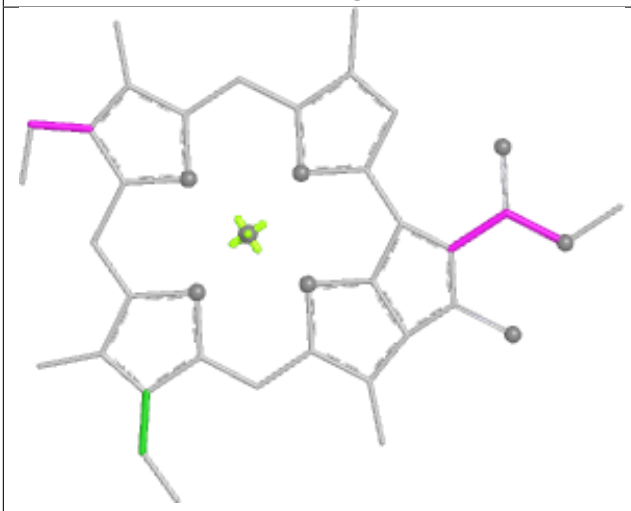
Ligand CLA 2 609



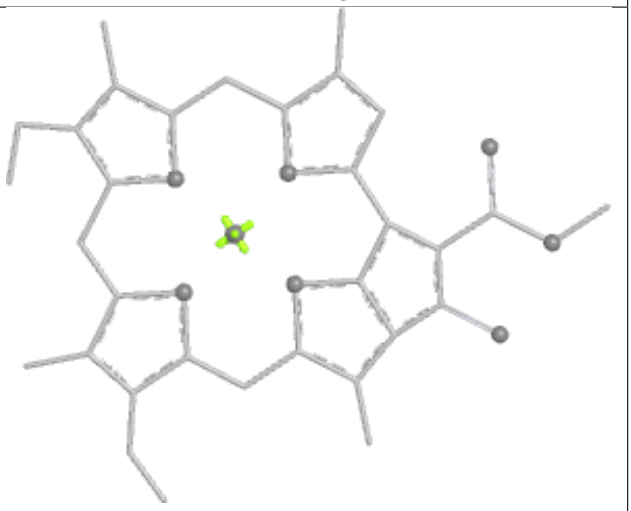
Bond lengths



Bond angles

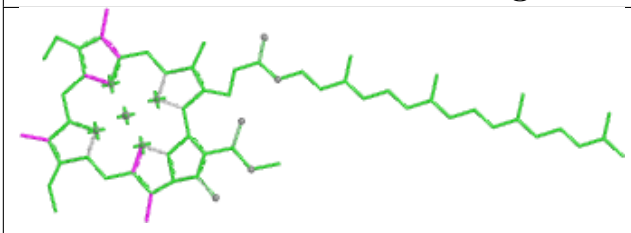


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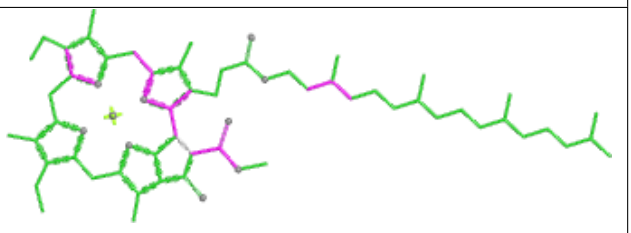


Rings

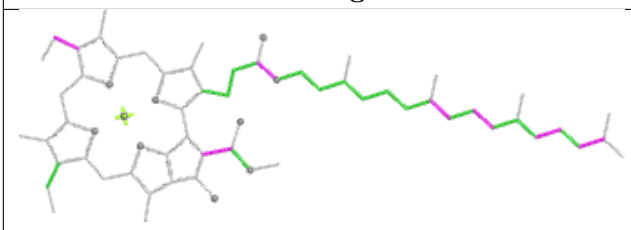
Ligand CLA CC 508



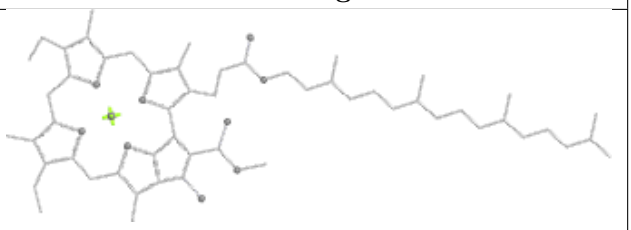
Bond lengths



Bond angles

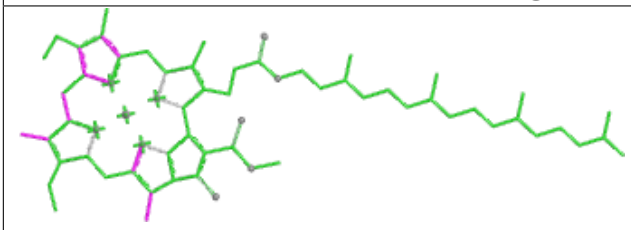


Torsions

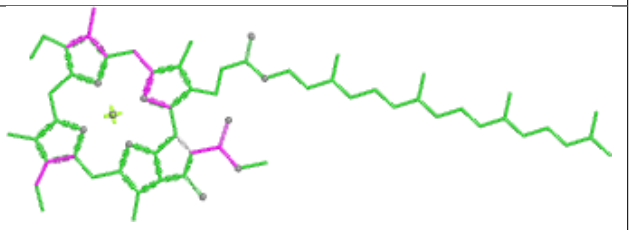


Rings

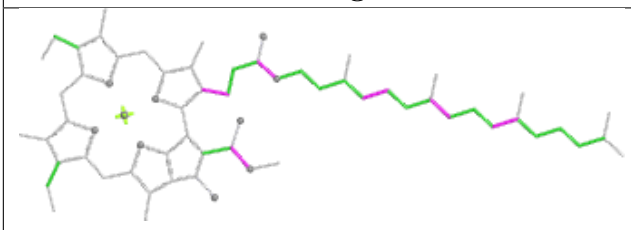
Ligand CLA d 401



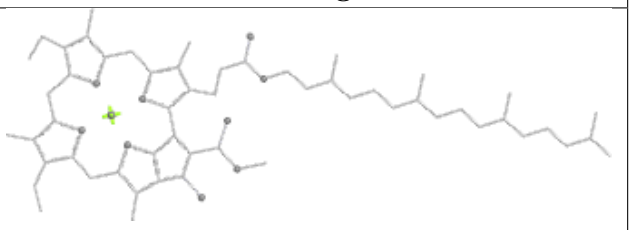
Bond lengths



Bond angles

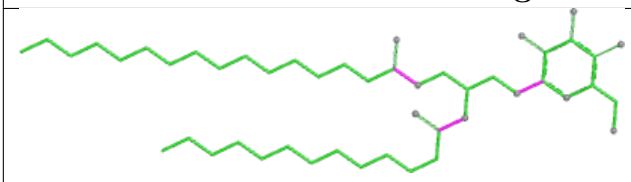


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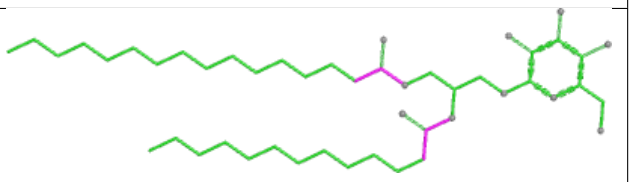


Rings

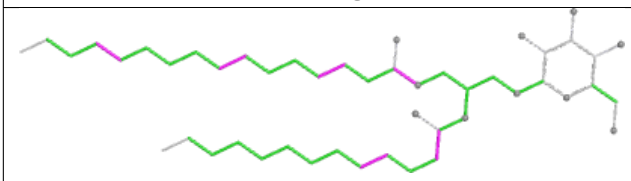
Ligand LMG W 201



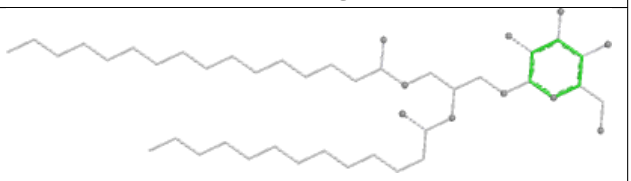
Bond lengths



Bond angles

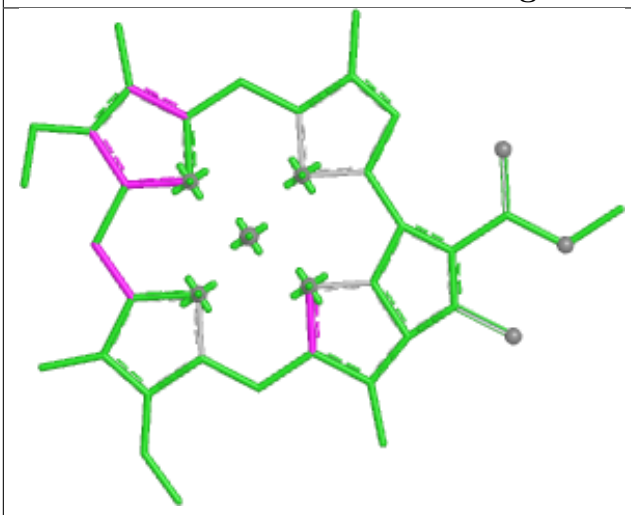


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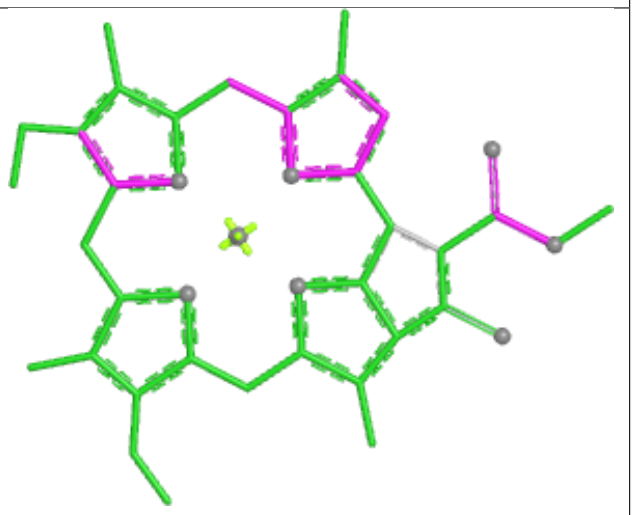


Rings

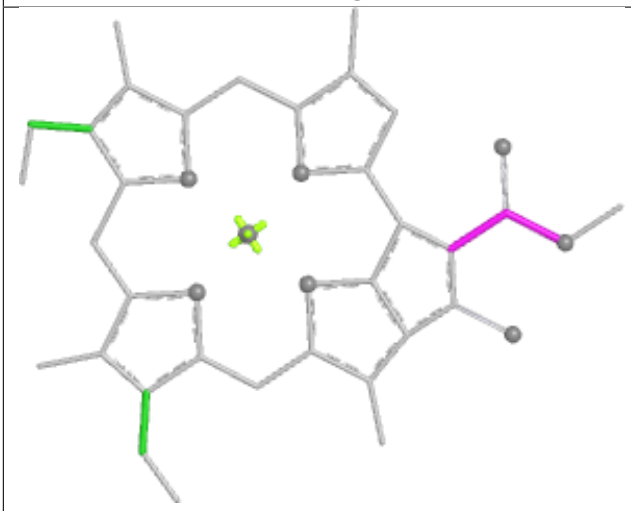
Ligand CLA 11 602



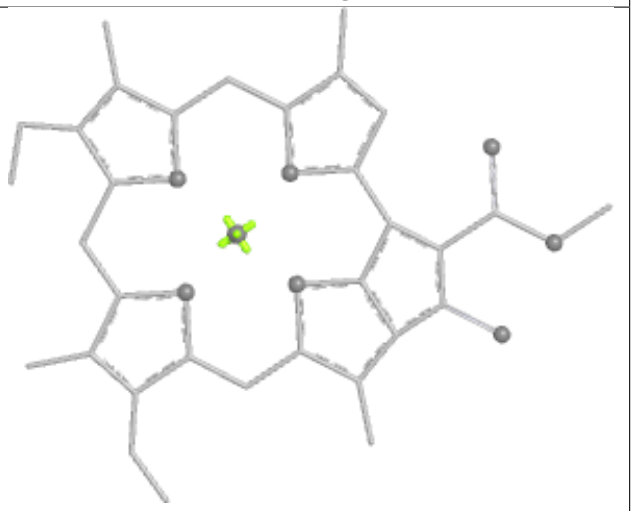
Bond lengths



Bond angles

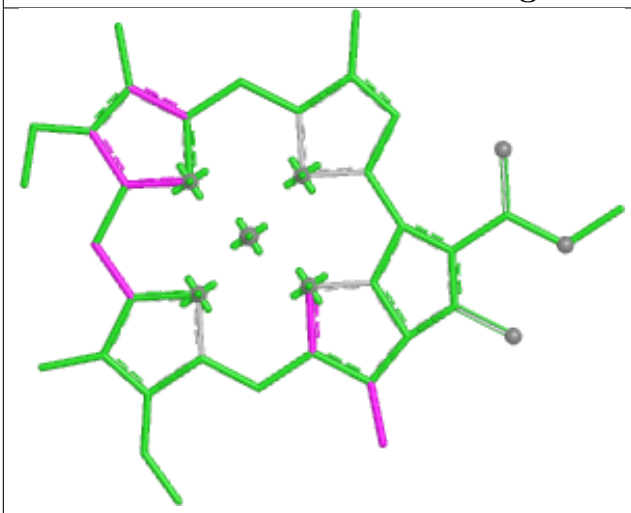


Torsions

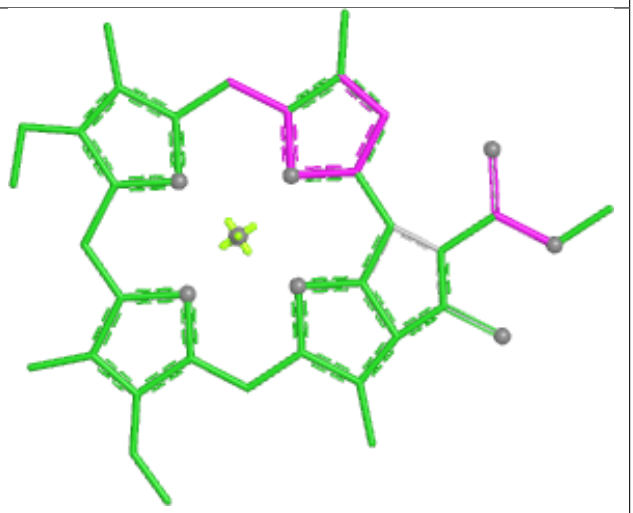


Rings

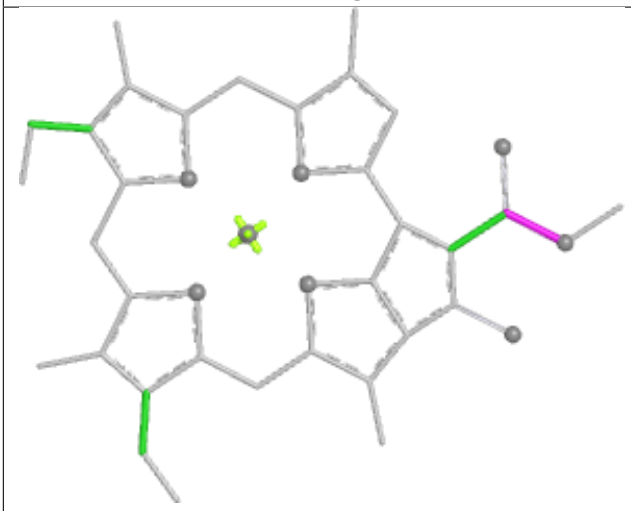
Ligand CLA 11 611



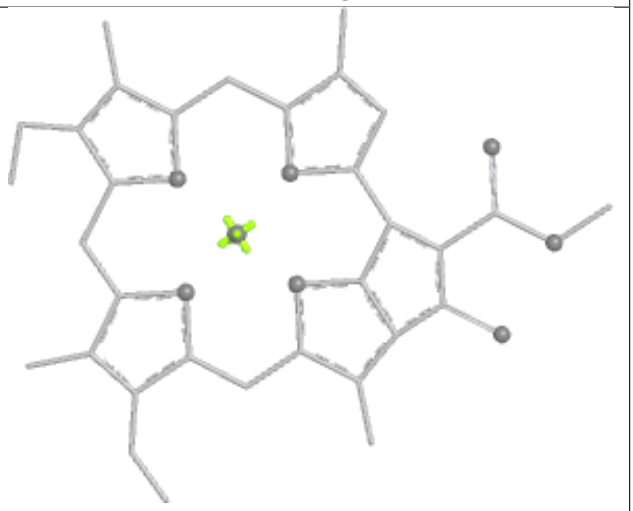
Bond lengths



Bond angles

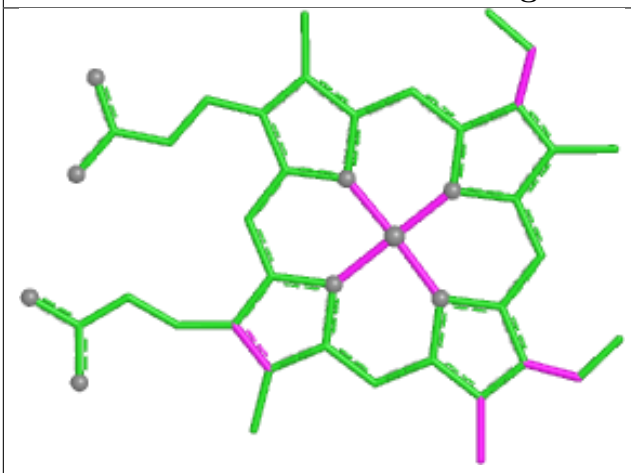


Torsions

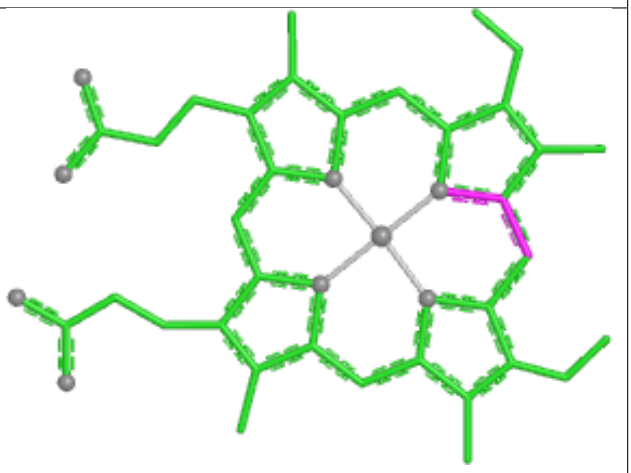


Rings

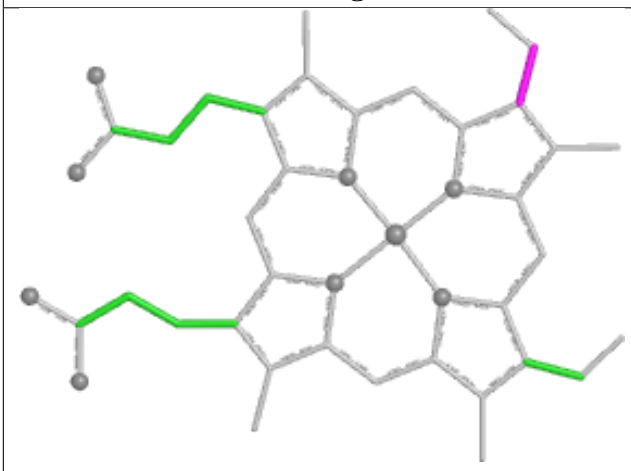
Ligand HEM E 101



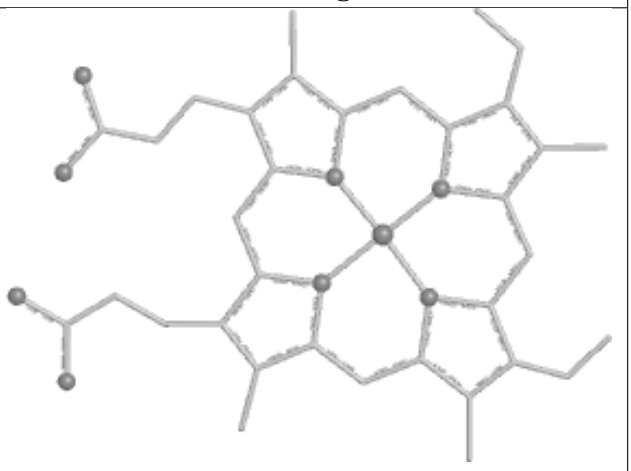
Bond lengths



Bond angles

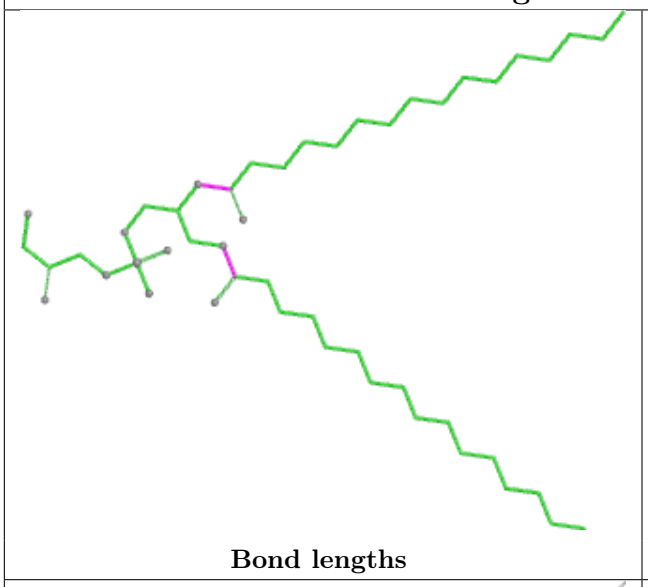


Torsions

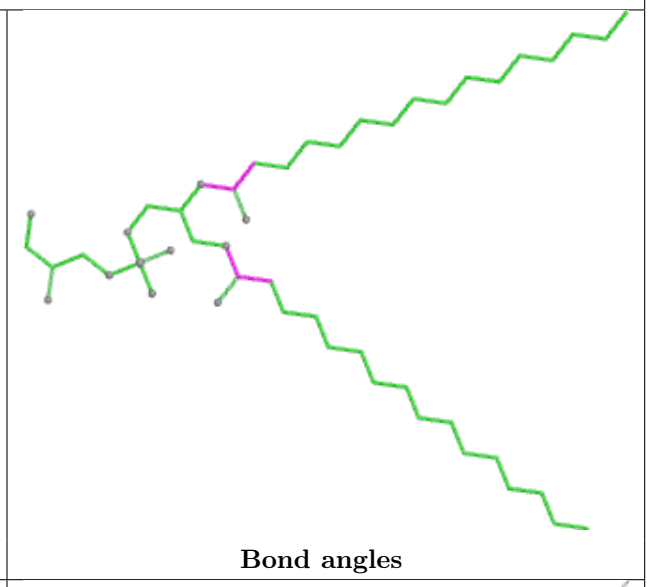


Rings

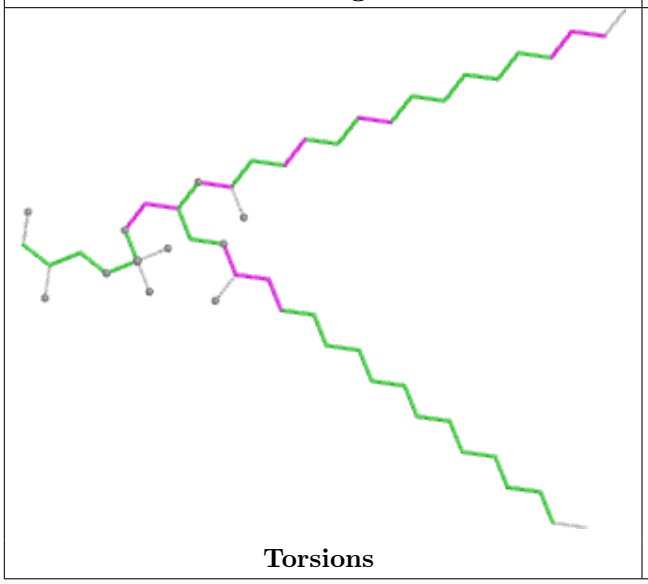
Ligand LHG Nn 310



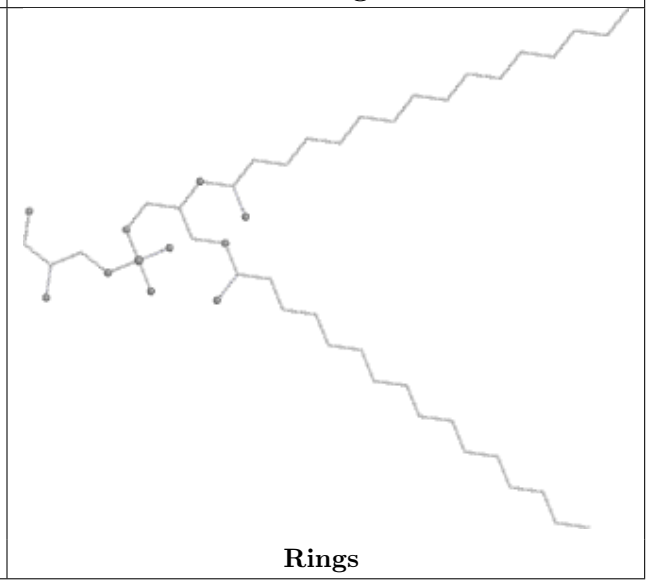
Bond lengths



Bond angles

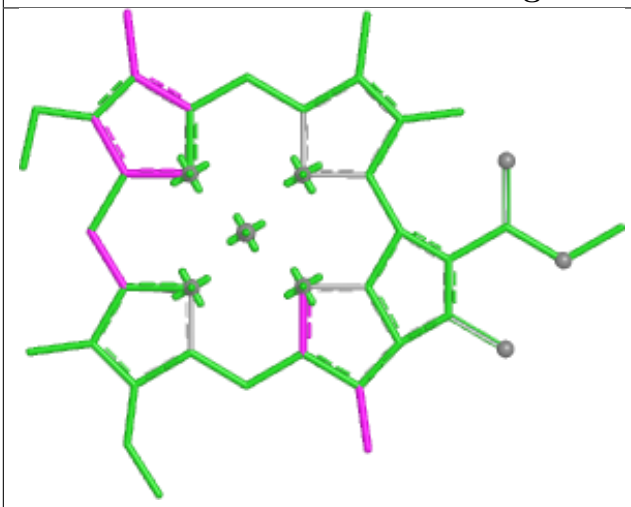


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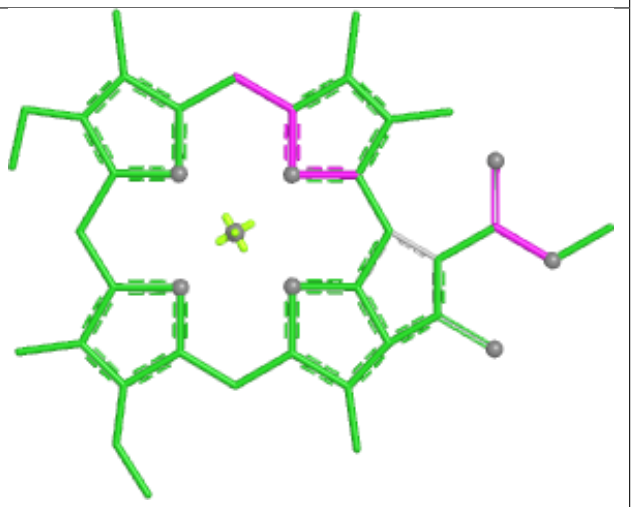


Rings

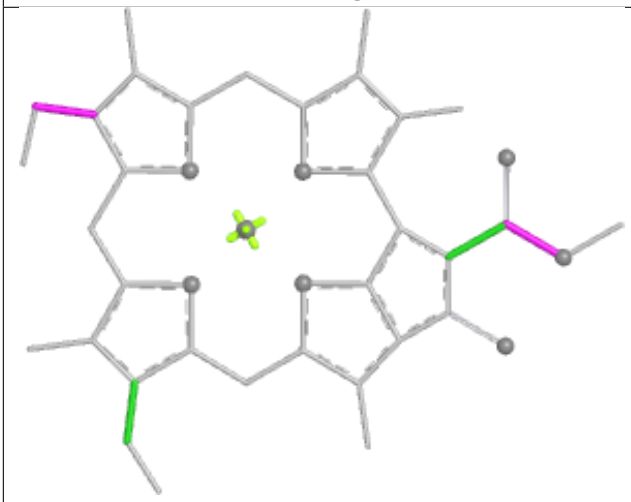
Ligand CLA N 614



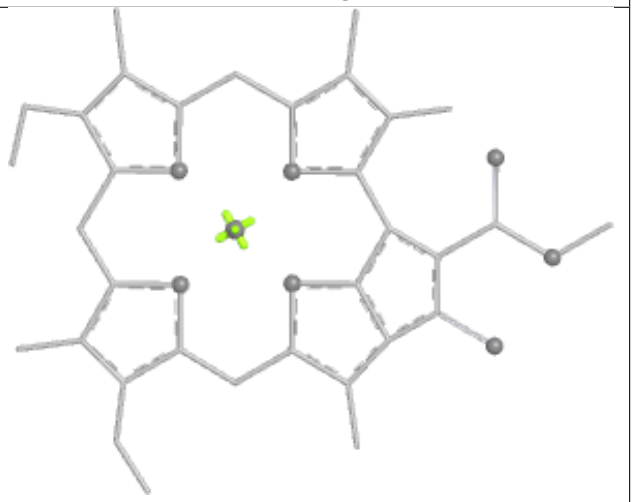
Bond lengths



Bond angles

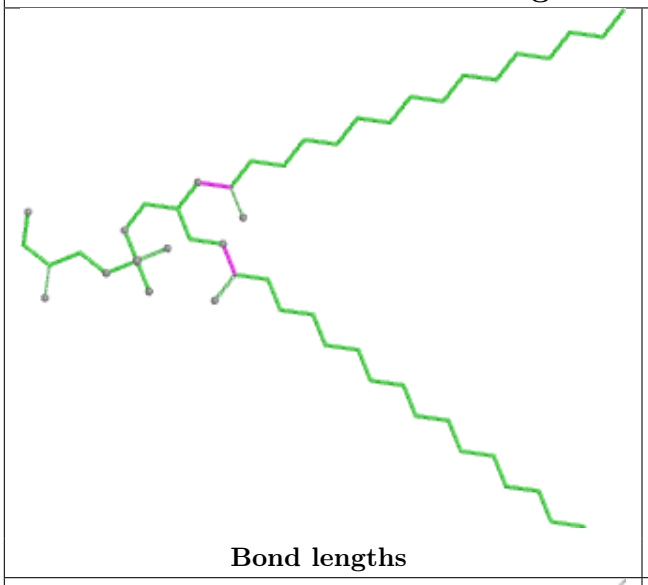


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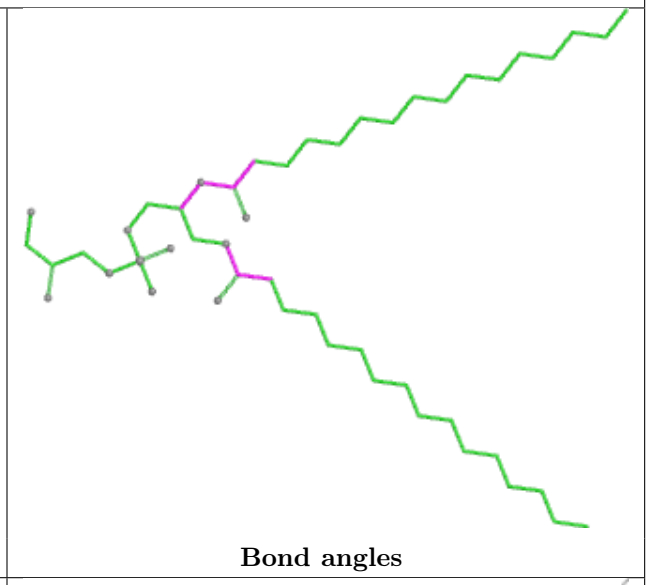


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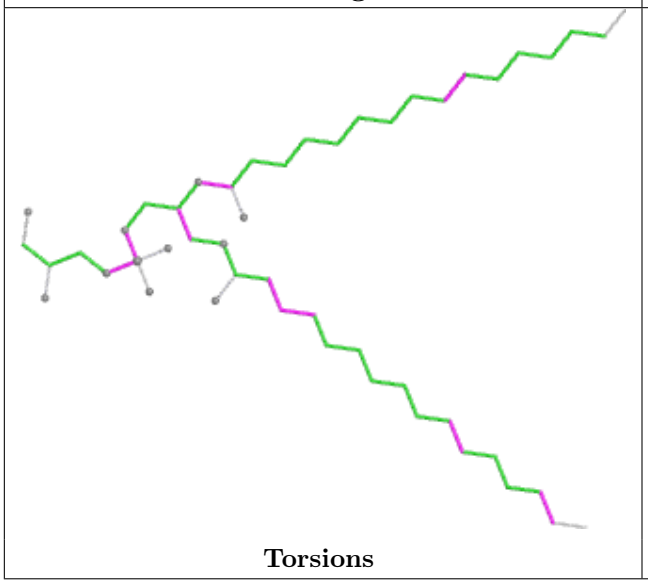
Ligand LHG l 101



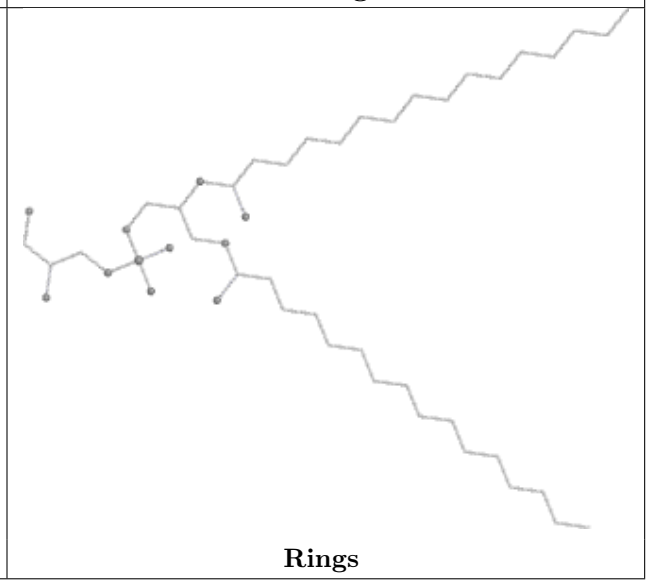
Bond lengths



Bond angles

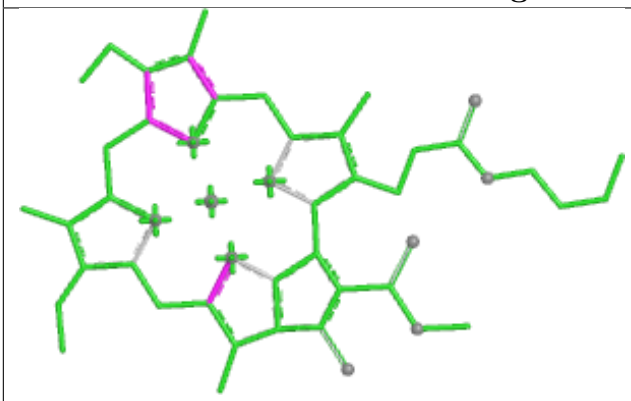


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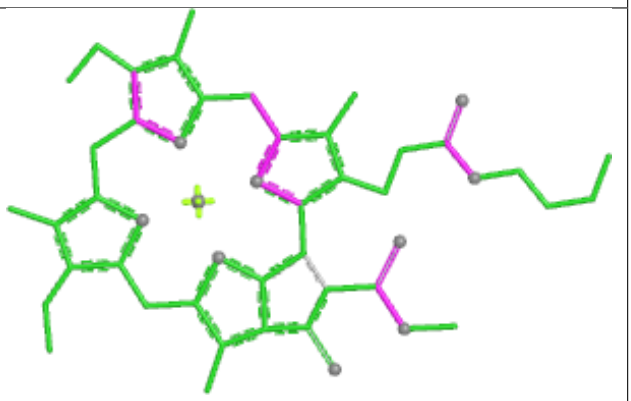


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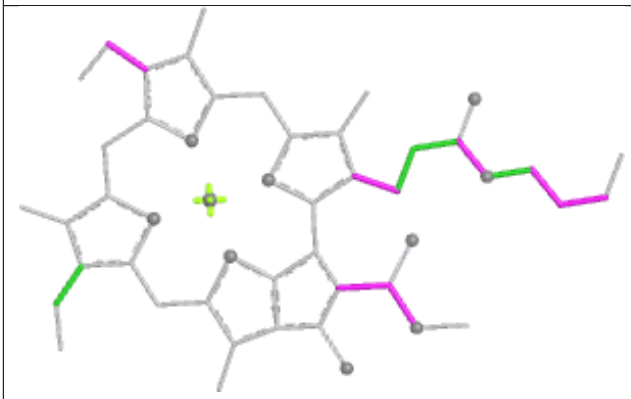
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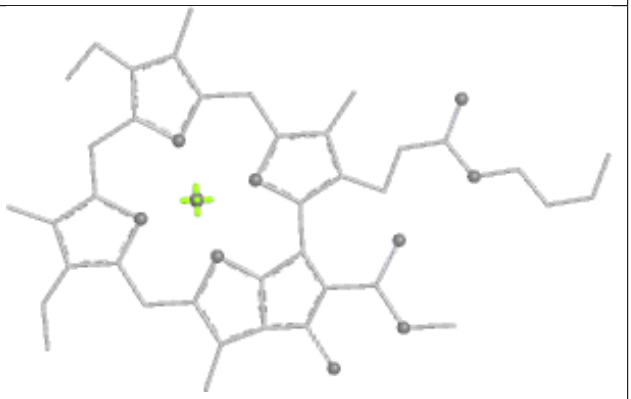
Bond lengths



Bond angles



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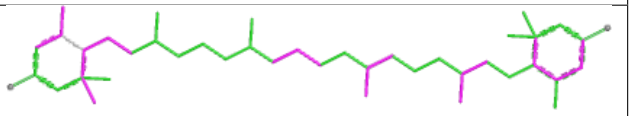


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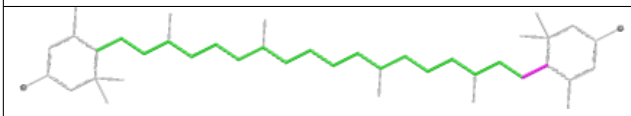
Ligand LUT r 614



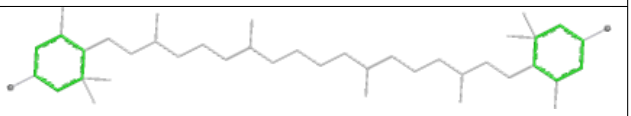
Bond lengths



Bond angles

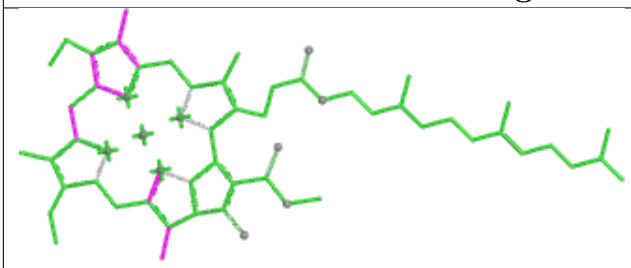


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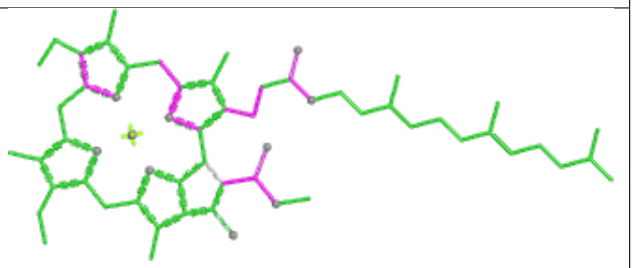


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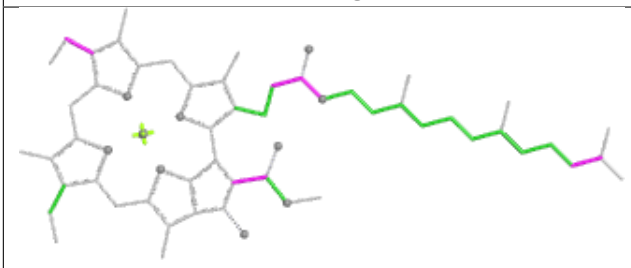
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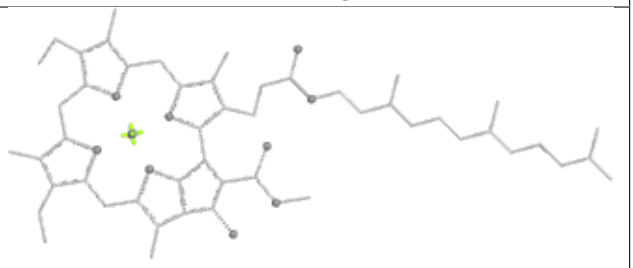
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Bond angles

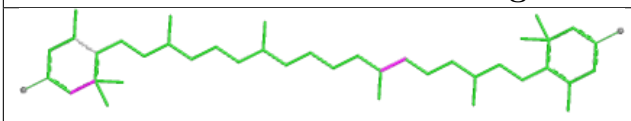


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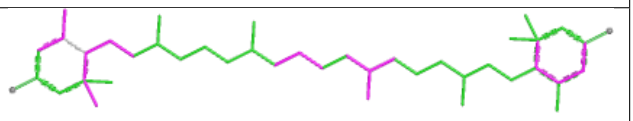


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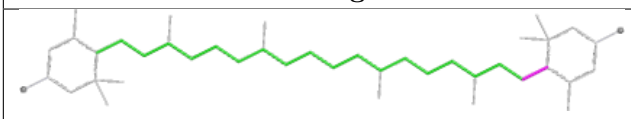
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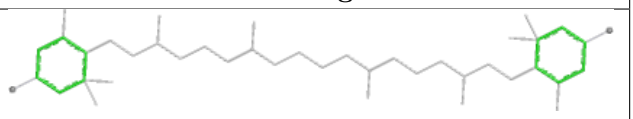
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Bond angles

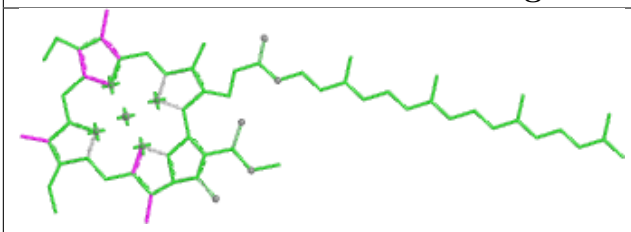


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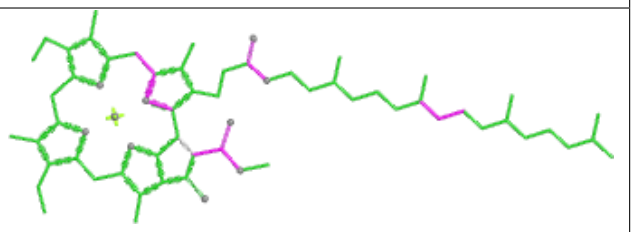


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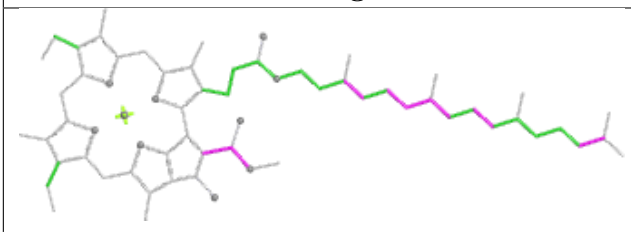
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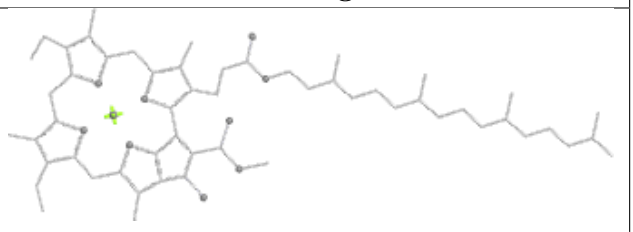
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Bond angles

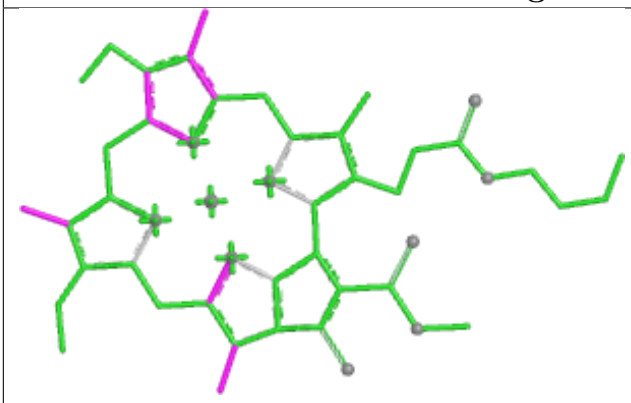


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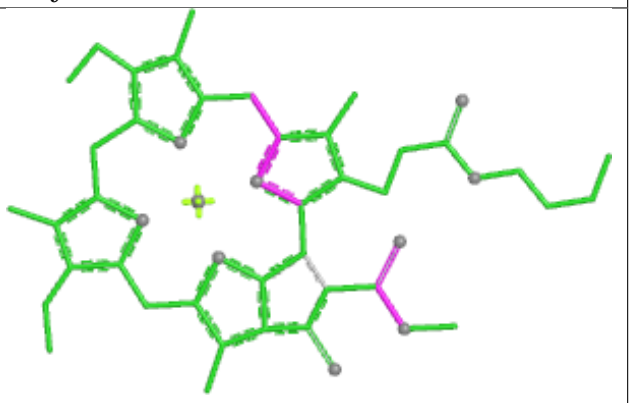


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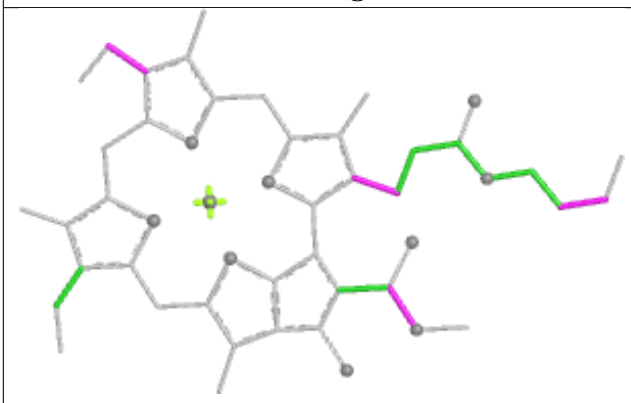
Ligand CLA y 305



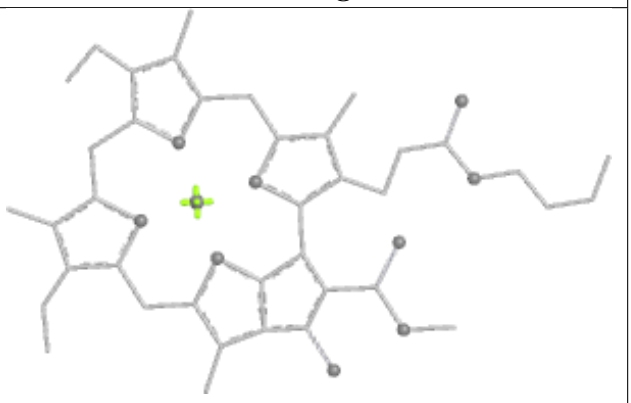
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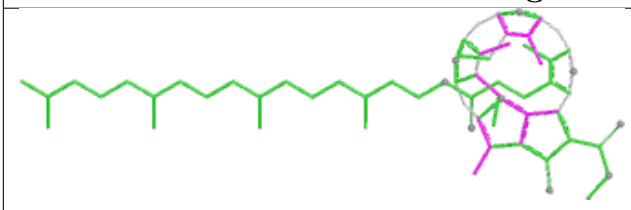


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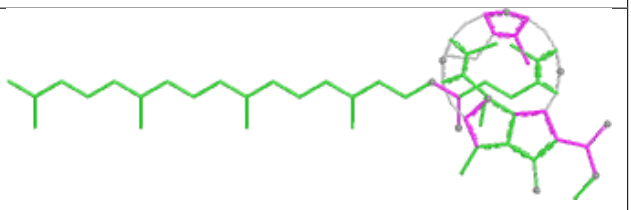


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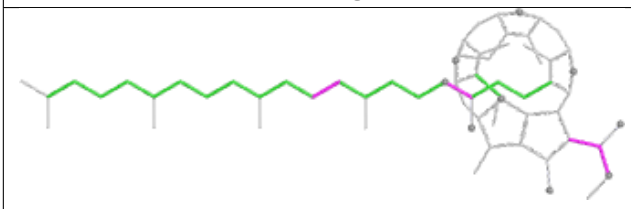
Ligand PHO a 408



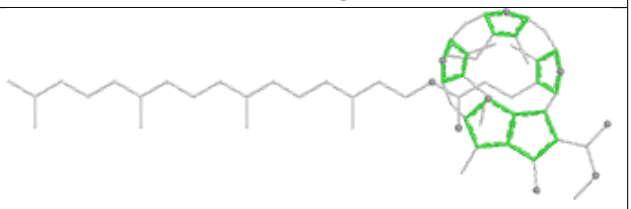
Bond lengths



Bond angles

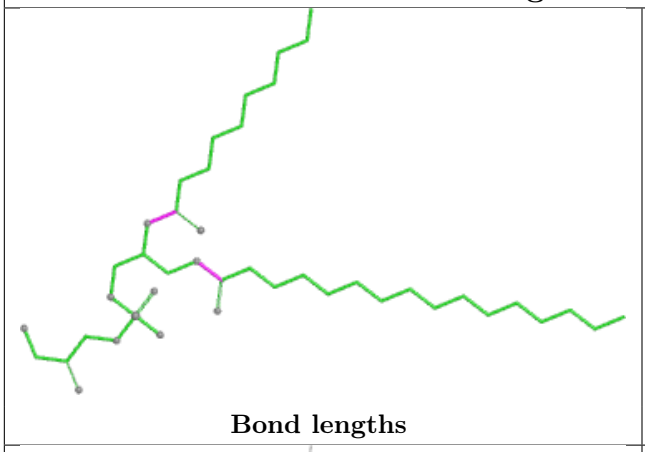


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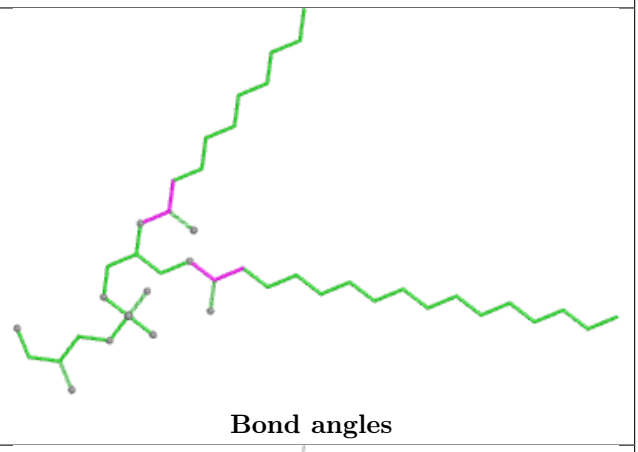


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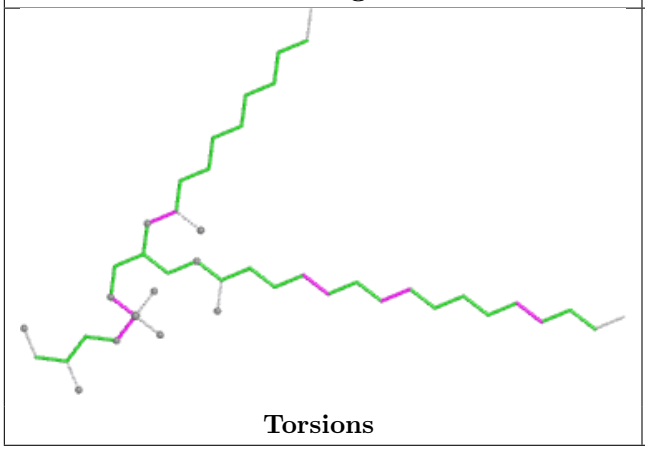
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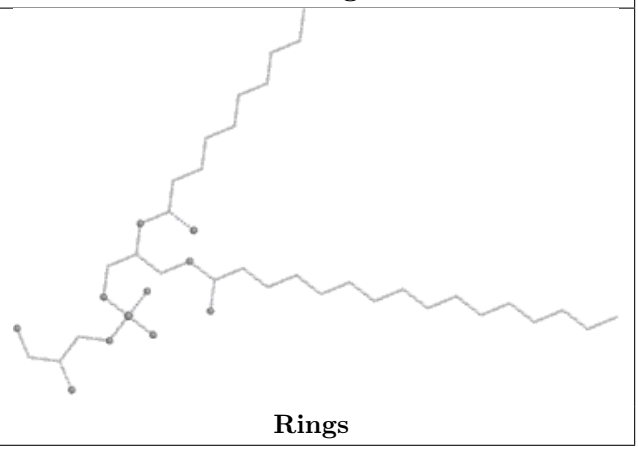
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Bond angles

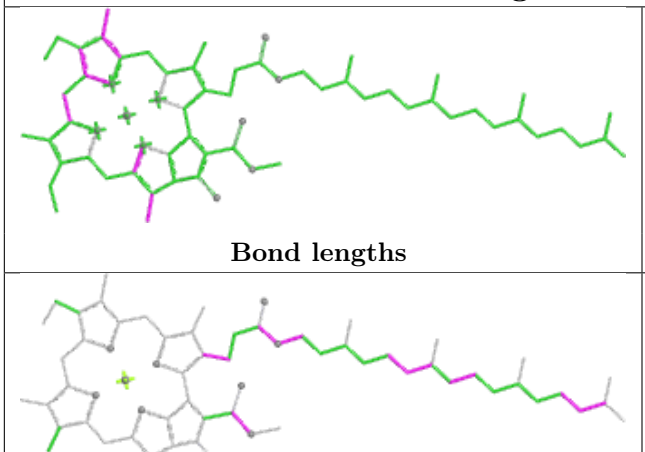


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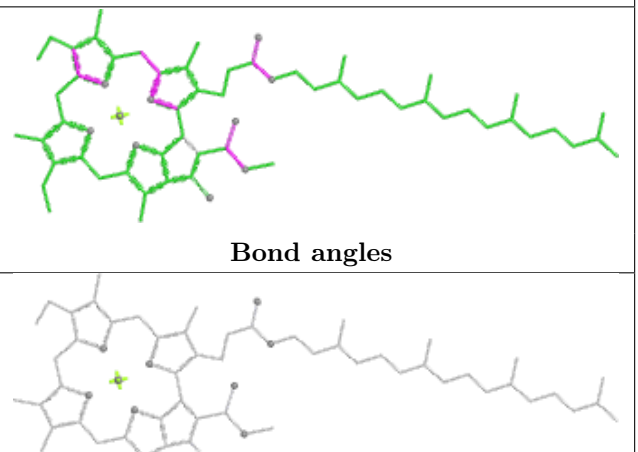


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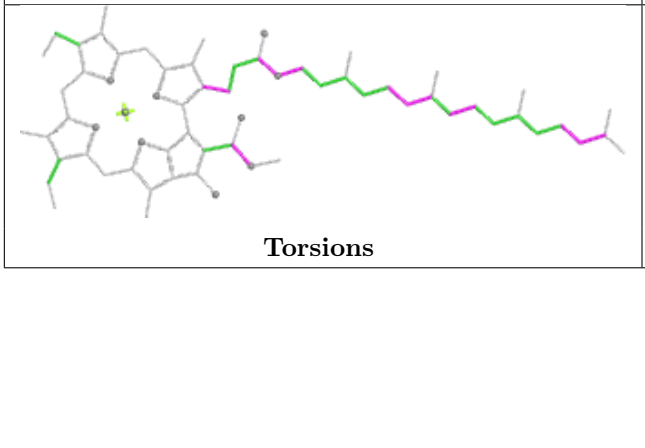
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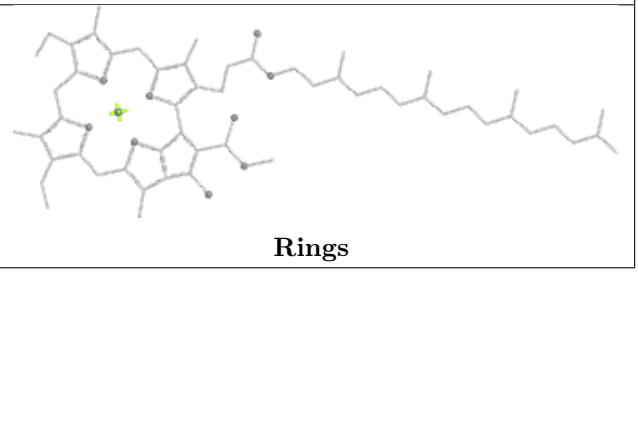
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Bond angles

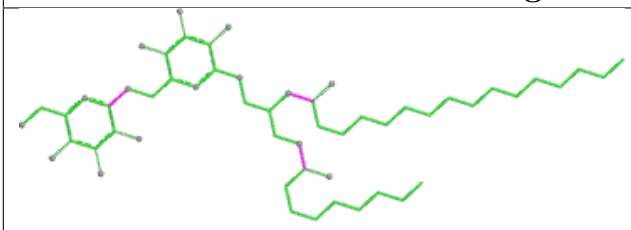


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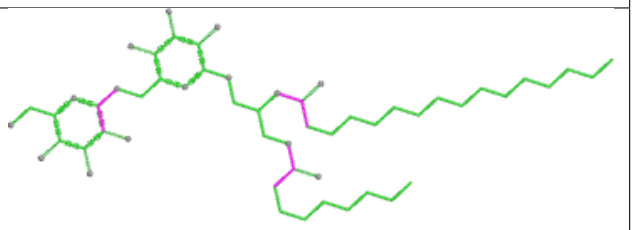


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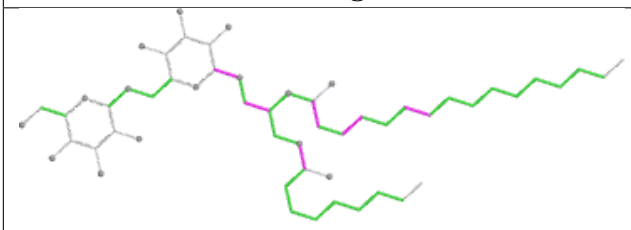
Ligand DGD a 415



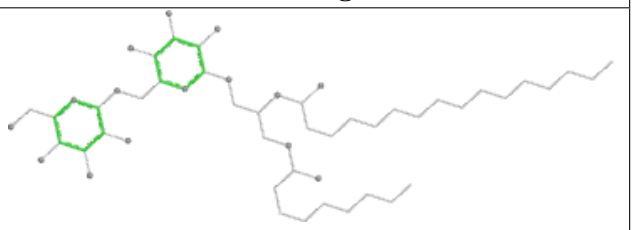
Bond lengths



Bond angles

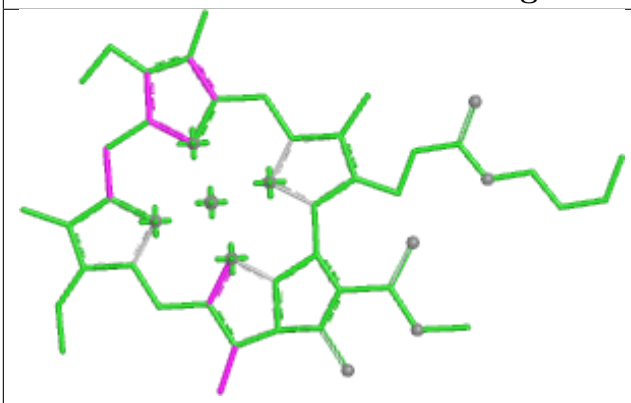


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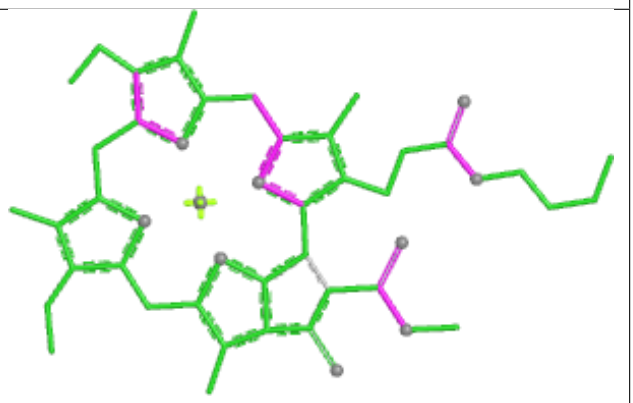


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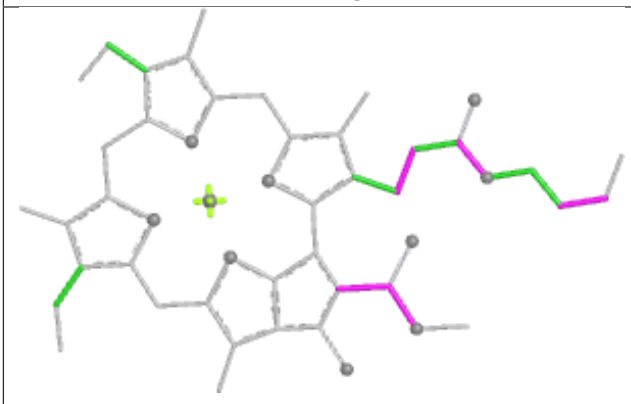
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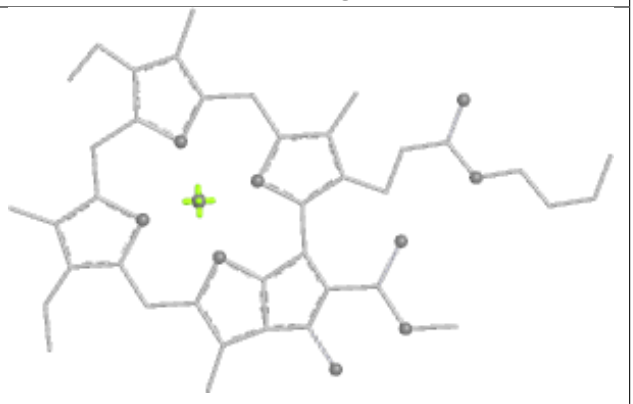
Bond lengths



Bond angles

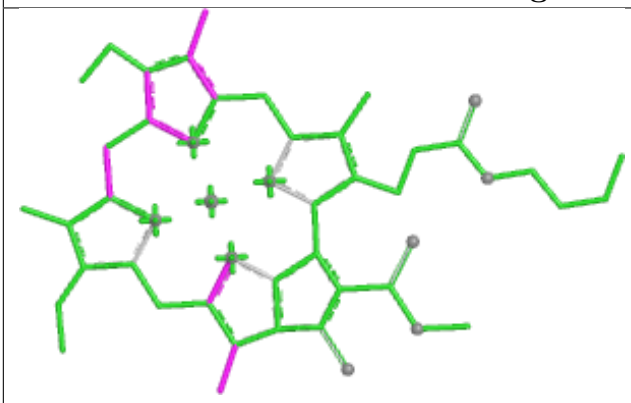


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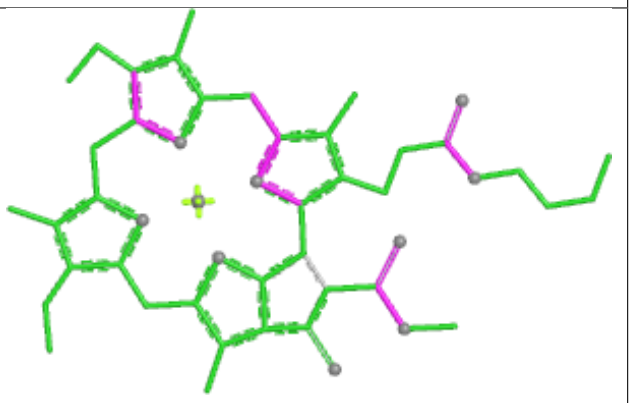


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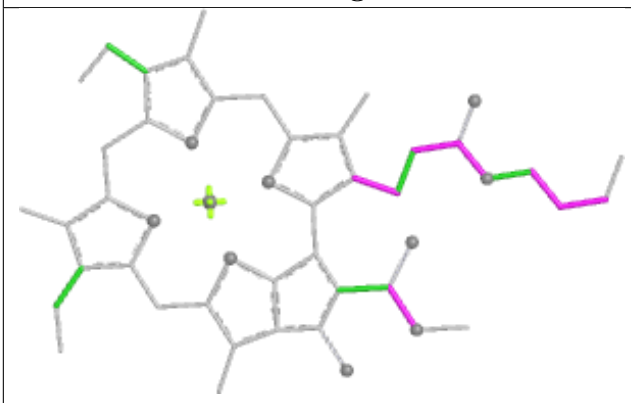
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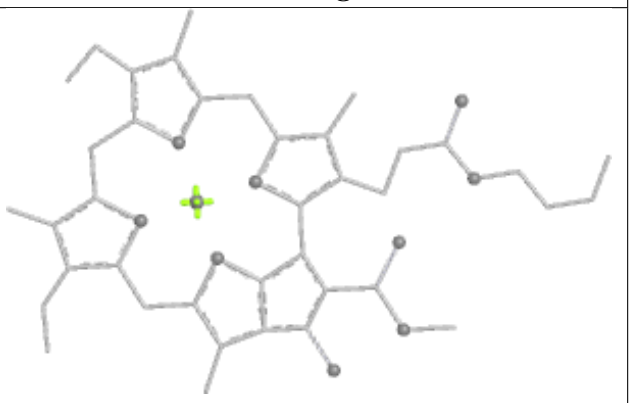
Bond lengths



Bond angles

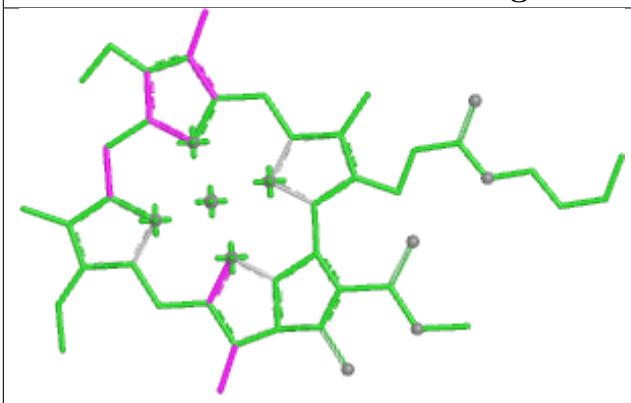


Torsions

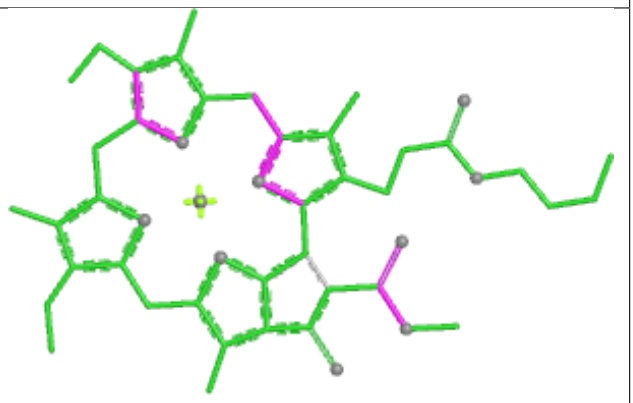


Rings

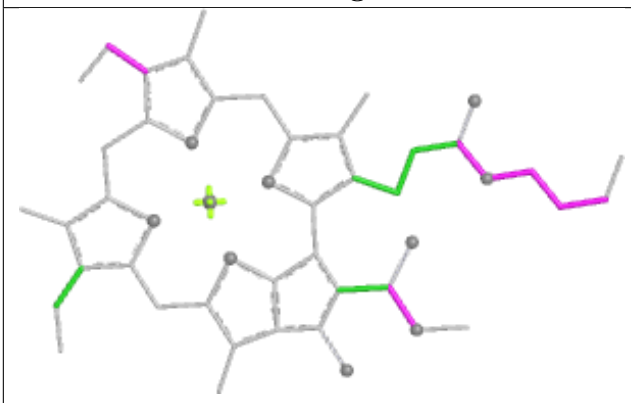
Ligand CLA RR 308



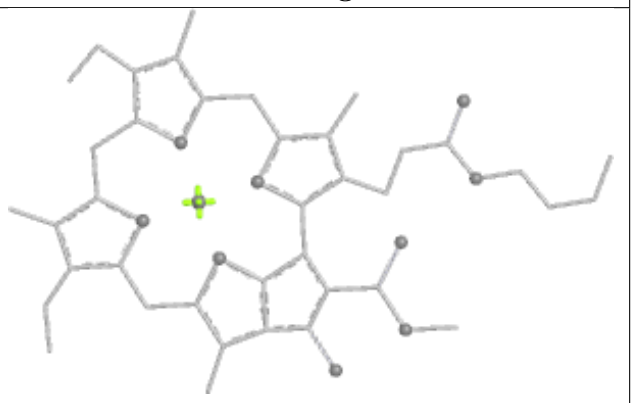
Bond lengths



Bond angles

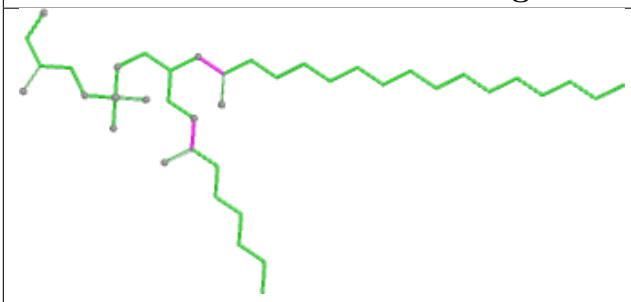


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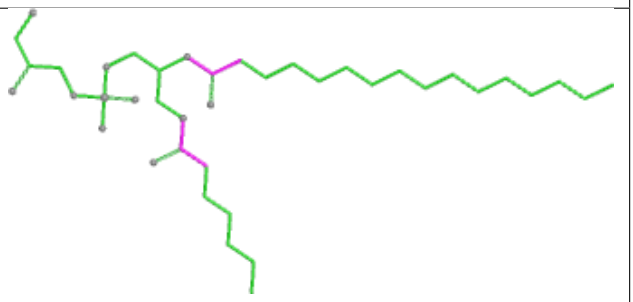


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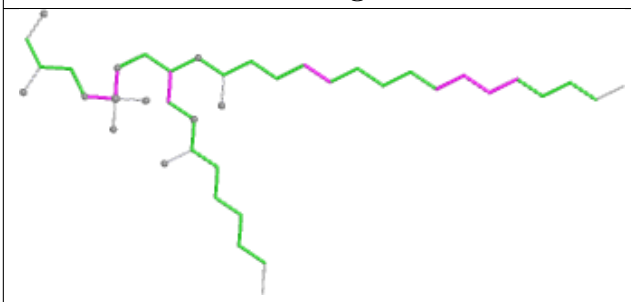
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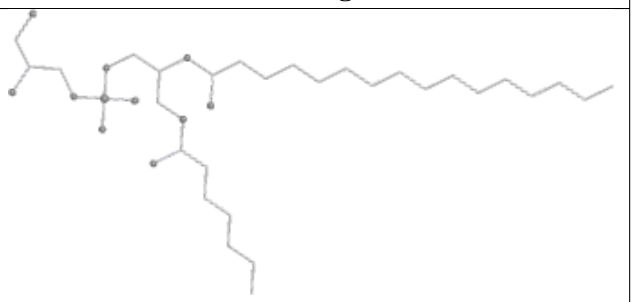
Bond lengths



Bond angles

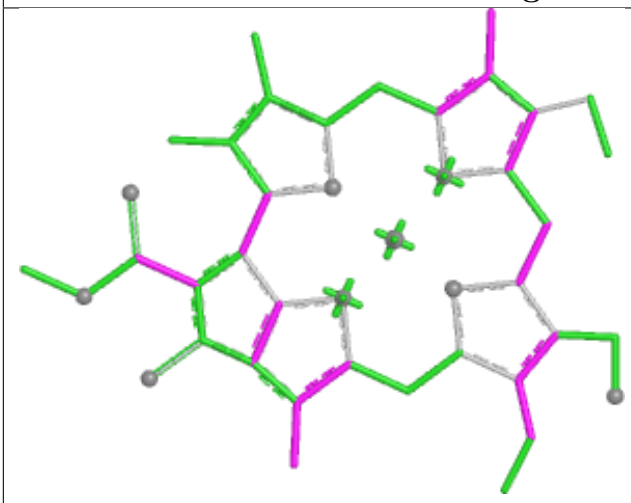


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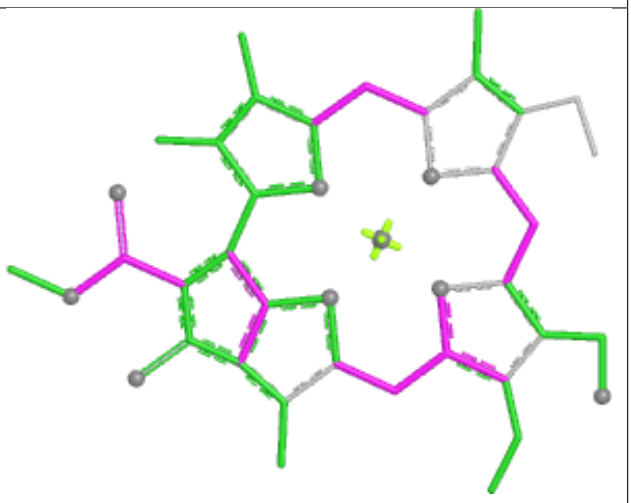


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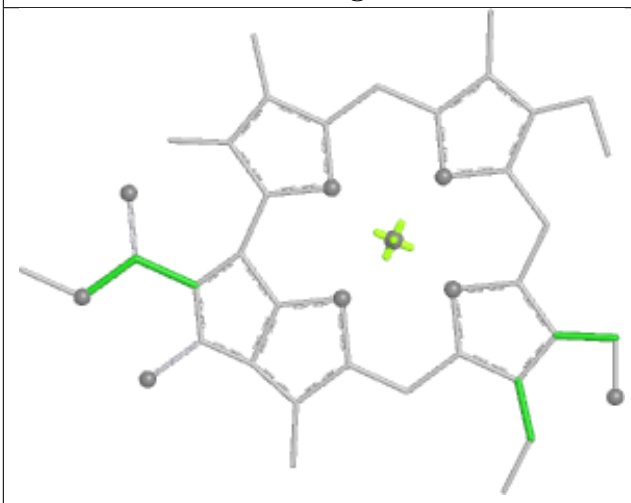
Ligand CHL N 606



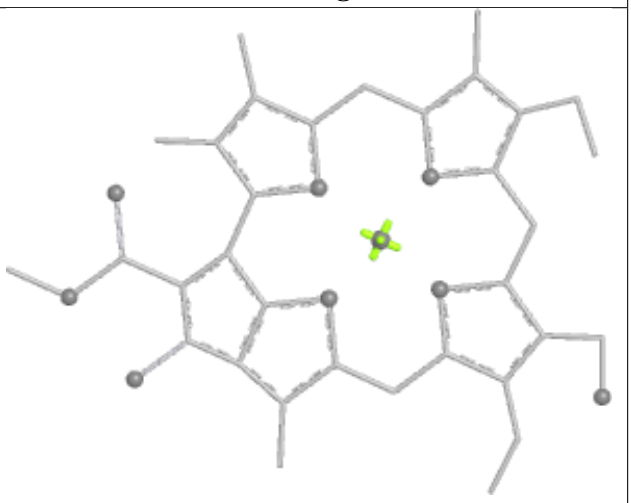
Bond lengths



Bond angles

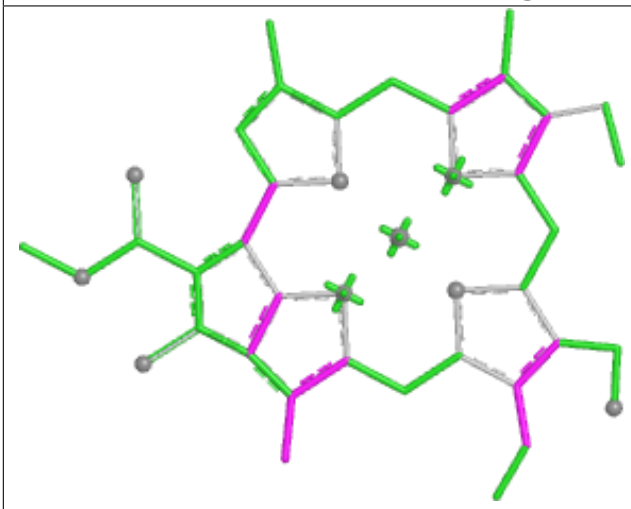


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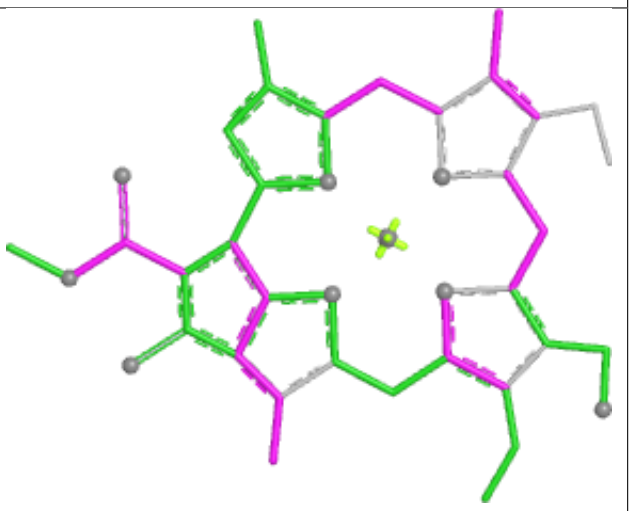


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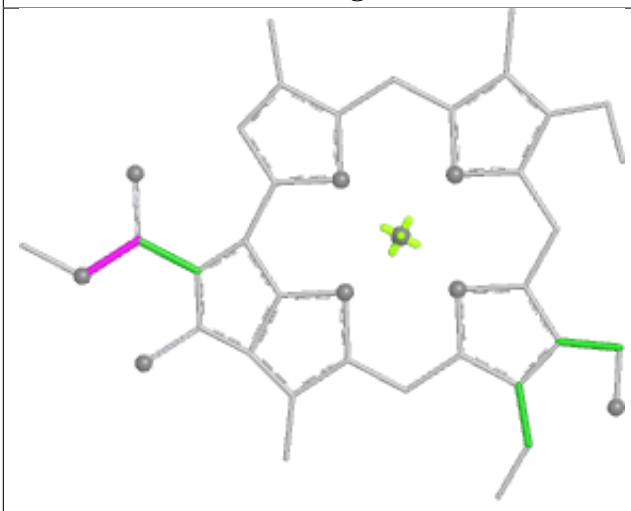
Ligand CHL 11 608



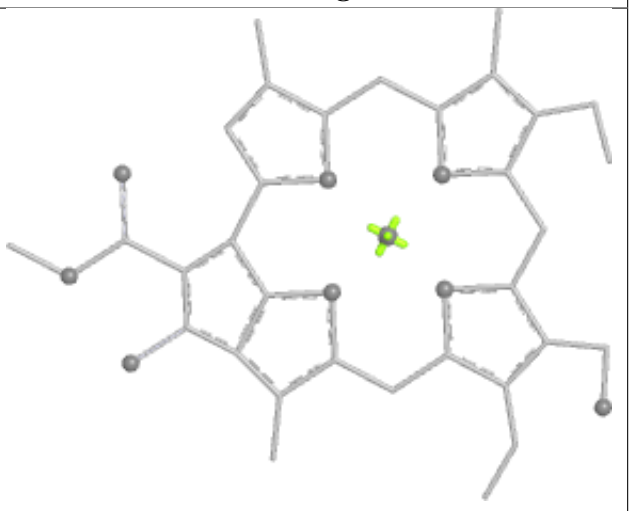
Bond lengths



Bond angles

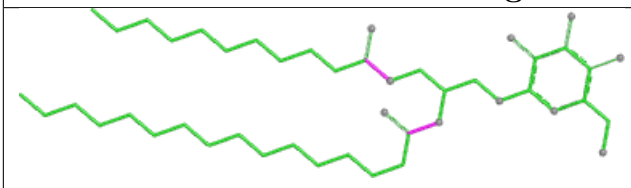


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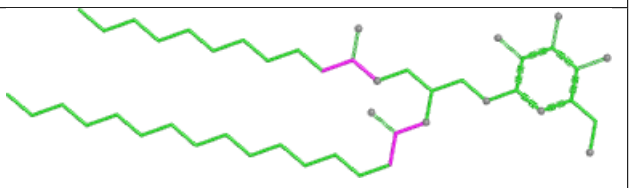


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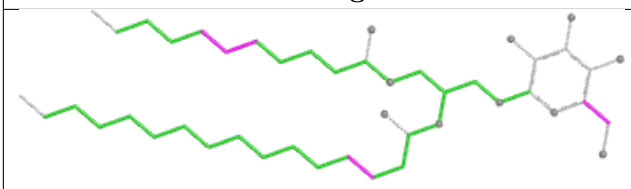
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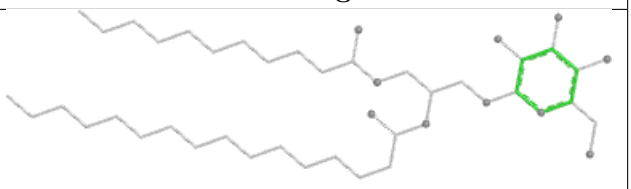
Bond lengths



Bond angles

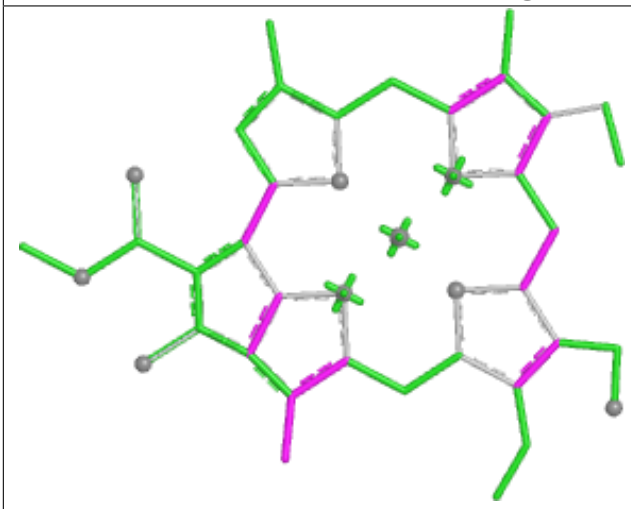


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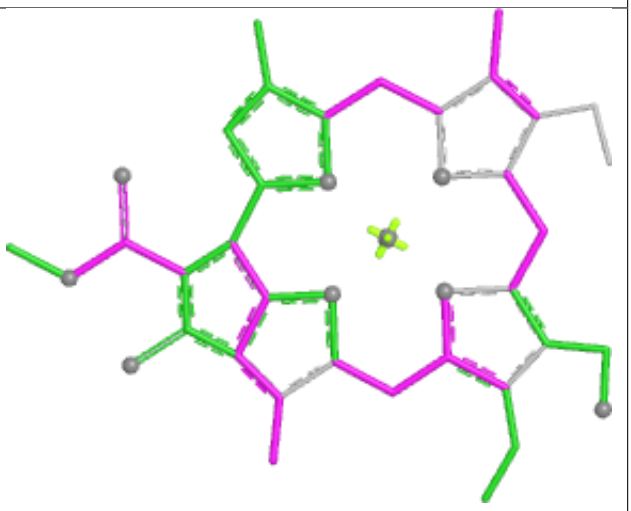


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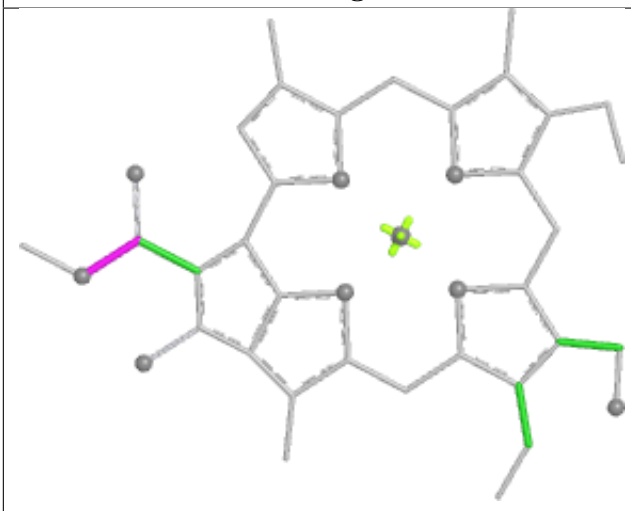
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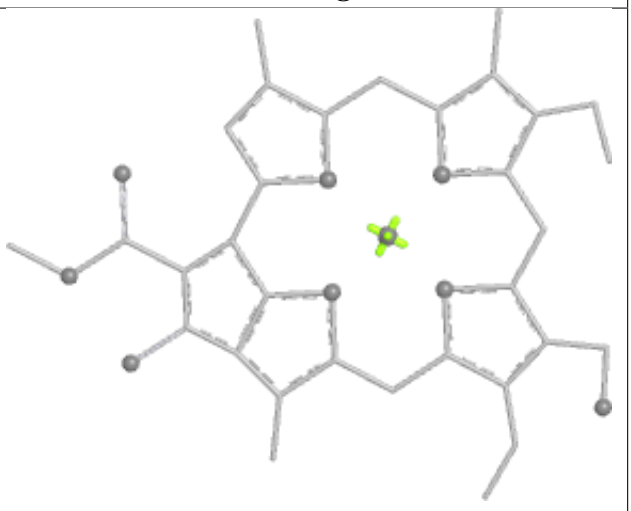
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Bond angles

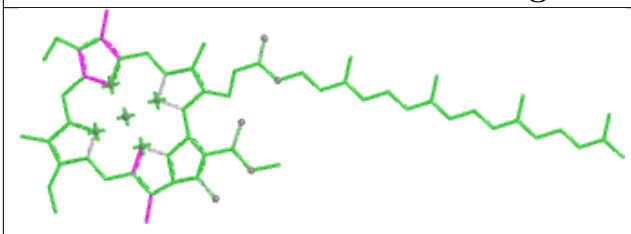


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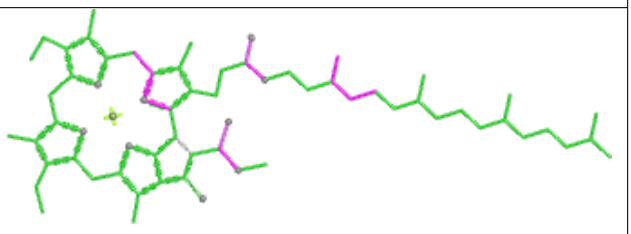


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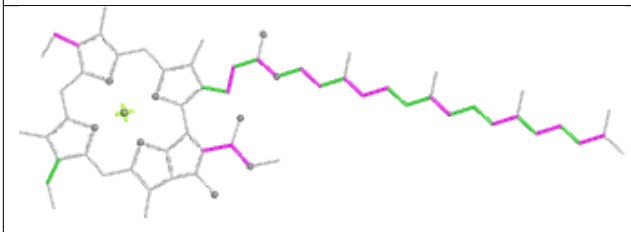
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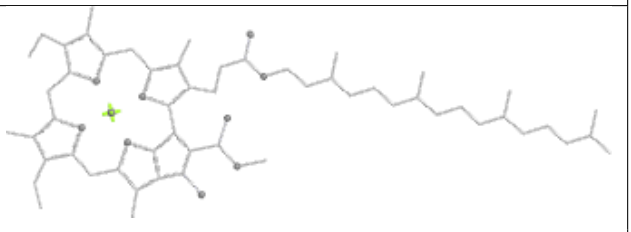
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Bond angles

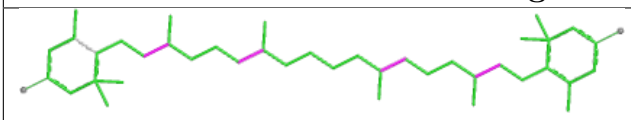


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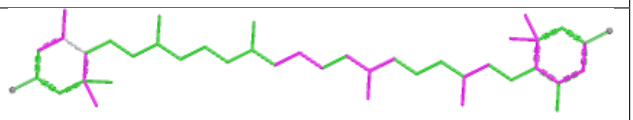


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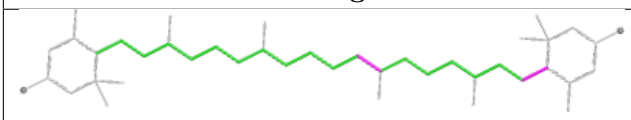
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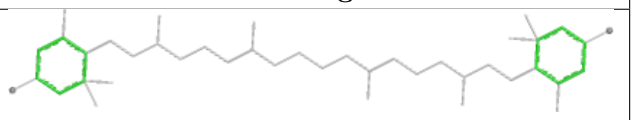
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Bond angles

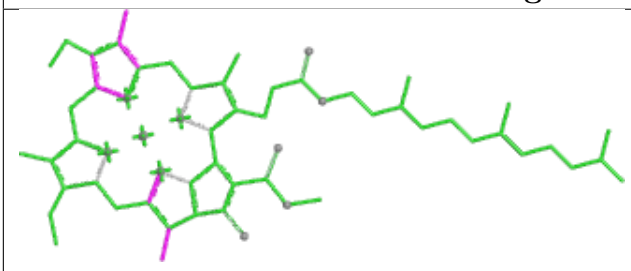


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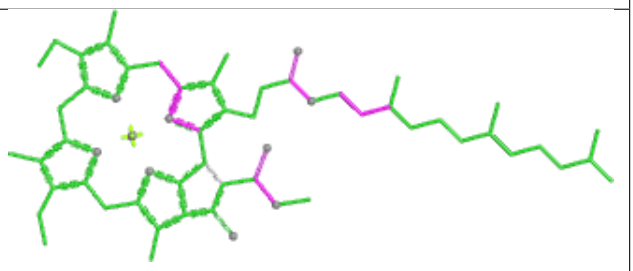


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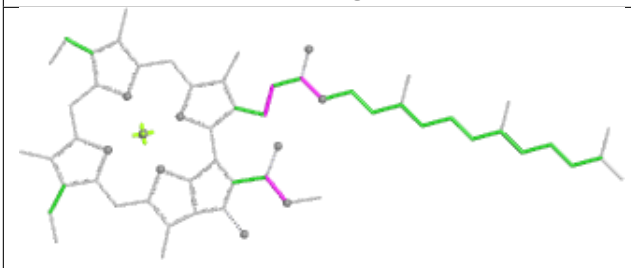
Ligand CLA B 609



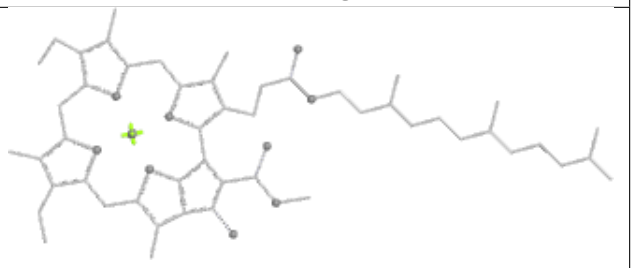
Bond lengths



Bond angles

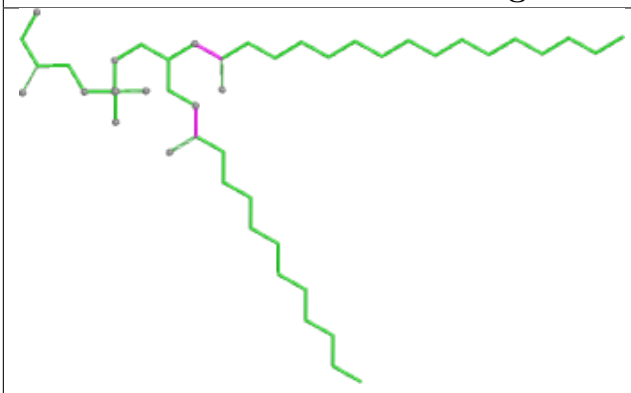


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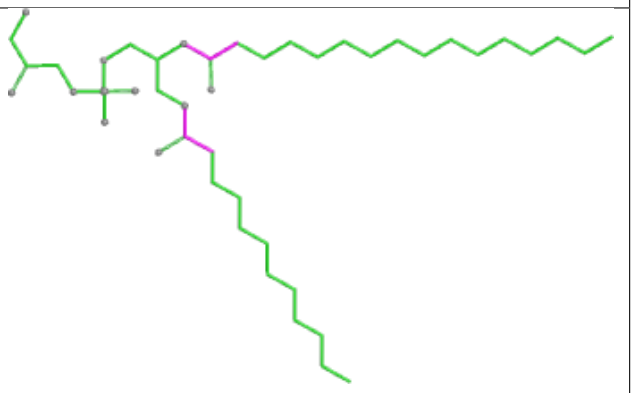


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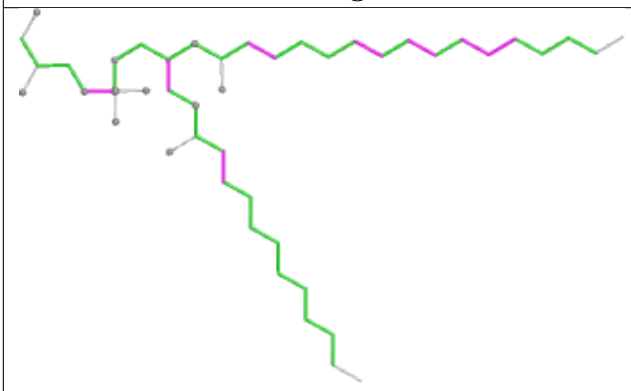
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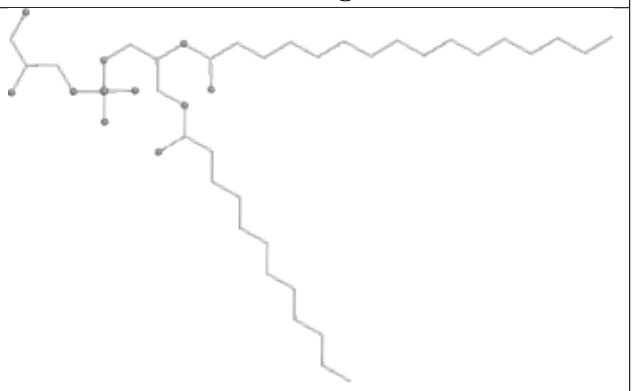
Bond lengths



Bond angles

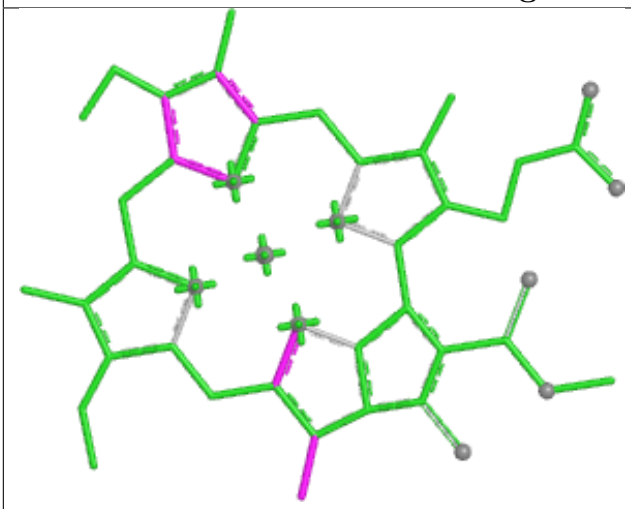


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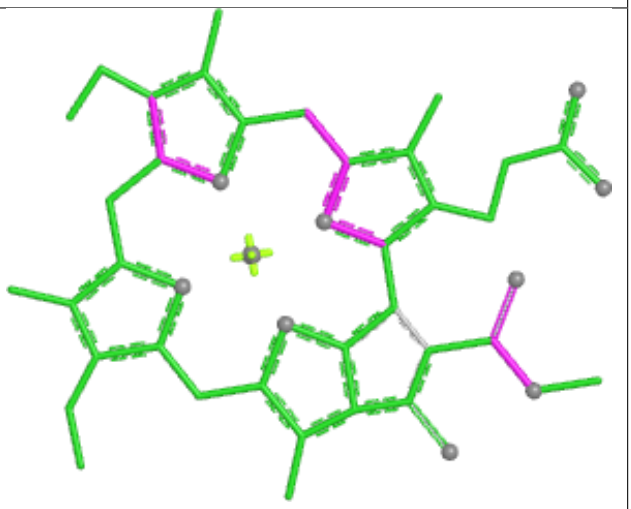


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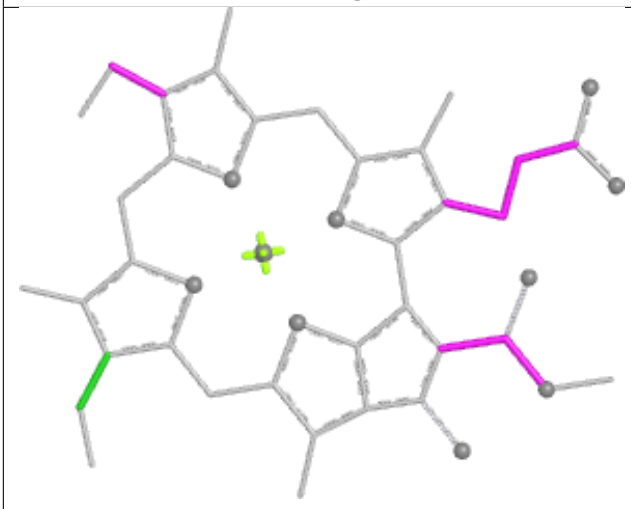
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Bond lengths



Bond angles

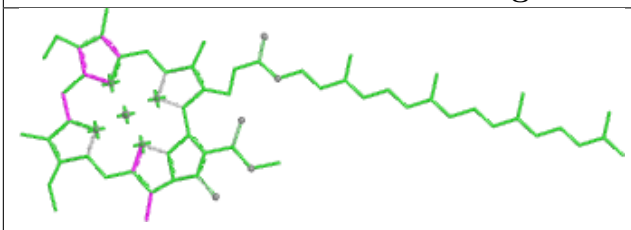


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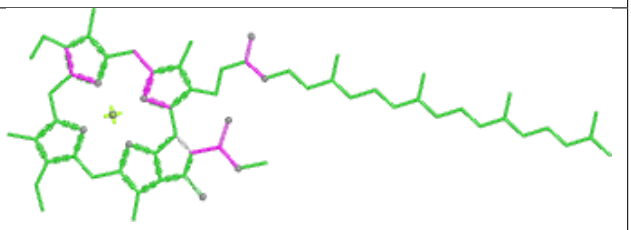


Rings

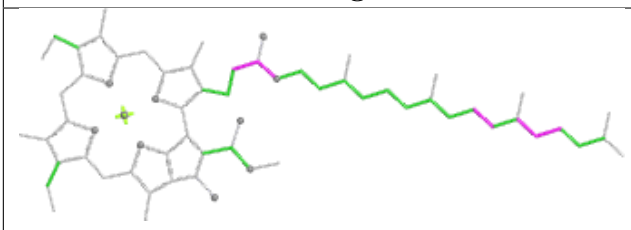
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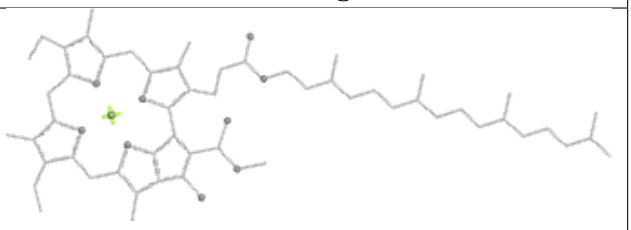
Bond lengths



Bond angles

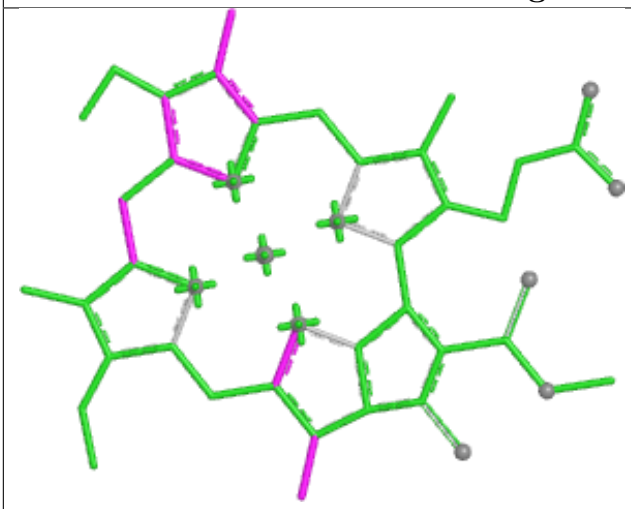


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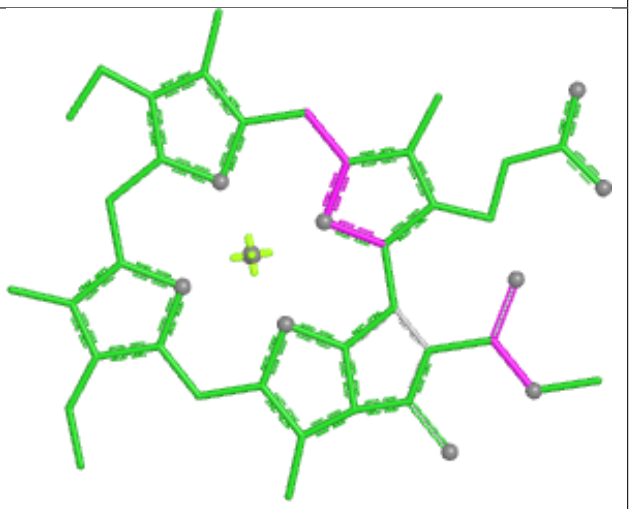


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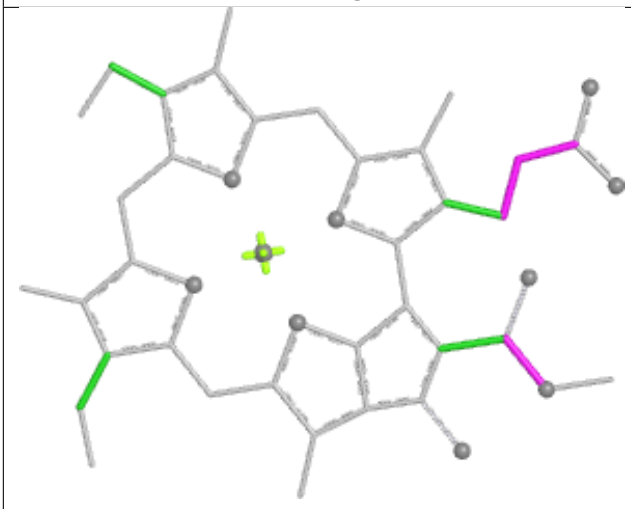
Ligand CLA 4 305



Bond lengths



Bond angles

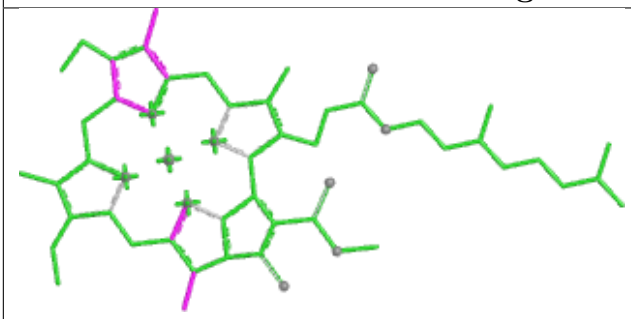


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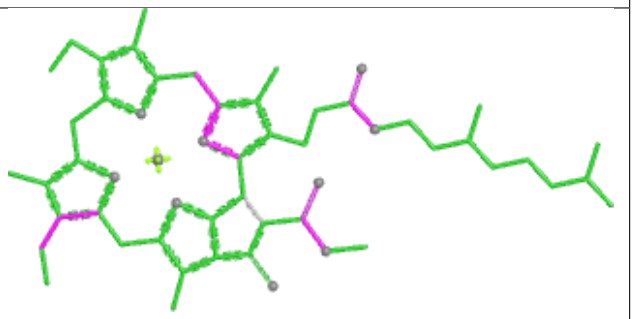


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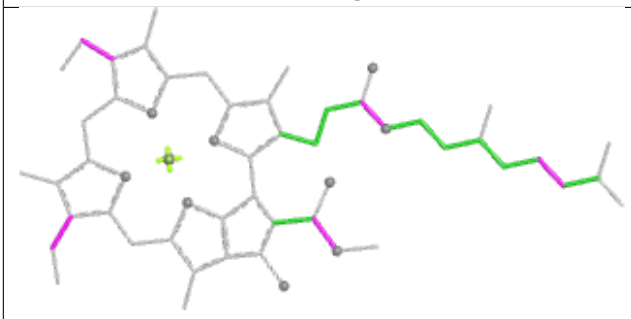
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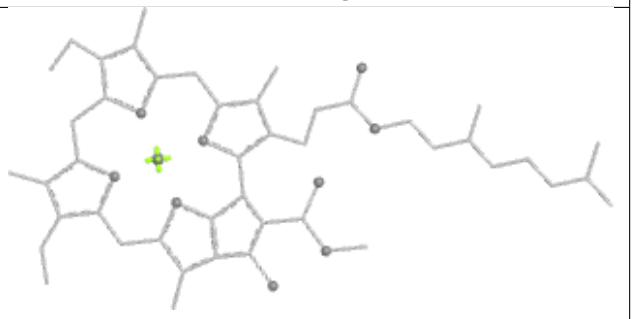
Bond lengths



Bond angles

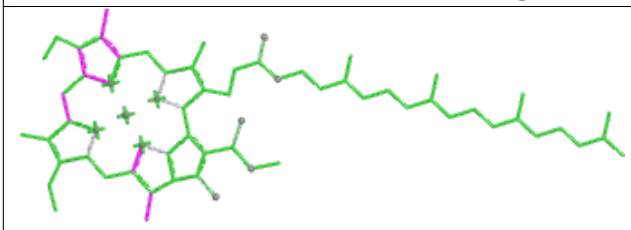


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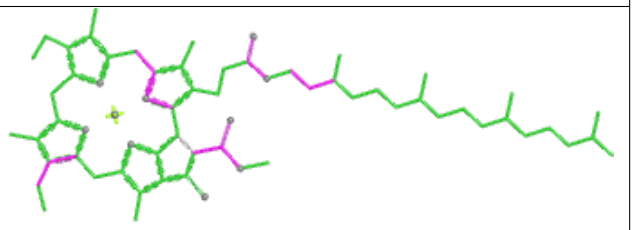


Rings

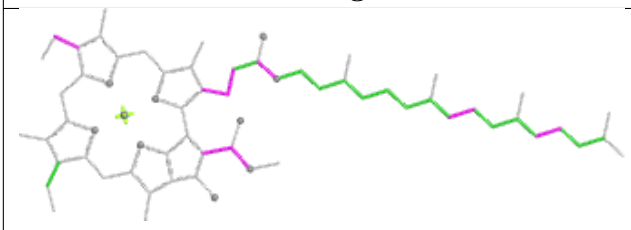
Ligand CLA Nn 312



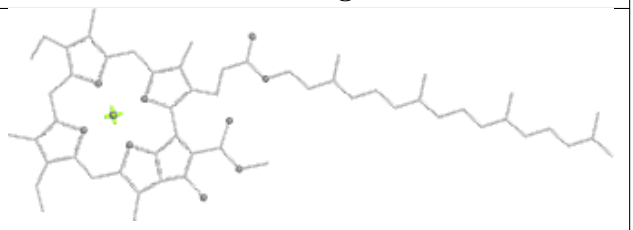
Bond lengths



Bond angles

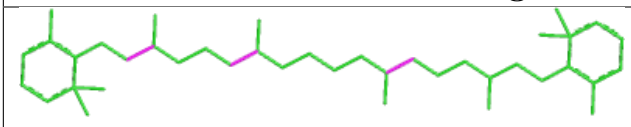


Torsions

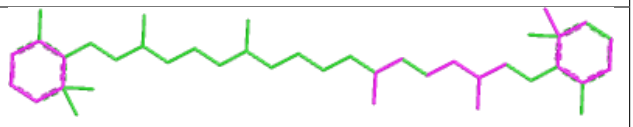


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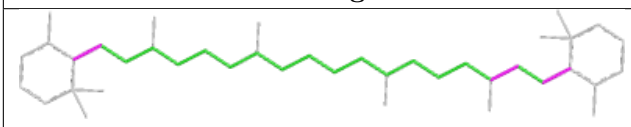
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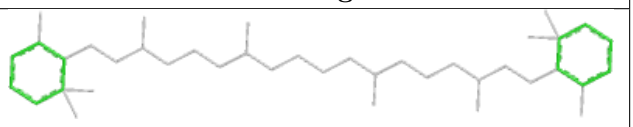
Bond lengths



Bond angles

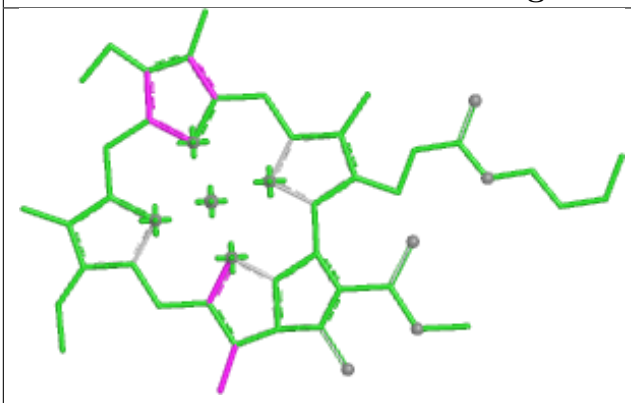


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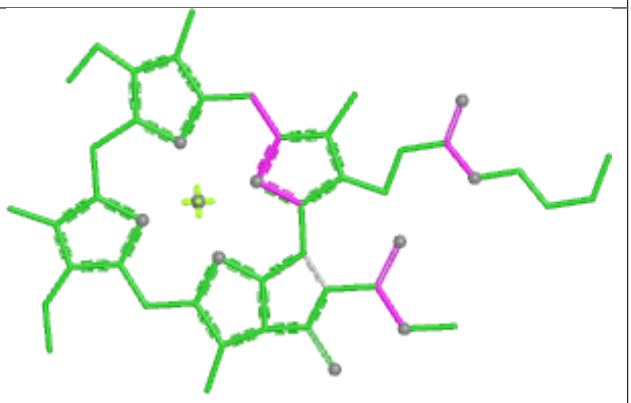


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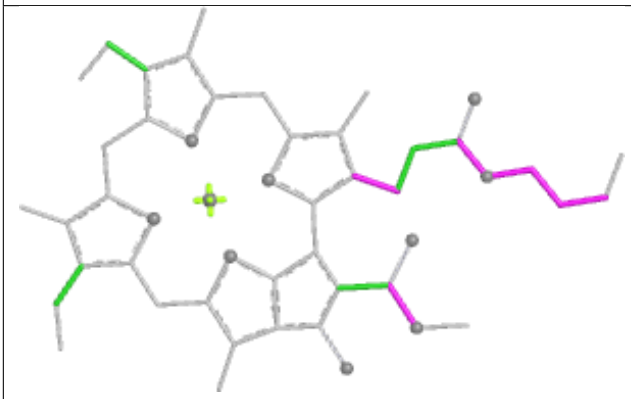
Ligand CLA n 603



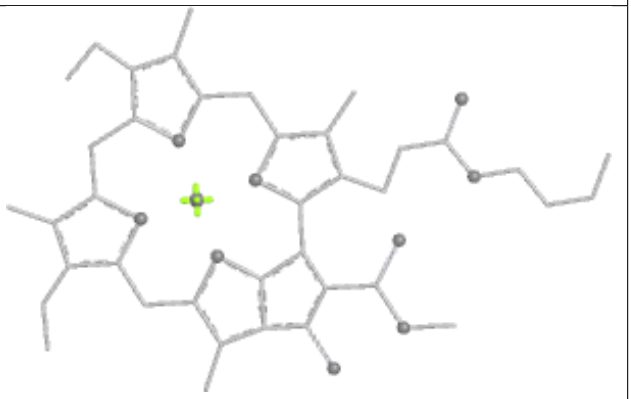
Bond lengths



Bond angles

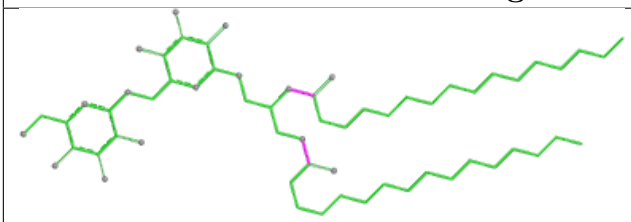


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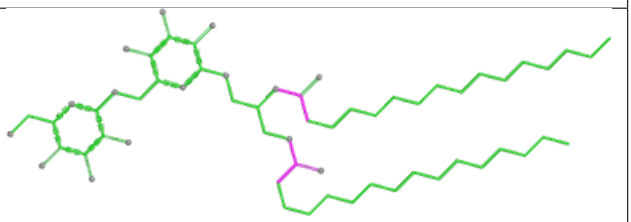


Rings

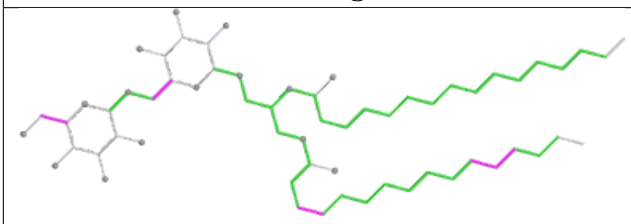
Ligand DGD CC 519



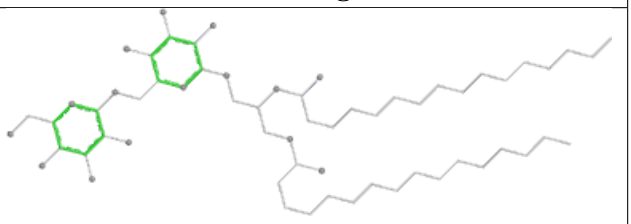
Bond lengths



Bond angles

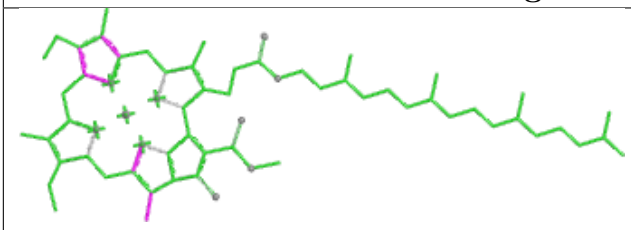


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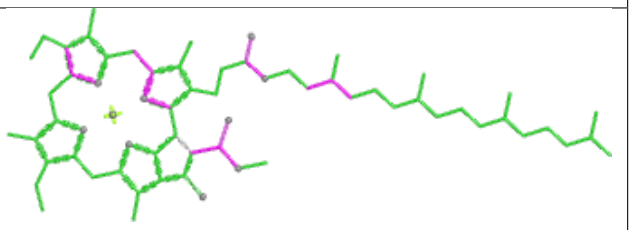


Rings

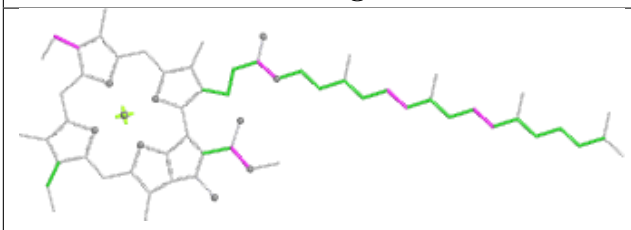
Ligand CLA B 610



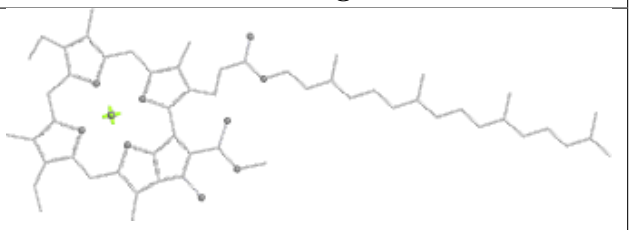
Bond lengths



Bond angles

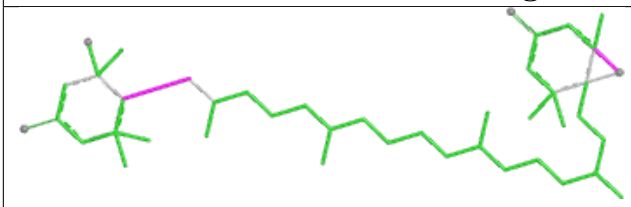


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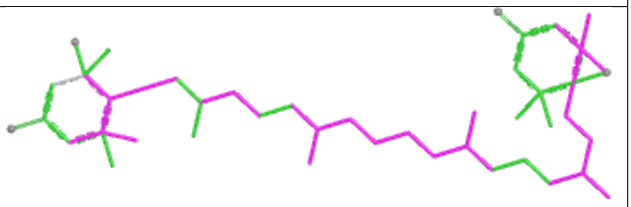


Rings

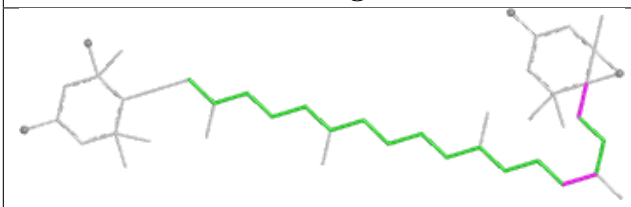
Ligand NEX Y 619



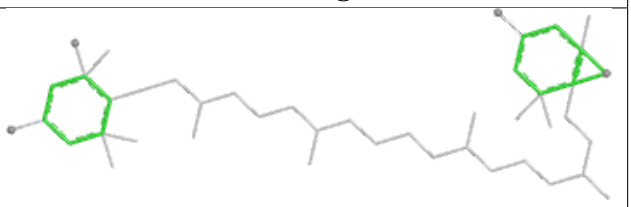
Bond lengths



Bond angles

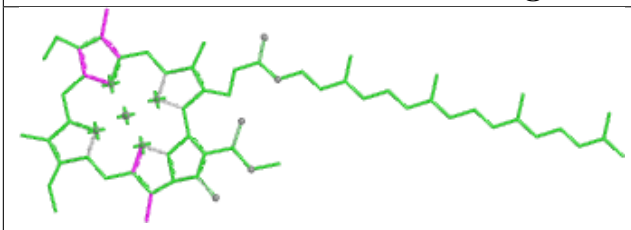


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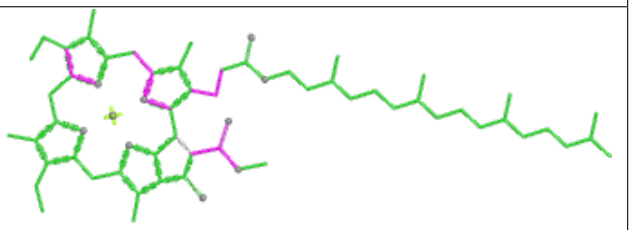


Rings

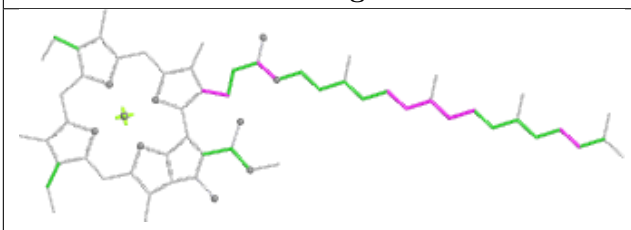
Ligand CLA C 503



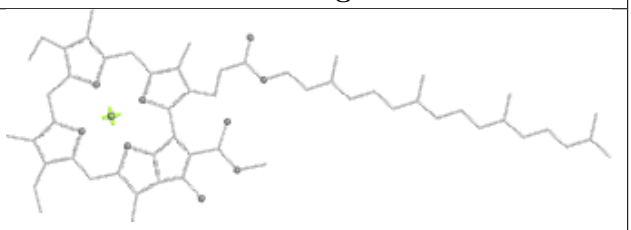
Bond lengths



Bond angles

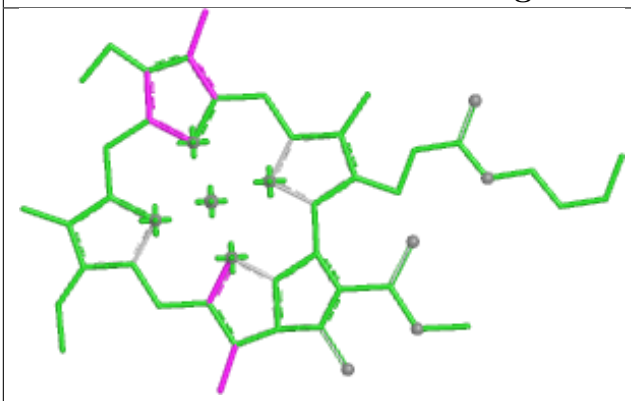


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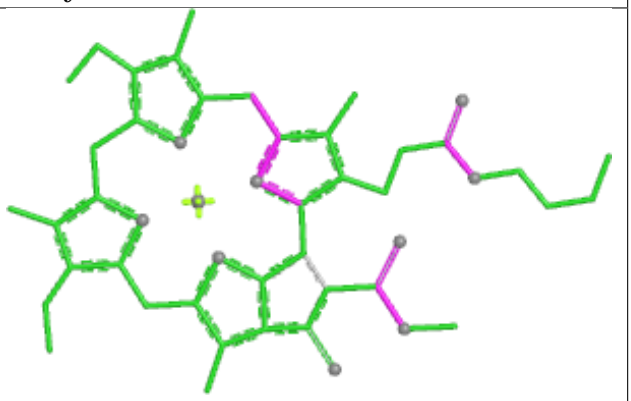


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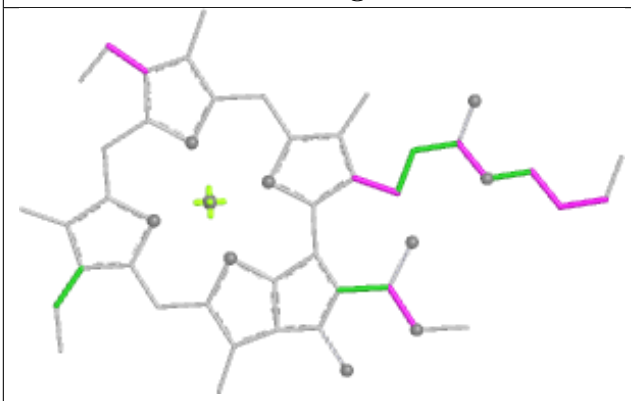
Ligand CLA Yy 614



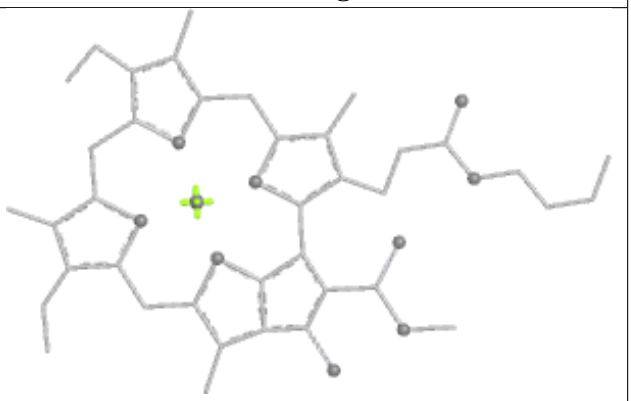
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Bond angles

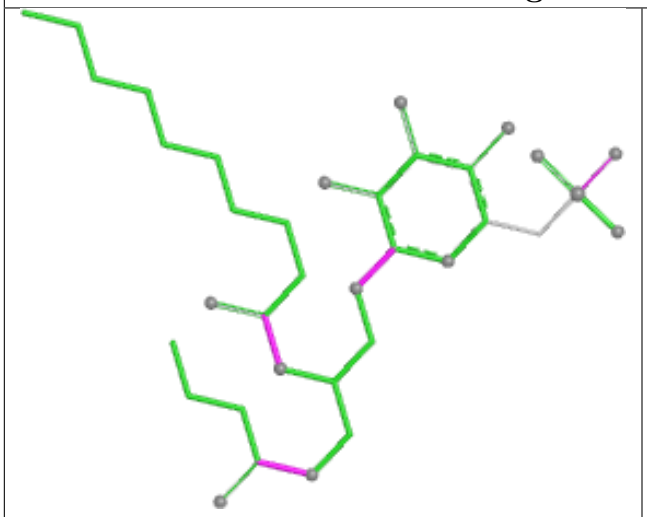


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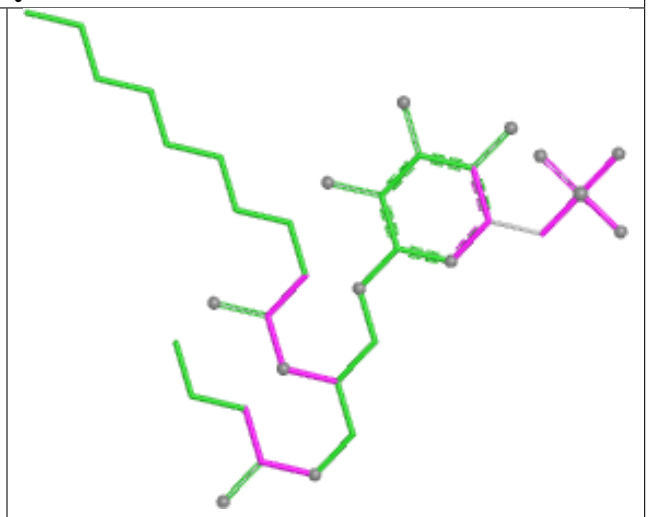


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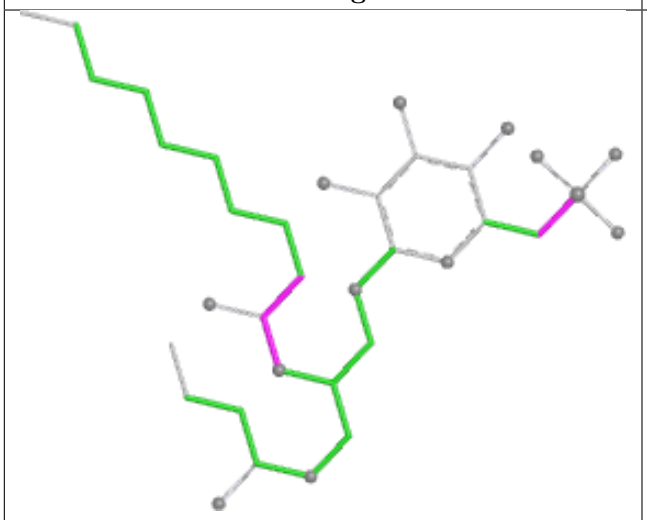
Ligand SQD B 617



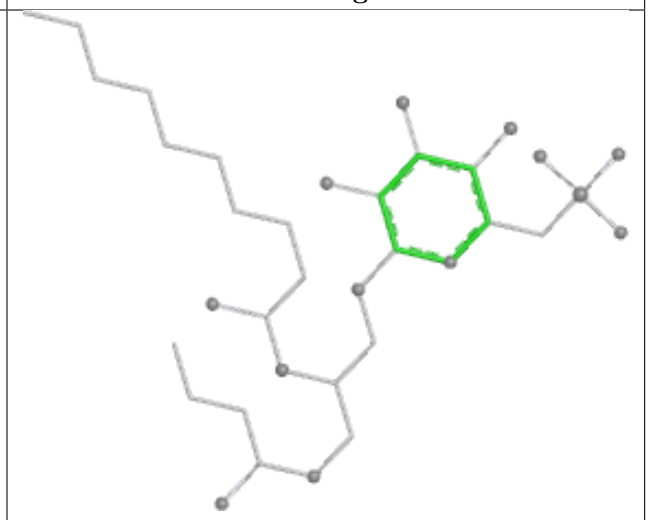
Bond lengths



Bond angles

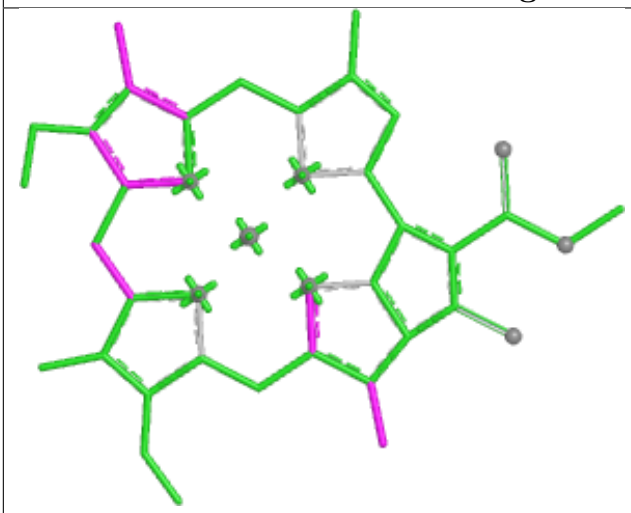


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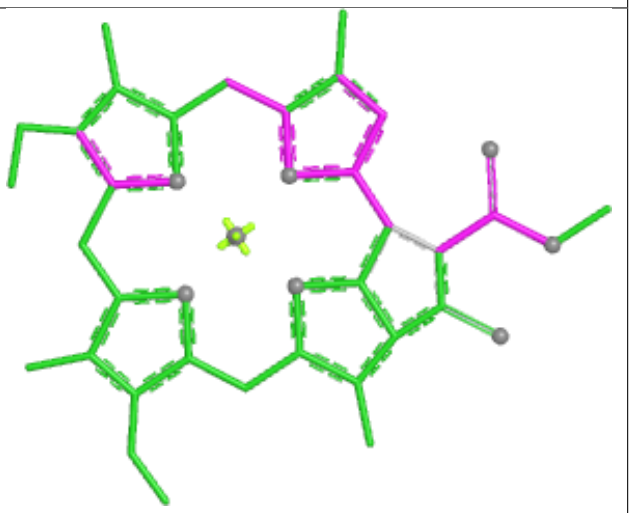


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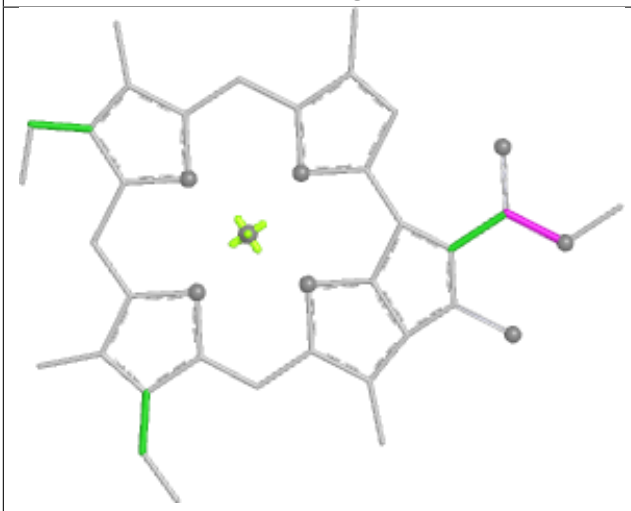
Ligand CLA 11 604



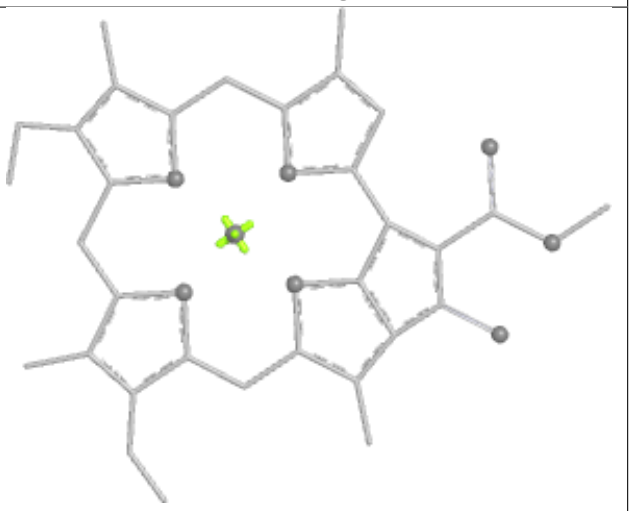
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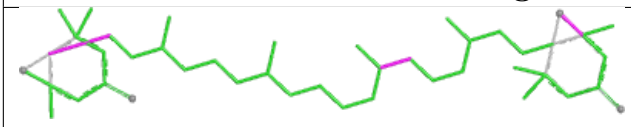


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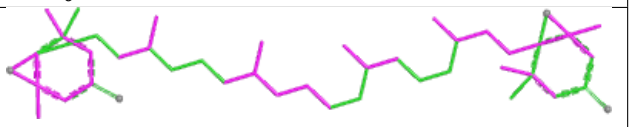


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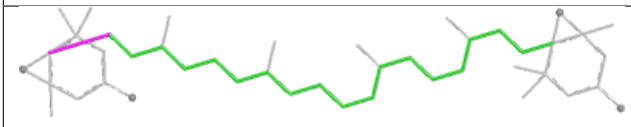
Ligand XAT Yy 619



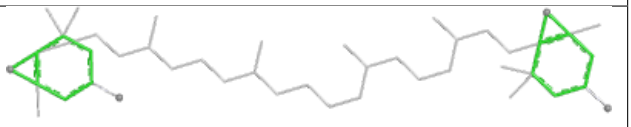
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Bond angles

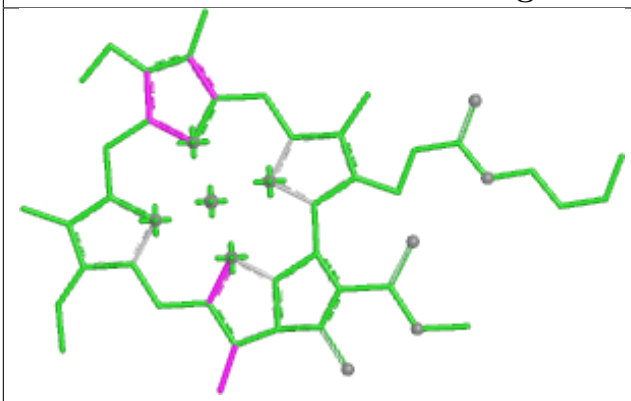


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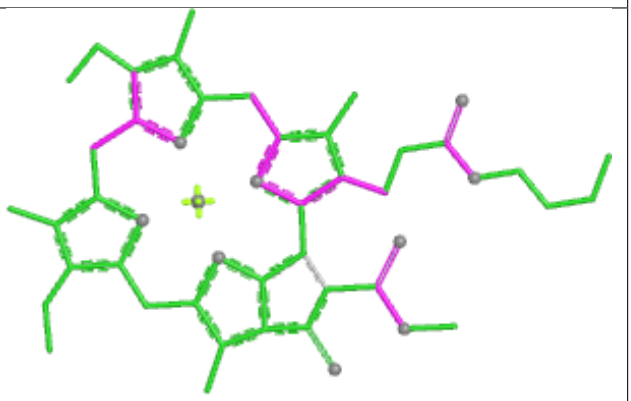


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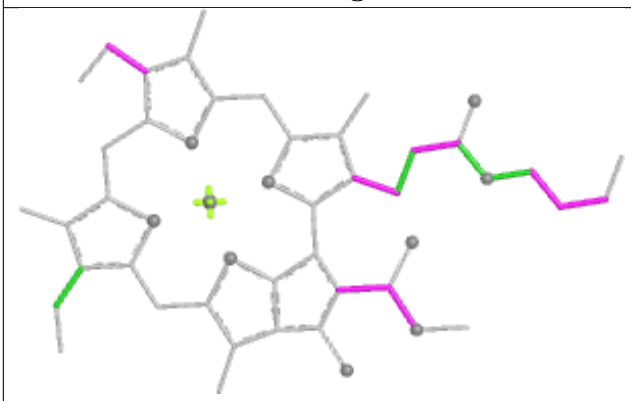
Ligand CLA Rr 604



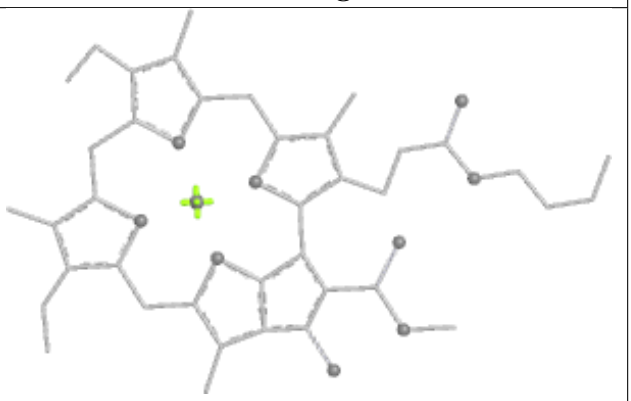
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Bond angles

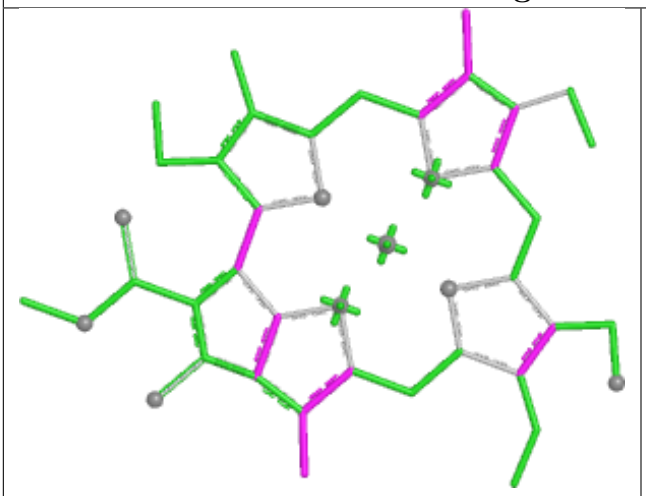


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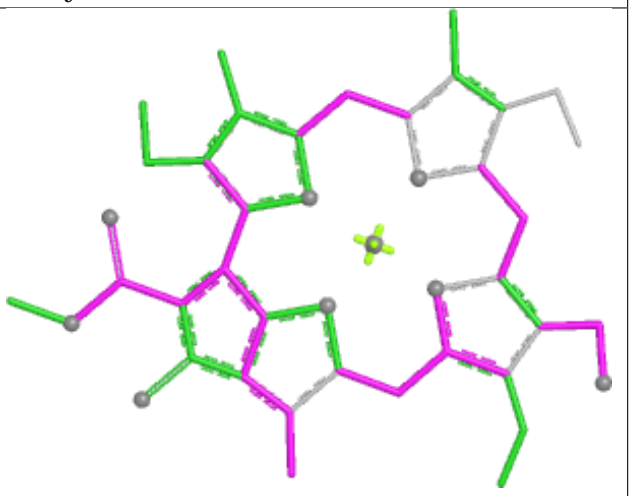


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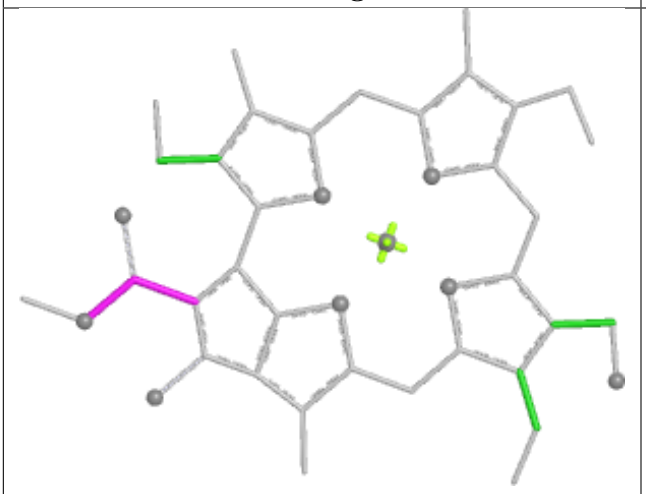
Ligand CHL Yy 607



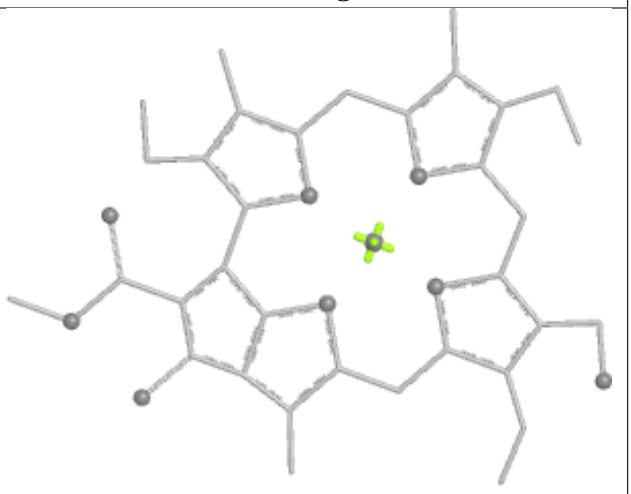
Bond lengths



Bond angles

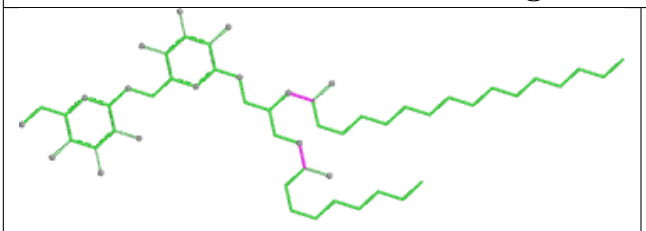


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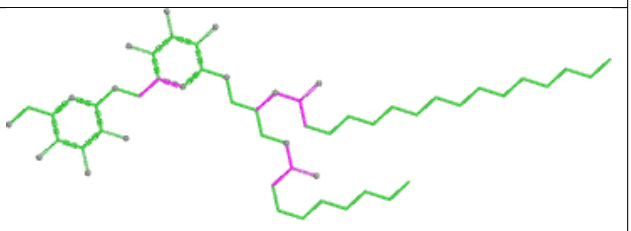


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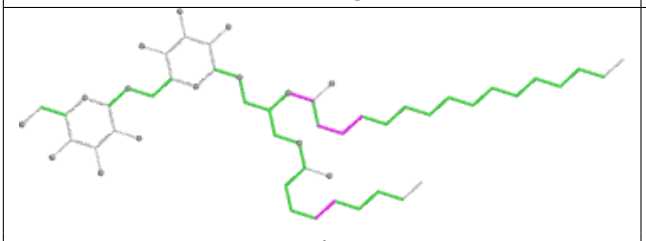
Ligand DGD c 517



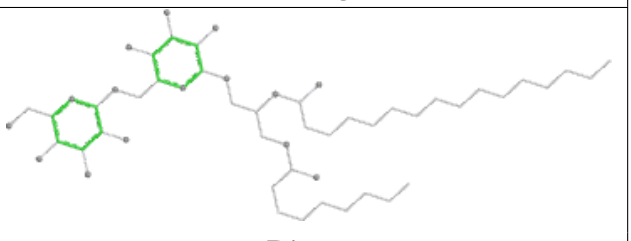
Bond lengths



Bond angles

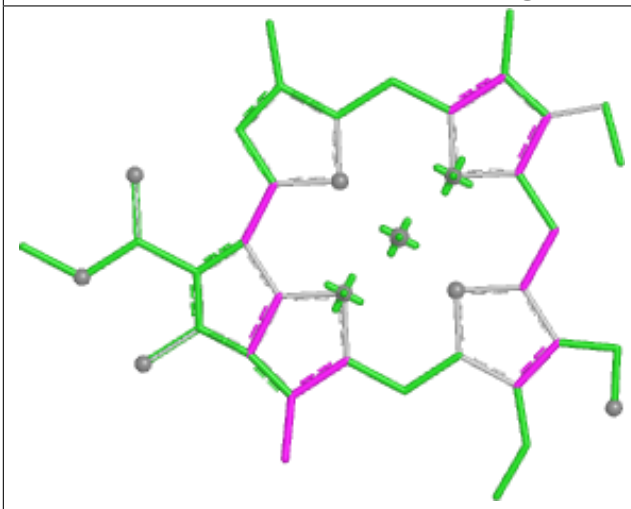


Torsions

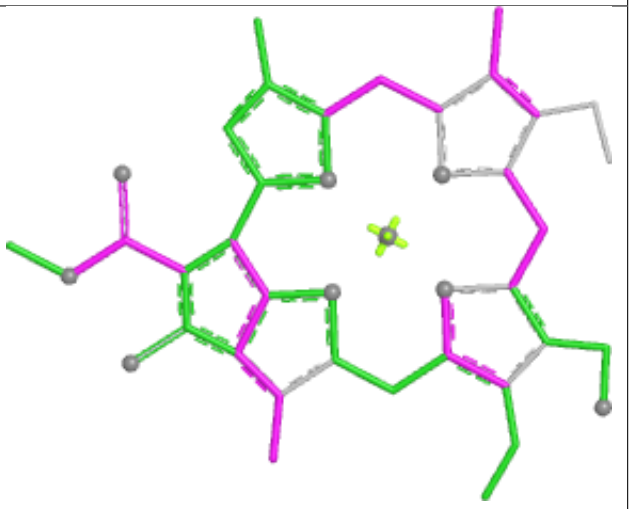


Rings

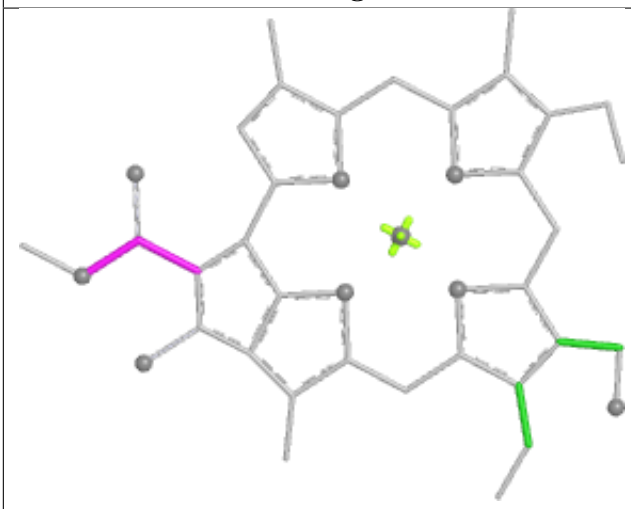
Ligand CHL 22 606



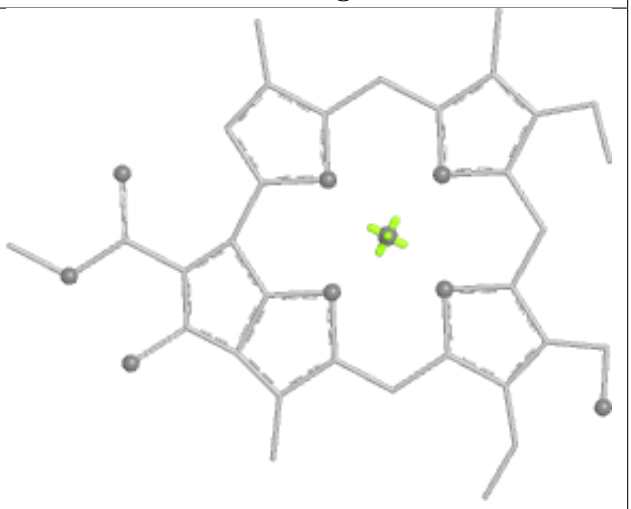
Bond lengths



Bond angles

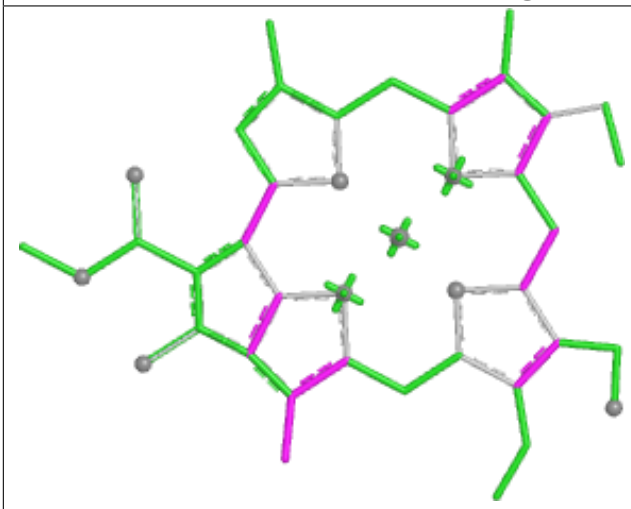


Torsions



Rings

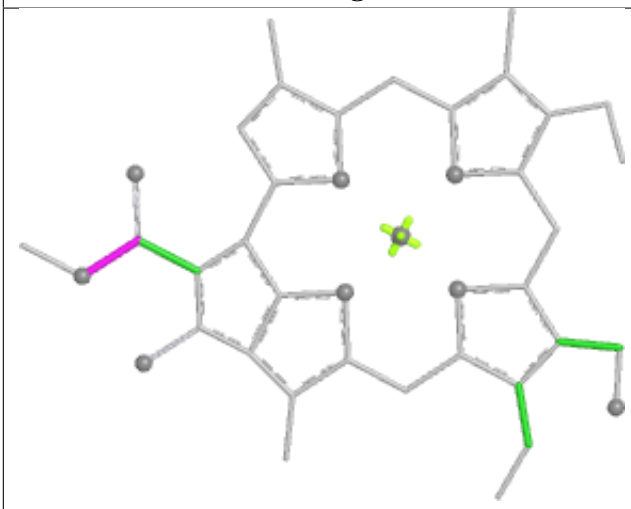
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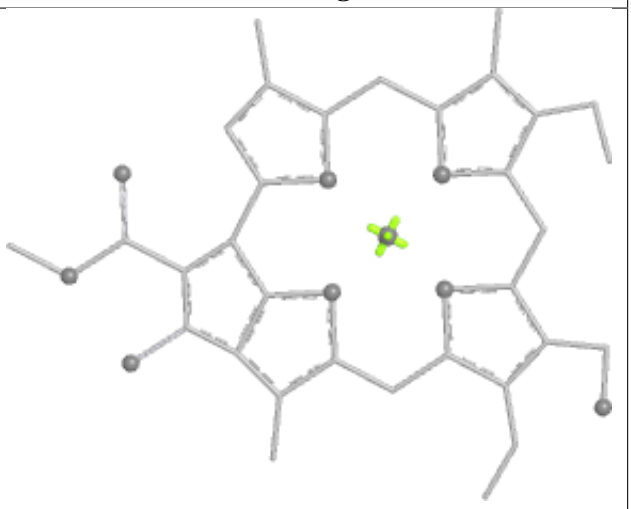
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Bond angles

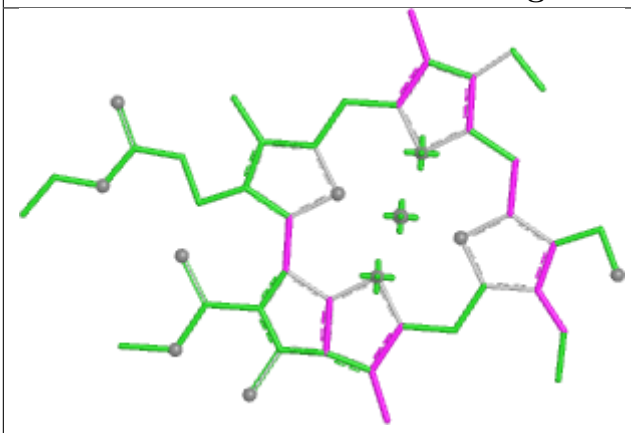


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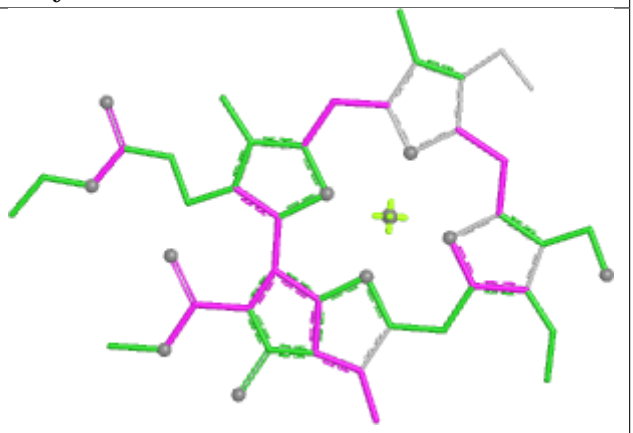


Rings

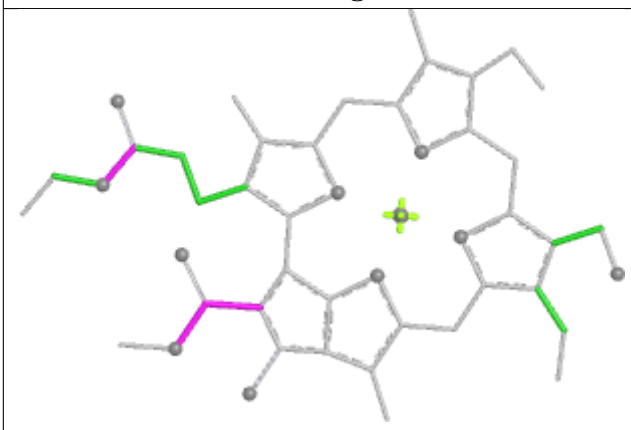
Ligand CHL y 307



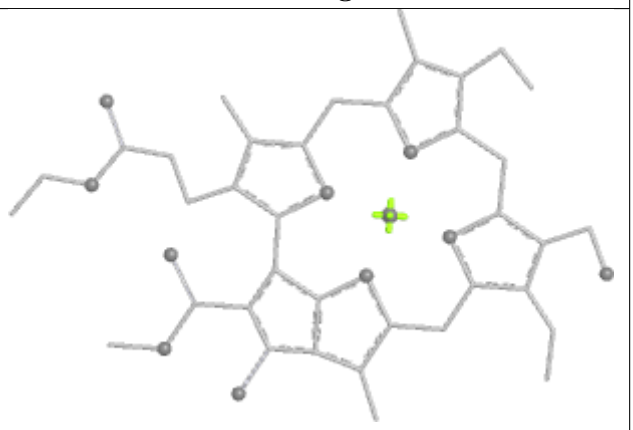
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Bond angles

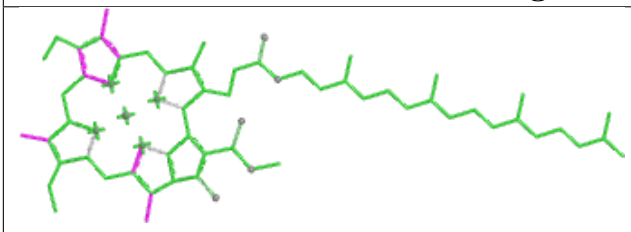


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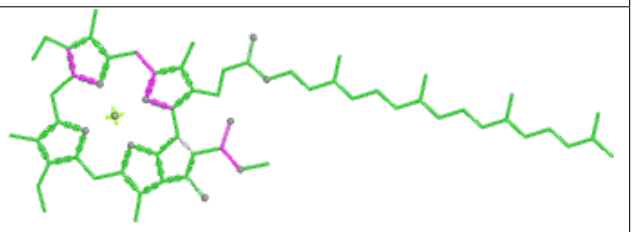


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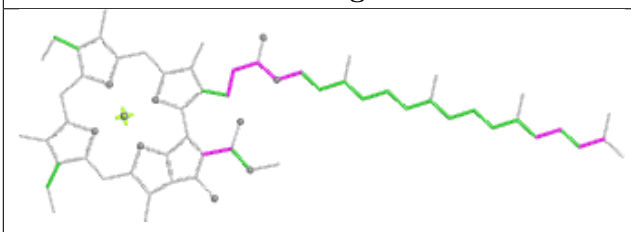
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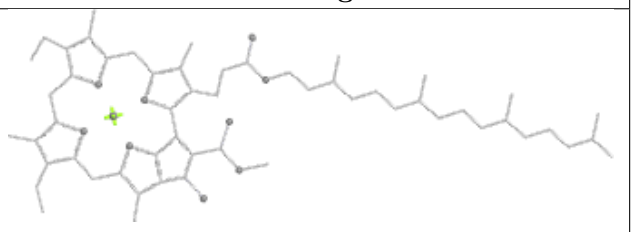
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Bond angles

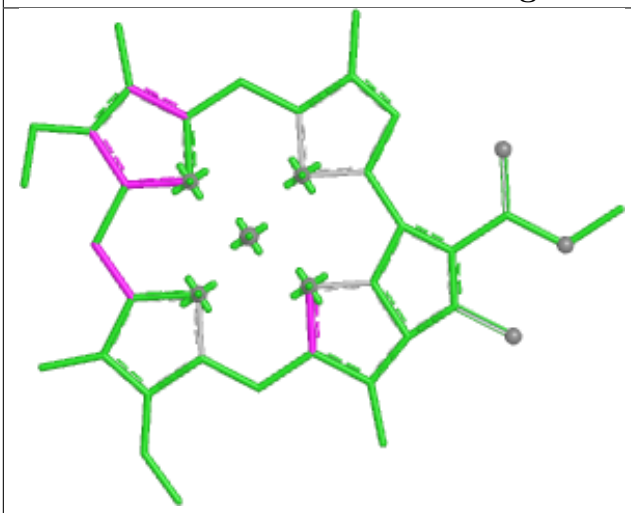


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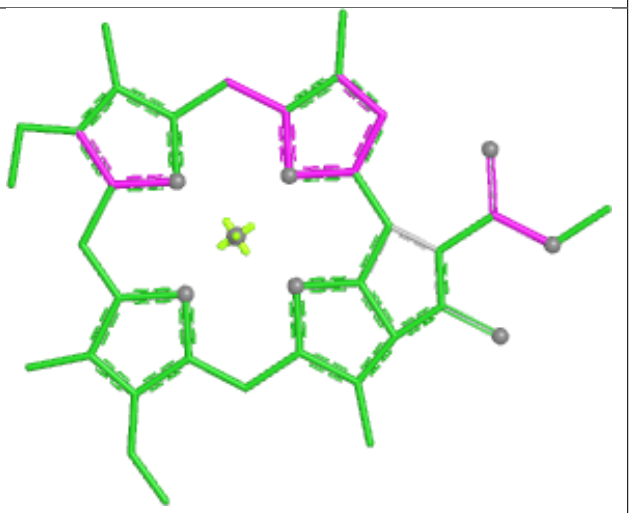


Rings

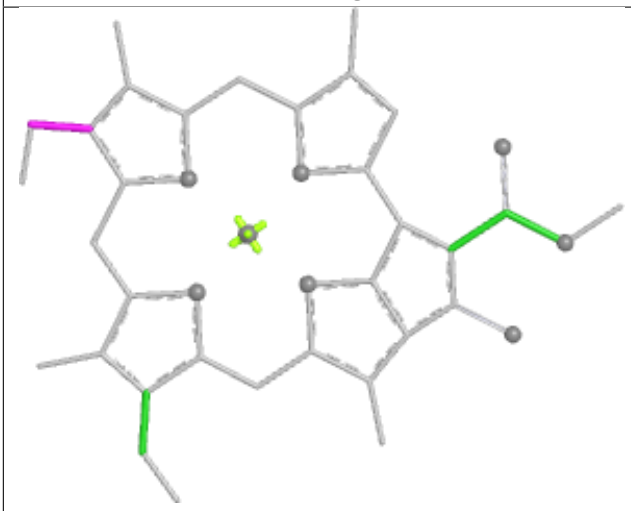
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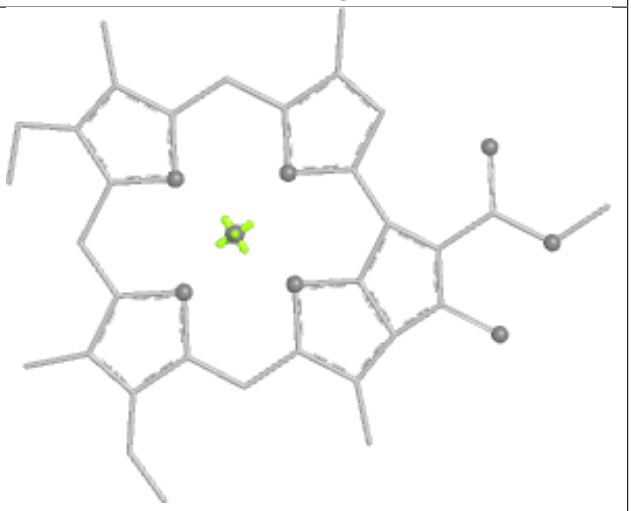
Bond lengths



Bond angles

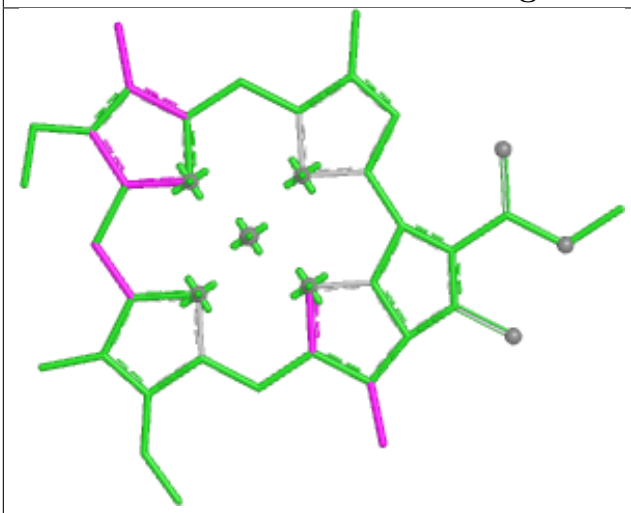


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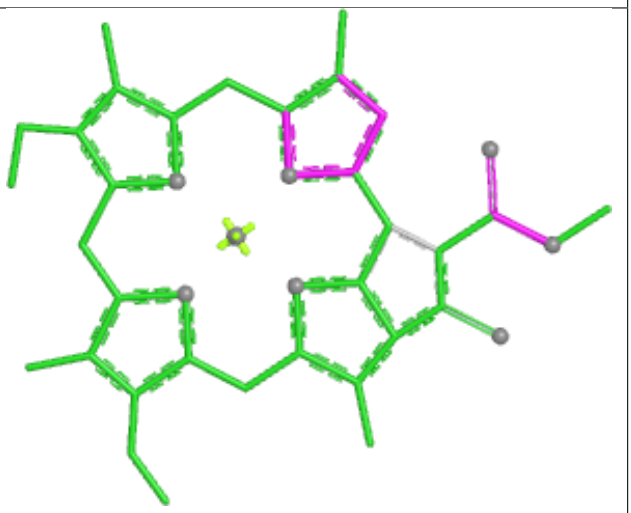


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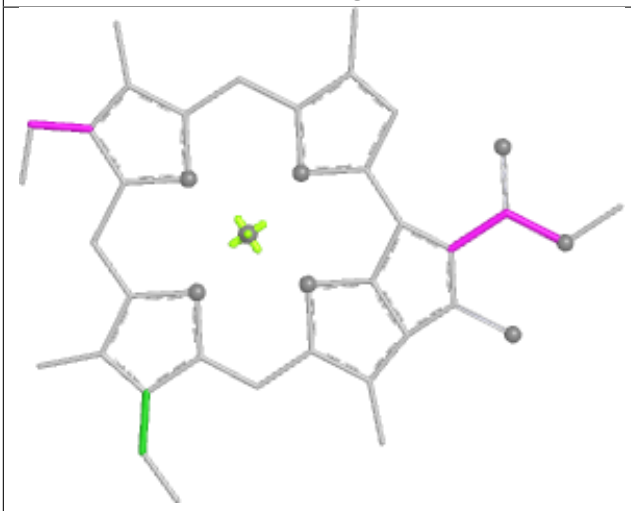
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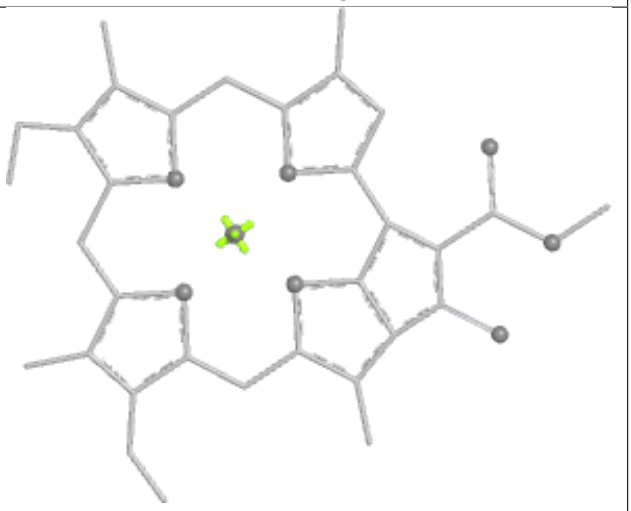
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Bond angles

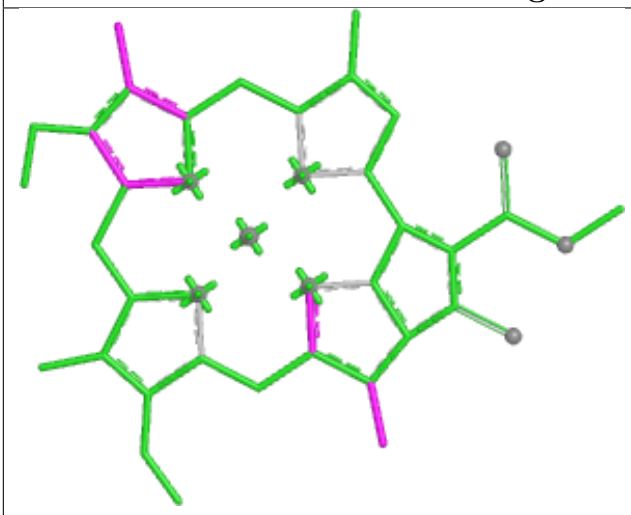


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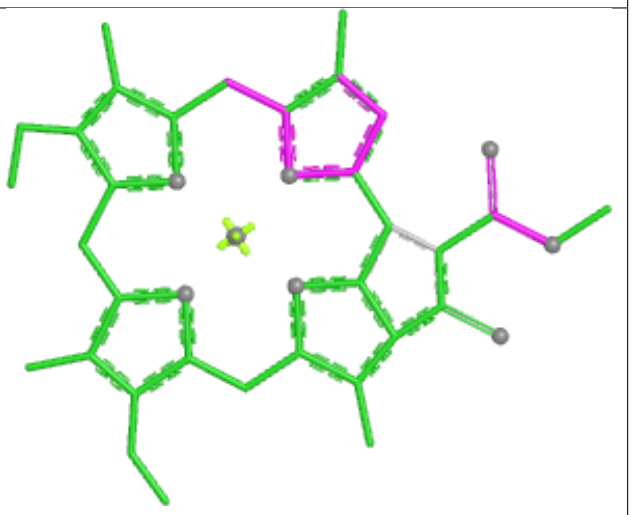


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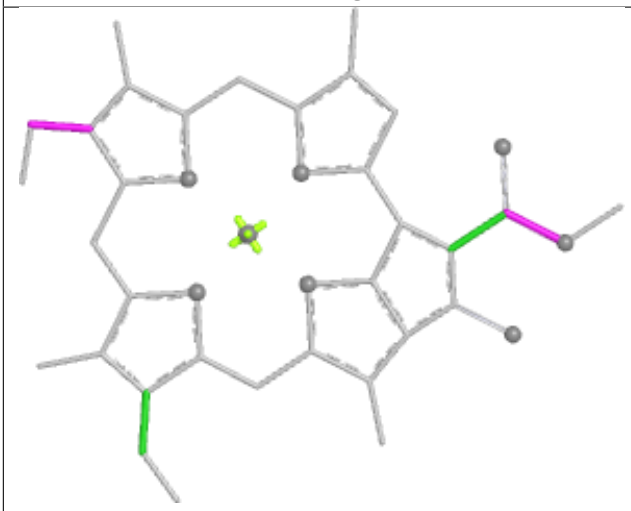
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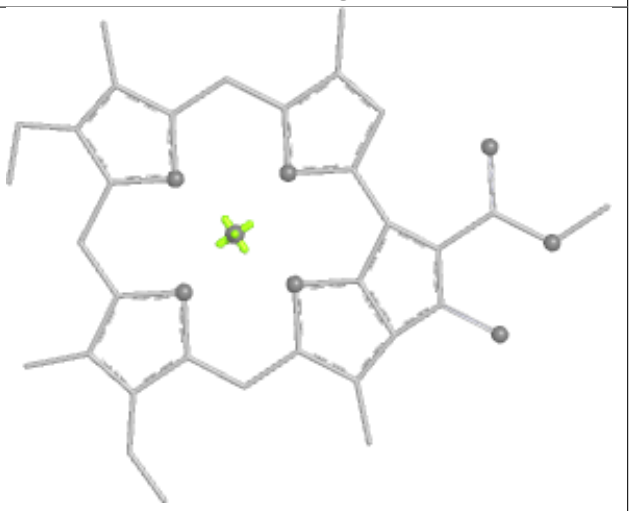
Bond lengths



Bond angles



Torsions

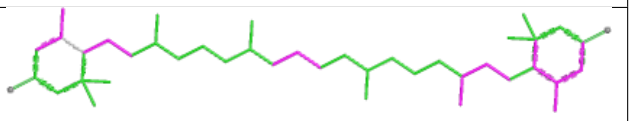


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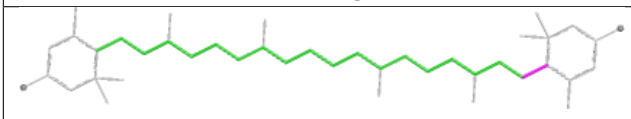
Ligand LUT S 614



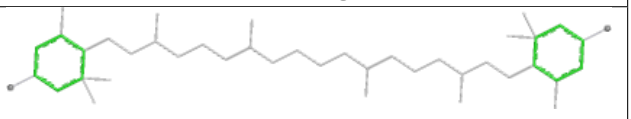
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Bond angles

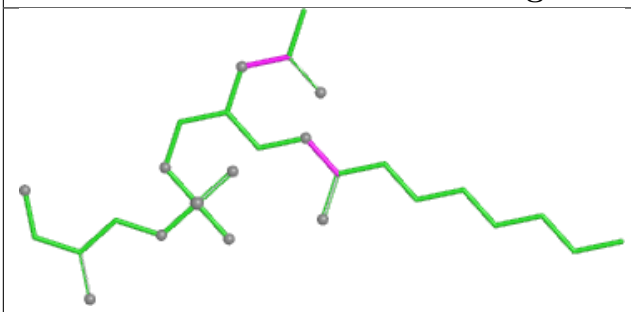


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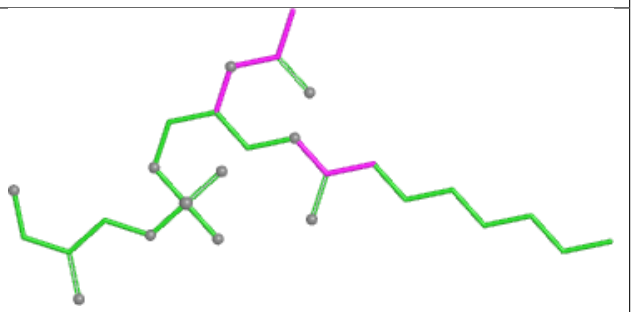


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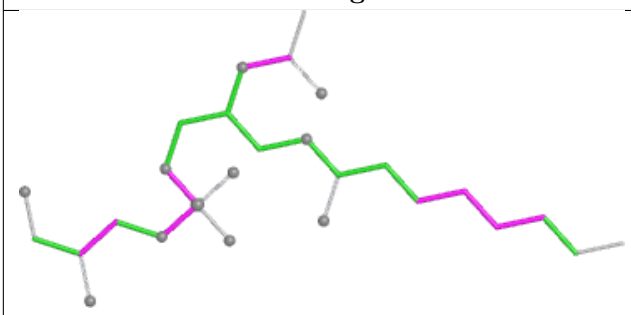
Ligand LHG J 101



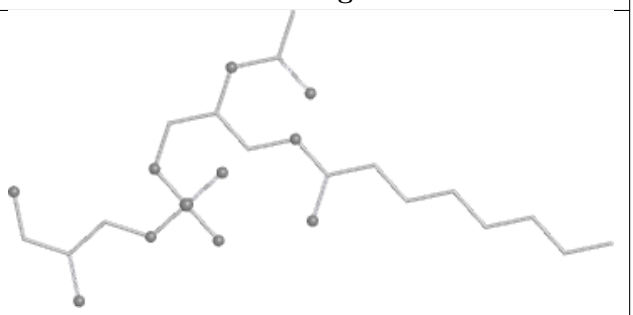
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Bond angles

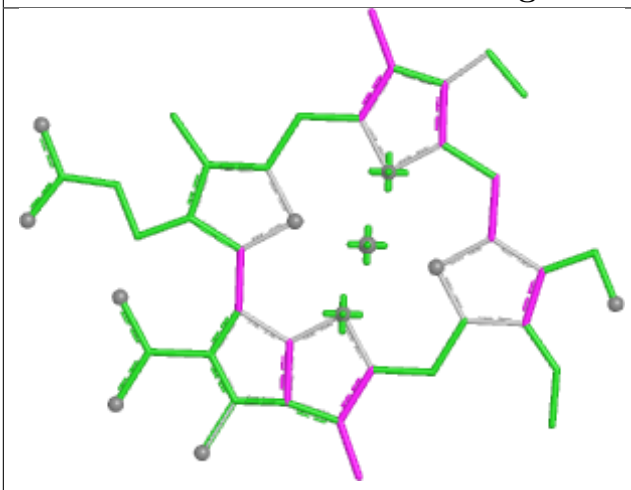


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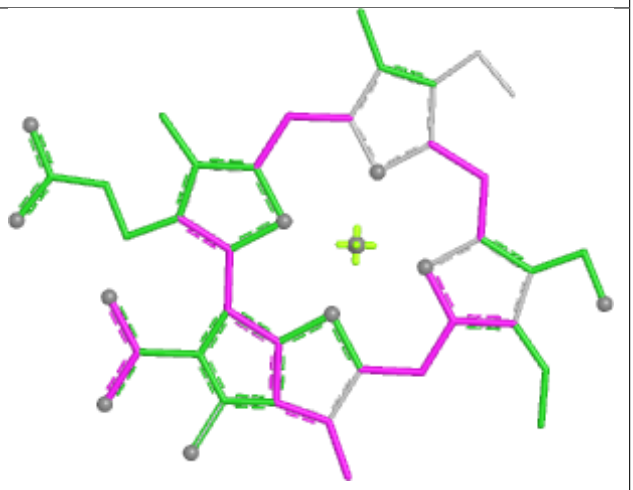


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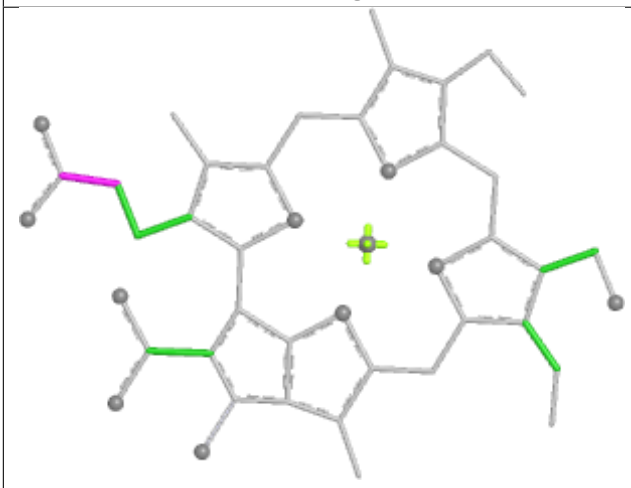
Ligand CHL 44 601



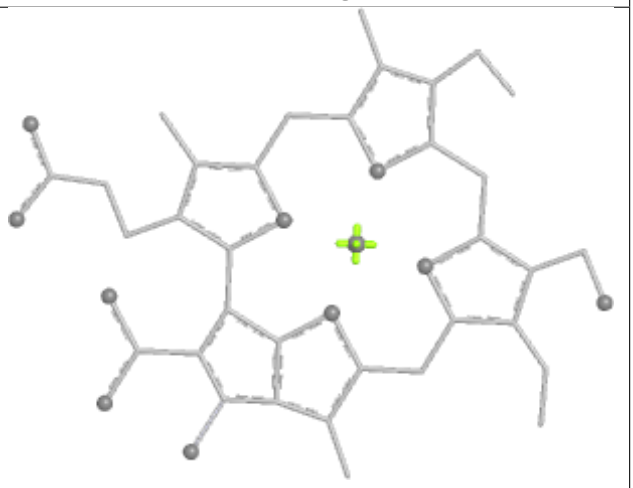
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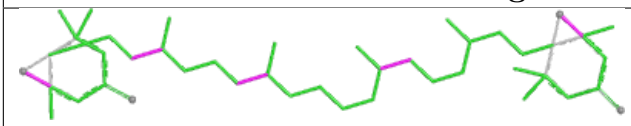


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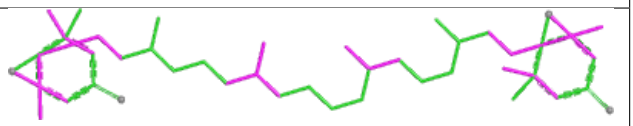


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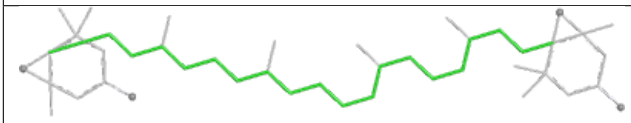
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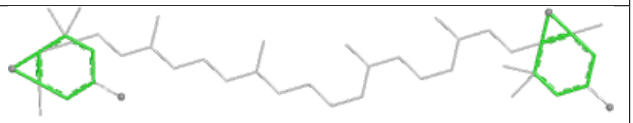
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Bond angles

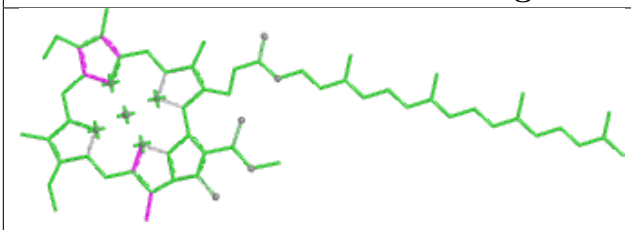


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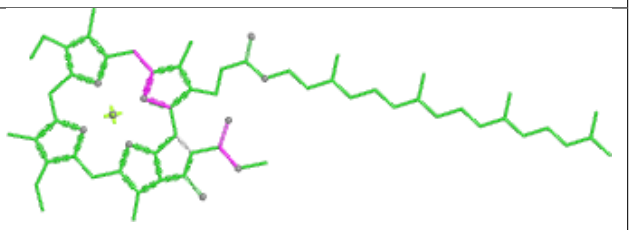


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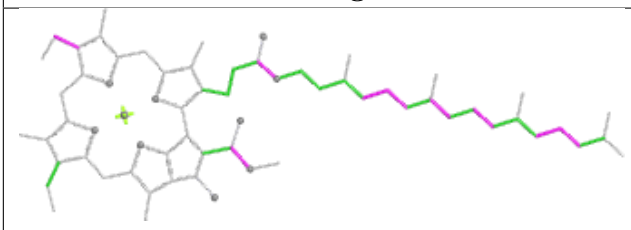
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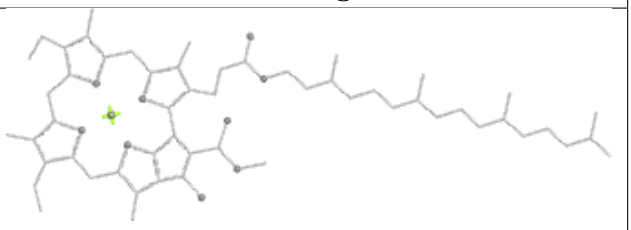
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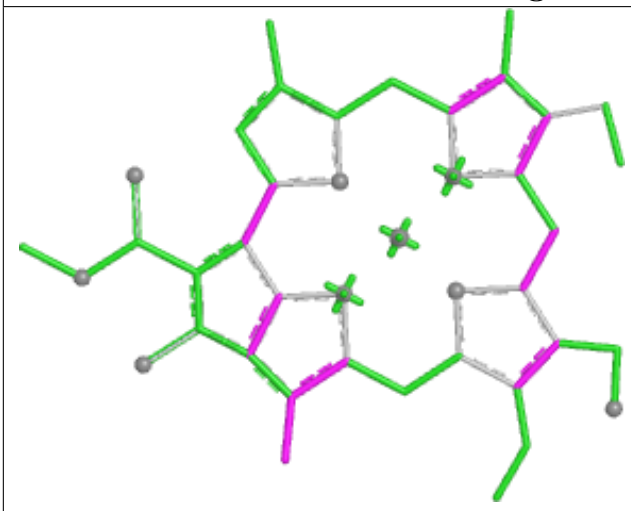


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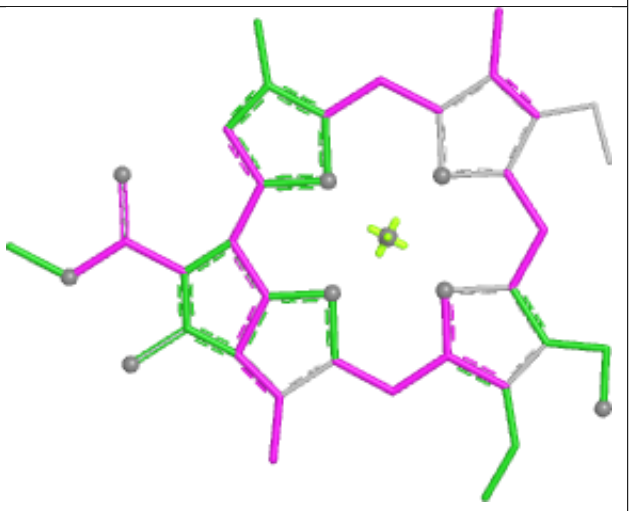


Rings

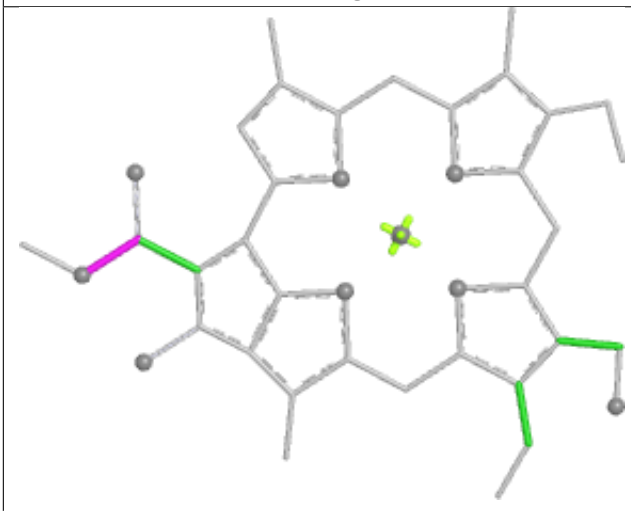
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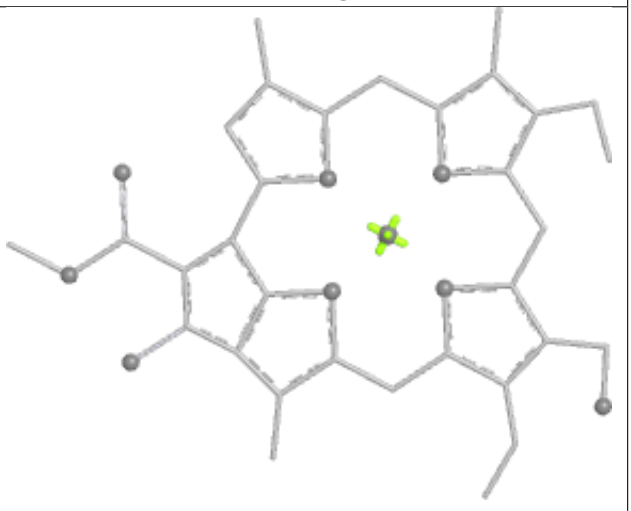
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Bond angles

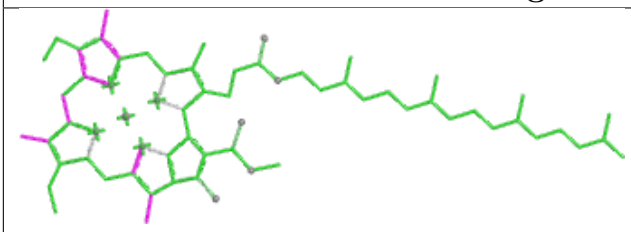


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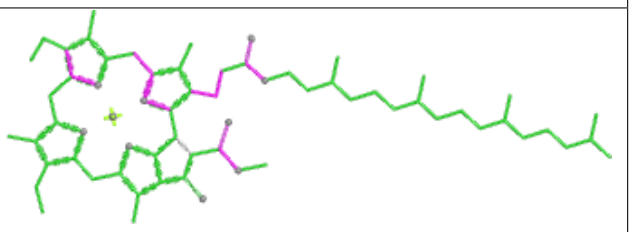


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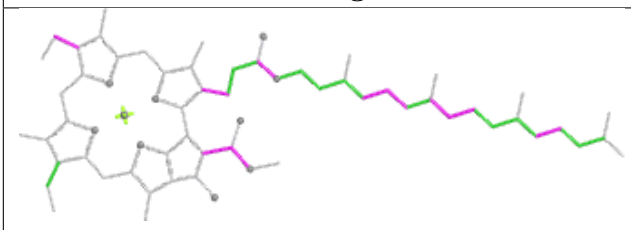
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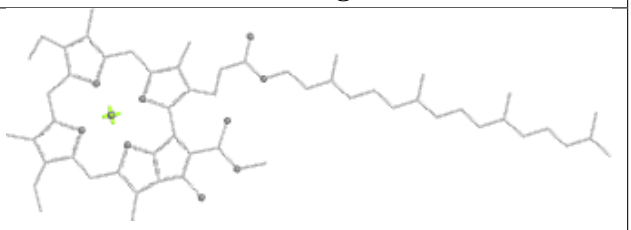
Bond lengths



Bond angles

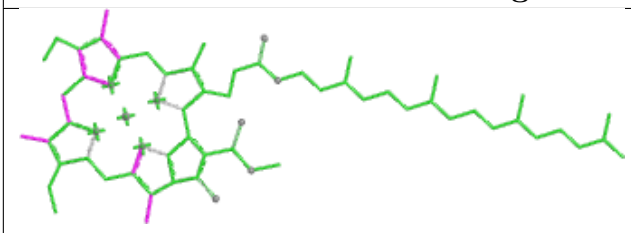


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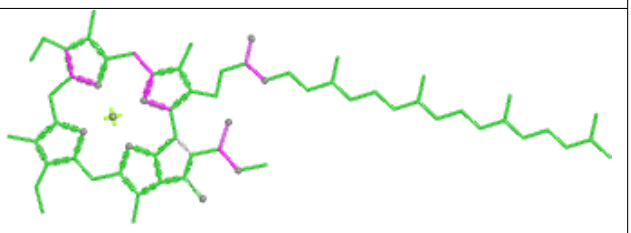


Rings

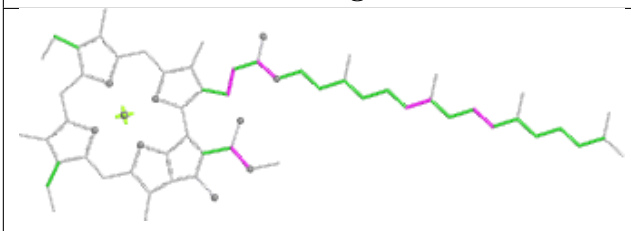
Ligand CLA CC 511



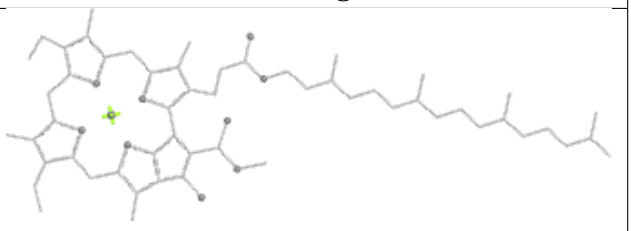
Bond lengths



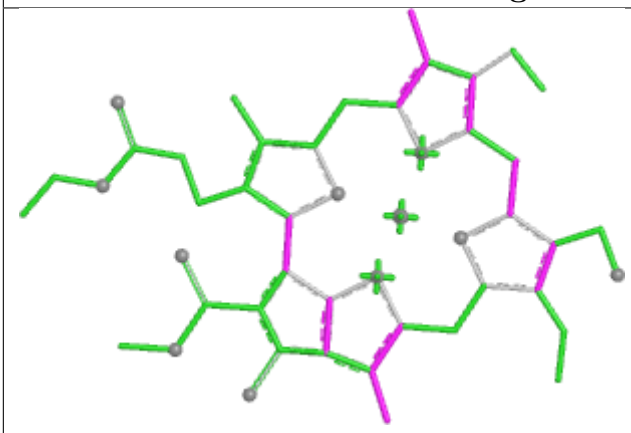
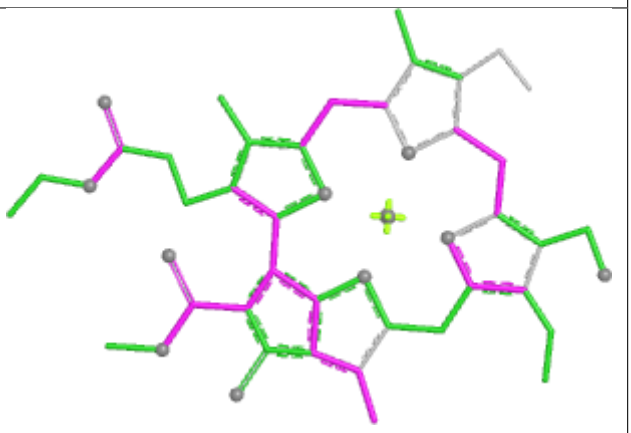
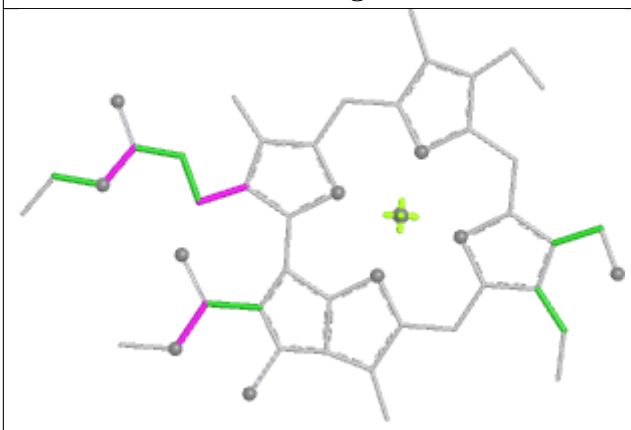
Bond angles



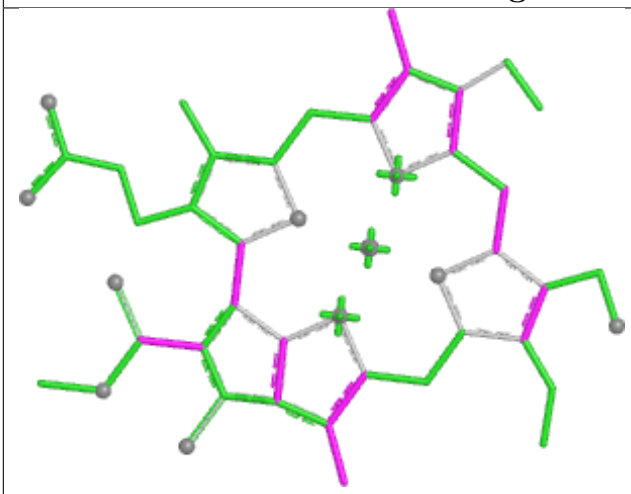
Torsions



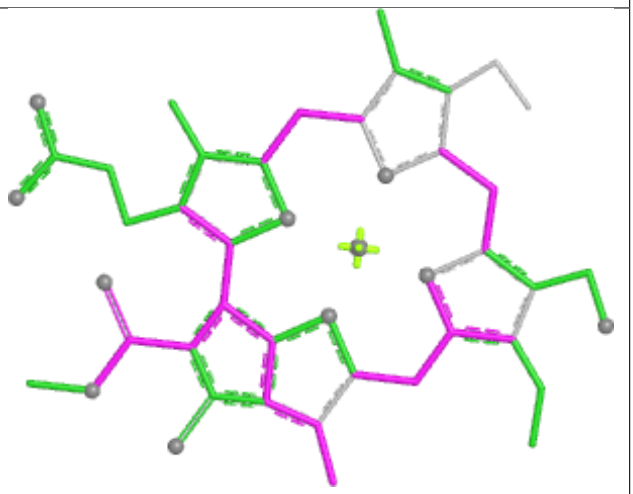
Rings

Ligand CHL YY 605	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

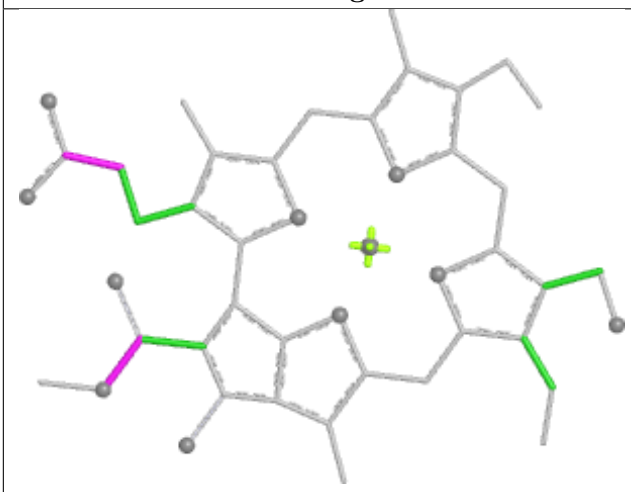
Ligand CHL GG 607



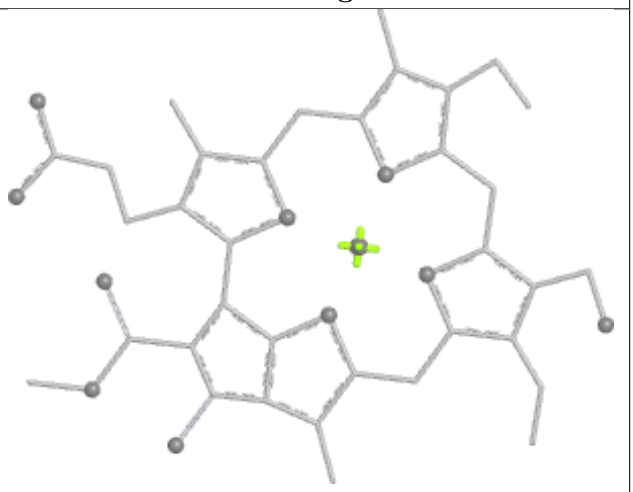
Bond lengths



Bond angles

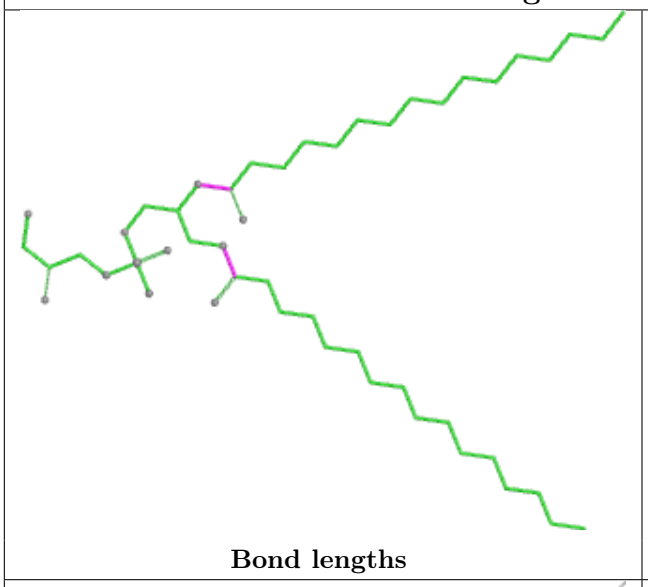


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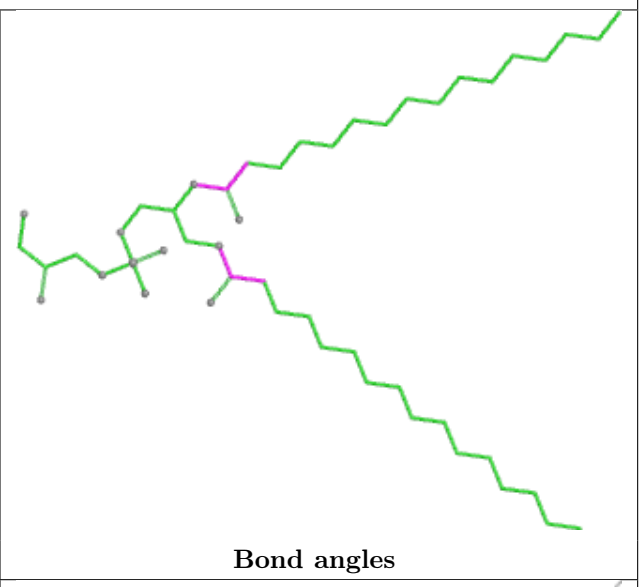


Rings

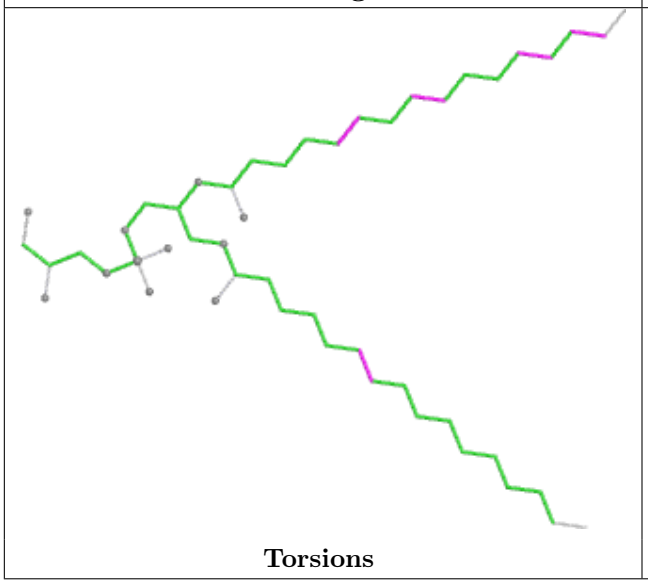
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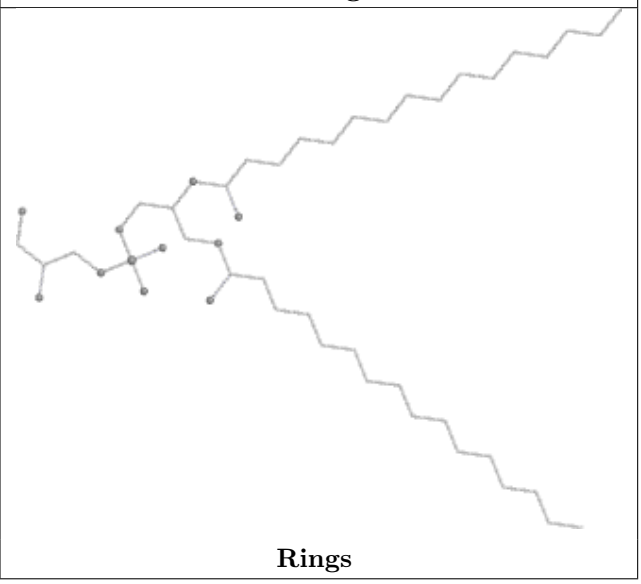
Bond lengths



Bond angles

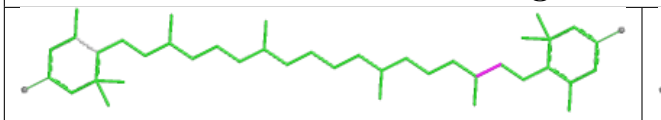


Torsions



Rings

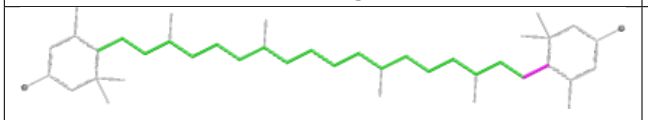
Ligand LUT s 615



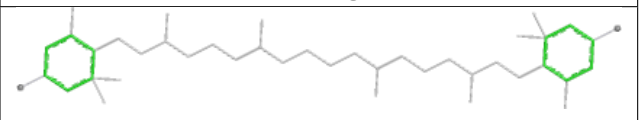
Bond lengths



Bond angles

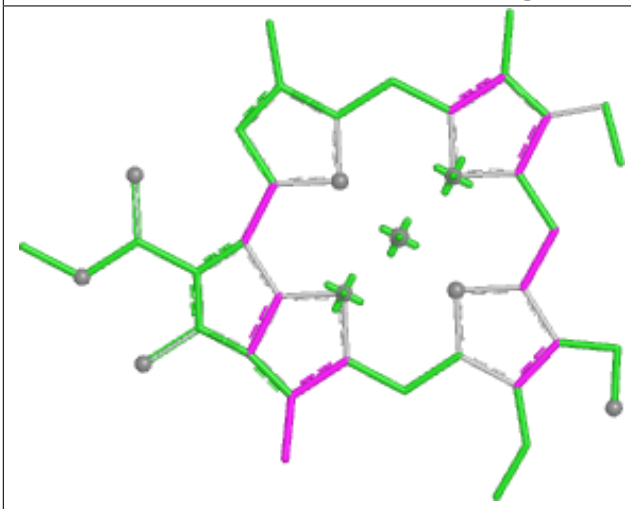


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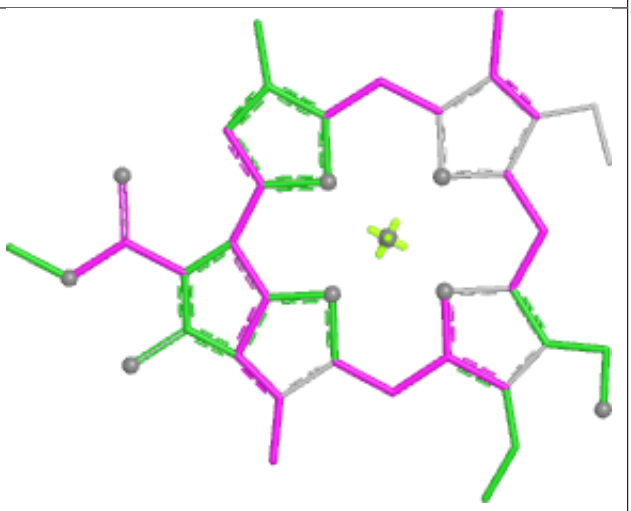


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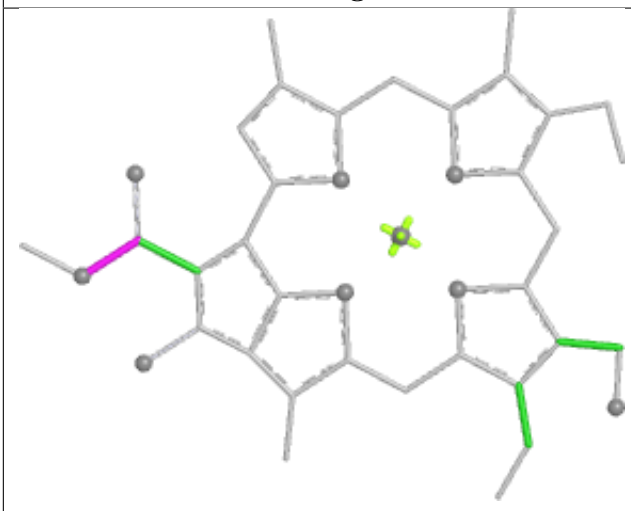
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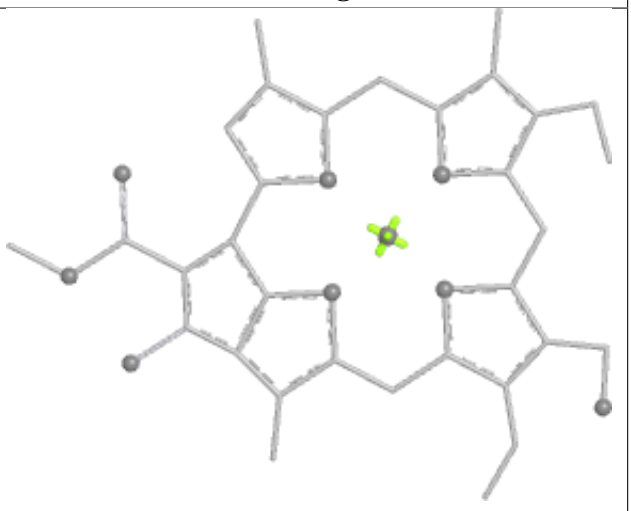
Bond lengths



Bond angles

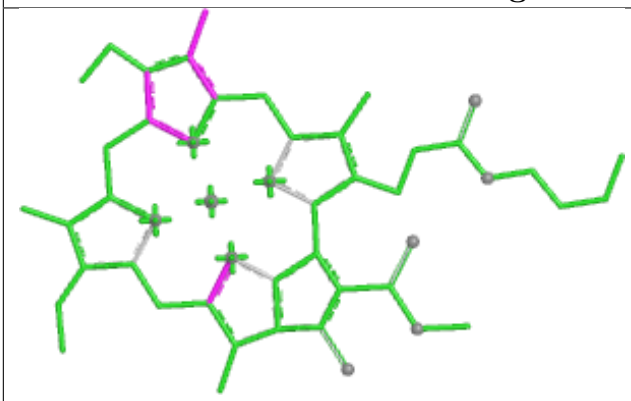


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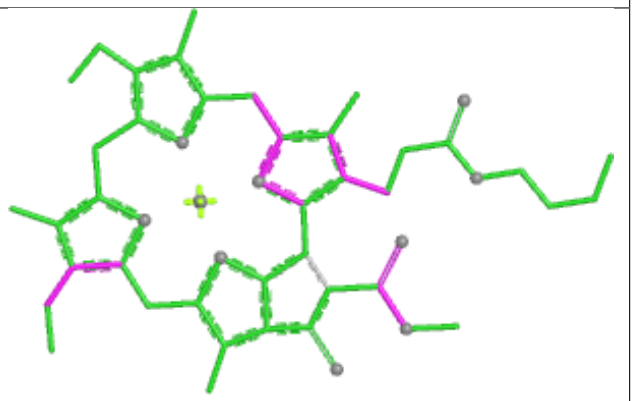


Rings

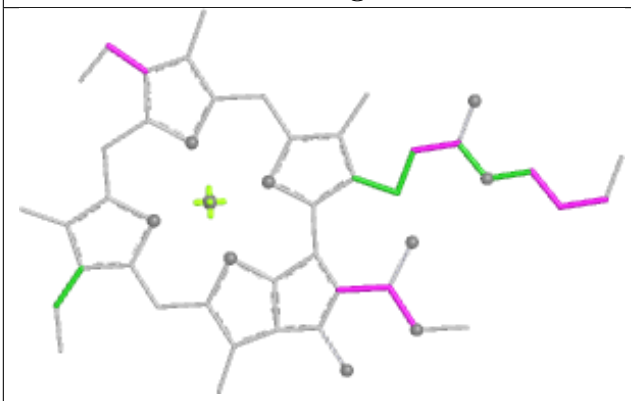
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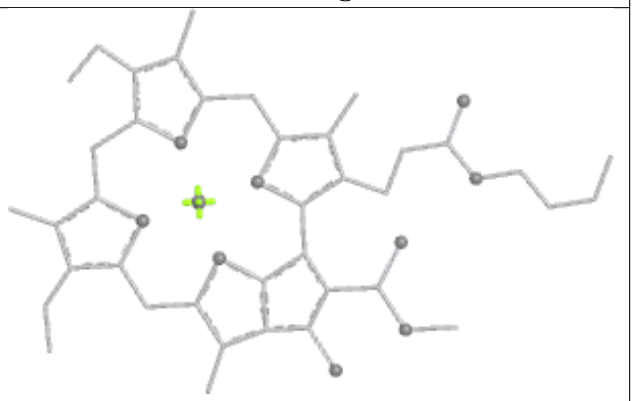
Bond lengths



Bond angles

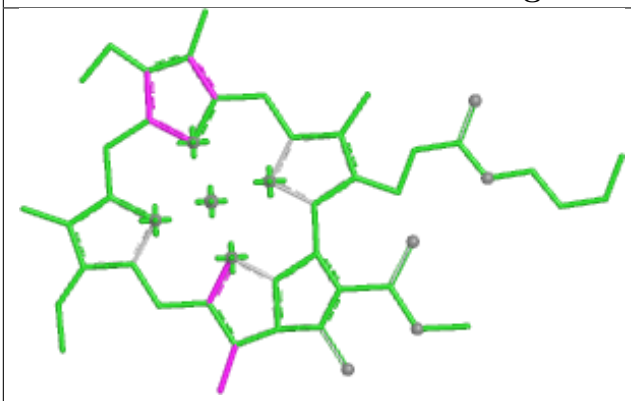


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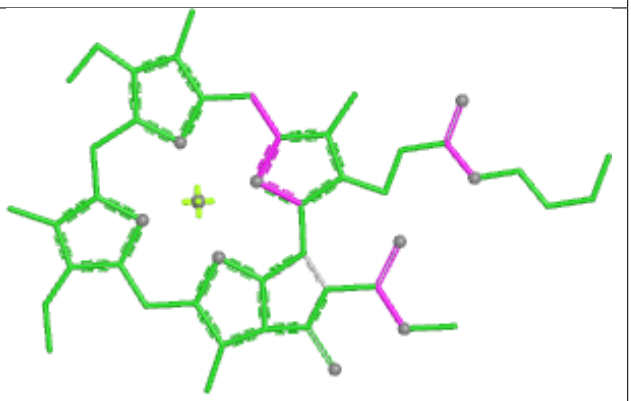


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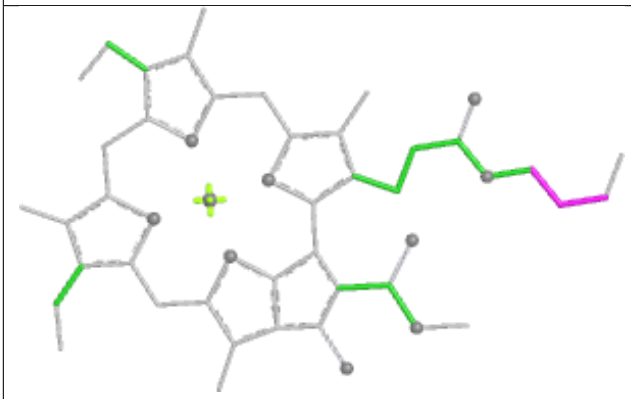
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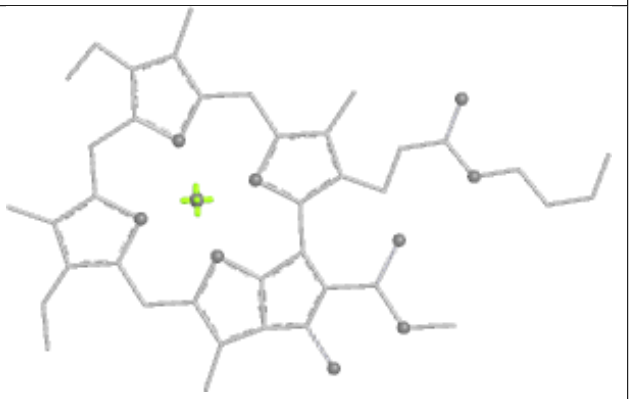
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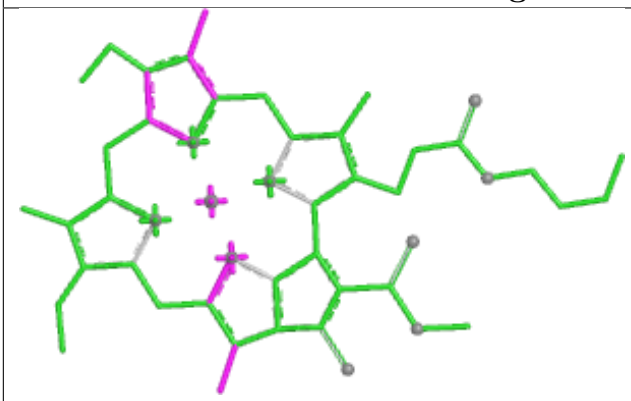


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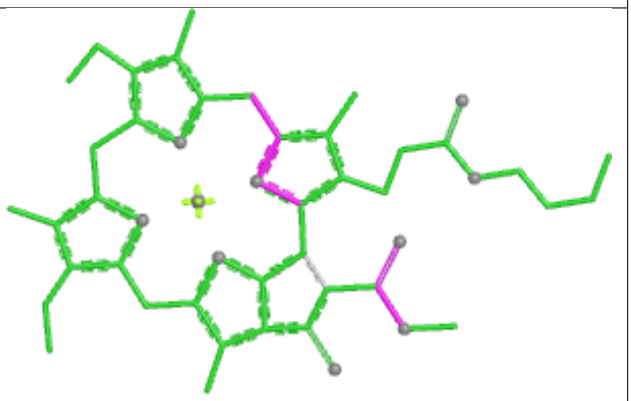


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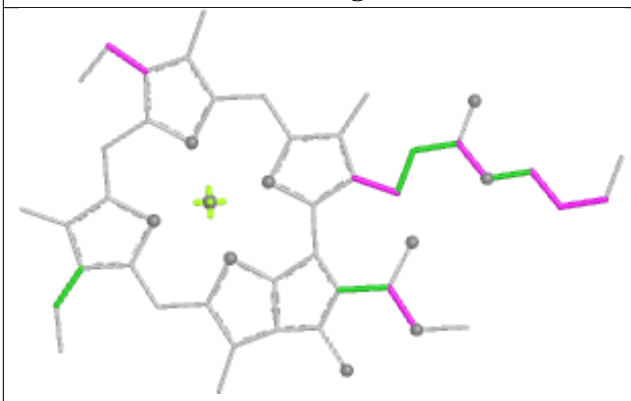
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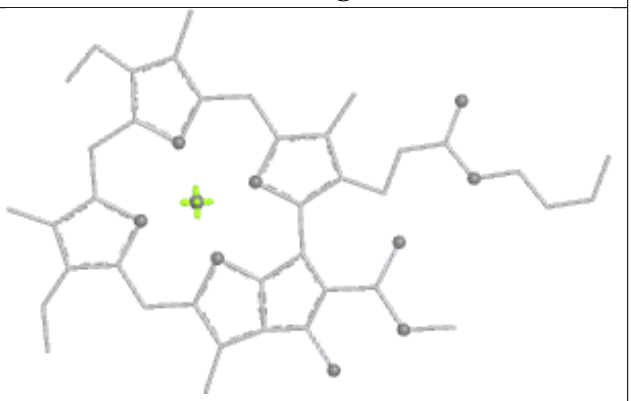
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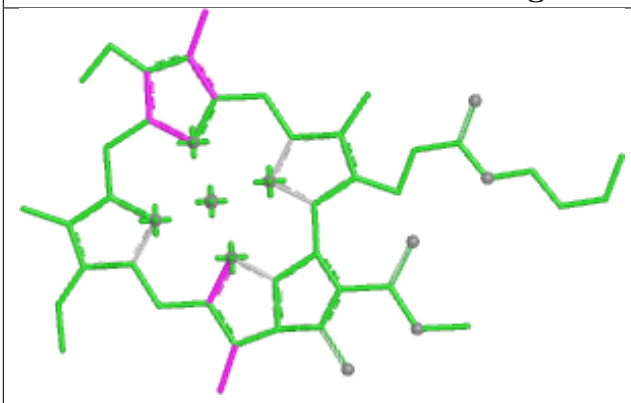


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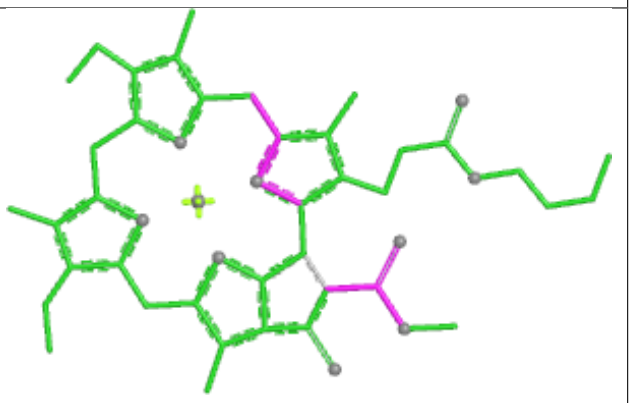


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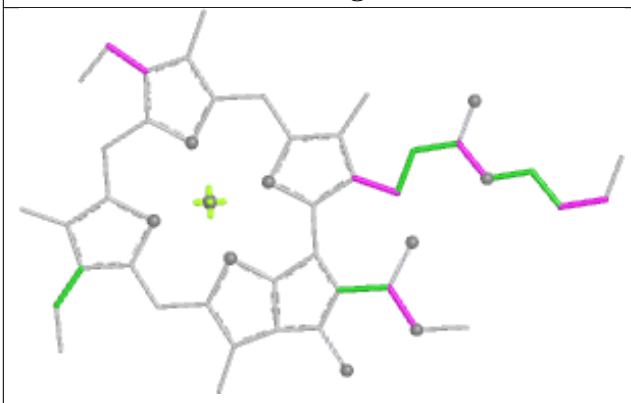
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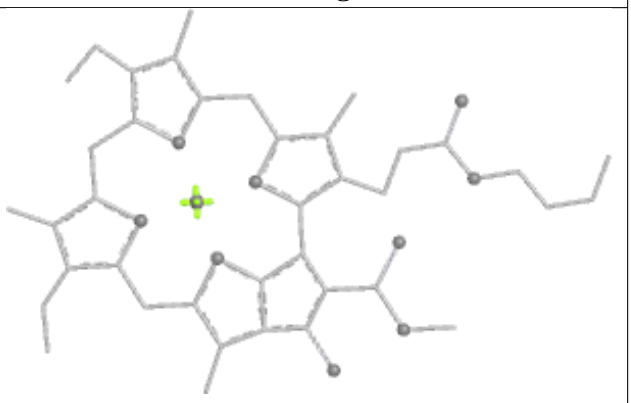
Bond lengths



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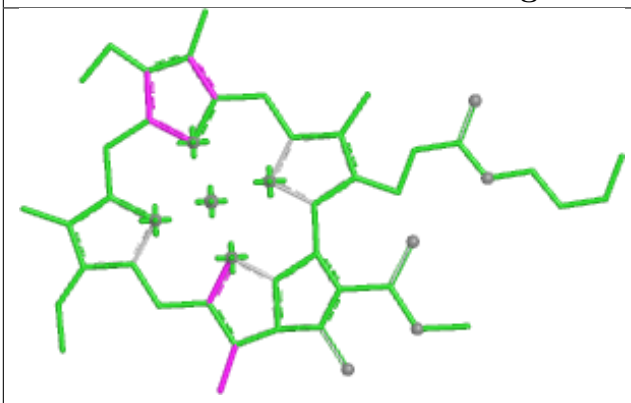


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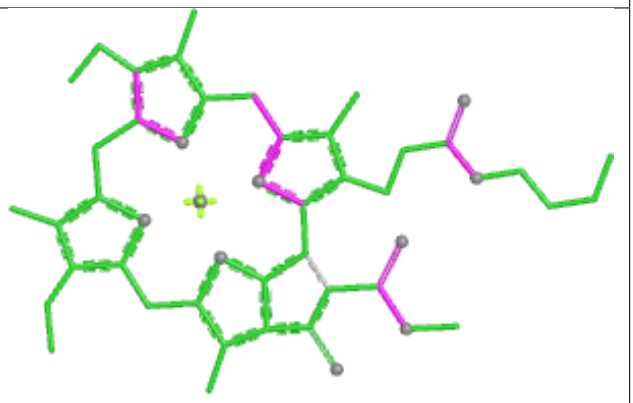


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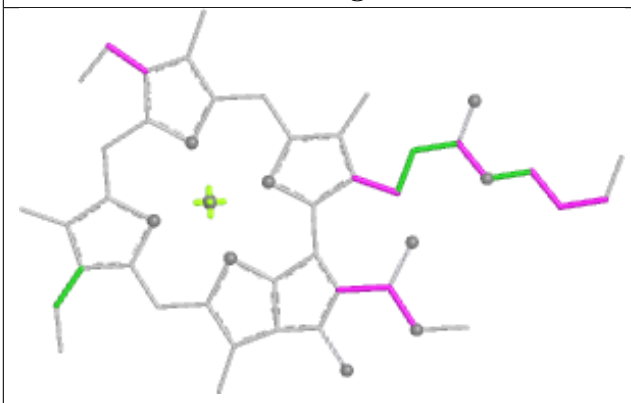
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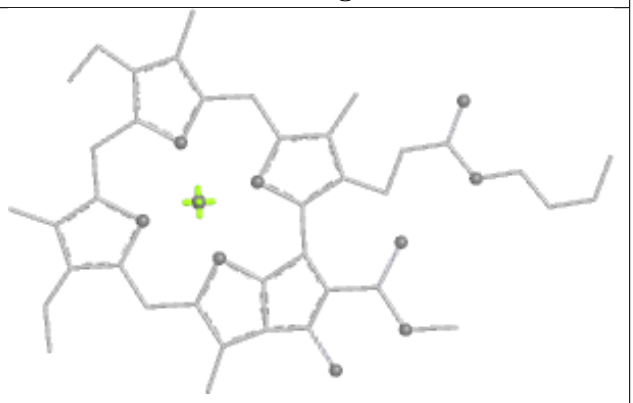
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Bond angles

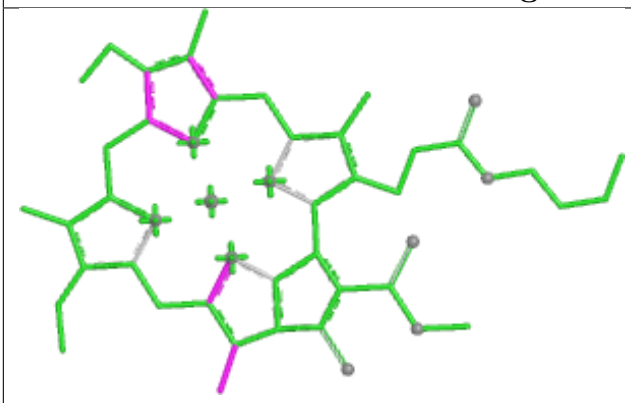


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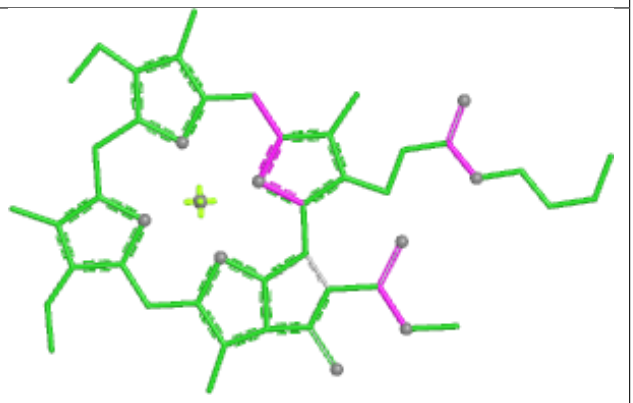


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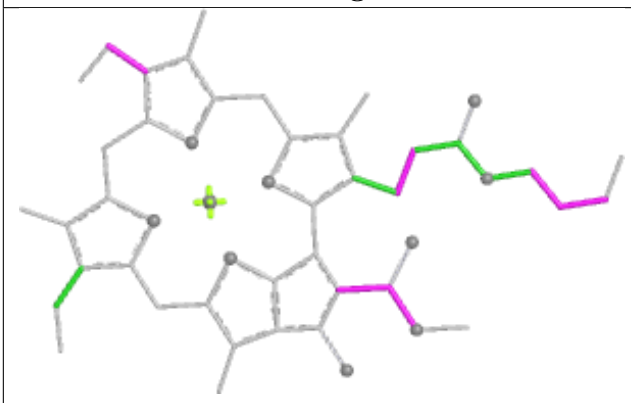
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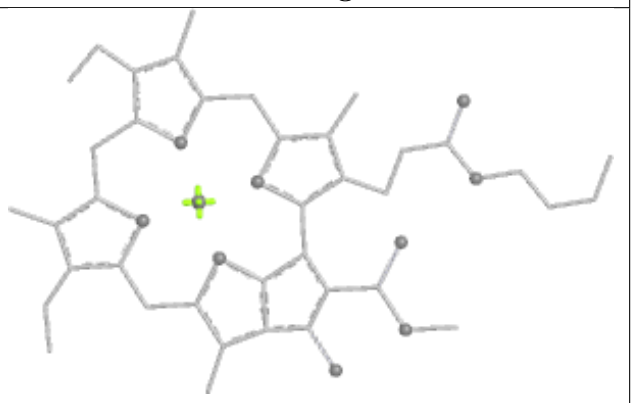
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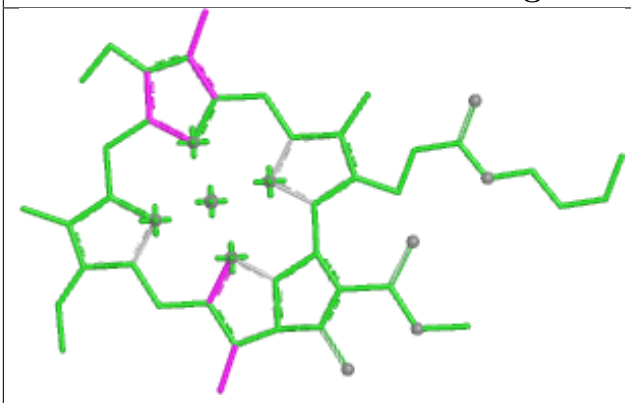


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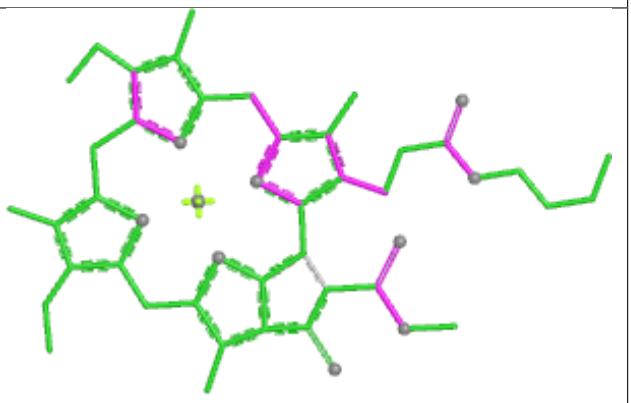


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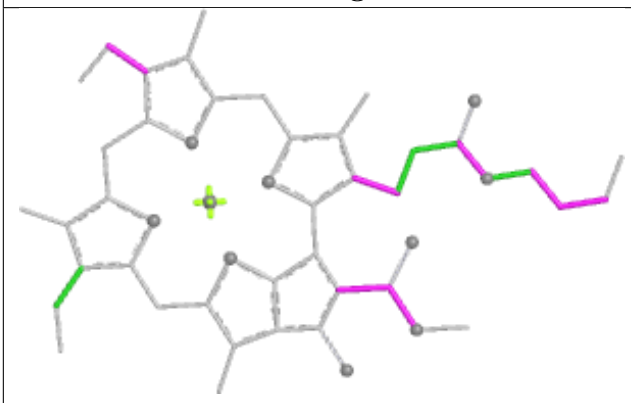
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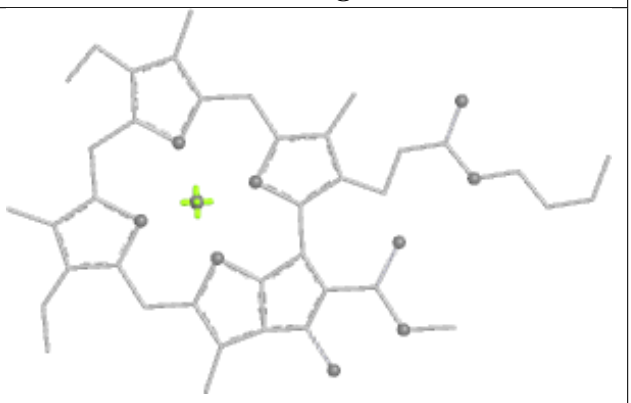
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Bond angles

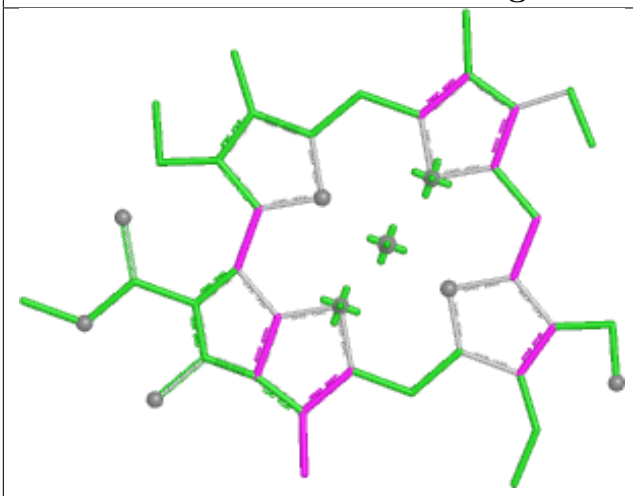


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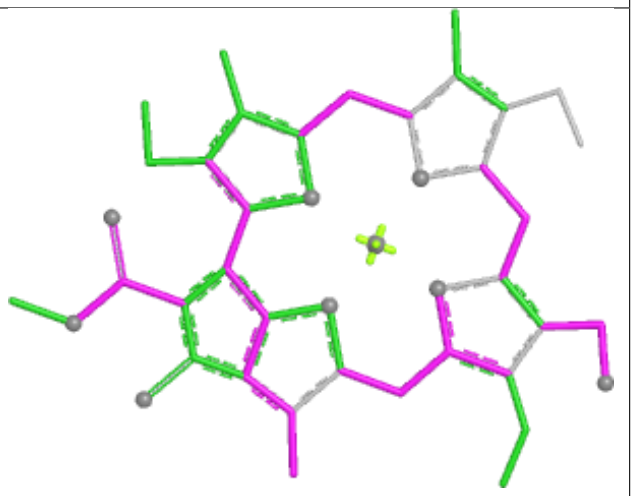


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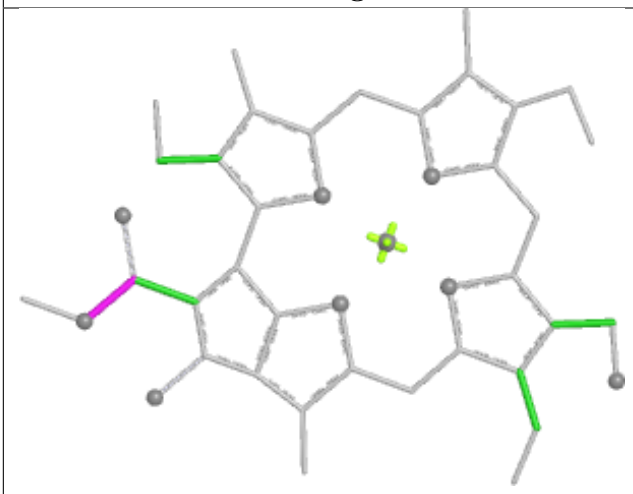
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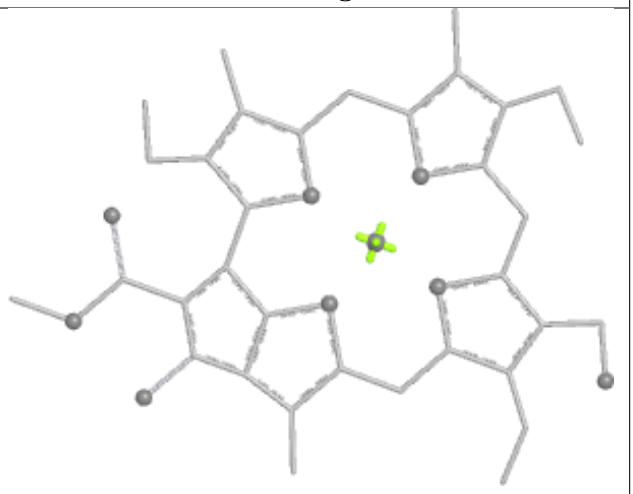
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Bond angles

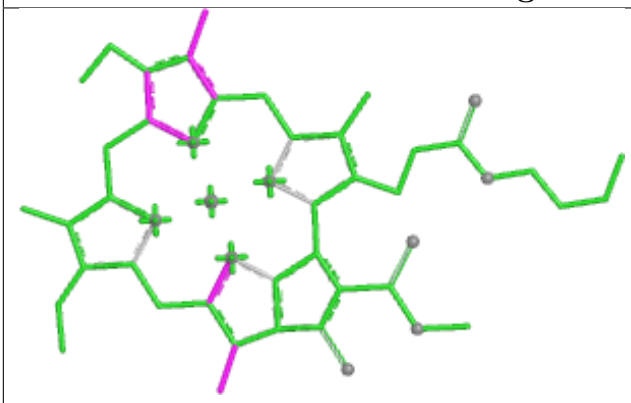


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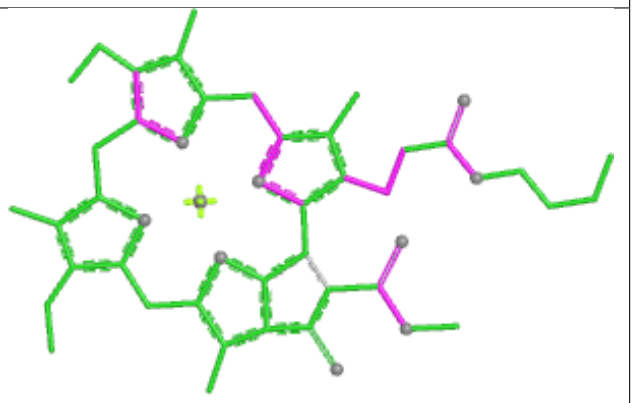


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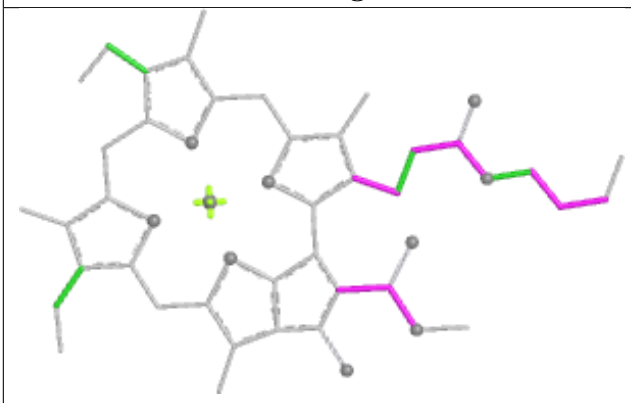
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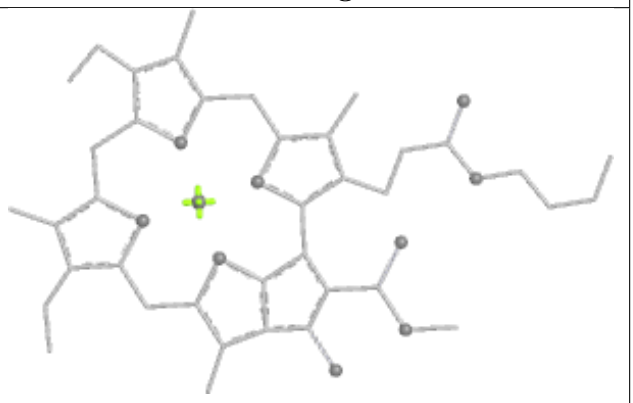
Bond lengths



Bond angles

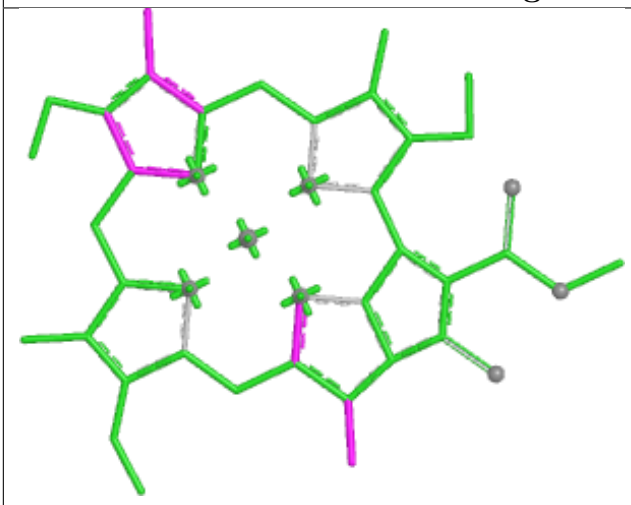


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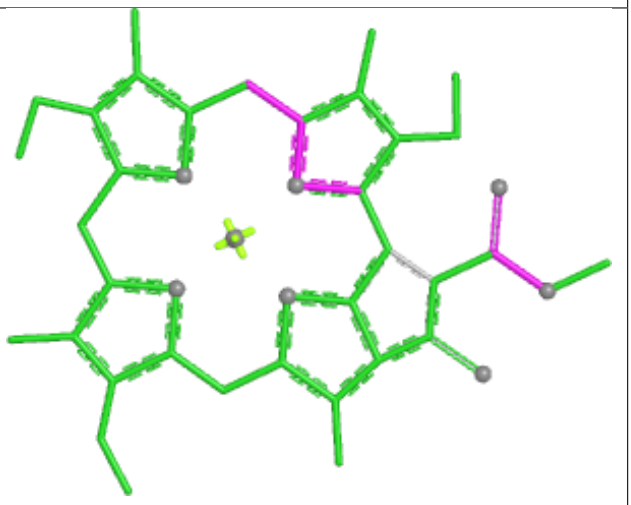


Rings

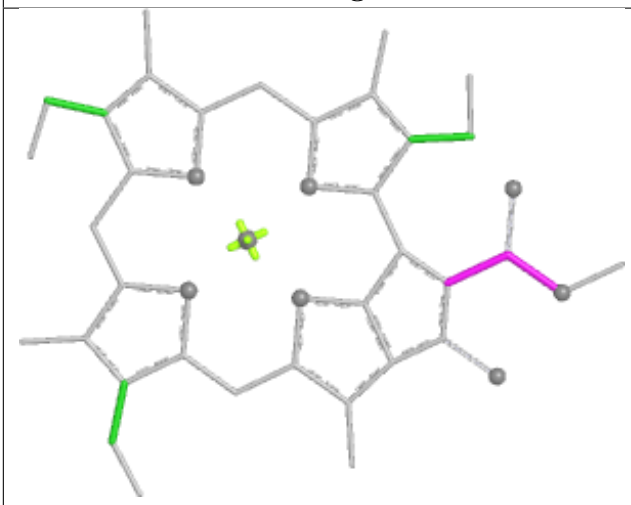
Ligand CLA N 603



Bond lengths



Bond angles

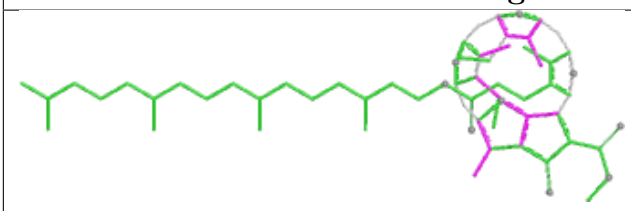


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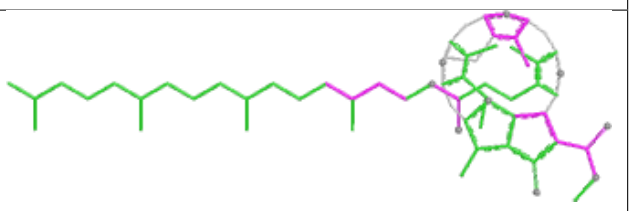


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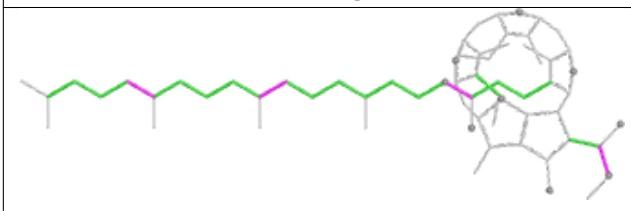
Ligand PHO AA 407



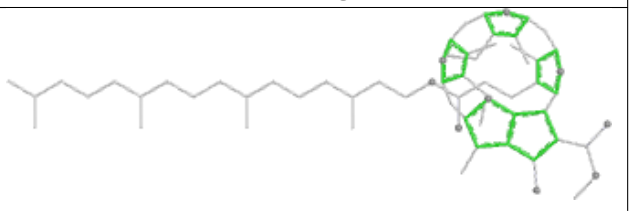
Bond lengths



Bond angles

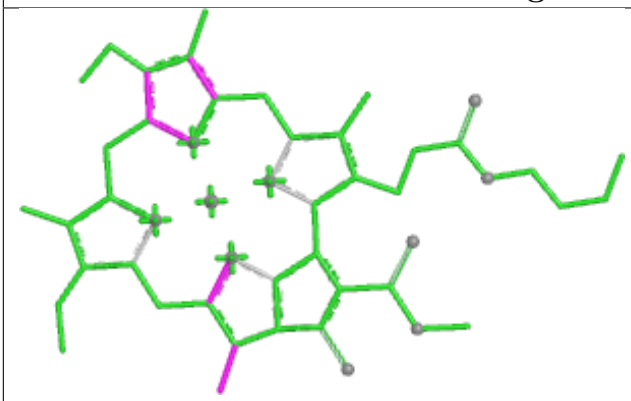


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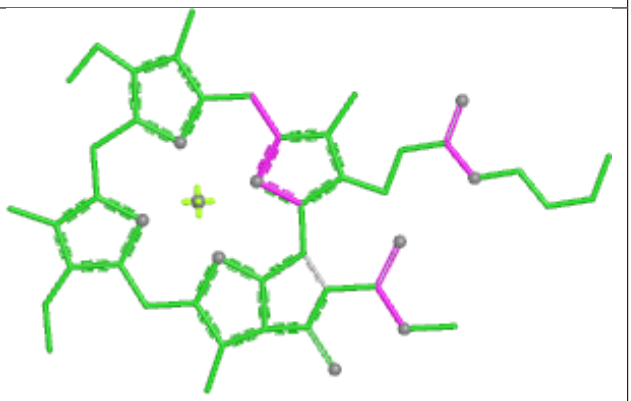


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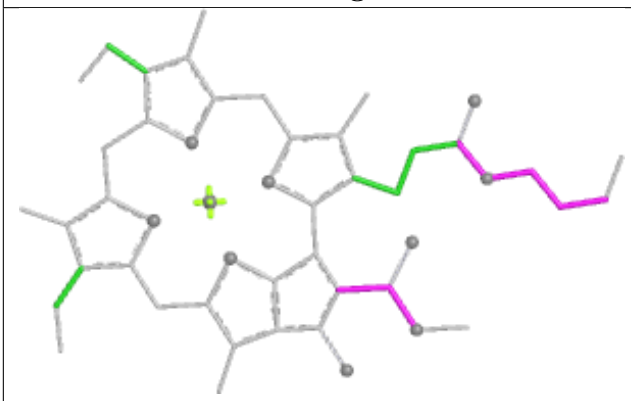
Ligand CLA S 611



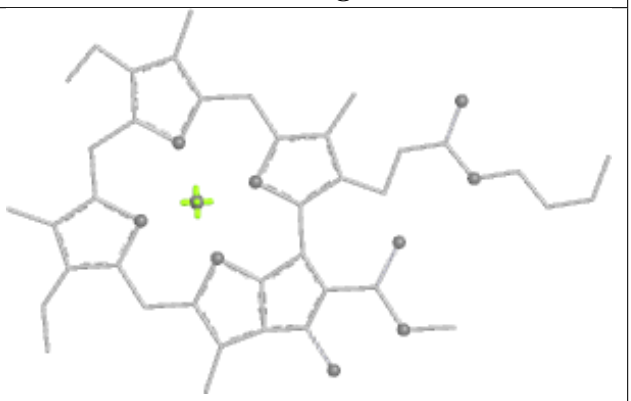
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Bond angles

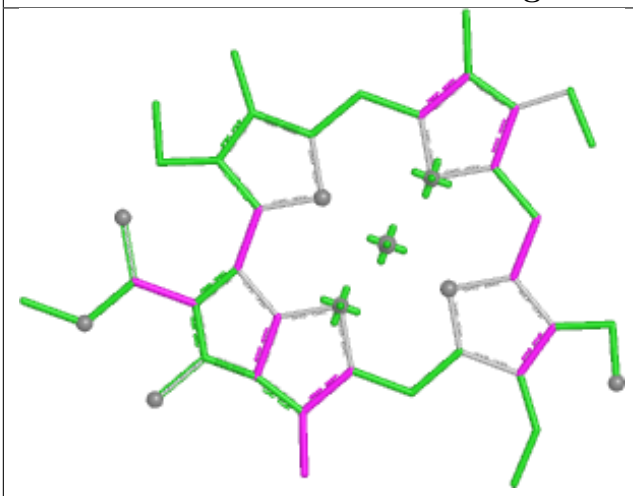


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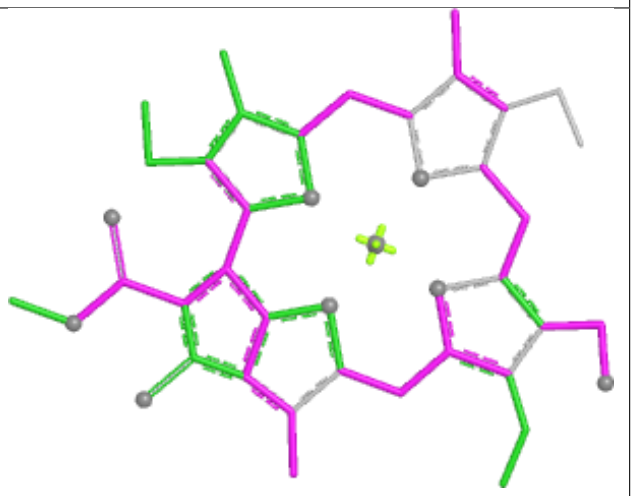


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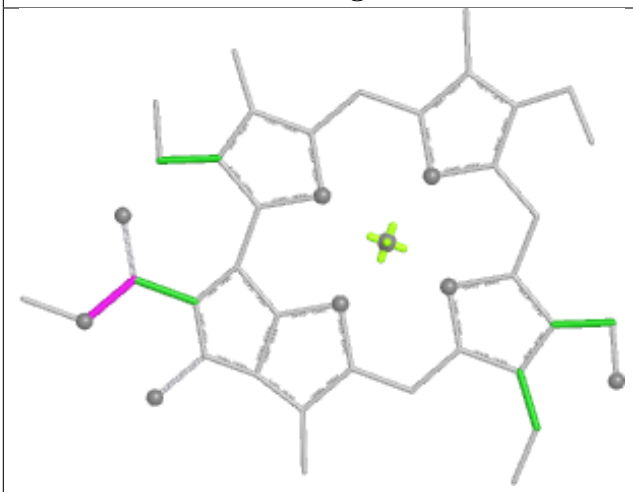
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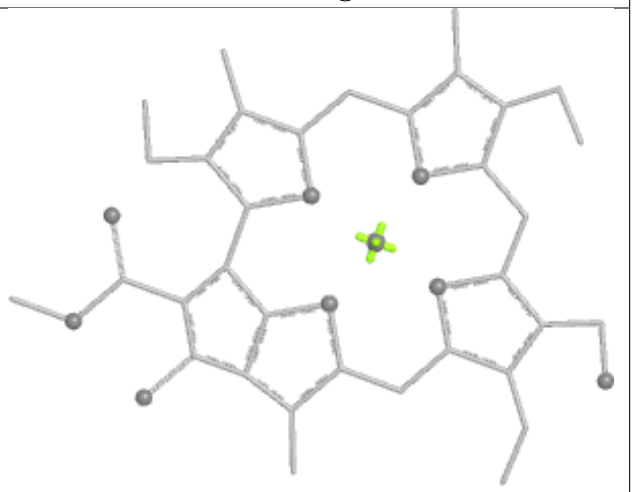
Bond lengths



Bond angles

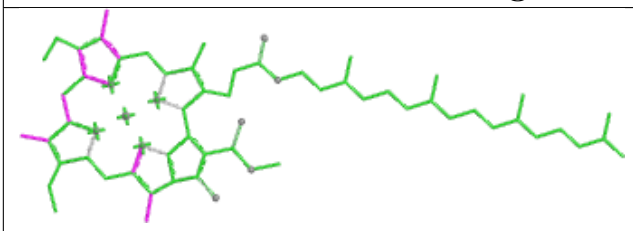


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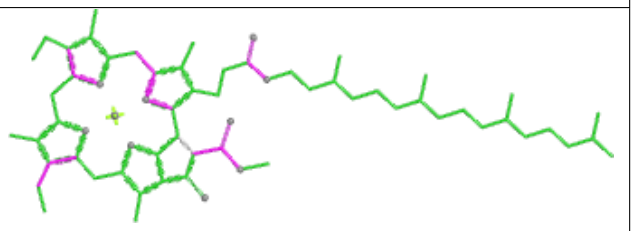


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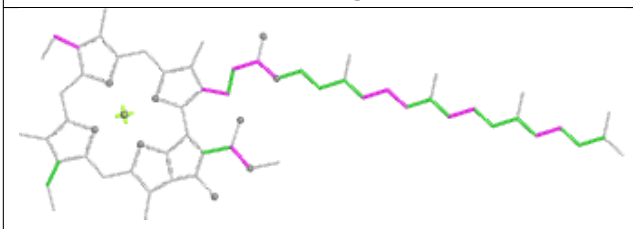
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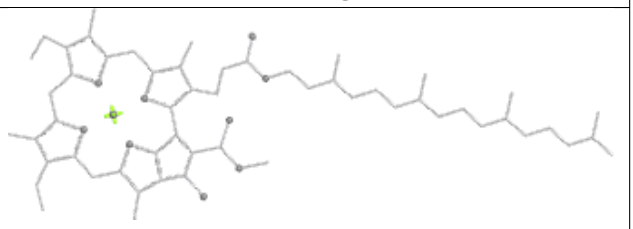
Bond lengths



Bond angles

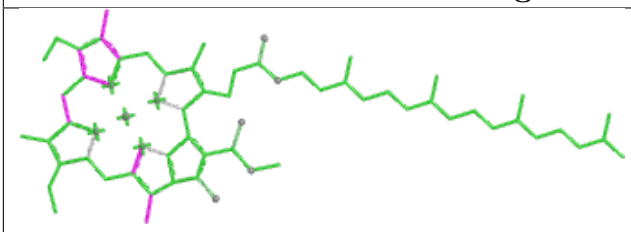


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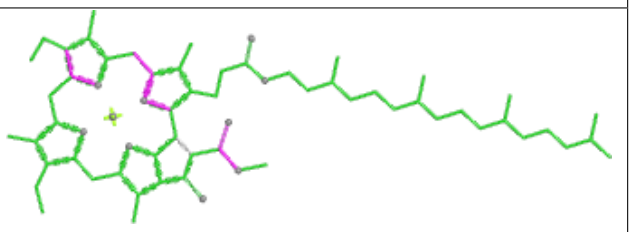


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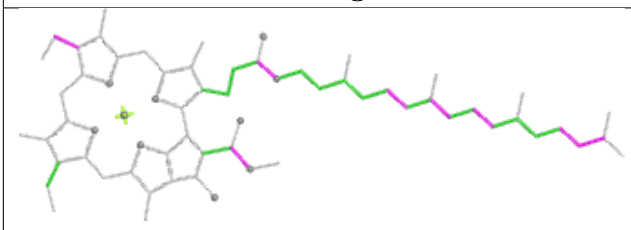
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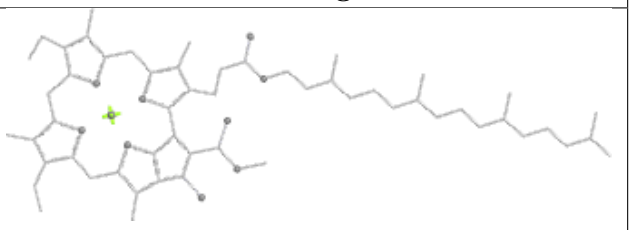
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Bond angles

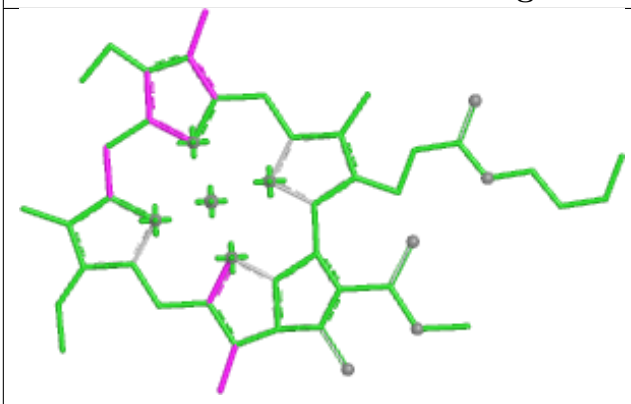


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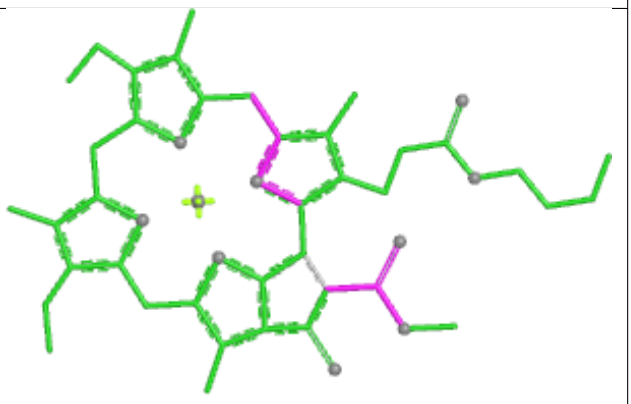


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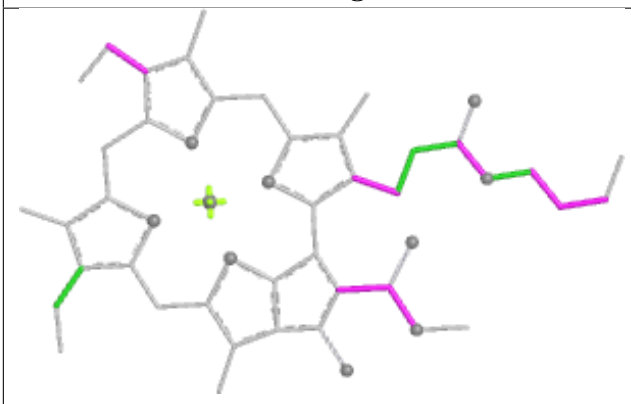
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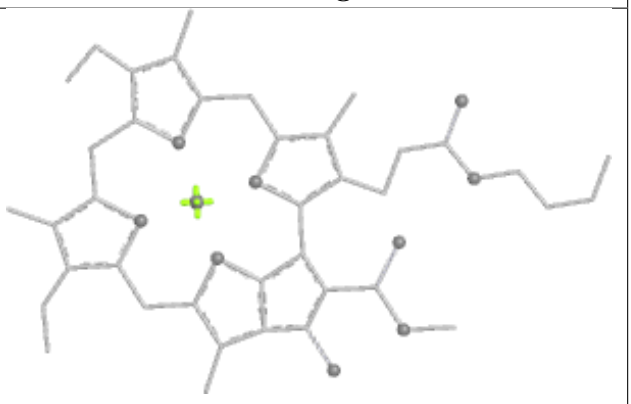
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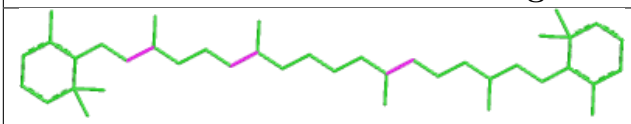


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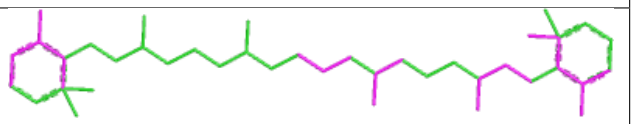


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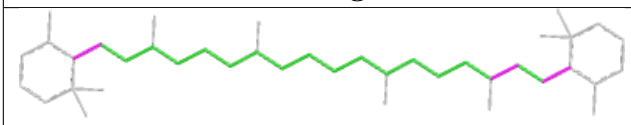
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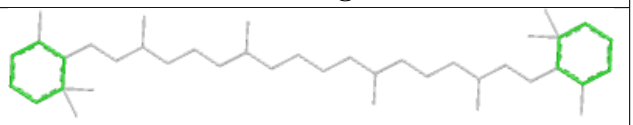
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Bond angles

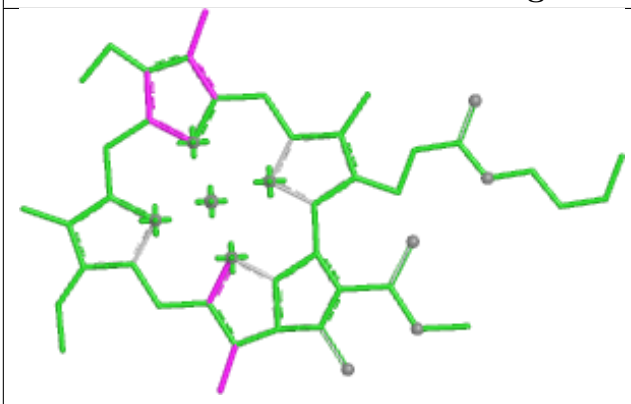


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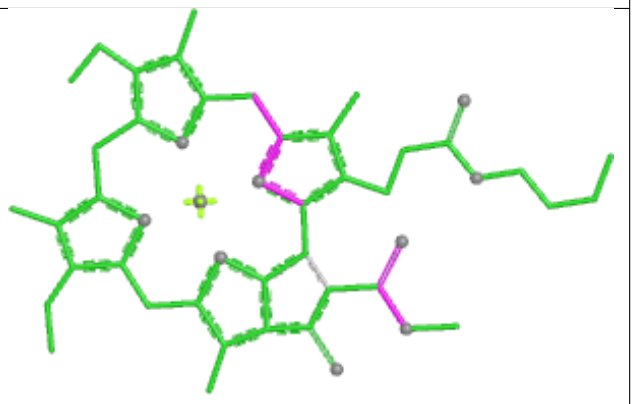


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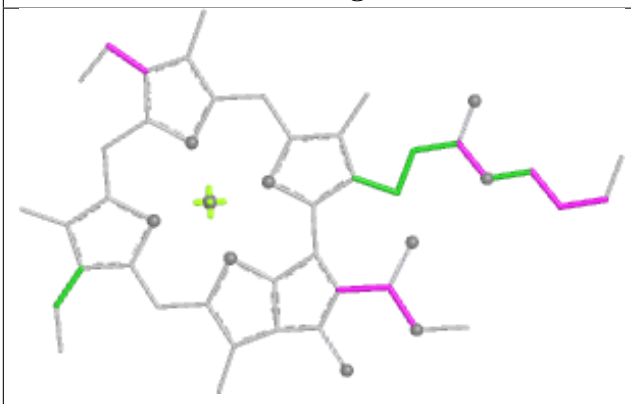
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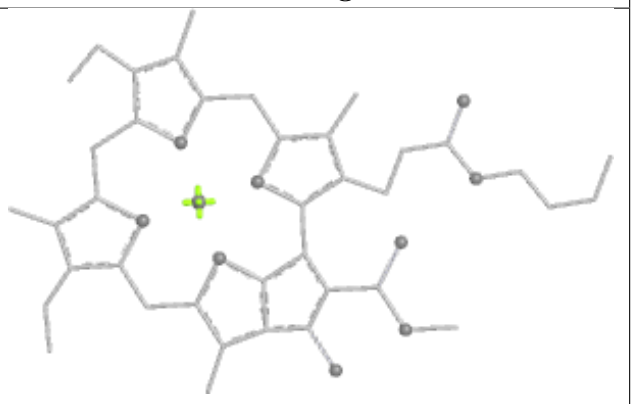
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Bond angles

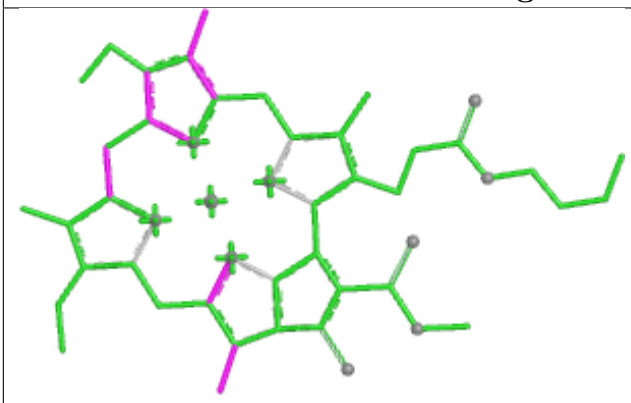


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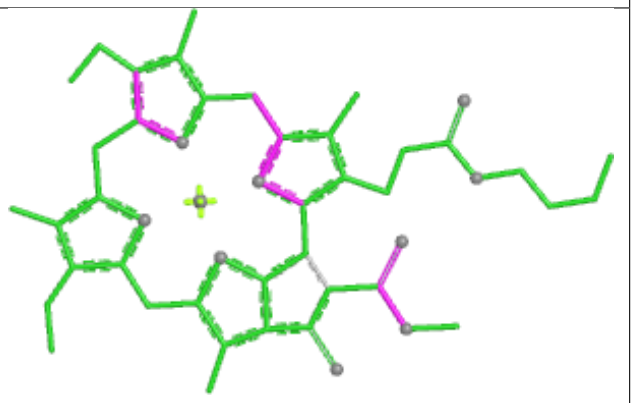


Rings

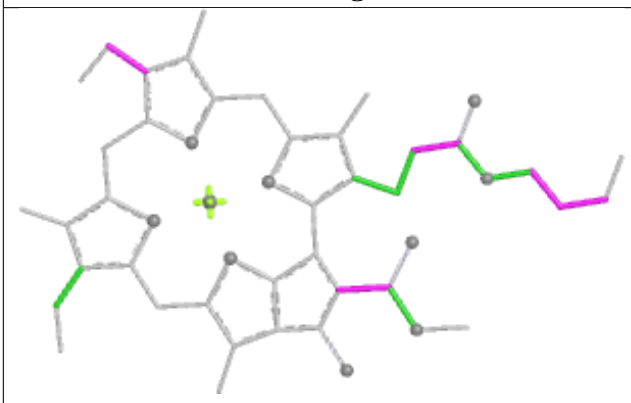
Ligand CLA Rr 603



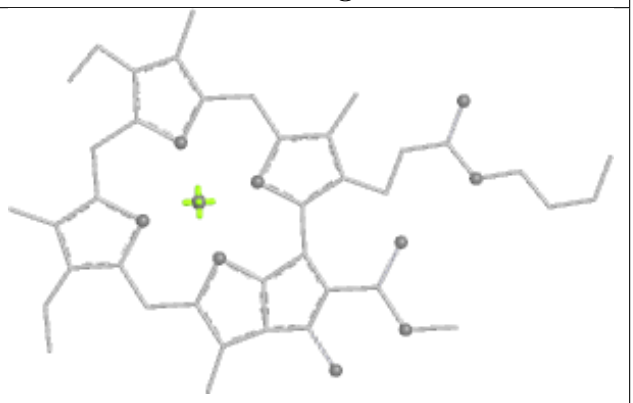
Bond lengths



Bond angles

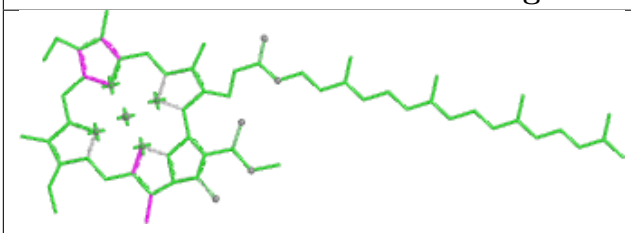


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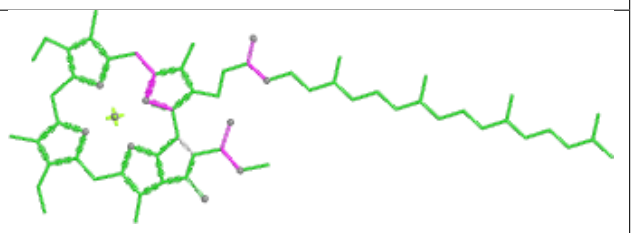


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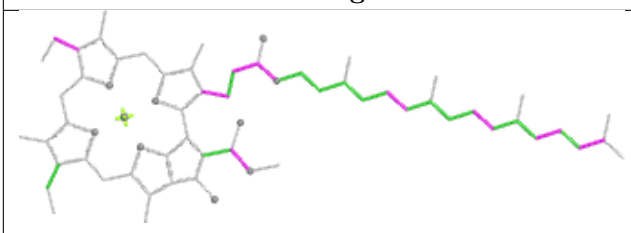
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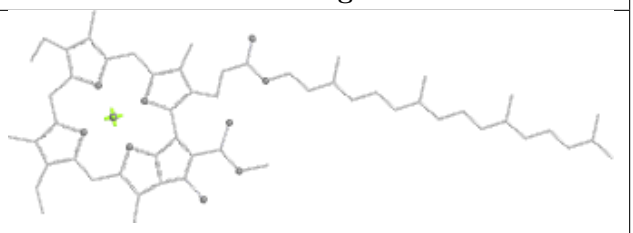
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Bond angles

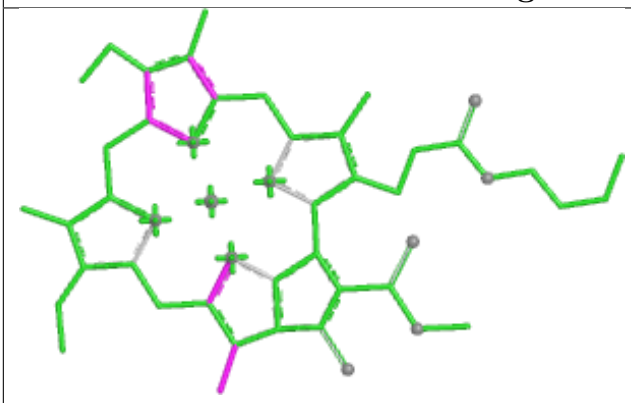


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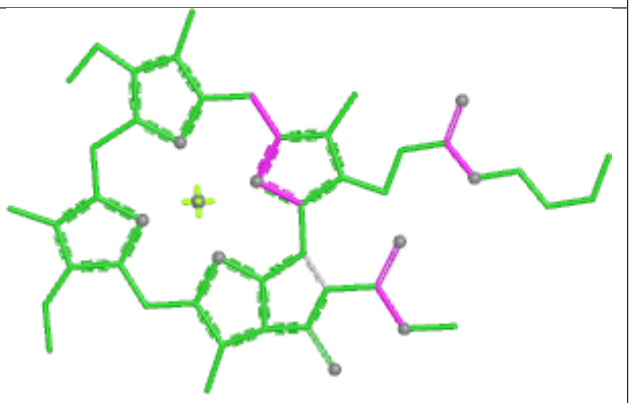


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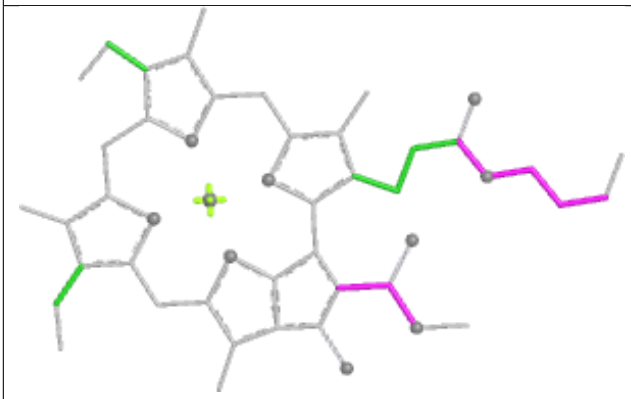
Ligand CLA SS 312



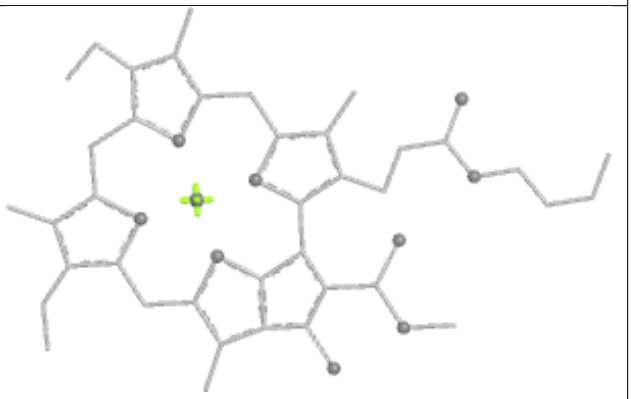
Bond lengths



Bond angles



Torsions

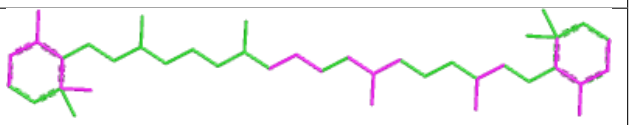


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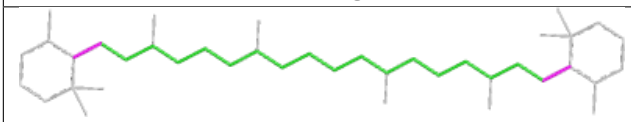
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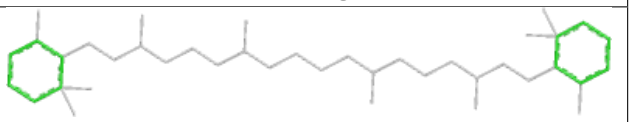
Bond lengths



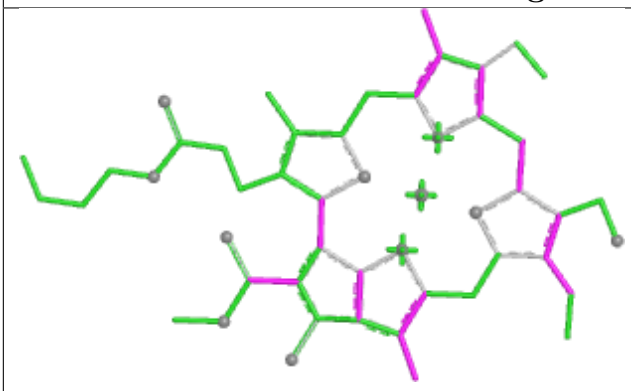
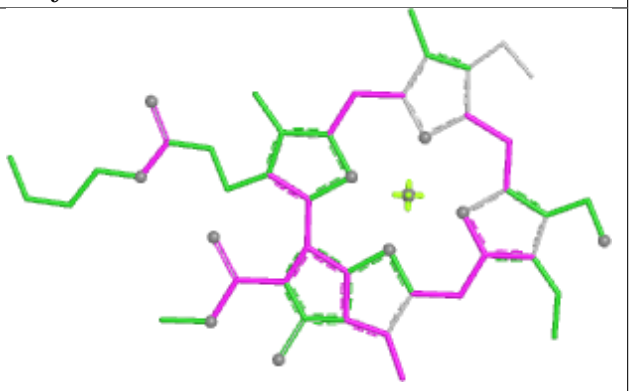
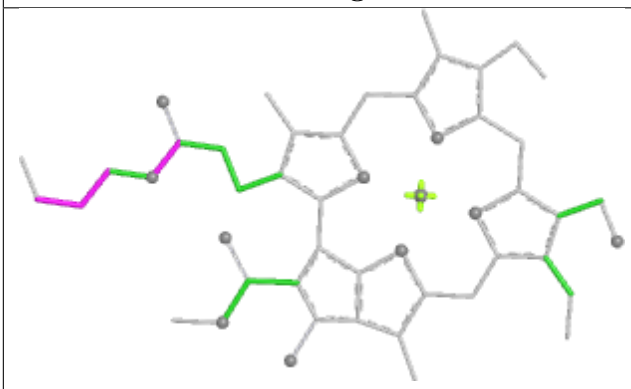
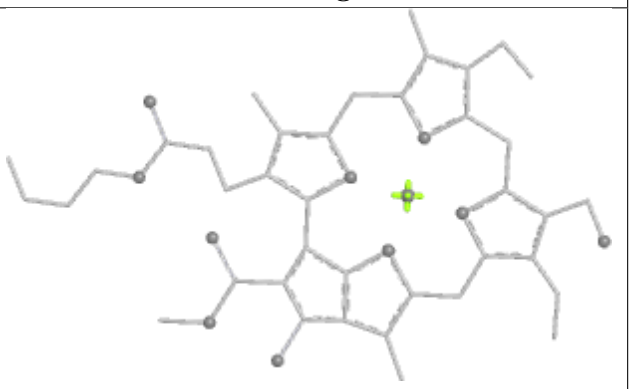
Bond angles

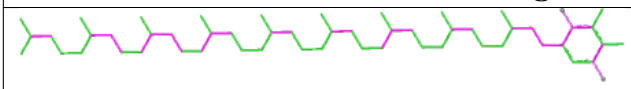
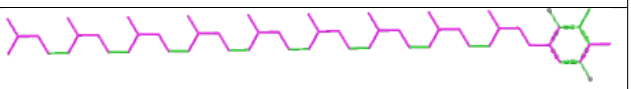
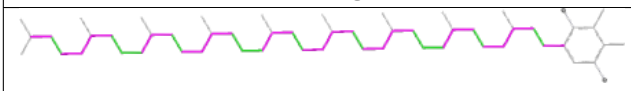
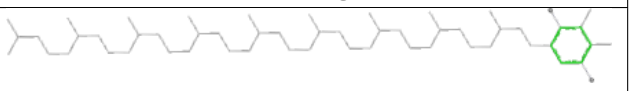


Torsions

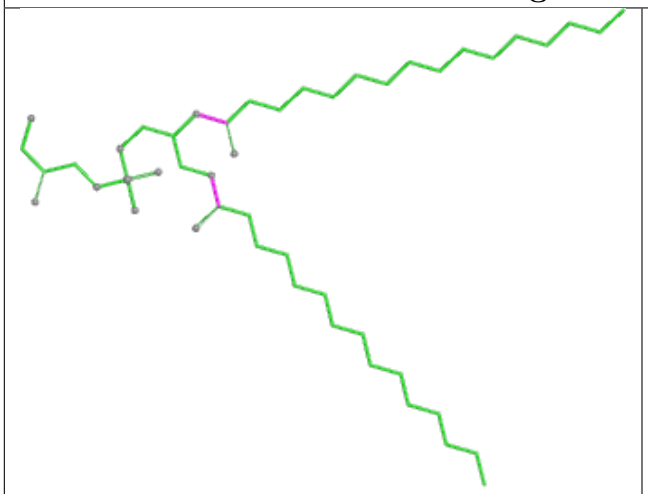


Rings

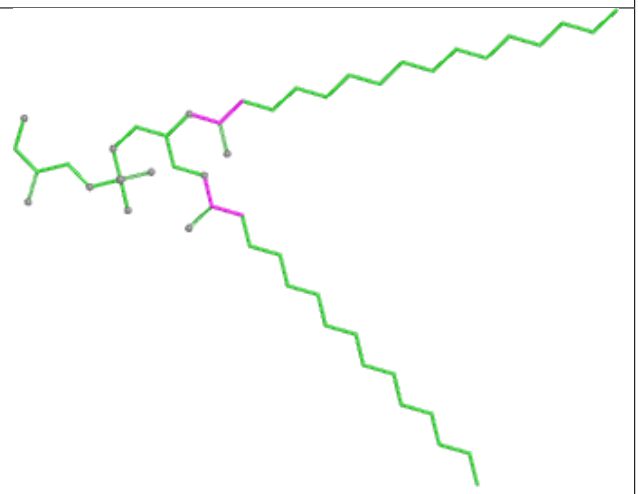
Ligand CHL y 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

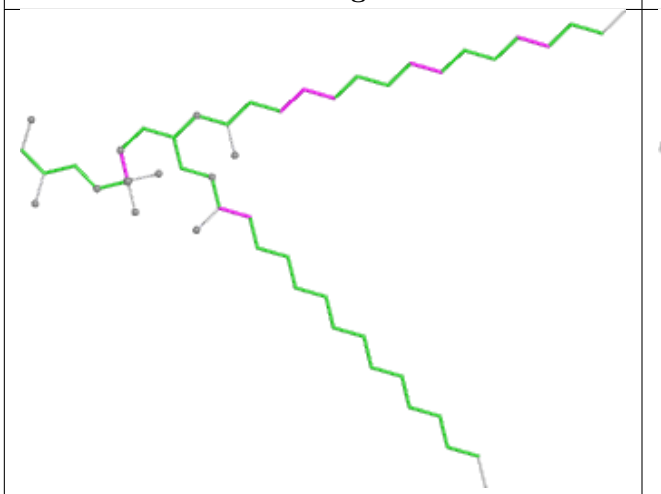
Ligand LHG s 616



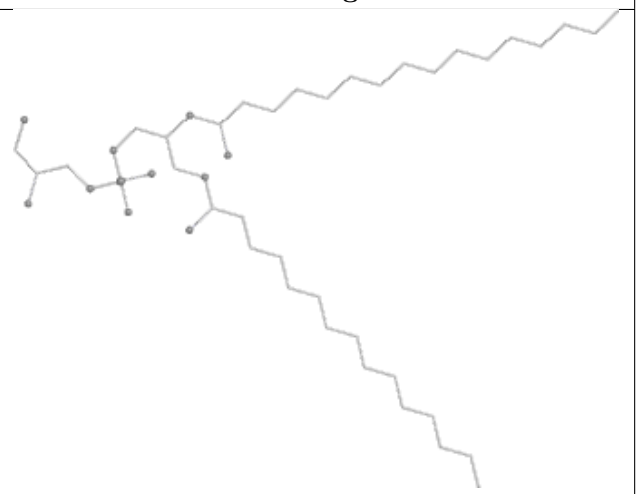
Bond lengths



Bond angles

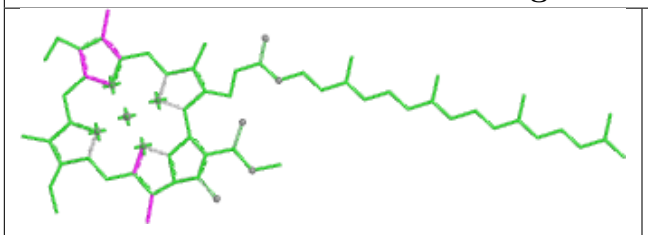


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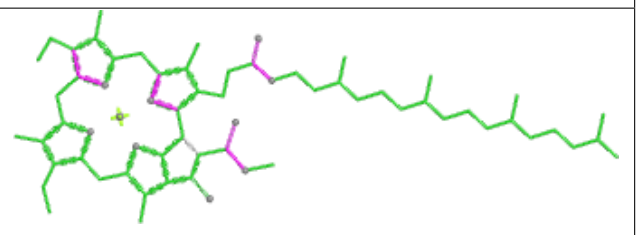


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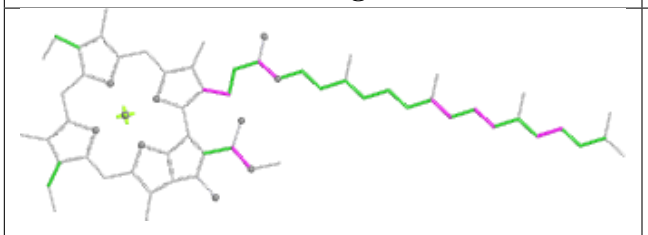
Ligand CLA c 503



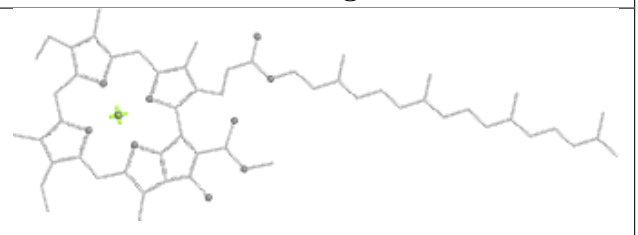
Bond lengths



Bond angles

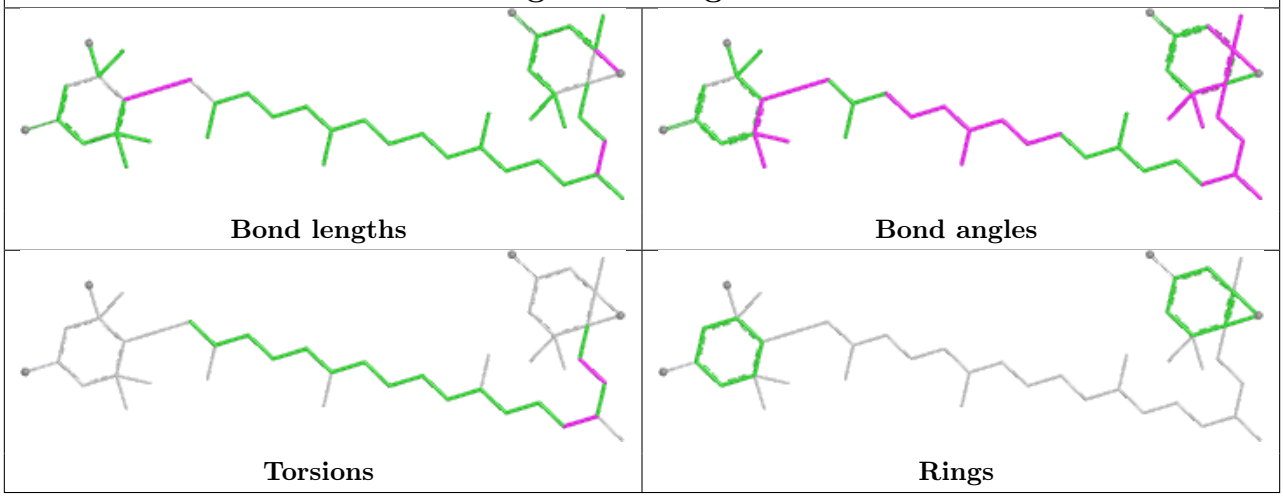


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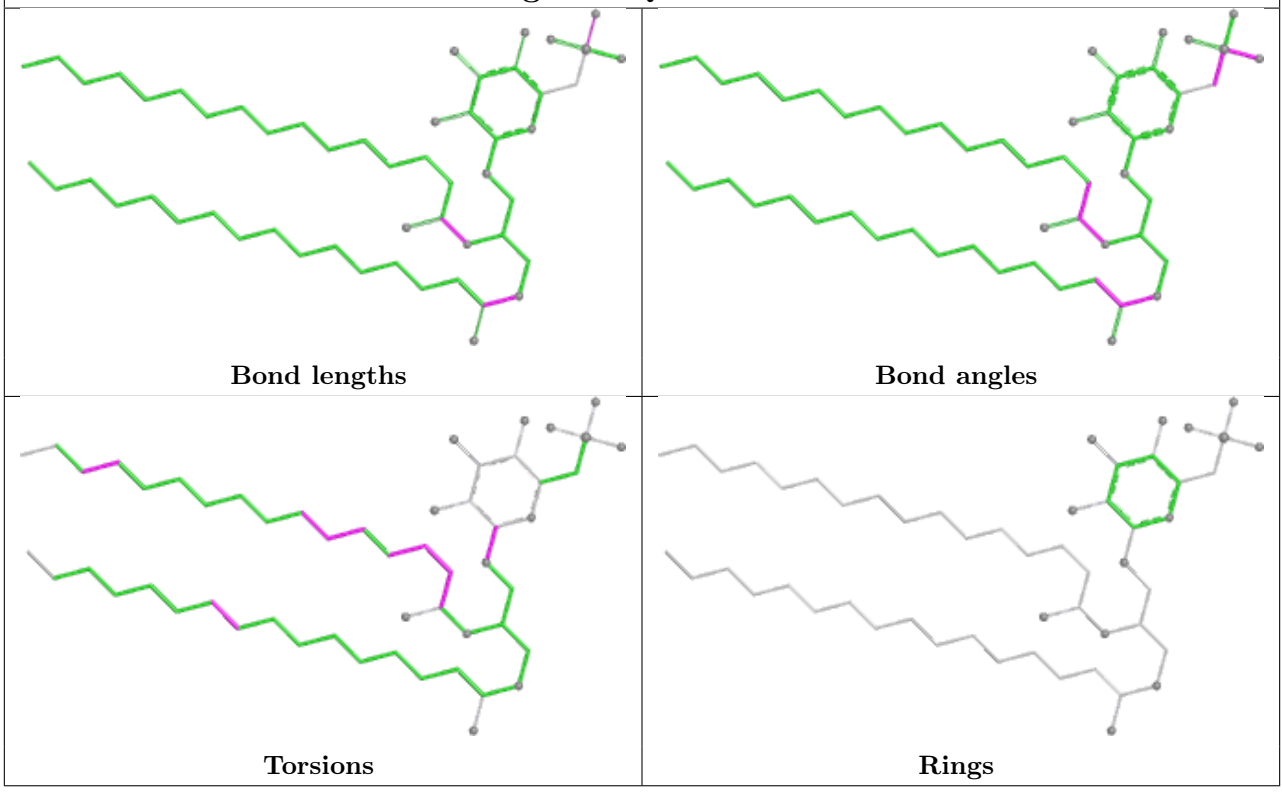


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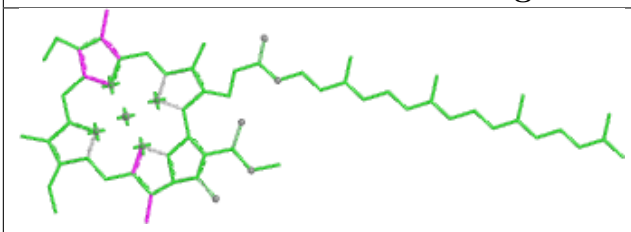
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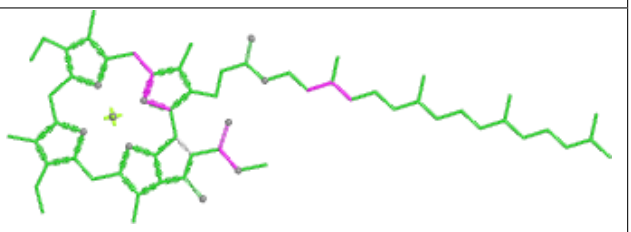
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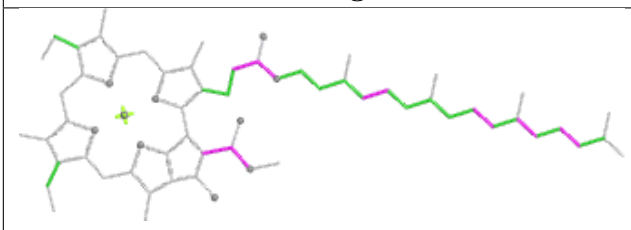
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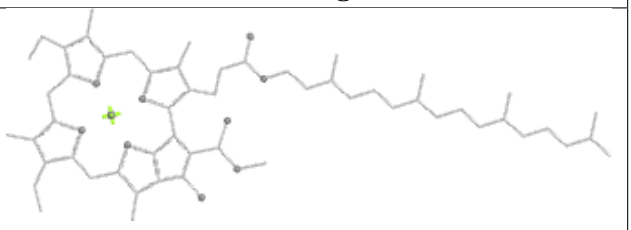
Bond lengths



Bond angles

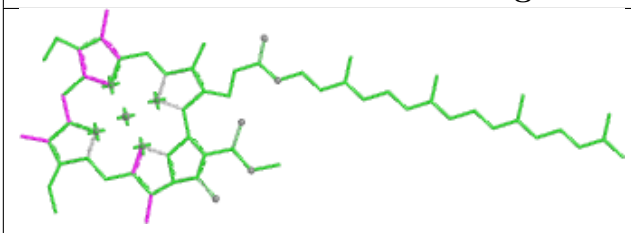


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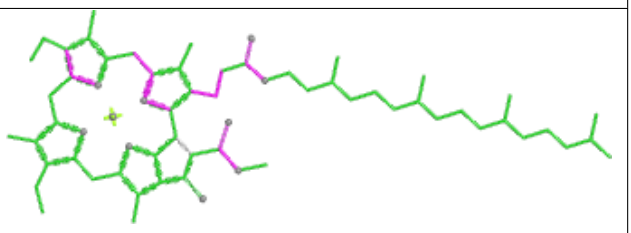


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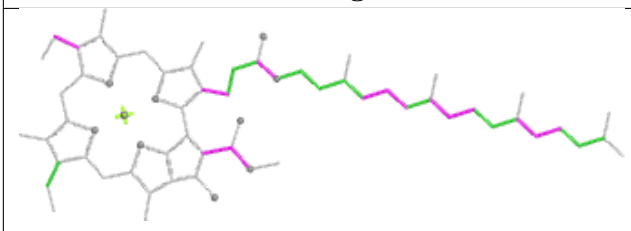
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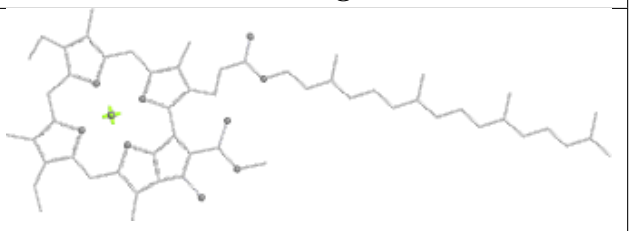
Bond lengths



Bond angles

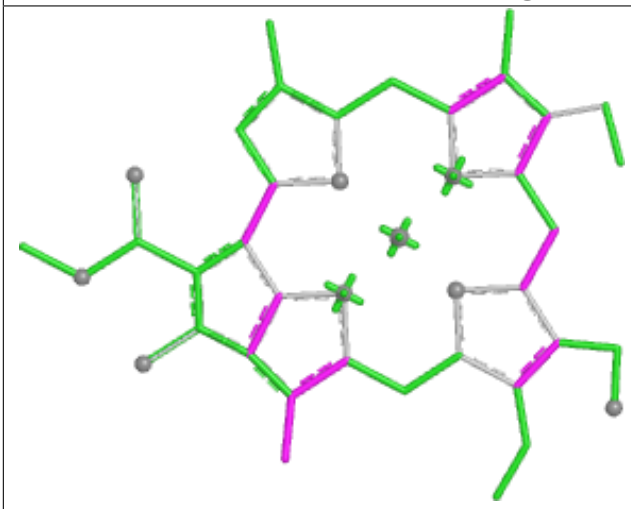


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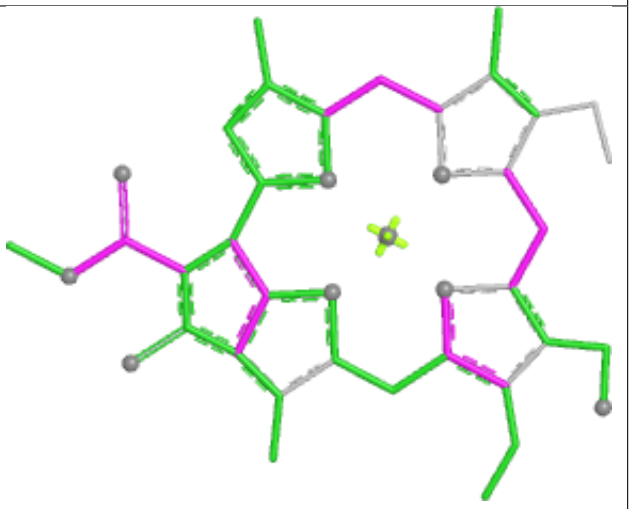


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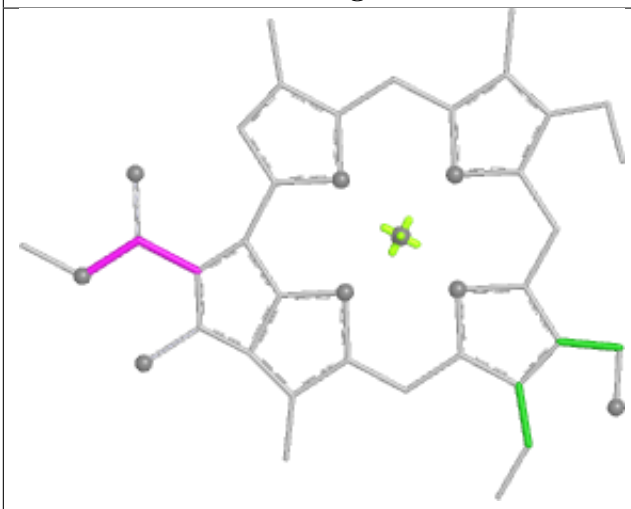
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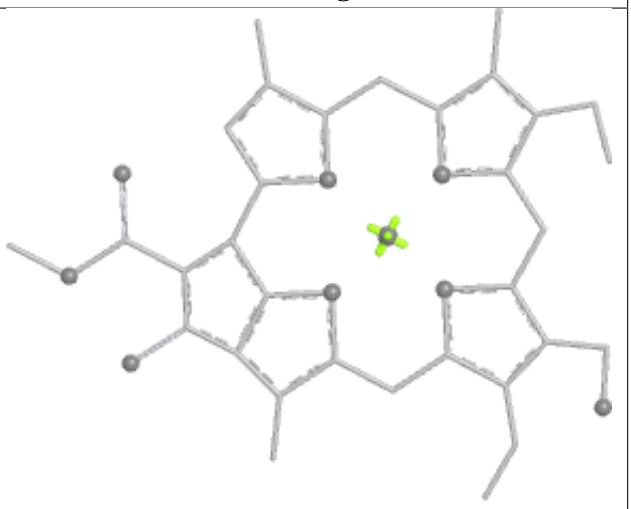
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Bond angles

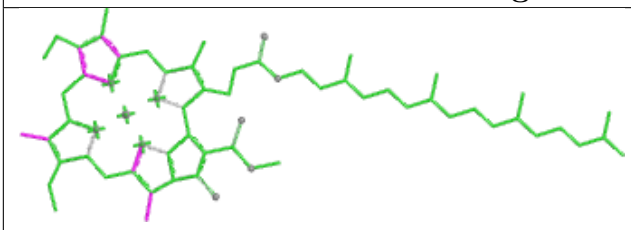


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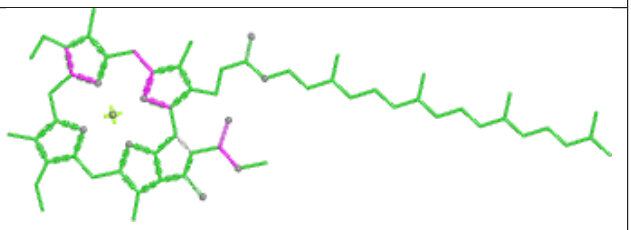


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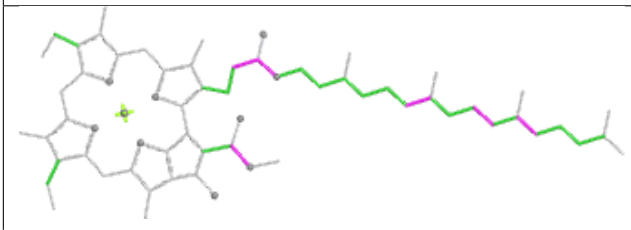
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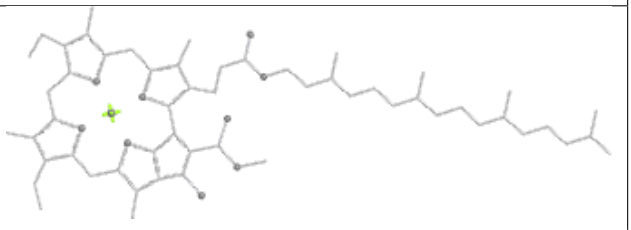
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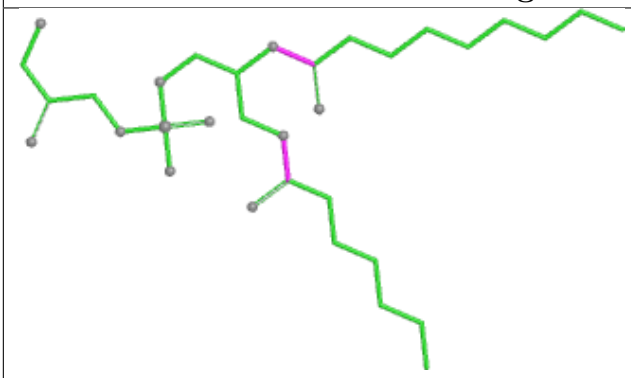


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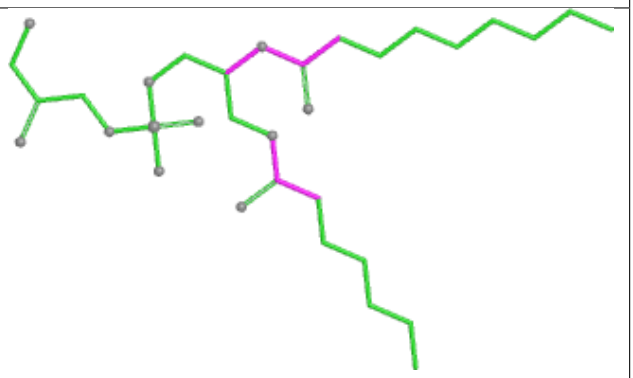


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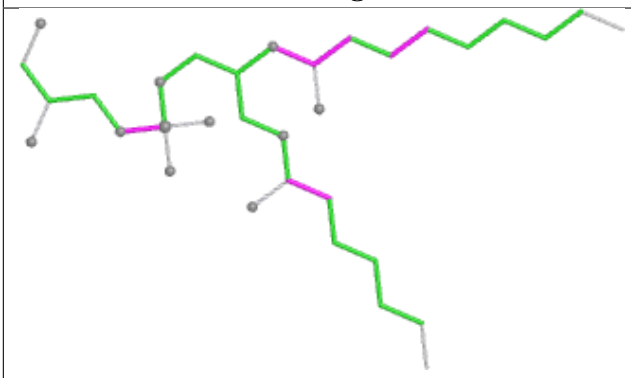
Ligand LHG JJ 101



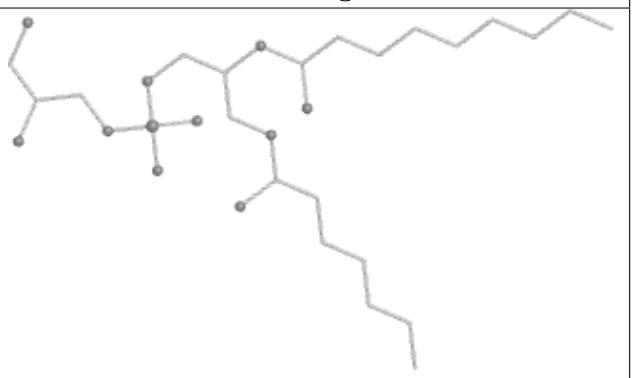
Bond lengths



Bond angles

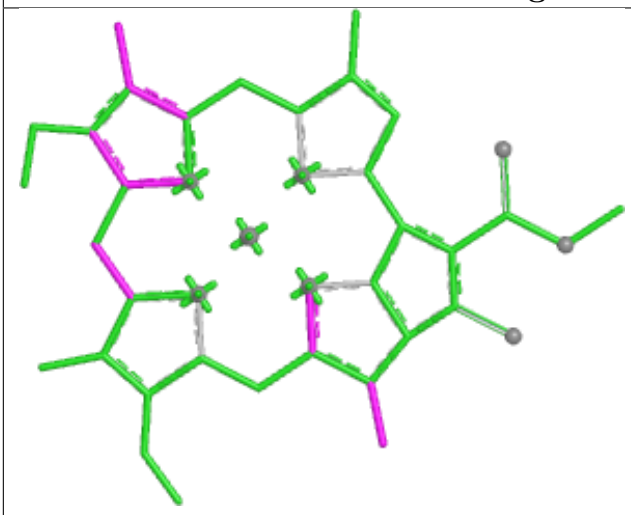


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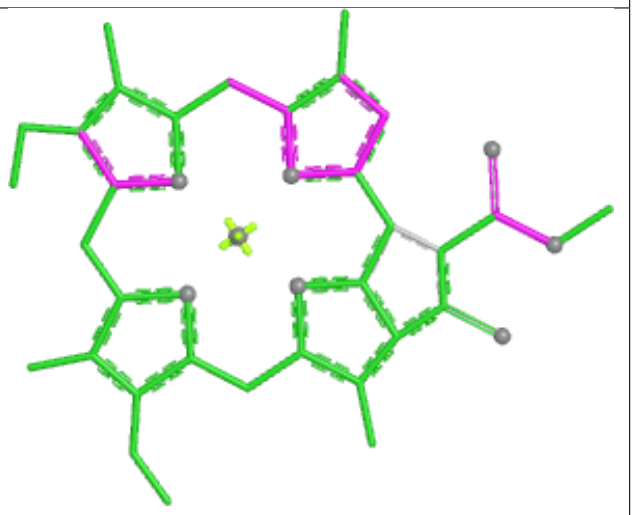


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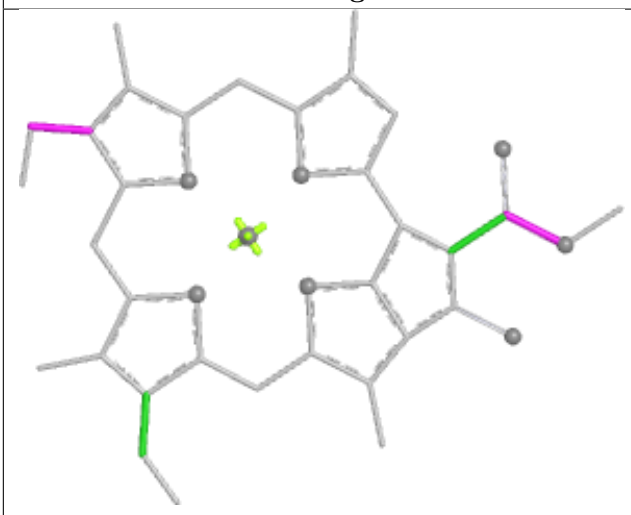
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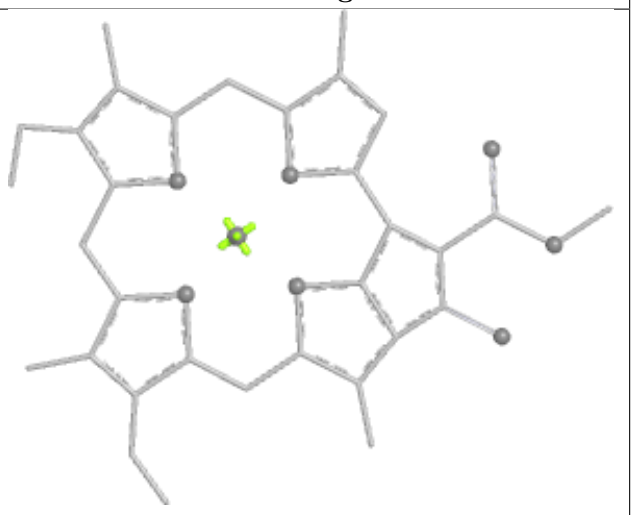
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Bond angles

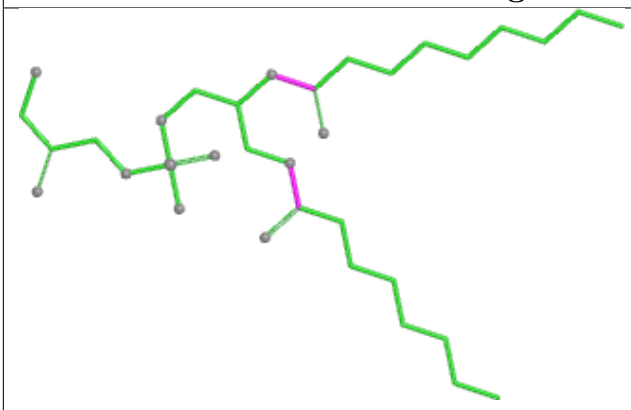


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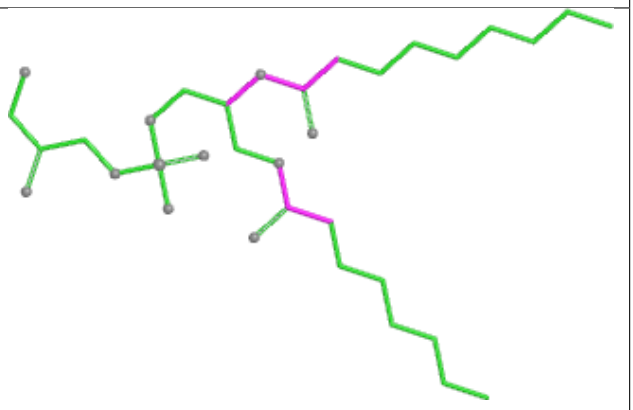


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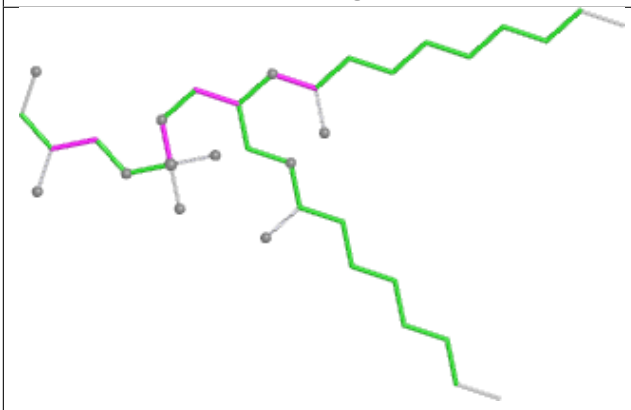
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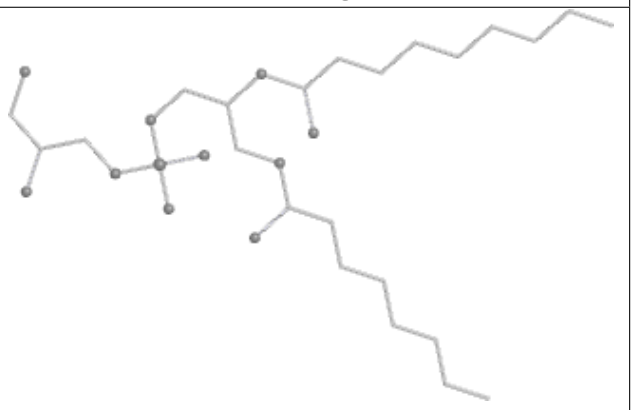
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Bond angles

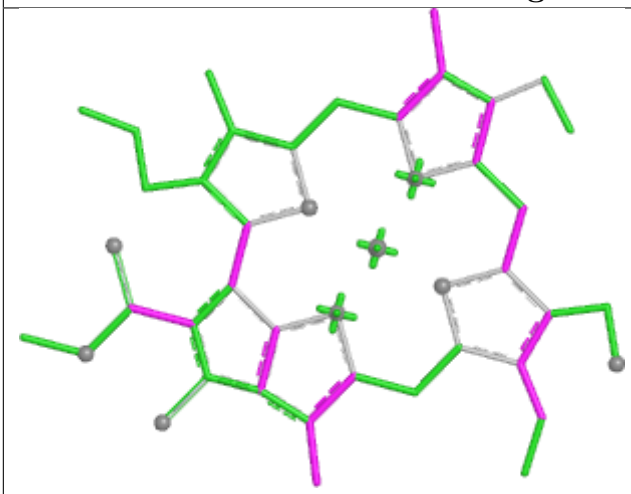


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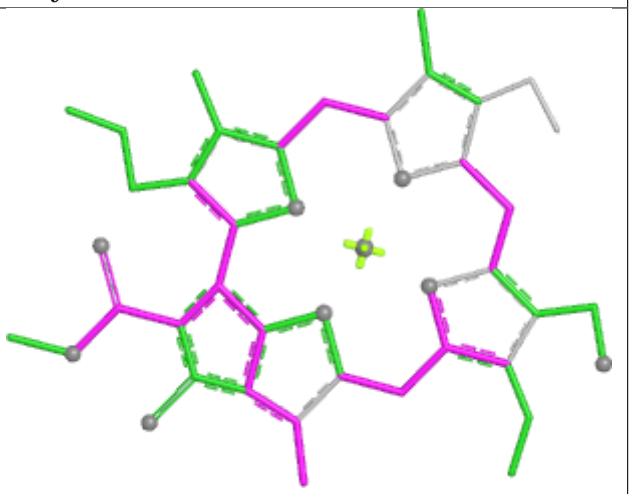


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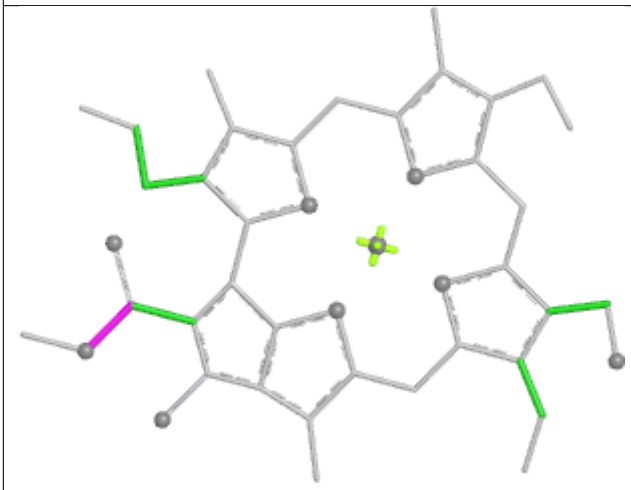
Ligand CHL y 308



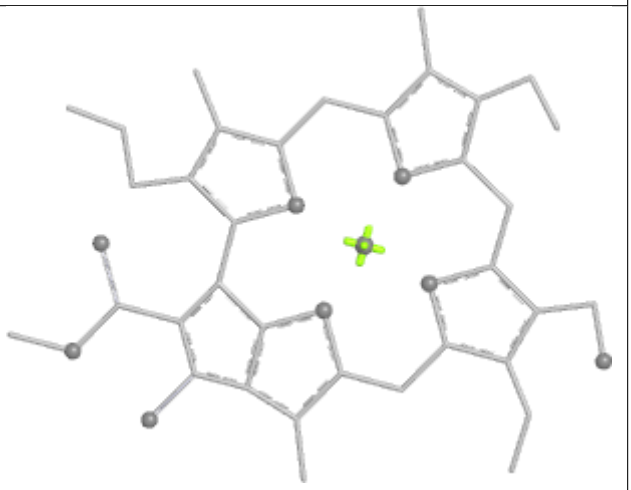
Bond lengths



Bond angles

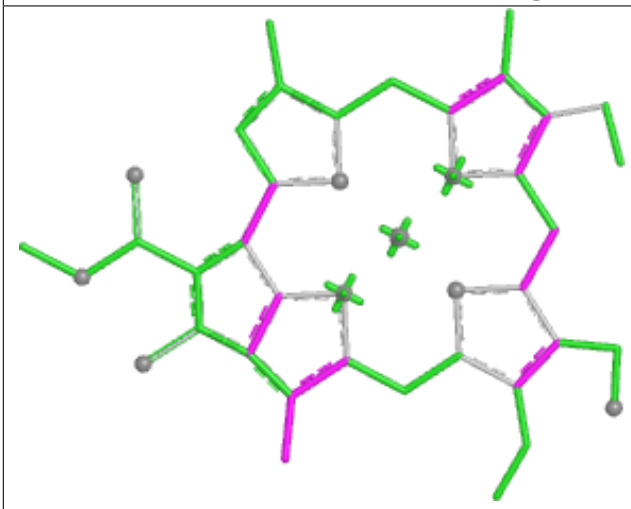


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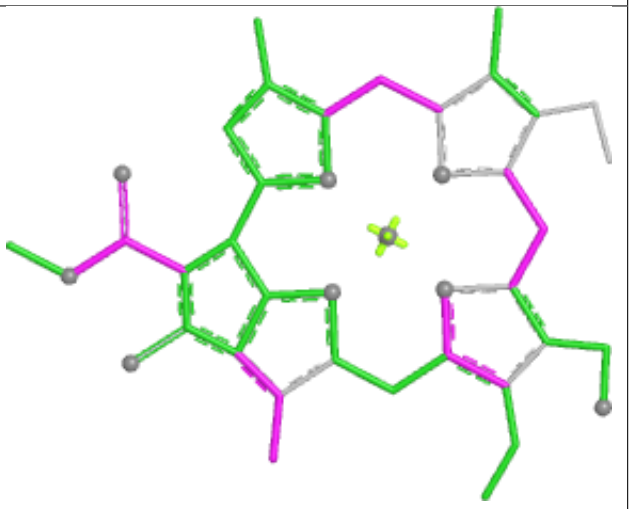


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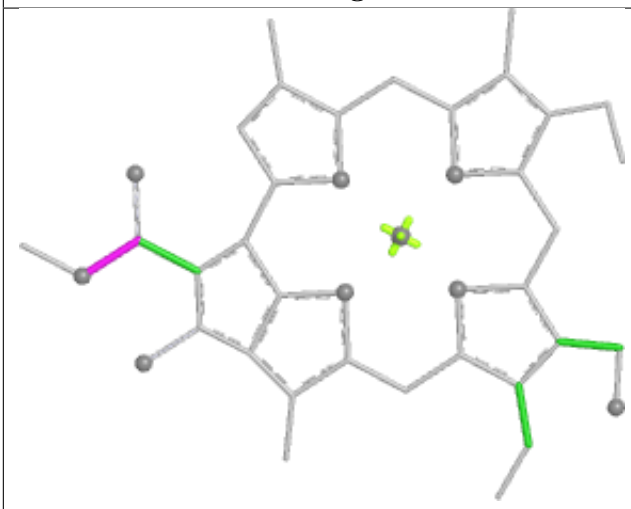
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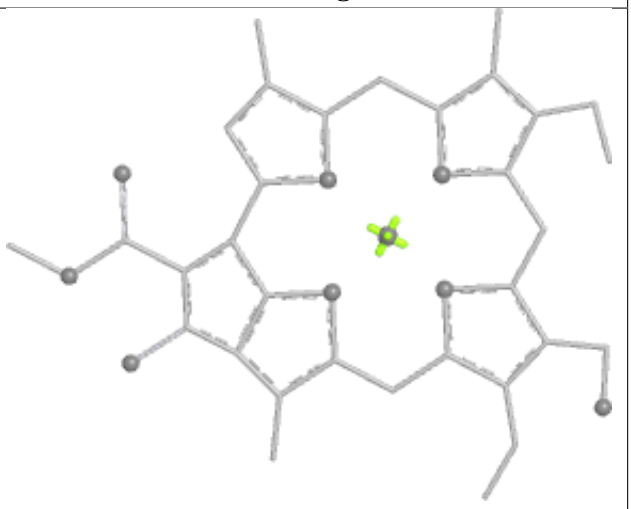
Bond lengths



Bond angles

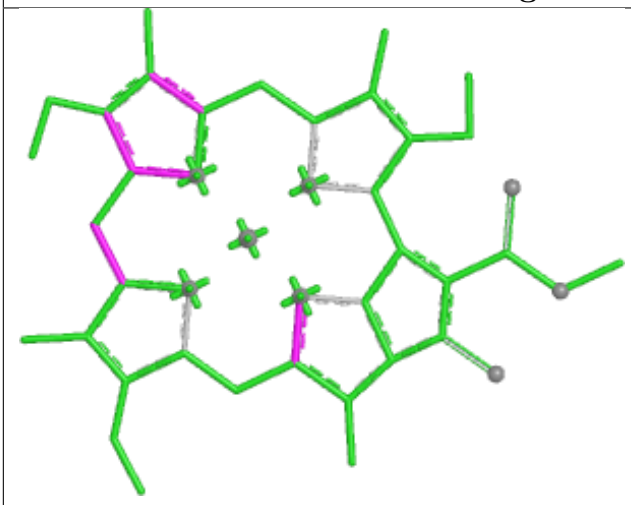


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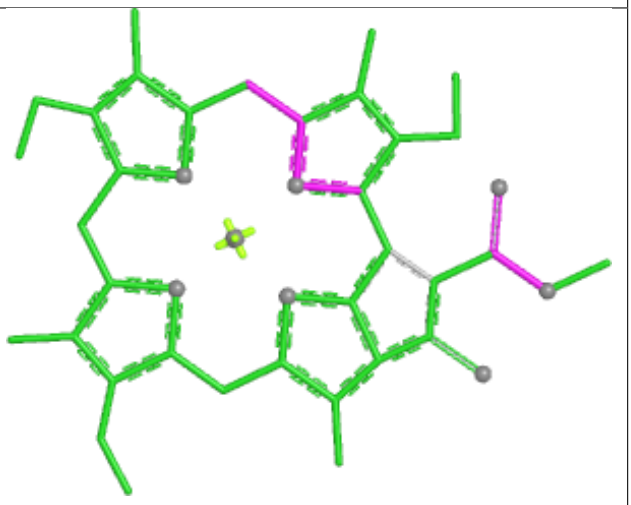


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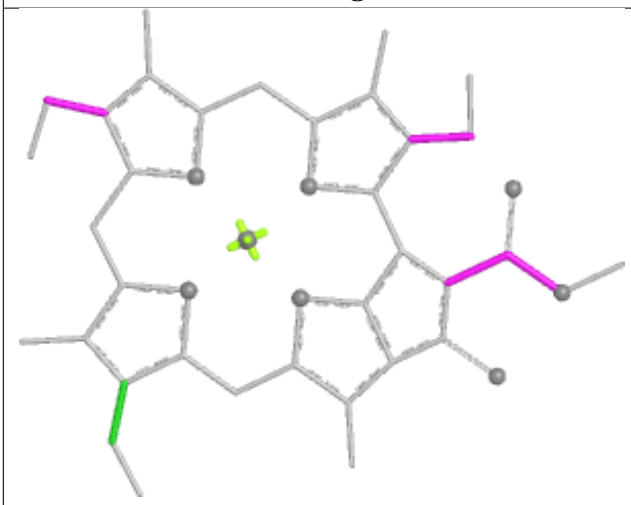
Ligand CLA 22 610



Bond lengths



Bond angles

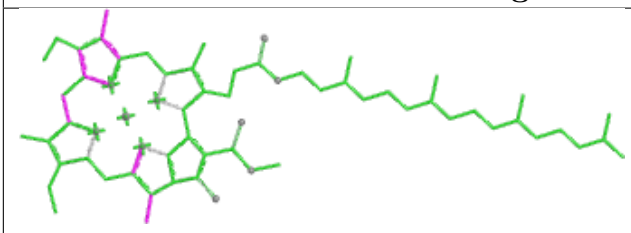


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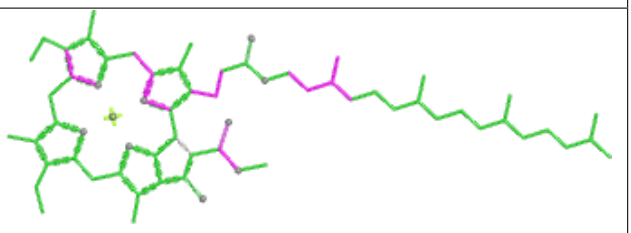


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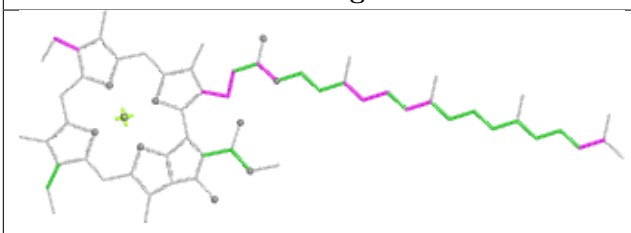
Ligand CLA CC 503



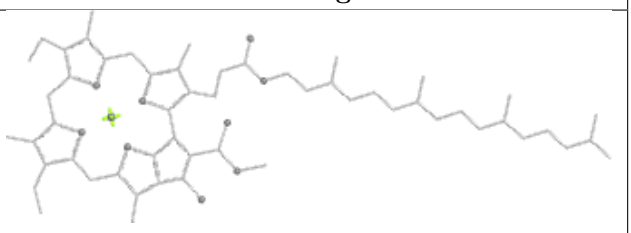
Bond lengths



Bond angles

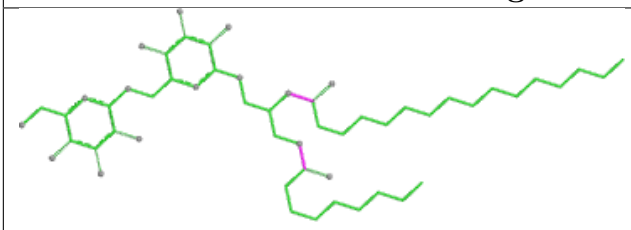


Torsions

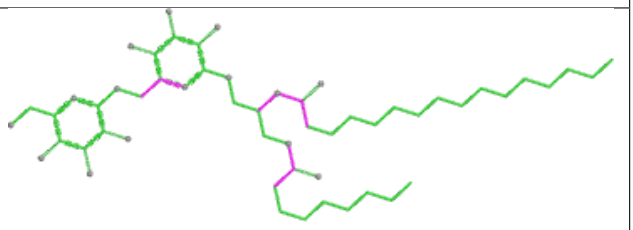


Rings

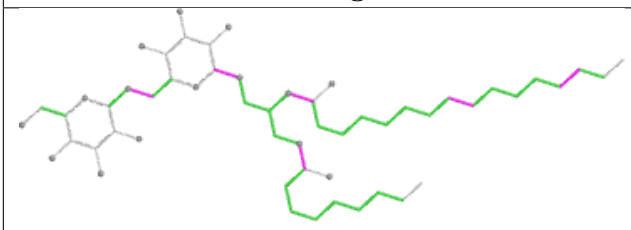
Ligand DGD BB 624



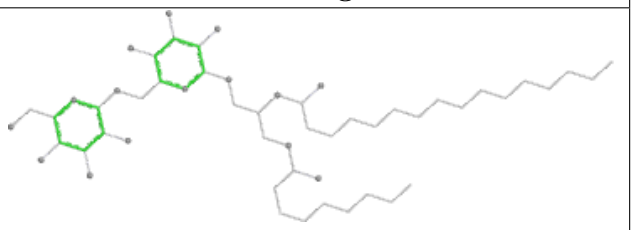
Bond lengths



Bond angles

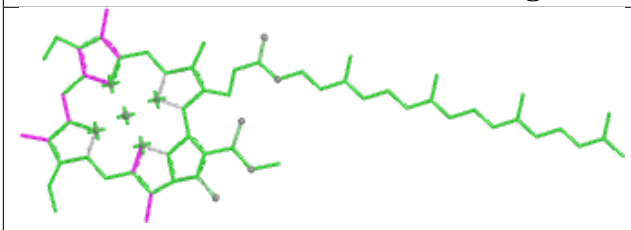


Torsions

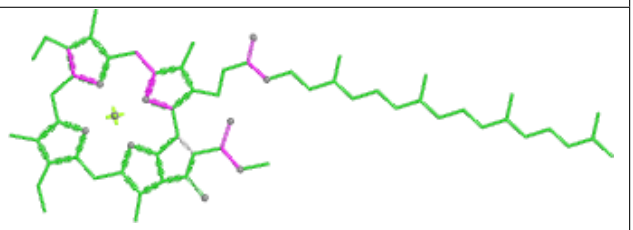


Rings

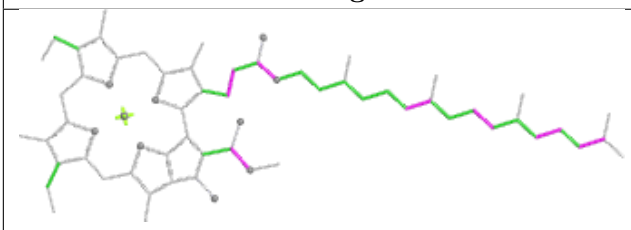
Ligand CLA C 512



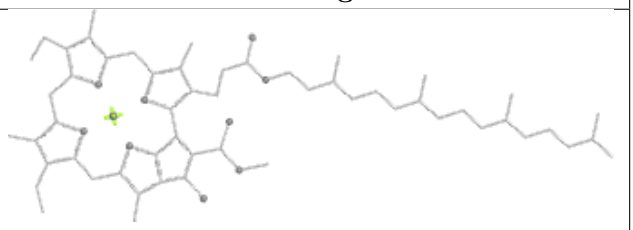
Bond lengths



Bond angles

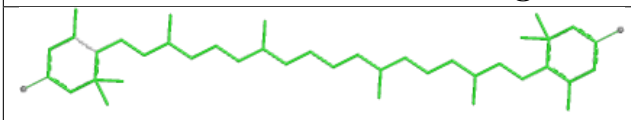


Torsions

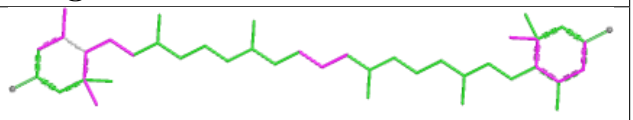


Rings

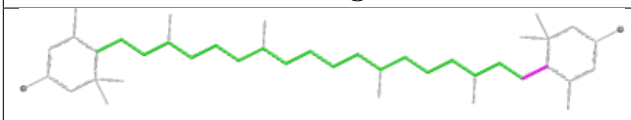
Ligand LUT Gg 316



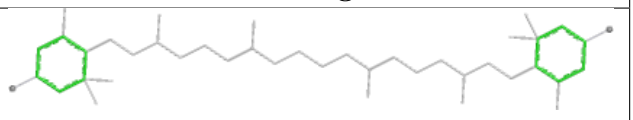
Bond lengths



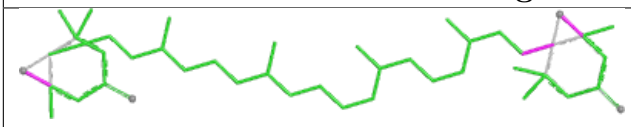
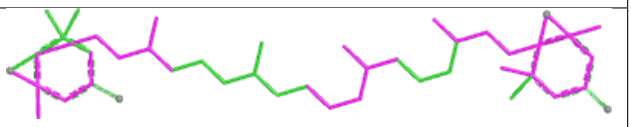
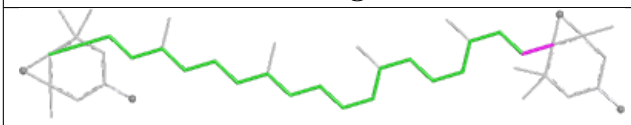
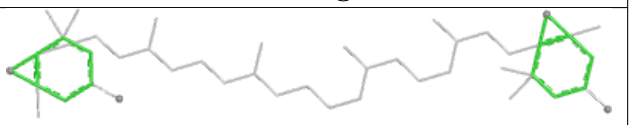
Bond angles

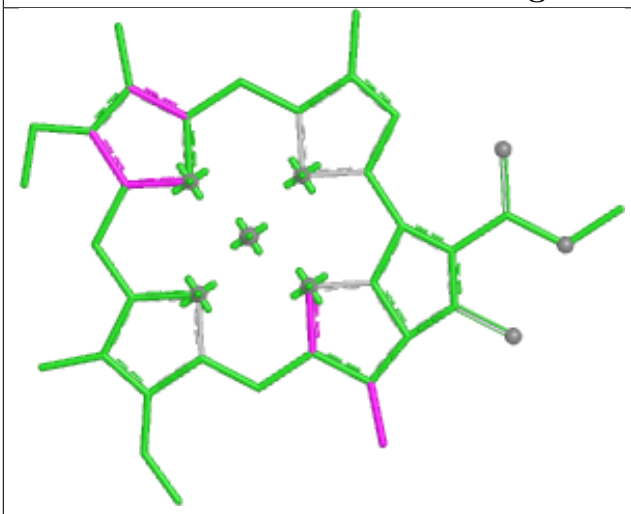
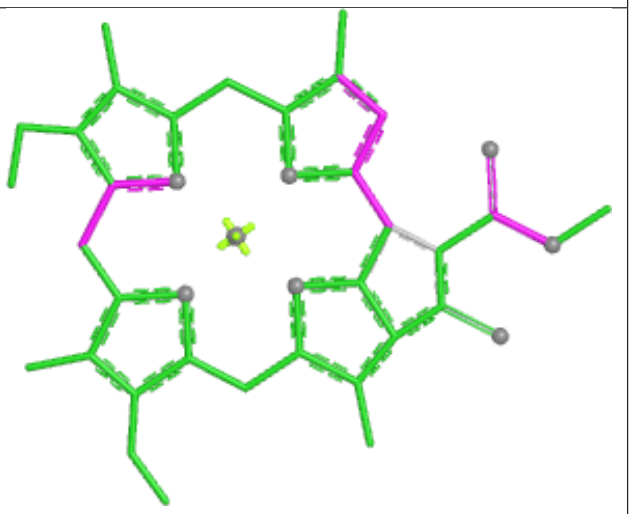
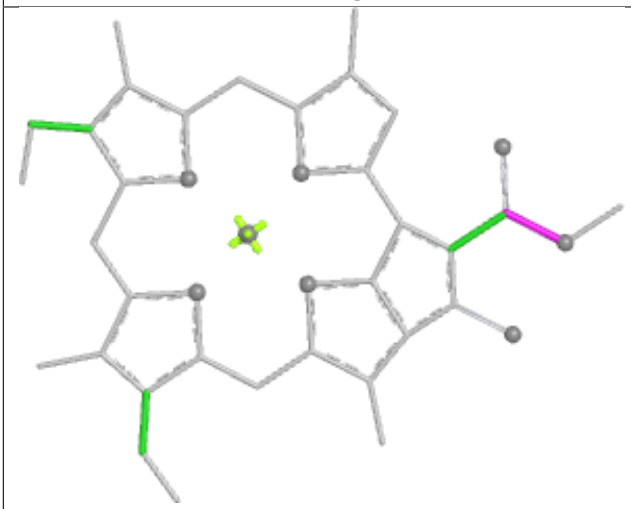
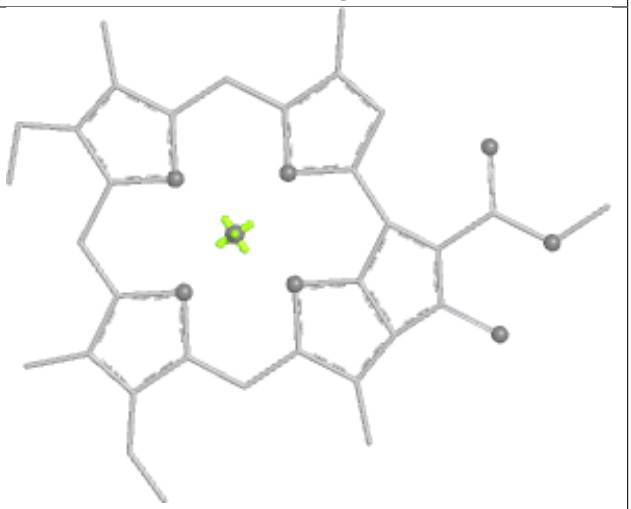


Torsions

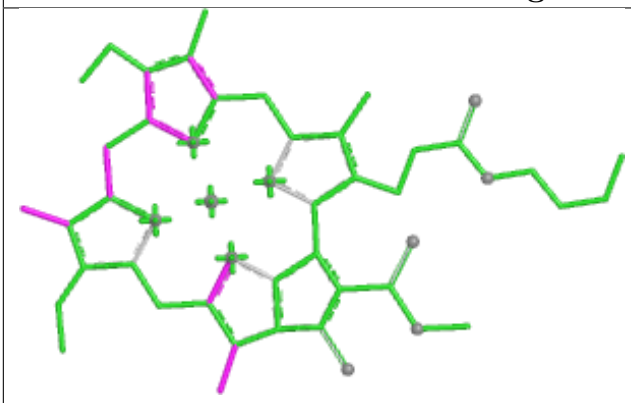


Rings

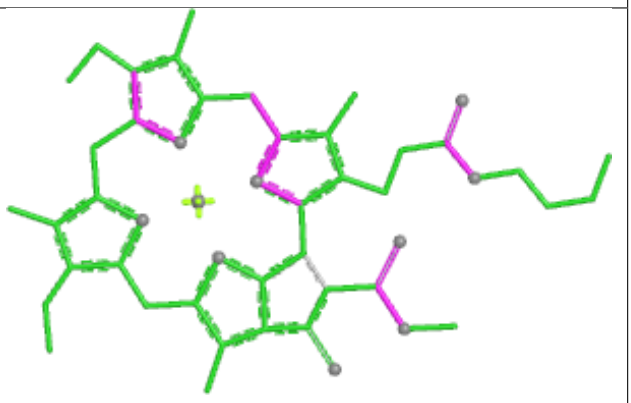
Ligand XAT Rr 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

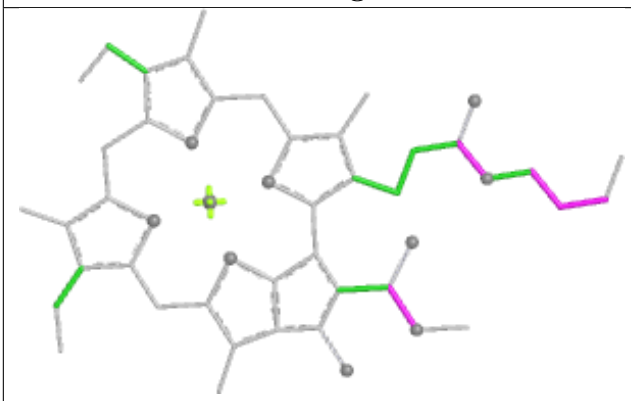
Ligand CLA n 604



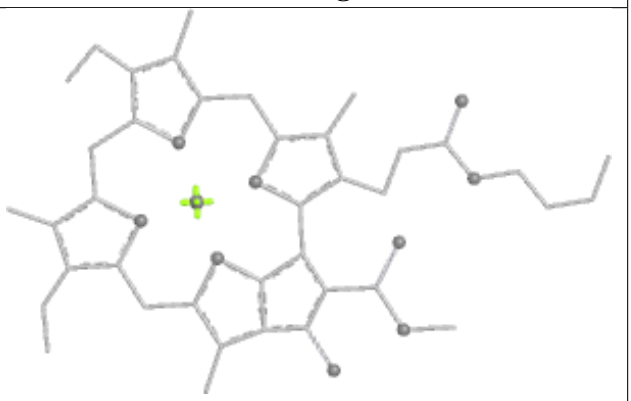
Bond lengths



Bond angles

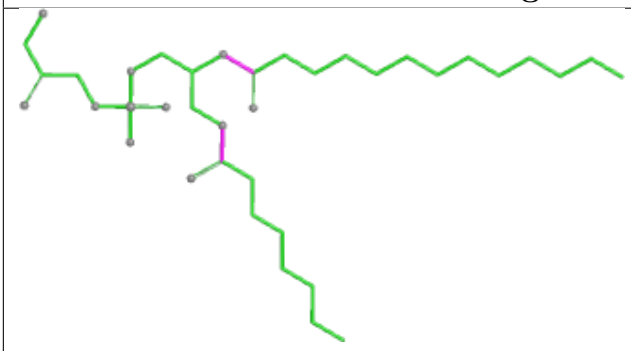


Torsions

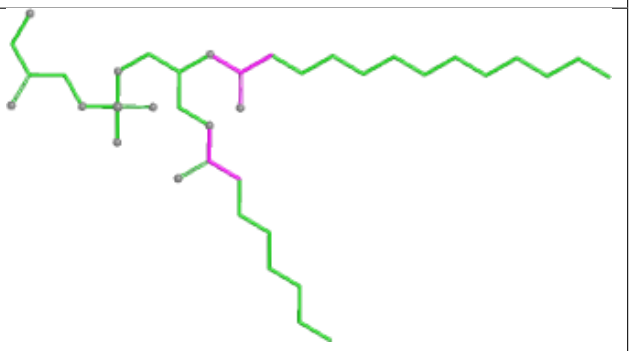


Rings

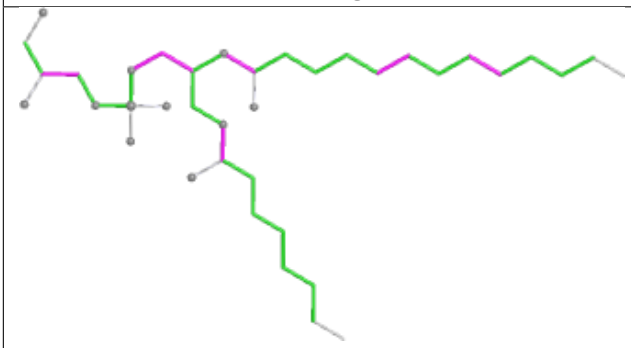
Ligand LHG N 619



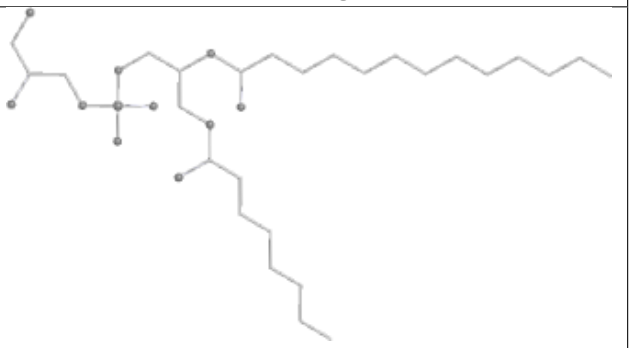
Bond lengths



Bond angles

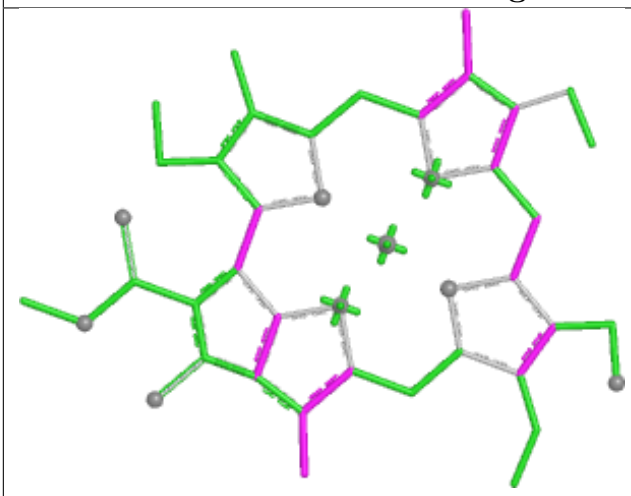


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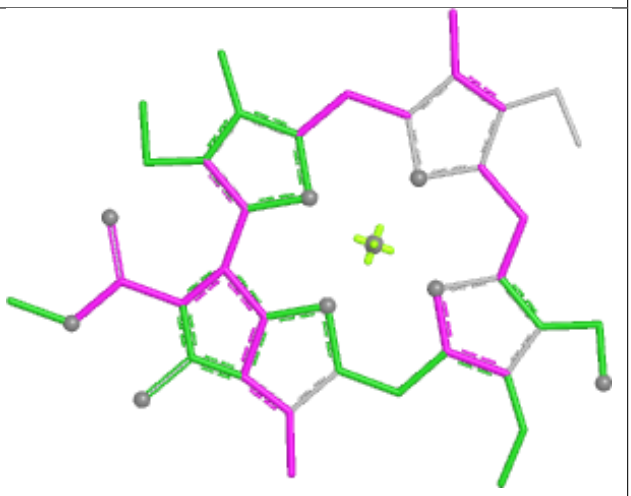


Rings

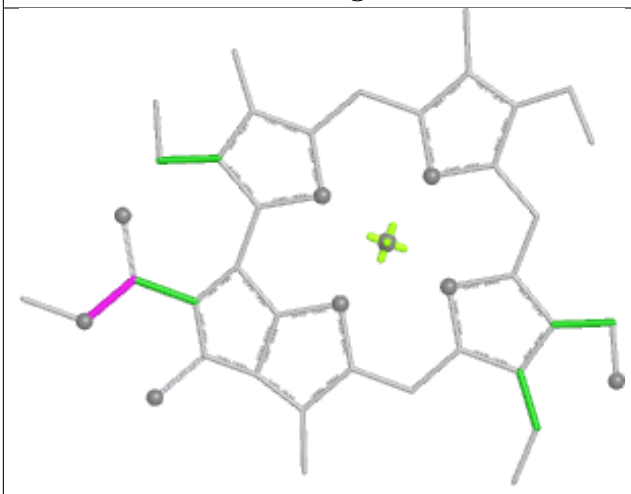
Ligand CHL GG 609



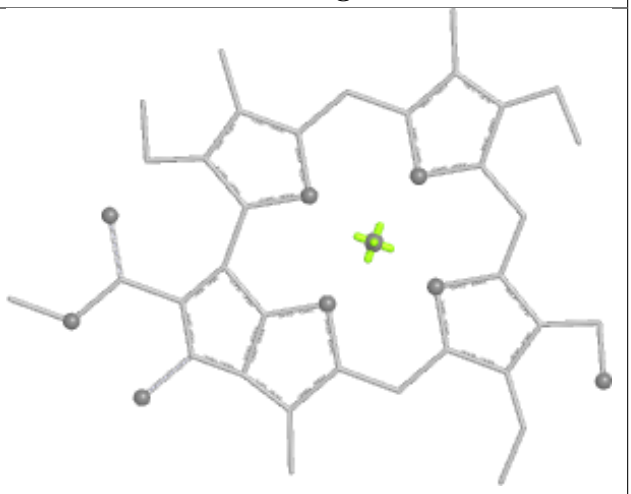
Bond lengths



Bond angles

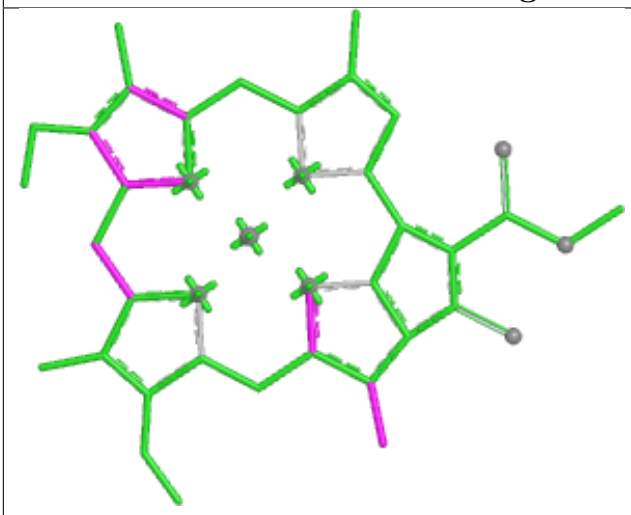


Torsions

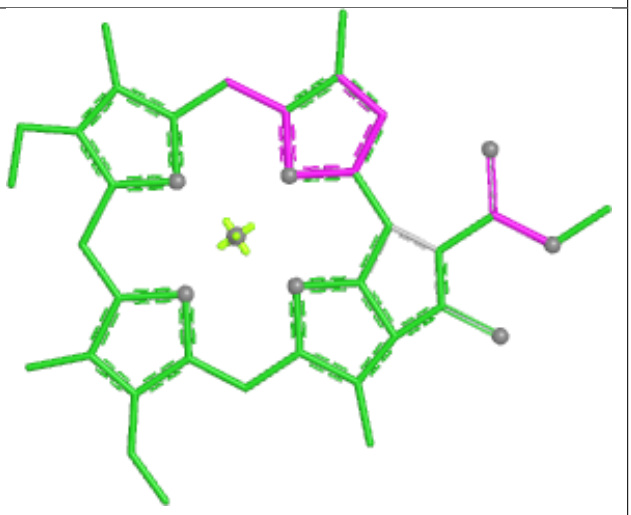


Rings

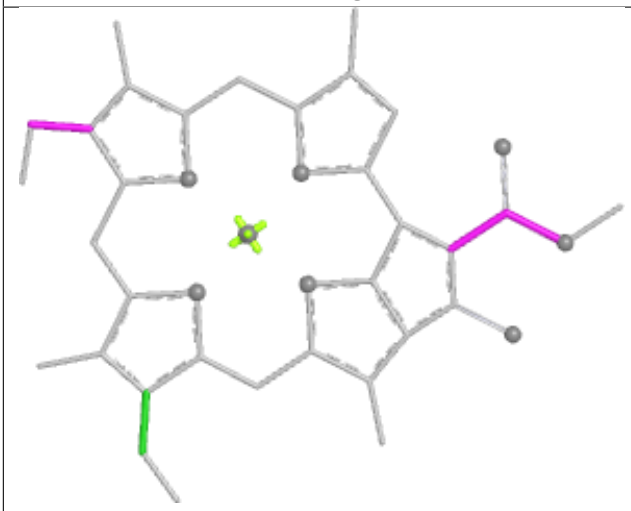
Ligand CLA 33 603



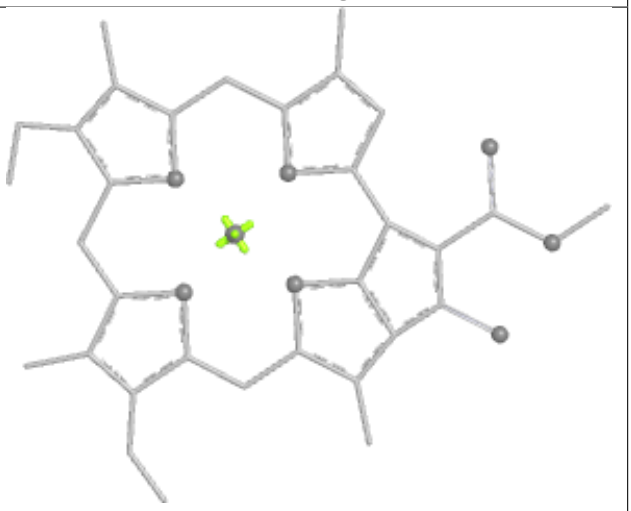
Bond lengths



Bond angles



Torsions

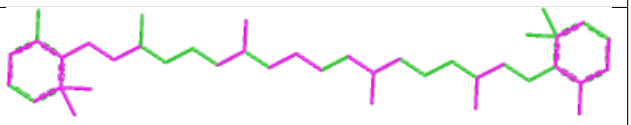


Rings

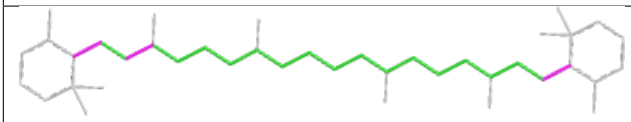
Ligand BCR XX 202



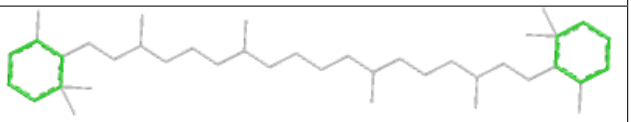
Bond lengths



Bond angles

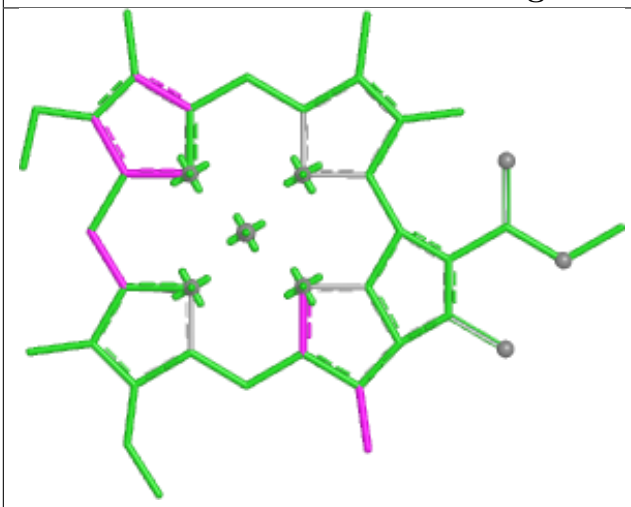


Torsions

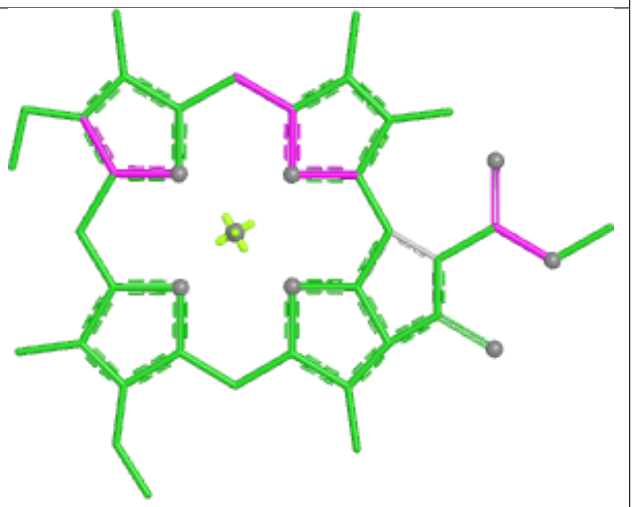


Rings

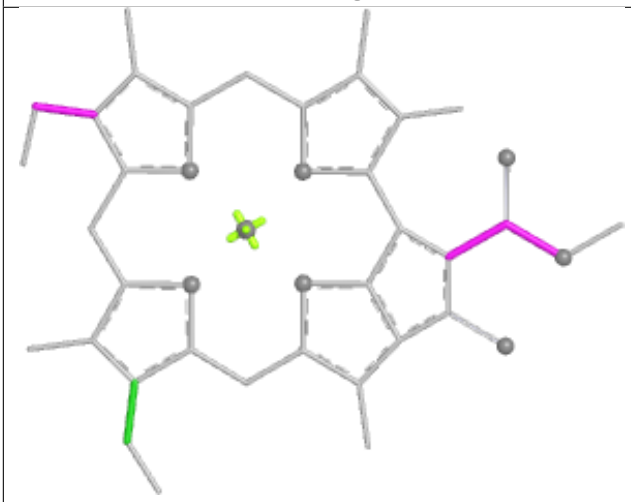
Ligand CLA S 608



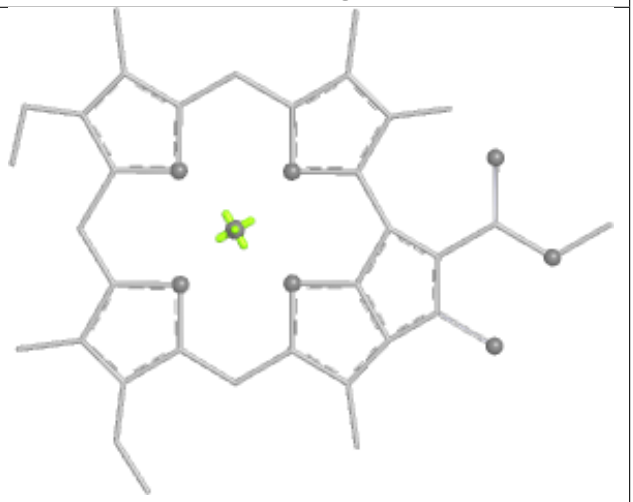
Bond lengths



Bond angles

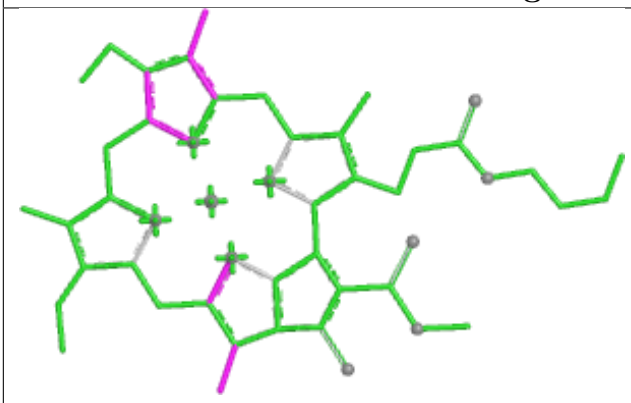


Torsions

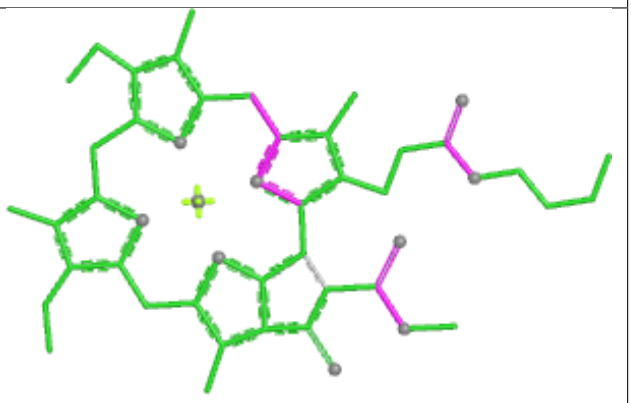


Rings

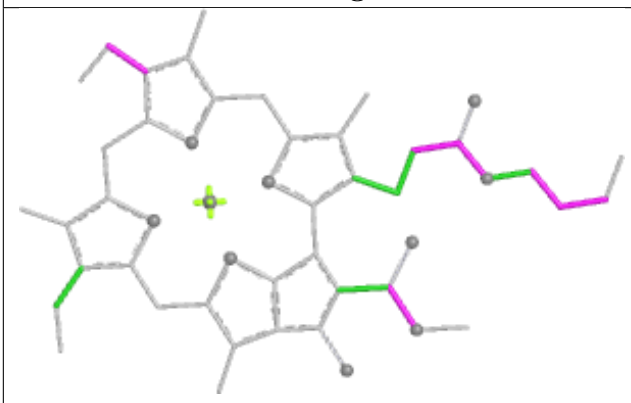
Ligand CLA Y 603



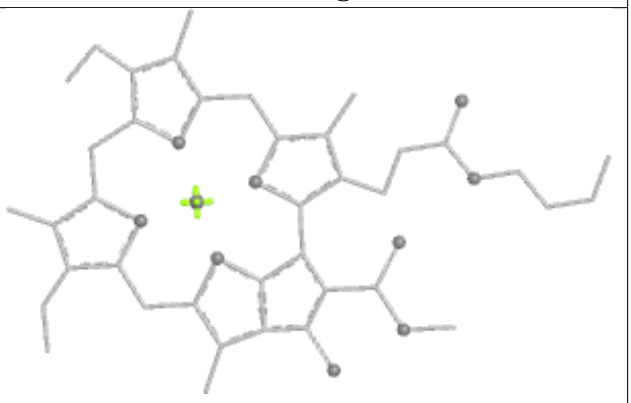
Bond lengths



Bond angles

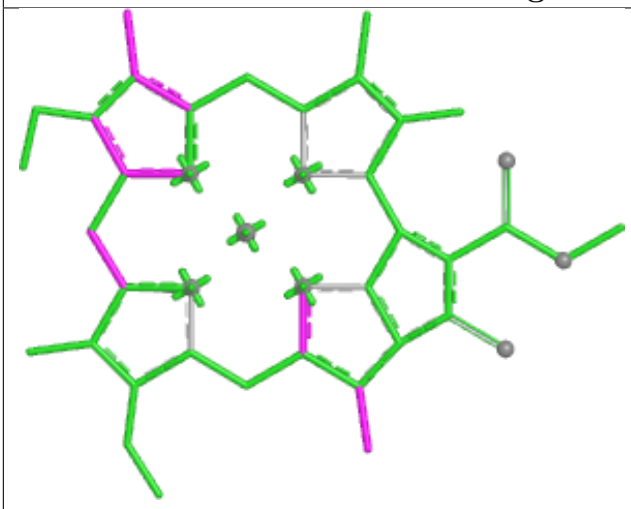


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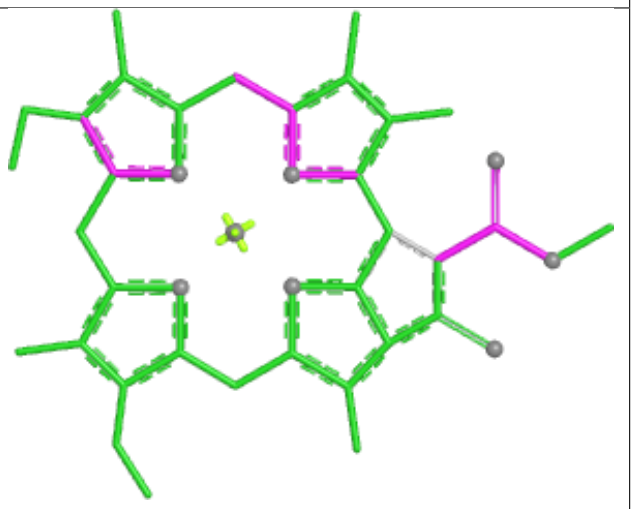


Rings

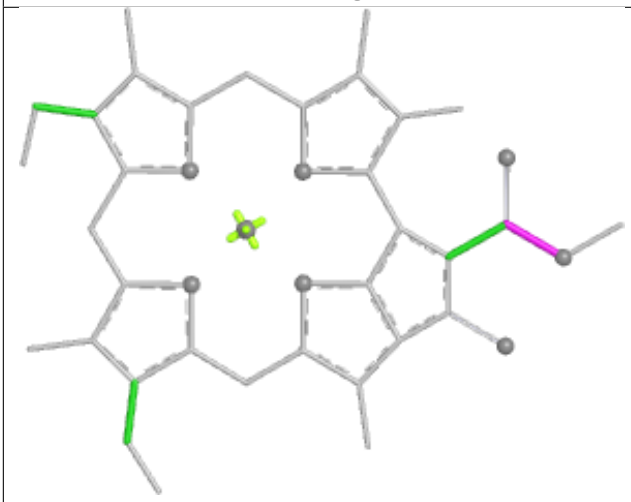
Ligand CLA S 609



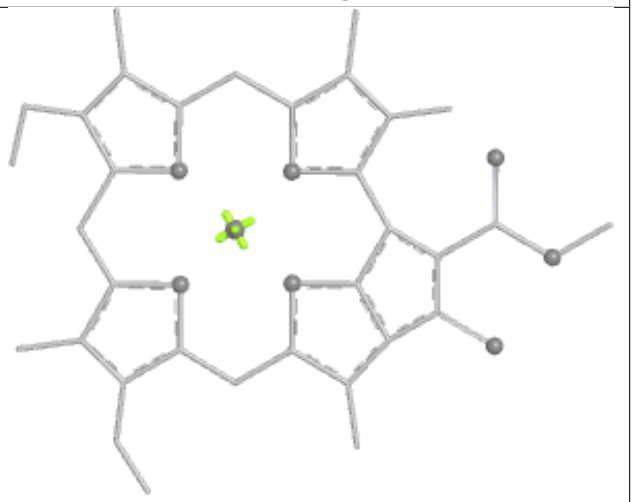
Bond lengths



Bond angles

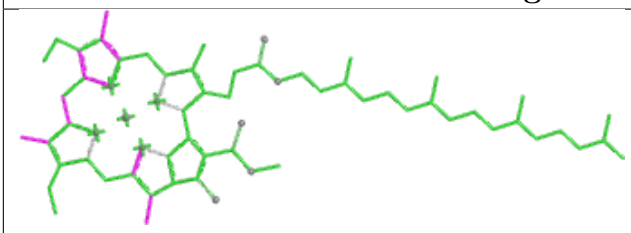


Torsions

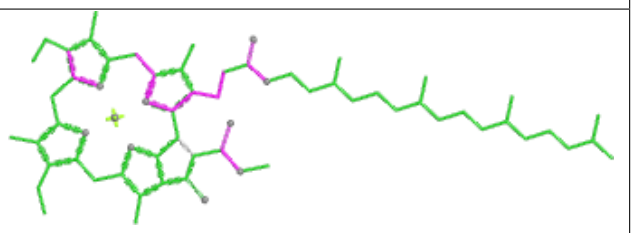


Rings

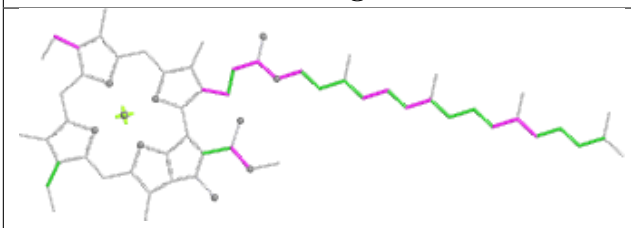
Ligand CLA Y 610



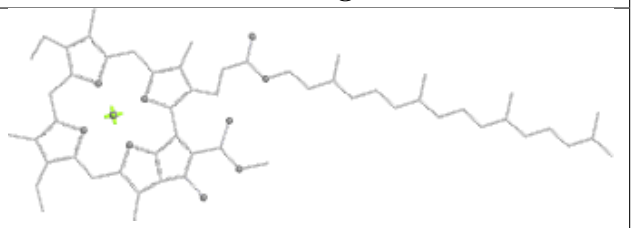
Bond lengths



Bond angles

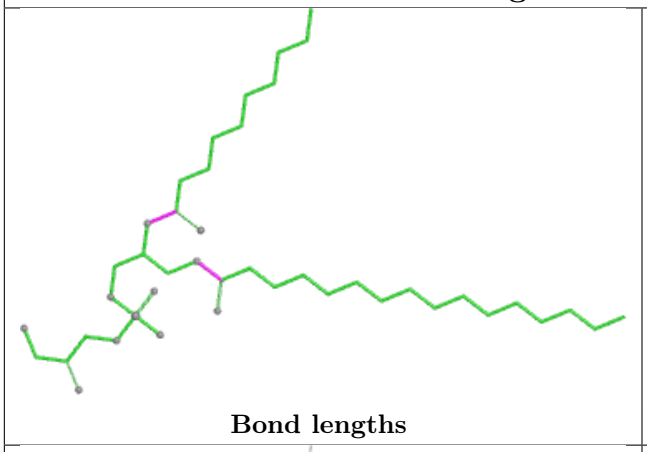


Torsions

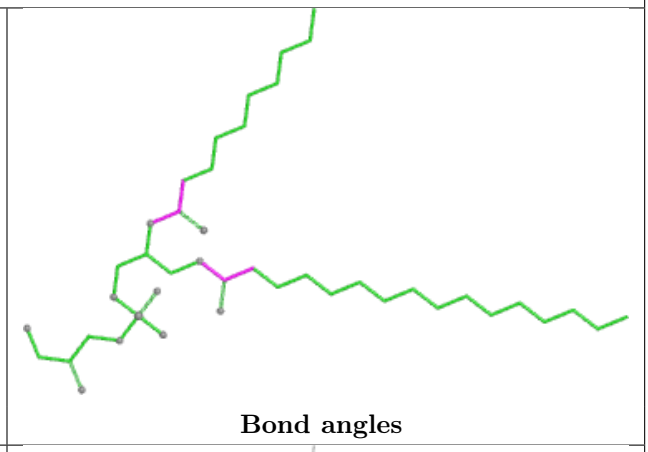


Rings

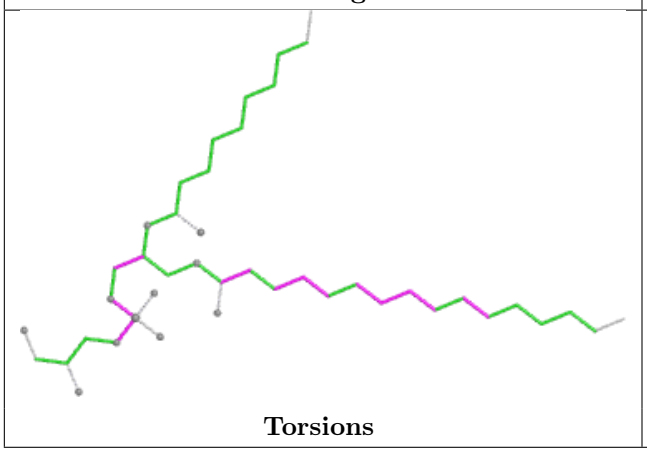
Ligand LHG DD 407



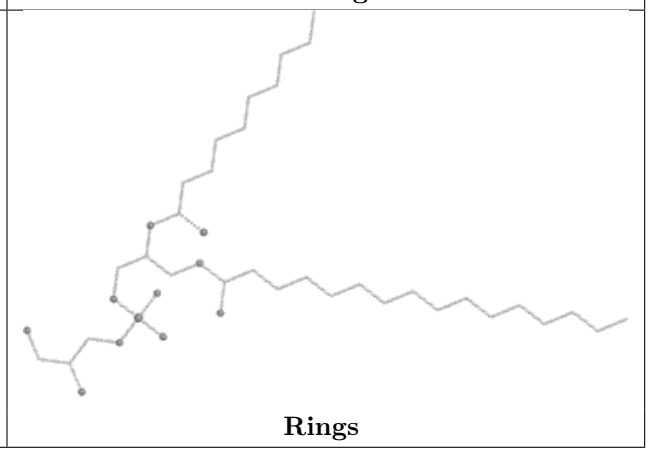
Bond lengths



Bond angles

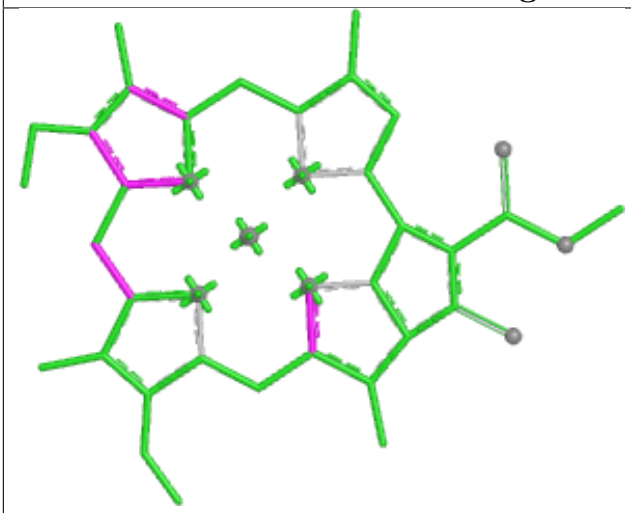


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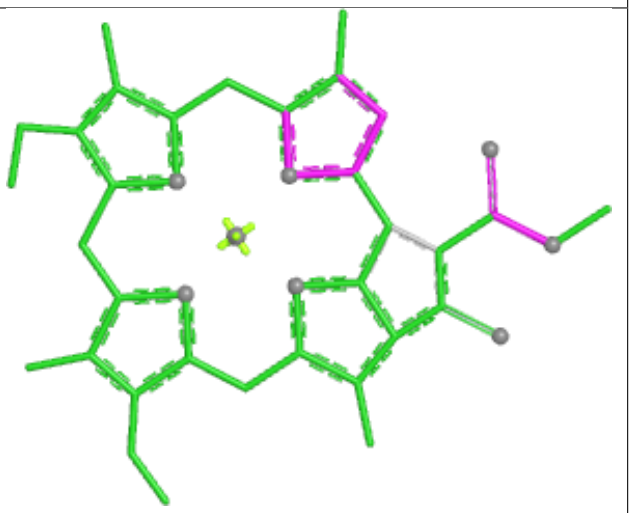


Rings

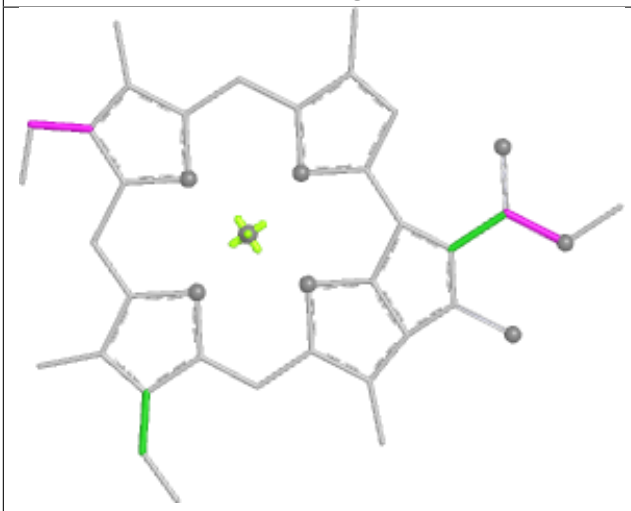
Ligand CLA 11 613



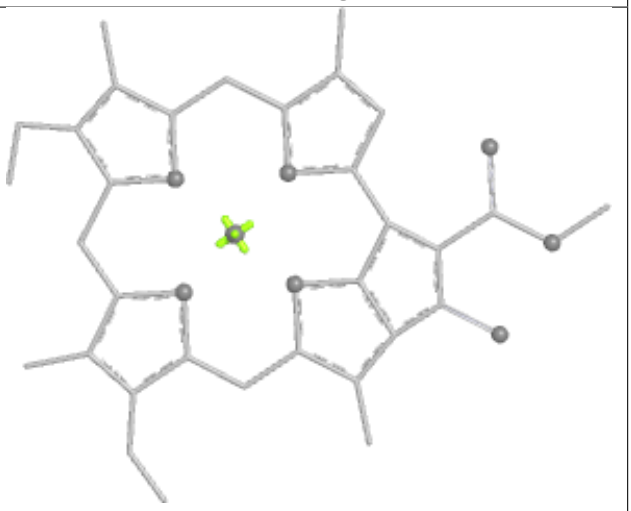
Bond lengths



Bond angles

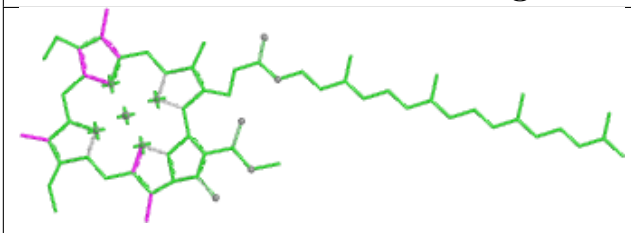


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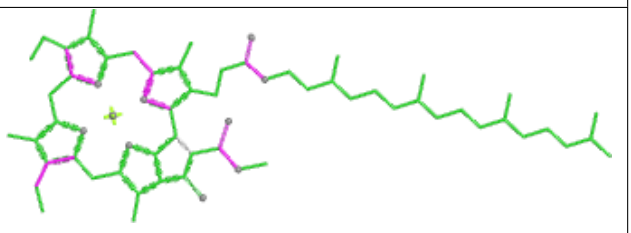


Rings

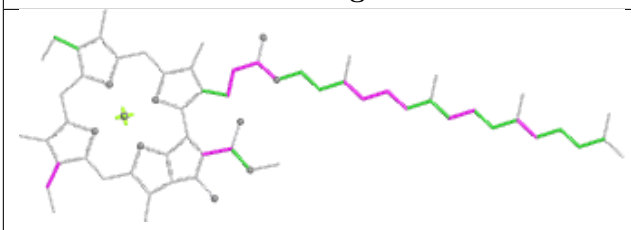
Ligand CLA CC 506



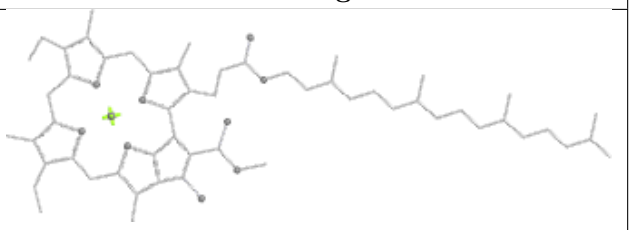
Bond lengths



Bond angles

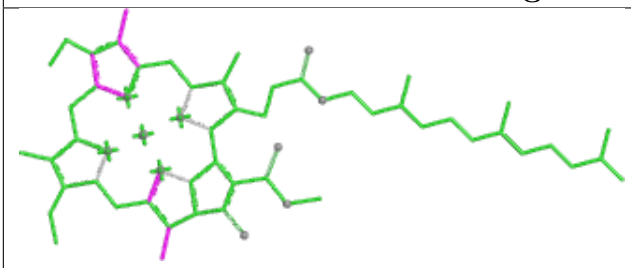


Torsions

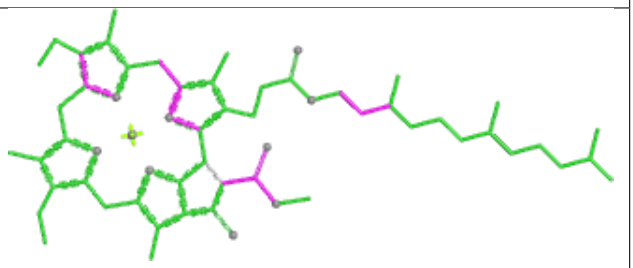


Rings

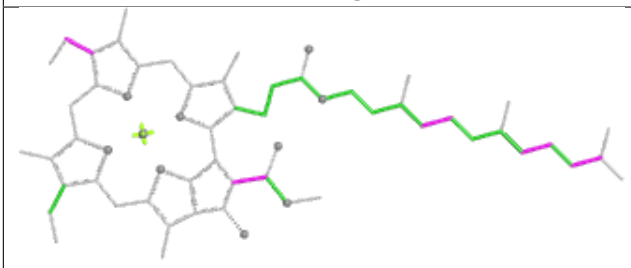
Ligand CLA A 408



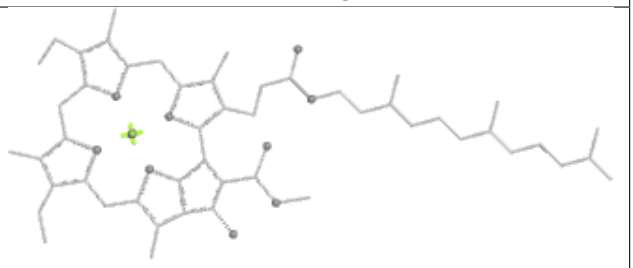
Bond lengths



Bond angles

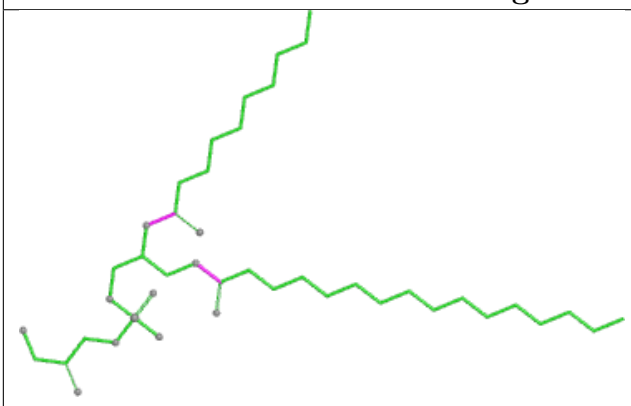


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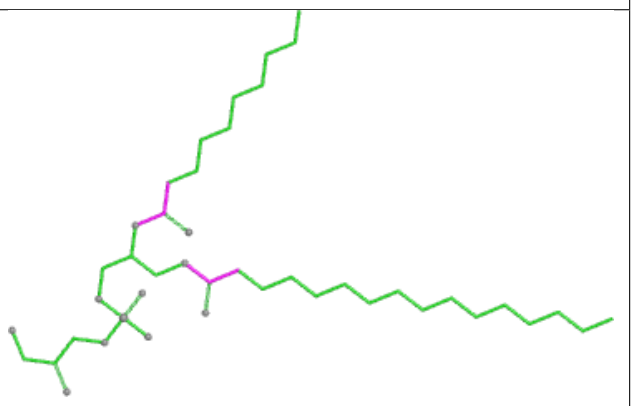


Rings

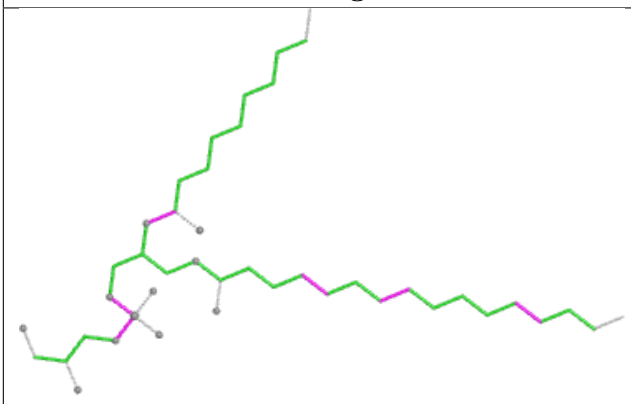
Ligand LHG Dd 405



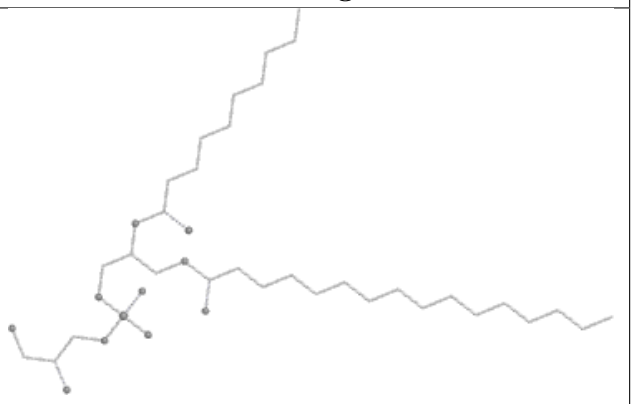
Bond lengths



Bond angles

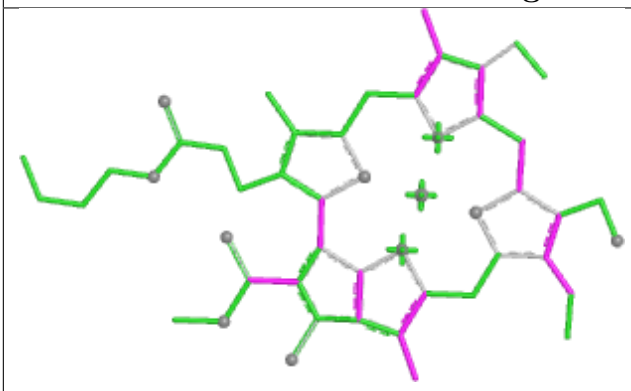


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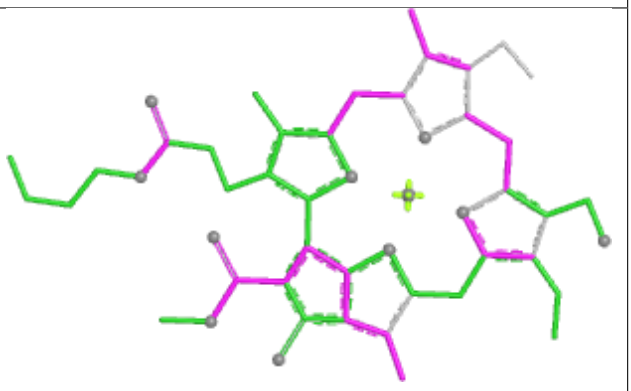


Rings

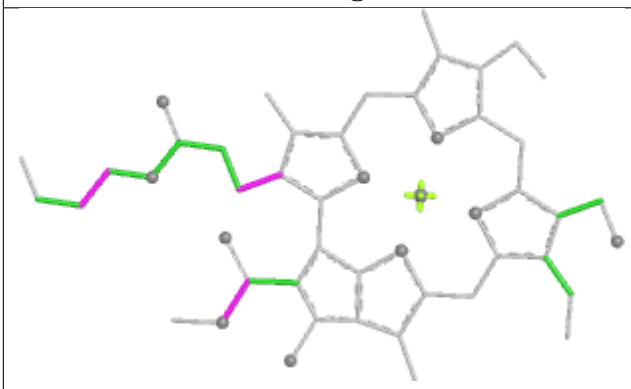
Ligand CHL N 609



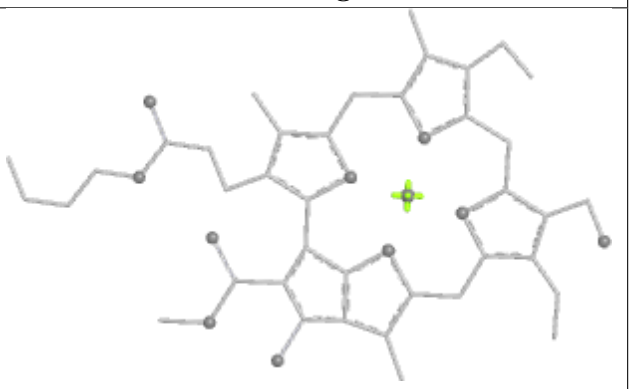
Bond lengths



Bond angles

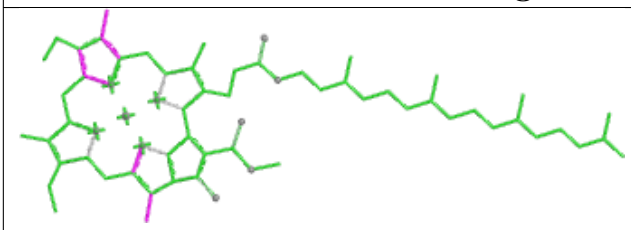


Torsions

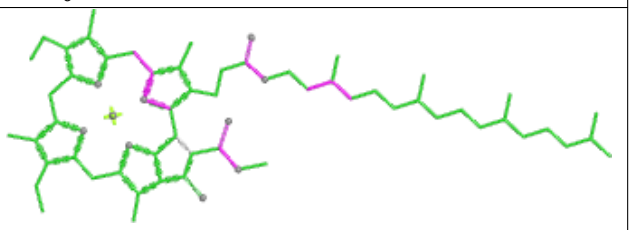


Rings

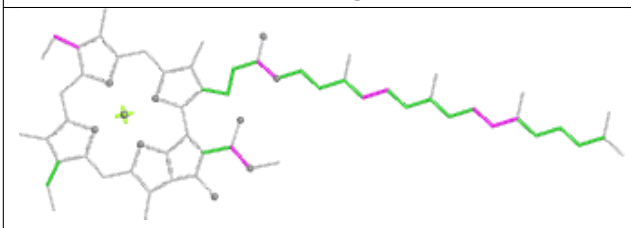
Ligand CLA Yy 612



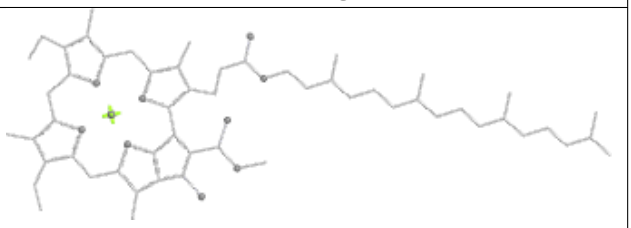
Bond lengths



Bond angles

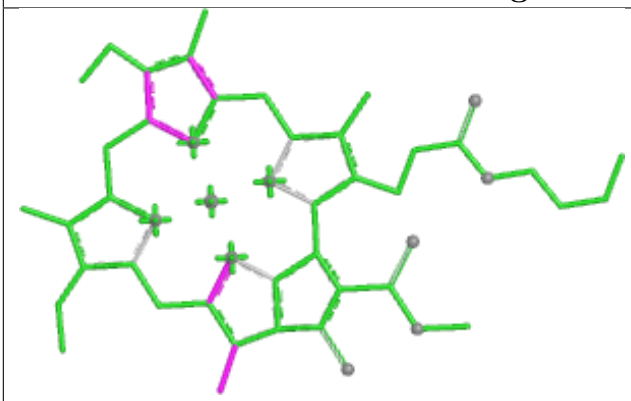


Torsions

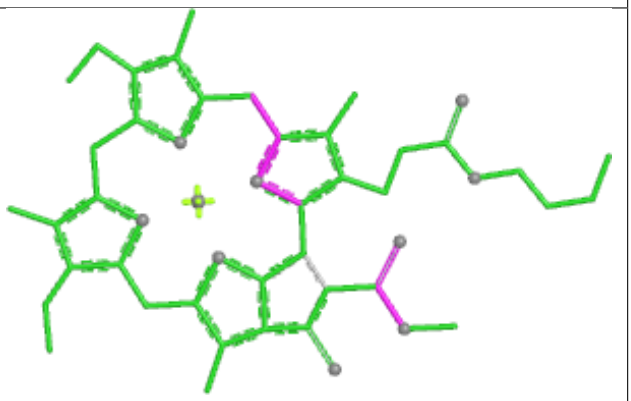


Rings

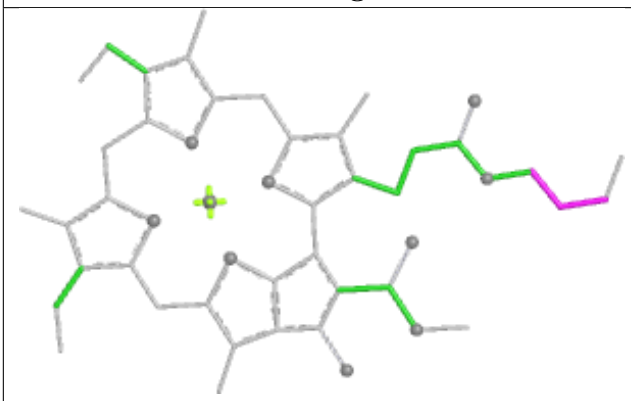
Ligand CLA RR 303



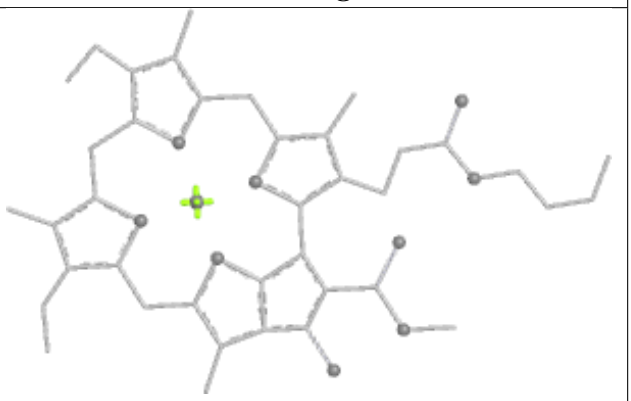
Bond lengths



Bond angles

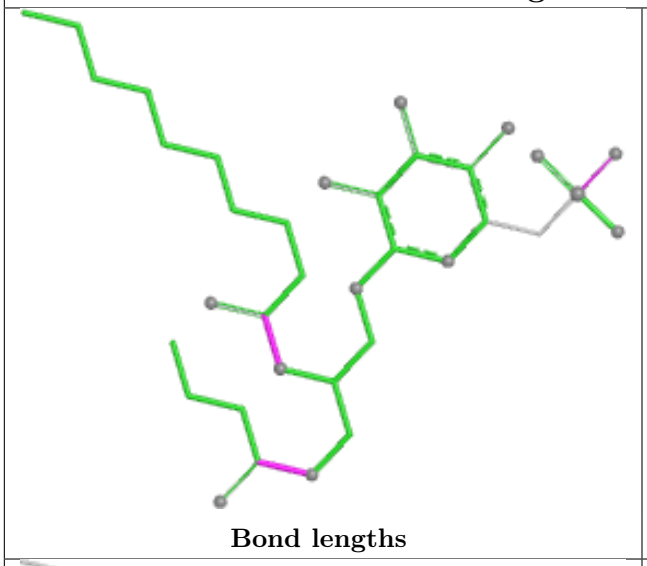


Torsions

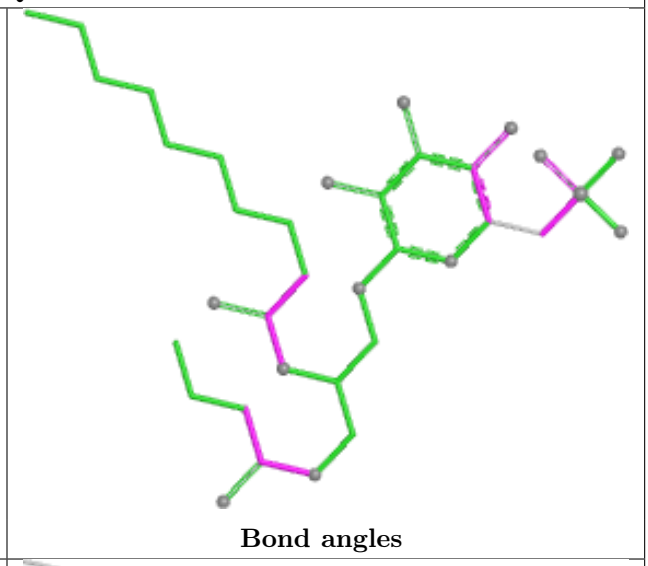


Rings

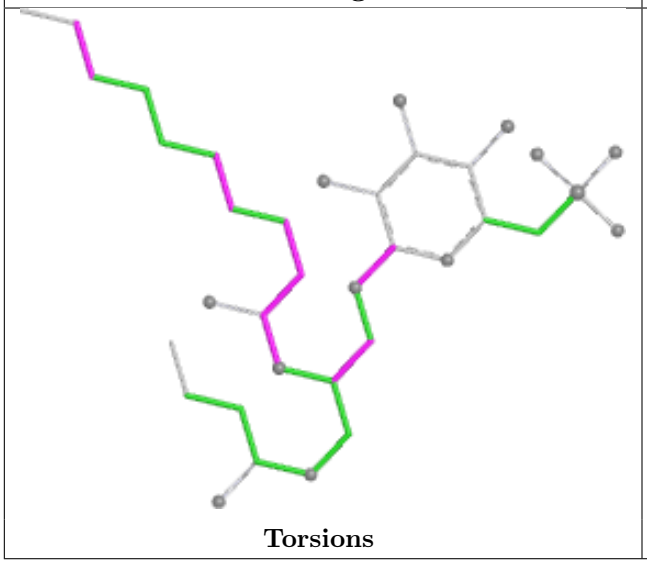
Ligand SQD L 102



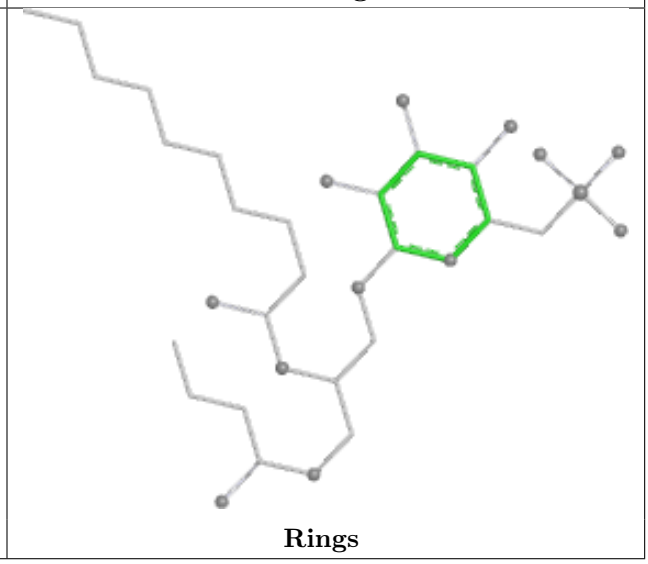
Bond lengths



Bond angles

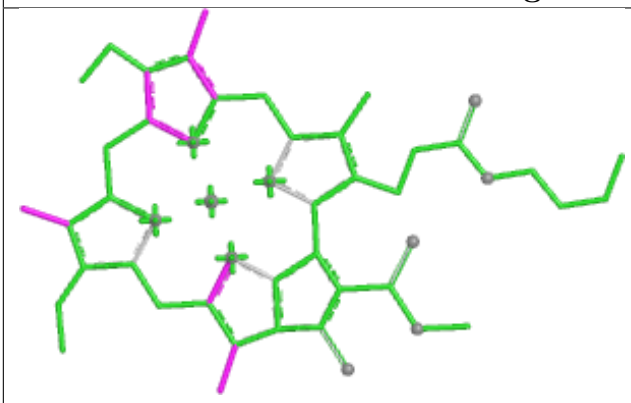


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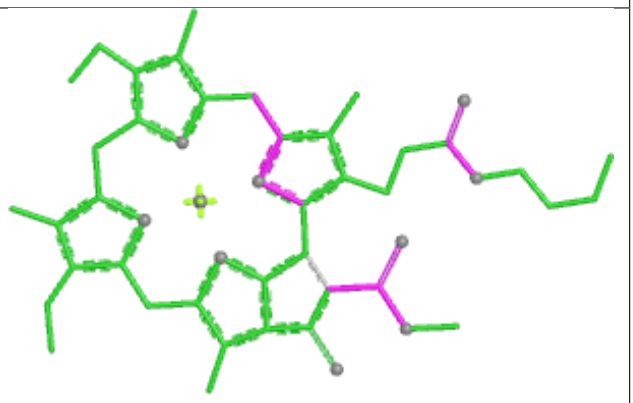


Rings

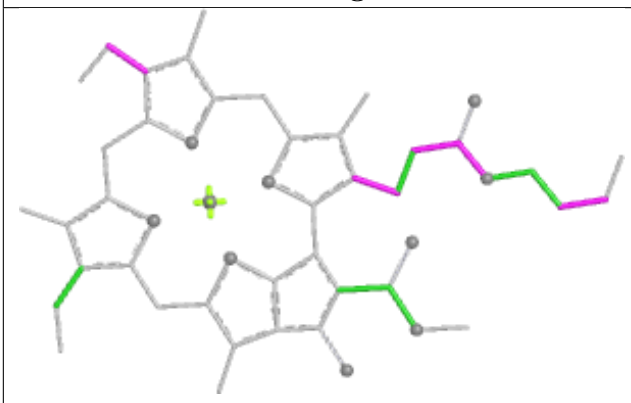
Ligand CLA A 406



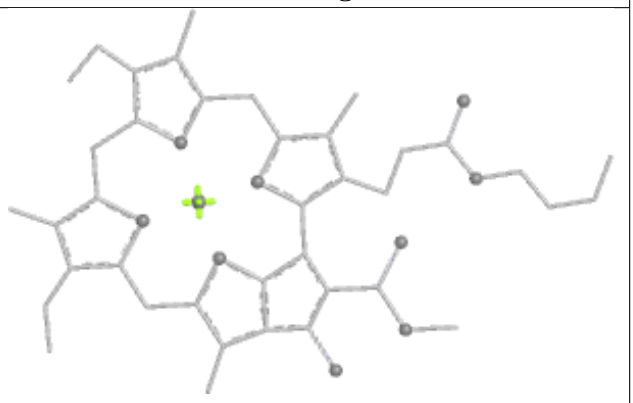
Bond lengths



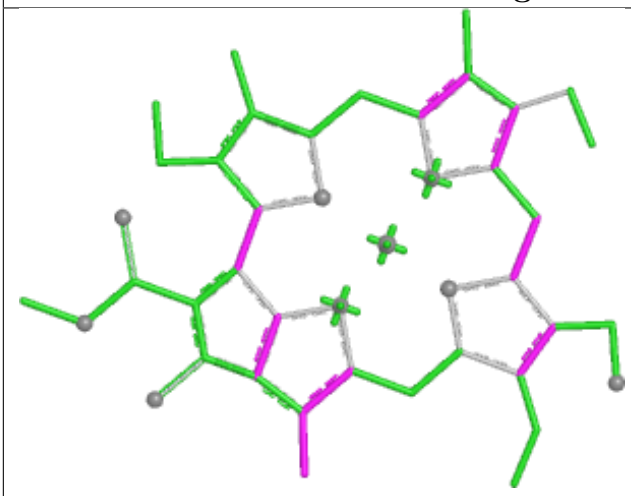
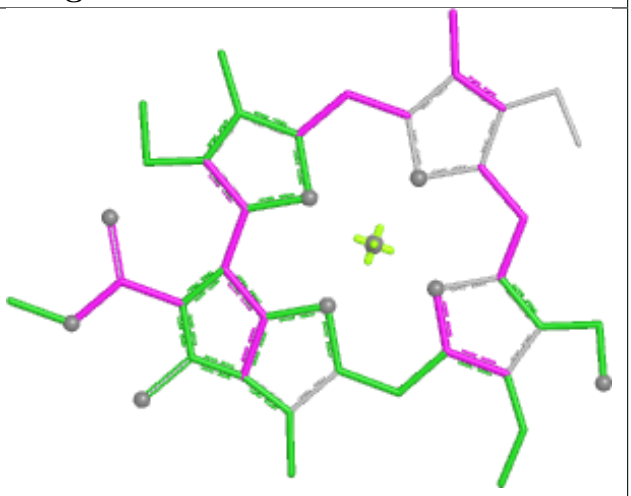
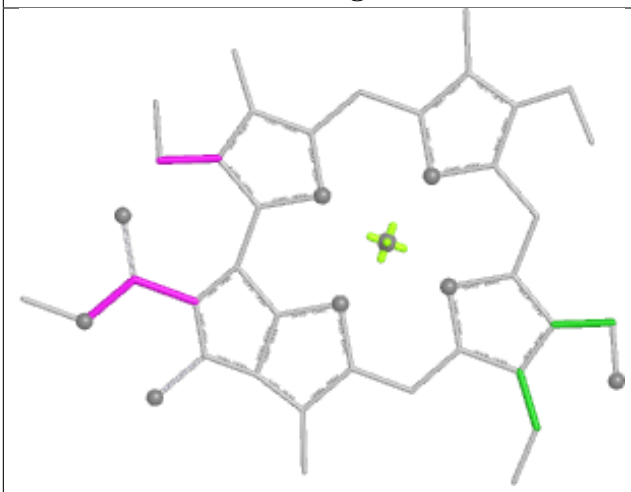
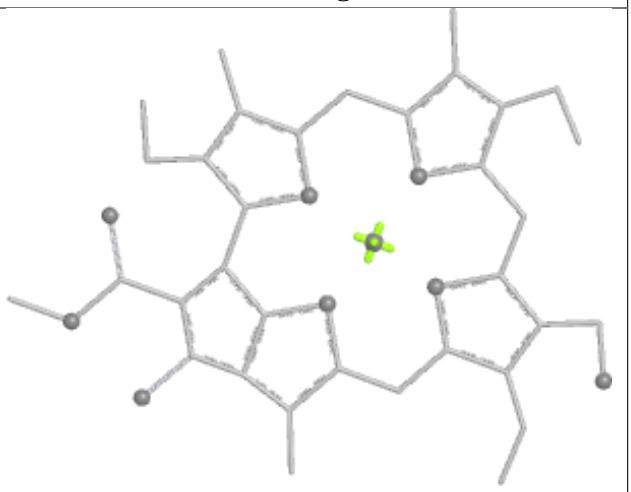
Bond angles

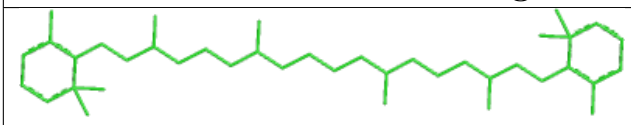
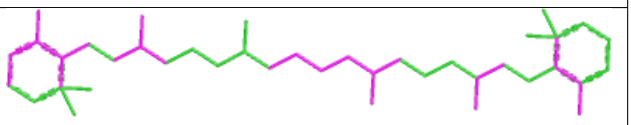
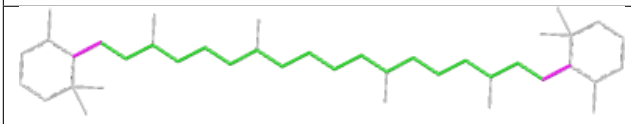
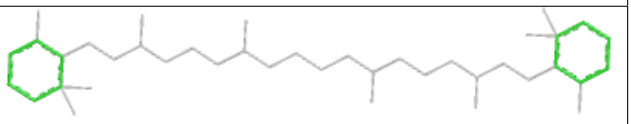


Torsions

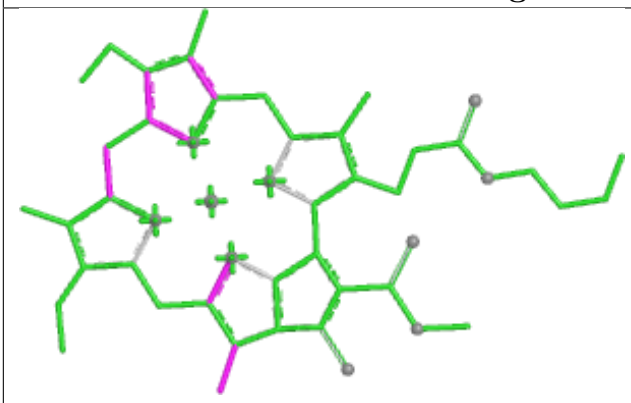


Rings

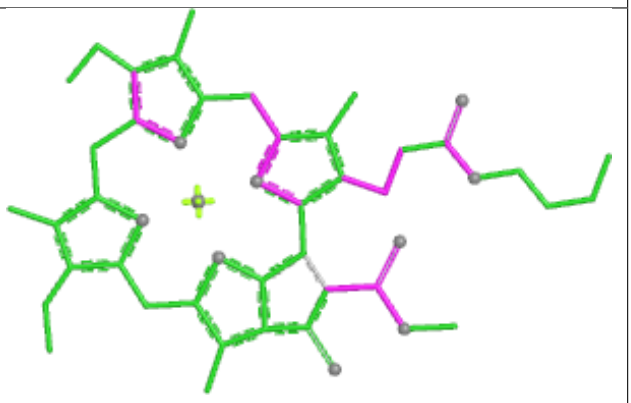
Ligand CHL Gg 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR Kk 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

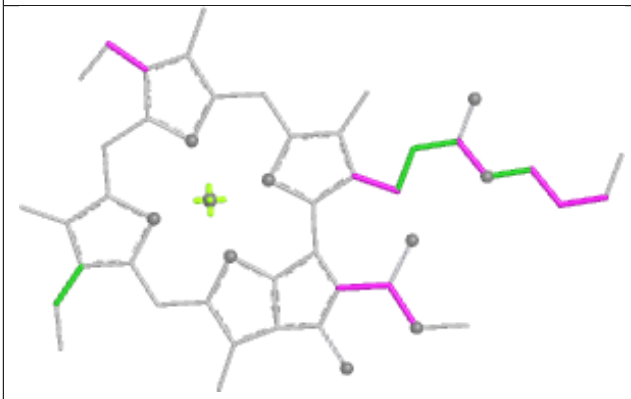
Ligand CLA NN 611



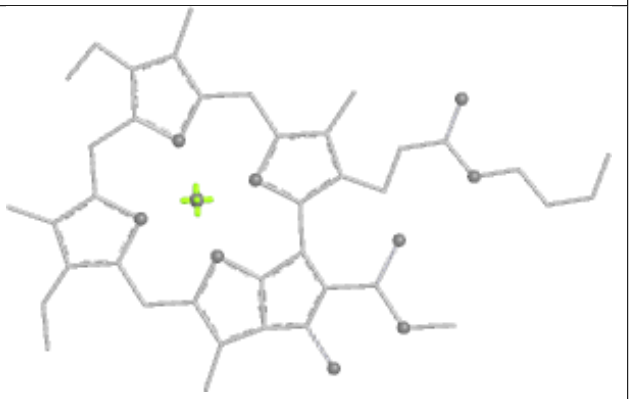
Bond lengths



Bond angles



Torsions

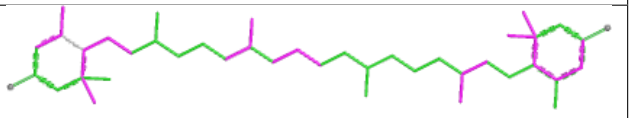


Rings

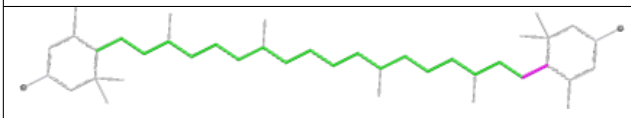
Ligand LUT Gg 317



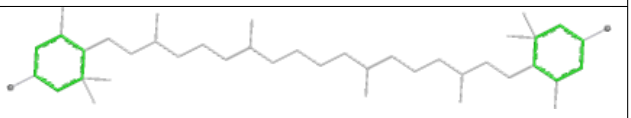
Bond lengths



Bond angles

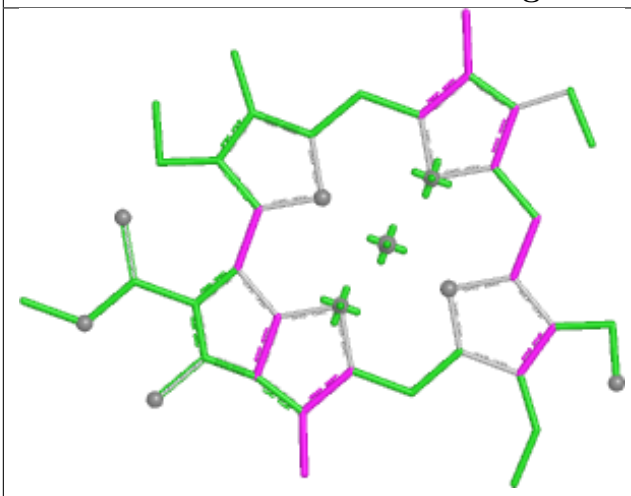


Torsions

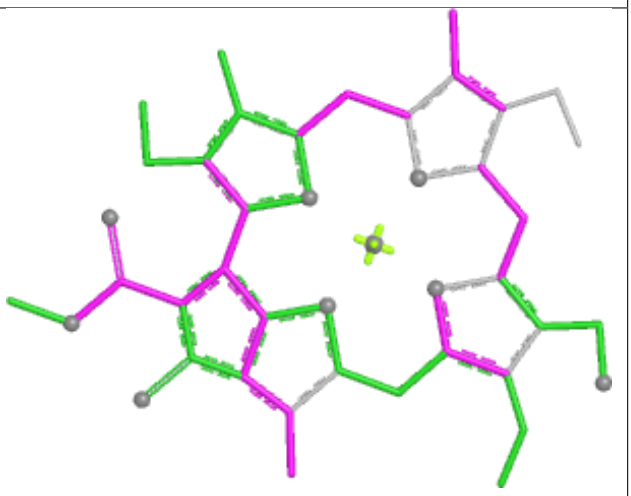


Rings

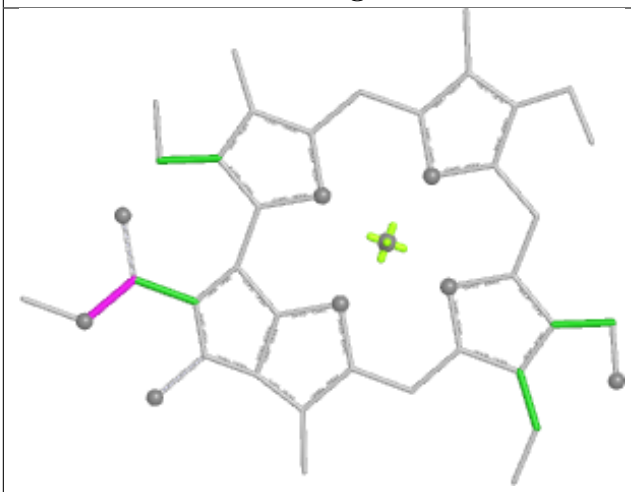
Ligand CHL G 609



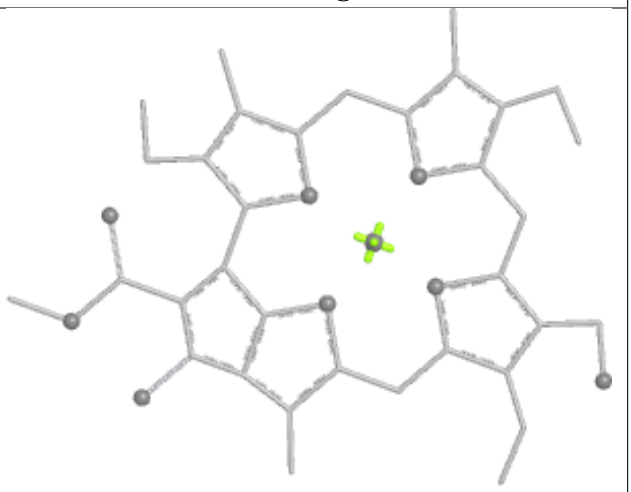
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Bond angles

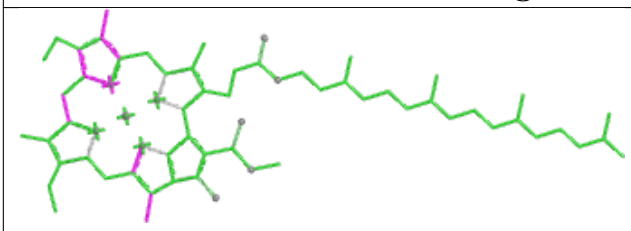


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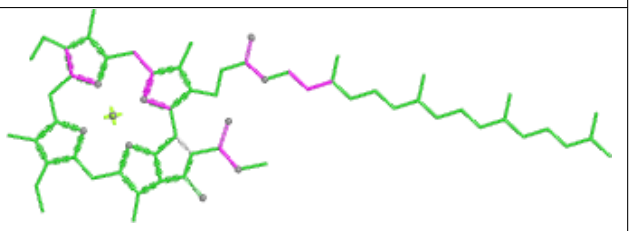


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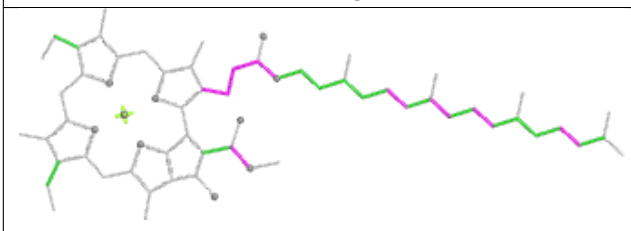
Ligand CLA Bb 609



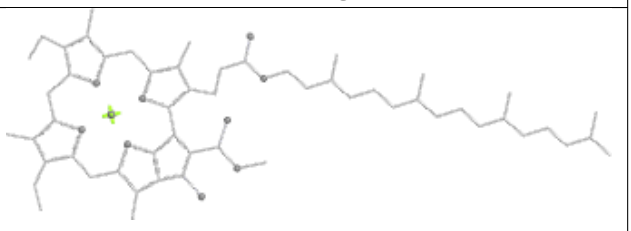
Bond lengths



Bond angles

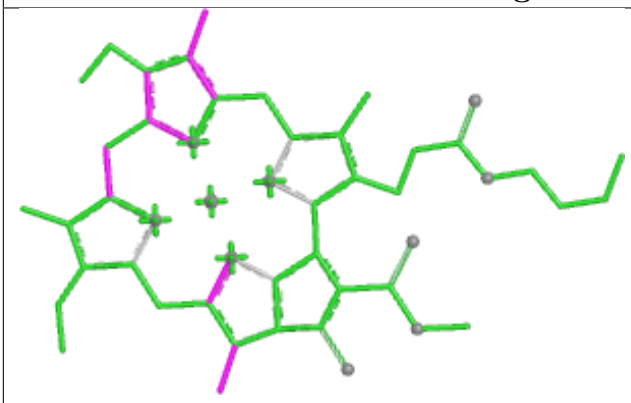


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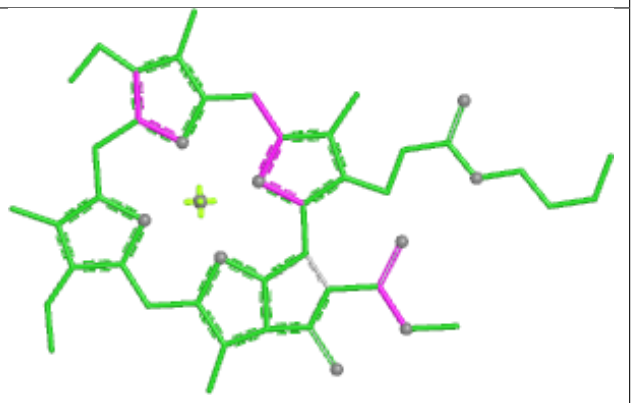


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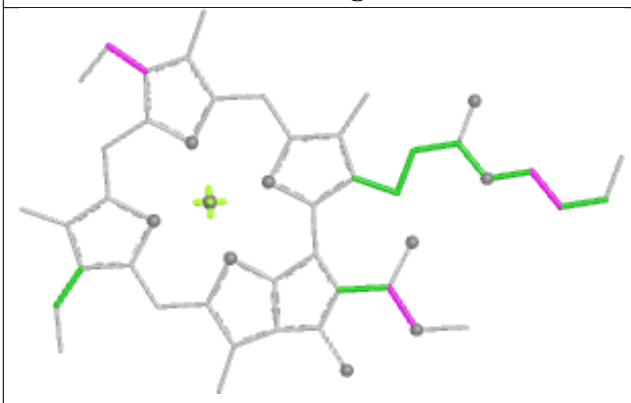
Ligand CLA Nn 302



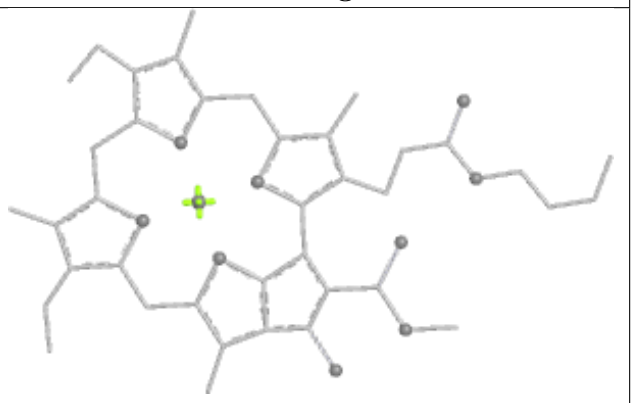
Bond lengths



Bond angles

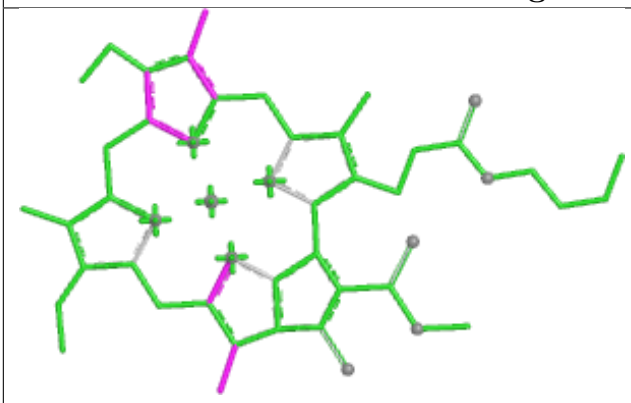


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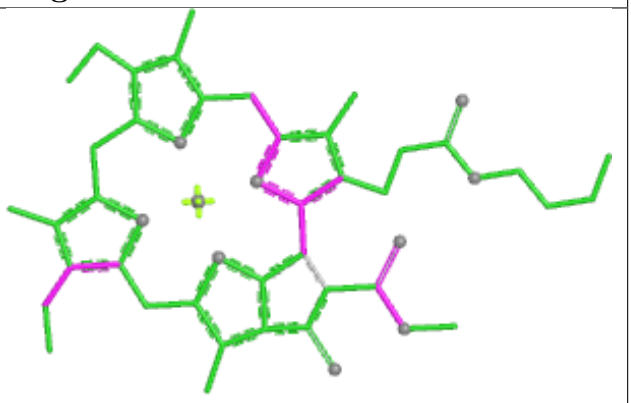


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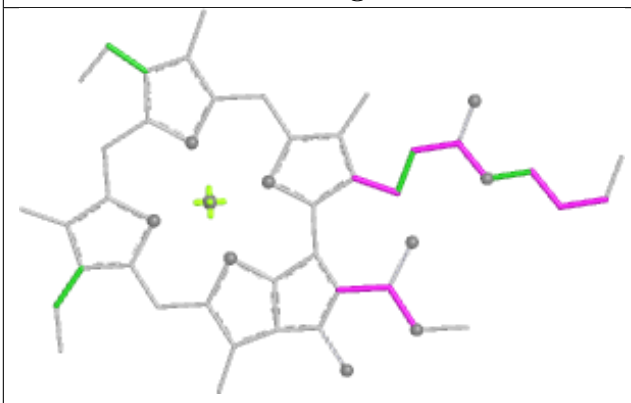
Ligand CLA g 612



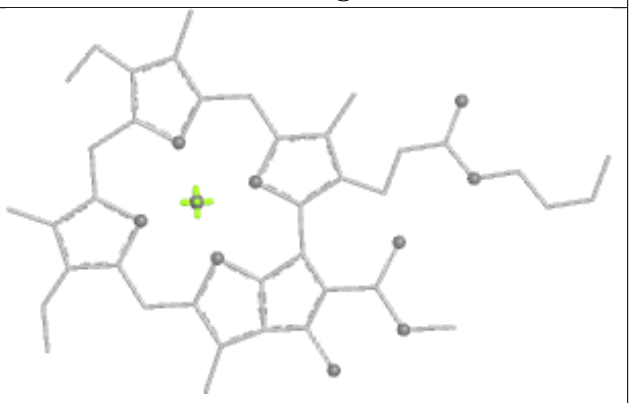
Bond lengths



Bond angles

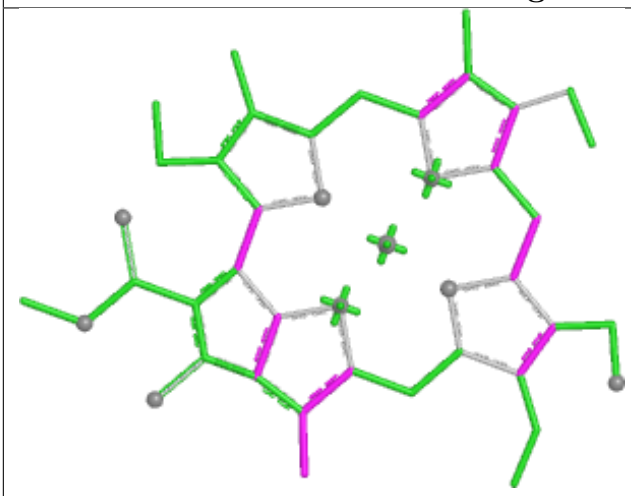


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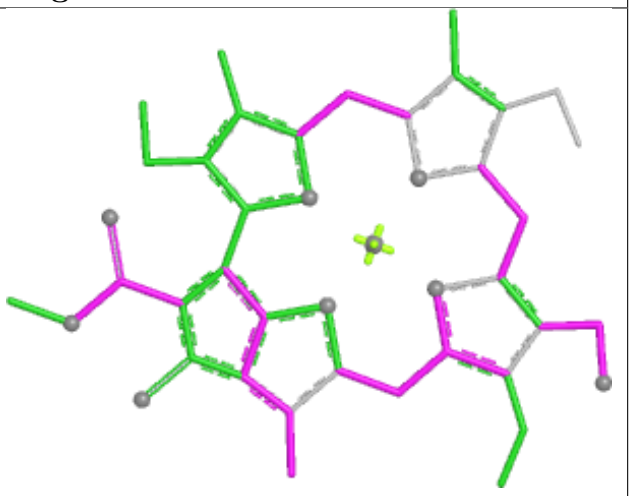


Rings

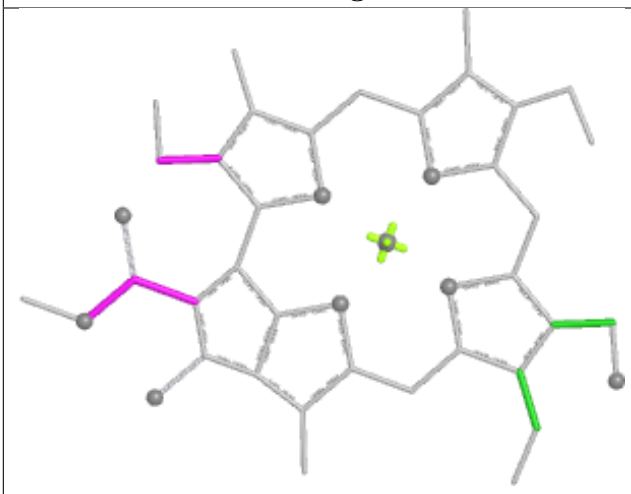
Ligand CHL g 605



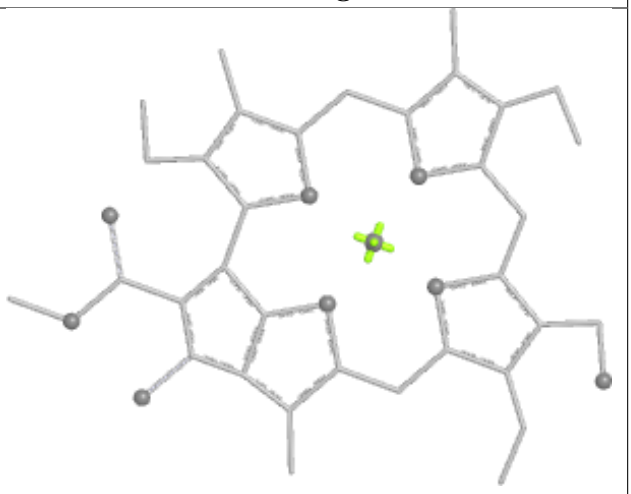
Bond lengths



Bond angles

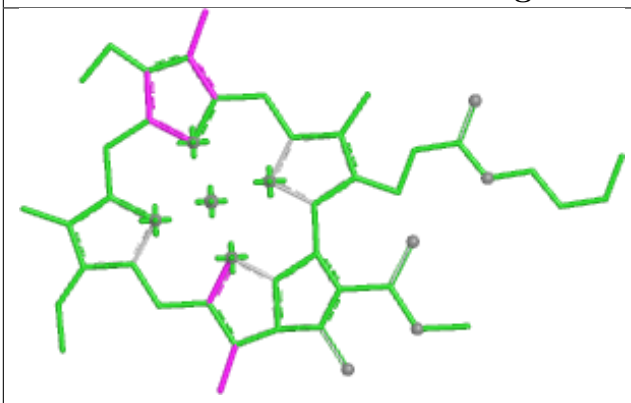


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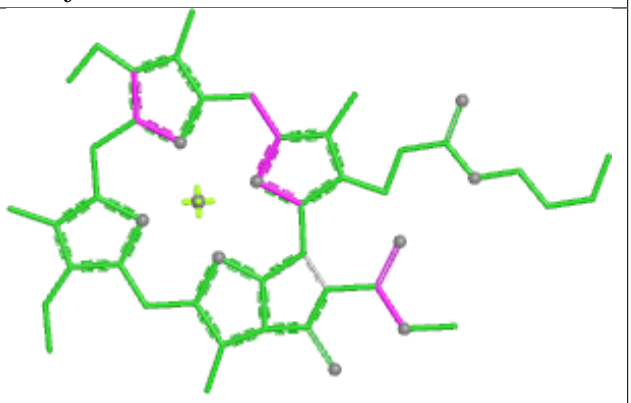


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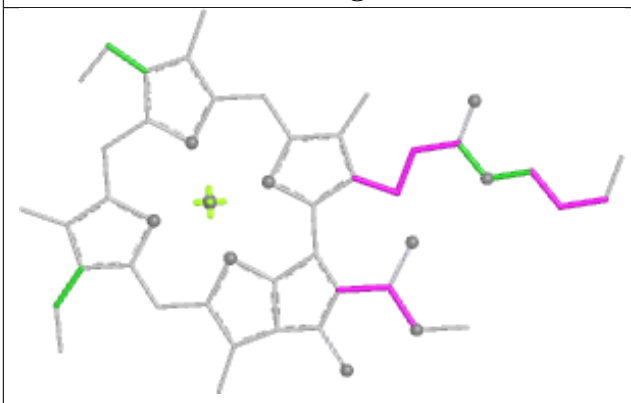
Ligand CLA Yy 604



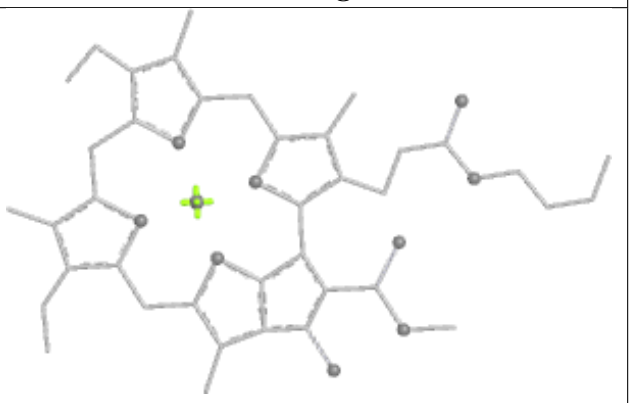
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Bond angles

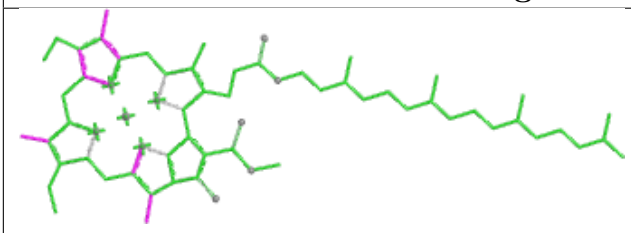


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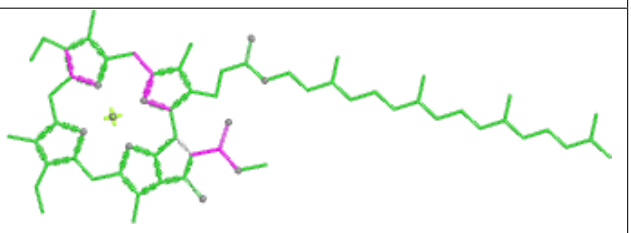


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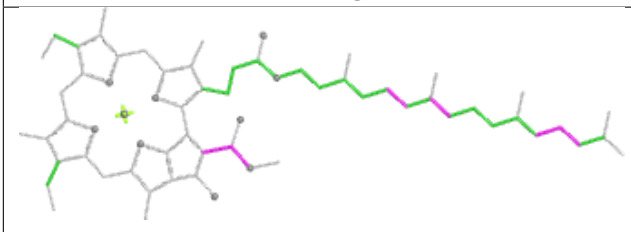
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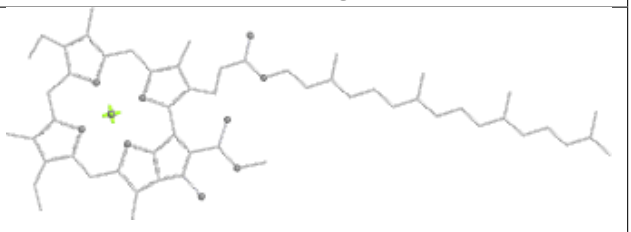
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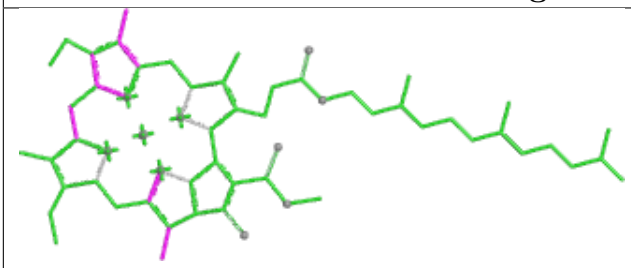


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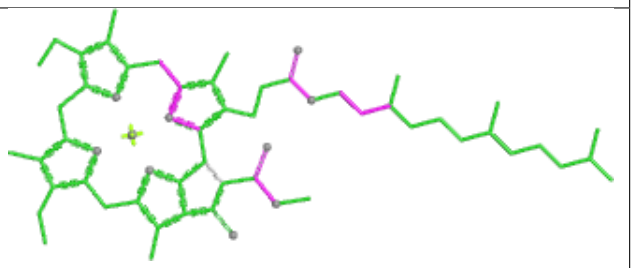


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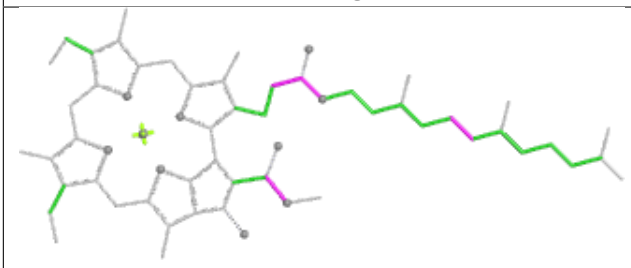
Ligand CLA c 508



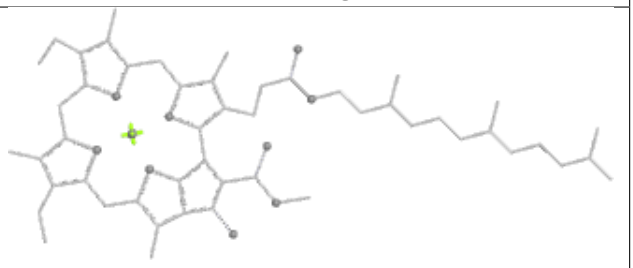
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Bond angles

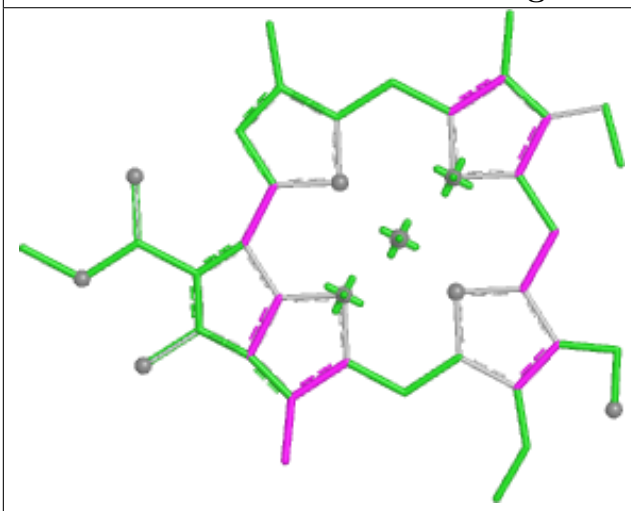


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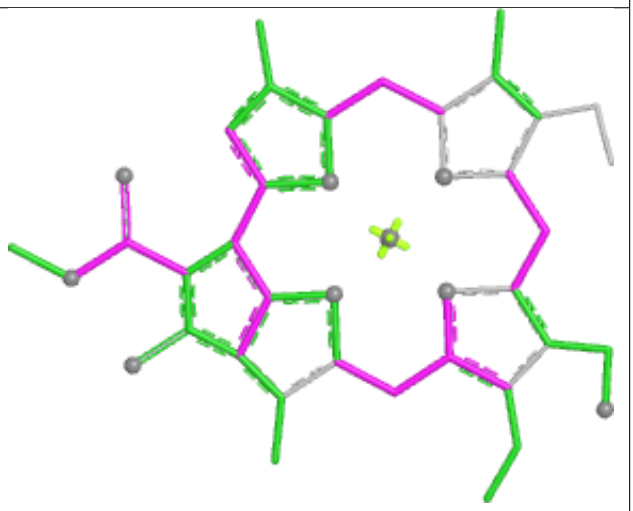


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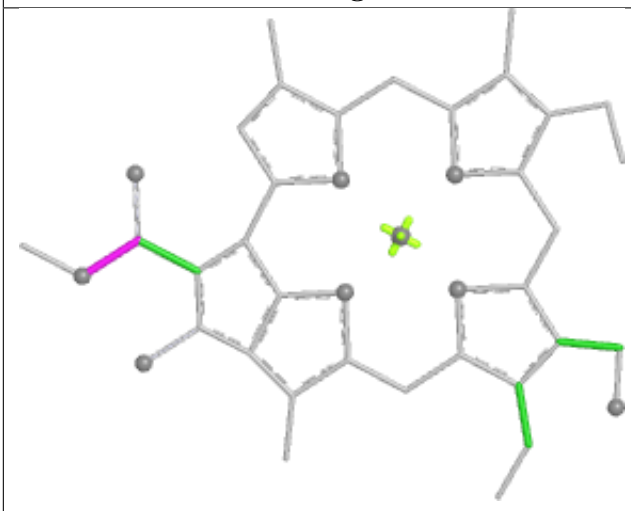
Ligand CHL 2 607



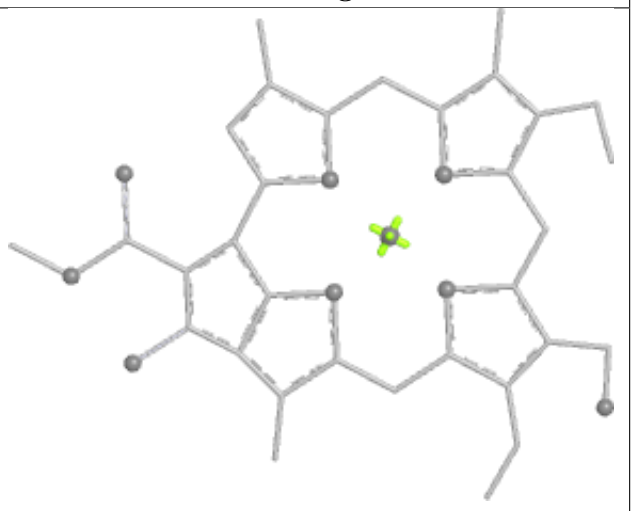
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Bond angles

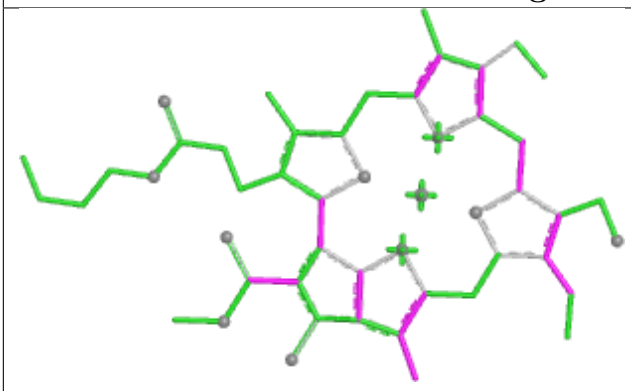


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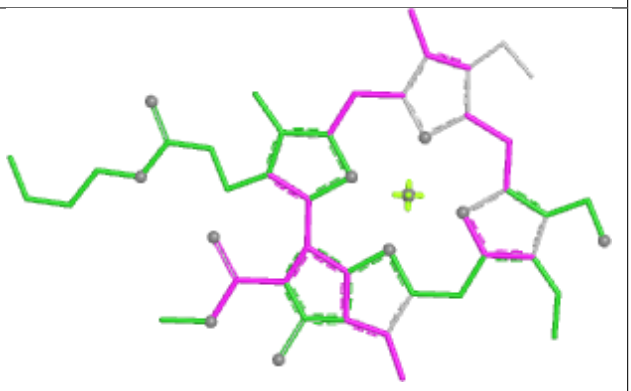


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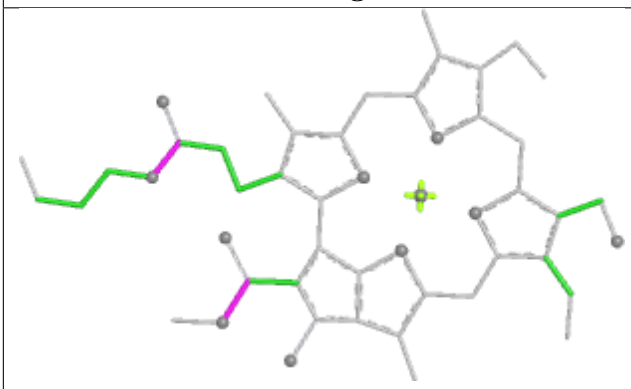
Ligand CHL r 606



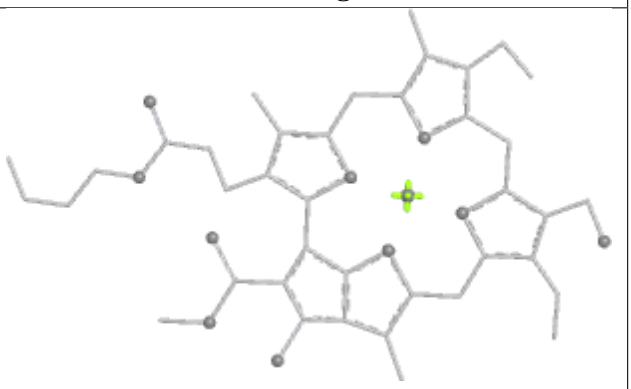
Bond lengths



Bond angles

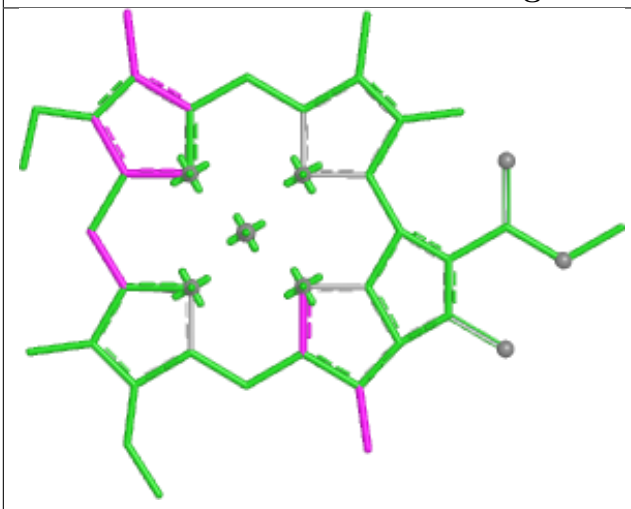


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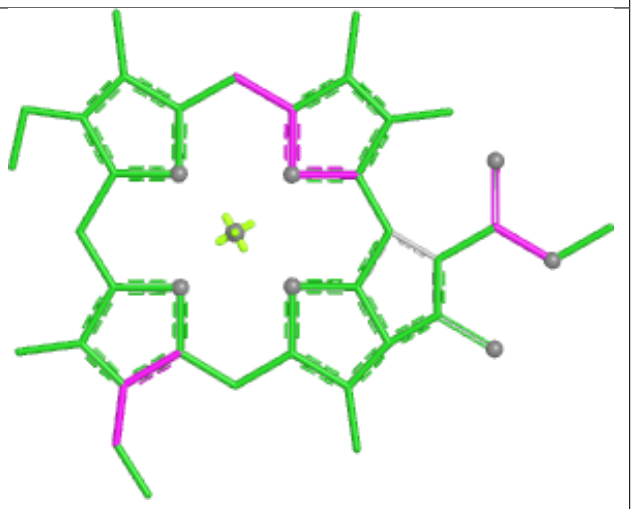


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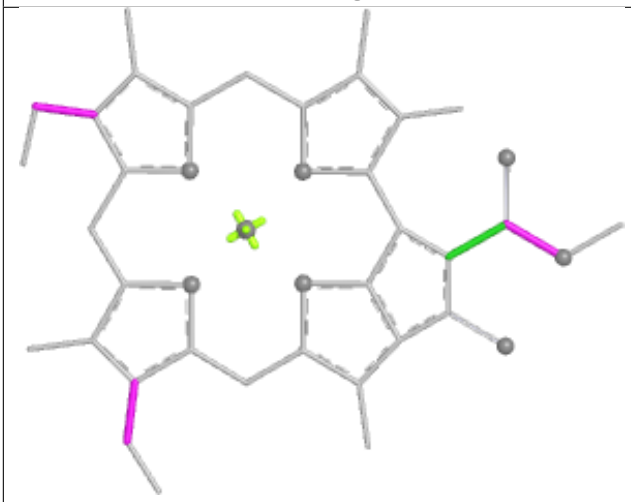
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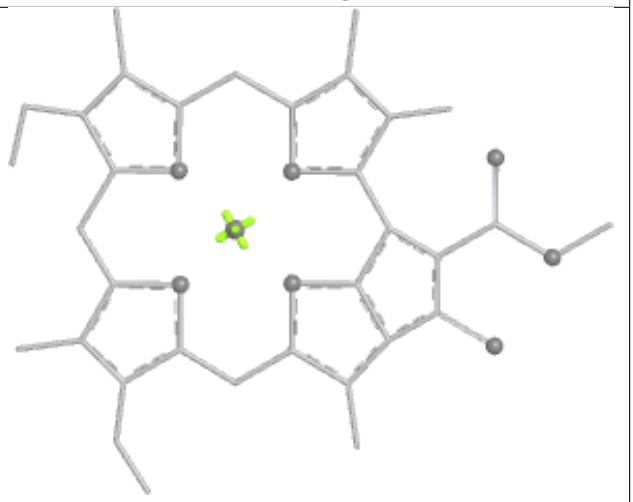
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Bond angles

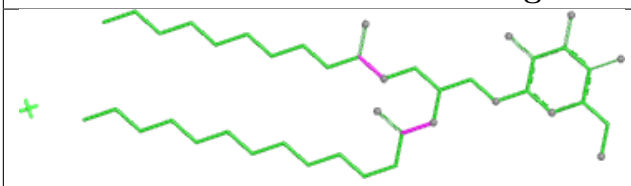


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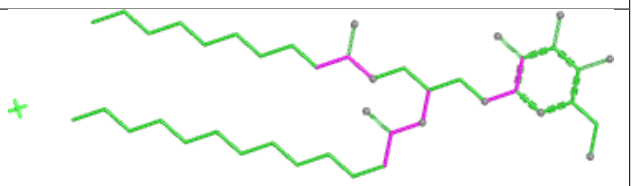


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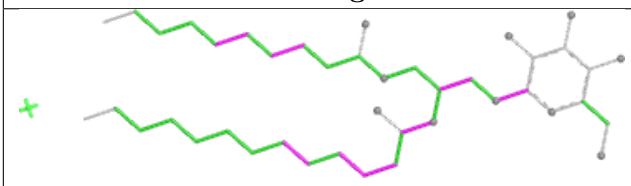
Ligand LMG a 412



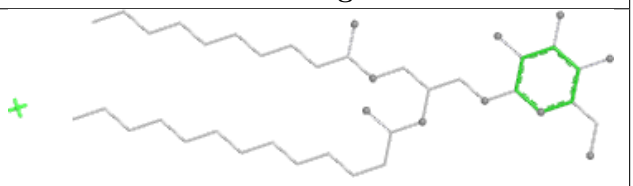
Bond lengths



Bond angles

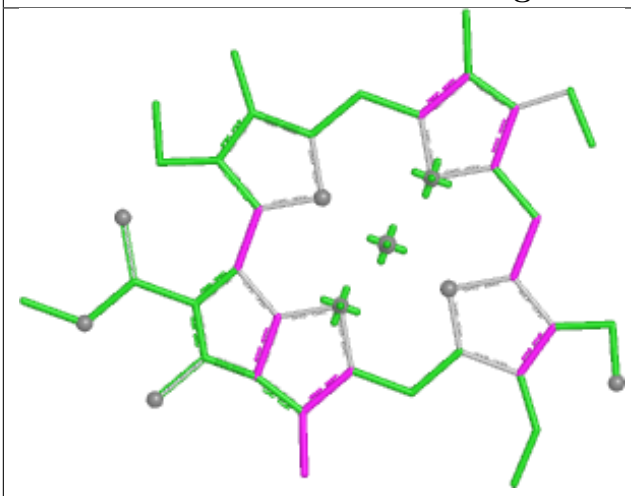


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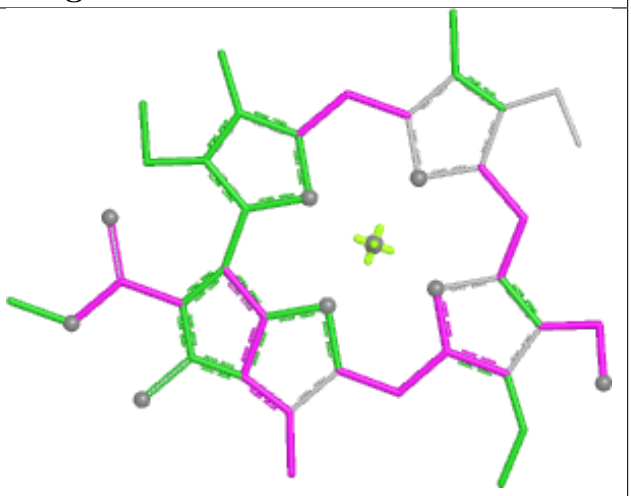


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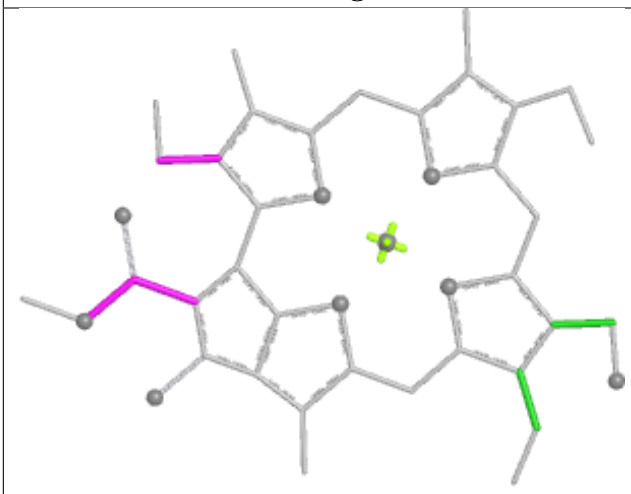
Ligand CHL Gg 306



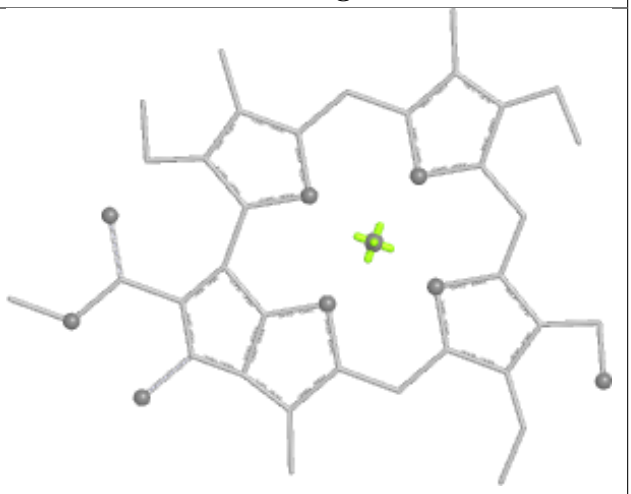
Bond lengths



Bond angles

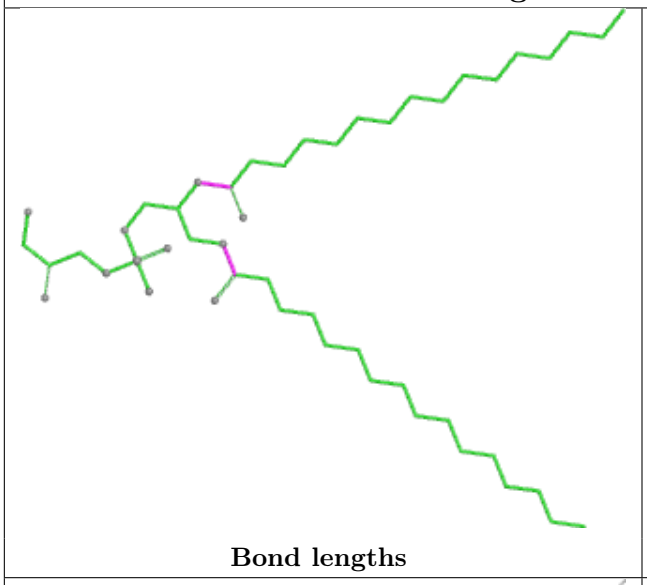


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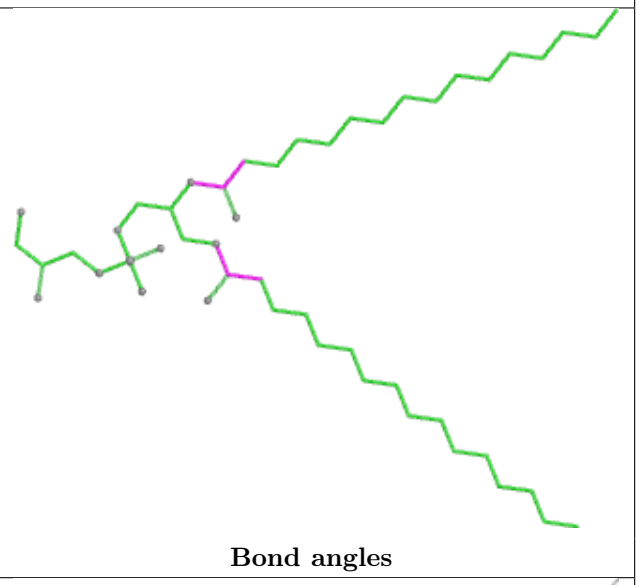


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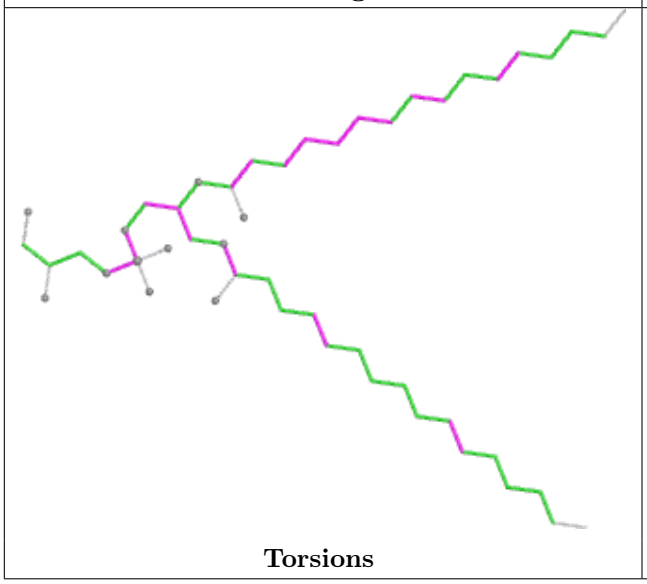
Ligand LHG YY 618



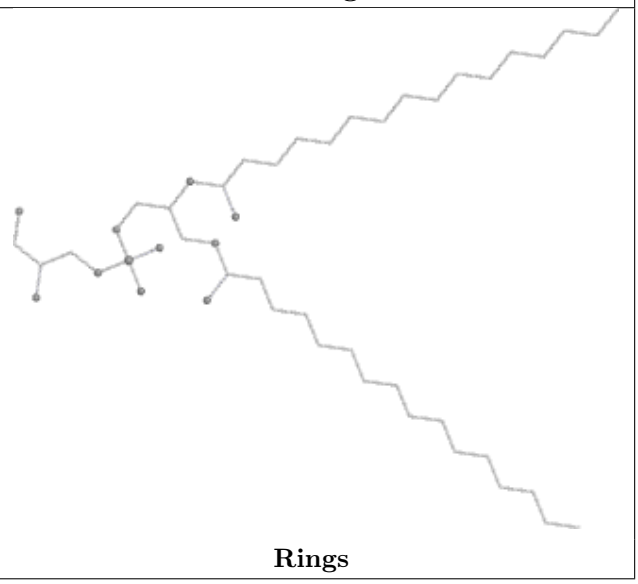
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR Bb 619



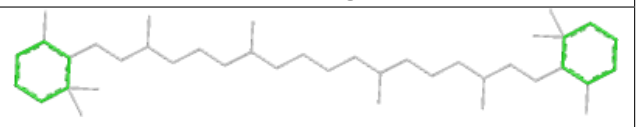
Bond lengths



Bond angles

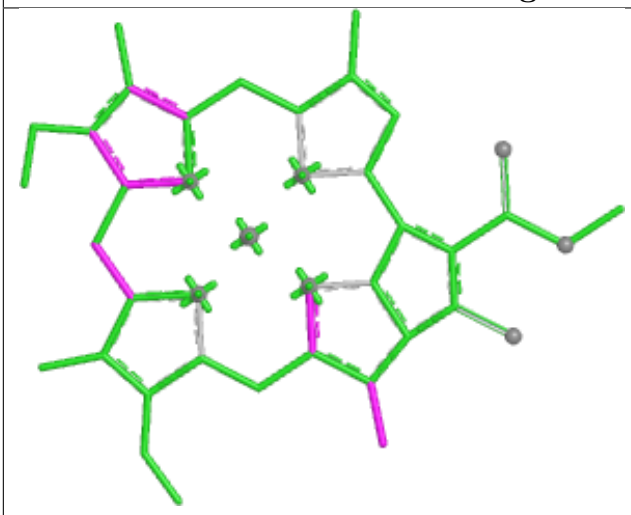


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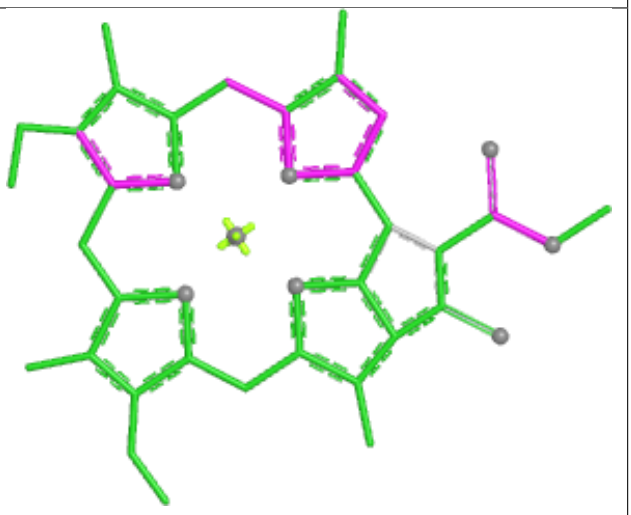


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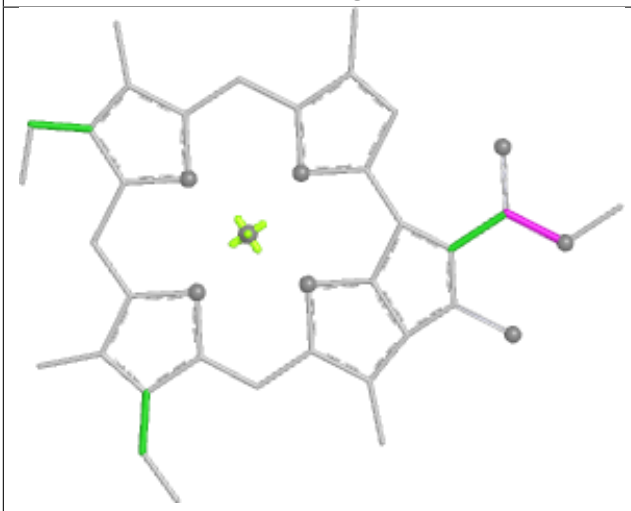
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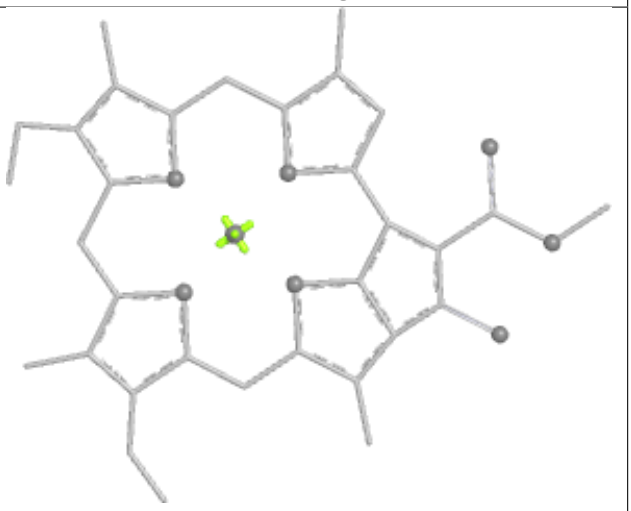
Bond lengths



Bond angles



Torsions



Rings

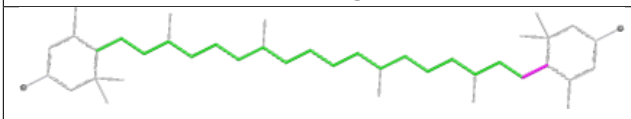
Ligand LUT GG 616



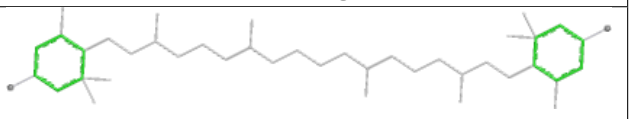
Bond lengths



Bond angles

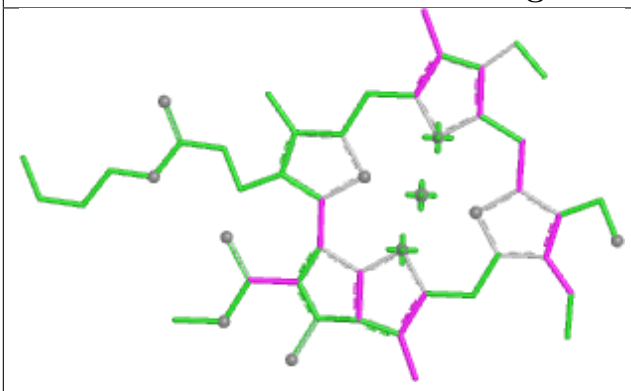


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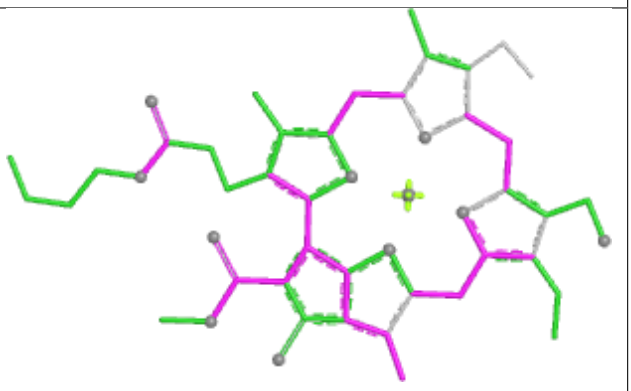


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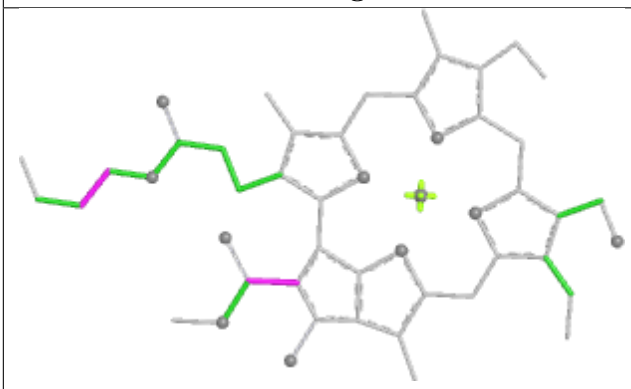
Ligand CHL n 606



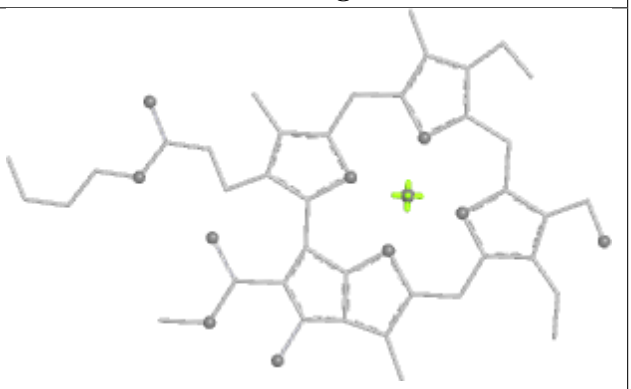
Bond lengths



Bond angles

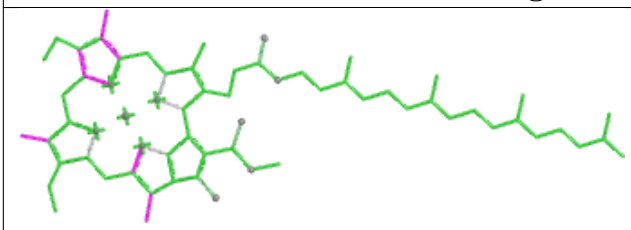


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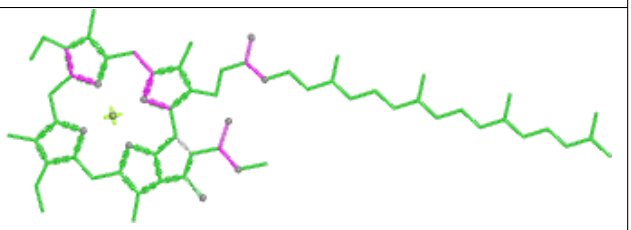


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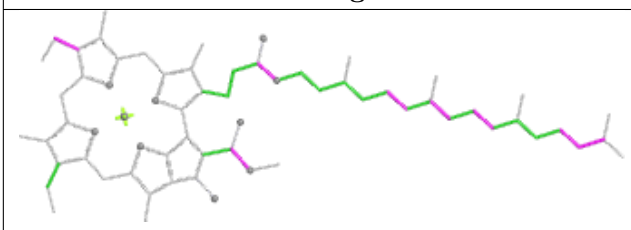
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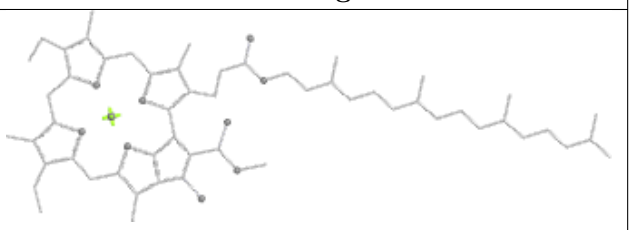
Bond lengths



Bond angles

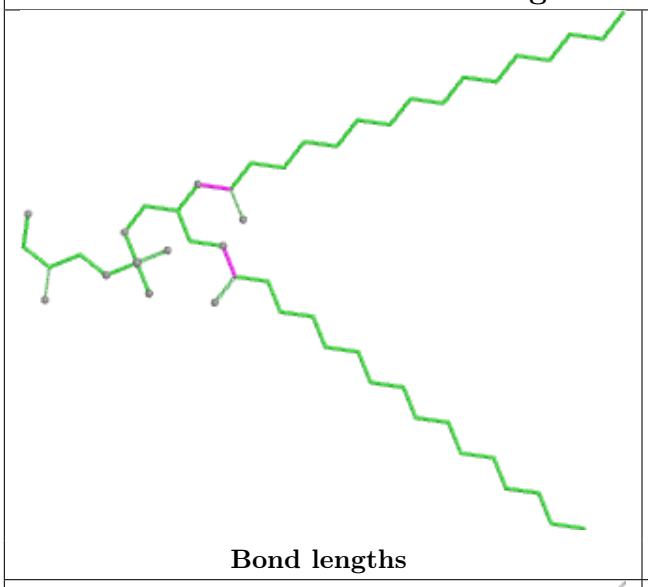


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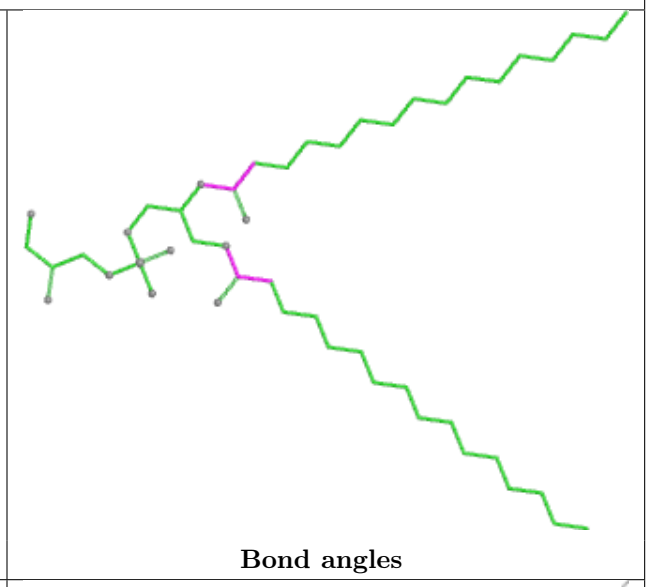


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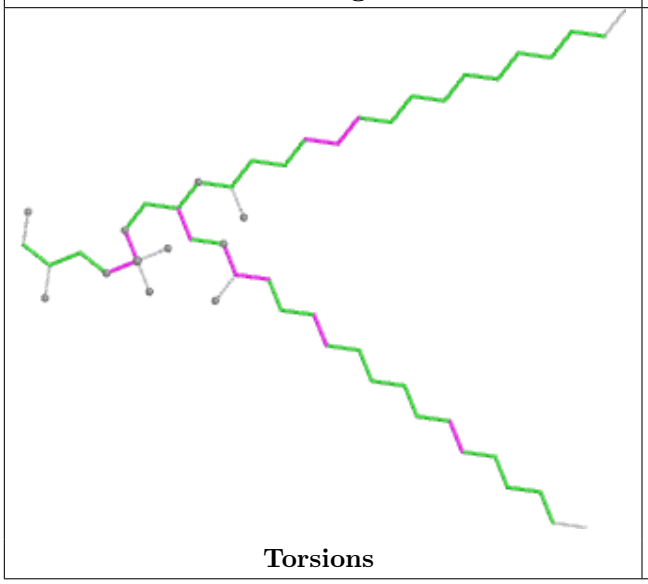
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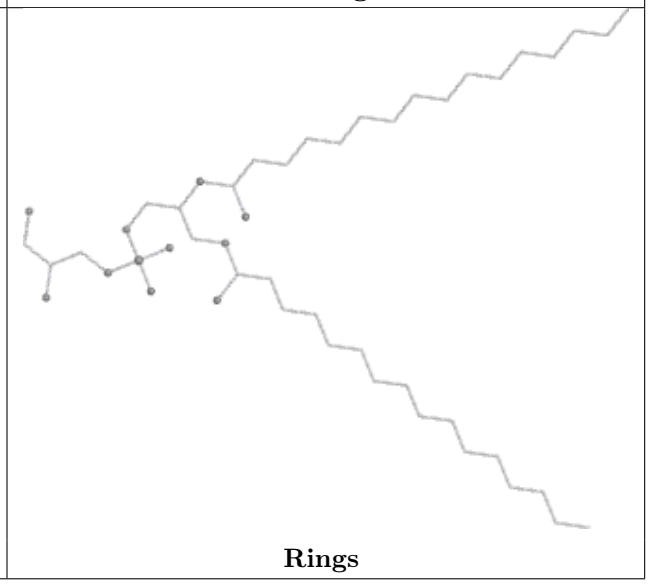
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Bond angles

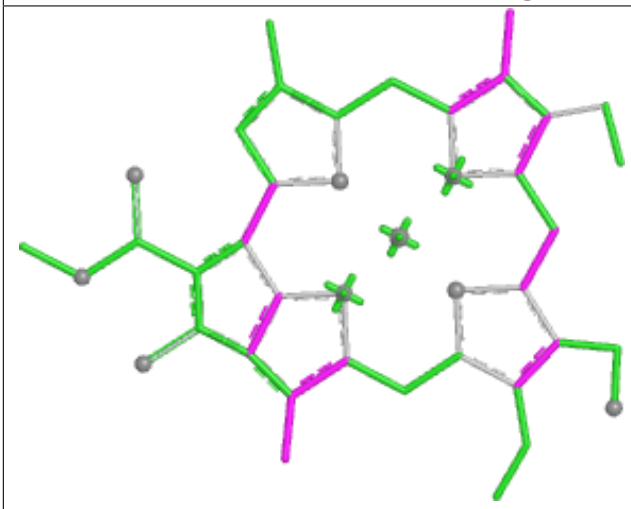


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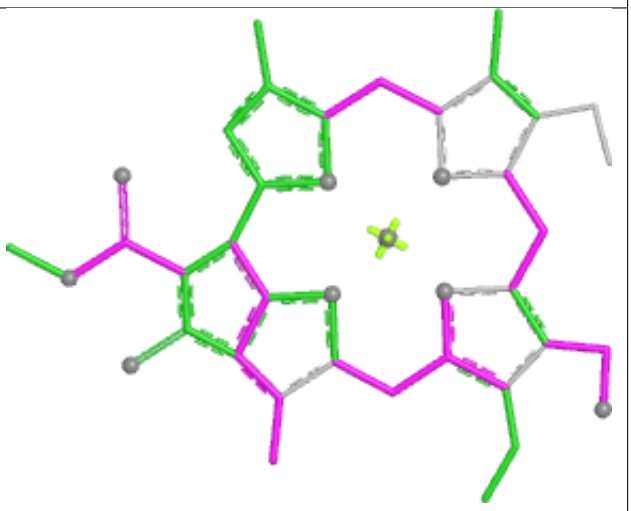


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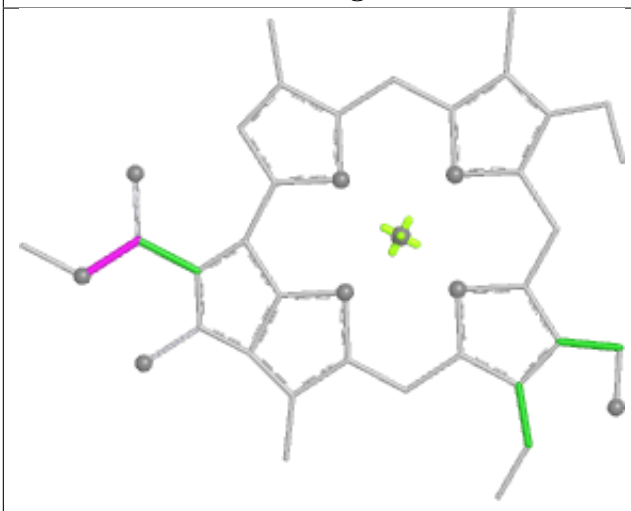
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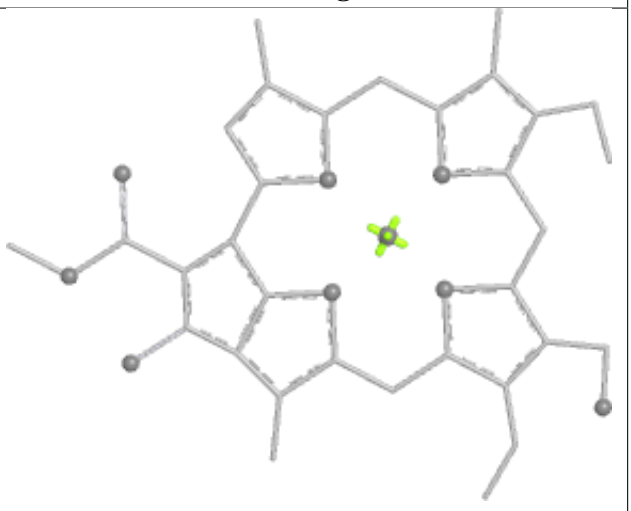
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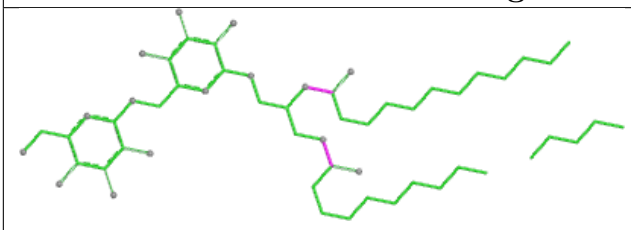


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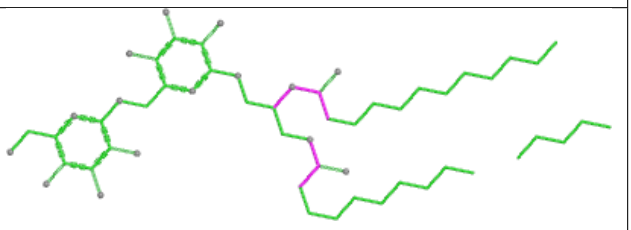


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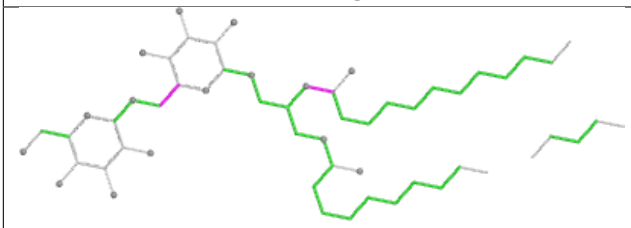
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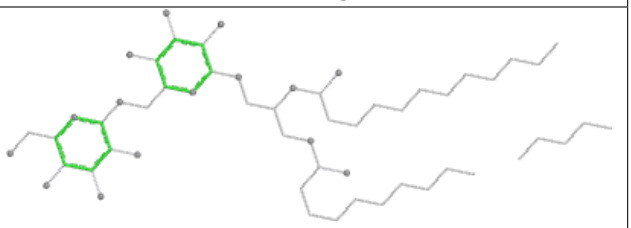
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Bond angles

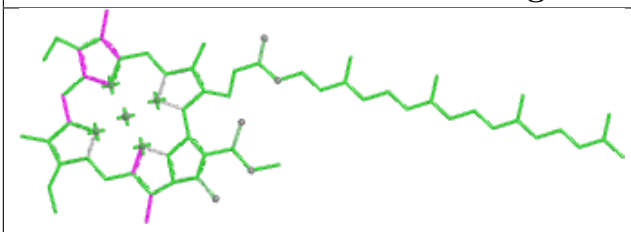


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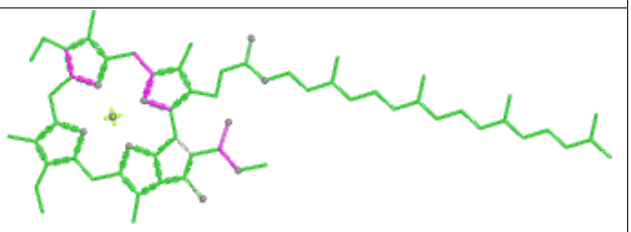


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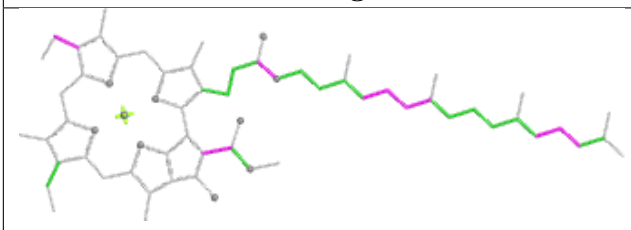
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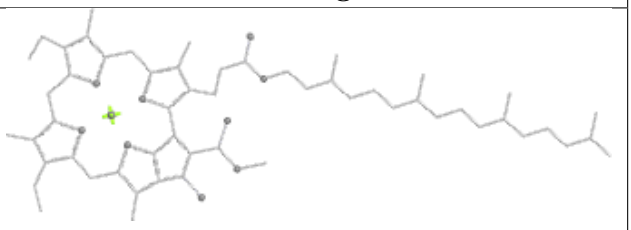
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Bond angles



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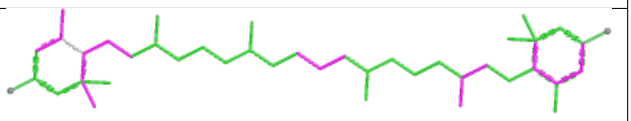


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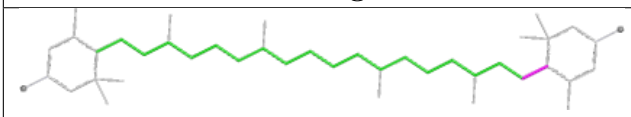
Ligand LUT 4 313



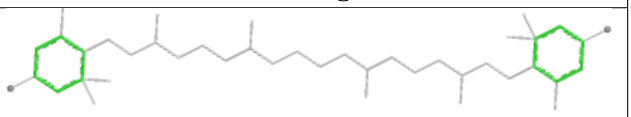
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Bond angles

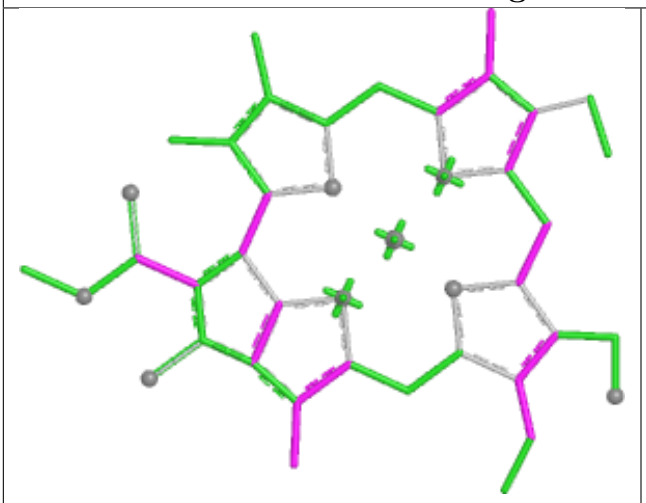


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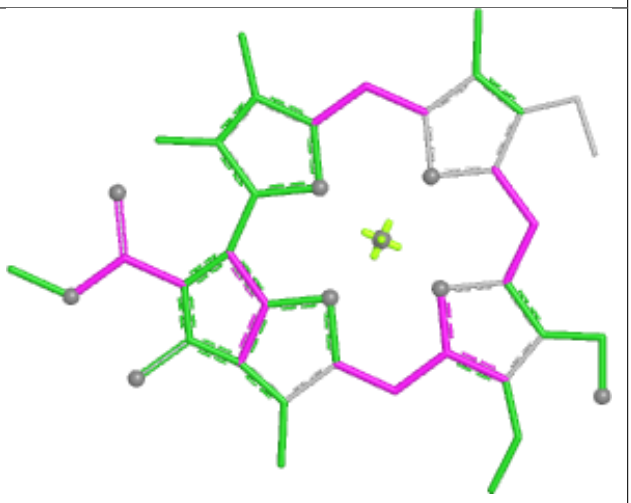


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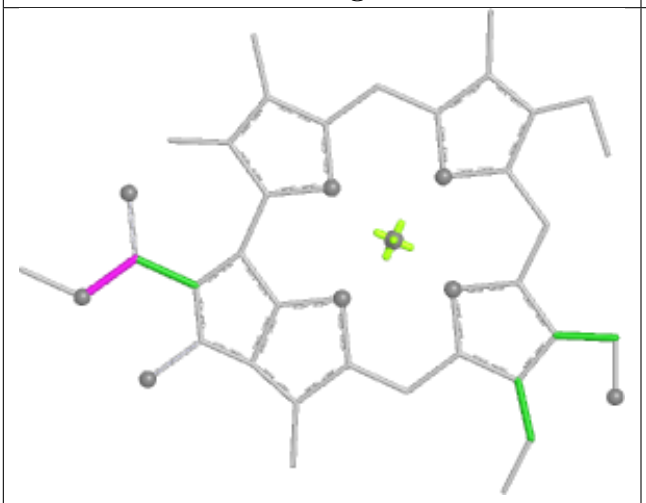
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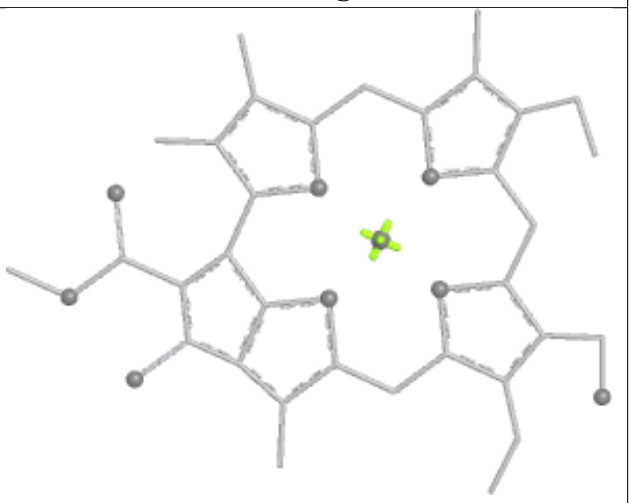
Bond lengths



Bond angles

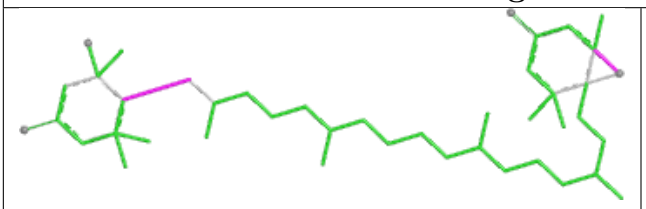


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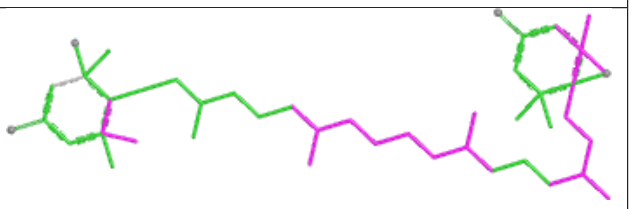


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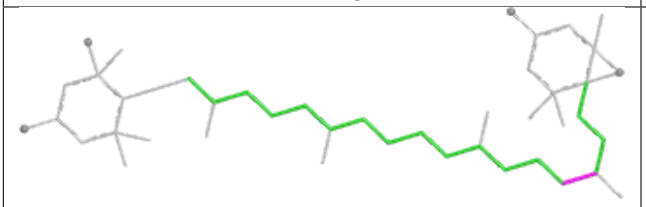
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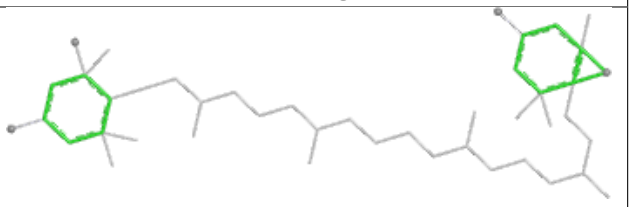
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Bond angles

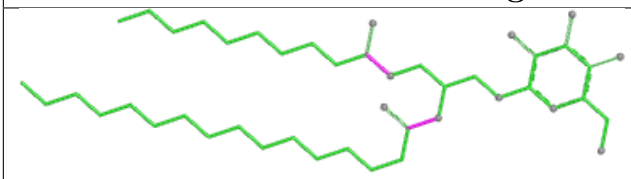


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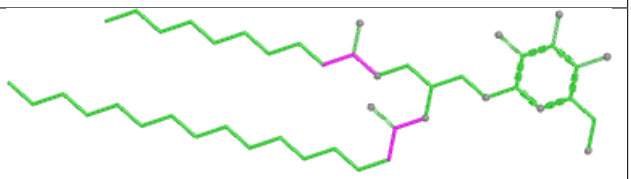


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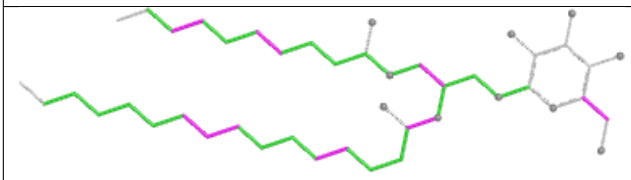
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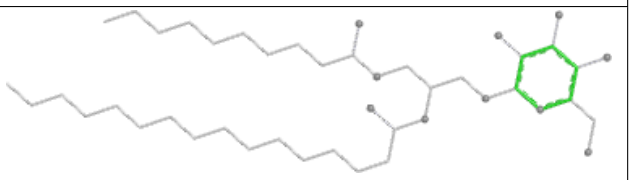
Bond lengths



Bond angles

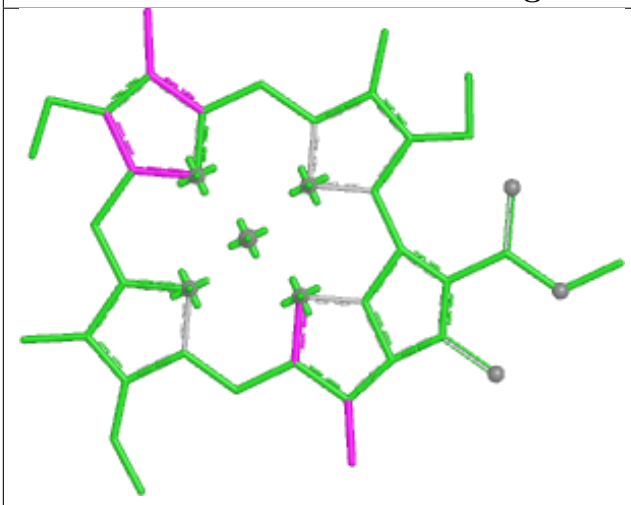


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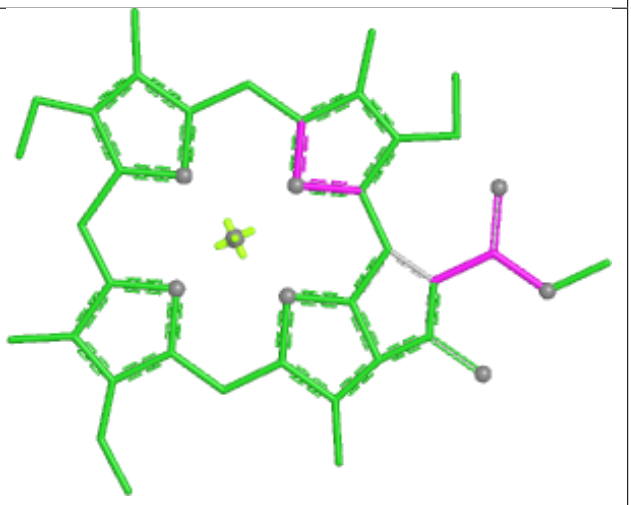


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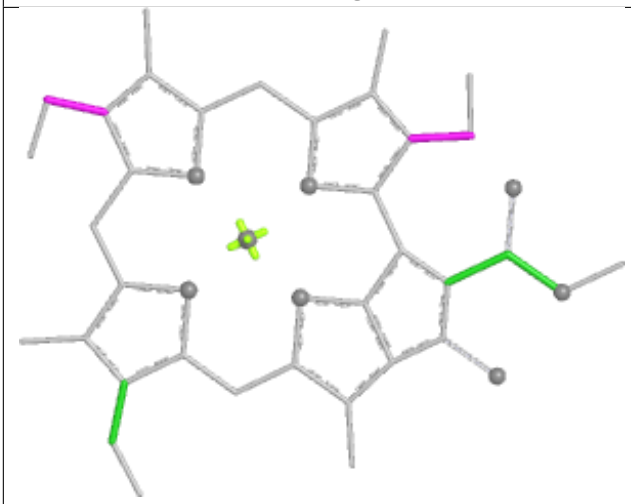
Ligand CLA R 612



Bond lengths



Bond angles

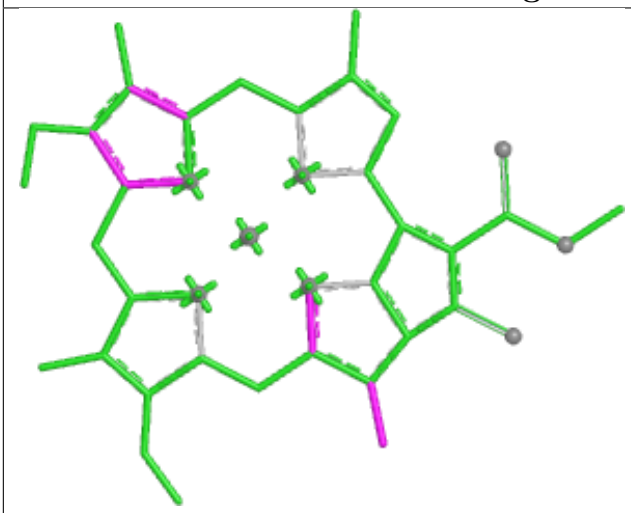


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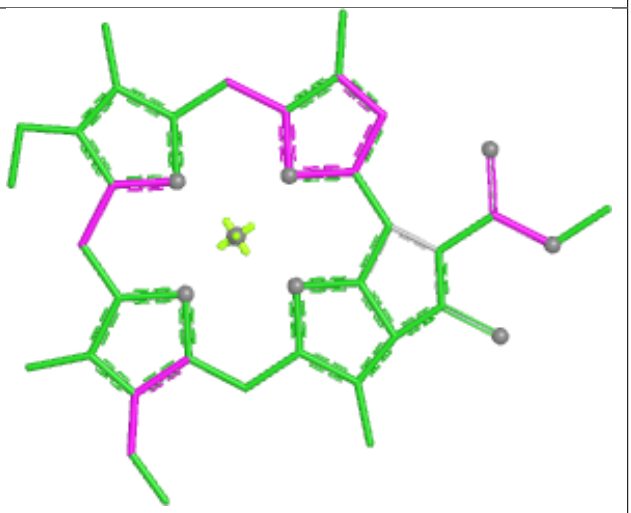


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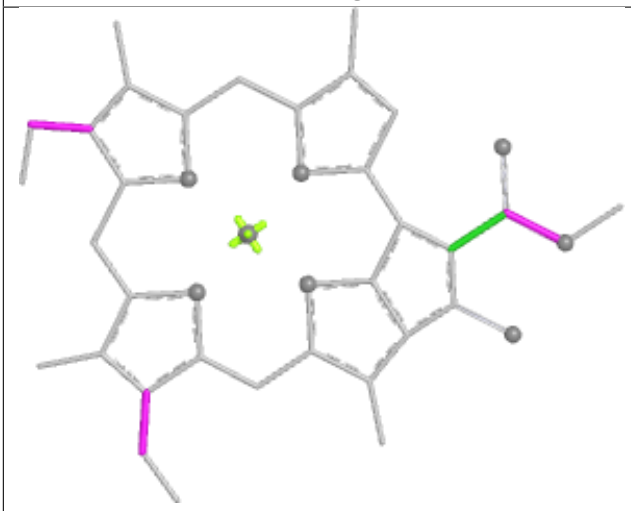
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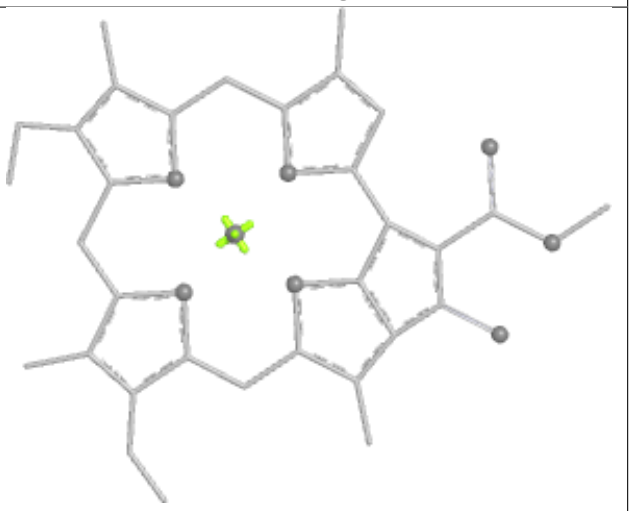
Bond lengths



Bond angles

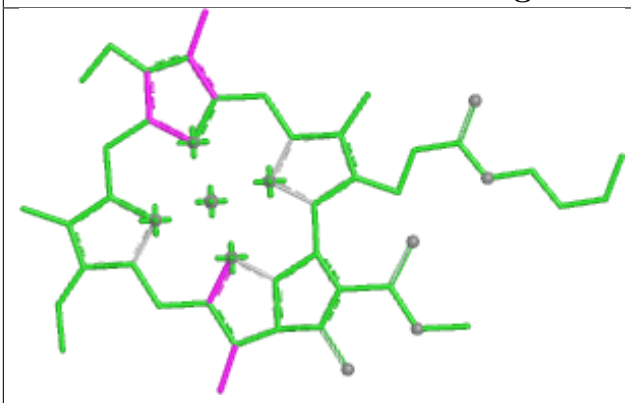


Torsions

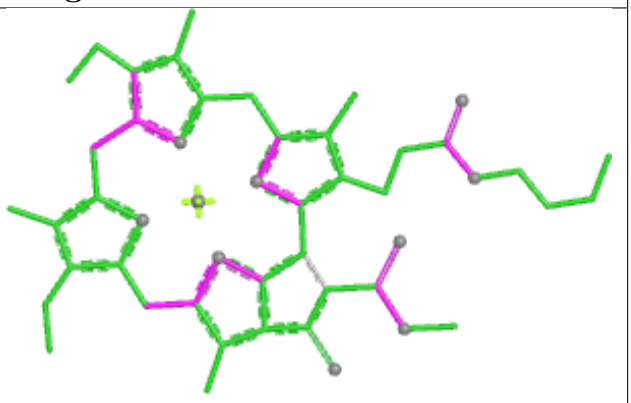


Rings

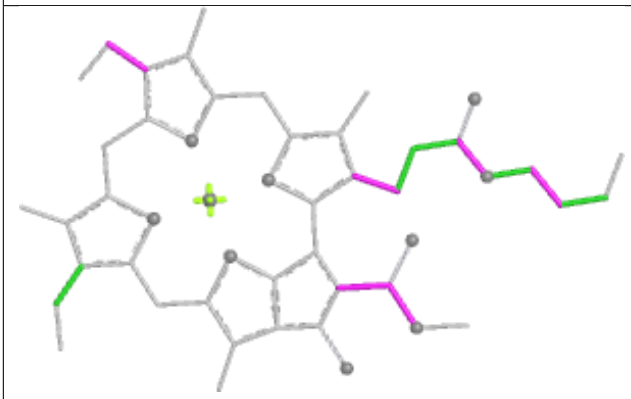
Ligand CLA Gg 303



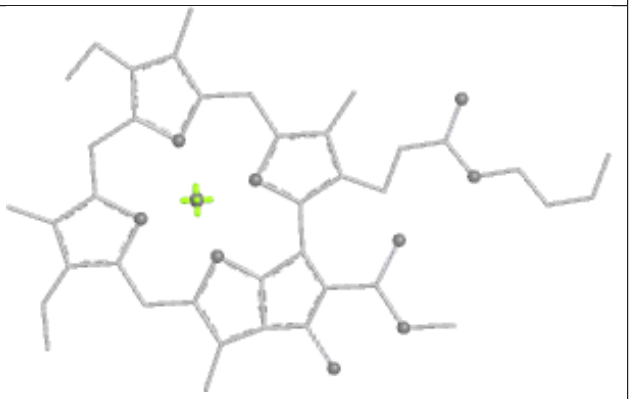
Bond lengths



Bond angles



Torsions

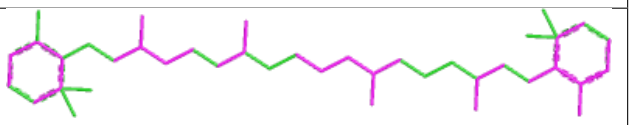


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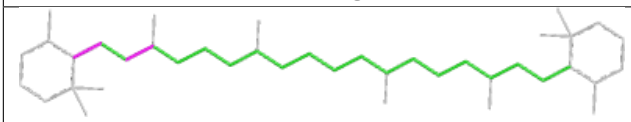
Ligand BCR Cc 516



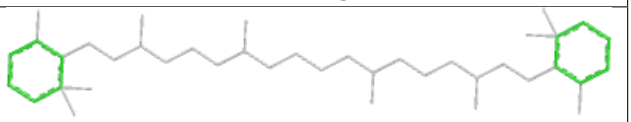
Bond lengths



Bond angles

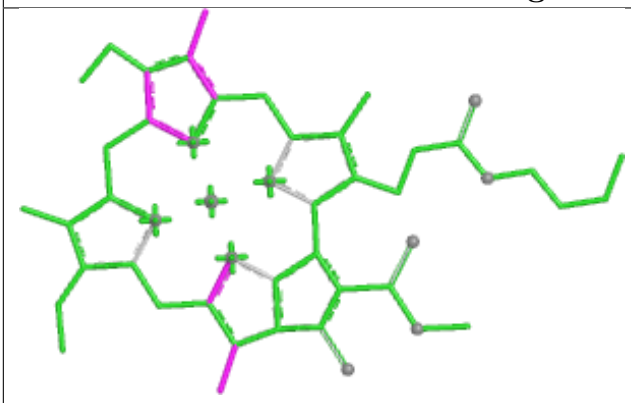


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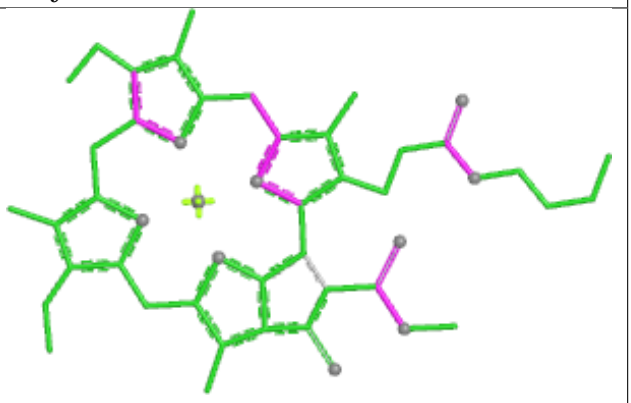


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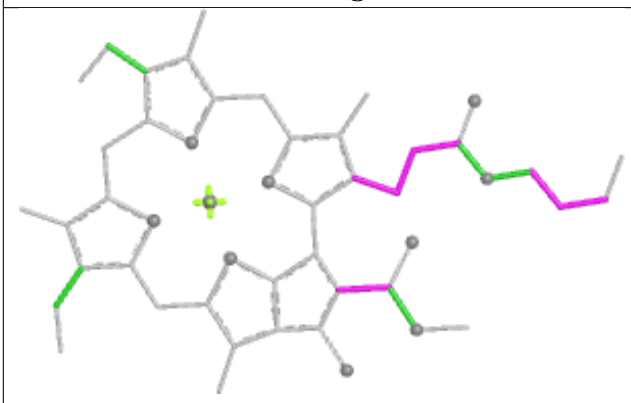
Ligand CLA y 306



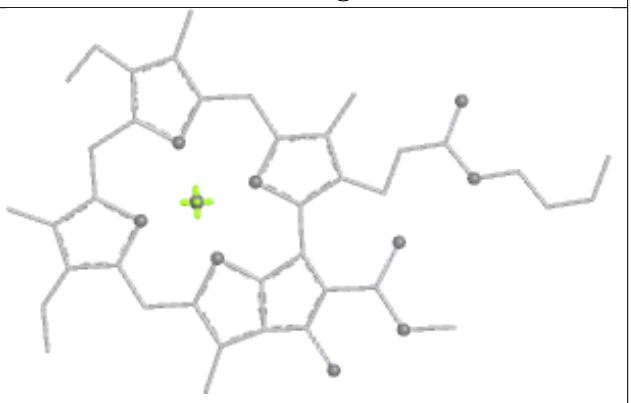
Bond lengths



Bond angles

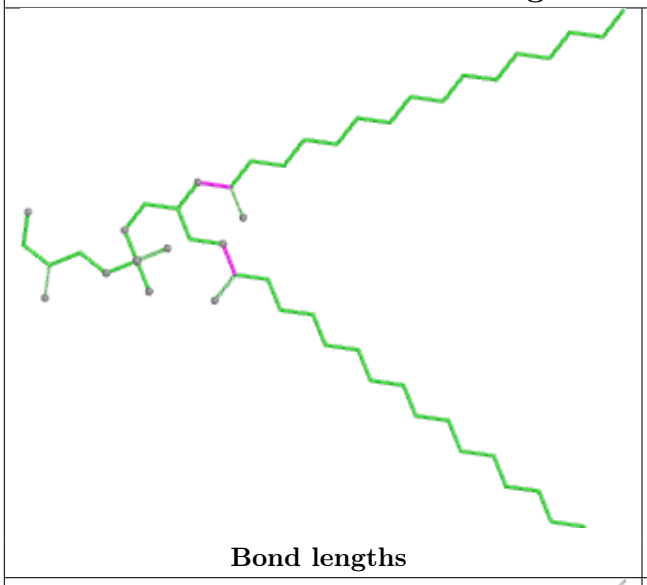


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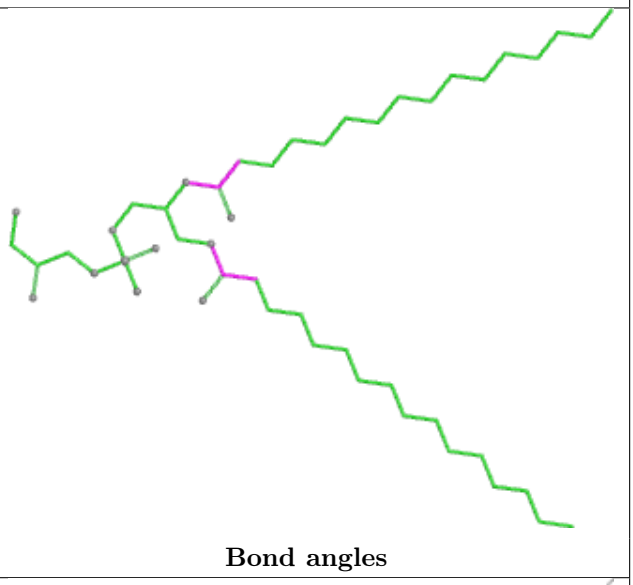


Rings

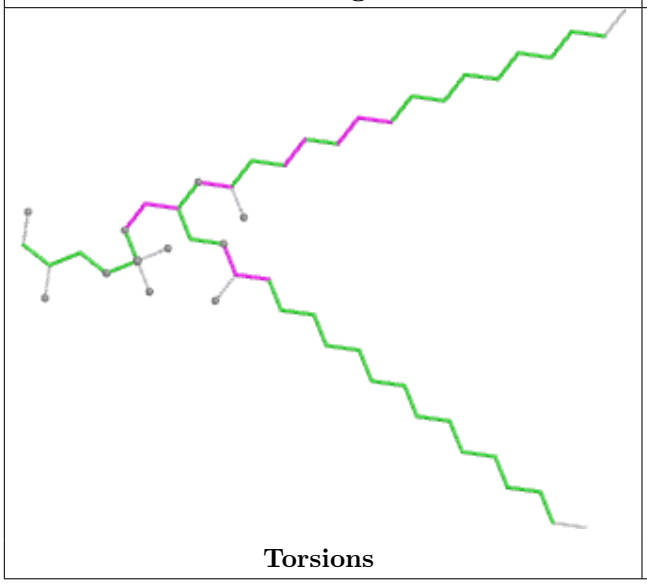
Ligand LHG n 618



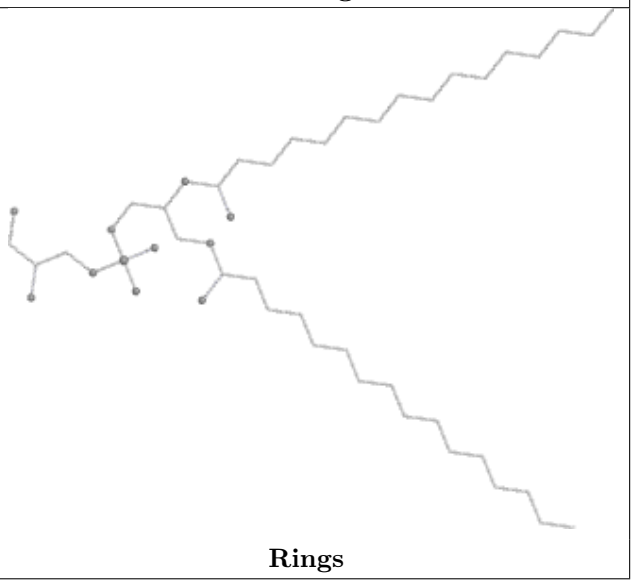
Bond lengths



Bond angles

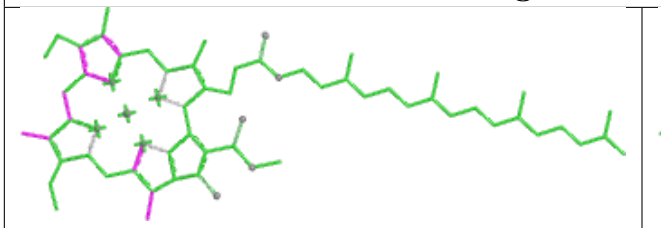


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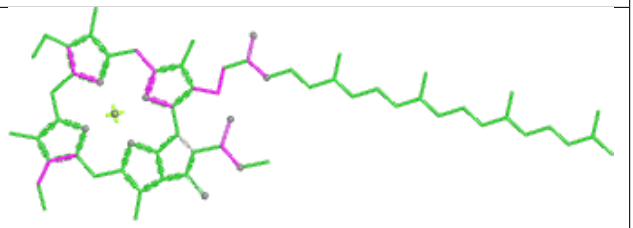


Rings

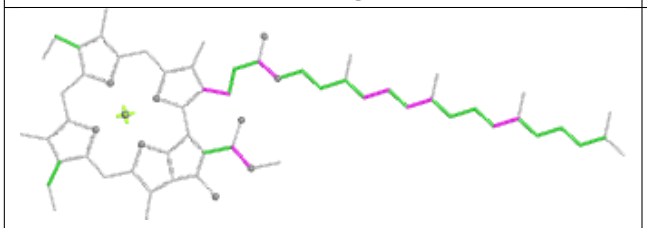
Ligand CLA Nn 301



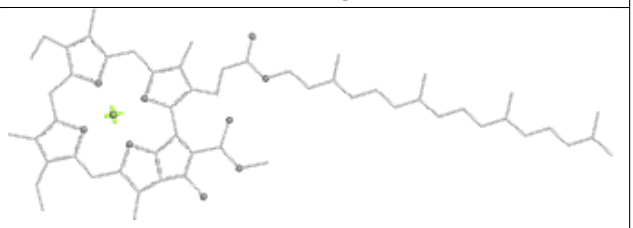
Bond lengths



Bond angles

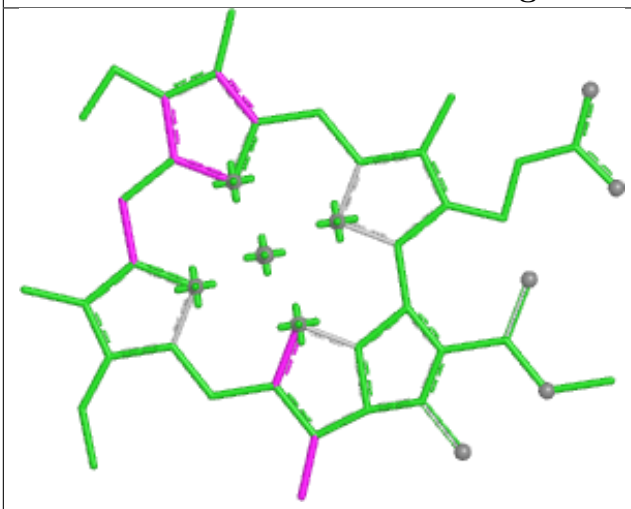


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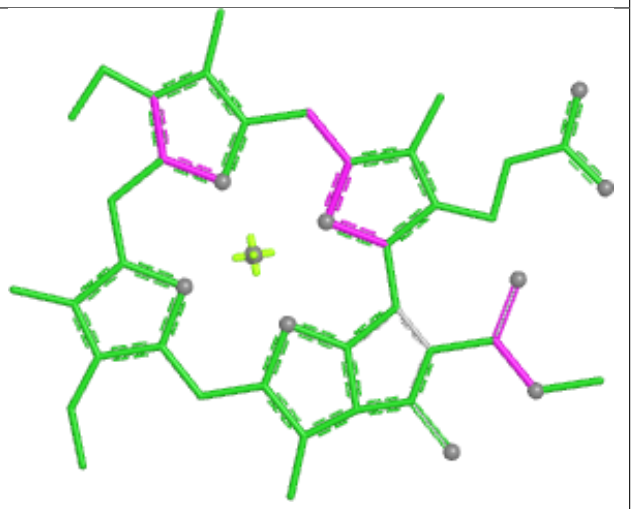


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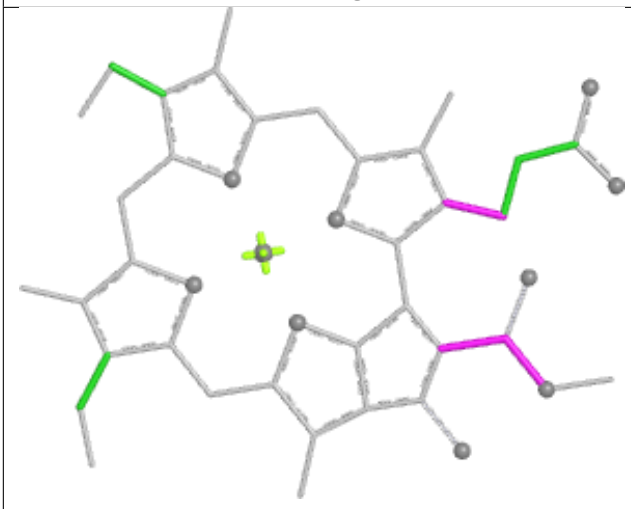
Ligand CLA 44 609



Bond lengths



Bond angles

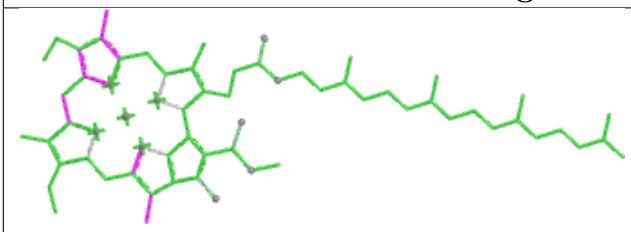


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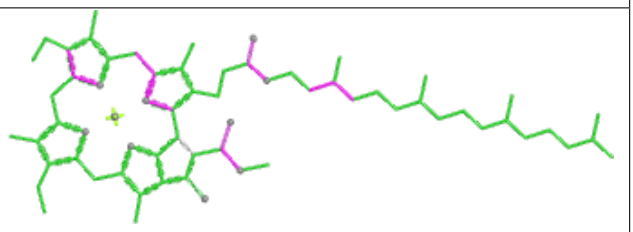


Rings

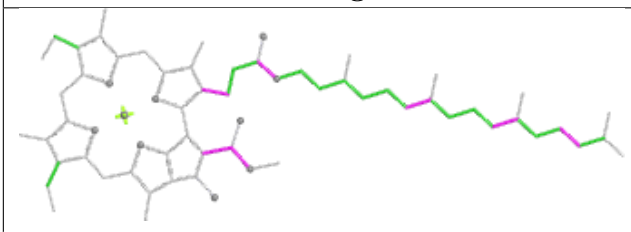
Ligand CLA Cc 504



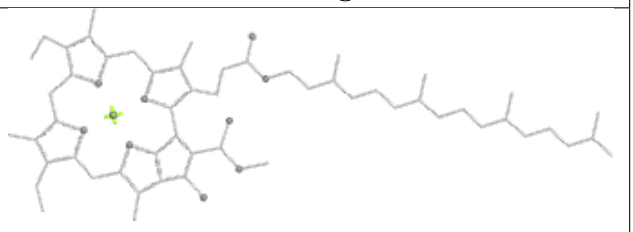
Bond lengths



Bond angles

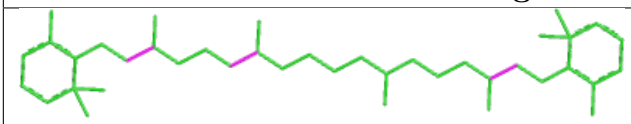


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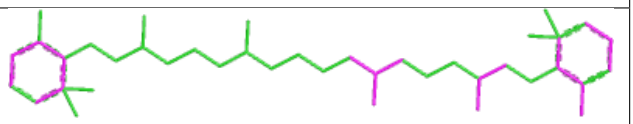


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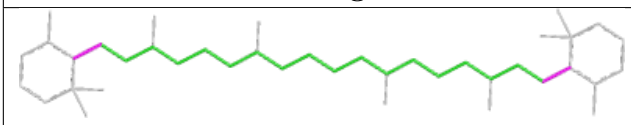
Ligand BCR Aa 411



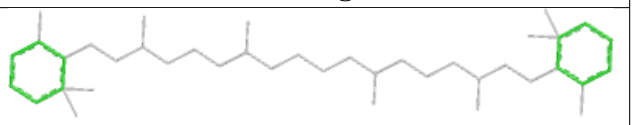
Bond lengths



Bond angles

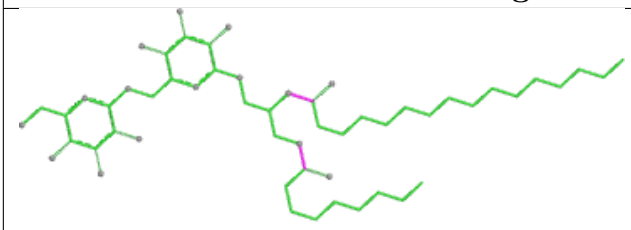


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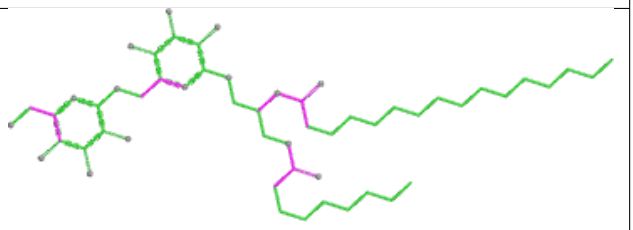


Rings

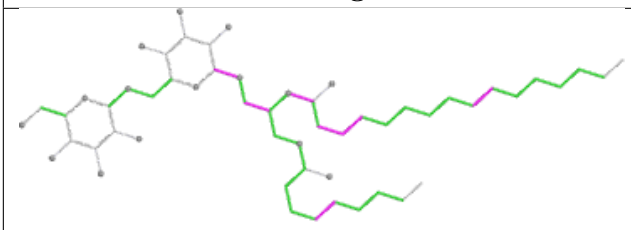
Ligand DGD Cc 519



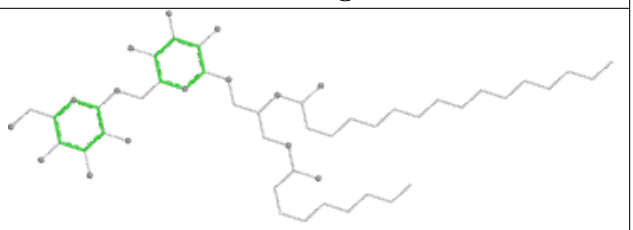
Bond lengths



Bond angles

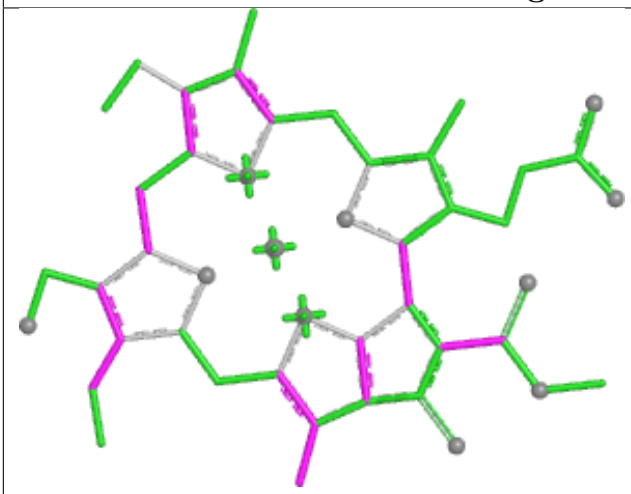


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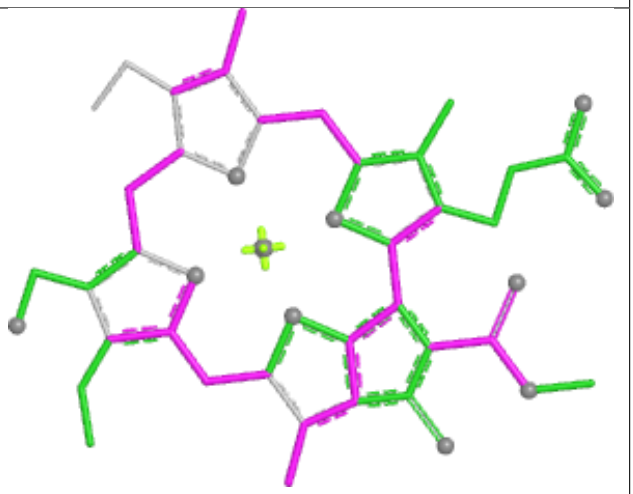


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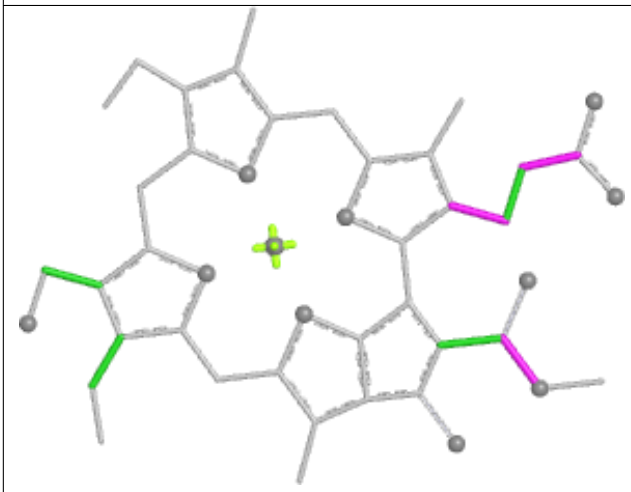
Ligand CHL 4 308



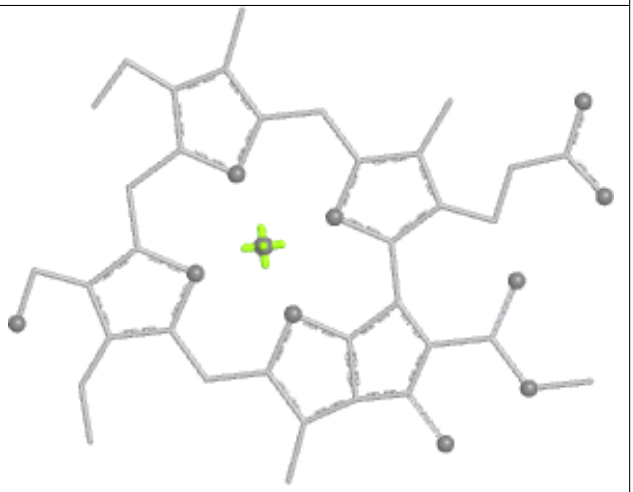
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Bond angles

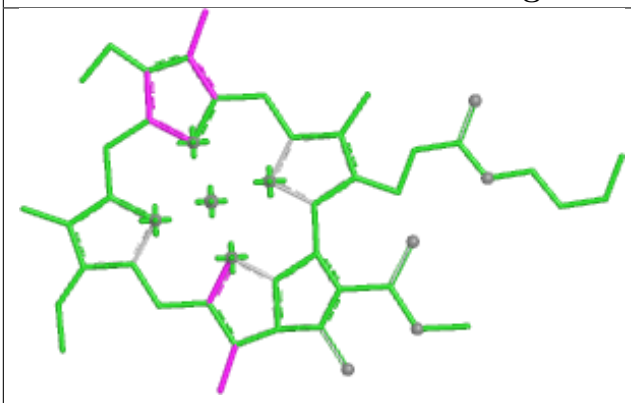


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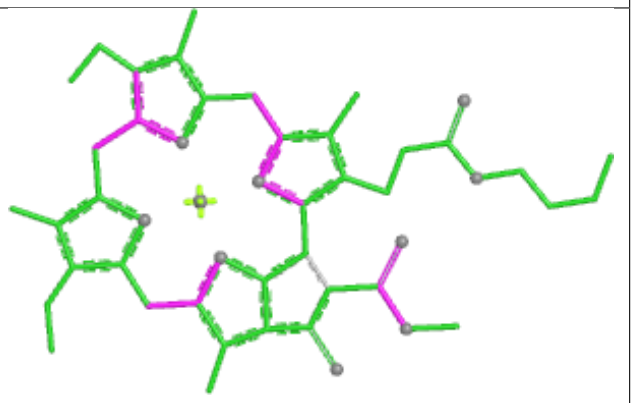


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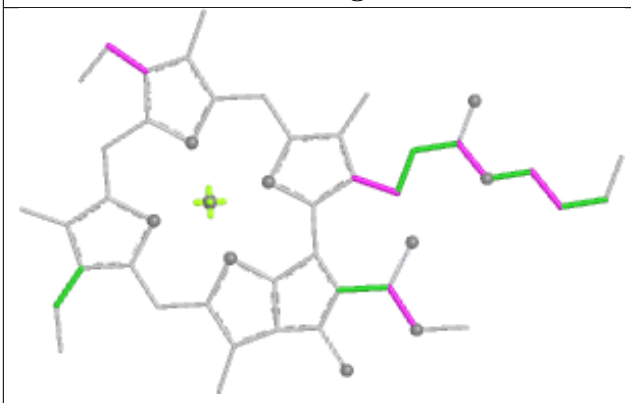
Ligand CLA G 602



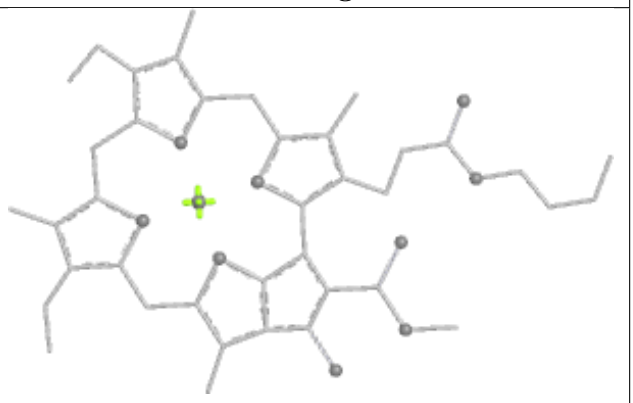
Bond lengths



Bond angles



Torsions

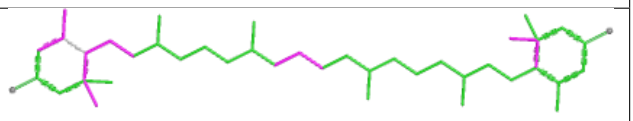


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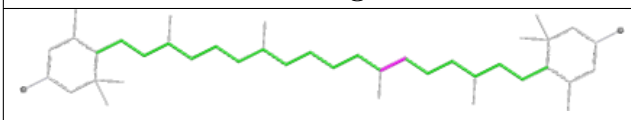
Ligand LUT n 615



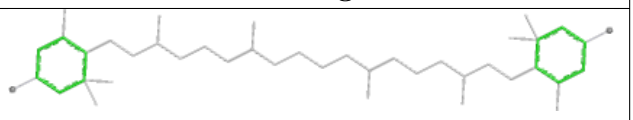
Bond lengths



Bond angles

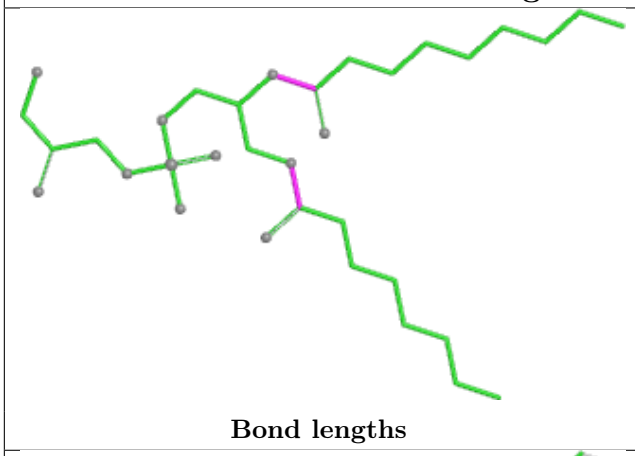


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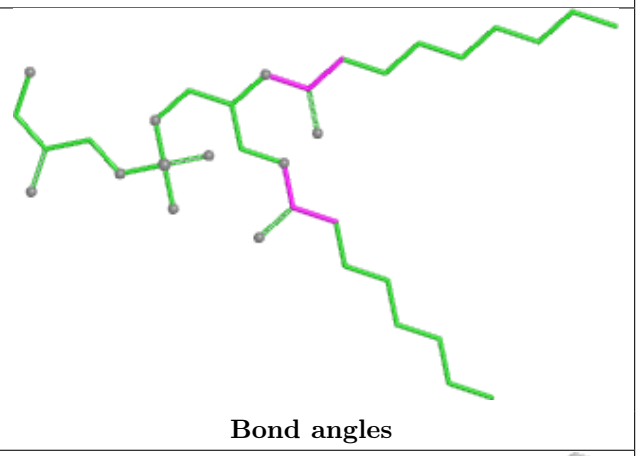


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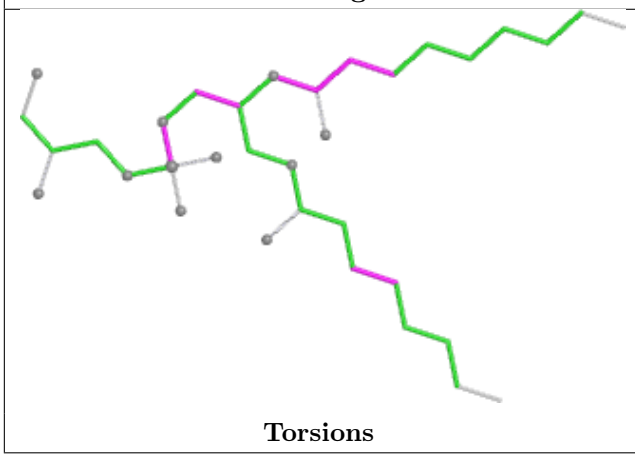
Ligand LHG II 101



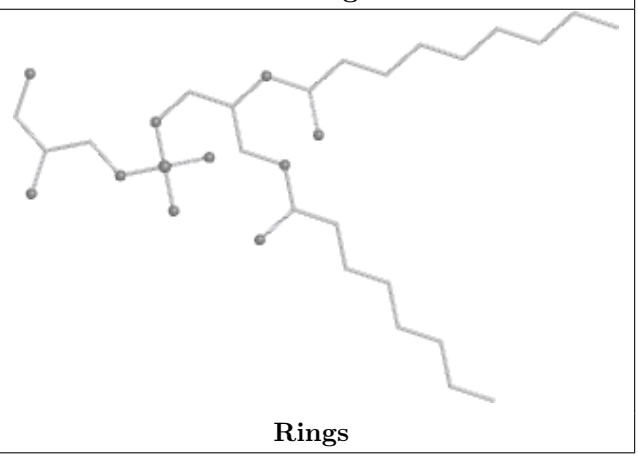
Bond lengths



Bond angles

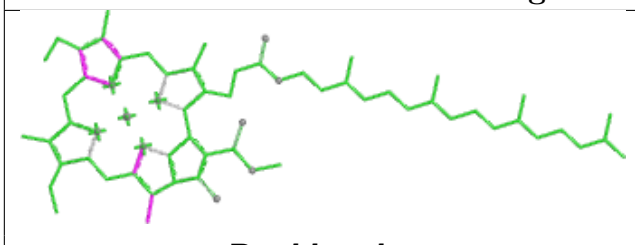


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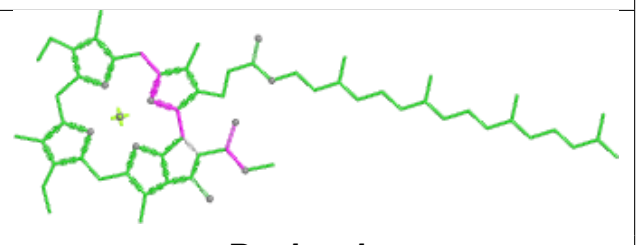


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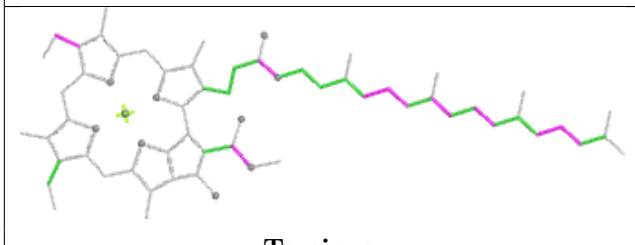
Ligand CLA b 615



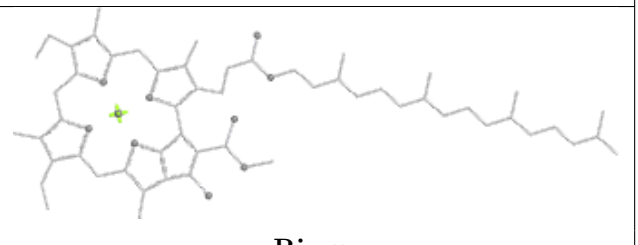
Bond lengths



Bond angles



Torsions

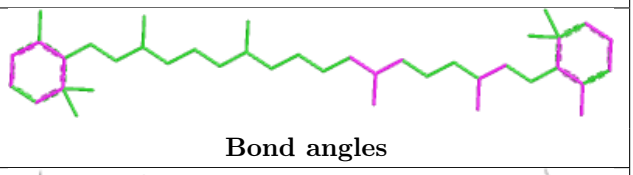


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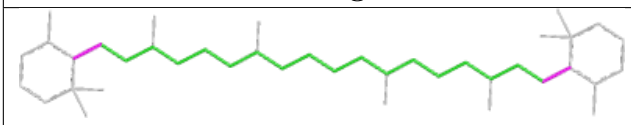
Ligand BCR a 411



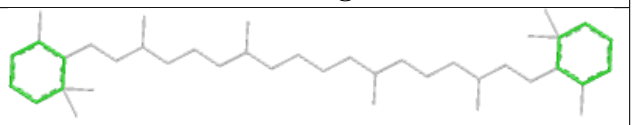
Bond lengths



Bond angles

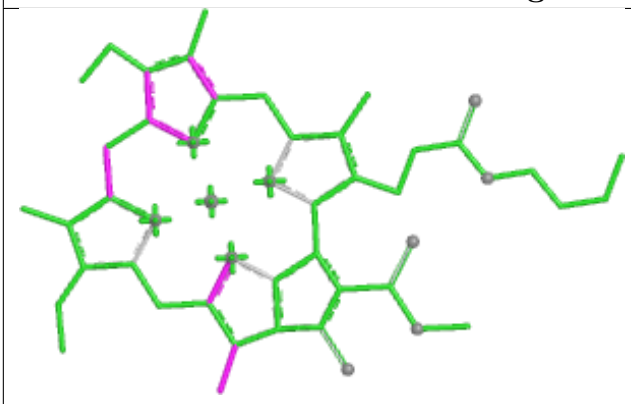


Torsions

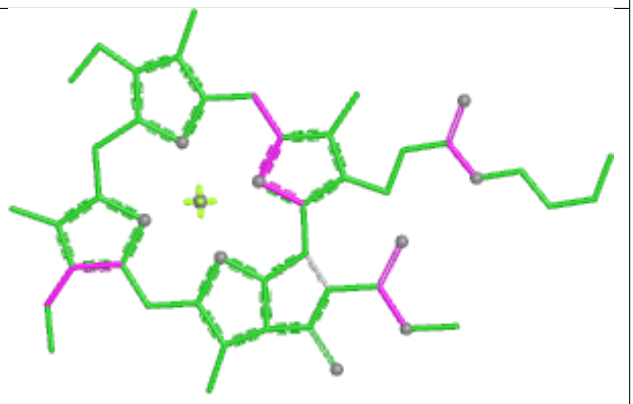


Rings

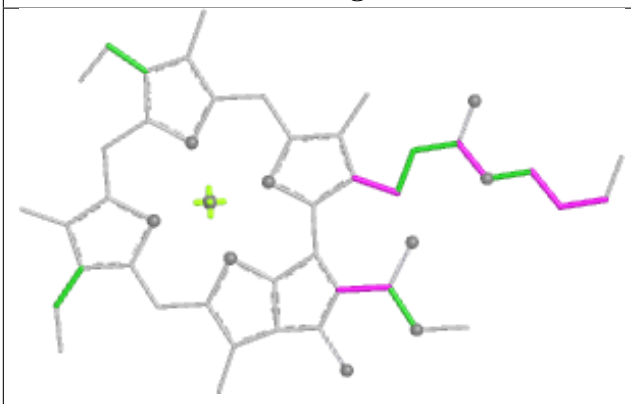
Ligand CLA S 604



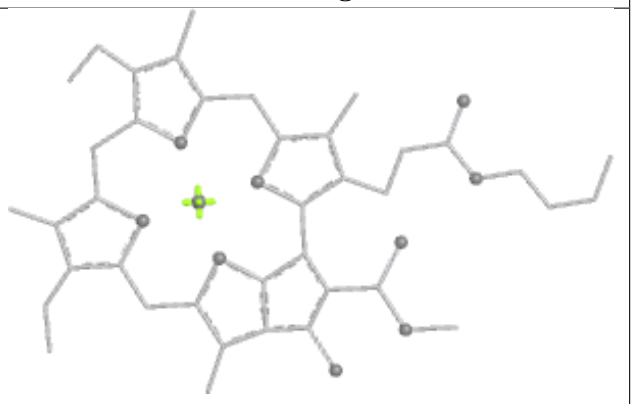
Bond lengths



Bond angles

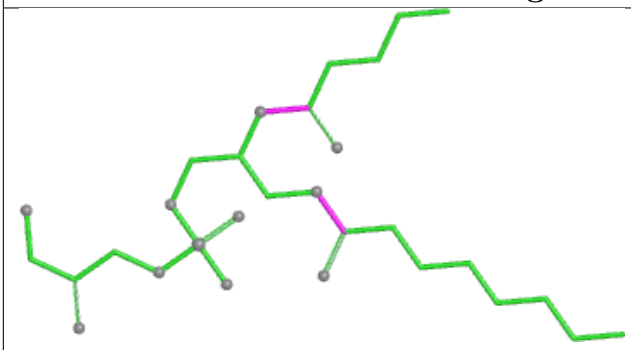


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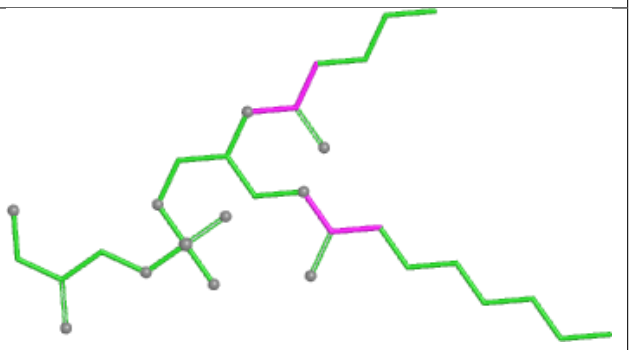


Rings

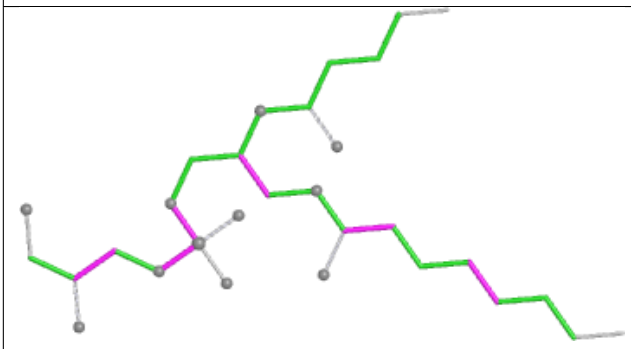
Ligand LHG 1 614



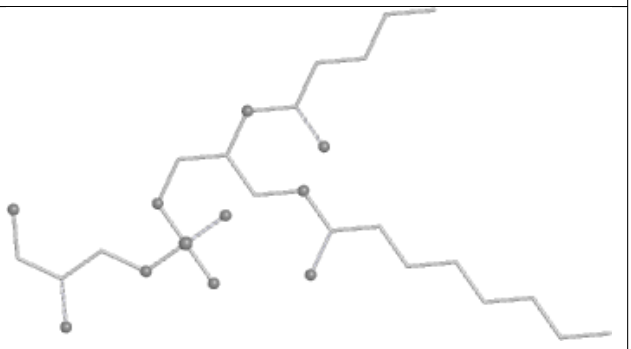
Bond lengths



Bond angles

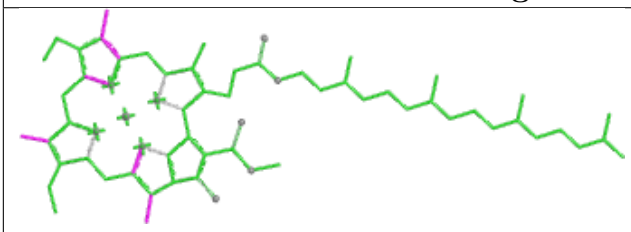


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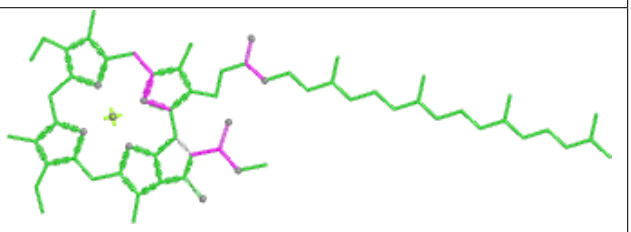


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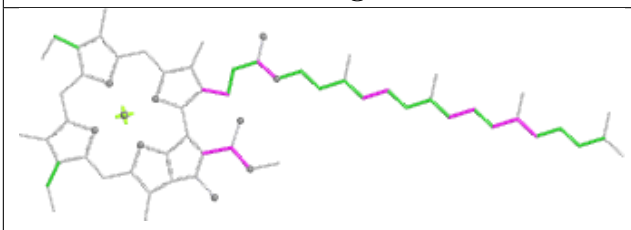
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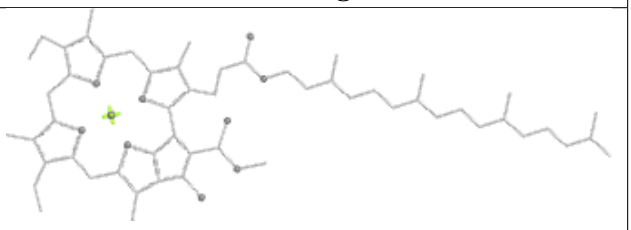
Bond lengths



Bond angles

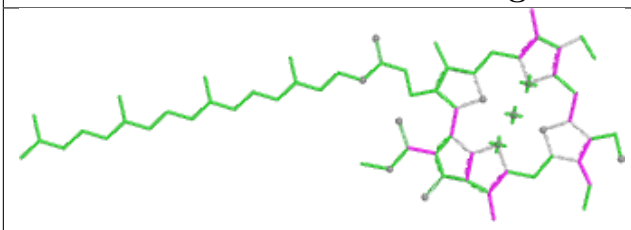


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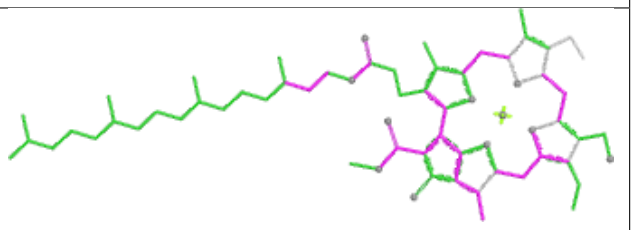


Rings

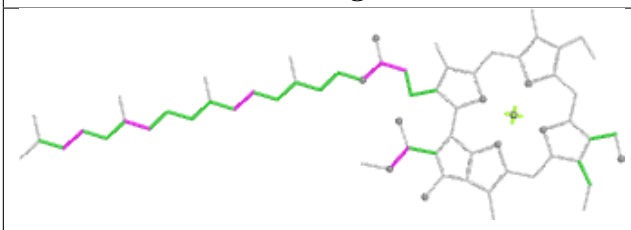
Ligand CHL GG 601



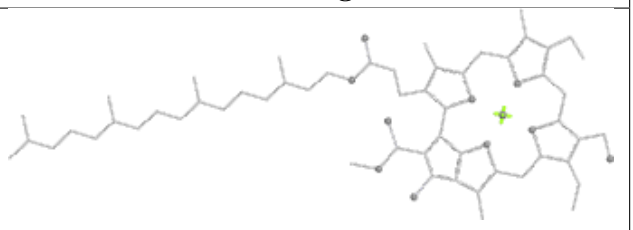
Bond lengths



Bond angles

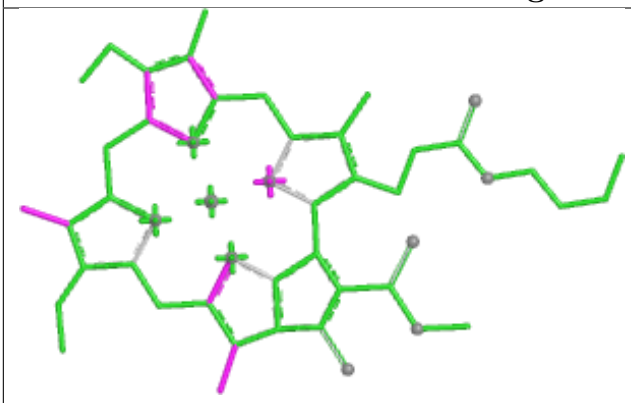


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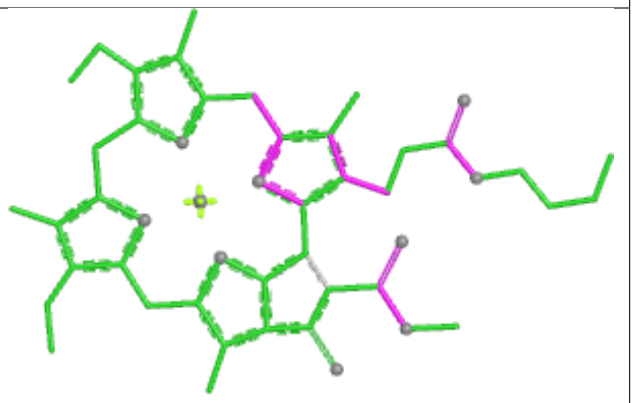


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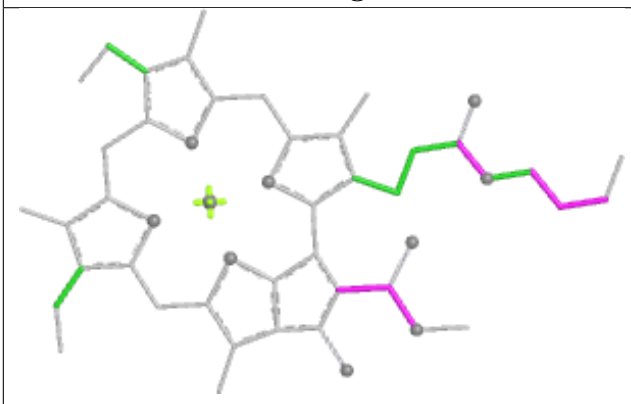
Ligand CLA n 612



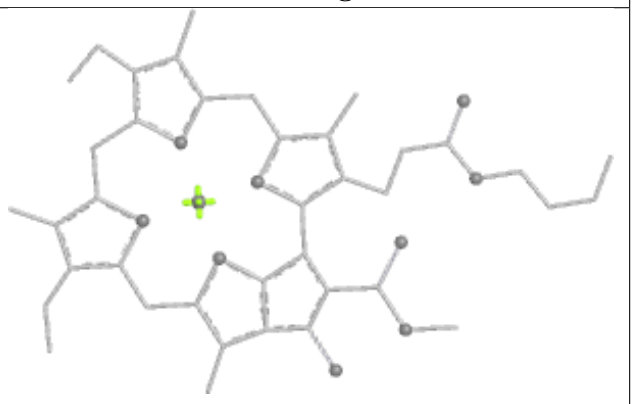
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Bond angles

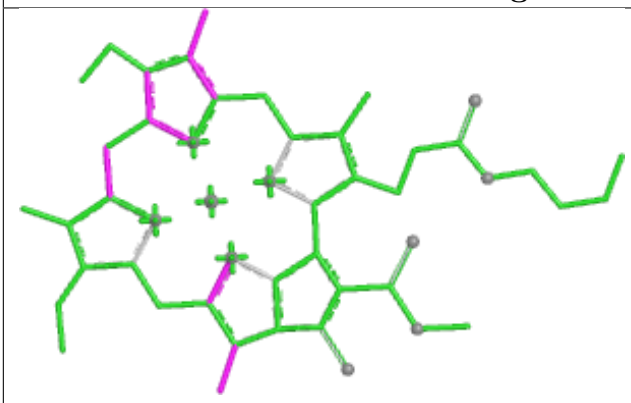


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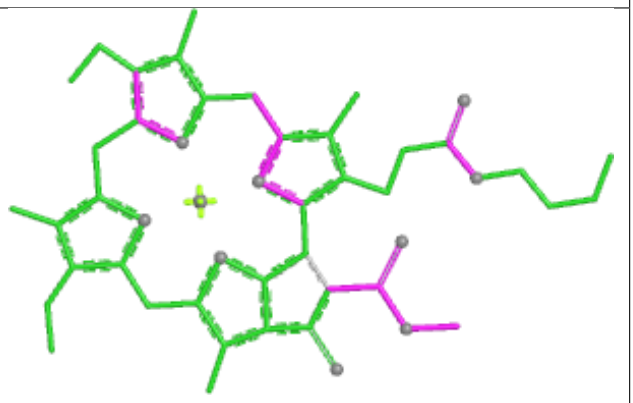


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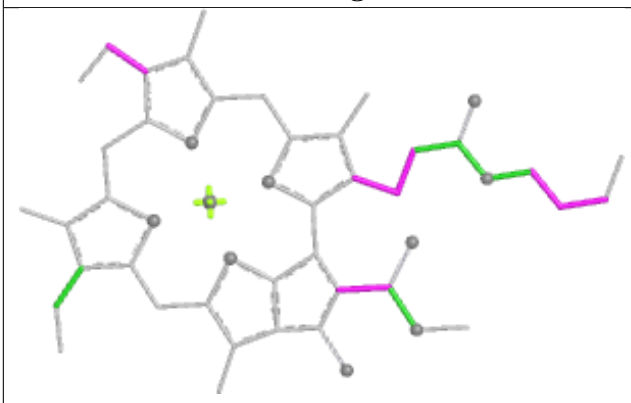
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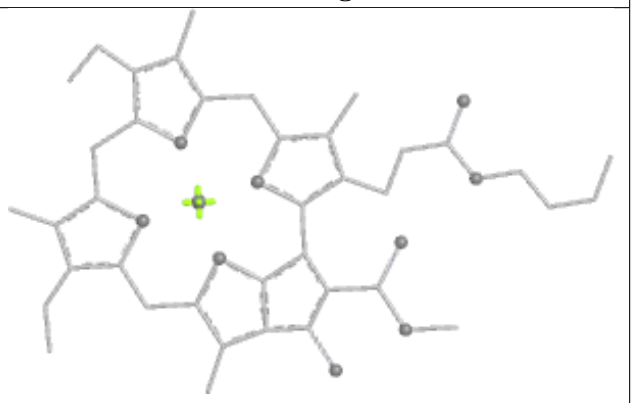
Bond lengths



Bond angles

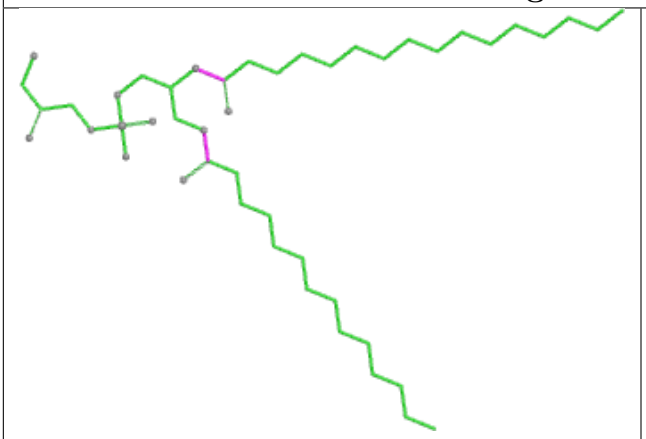


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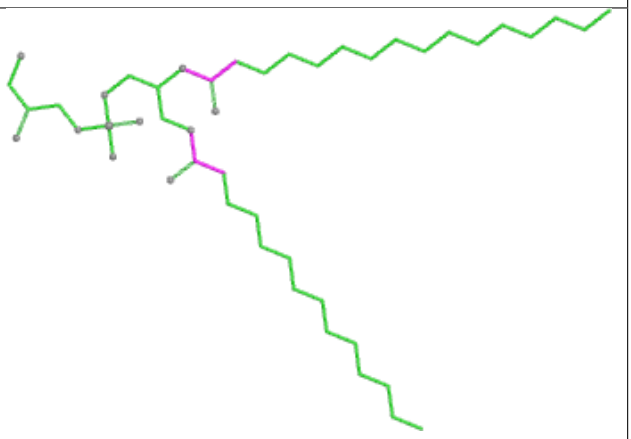


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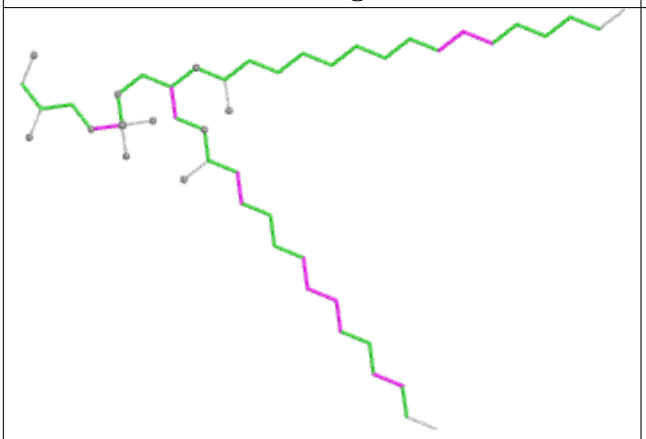
Ligand LHG 0 201



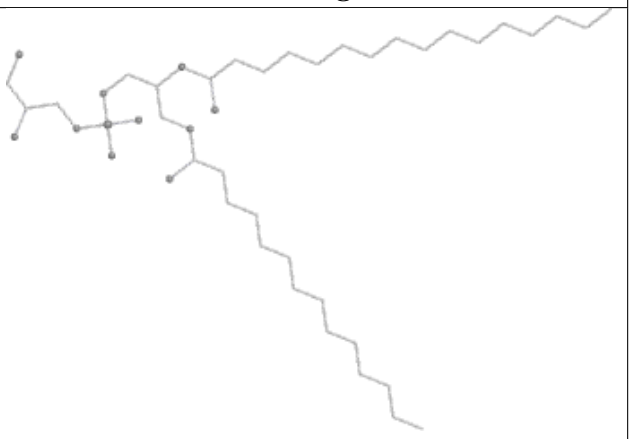
Bond lengths



Bond angles

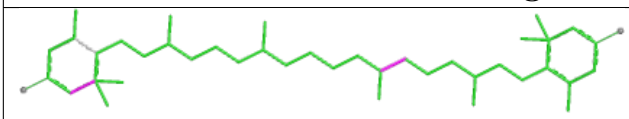


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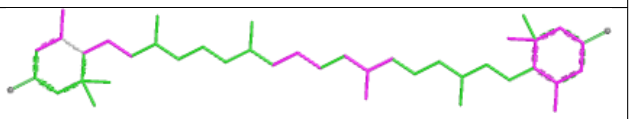


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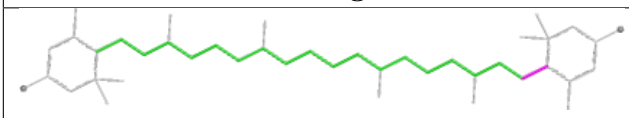
Ligand LUT N 615



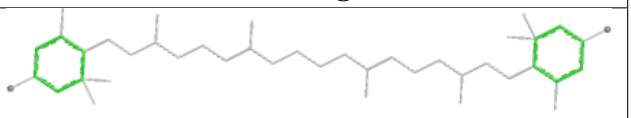
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Bond angles

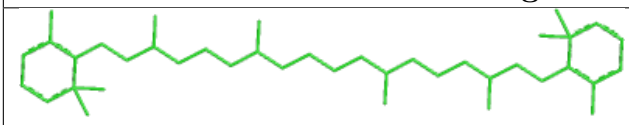


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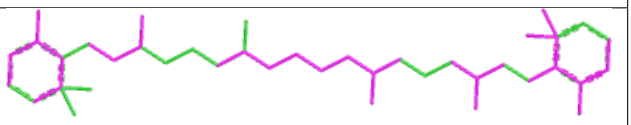


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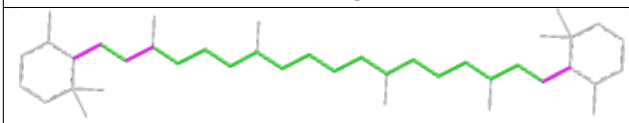
Ligand BCR K 102



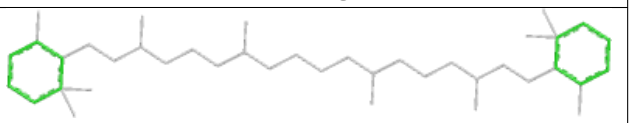
Bond lengths



Bond angles

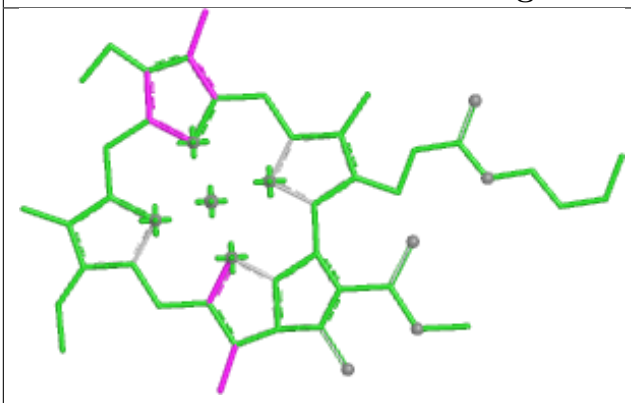


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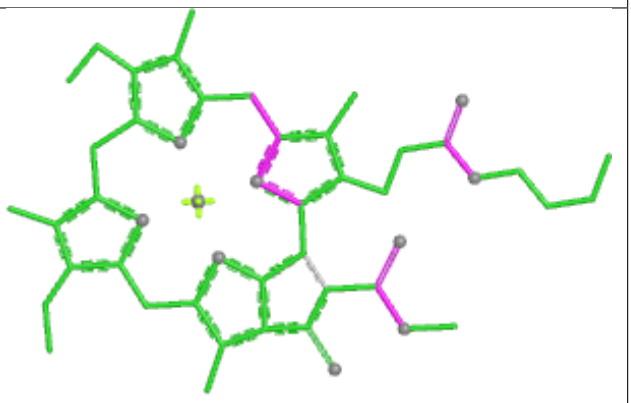


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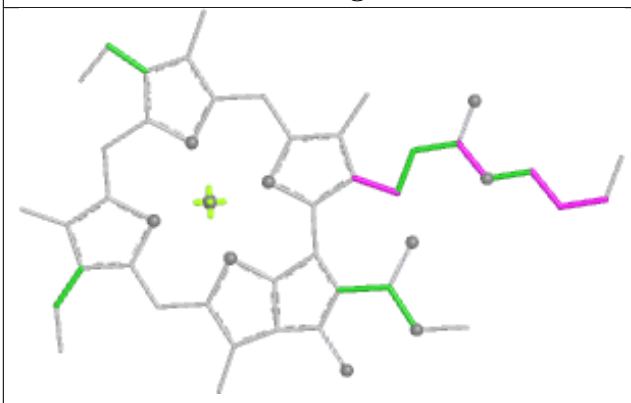
Ligand CLA Rr 612



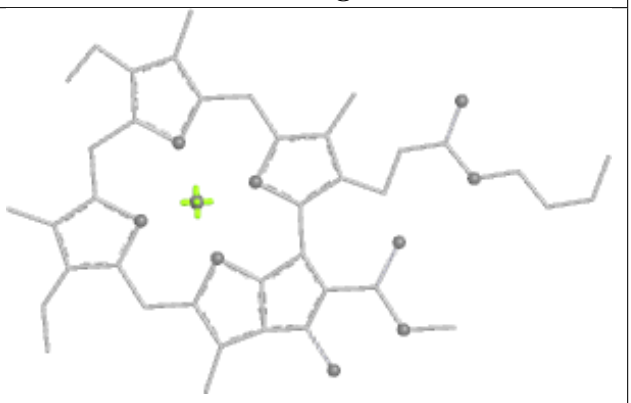
Bond lengths



Bond angles

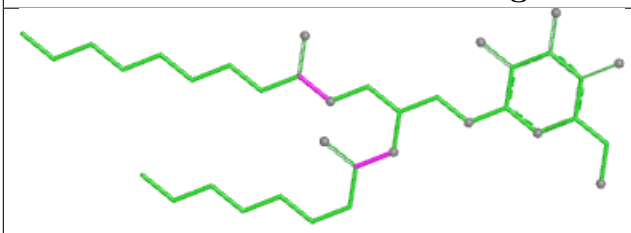


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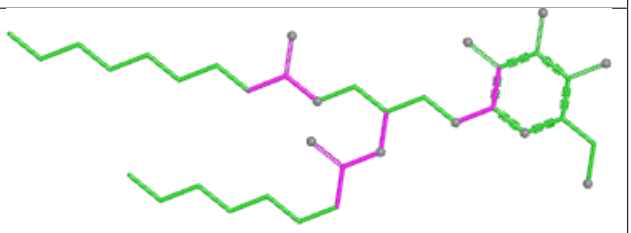


Rings

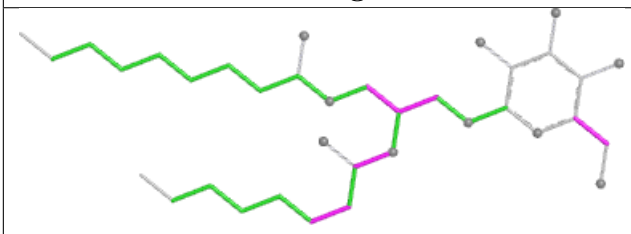
Ligand LMG Bb 621



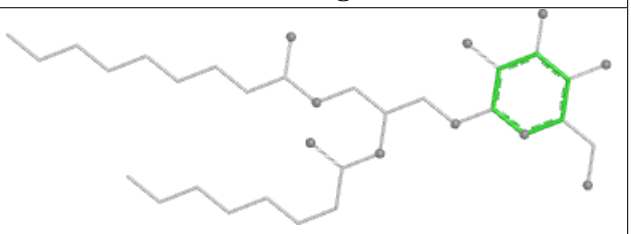
Bond lengths



Bond angles

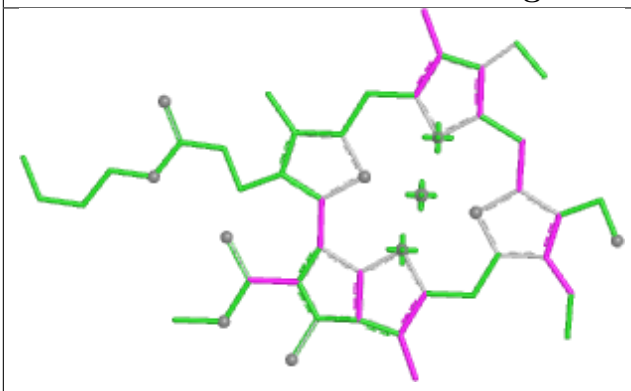


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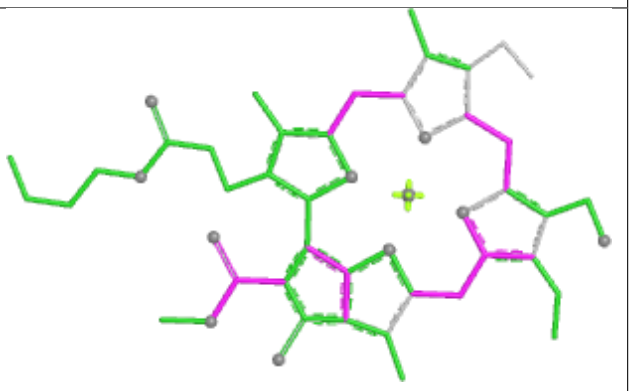


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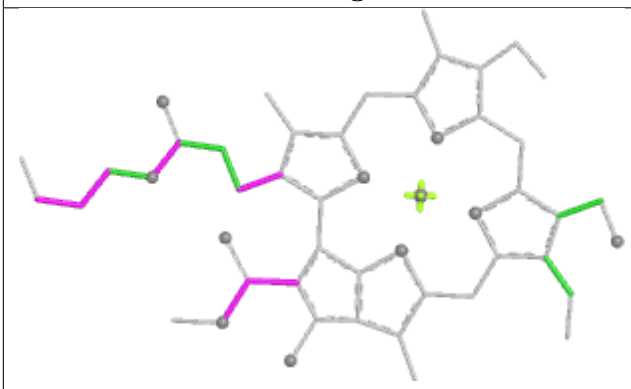
Ligand CHL R 606



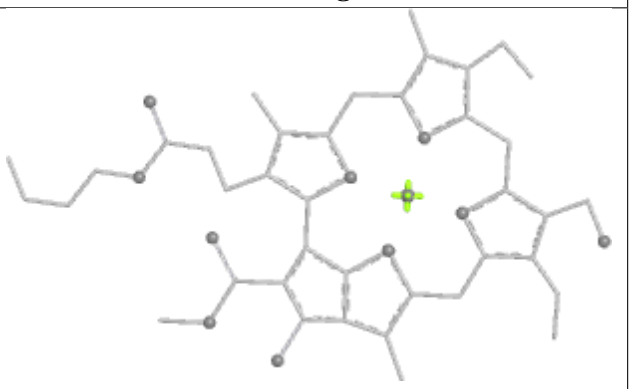
Bond lengths



Bond angles

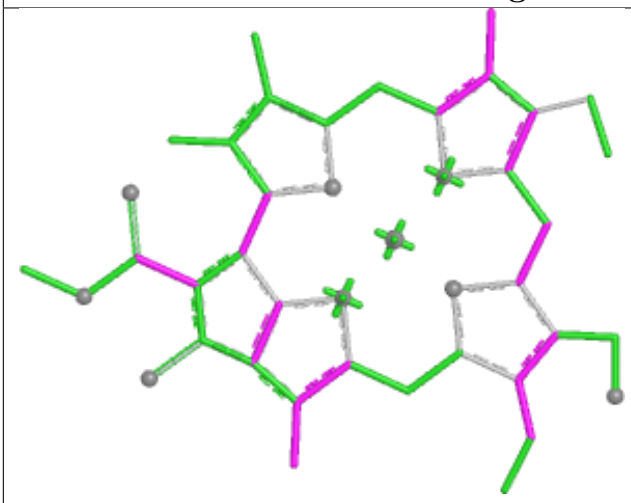


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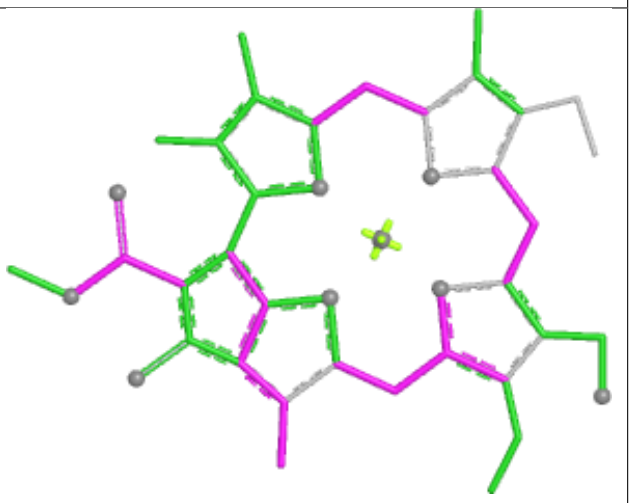


Rings

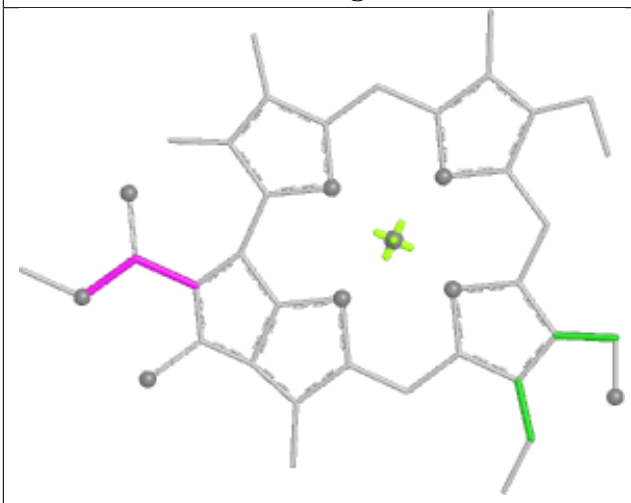
Ligand CHL GG 608



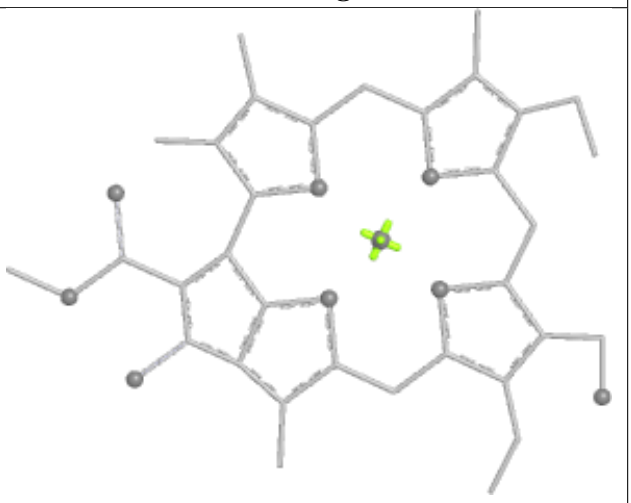
Bond lengths



Bond angles

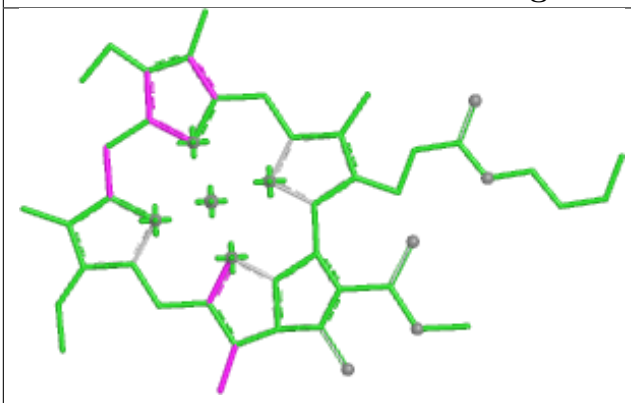


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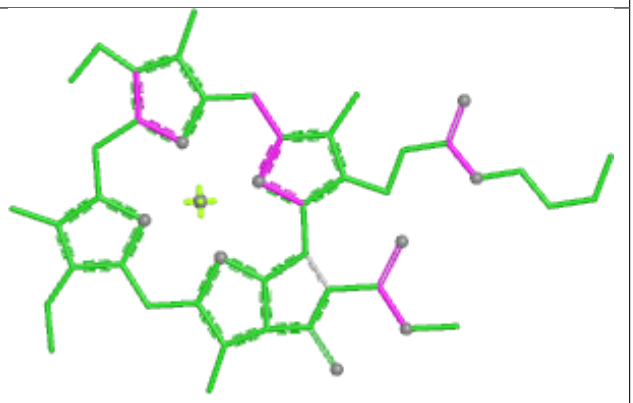


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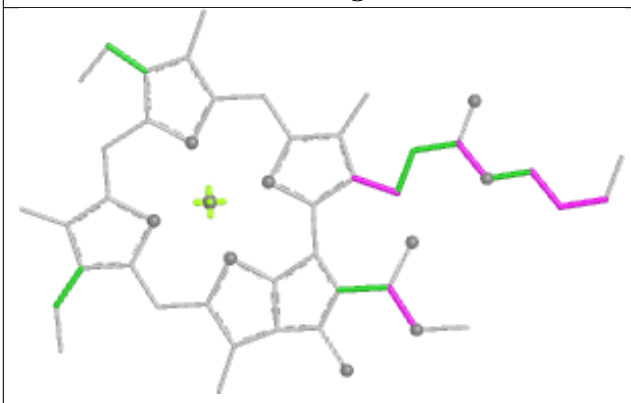
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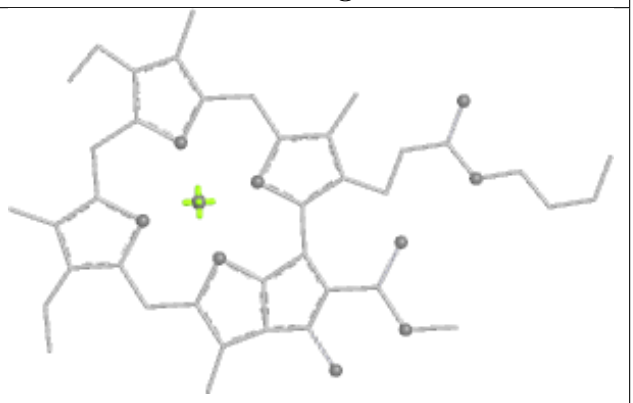
Bond lengths



Bond angles

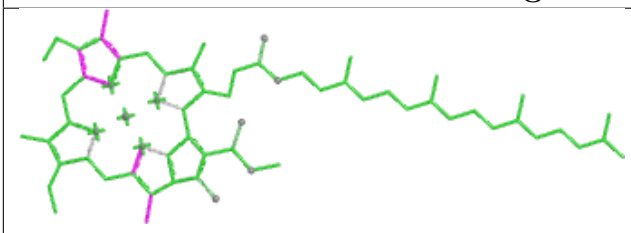


Torsions

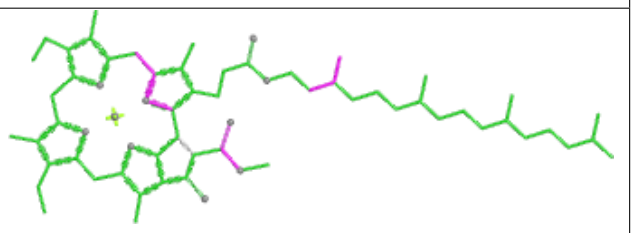


Rings

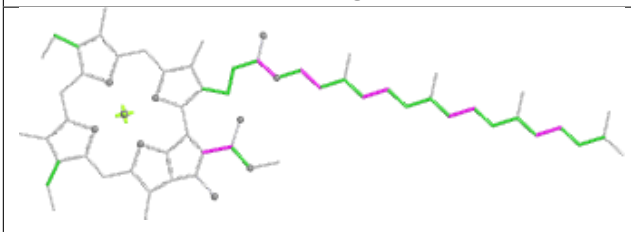
Ligand CLA C 514



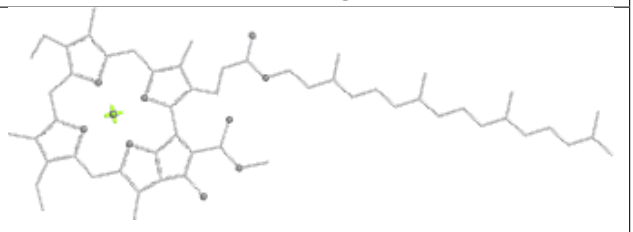
Bond lengths



Bond angles

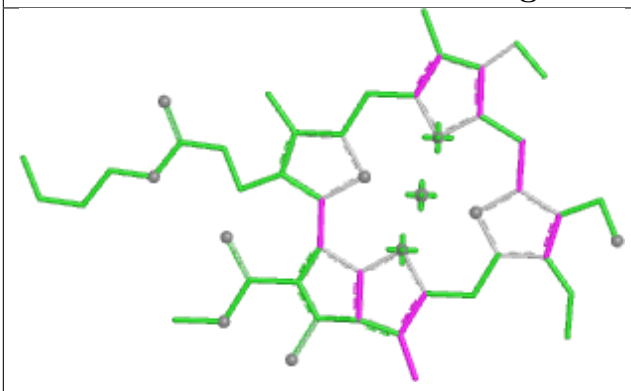


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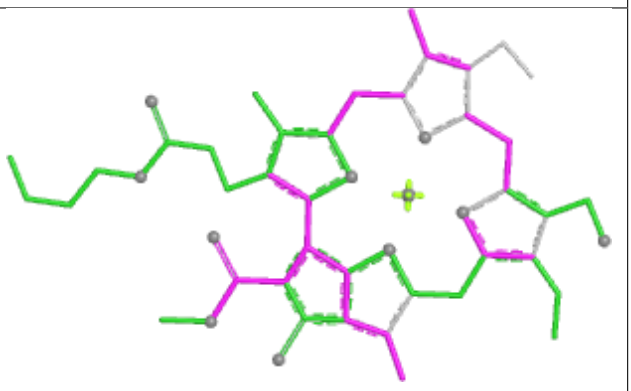


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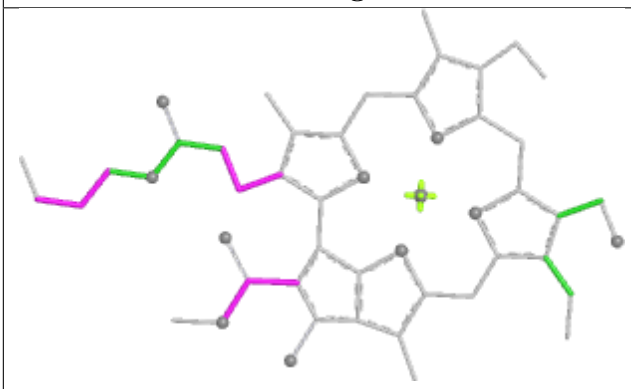
Ligand CHL Ss 606



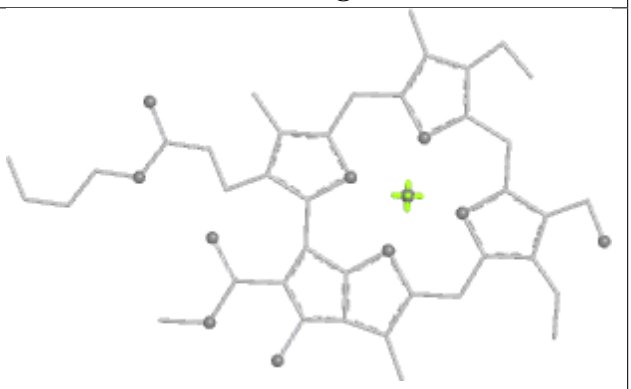
Bond lengths



Bond angles

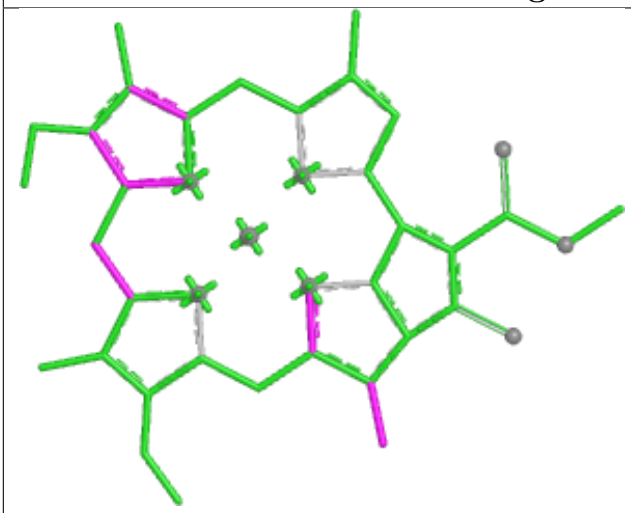


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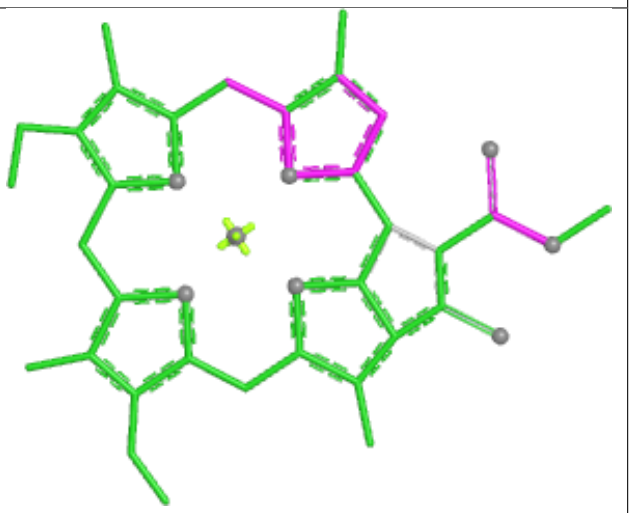


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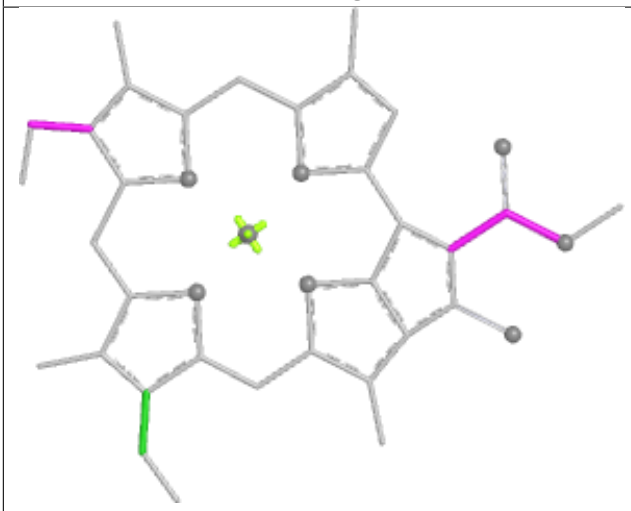
Ligand CLA 3 611



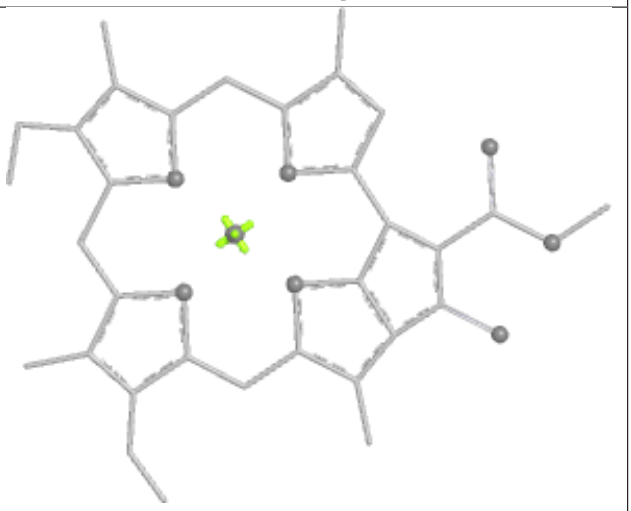
Bond lengths



Bond angles

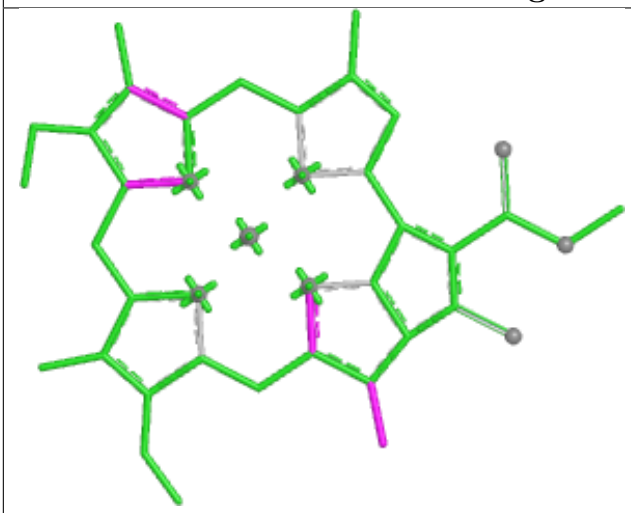


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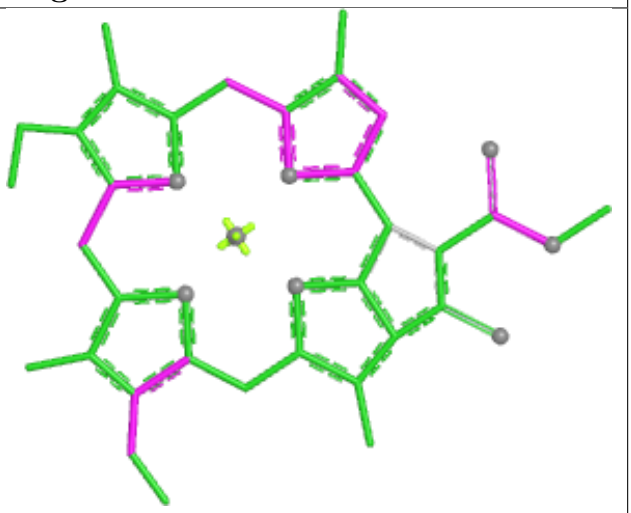


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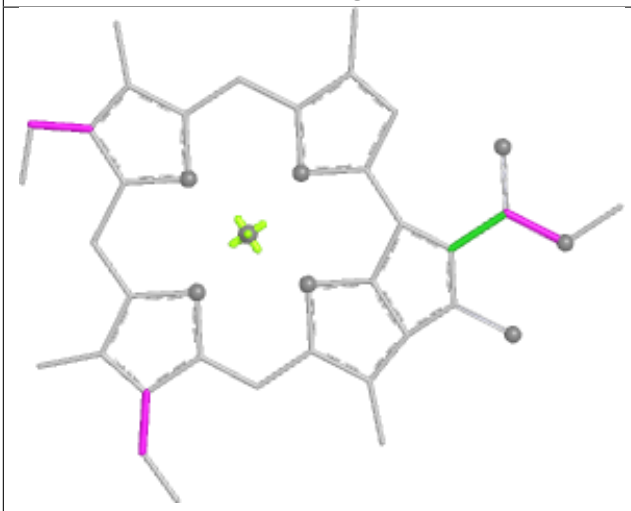
Ligand CLA g 613



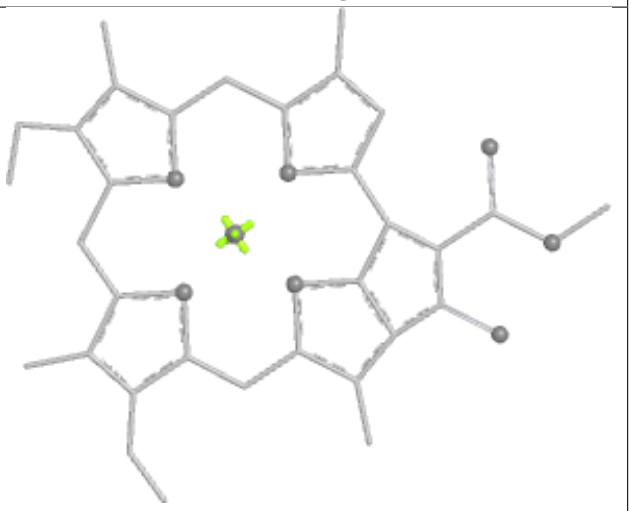
Bond lengths



Bond angles

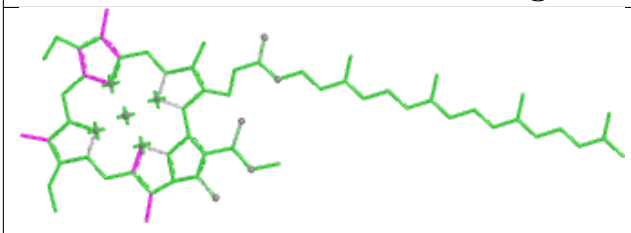


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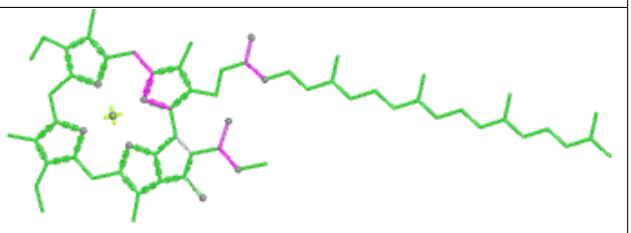


Rings

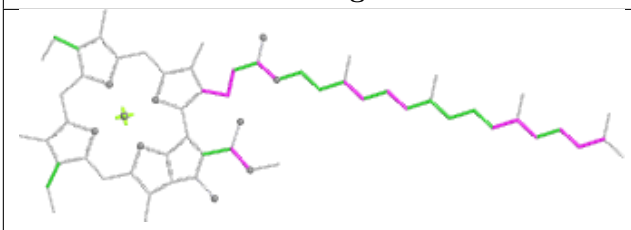
Ligand CLA c 510



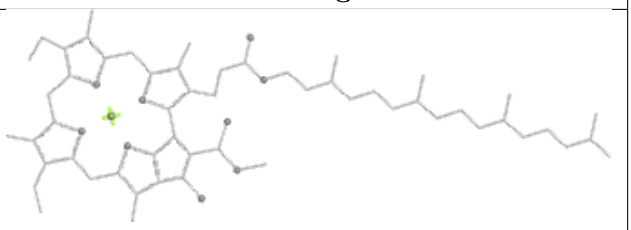
Bond lengths



Bond angles

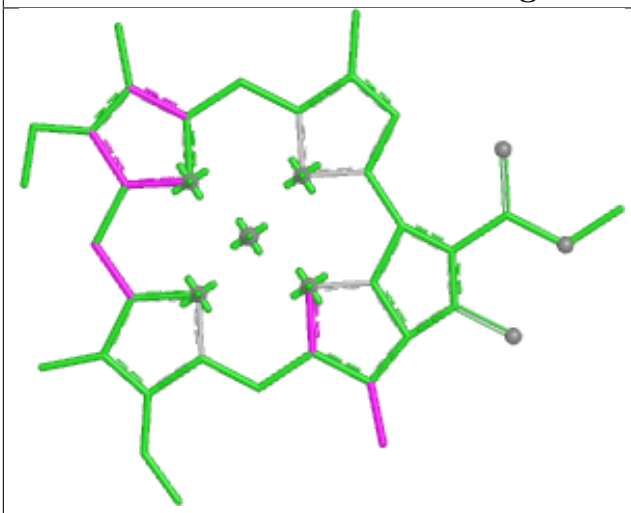


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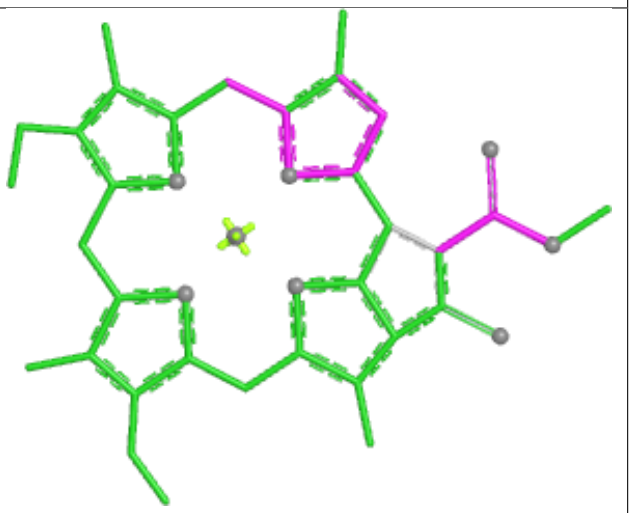


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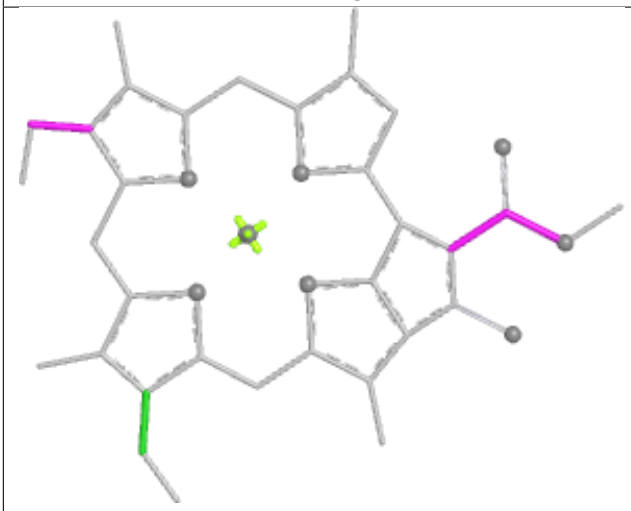
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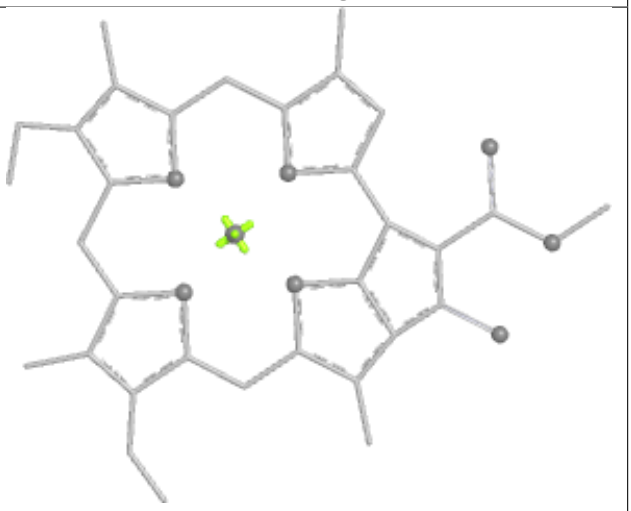
Bond lengths



Bond angles



Torsions

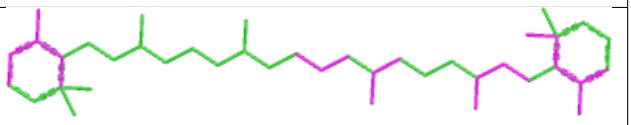


Rings

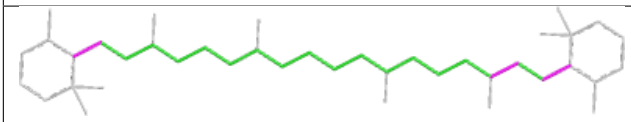
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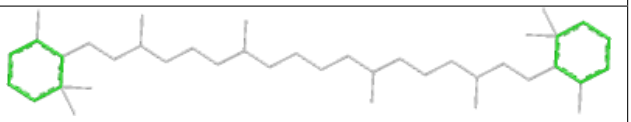
Bond lengths



Bond angles

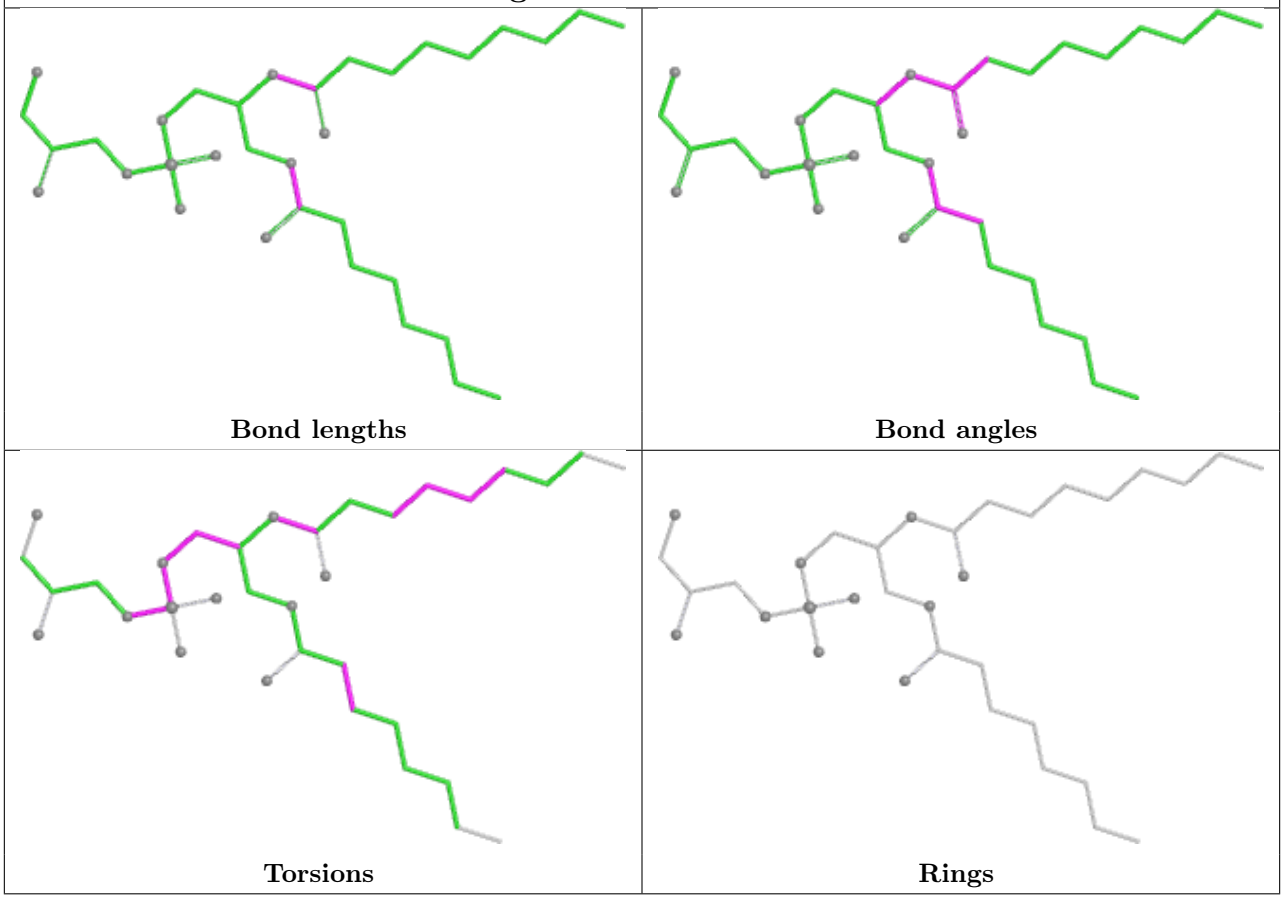


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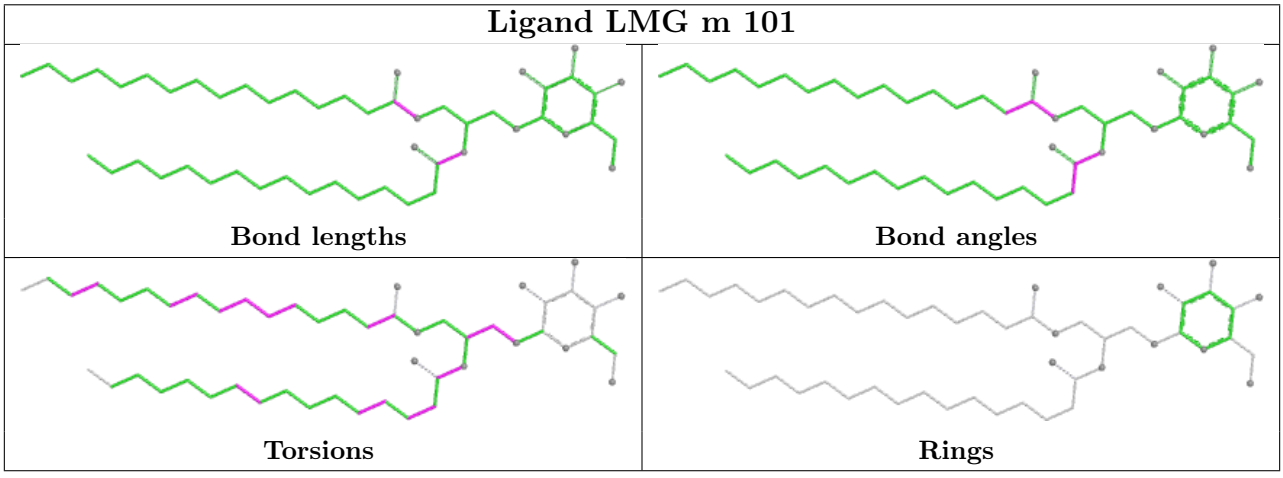


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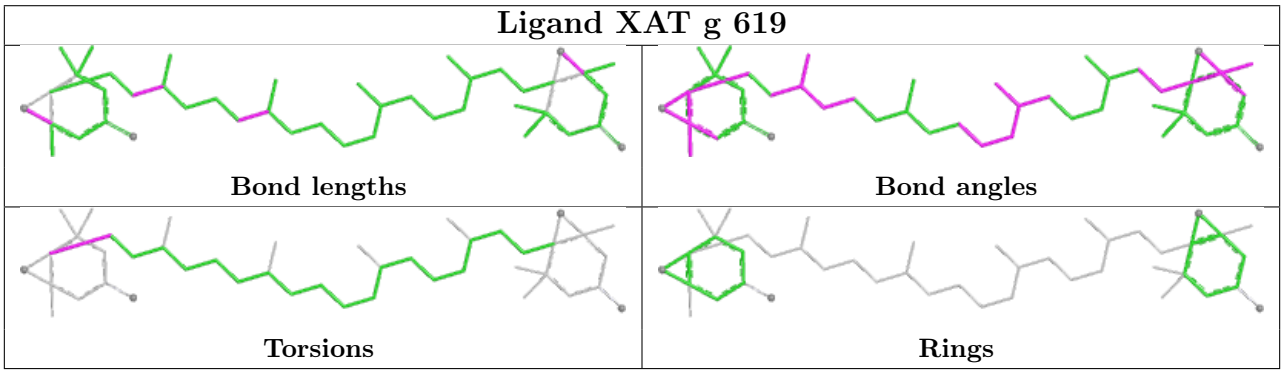
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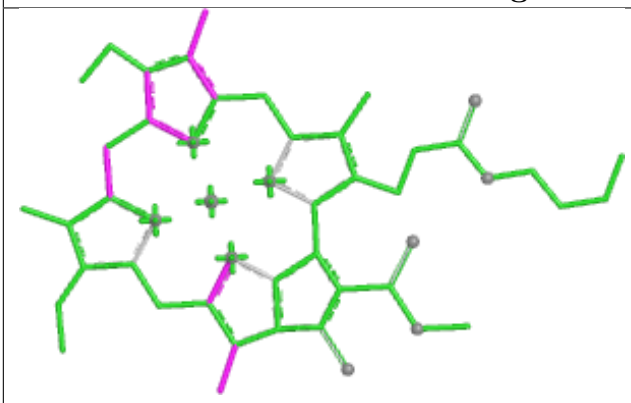
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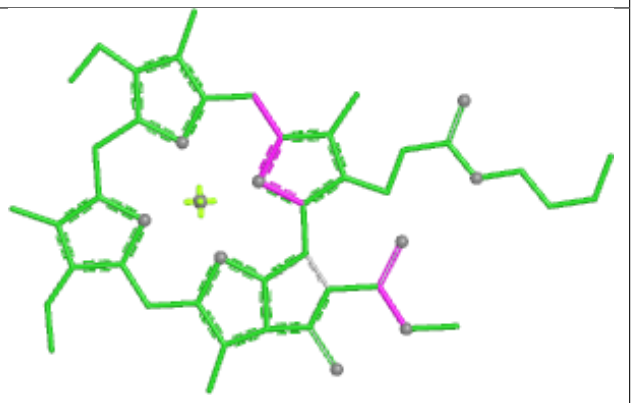
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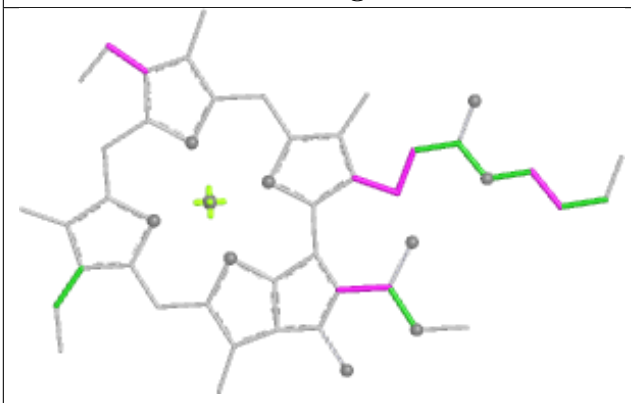
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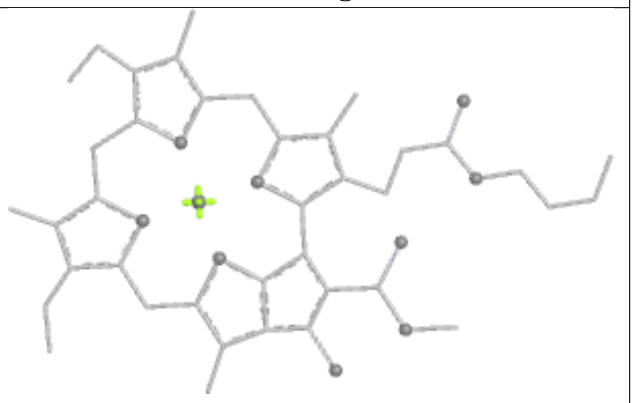
Bond lengths



Bond angles

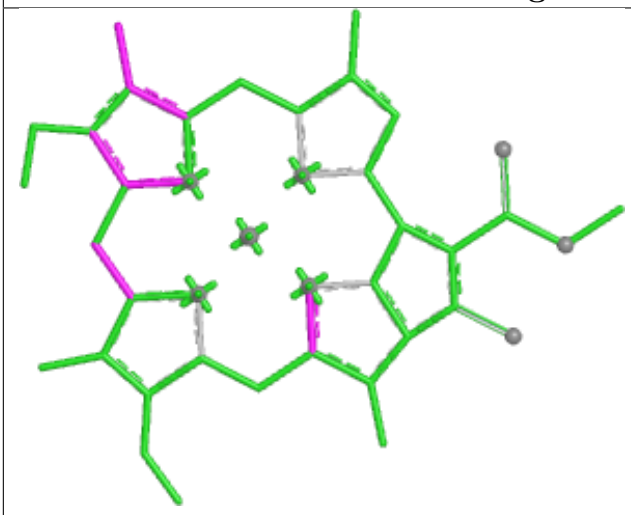


Torsions

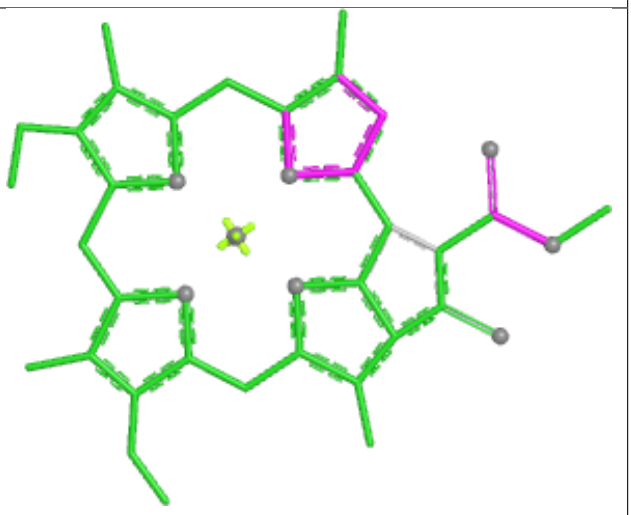


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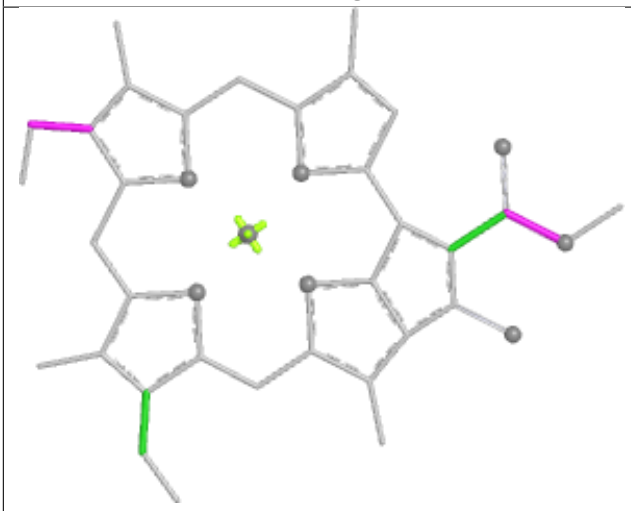
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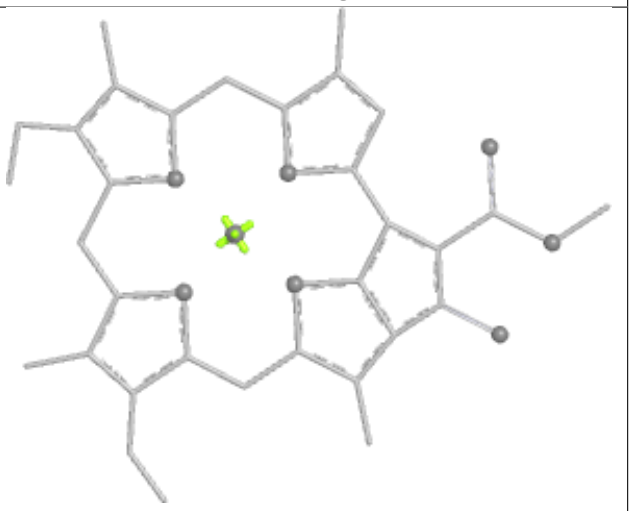
Bond lengths



Bond angles



Torsions



Rings

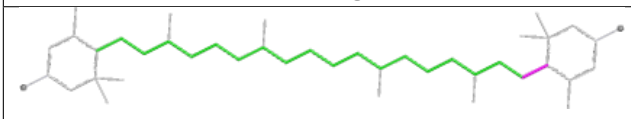
Ligand LUT G 616



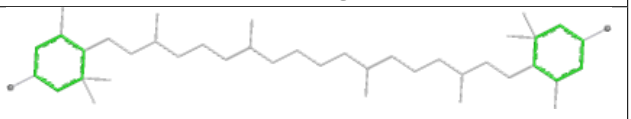
Bond lengths



Bond angles

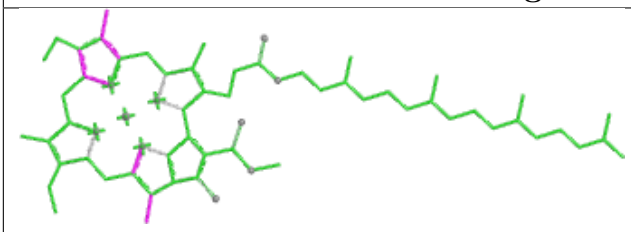


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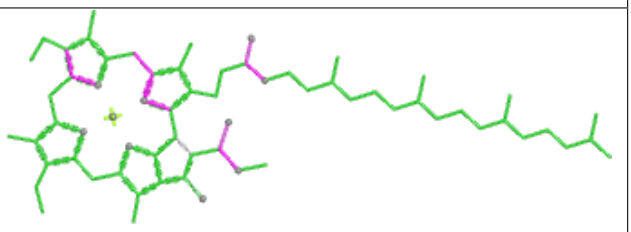


Rings

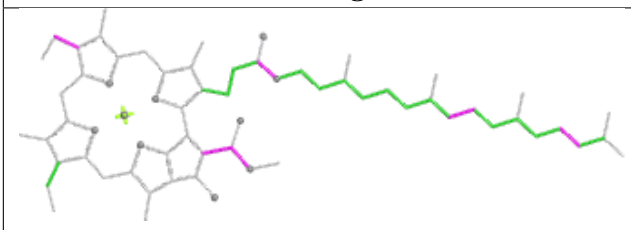
Ligand CLA C 506



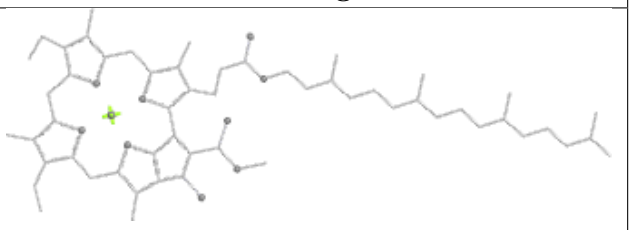
Bond lengths



Bond angles

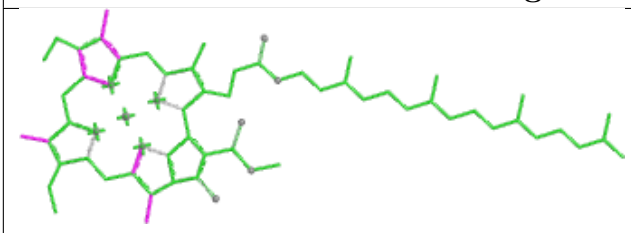


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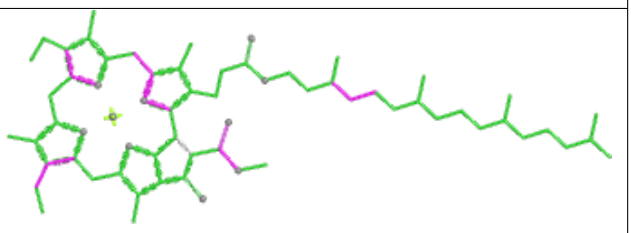


Rings

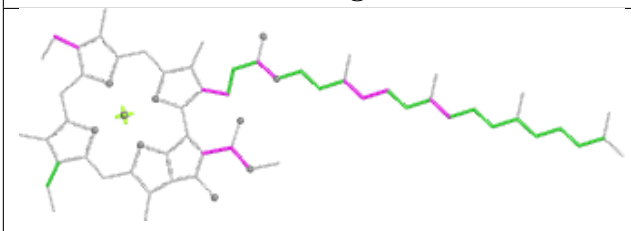
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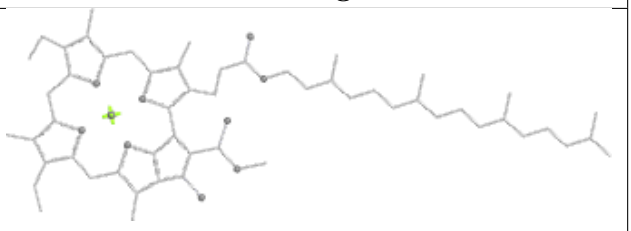
Bond lengths



Bond angles

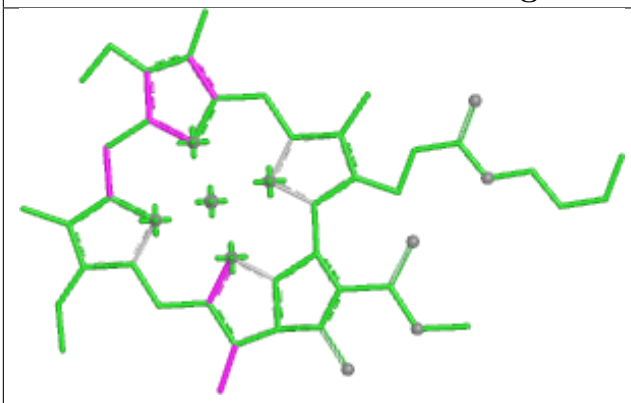


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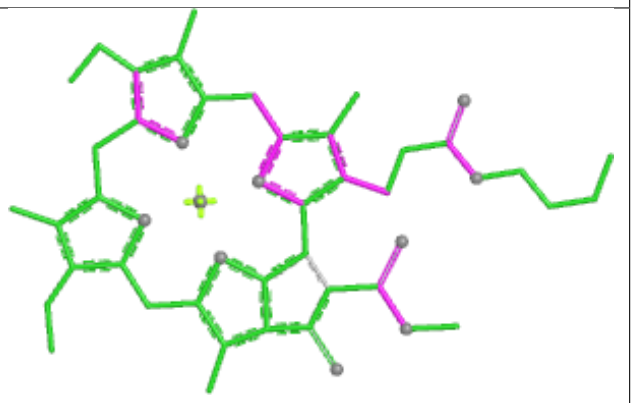


Rings

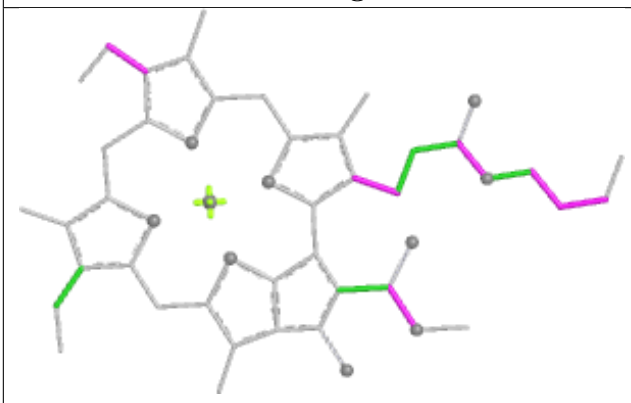
Ligand CLA Ss 608



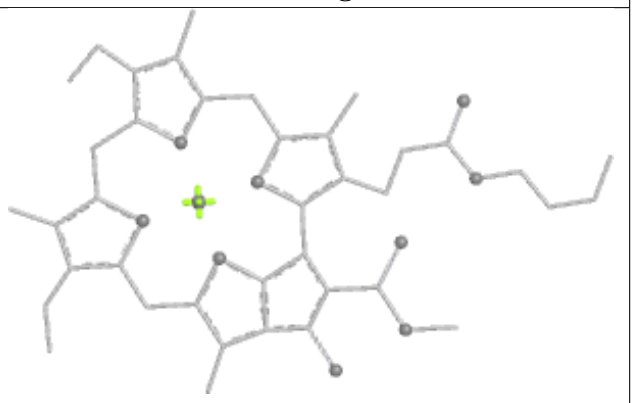
Bond lengths



Bond angles

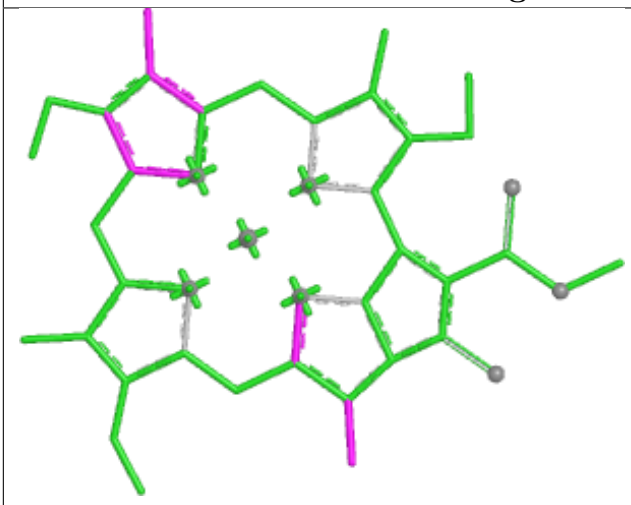


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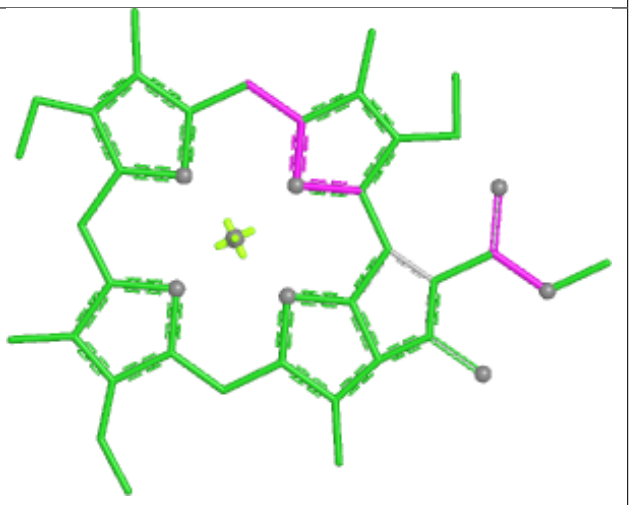


Rings

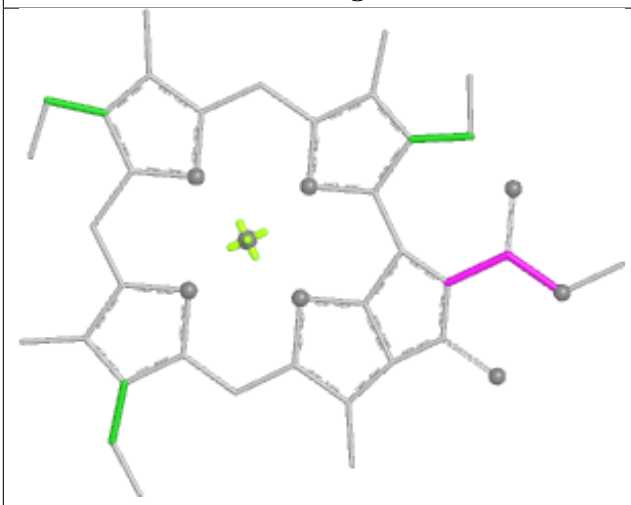
Ligand CLA GG 604



Bond lengths



Bond angles

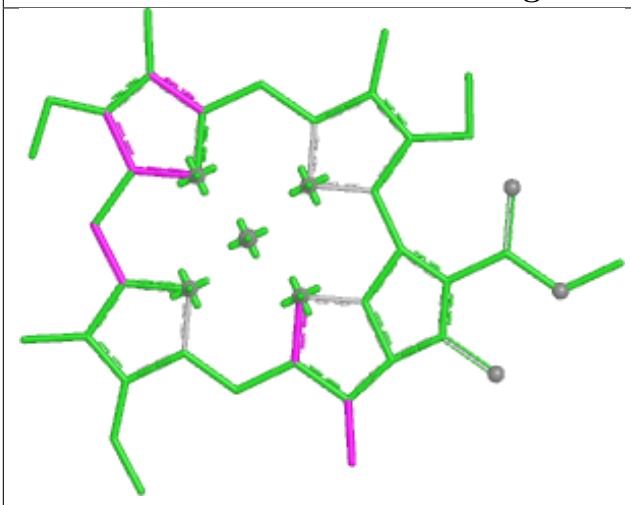


Torsions

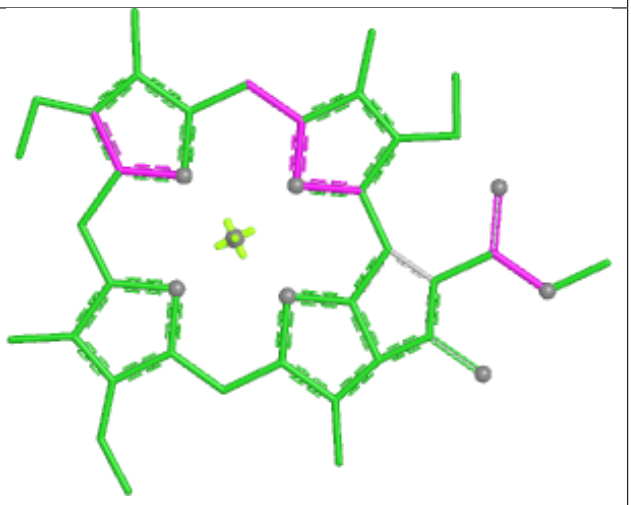


Rings

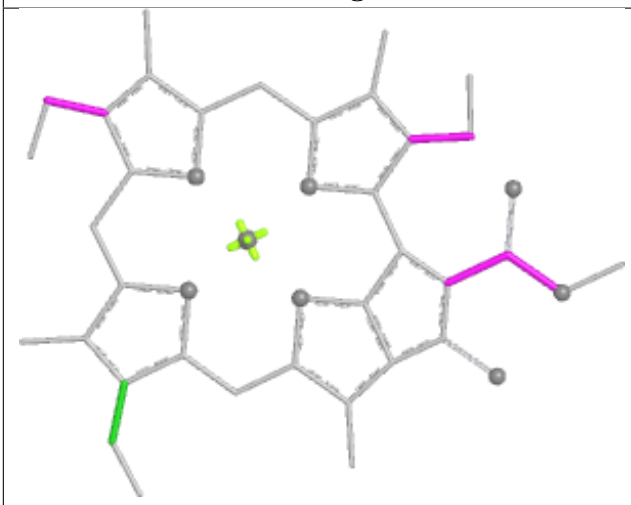
Ligand CLA G 604



Bond lengths



Bond angles

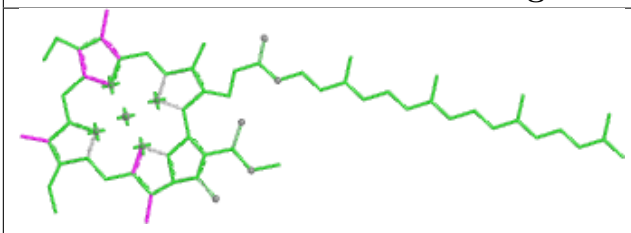


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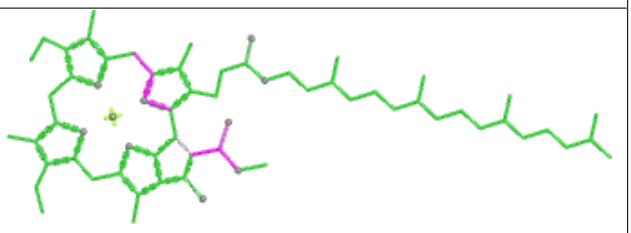


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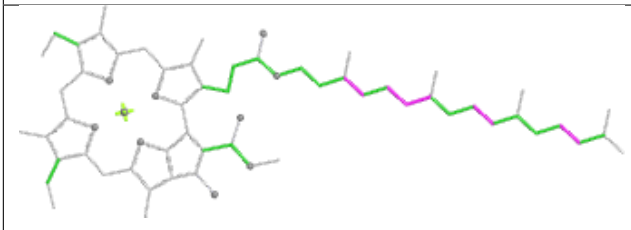
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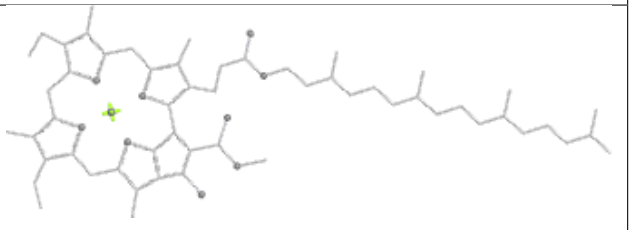
Bond lengths



Bond angles

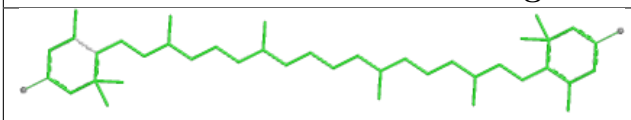


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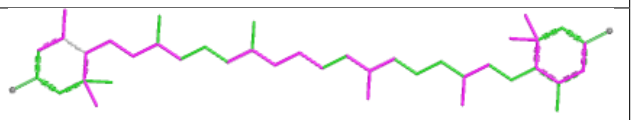


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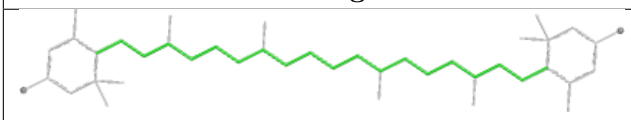
Ligand LUT R 615



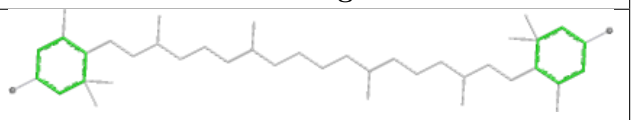
Bond lengths



Bond angles

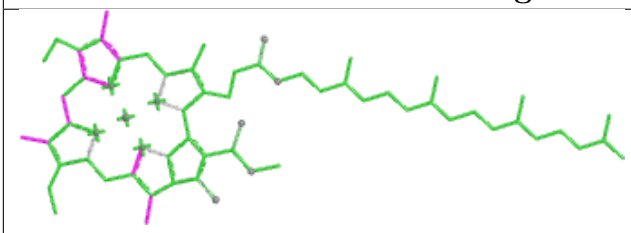


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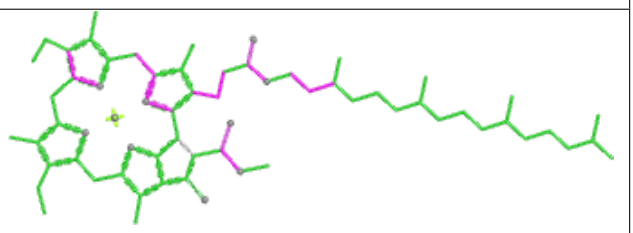


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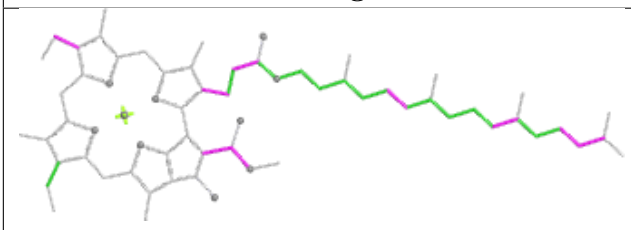
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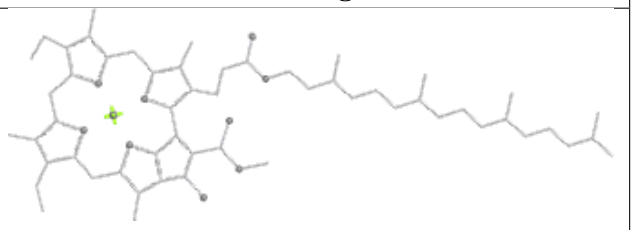
Bond lengths



Bond angles

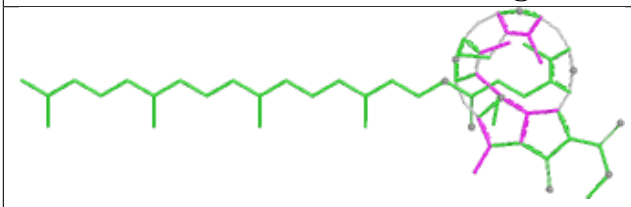


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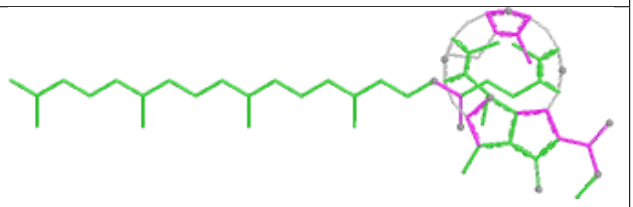


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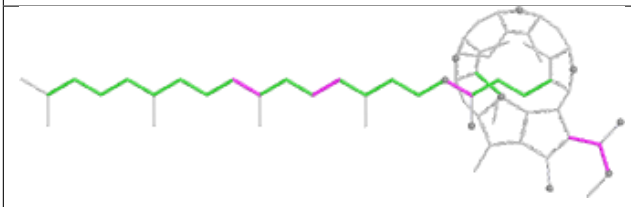
Ligand PHO Aa 408



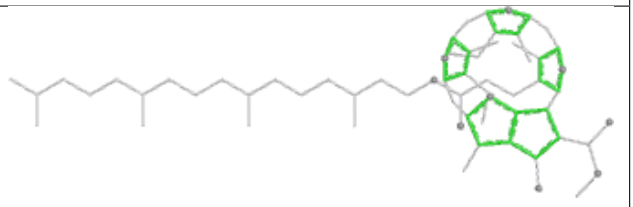
Bond lengths



Bond angles

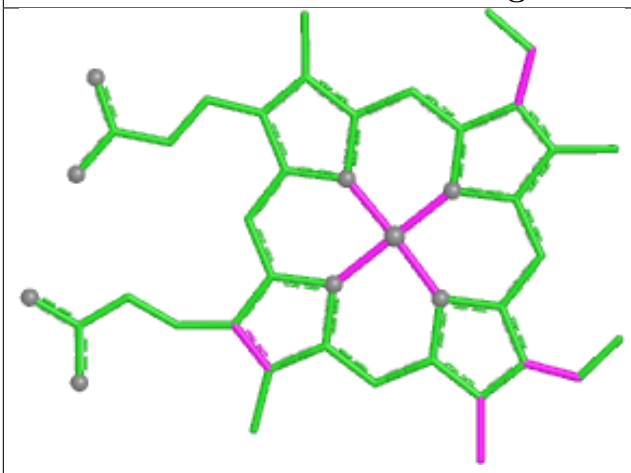


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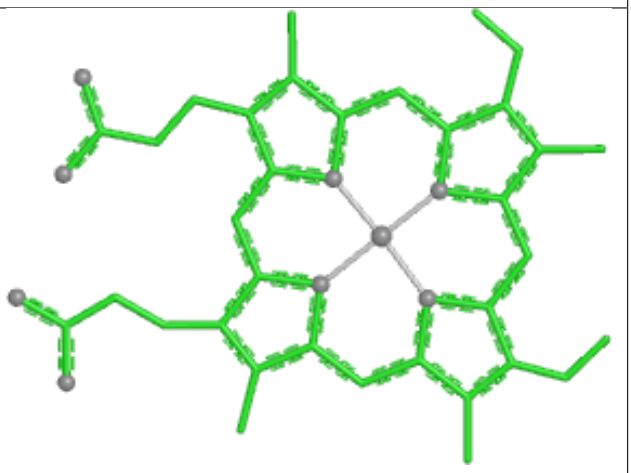


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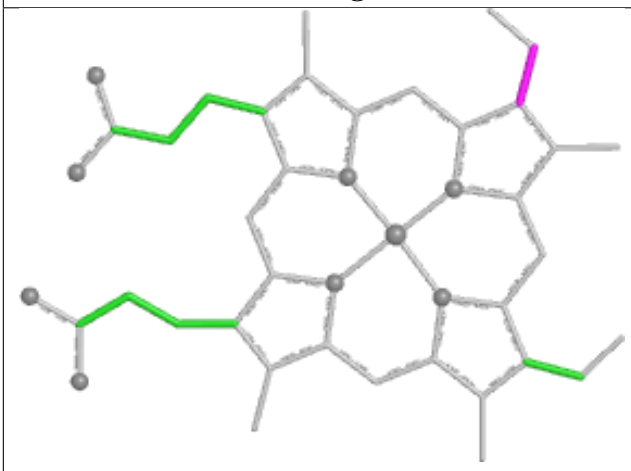
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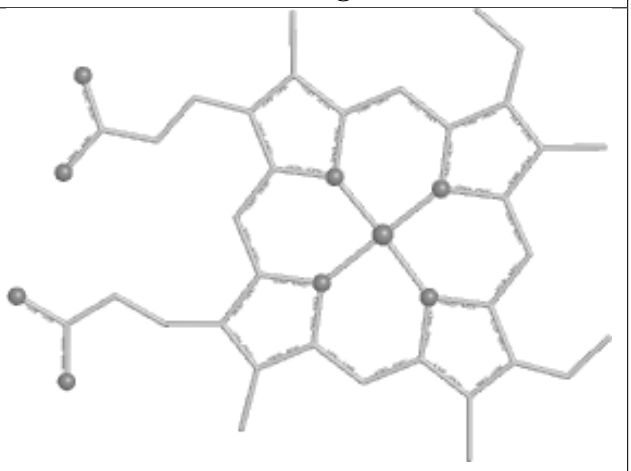
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Bond angles

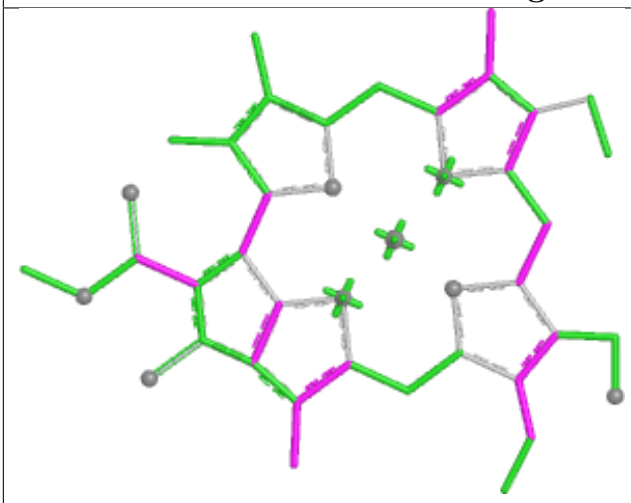


Torsions



Rings

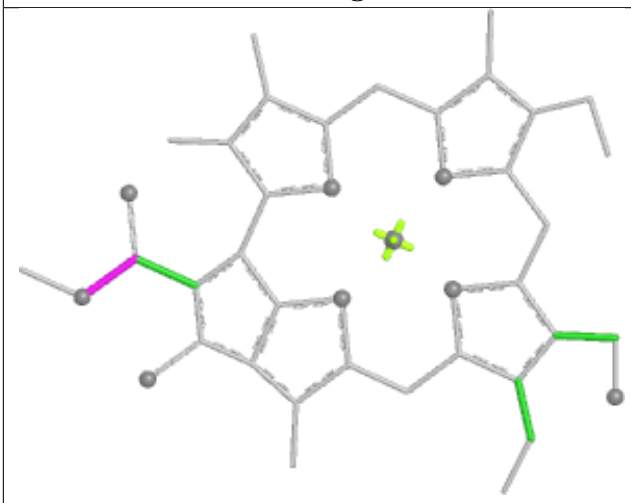
Ligand CHL g 608



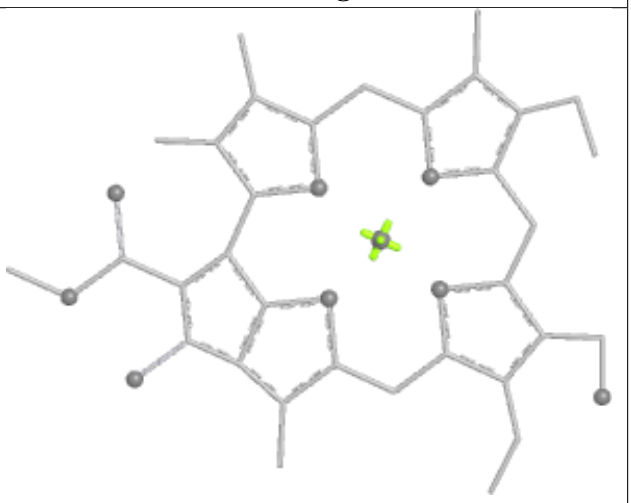
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Bond angles

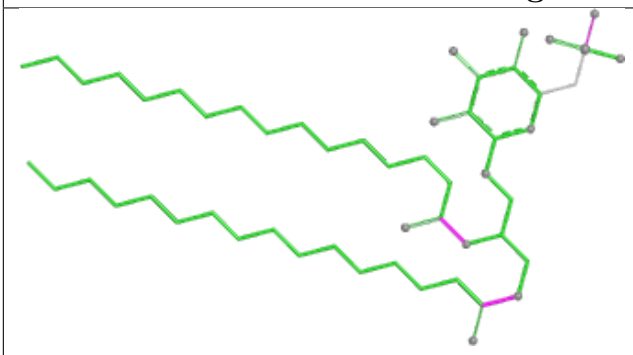


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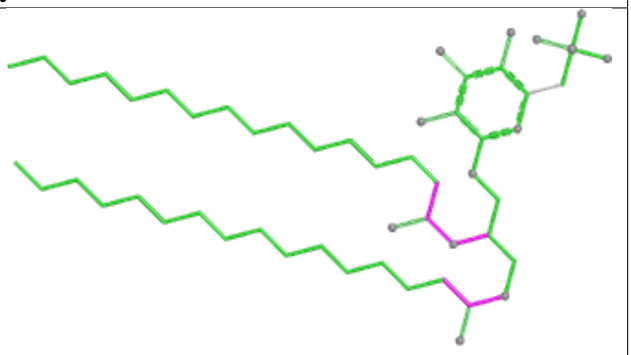


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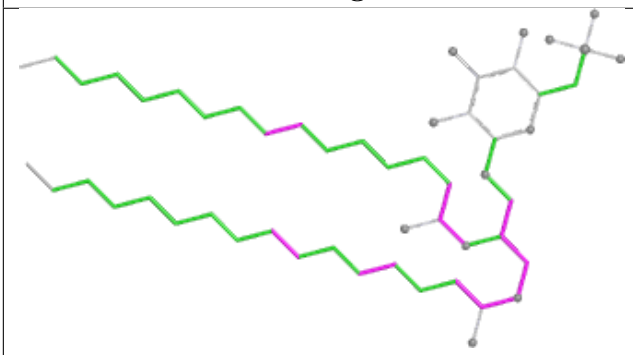
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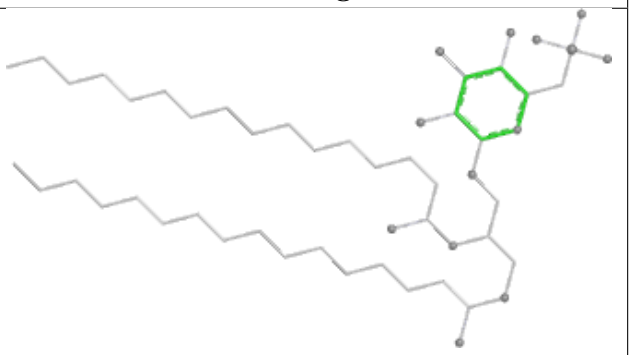
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Bond angles

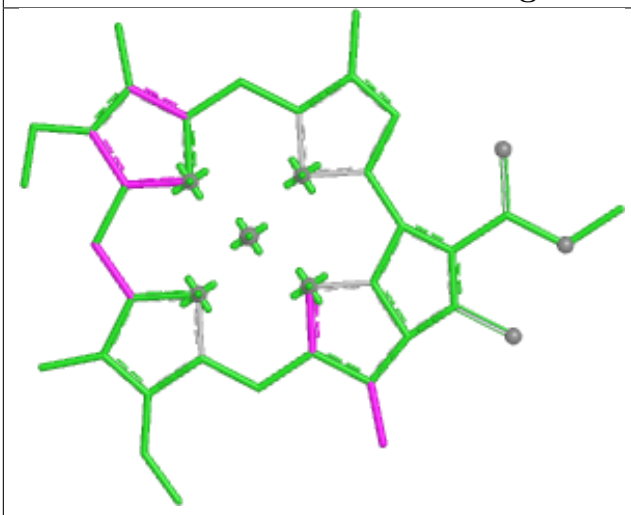


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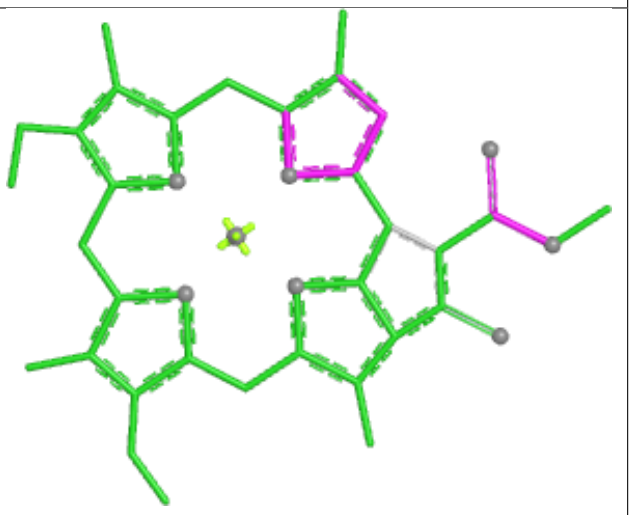


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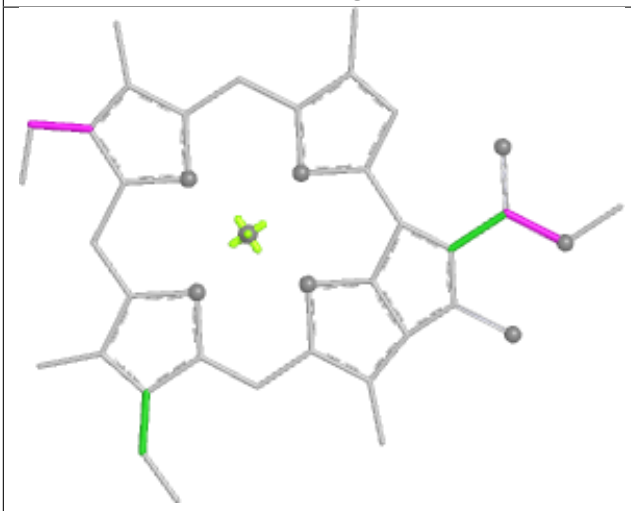
Ligand CLA 33 612



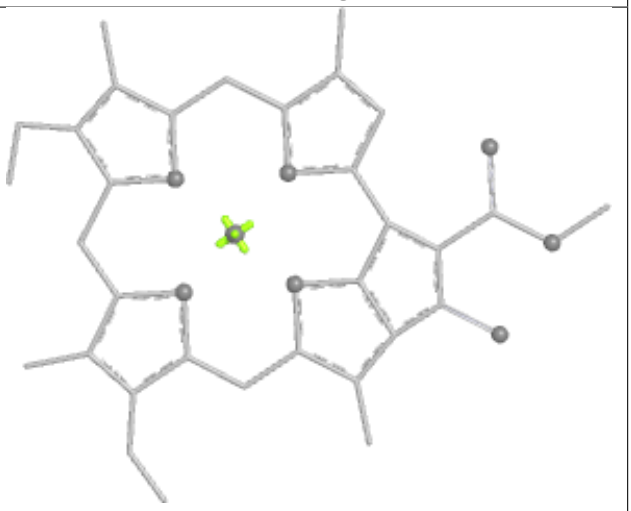
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Bond angles

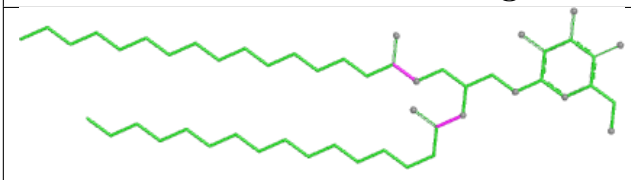


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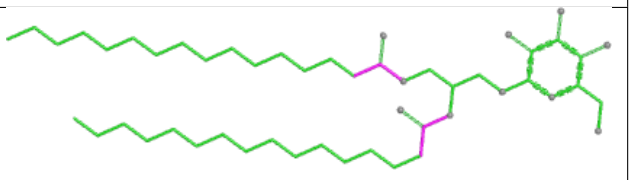


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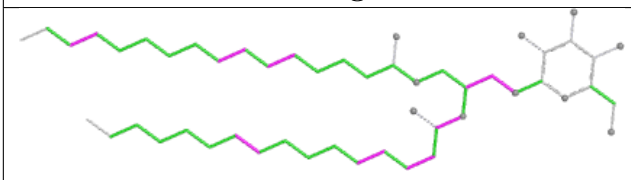
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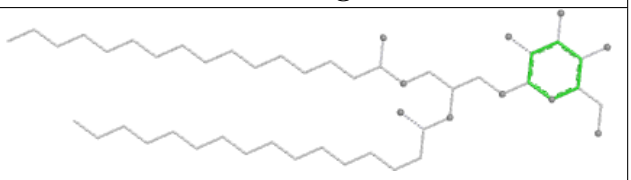
Bond lengths



Bond angles

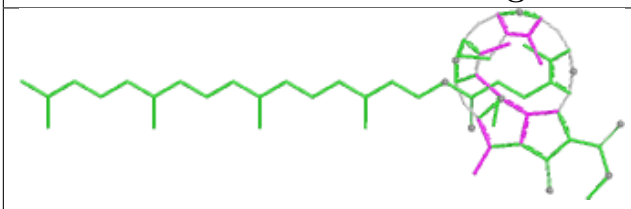


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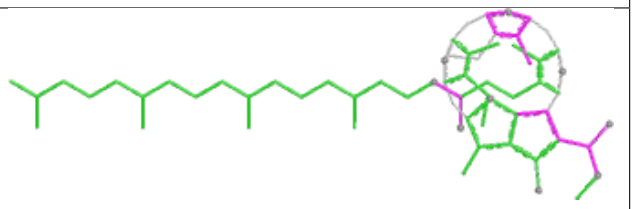


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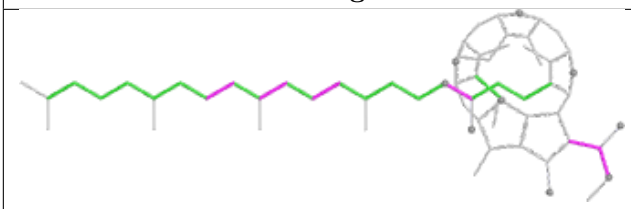
Ligand PHO DD 402



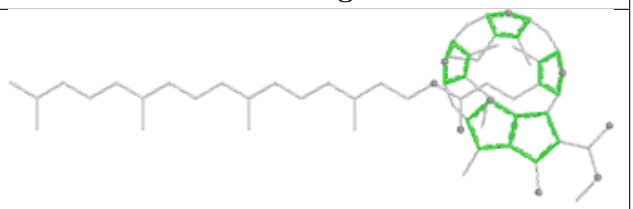
Bond lengths



Bond angles

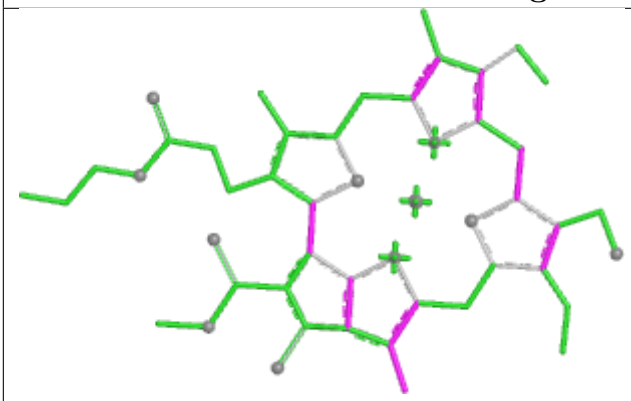


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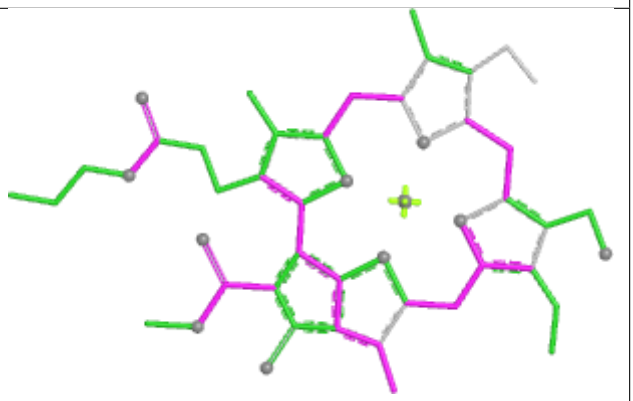


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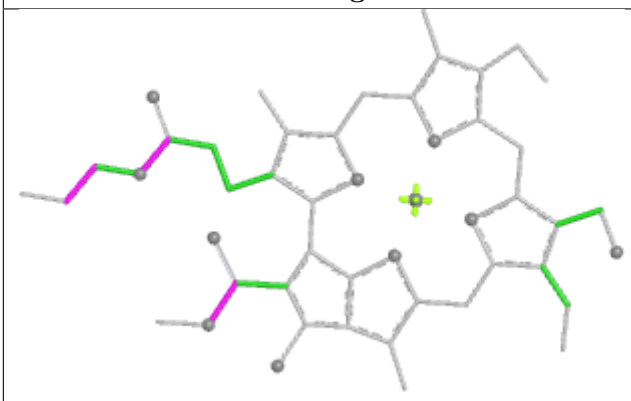
Ligand CHL s 607



Bond lengths



Bond angles

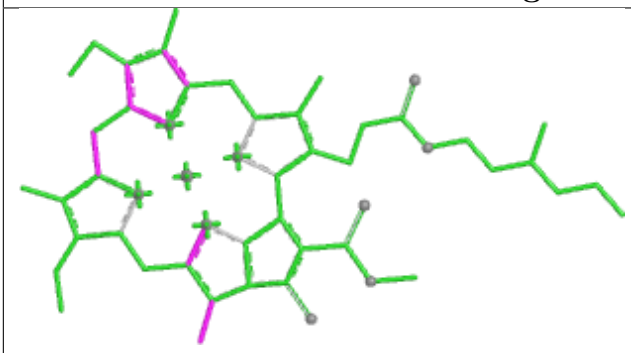


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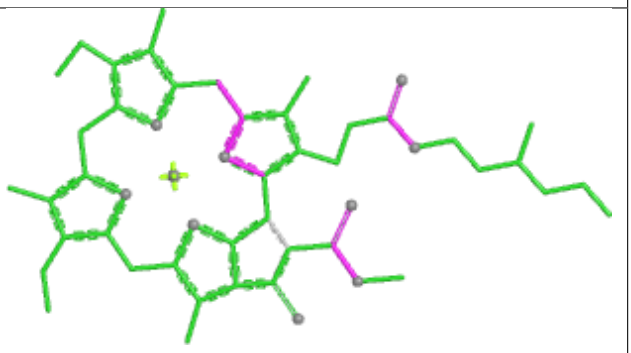


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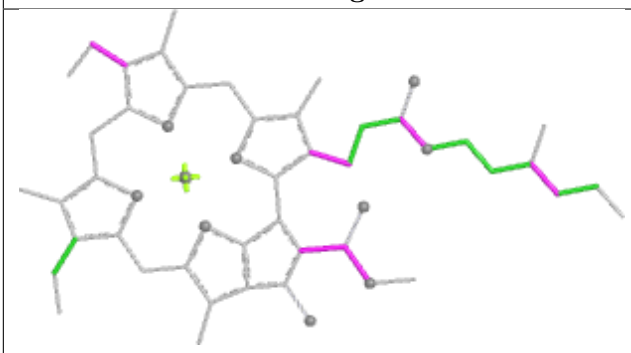
Ligand CLA G 611



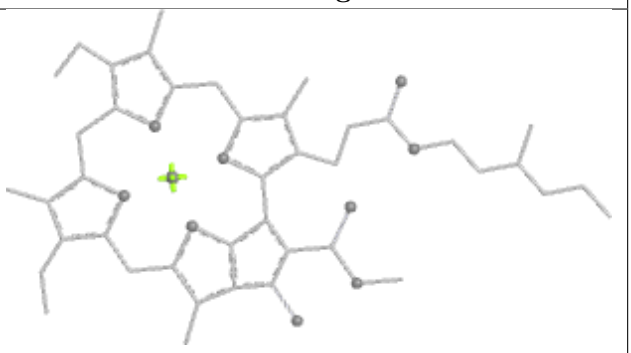
Bond lengths



Bond angles

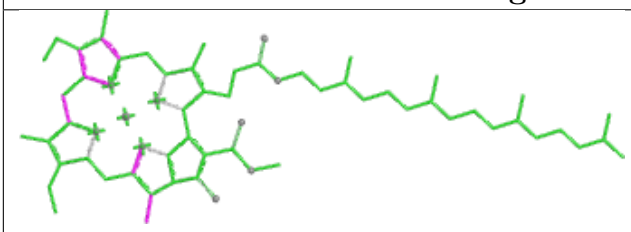


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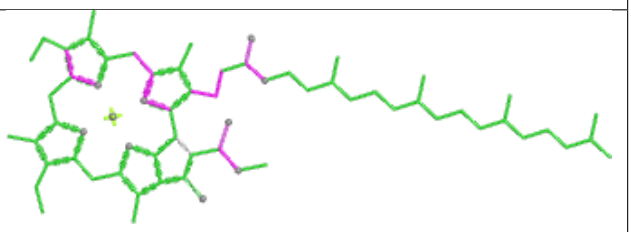


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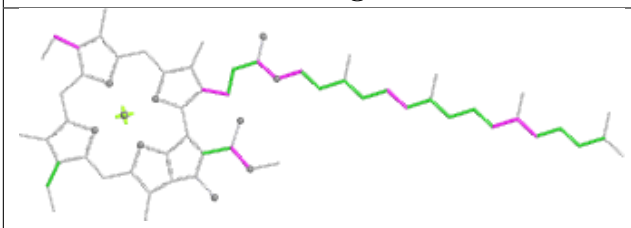
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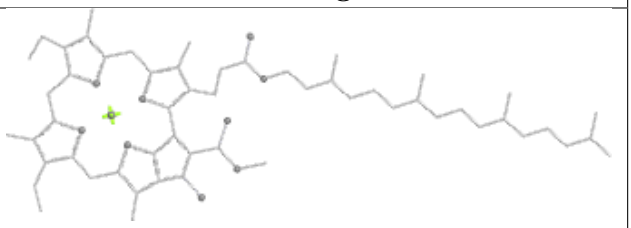
Bond lengths



Bond angles

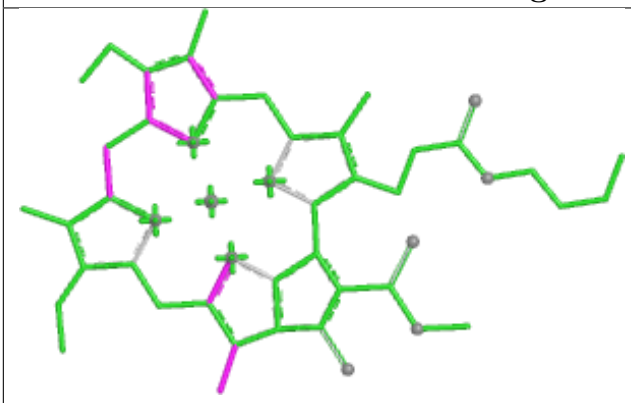


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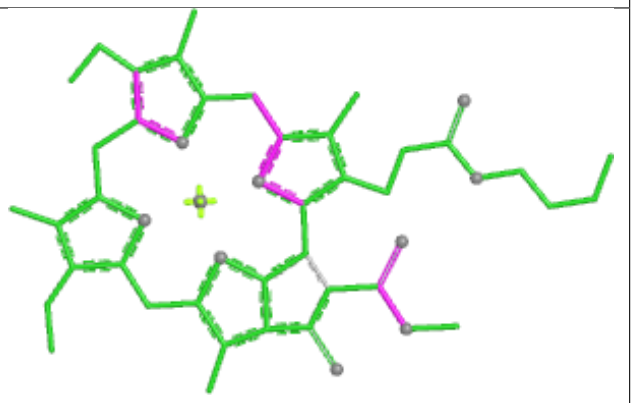


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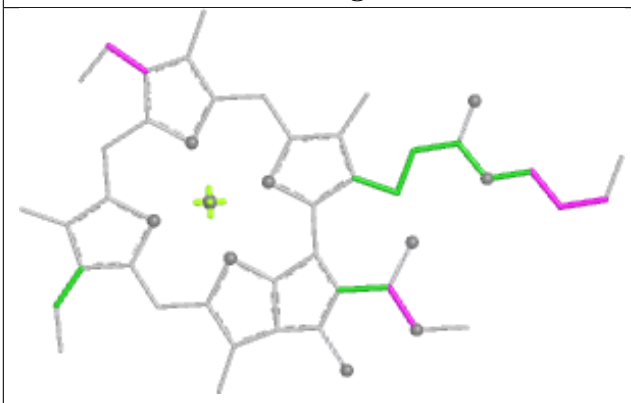
Ligand CLA s 613



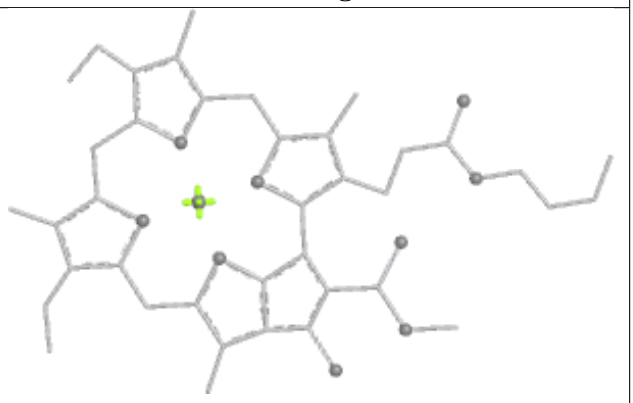
Bond lengths



Bond angles

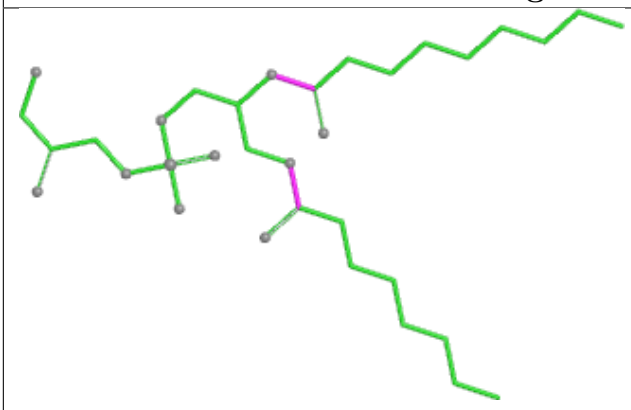


Torsions

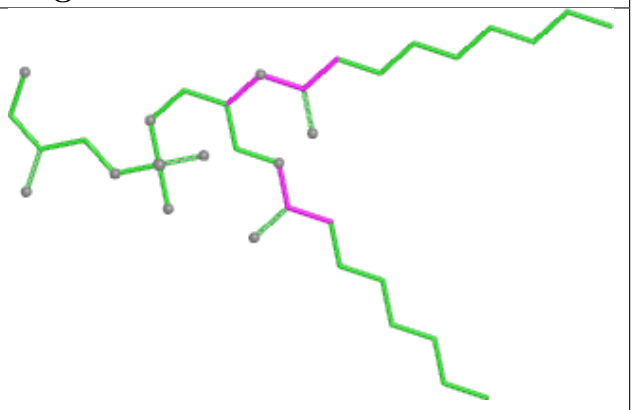


Rings

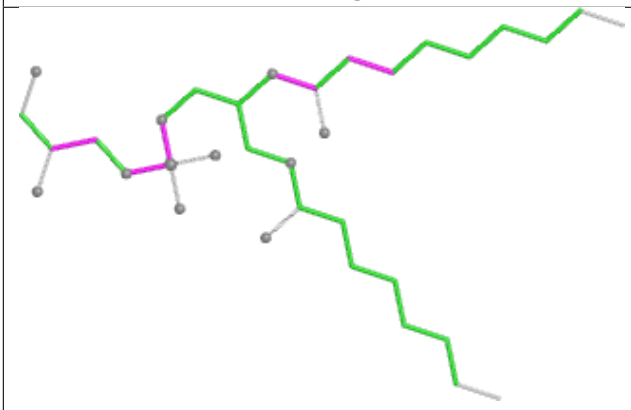
Ligand LHG g 618



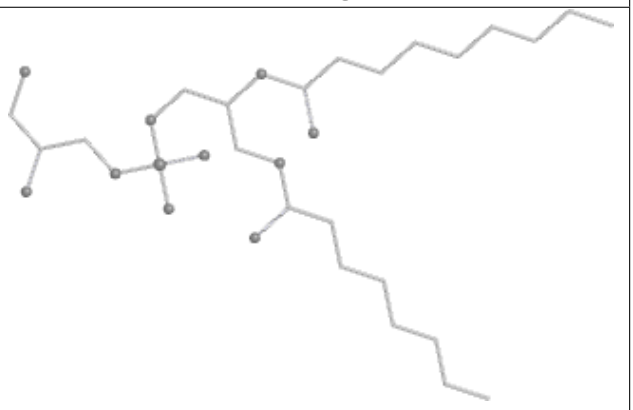
Bond lengths



Bond angles

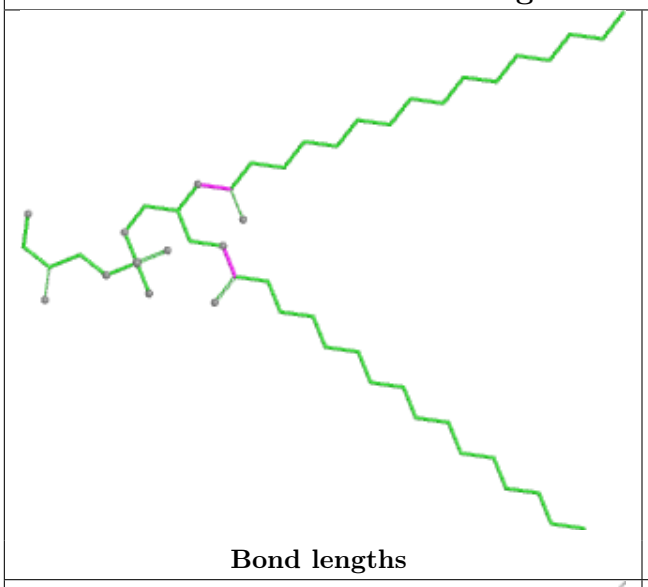


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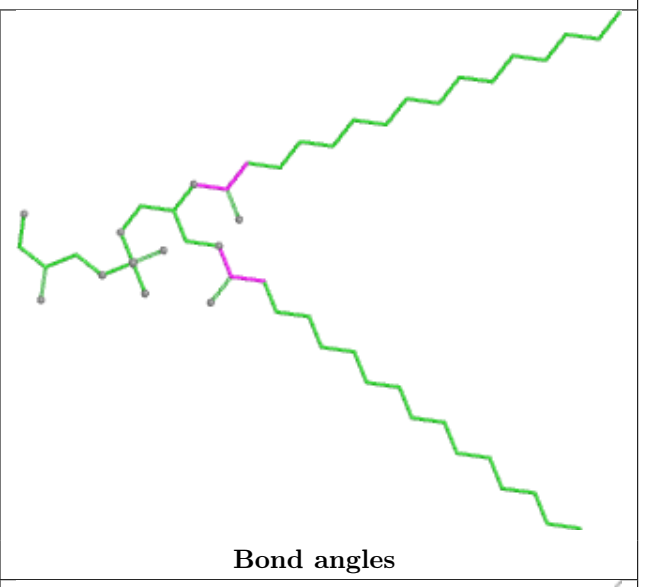


Rings

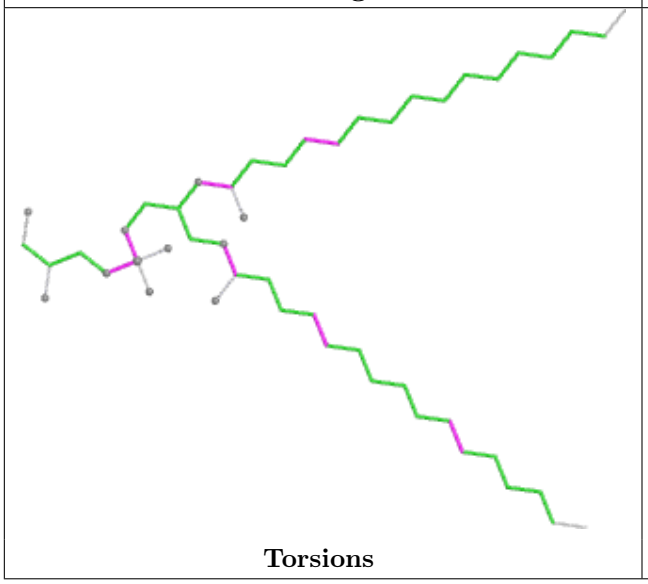
Ligand LHG Rr 617



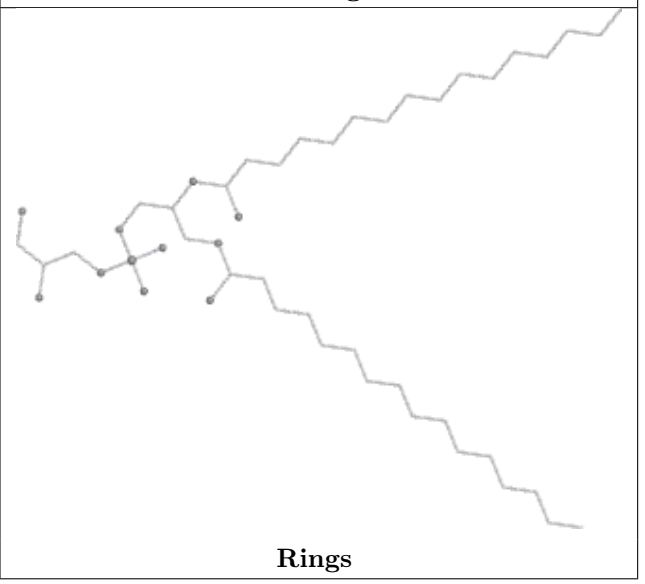
Bond lengths



Bond angles

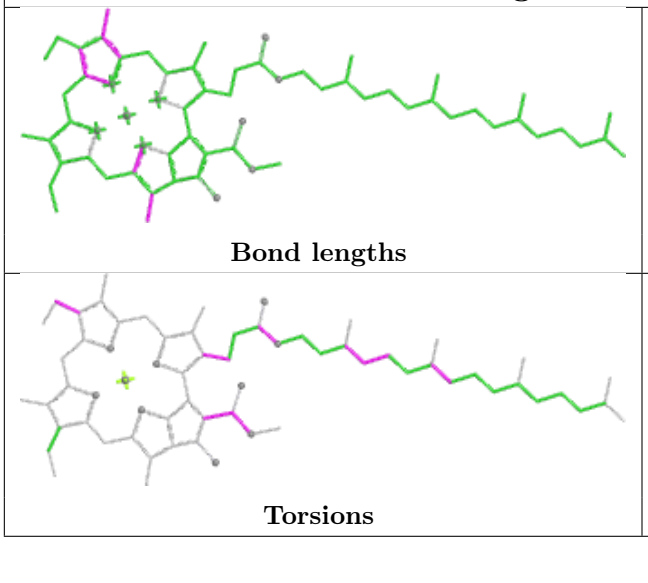


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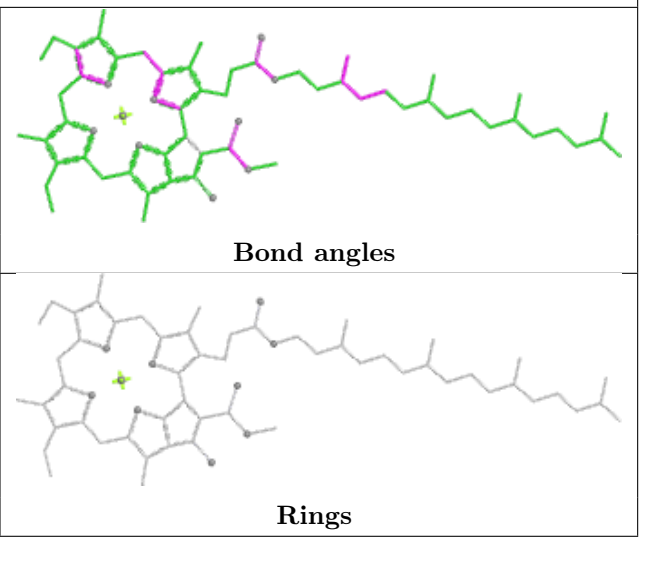


Rings

Ligand CLA BB 604



Bond lengths

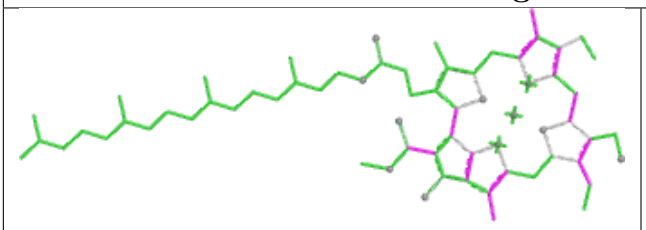


Bond angles

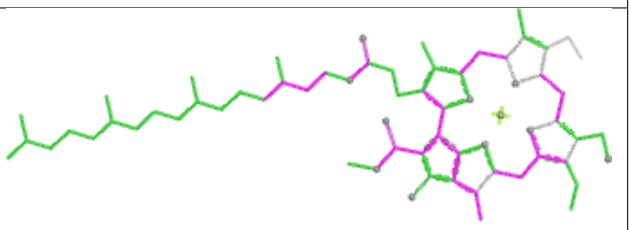
Torsions

Rings

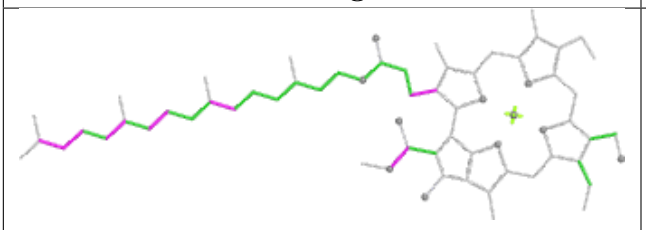
Ligand CHL Nn 317



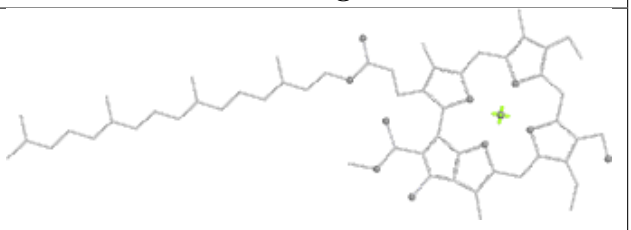
Bond lengths



Bond angles

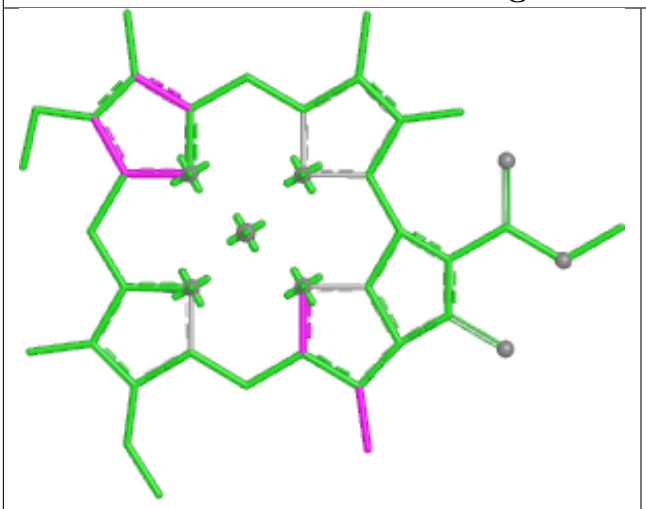


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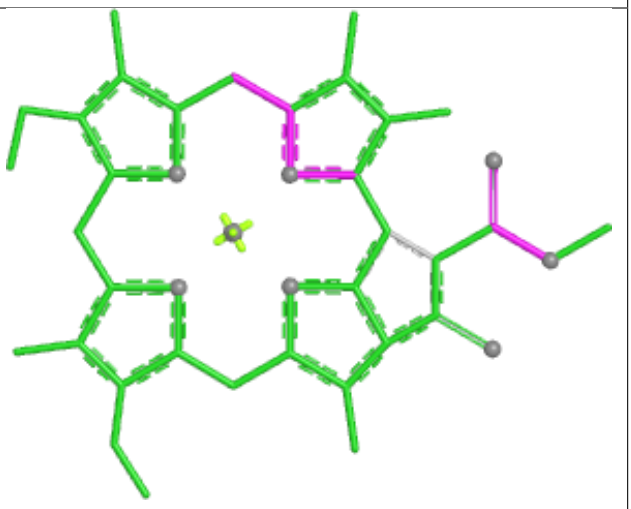


Rings

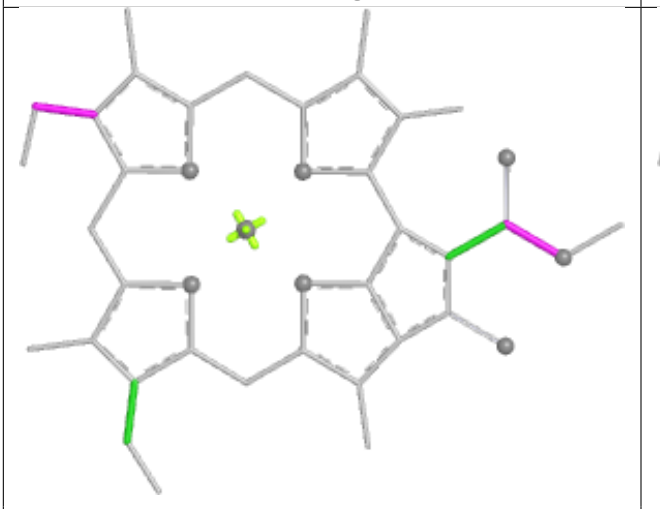
Ligand CLA GG 614



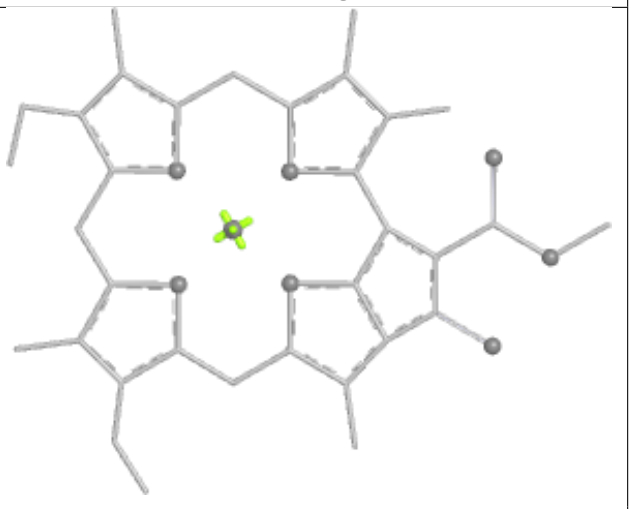
Bond lengths



Bond angles

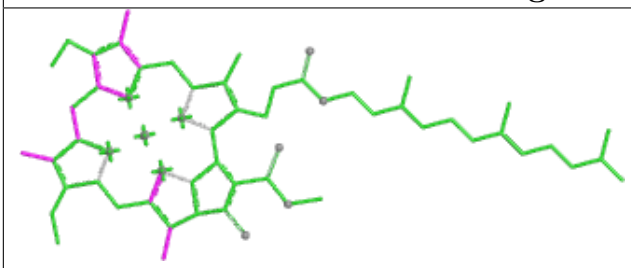


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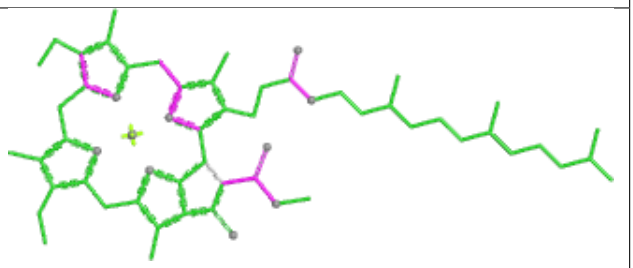


Rings

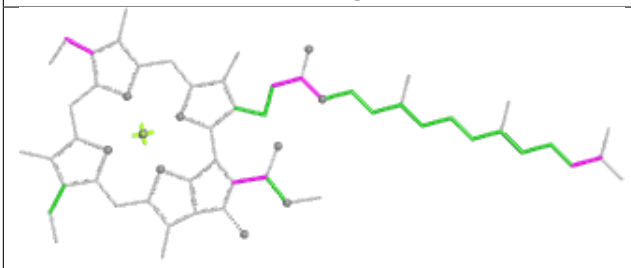
Ligand CLA a 410



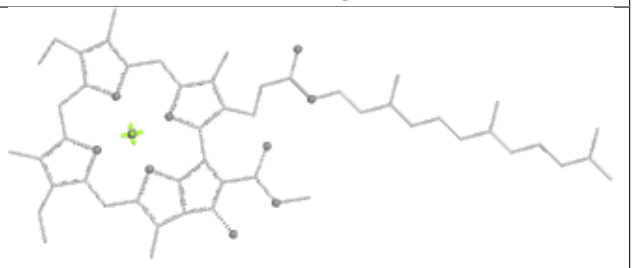
Bond lengths



Bond angles

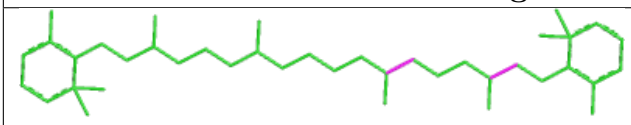


Torsions

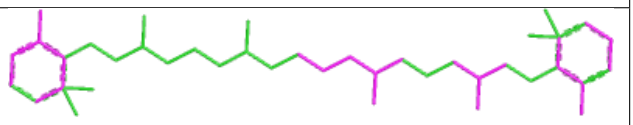


Rings

Ligand BCR BB 617



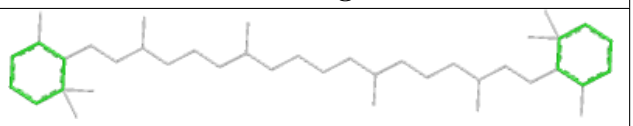
Bond lengths



Bond angles

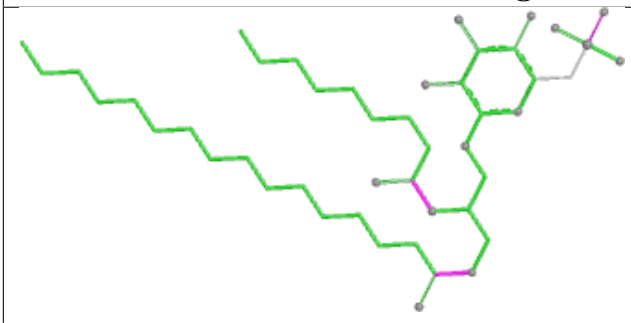


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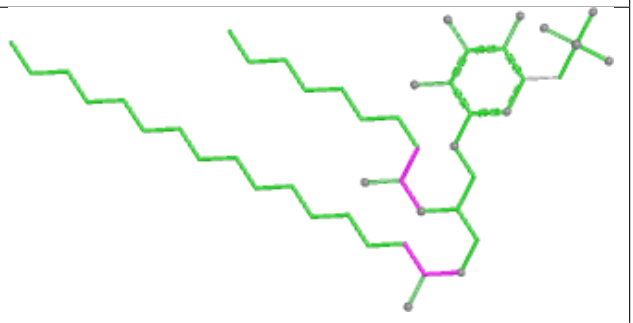


Rings

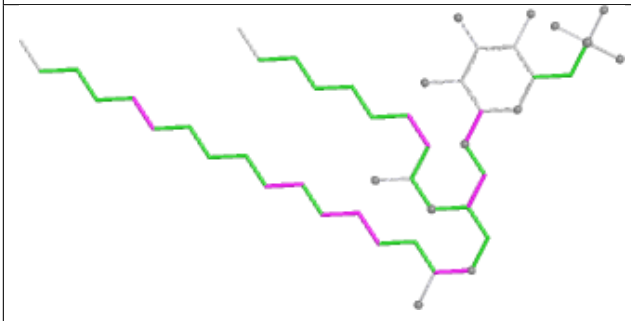
Ligand SQD Aa 413



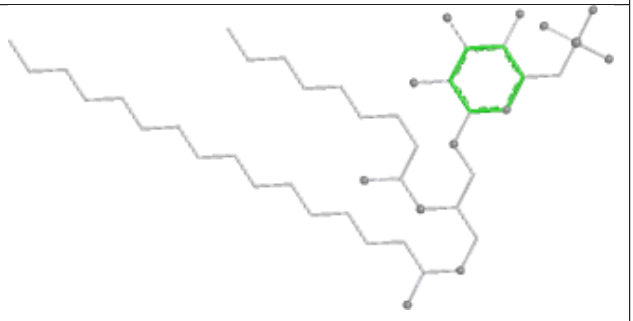
Bond lengths



Bond angles

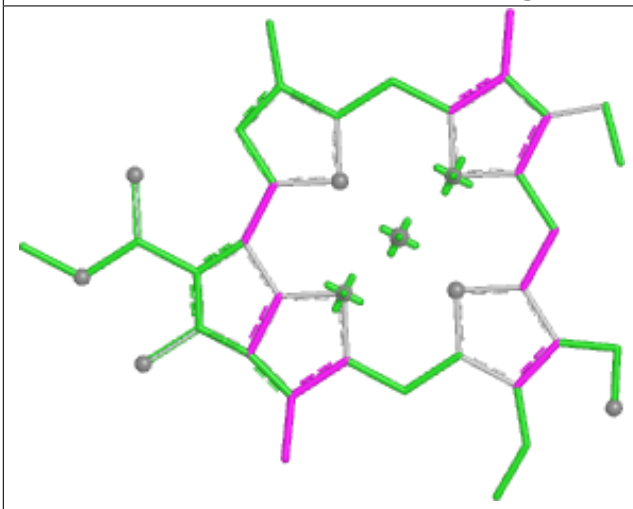


Torsions



Rings

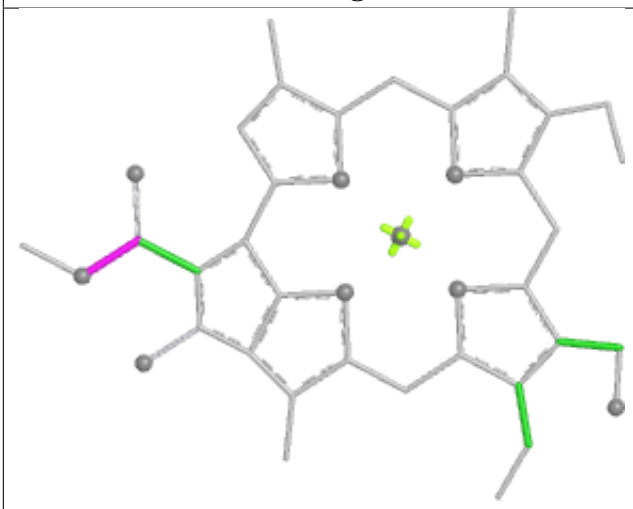
Ligand CHL 22 601



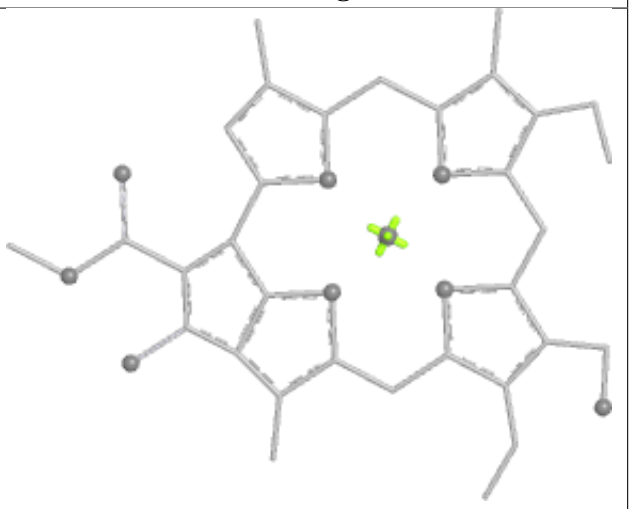
Bond lengths



Bond angles

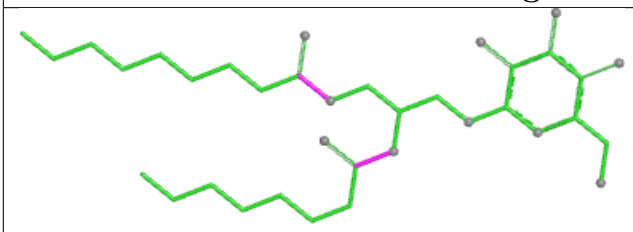


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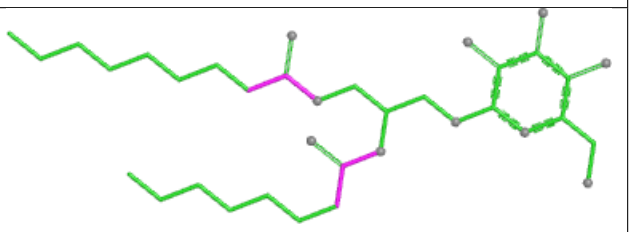


Rings

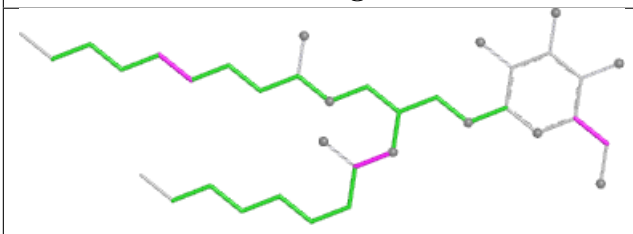
Ligand LMG b 620



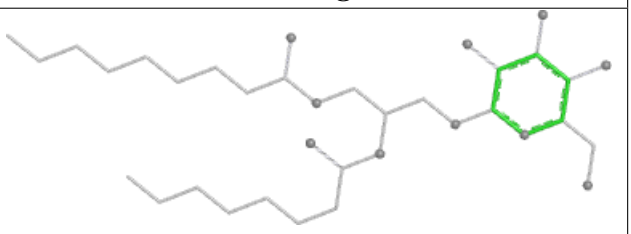
Bond lengths



Bond angles

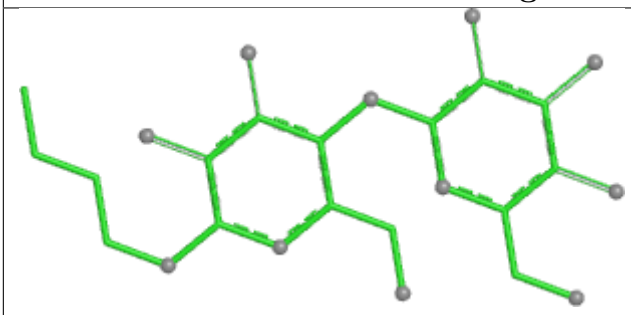


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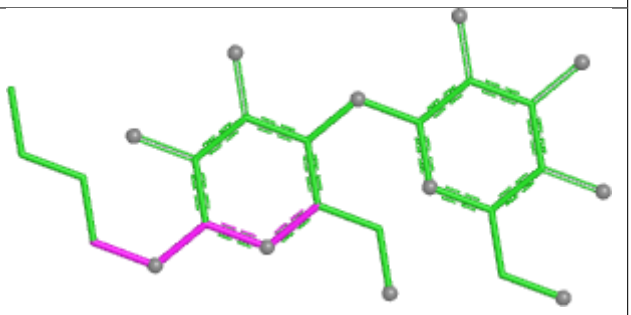


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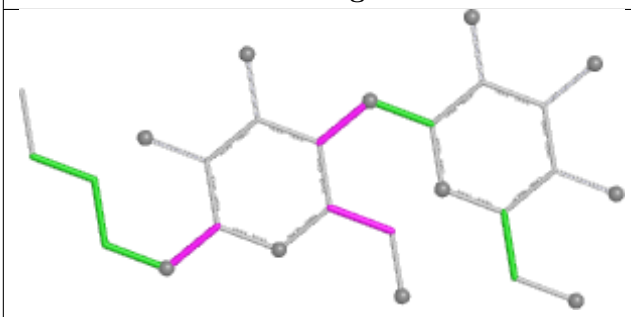
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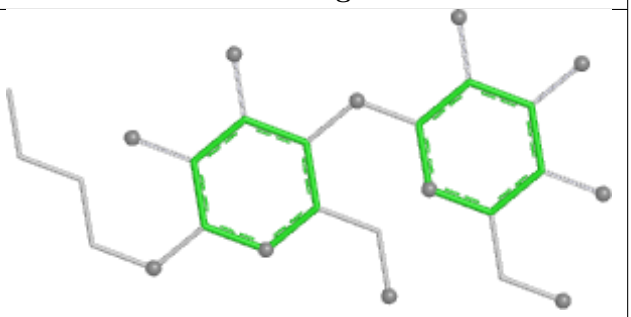
Bond lengths



Bond angles

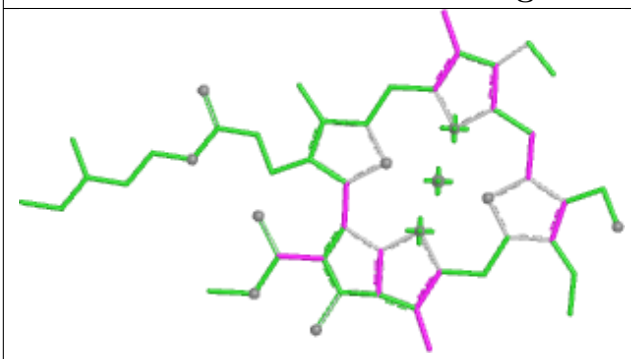


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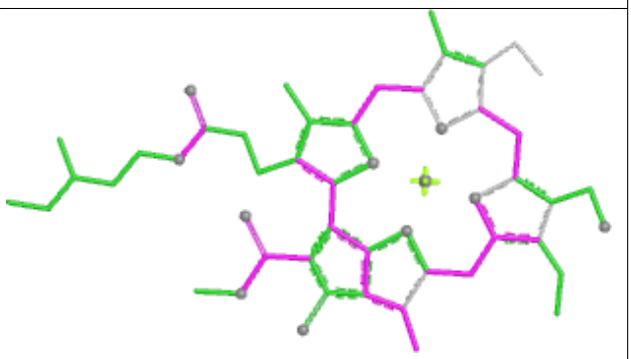


Rings

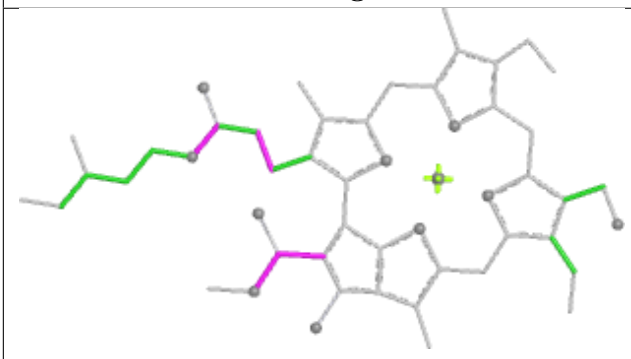
Ligand CHL SS 302



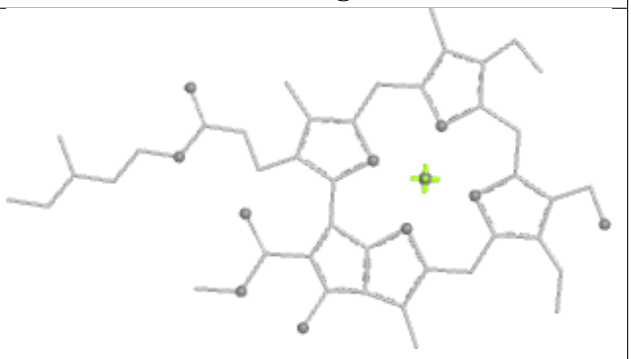
Bond lengths



Bond angles

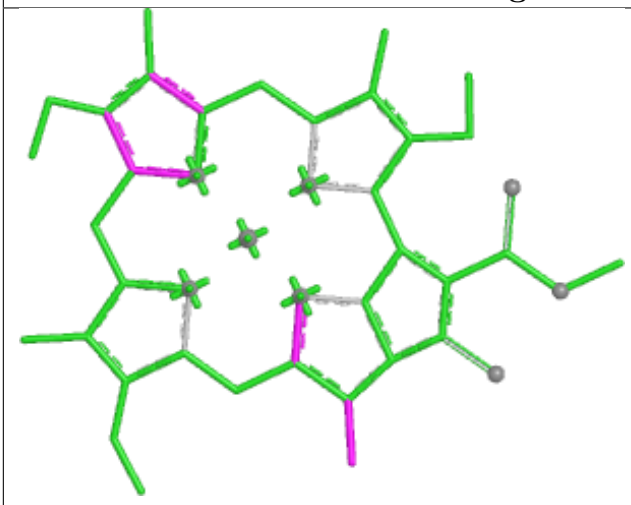


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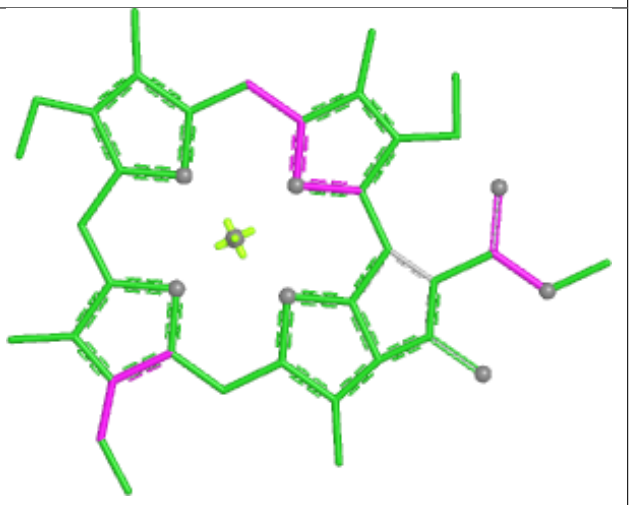


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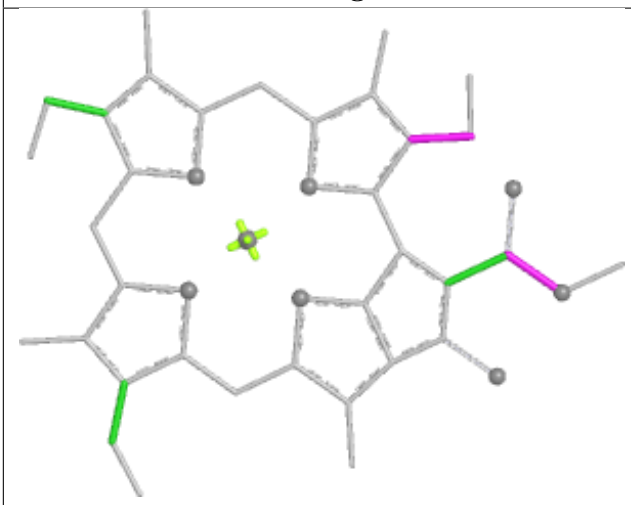
Ligand CLA NN 612



Bond lengths



Bond angles

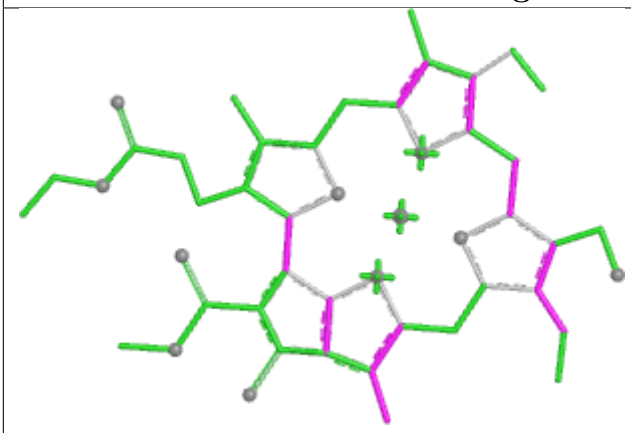


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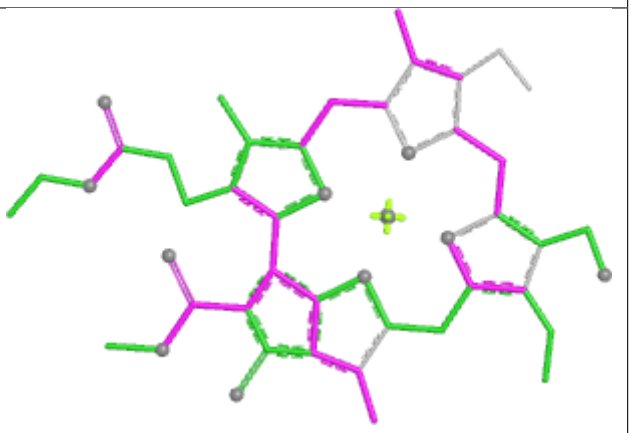


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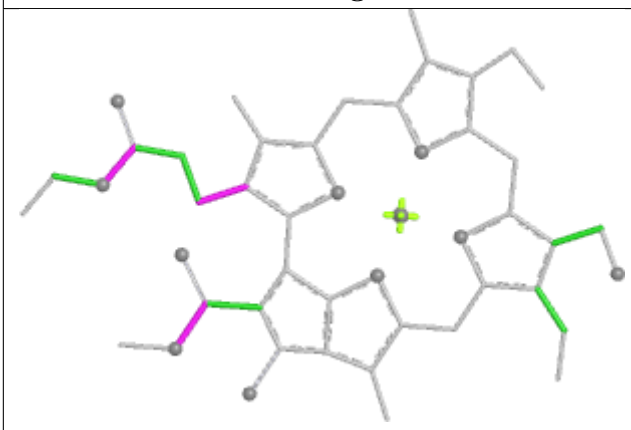
Ligand CHL Nn 315



Bond lengths



Bond angles

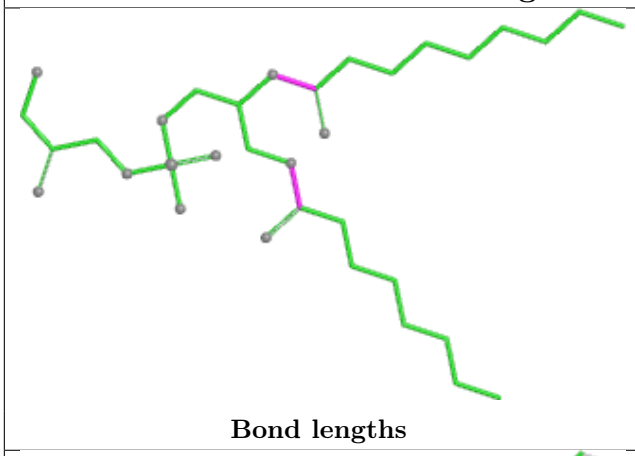


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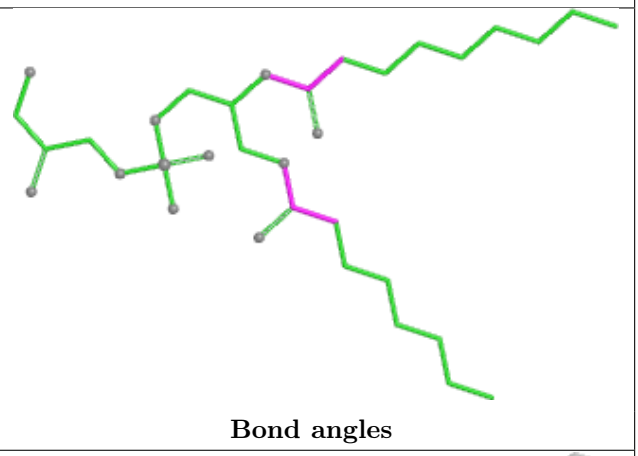


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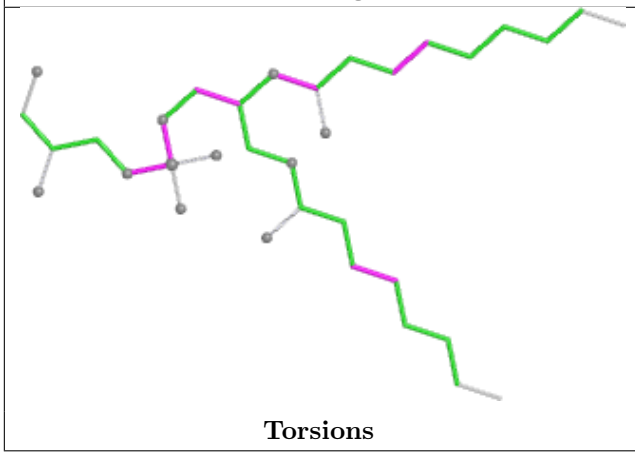
Ligand LHG 33 614



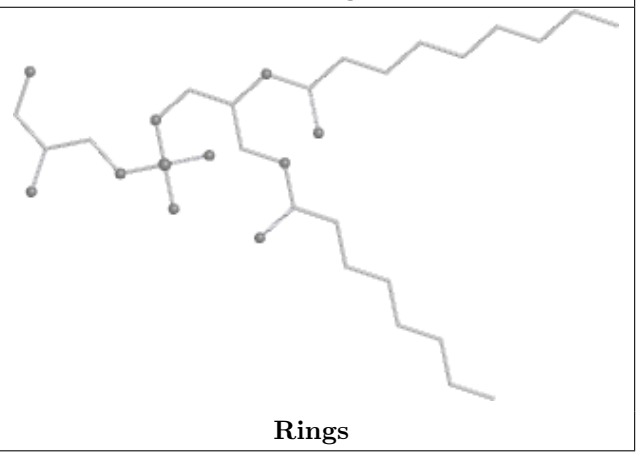
Bond lengths



Bond angles

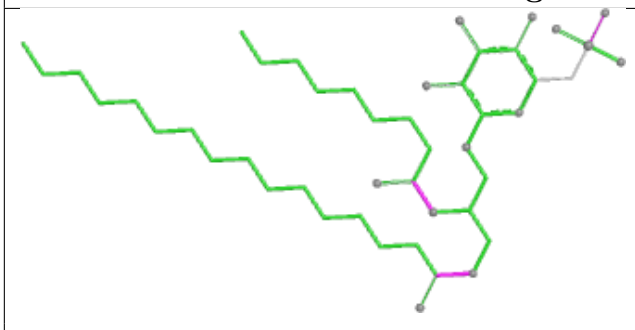


Torsions

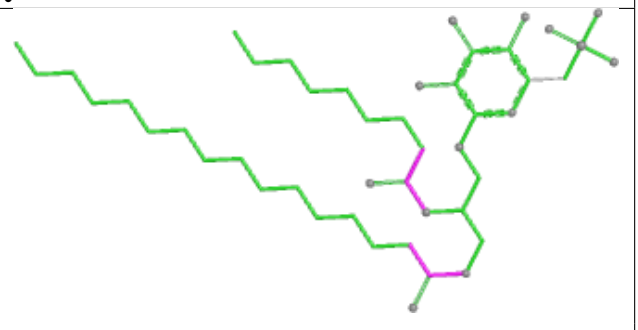


Rings

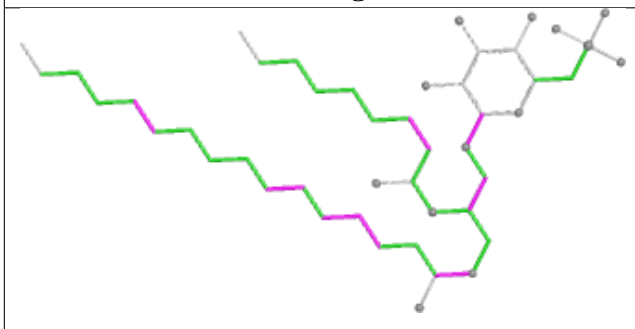
Ligand SQD B 602



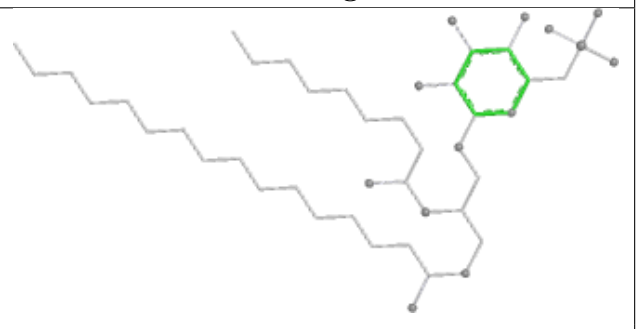
Bond lengths



Bond angles

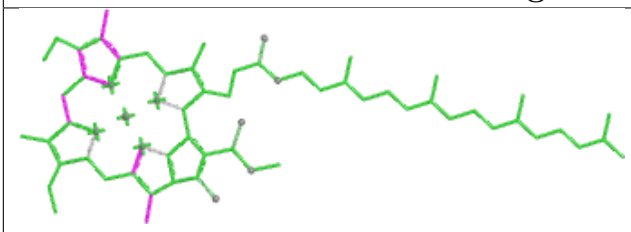


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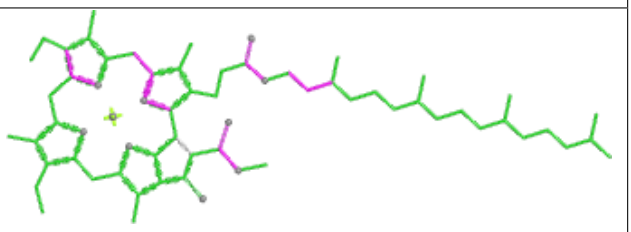


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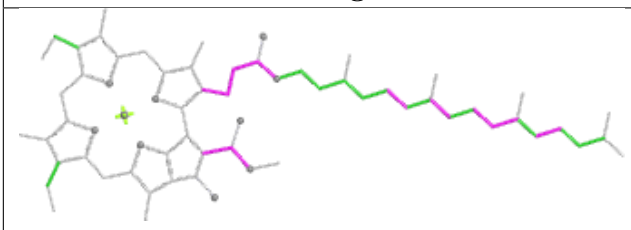
Ligand CLA b 609



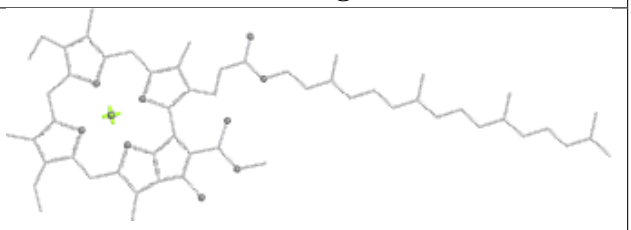
Bond lengths



Bond angles

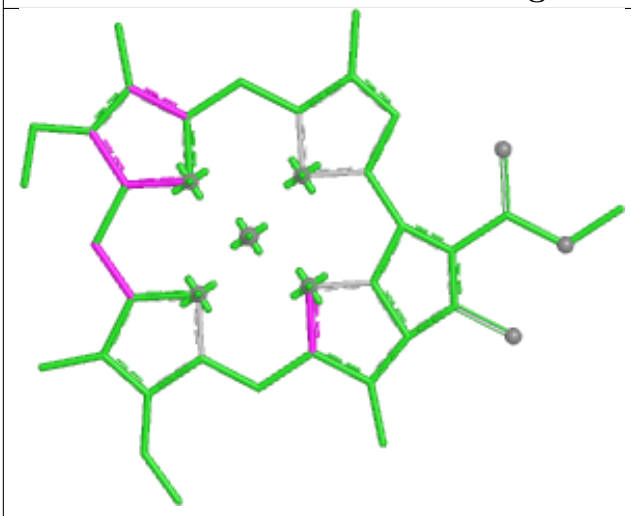


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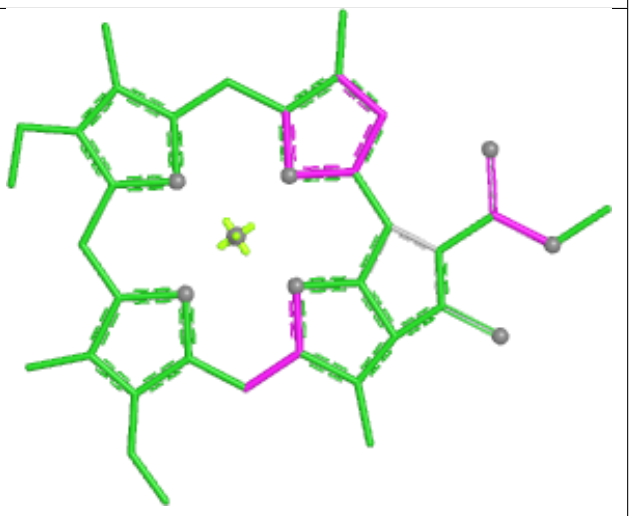


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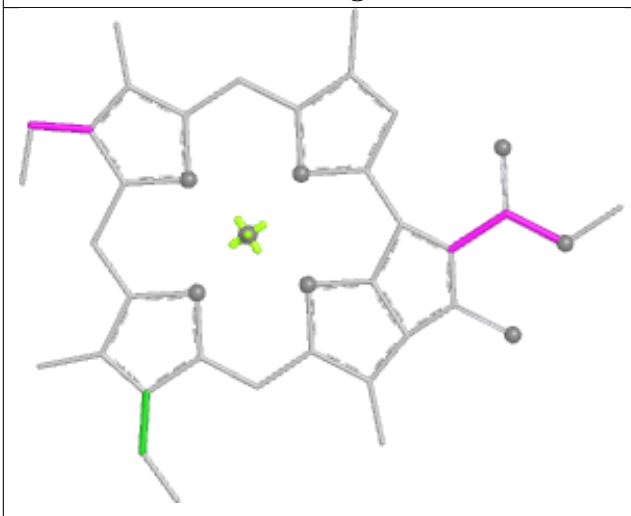
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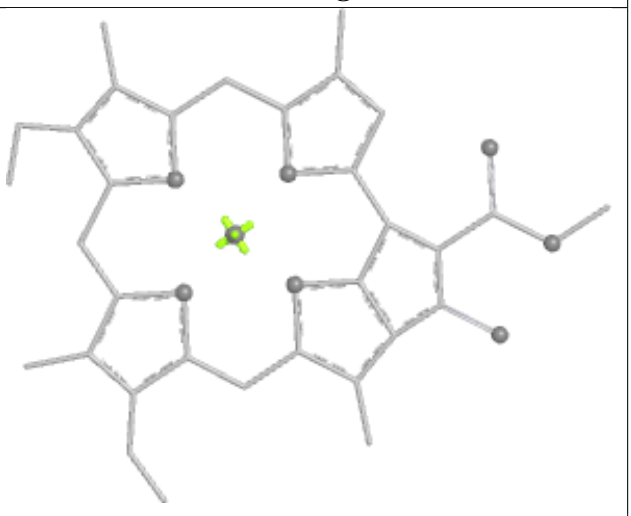
Bond lengths



Bond angles

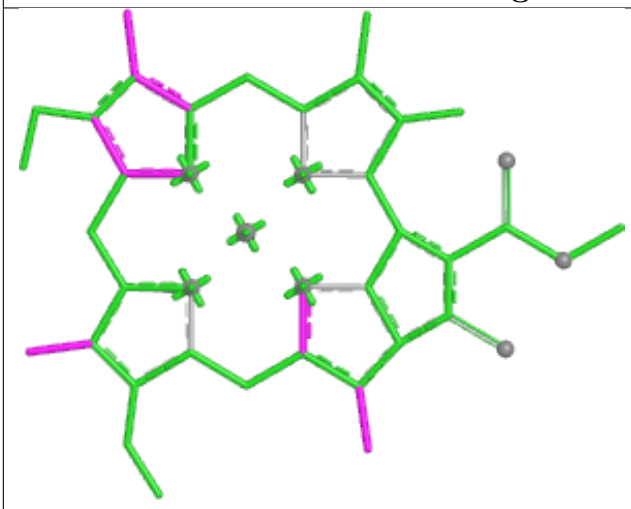


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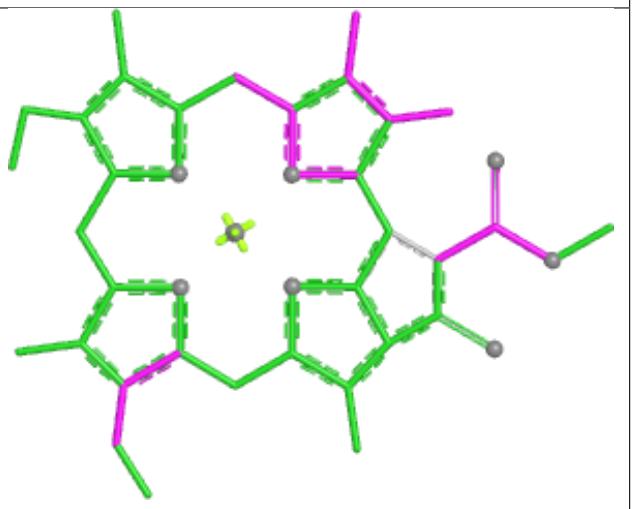


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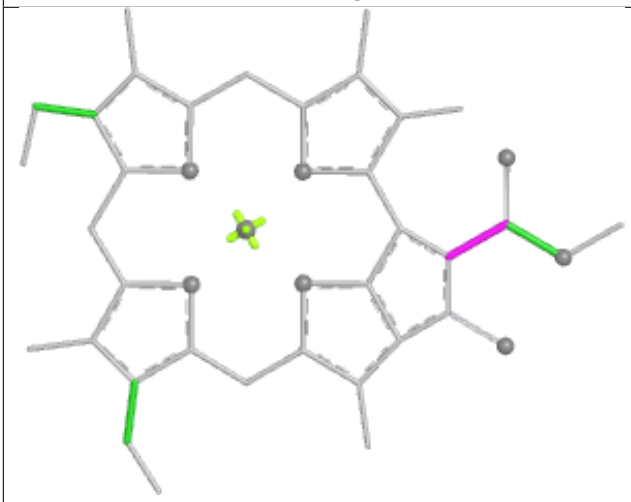
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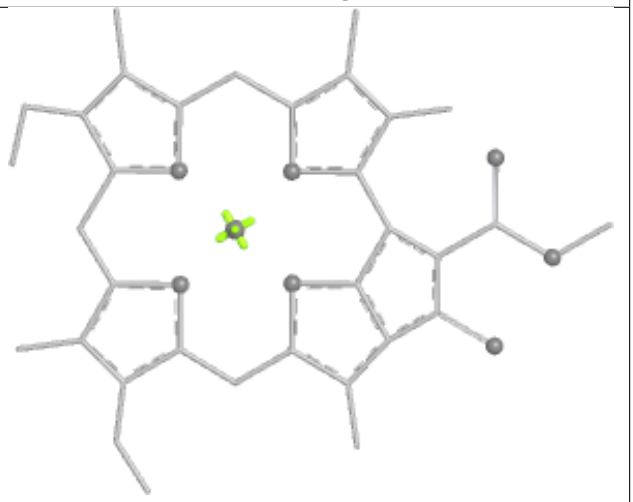
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Bond angles

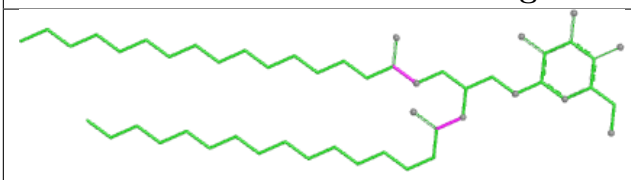


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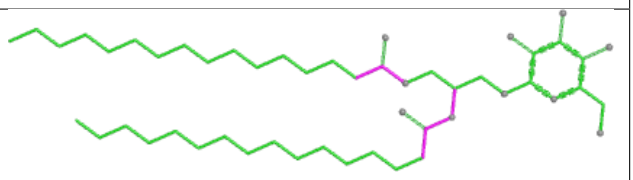


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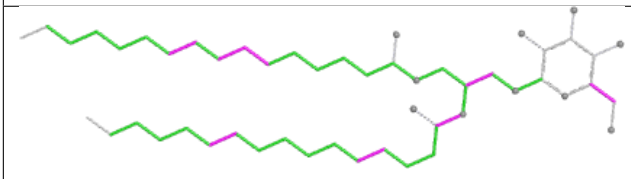
Ligand LMG C 521



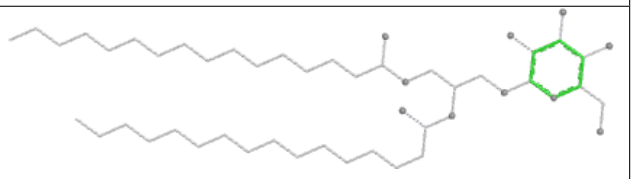
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Bond angles

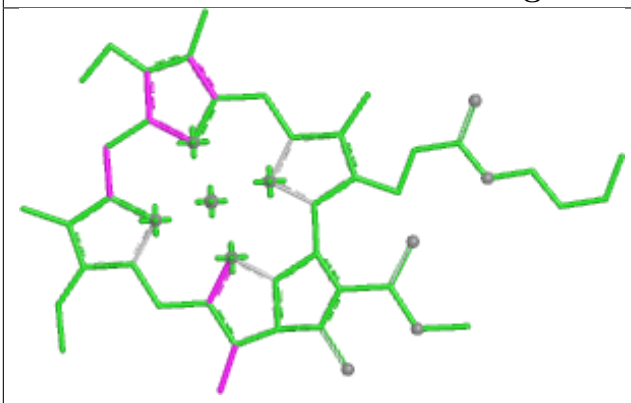


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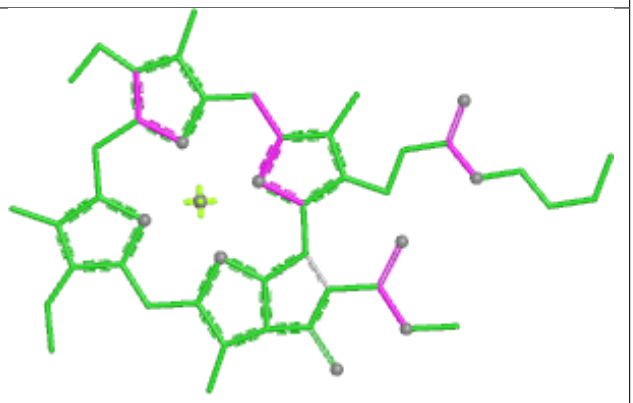


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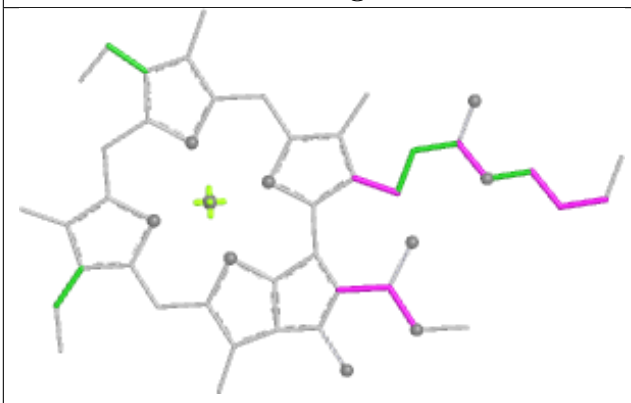
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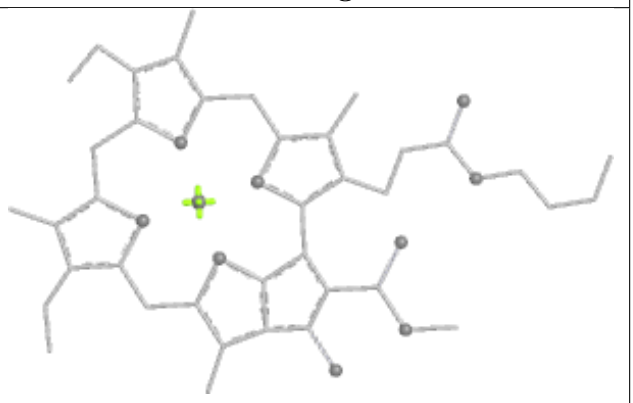
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Bond angles

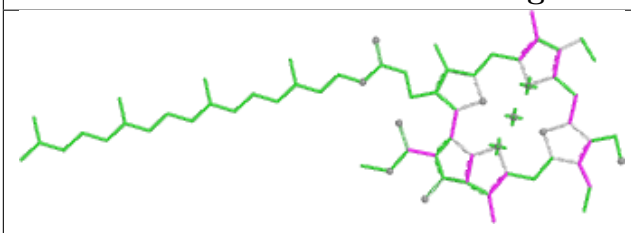


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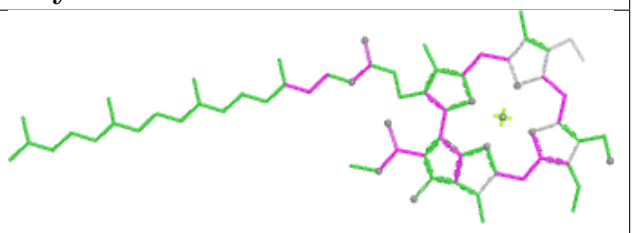


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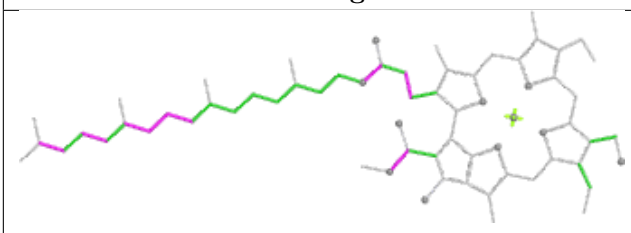
Ligand CHL y 303



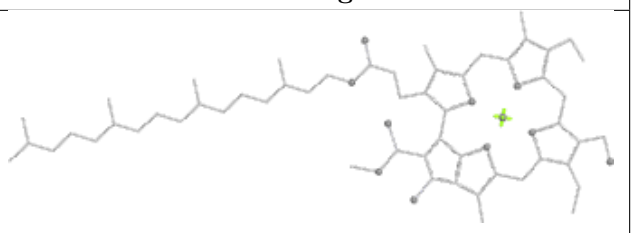
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Bond angles

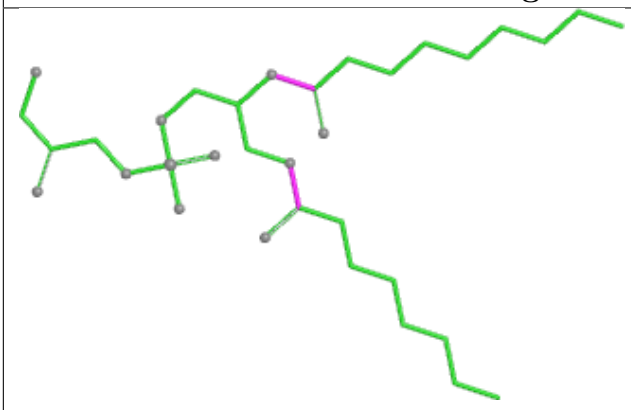


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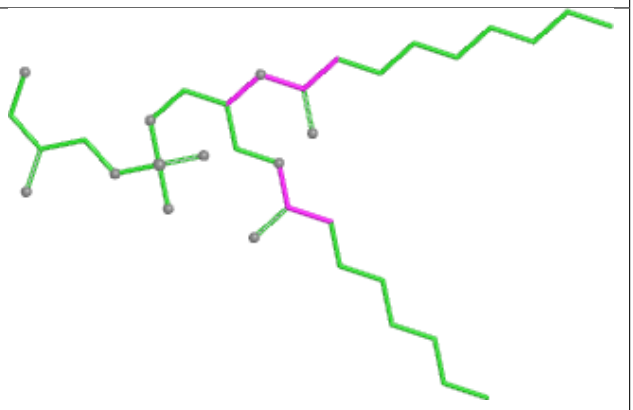


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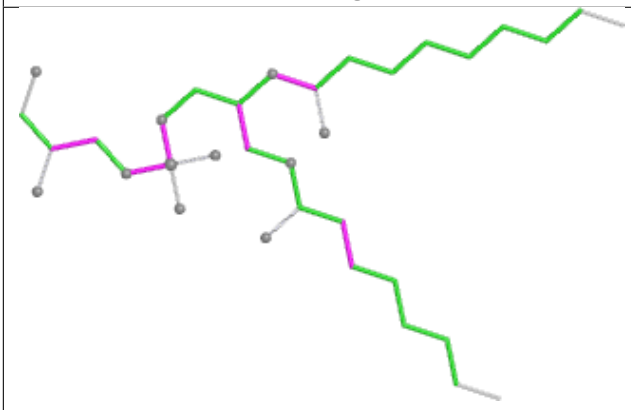
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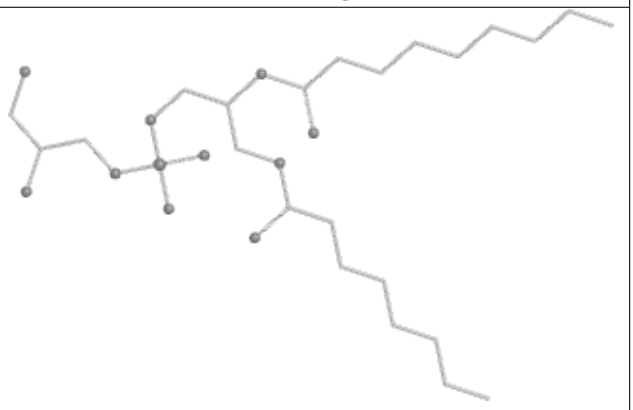
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Bond angles



Torsions

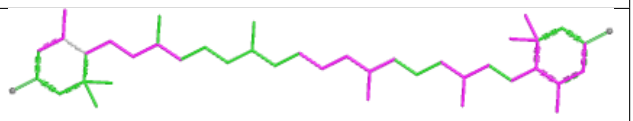


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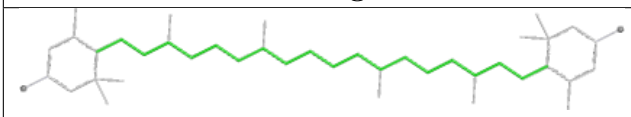
Ligand LUT Ss 615



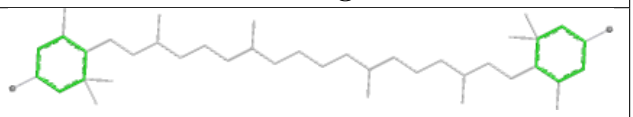
Bond lengths



Bond angles

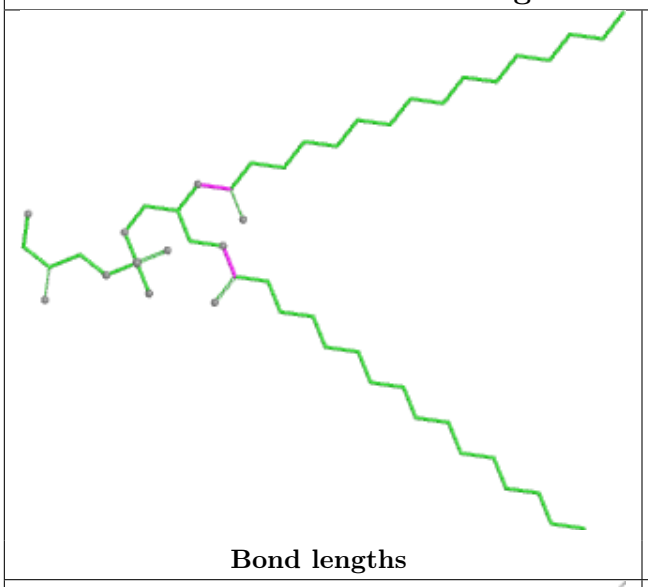


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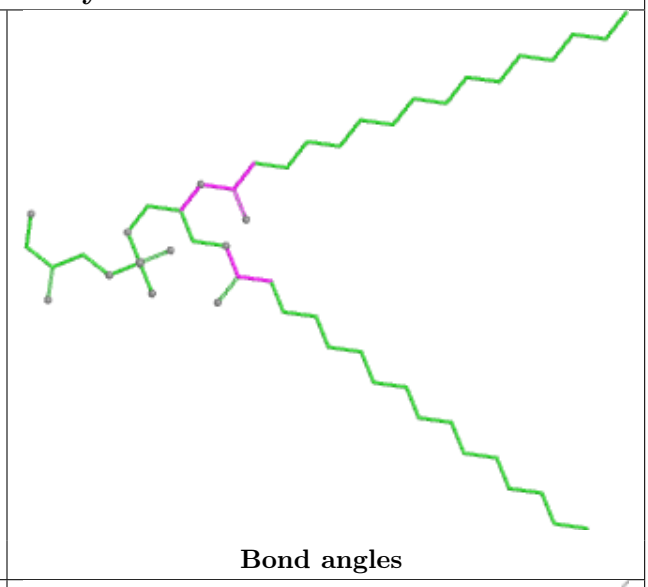


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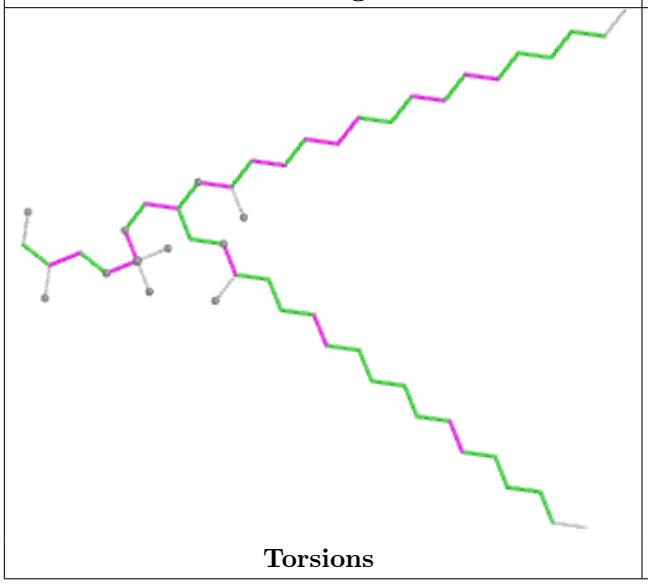
Ligand LHG Yy 618



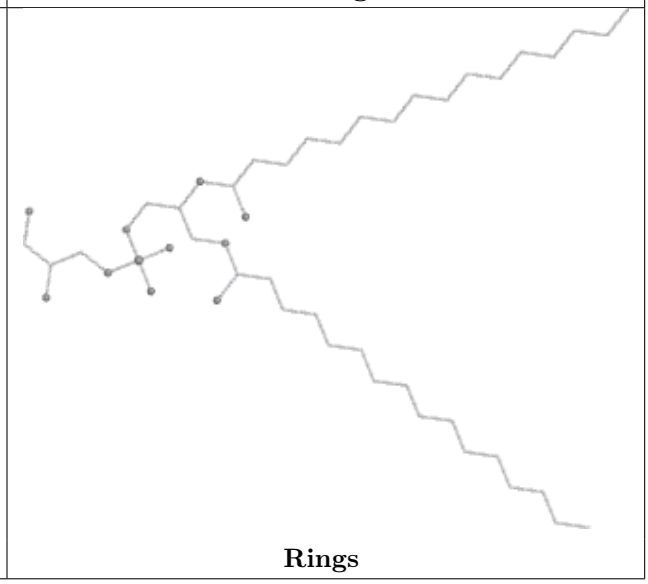
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Bond angles

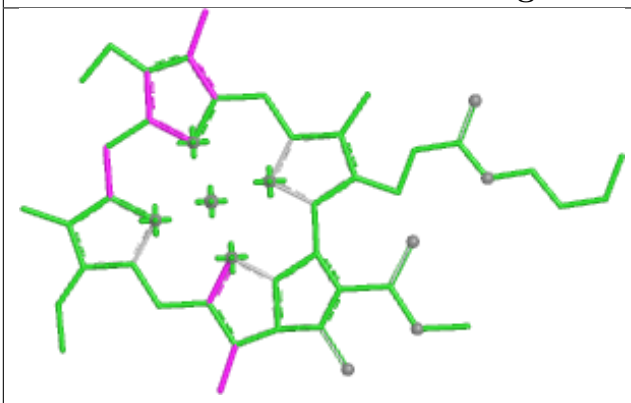


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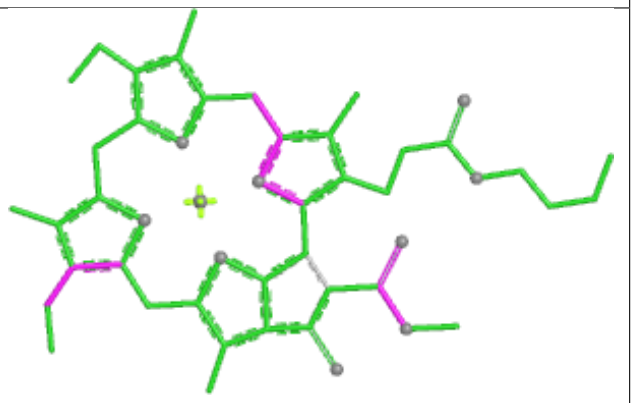


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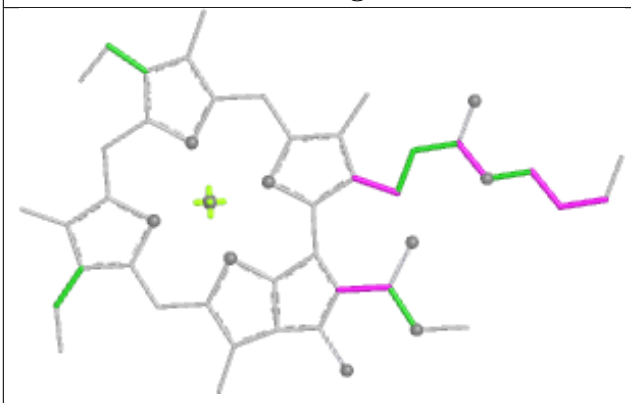
Ligand CLA SS 305



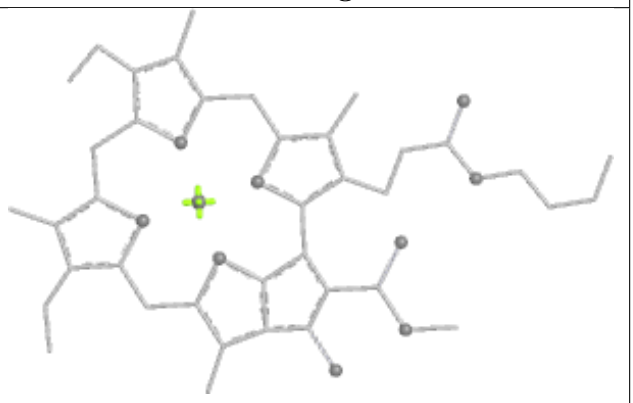
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Bond angles

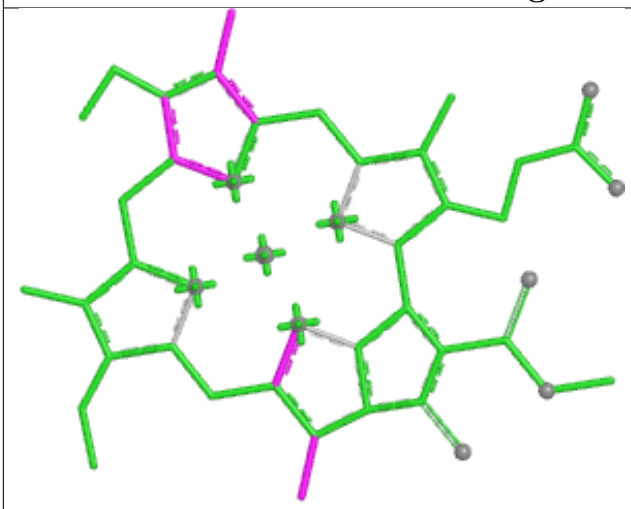


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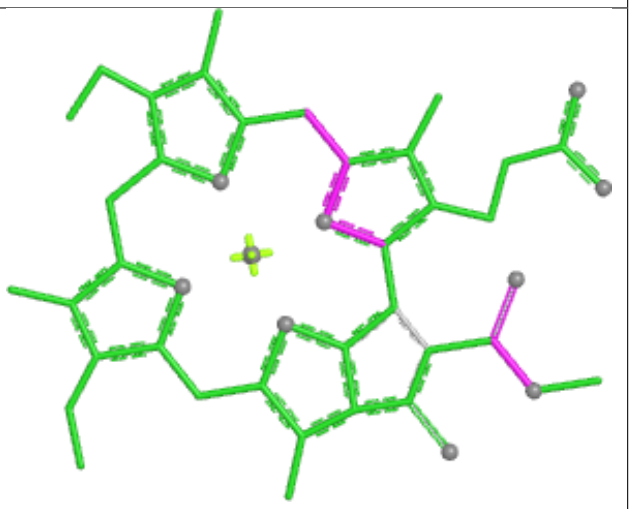


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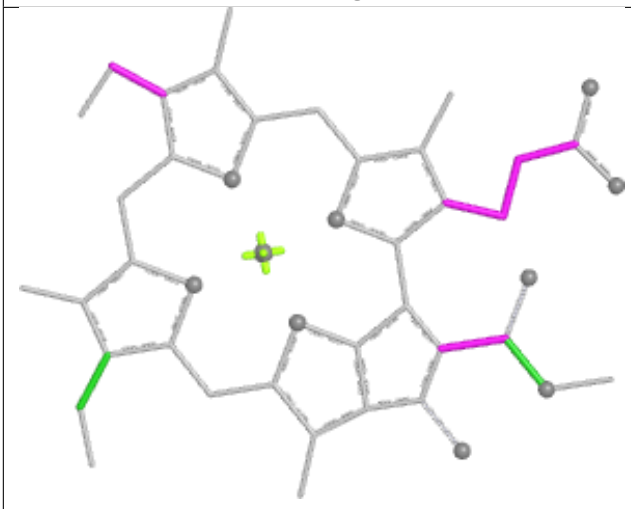
Ligand CLA 4 312



Bond lengths



Bond angles

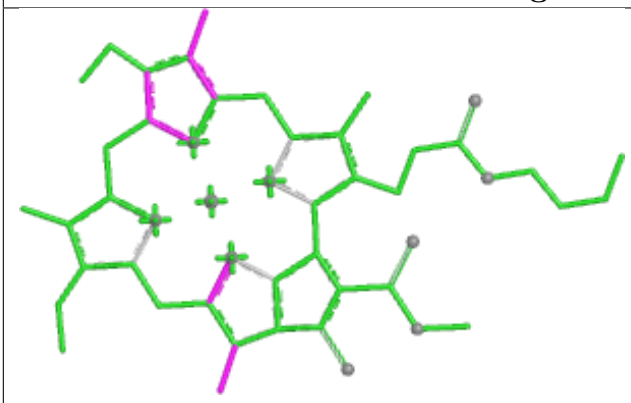


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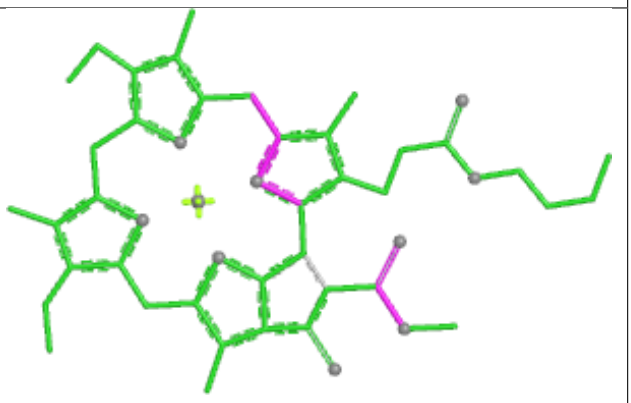


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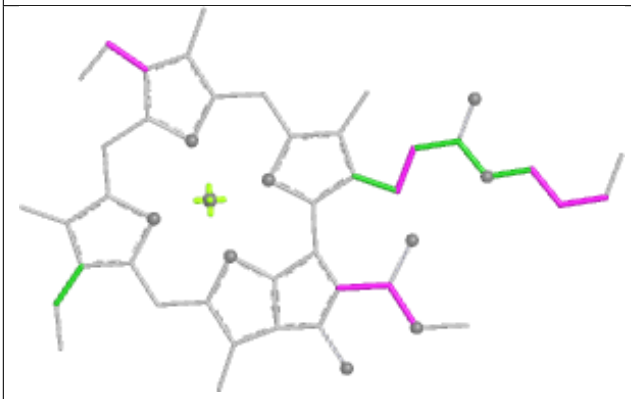
Ligand CLA s 610



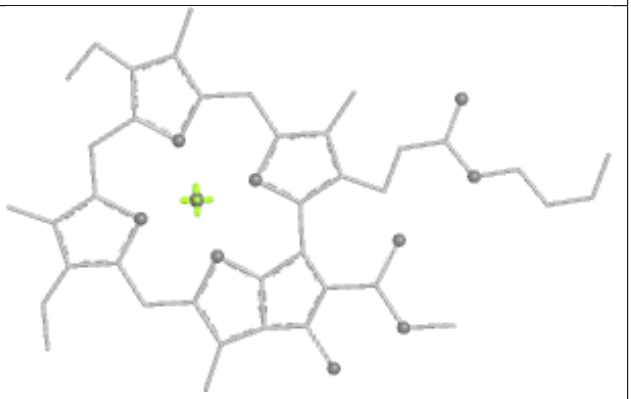
Bond lengths



Bond angles



Torsions

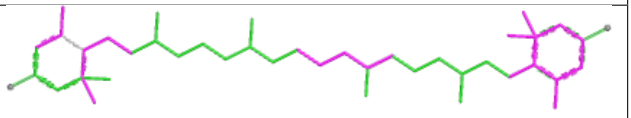


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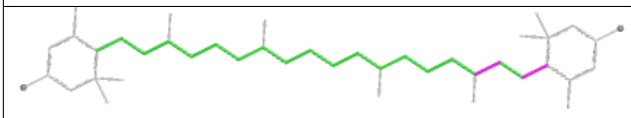
Ligand LUT Yy 615



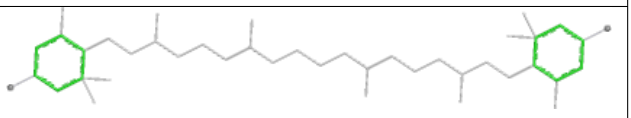
Bond lengths



Bond angles

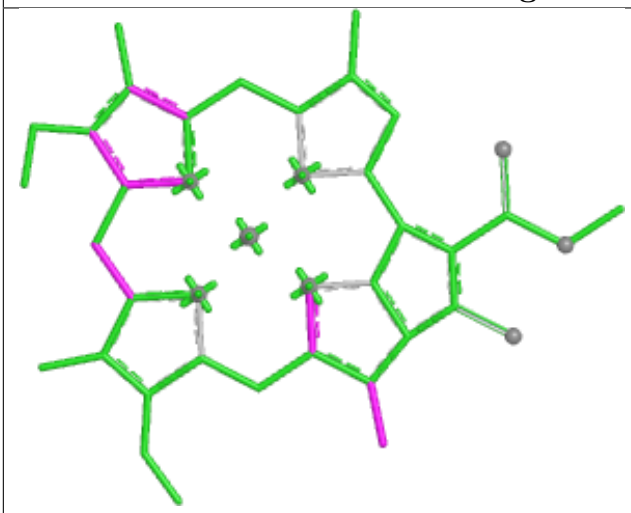


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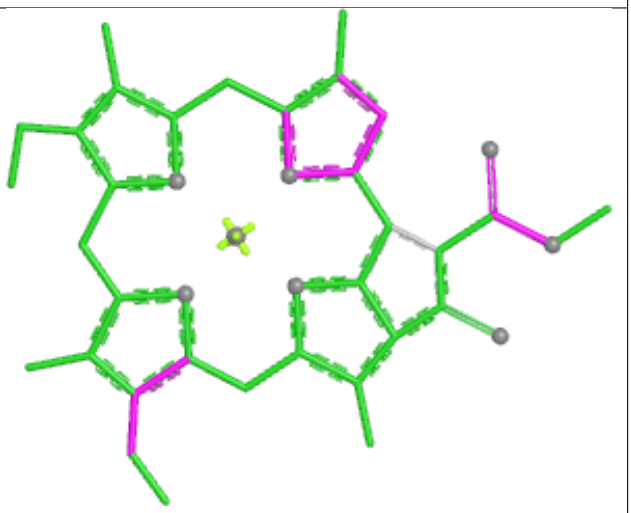


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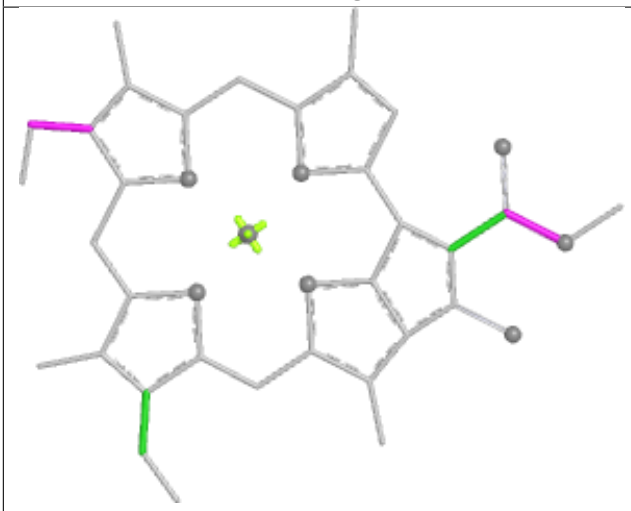
Ligand CLA 11 609



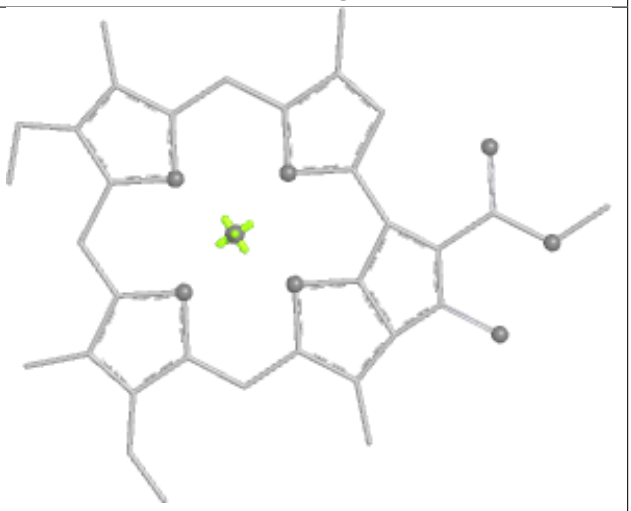
Bond lengths



Bond angles

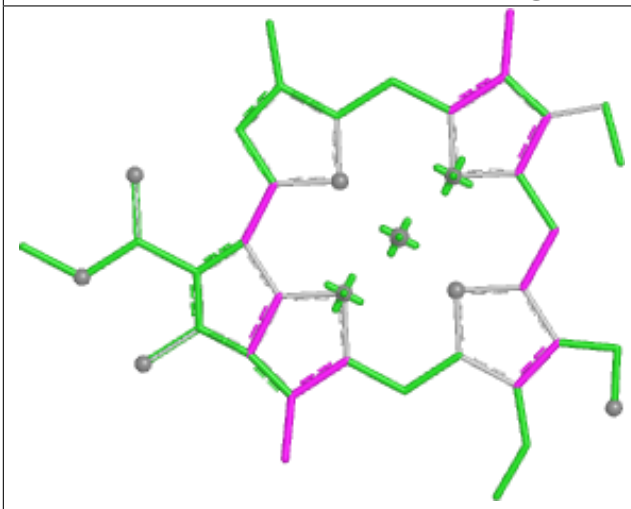


Torsions



Rings

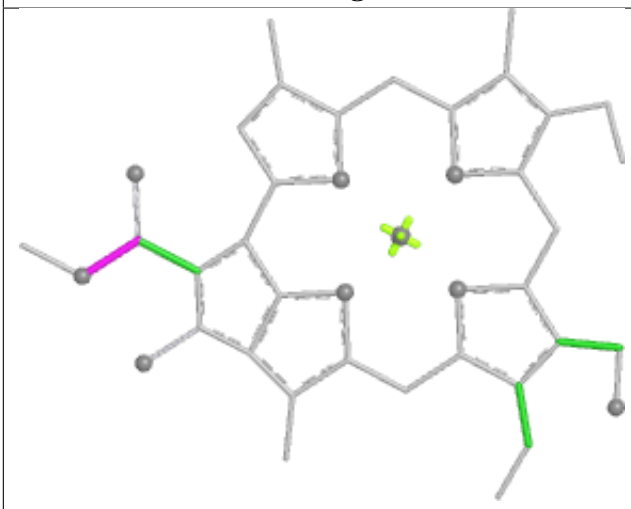
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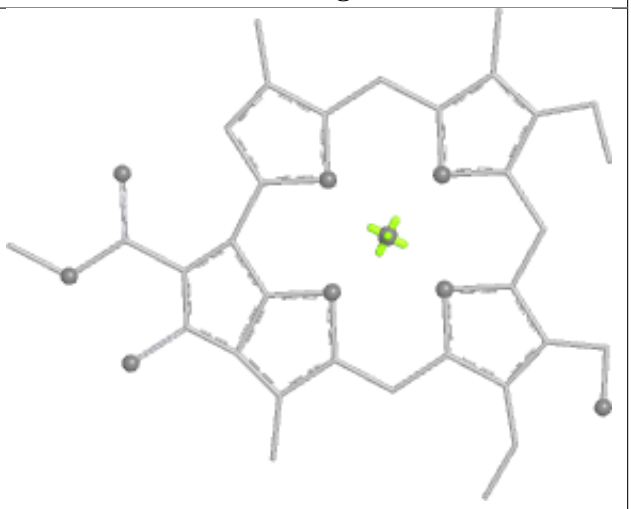
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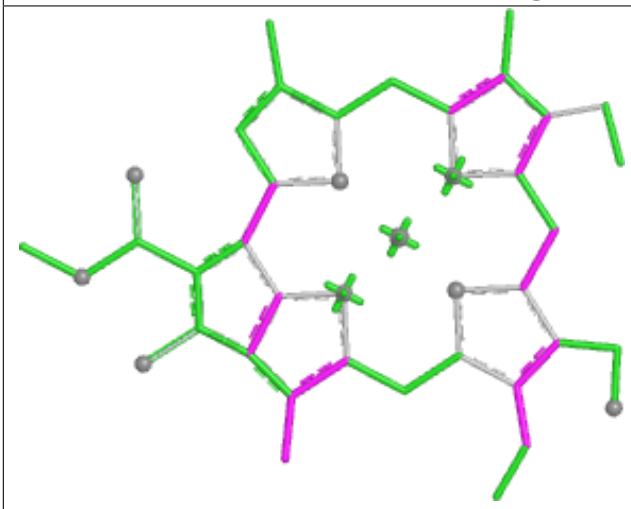


Torsions



Rings

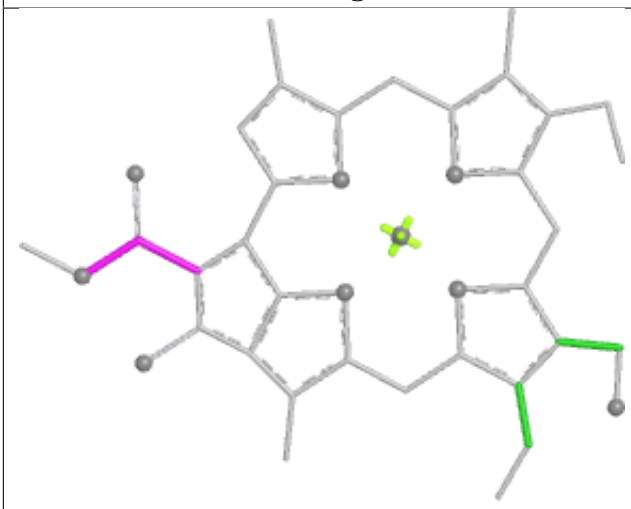
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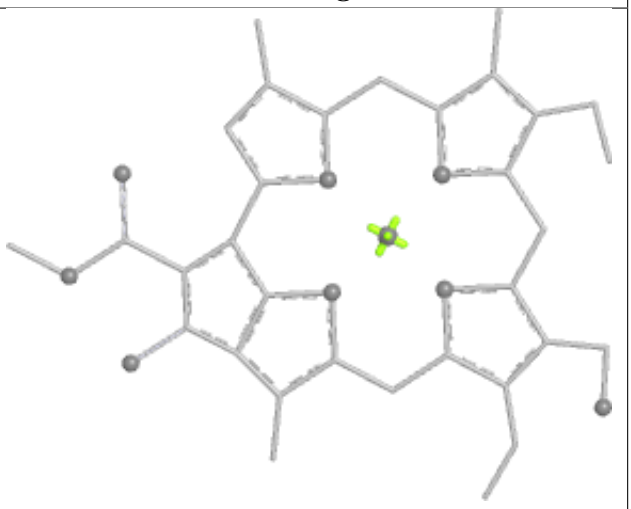
Bond lengths



Bond angles

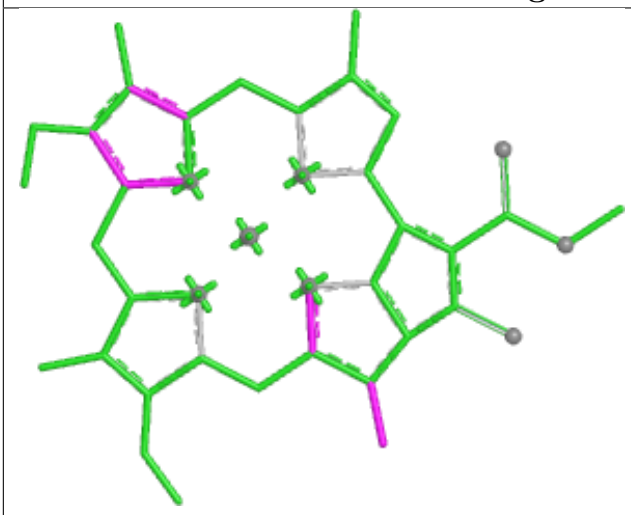


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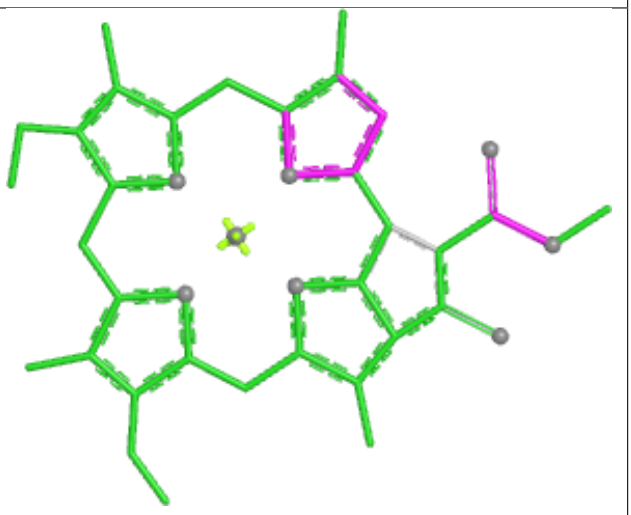


Rings

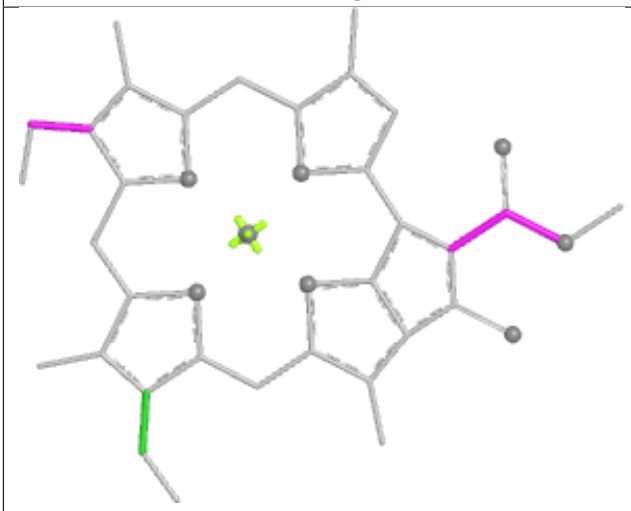
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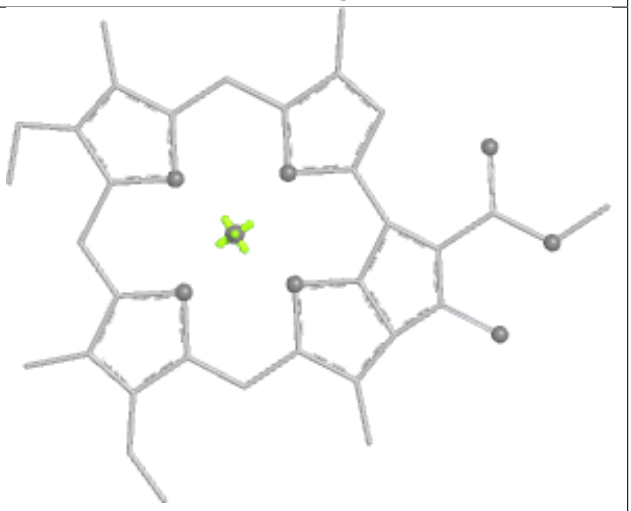
Bond lengths



Bond angles

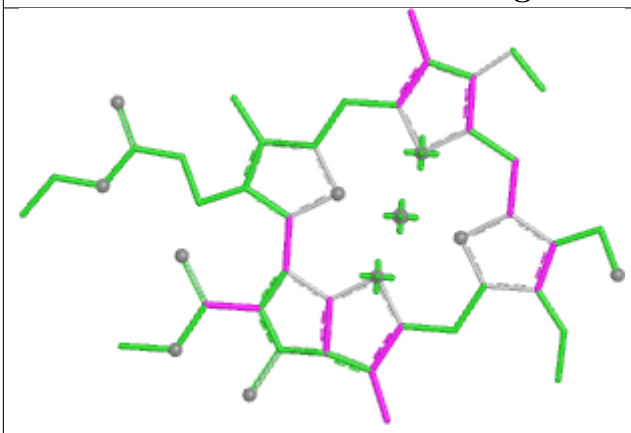


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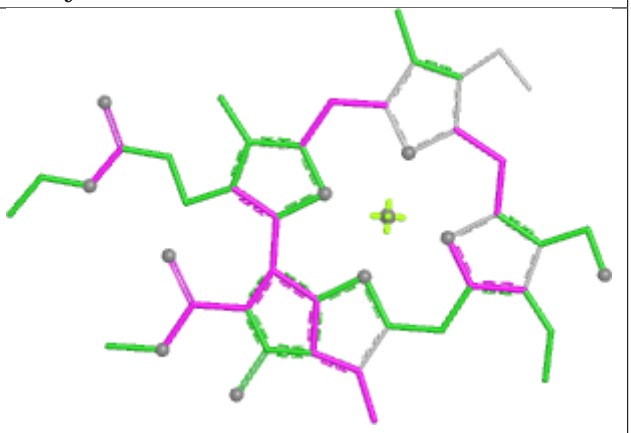


Rings

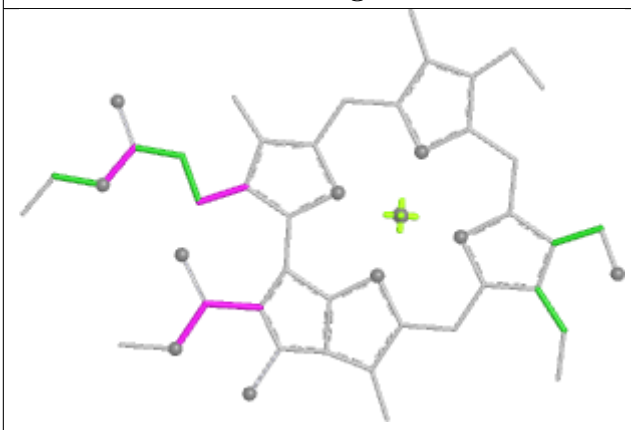
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Bond lengths



Bond angles

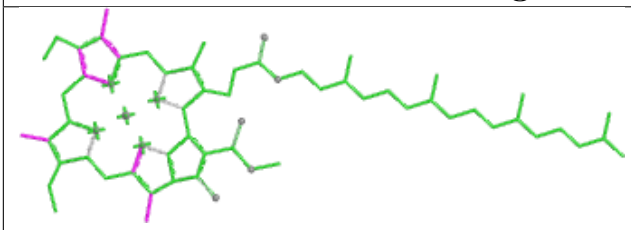


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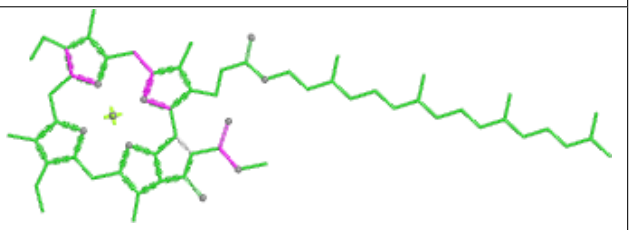


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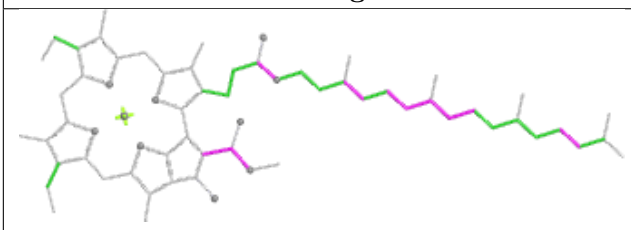
Ligand CLA CC 512



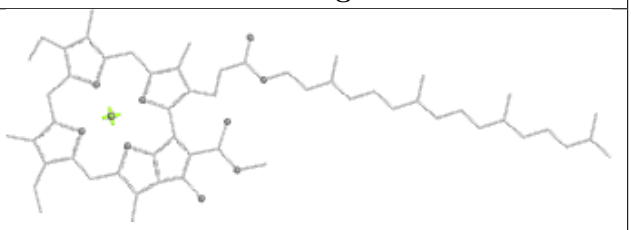
Bond lengths



Bond angles

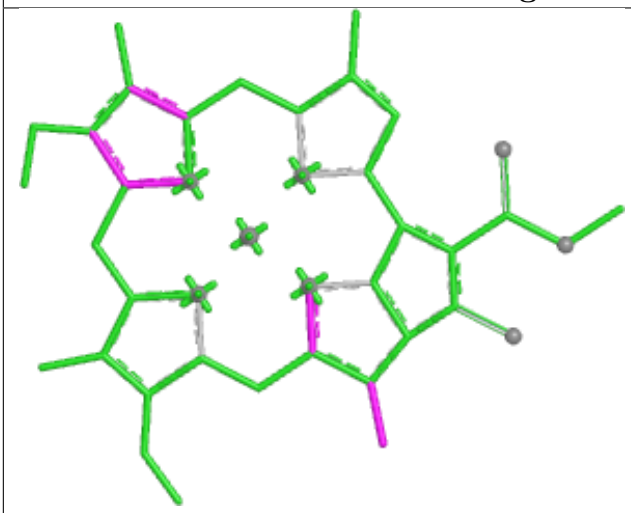


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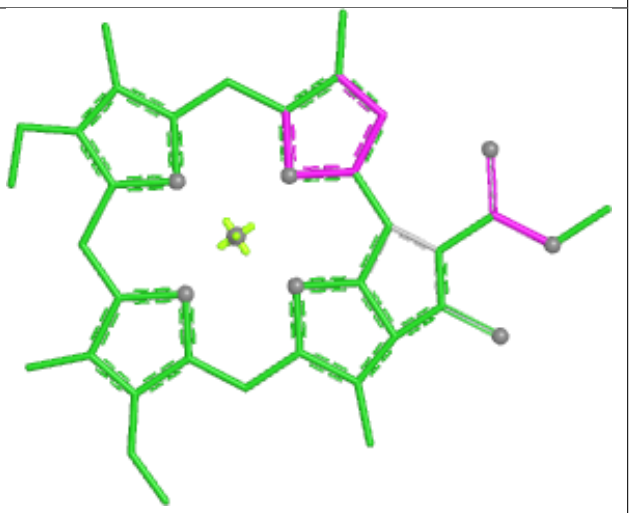


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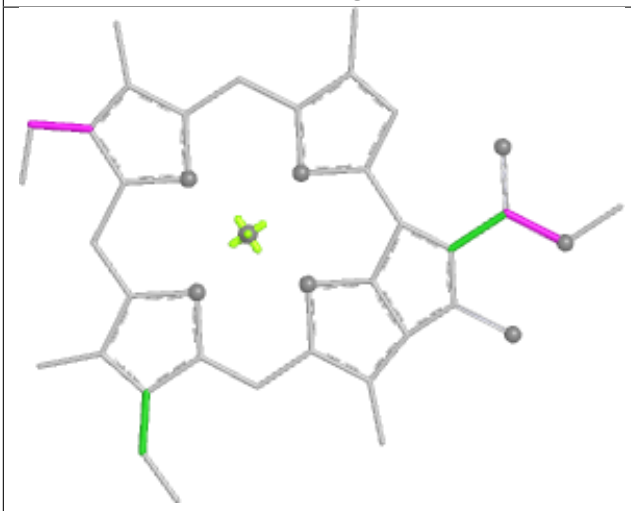
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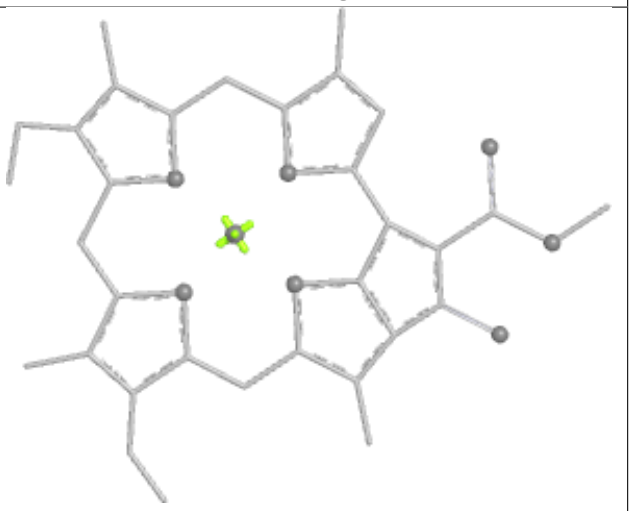
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Bond angles

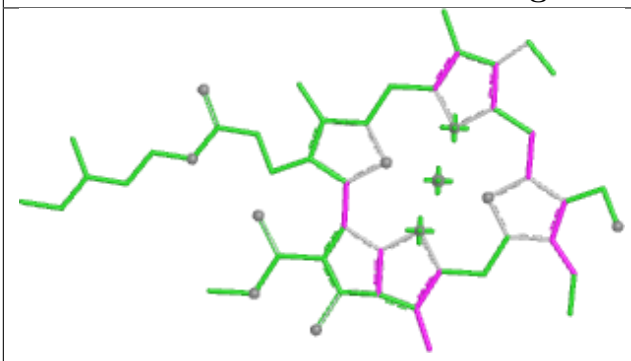


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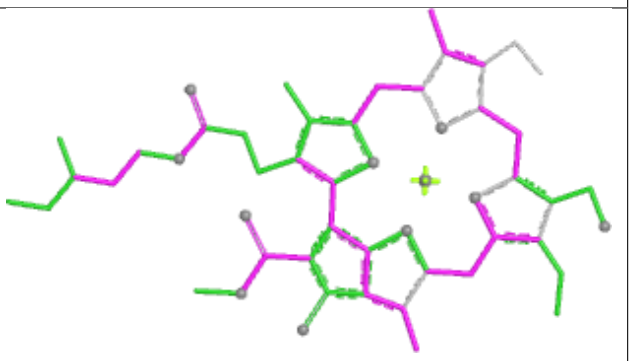


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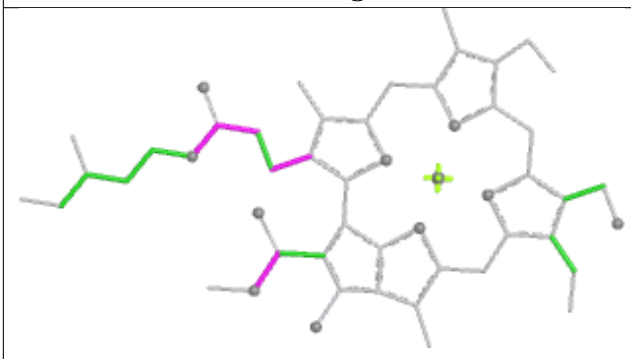
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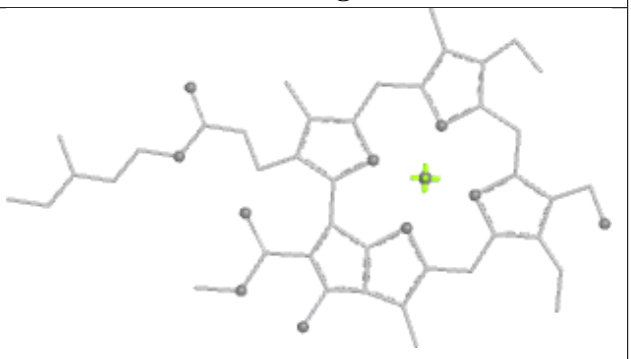
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Bond angles

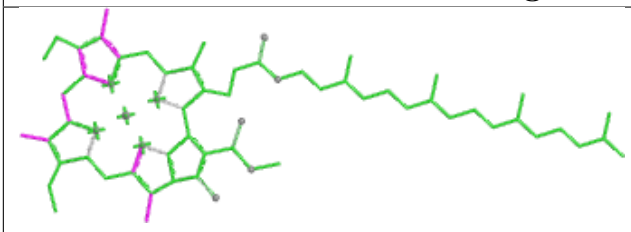


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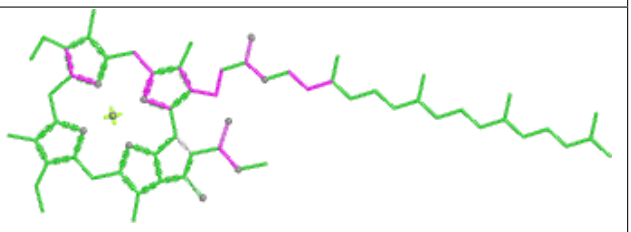


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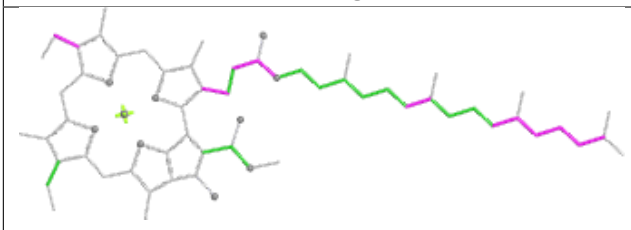
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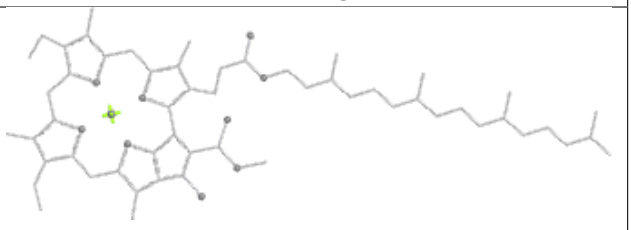
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Bond angles

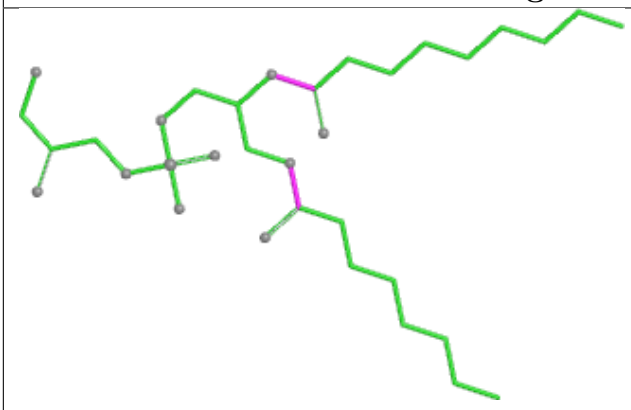


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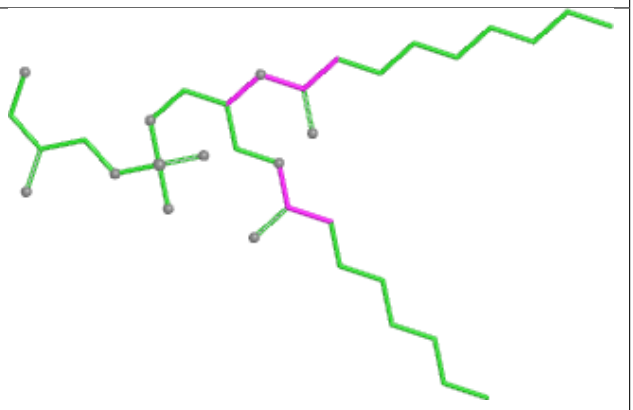


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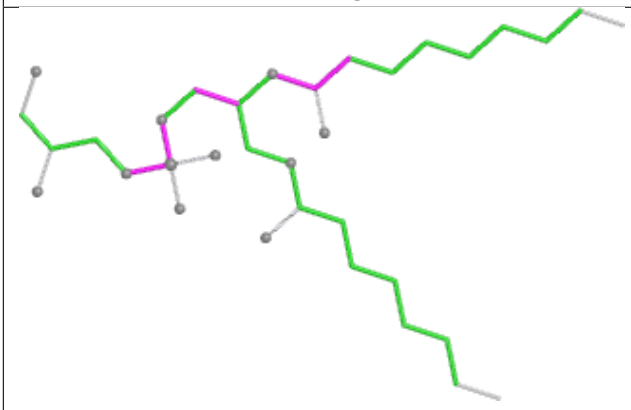
Ligand LHG 3 614



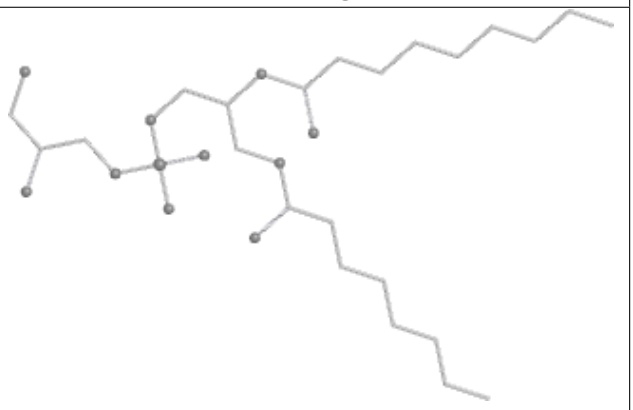
Bond lengths



Bond angles

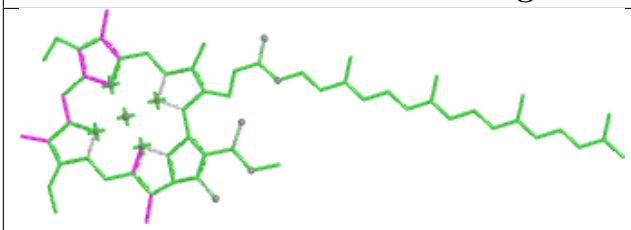


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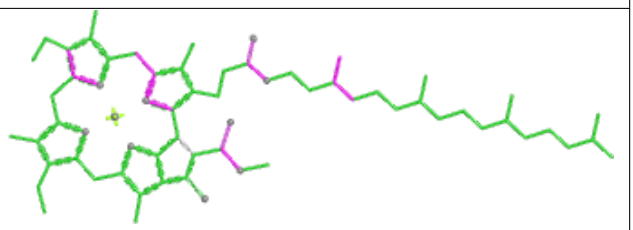


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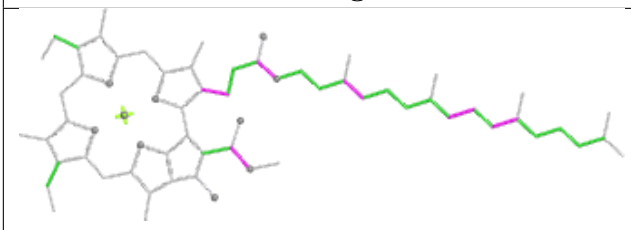
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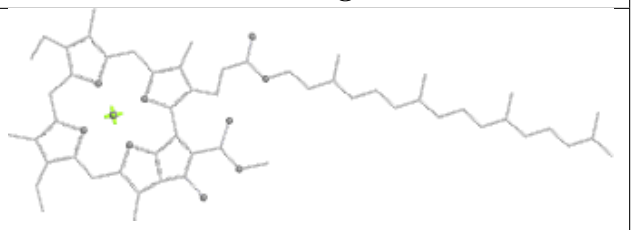
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Bond angles

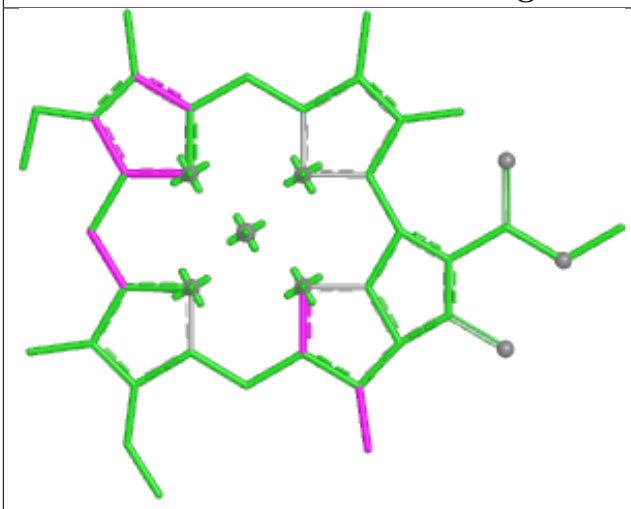


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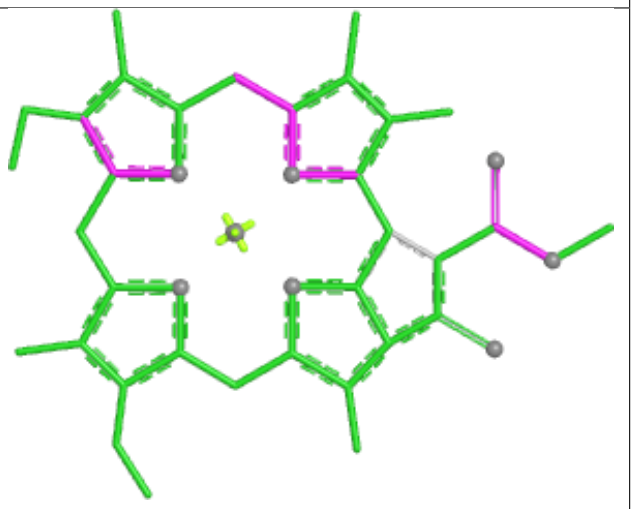


Rings

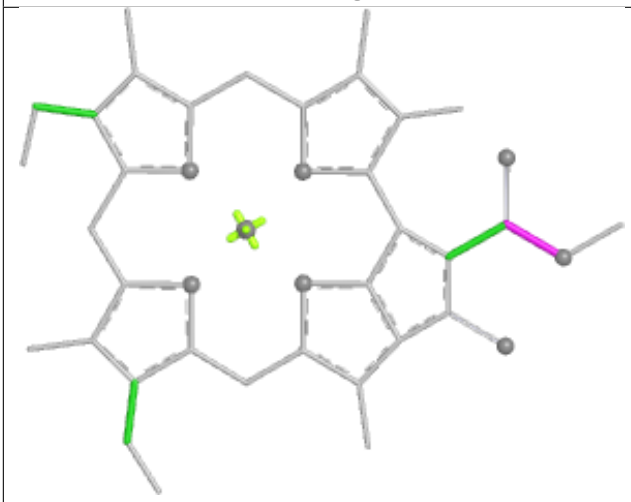
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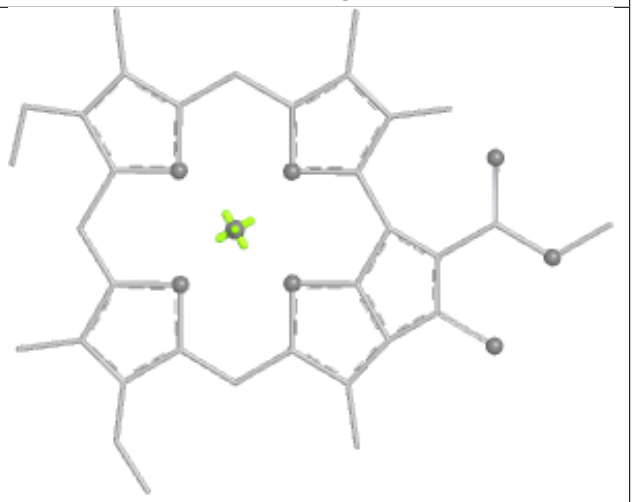
Bond lengths



Bond angles

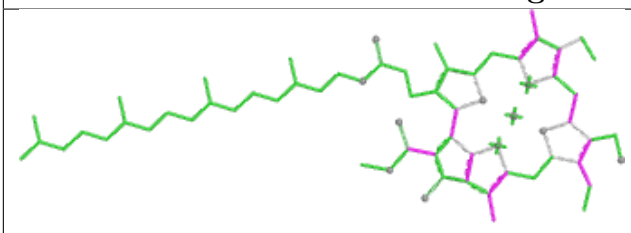


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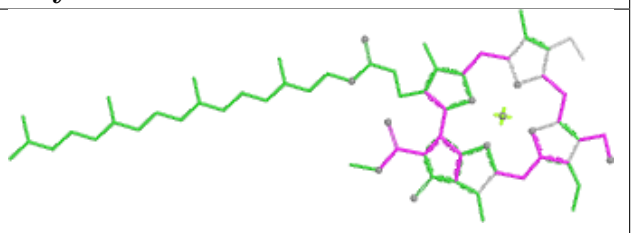


Rings

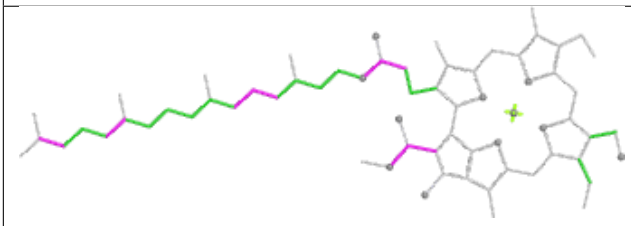
Ligand CHL y 311



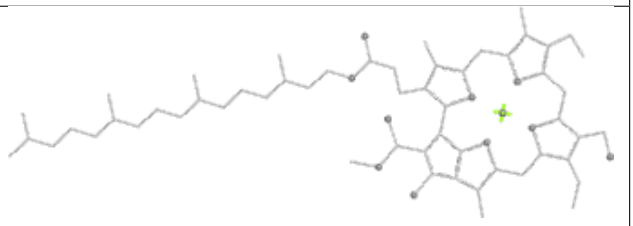
Bond lengths



Bond angles

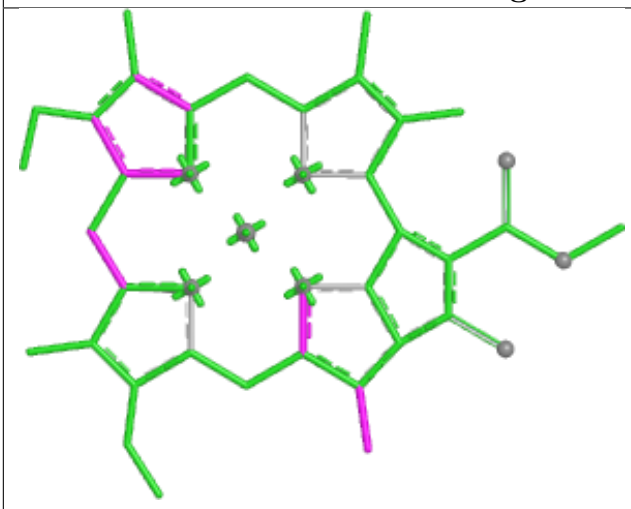


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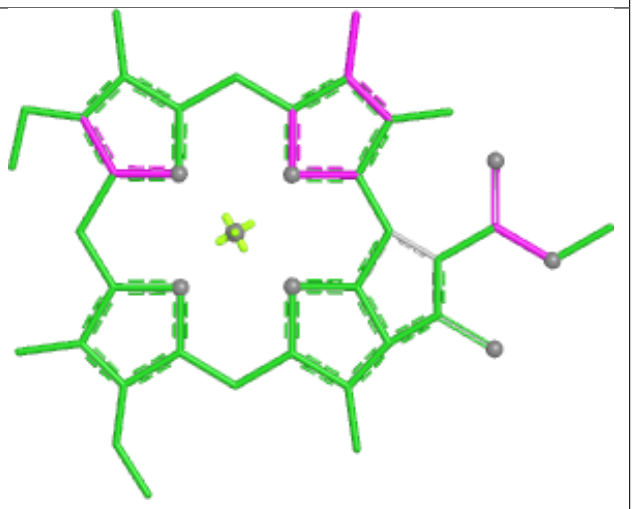


Rings

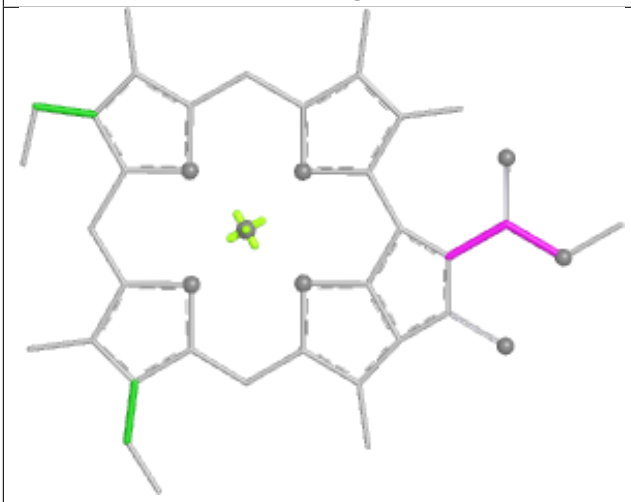
Ligand CLA XX 201



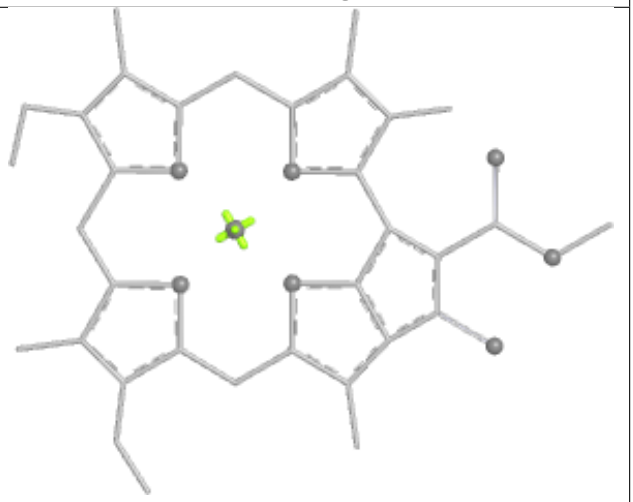
Bond lengths



Bond angles



Torsions

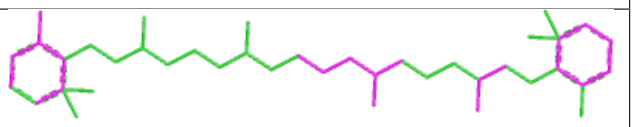


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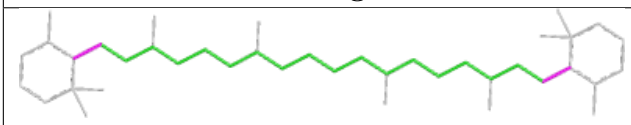
Ligand BCR Bb 618



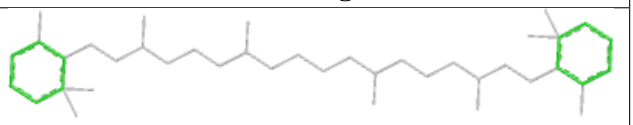
Bond lengths



Bond angles



Torsions

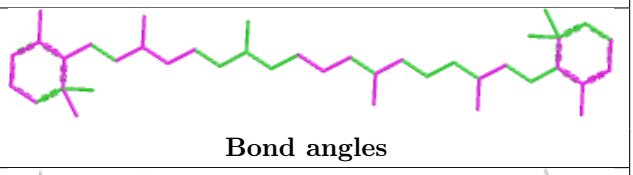


Rings

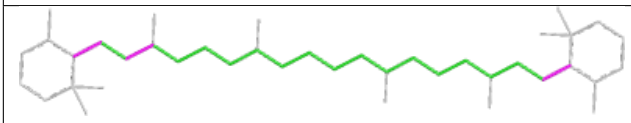
Ligand BCR CC 515



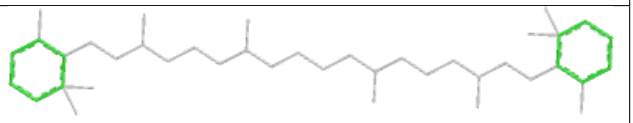
Bond lengths



Bond angles

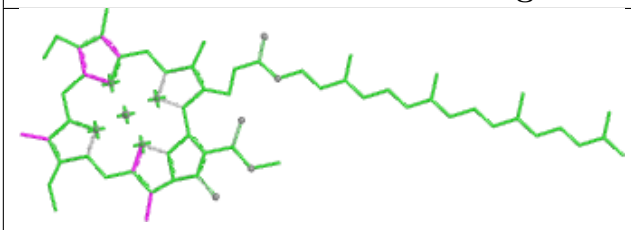


Torsions

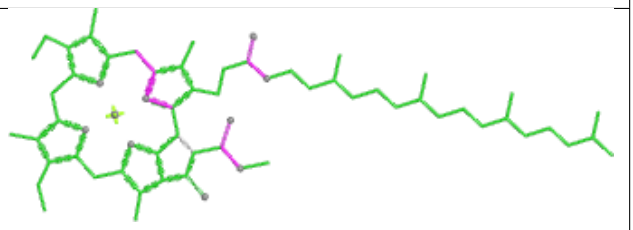


Rings

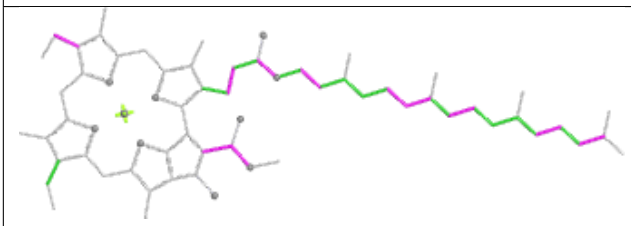
Ligand CLA Cc 503



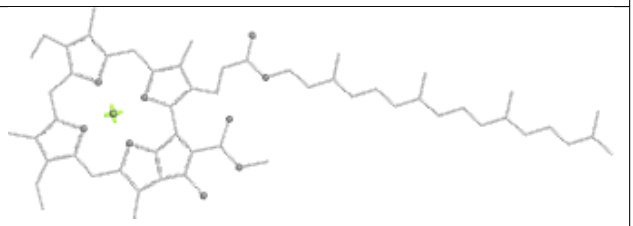
Bond lengths



Bond angles



Torsions

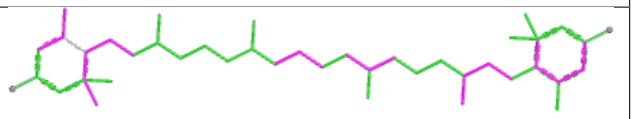


Rings

Ligand LUT n 616



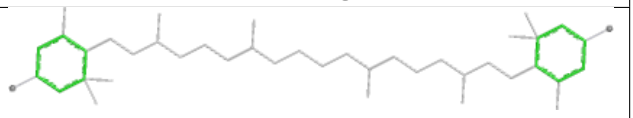
Bond lengths



Bond angles

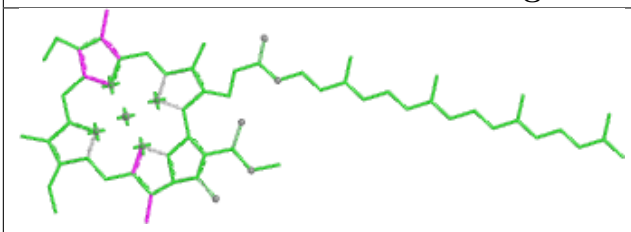


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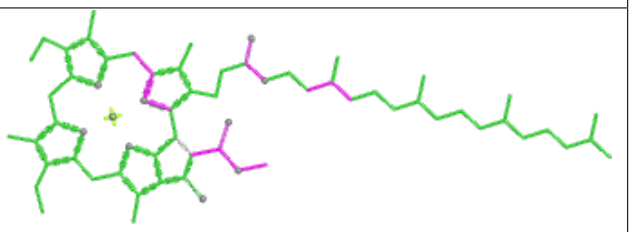


Rings

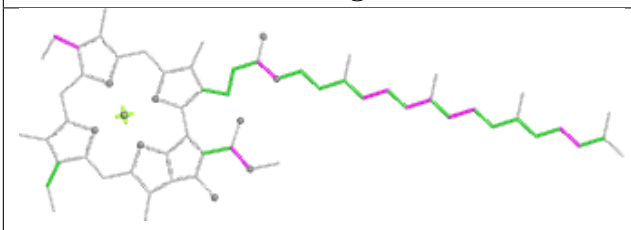
Ligand CLA Y 612



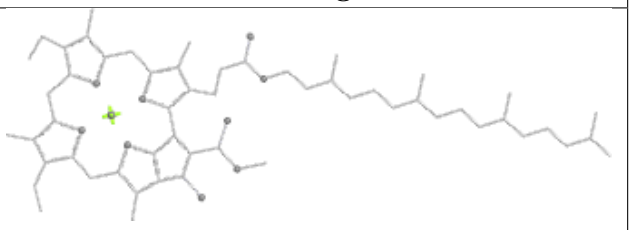
Bond lengths



Bond angles

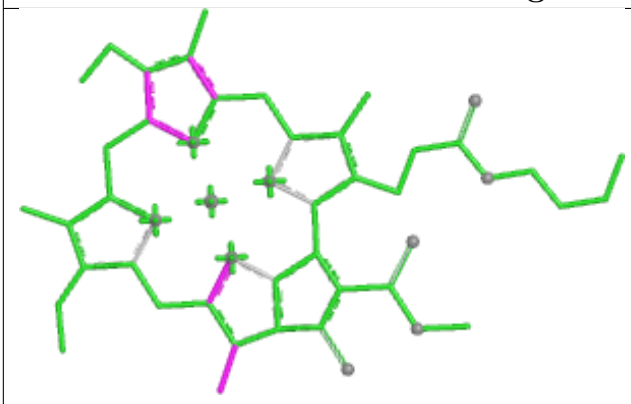


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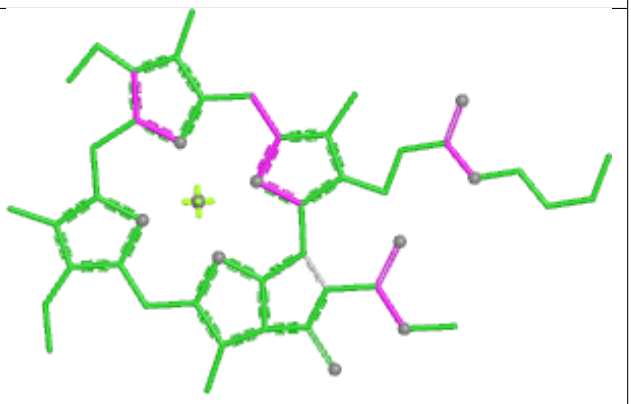


Rings

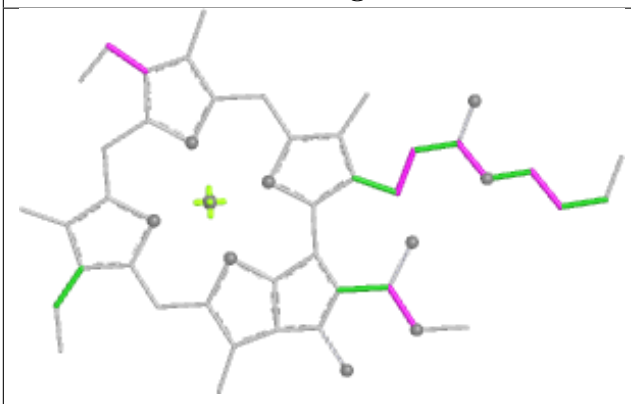
Ligand CLA S 612



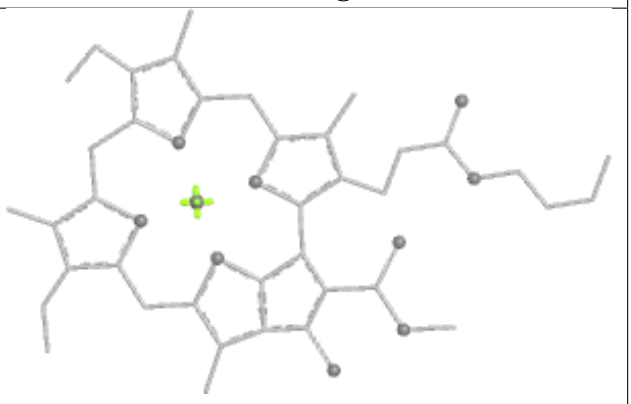
Bond lengths



Bond angles

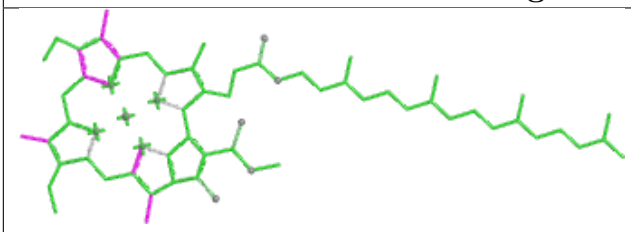


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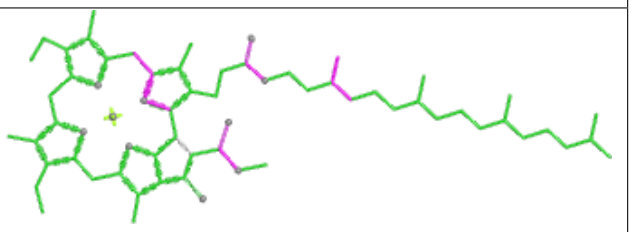


Rings

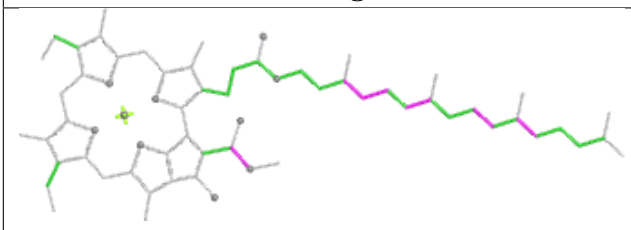
Ligand CLA b 604



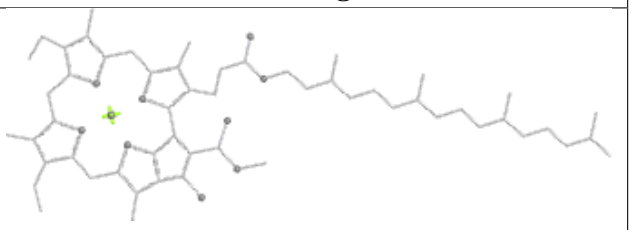
Bond lengths



Bond angles

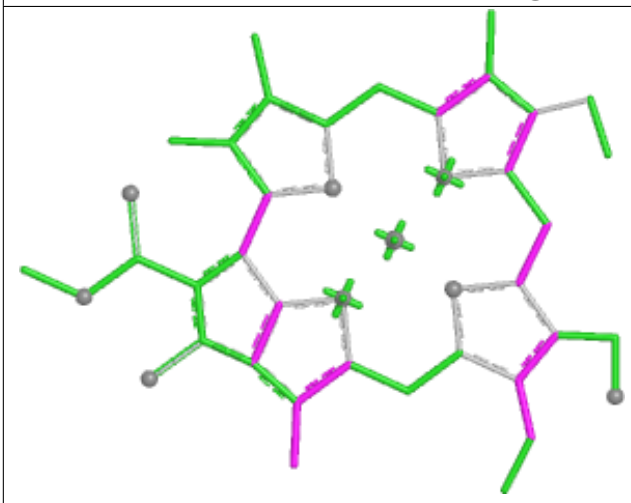


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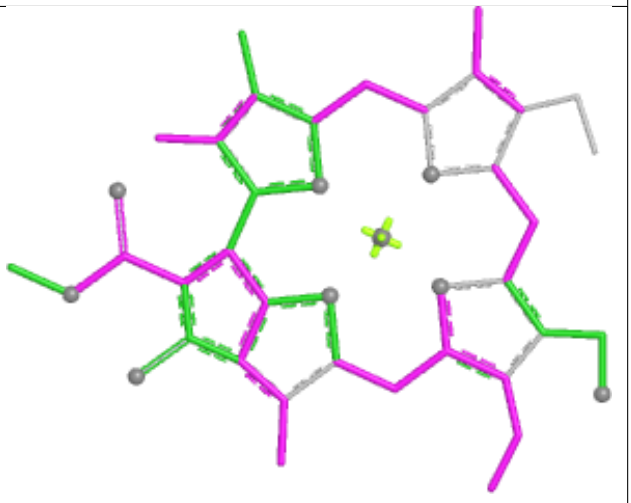


Rings

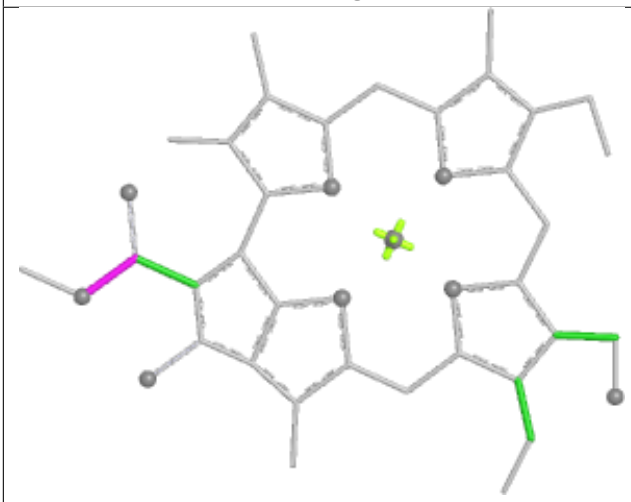
Ligand CHL S 605



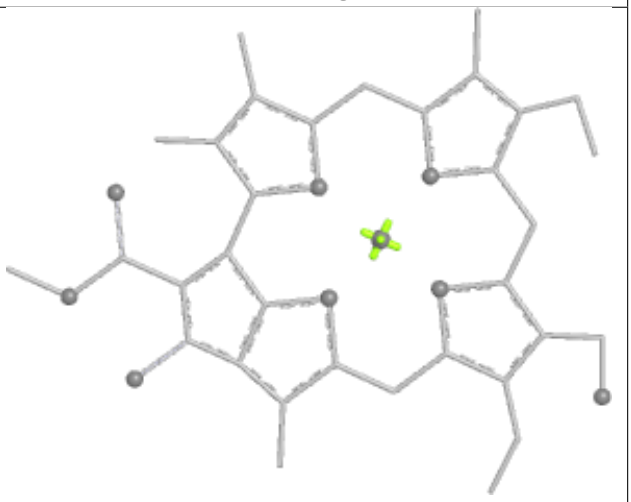
Bond lengths



Bond angles

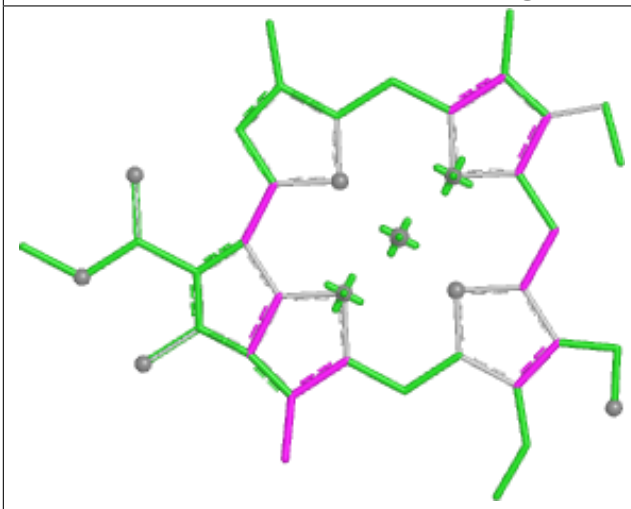


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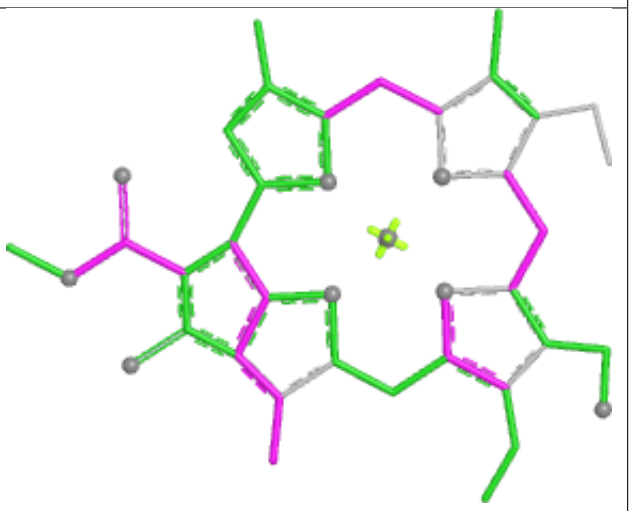


Rings

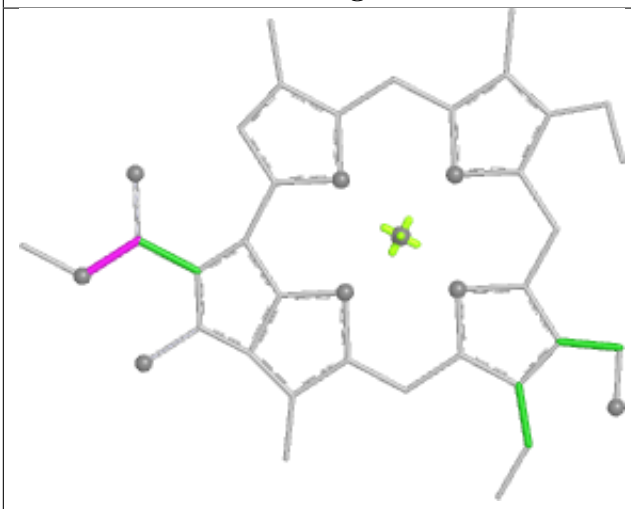
Ligand CHL 11 601



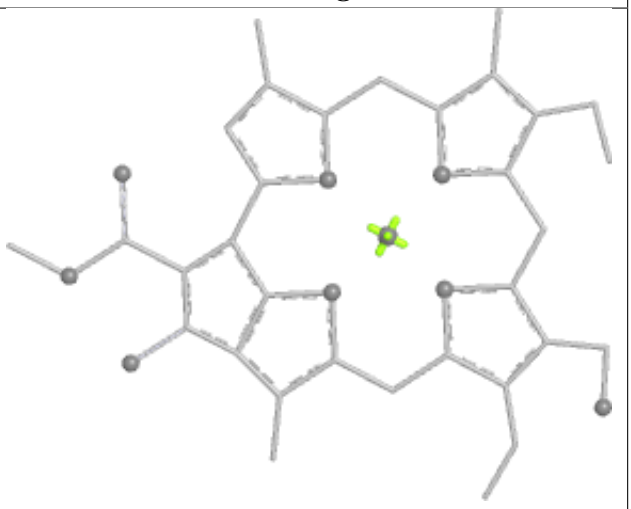
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Bond angles

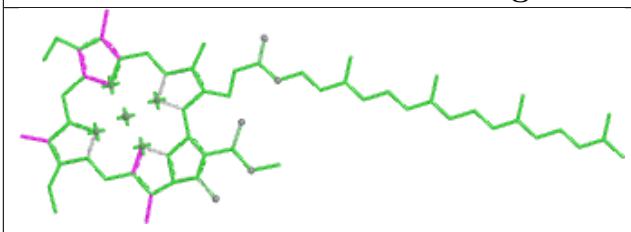


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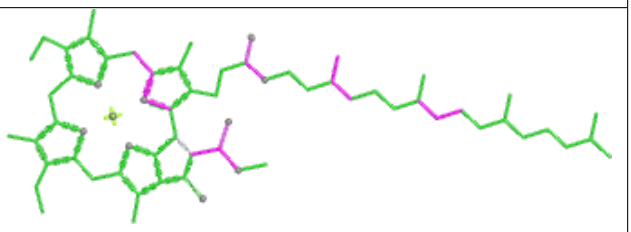


Rings

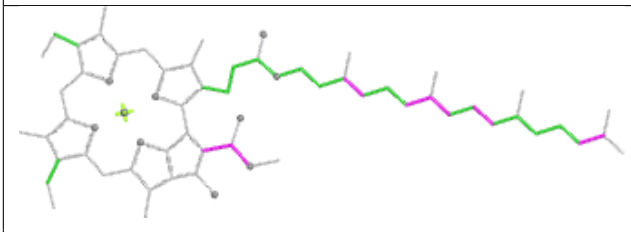
Ligand CLA BB 610



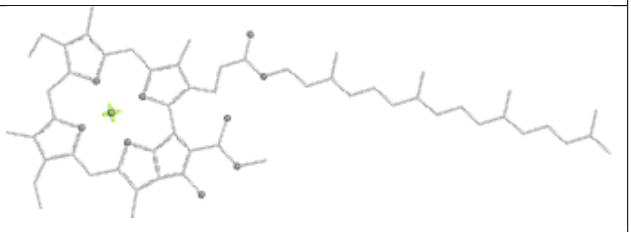
Bond lengths



Bond angles

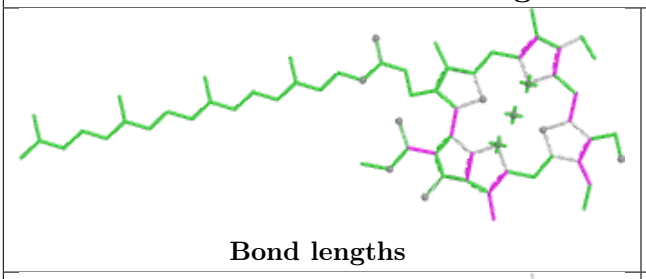


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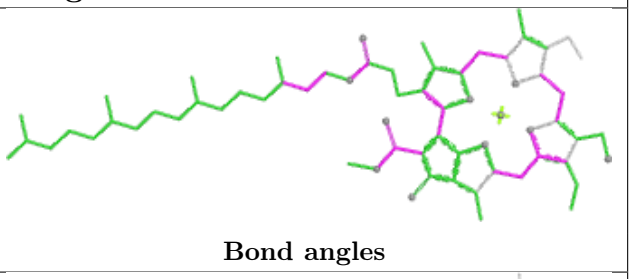


Rings

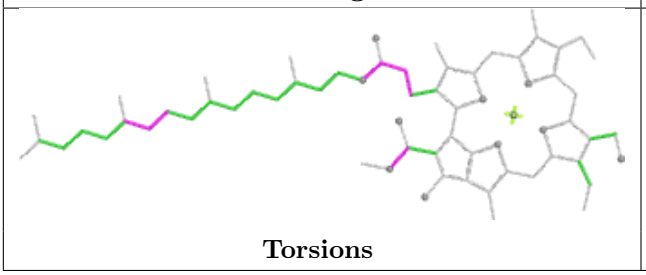
Ligand CHL Gg 302



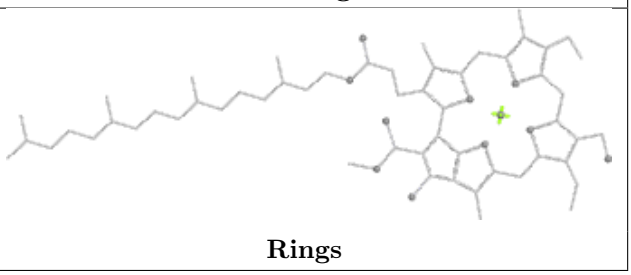
Bond lengths



Bond angles

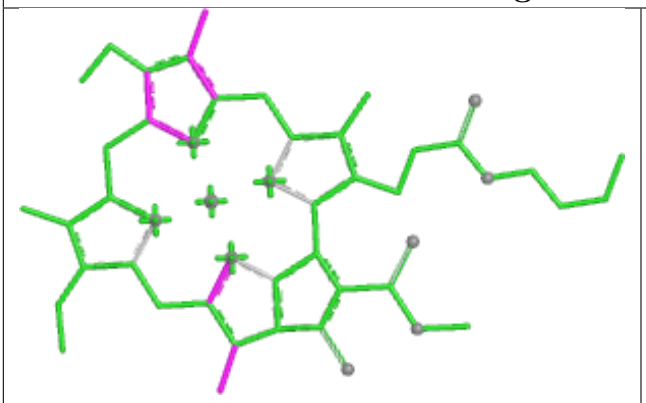


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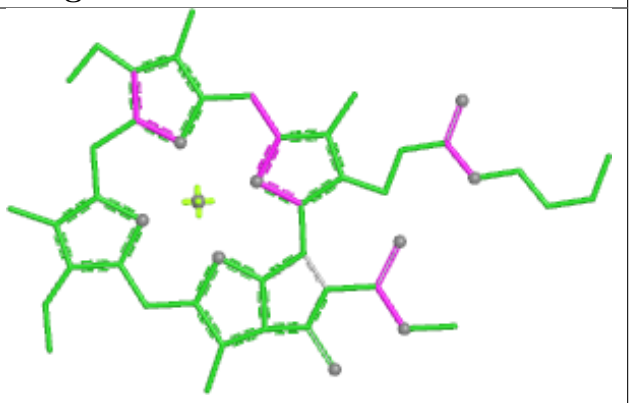


Rings

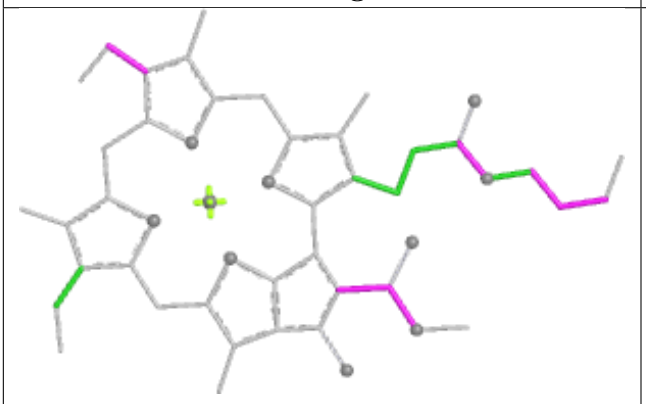
Ligand CLA Gg 315



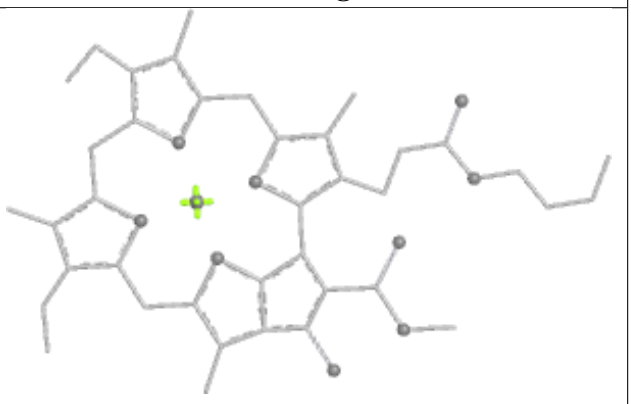
Bond lengths



Bond angles

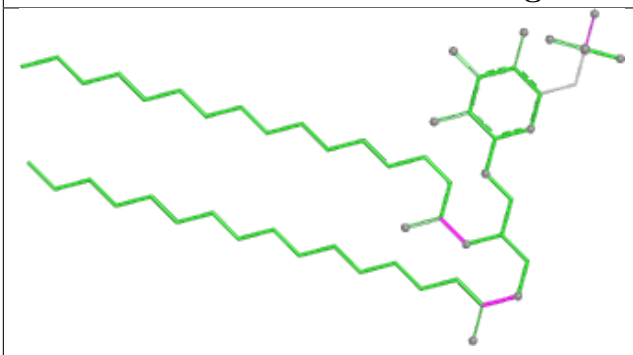


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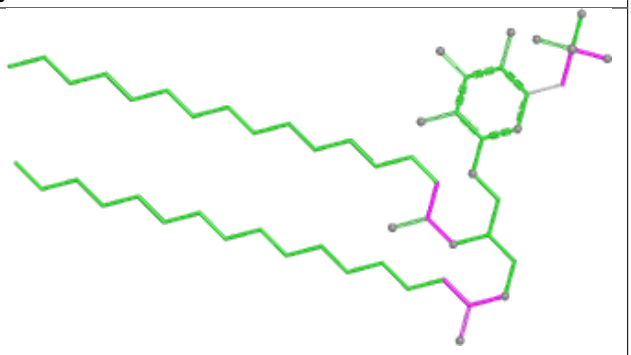


Rings

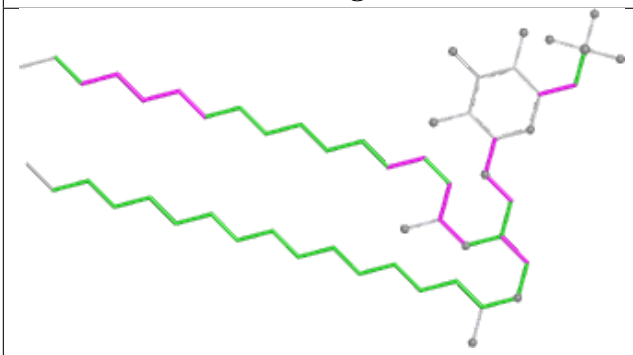
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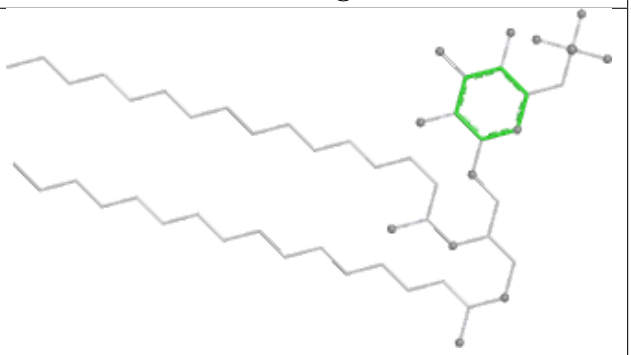
Bond lengths



Bond angles

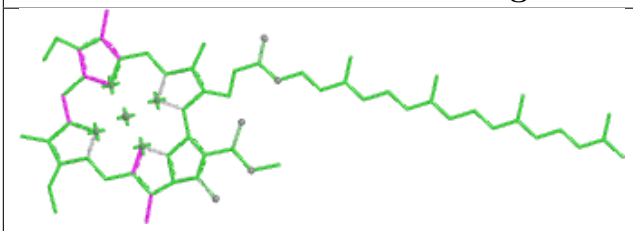


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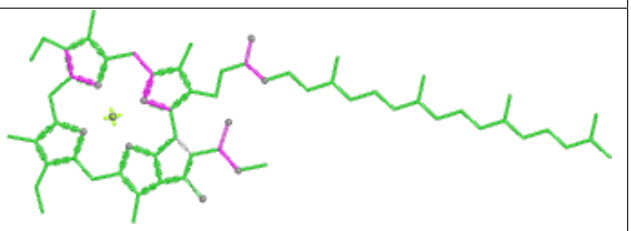


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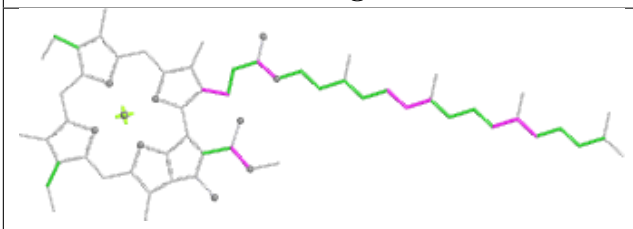
Ligand CLA YY 610



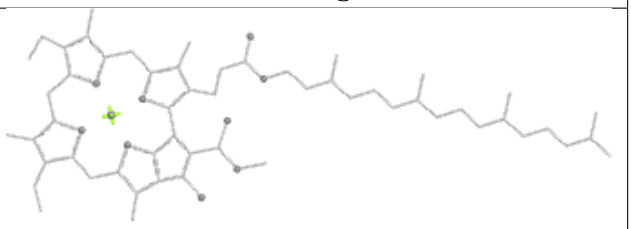
Bond lengths



Bond angles

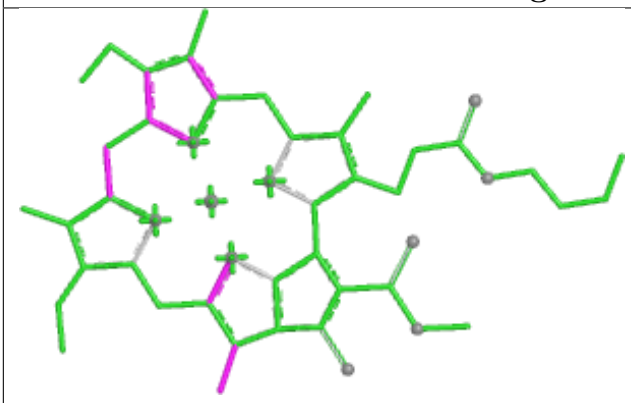


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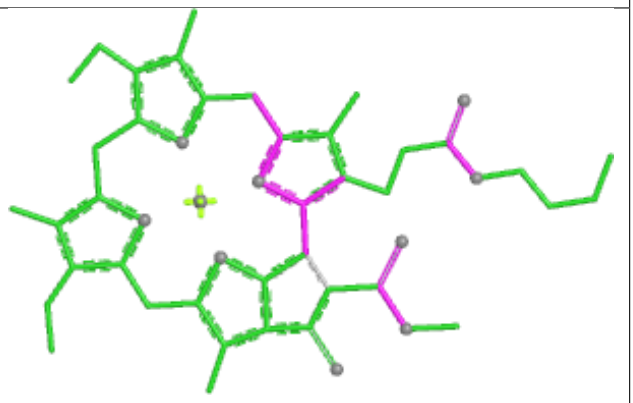


Rings

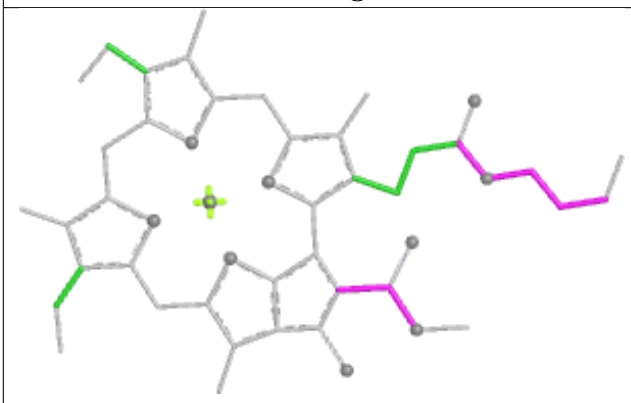
Ligand CLA s 611



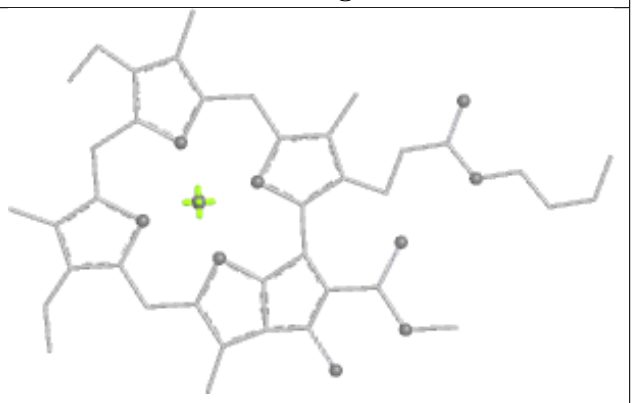
Bond lengths



Bond angles

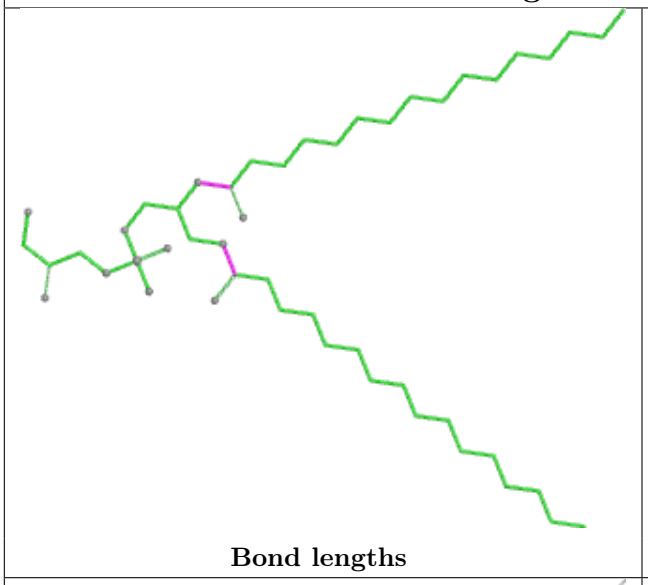


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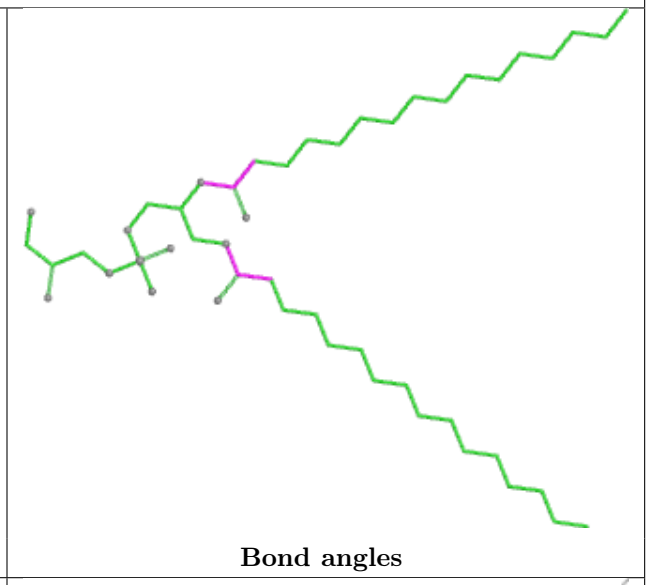


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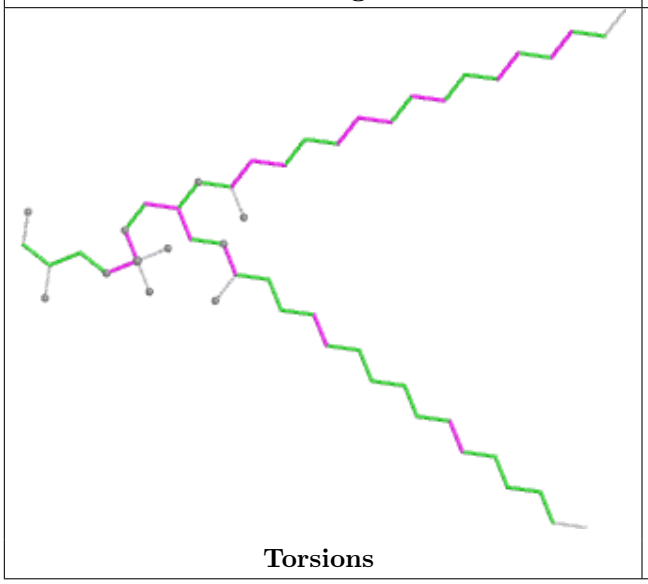
Ligand LHG Y 618



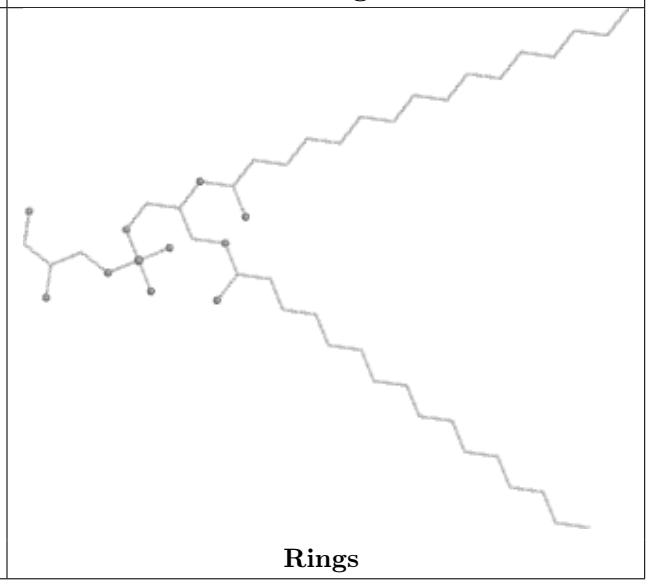
Bond lengths



Bond angles

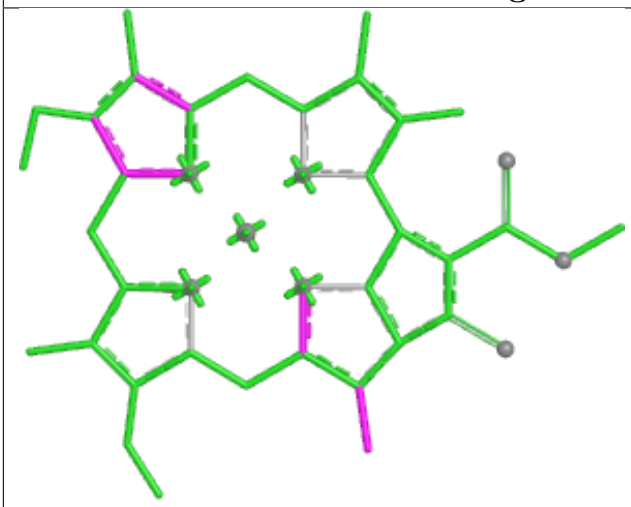


Torsions

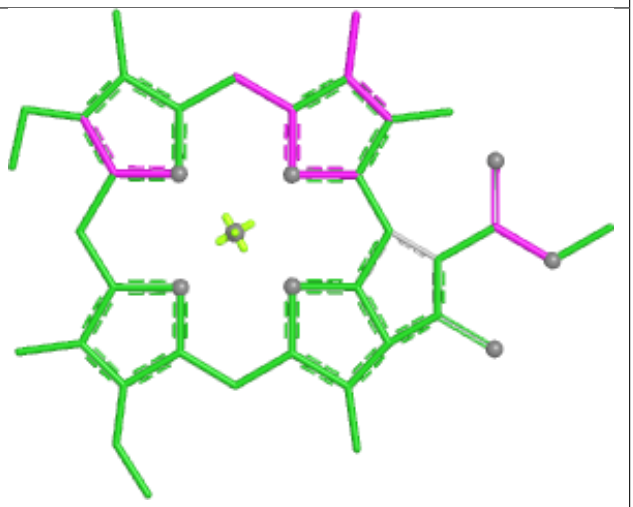


Rings

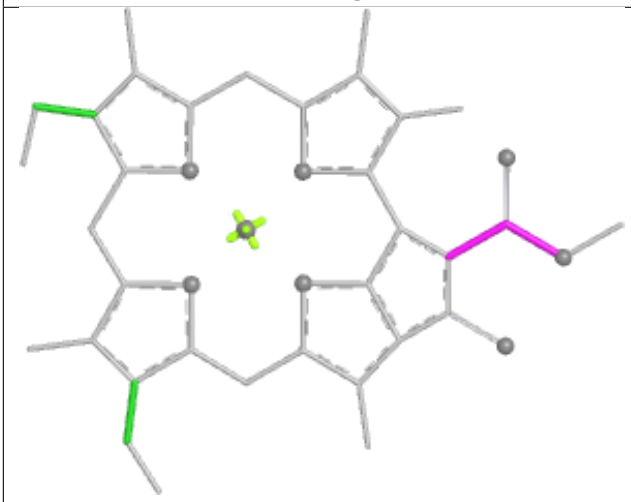
Ligand CLA NN 604



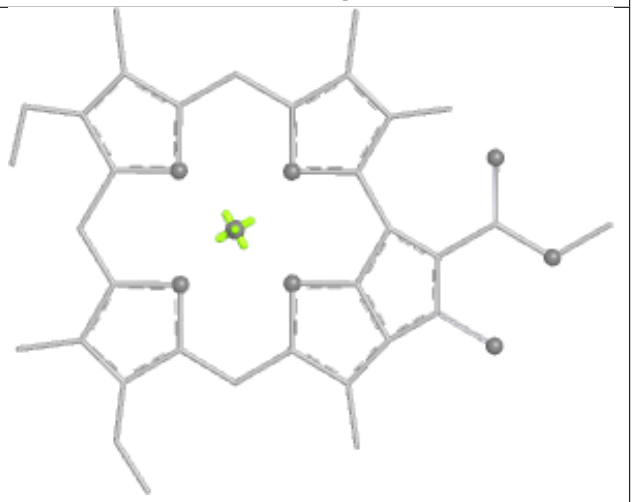
Bond lengths



Bond angles

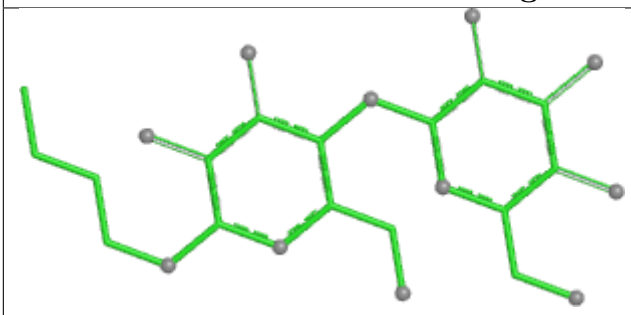


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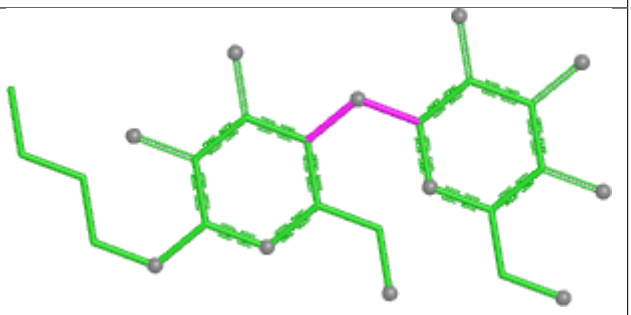


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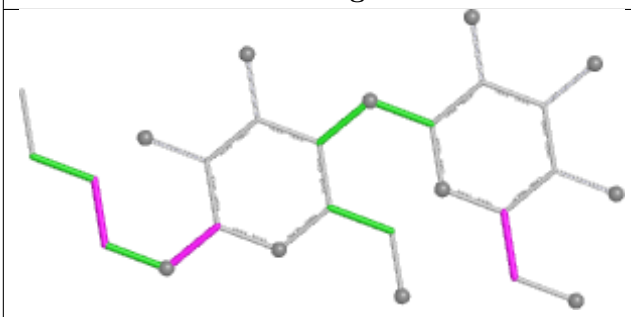
Ligand LMU C 502



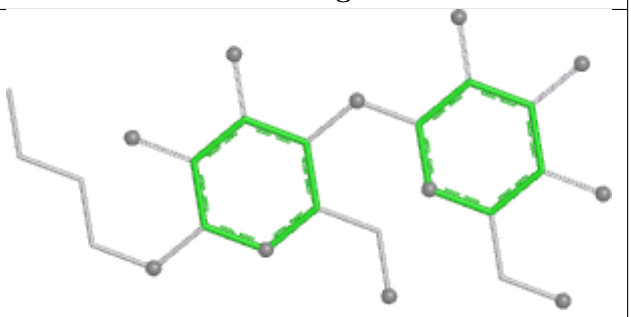
Bond lengths



Bond angles

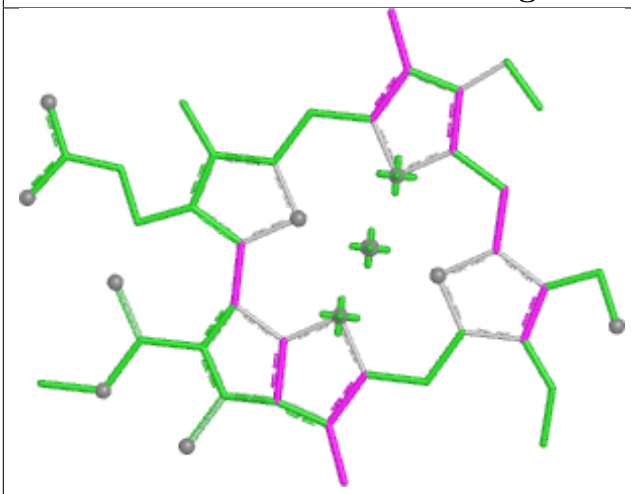


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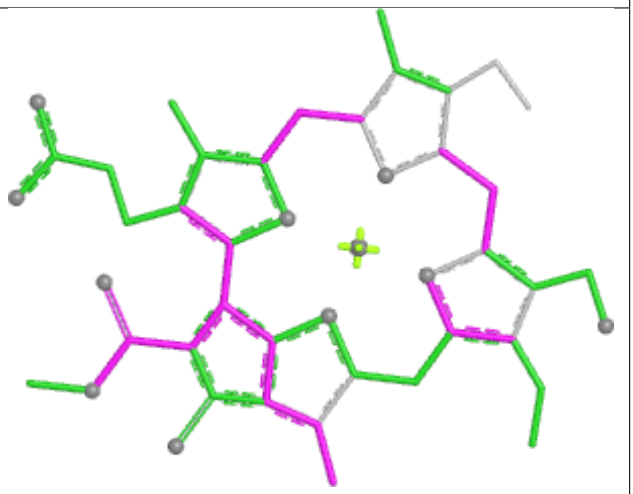


Rings

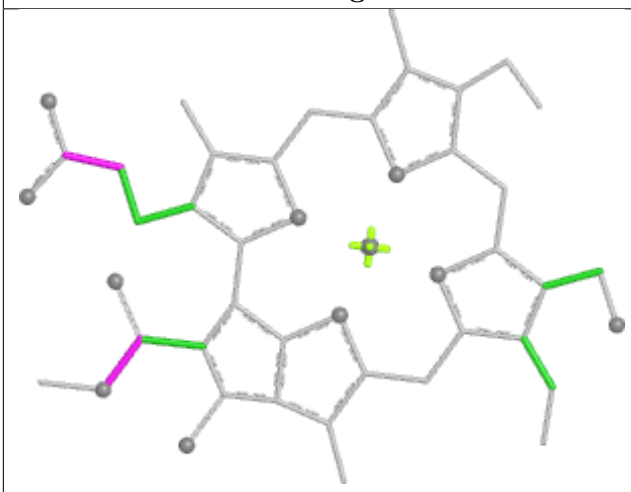
Ligand CHL 44 606



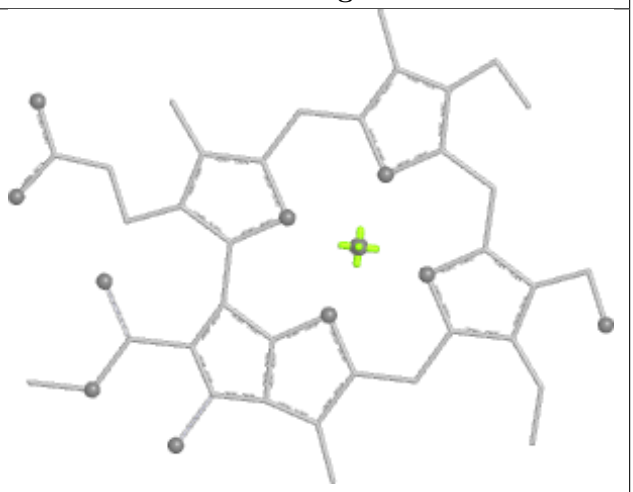
Bond lengths



Bond angles

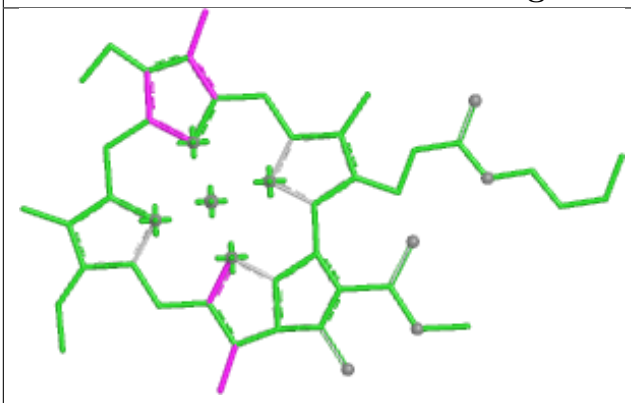


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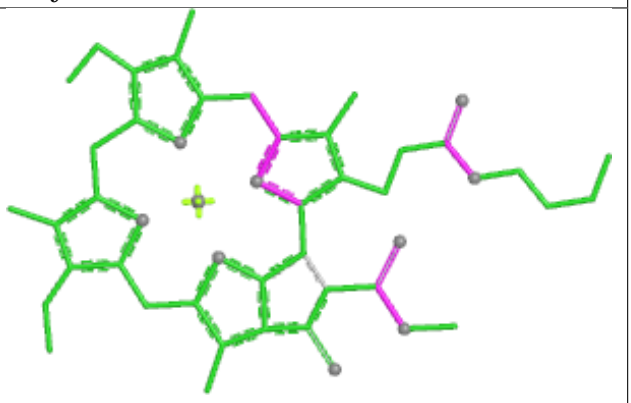


Rings

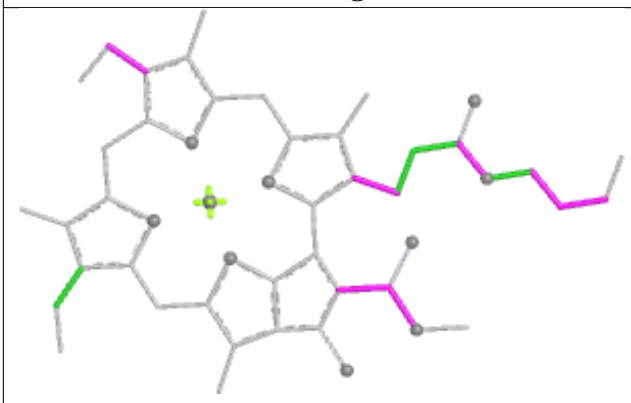
Ligand CLA y 316



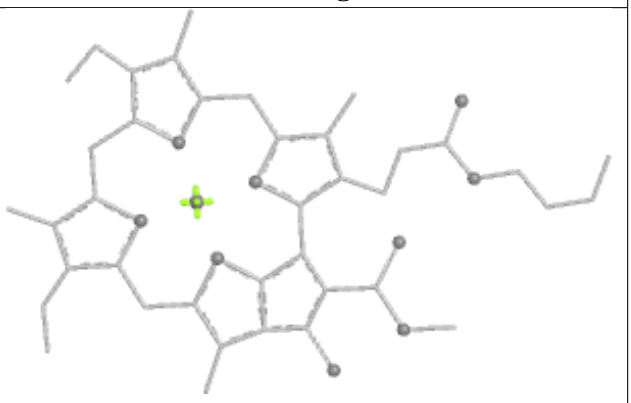
Bond lengths



Bond angles

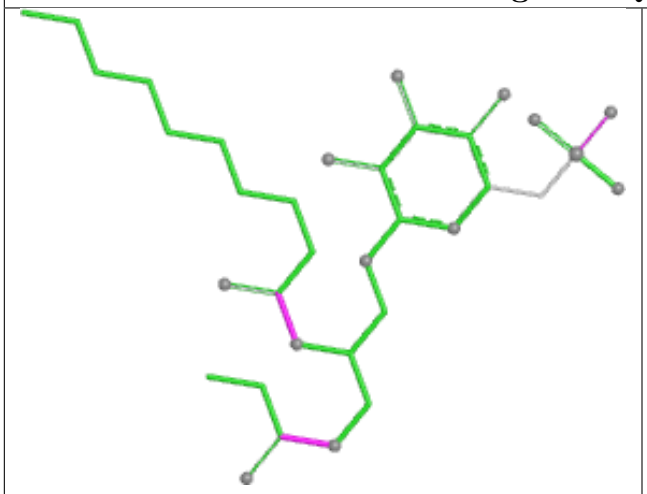


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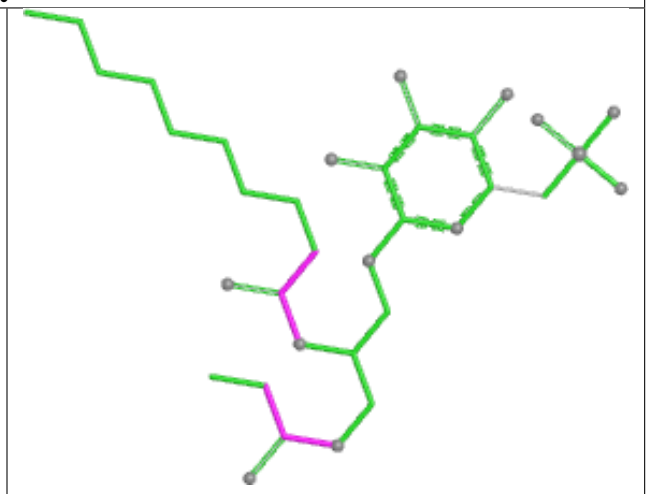


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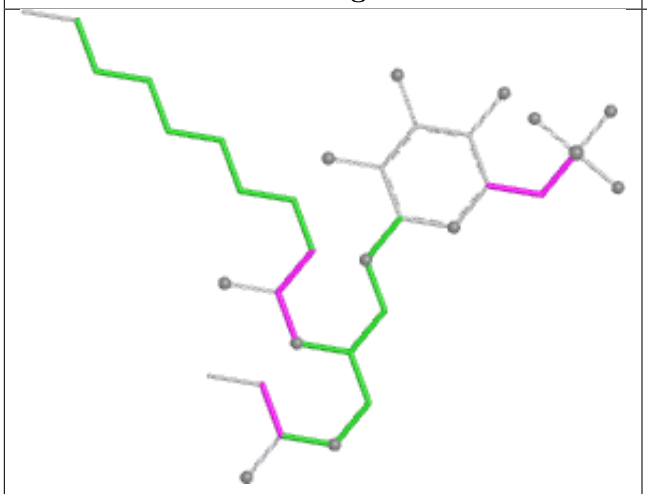
Ligand SQD AA 412



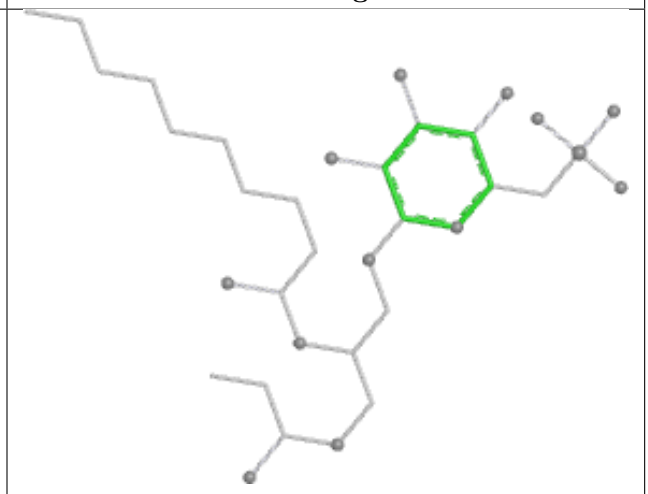
Bond lengths



Bond angles

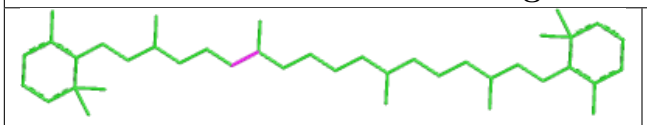


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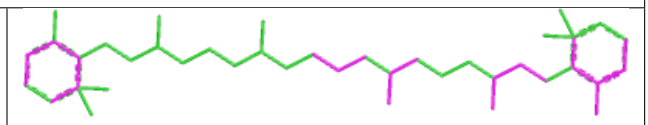


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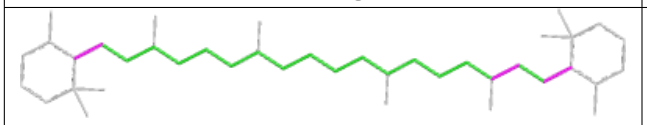
Ligand BCR C 517



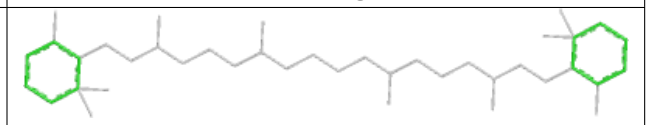
Bond lengths



Bond angles

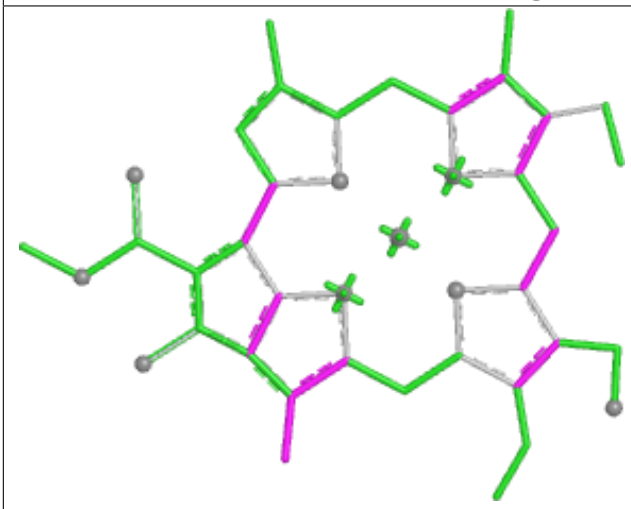


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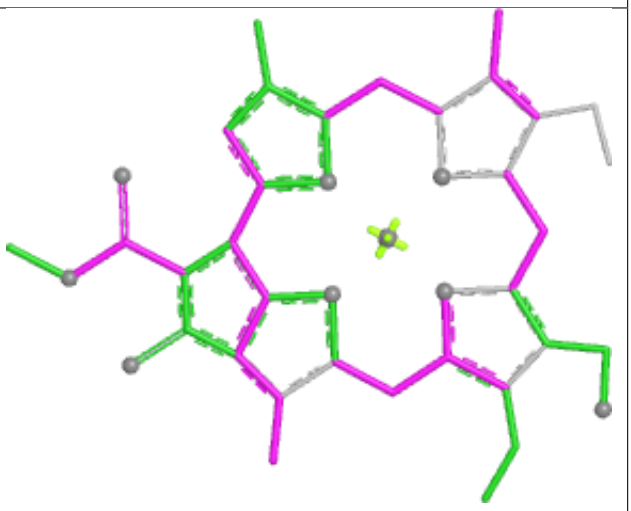


Rings

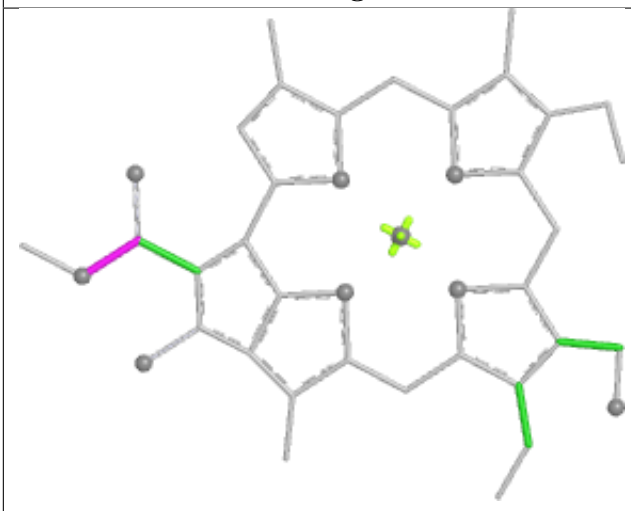
Ligand CHL 2 605



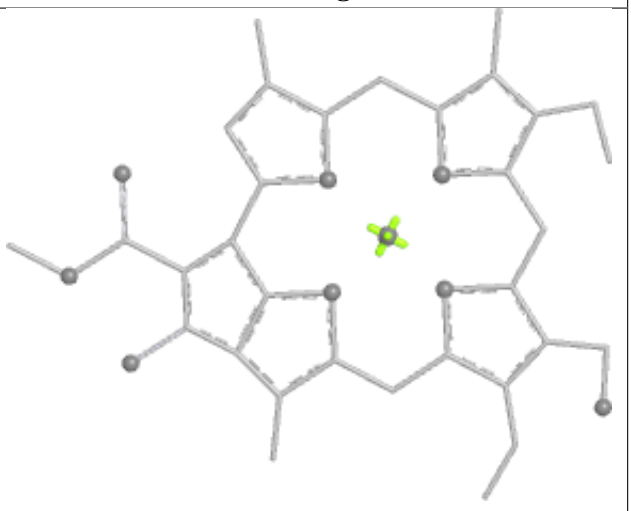
Bond lengths



Bond angles

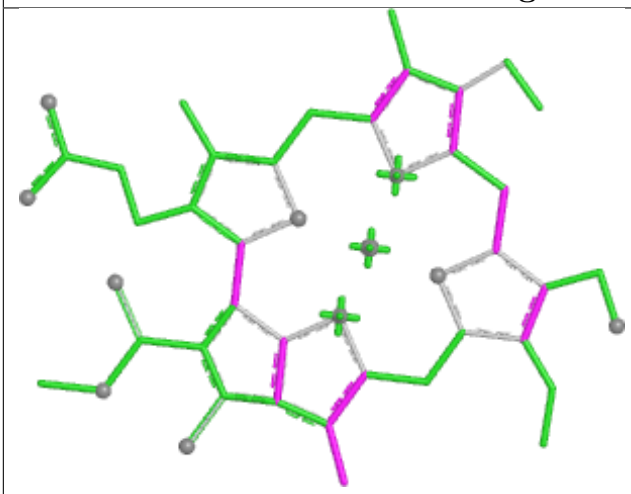


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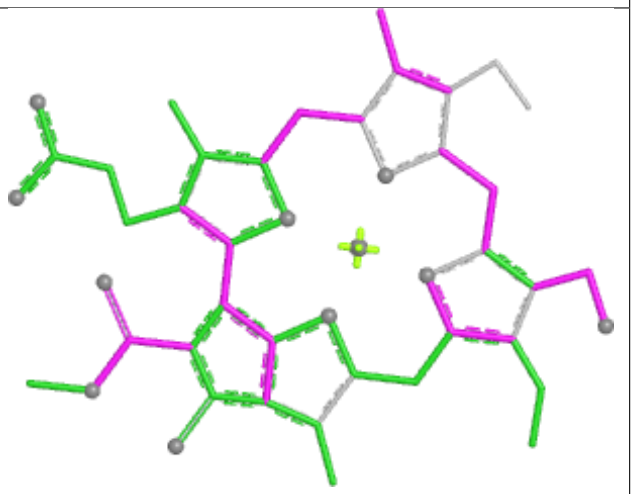


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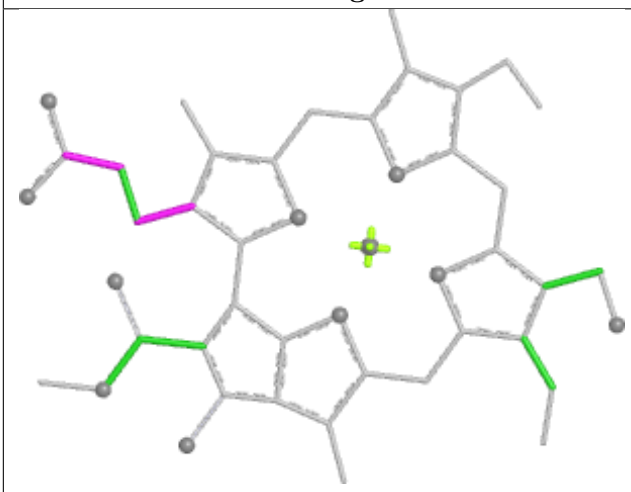
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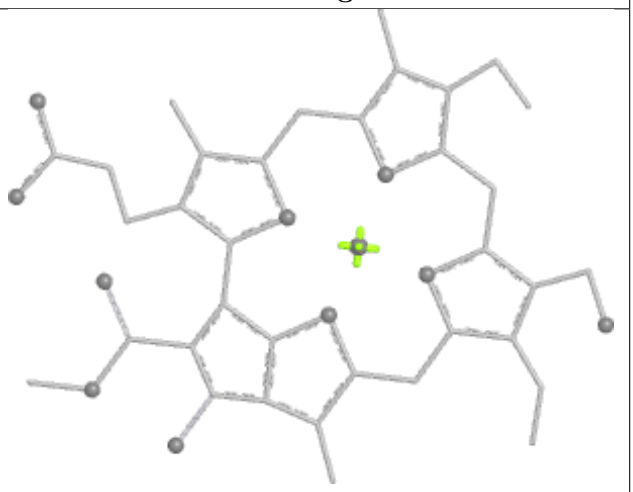
Bond lengths



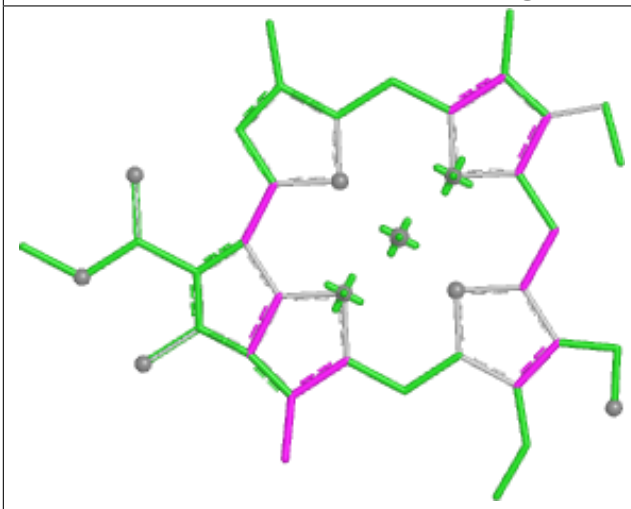
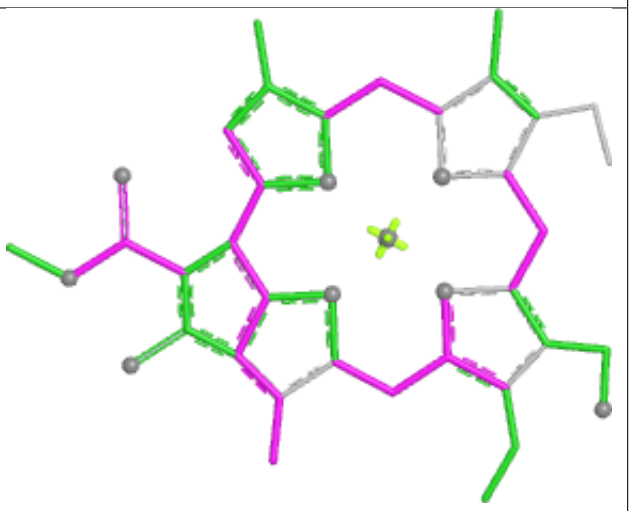
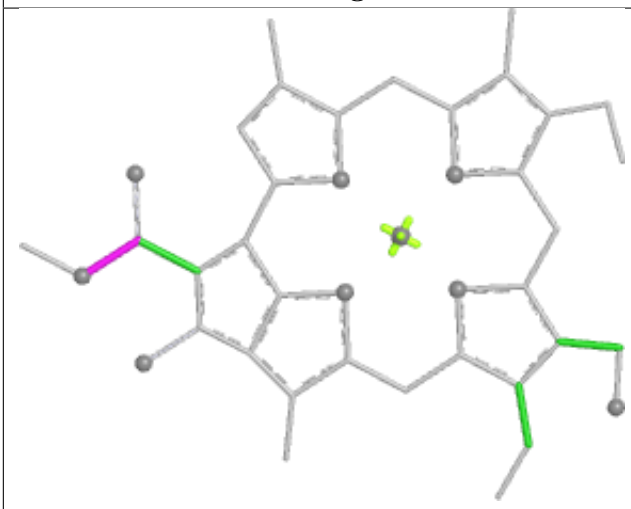
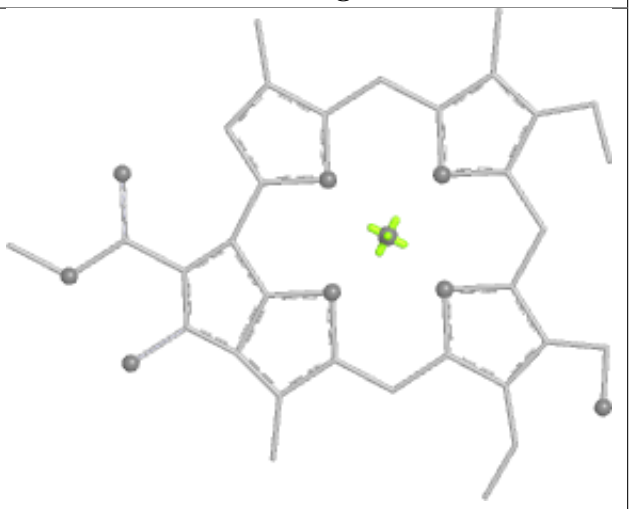
Bond angles

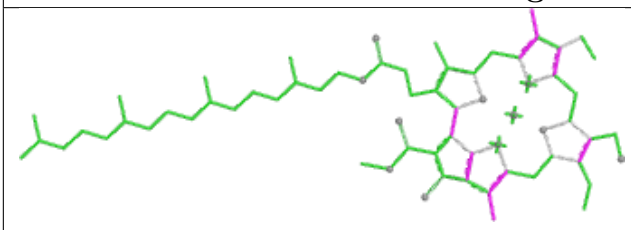
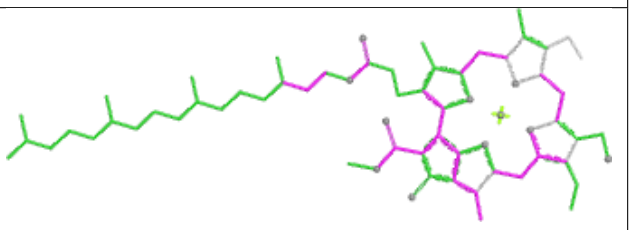
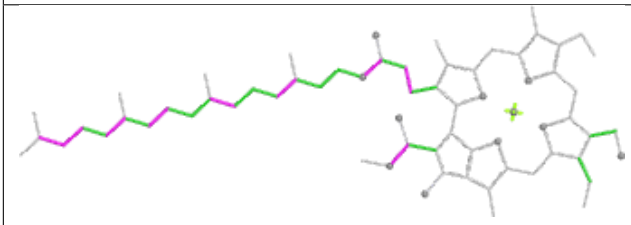
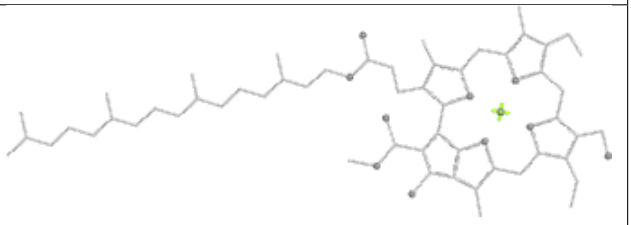


Torsions

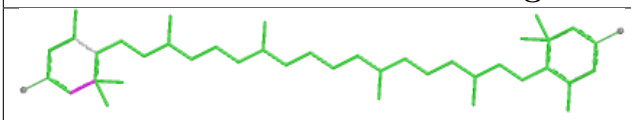


Rings

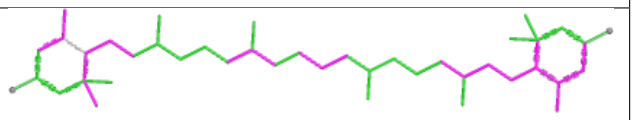
Ligand CHL 11 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL n 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

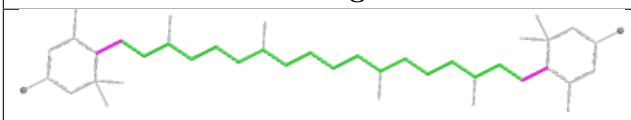
Ligand LUT Y 615



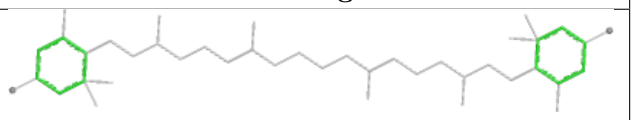
Bond lengths



Bond angles



Torsions

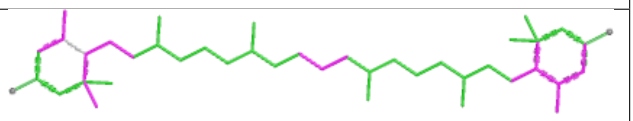


Rings

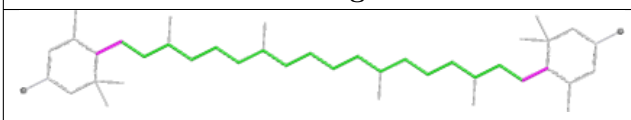
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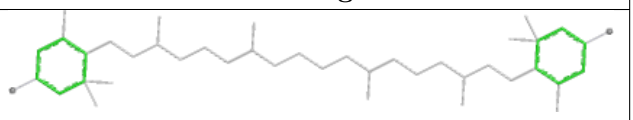
Bond lengths



Bond angles

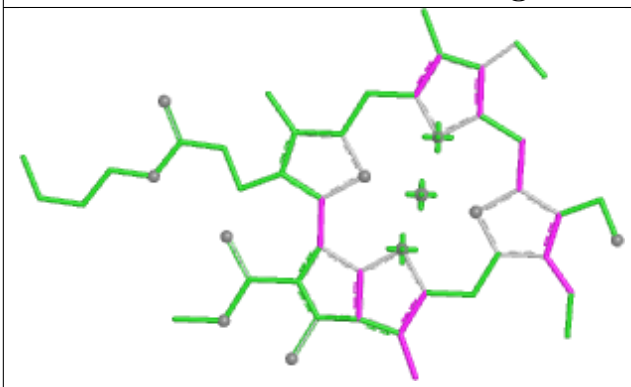


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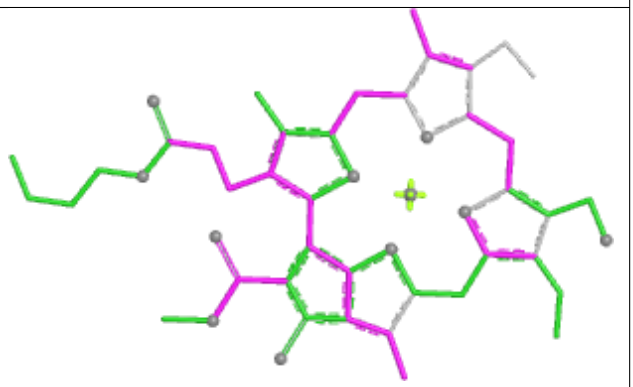


Rings

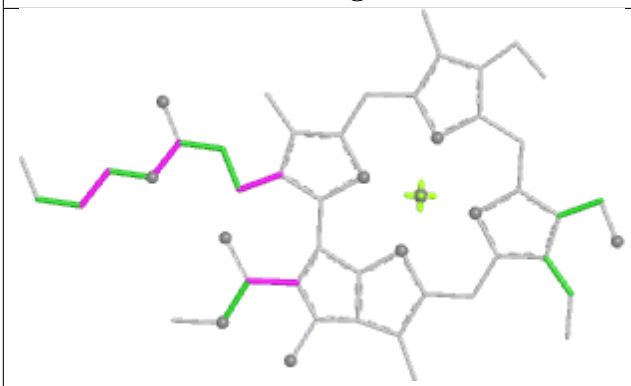
Ligand CHL RR 305



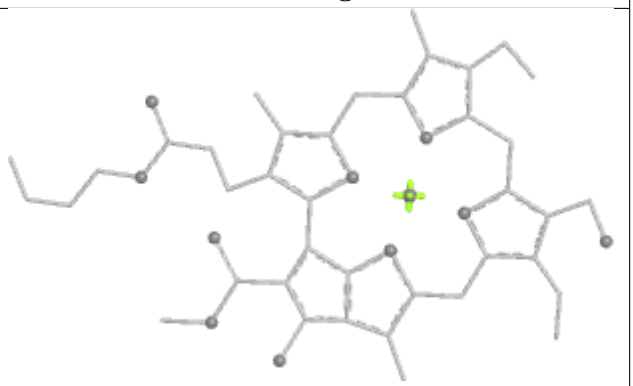
Bond lengths



Bond angles

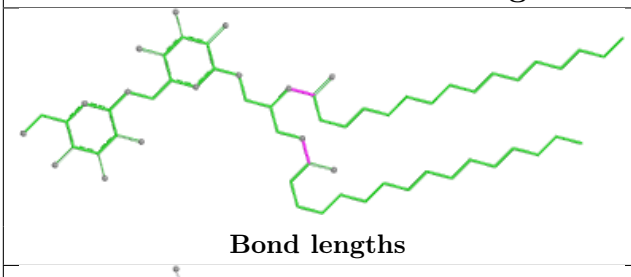


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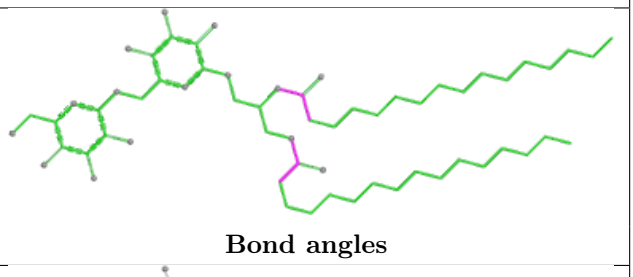


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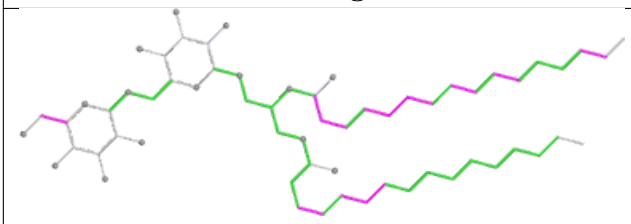
Ligand DGD Hh 102



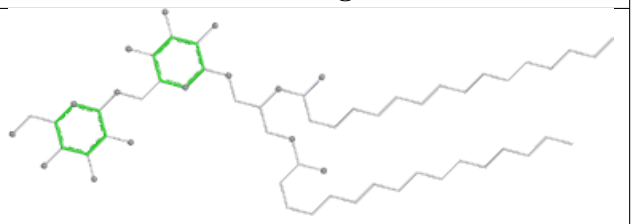
Bond lengths



Bond angles

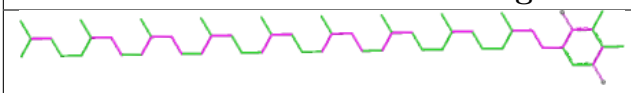


Torsions

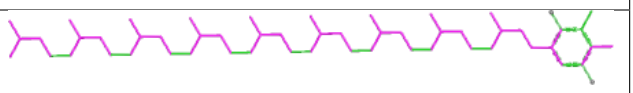


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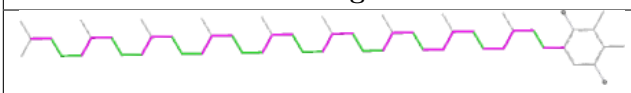
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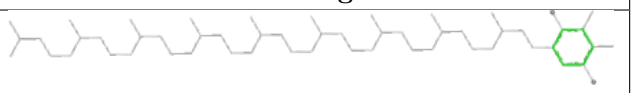
Bond lengths



Bond angles

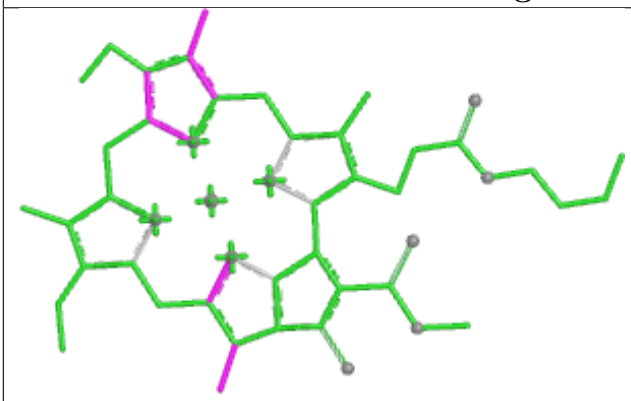


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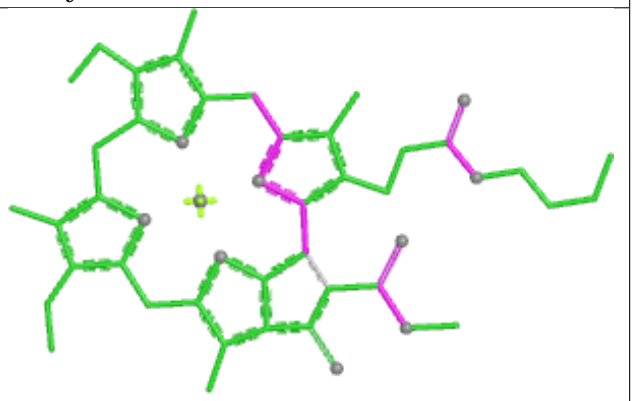


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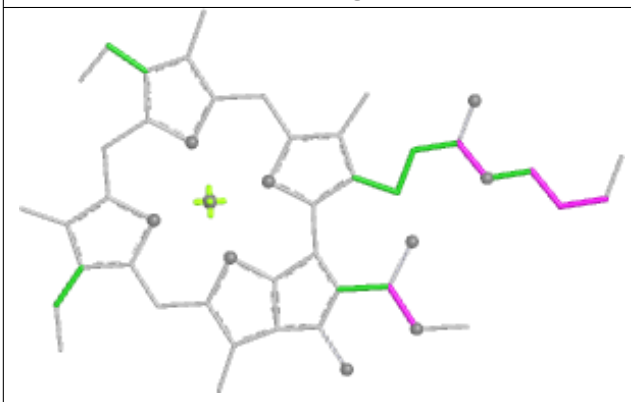
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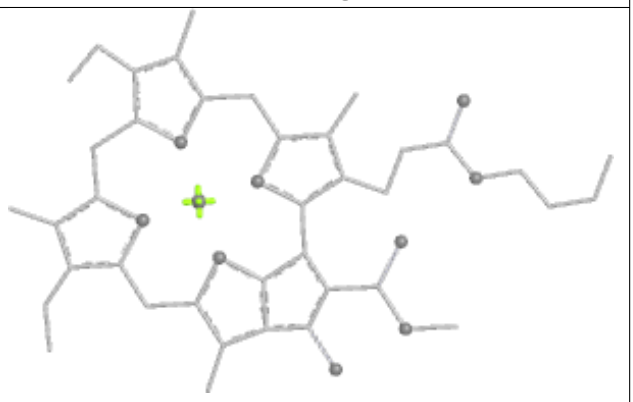
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Bond angles

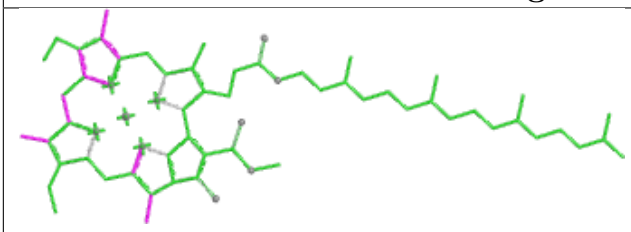


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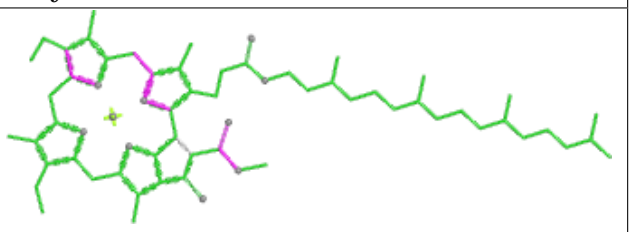


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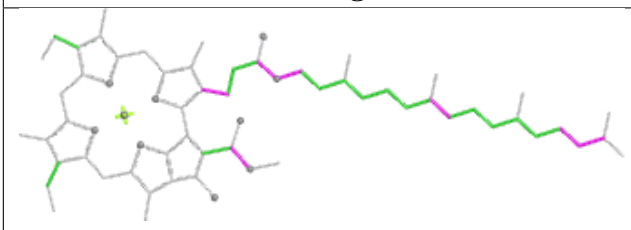
Ligand CLA y 304



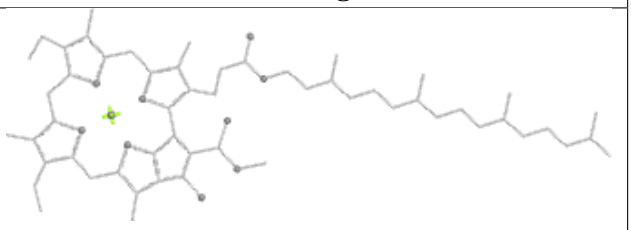
Bond lengths



Bond angles

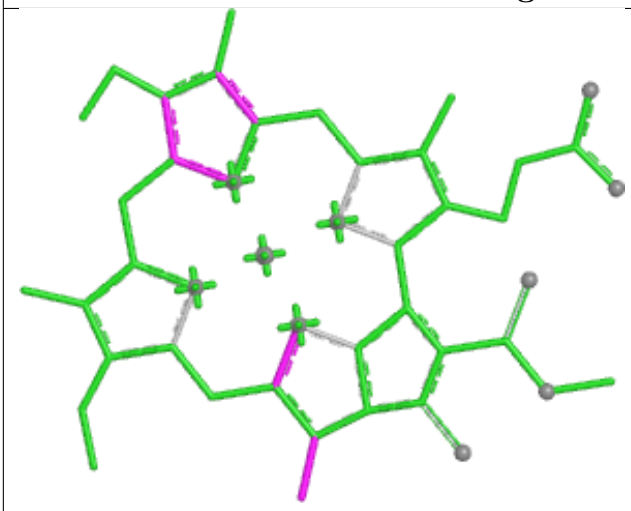


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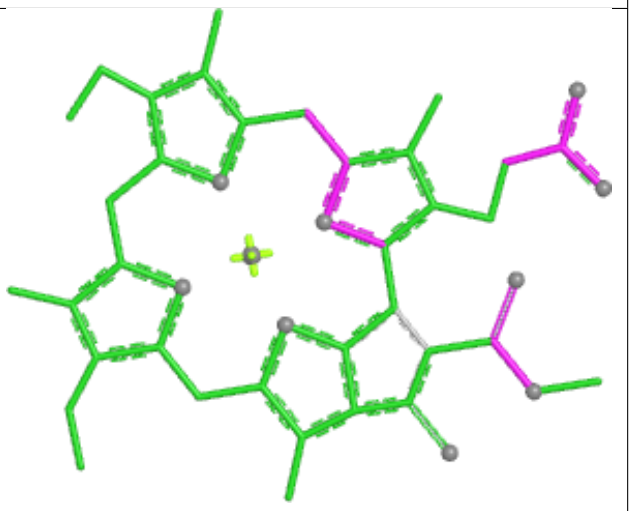


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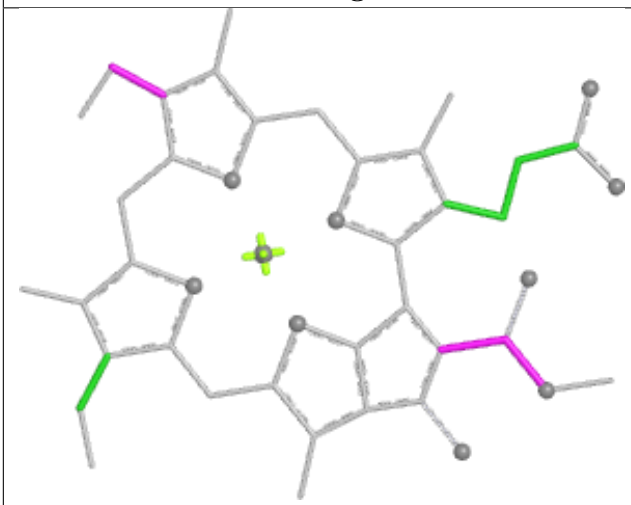
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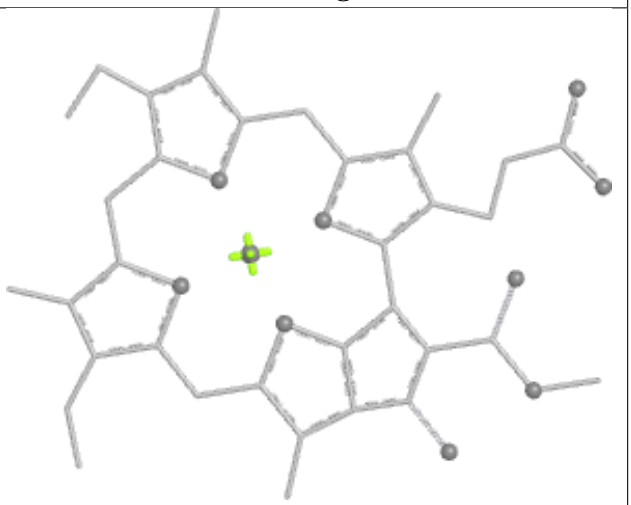
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Bond angles

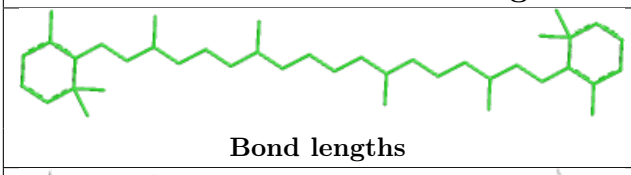


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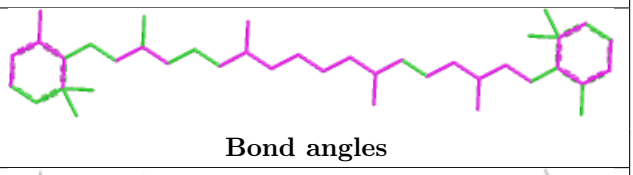


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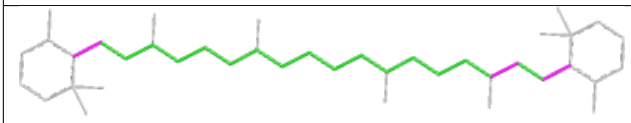
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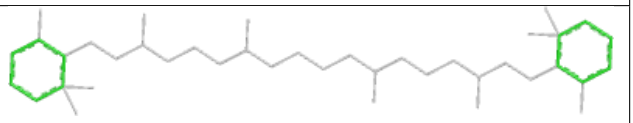
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Bond angles

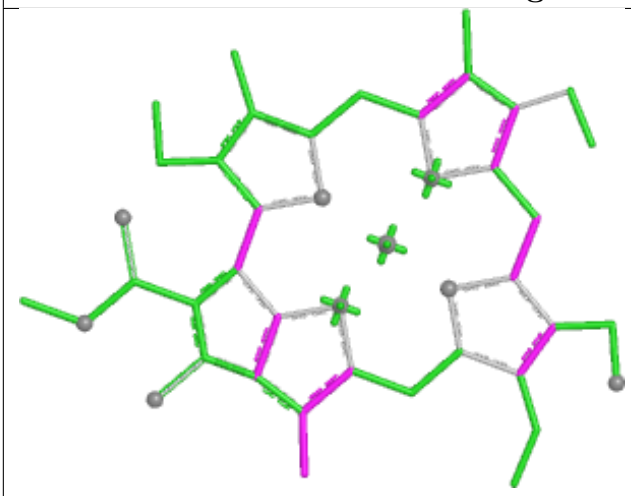


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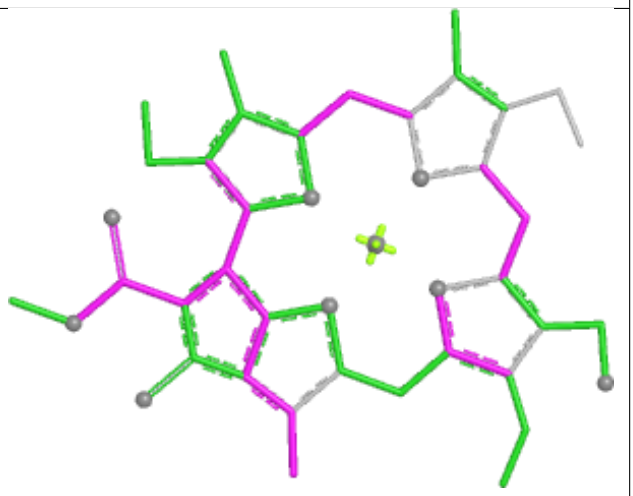


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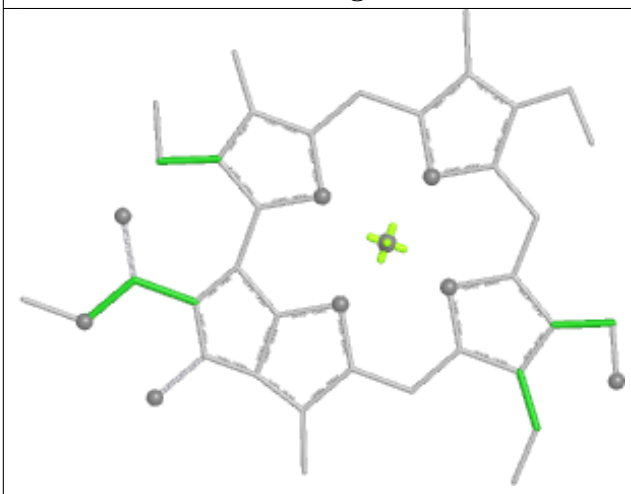
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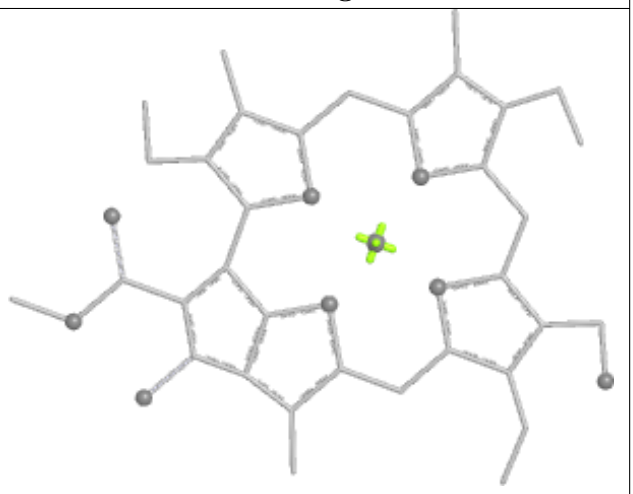
Bond lengths



Bond angles



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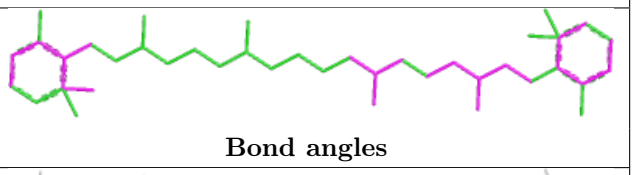


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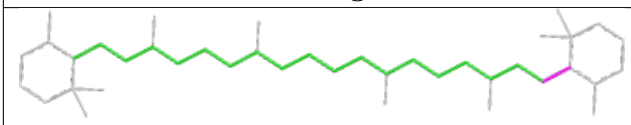
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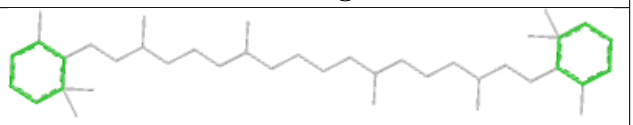
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Bond angles

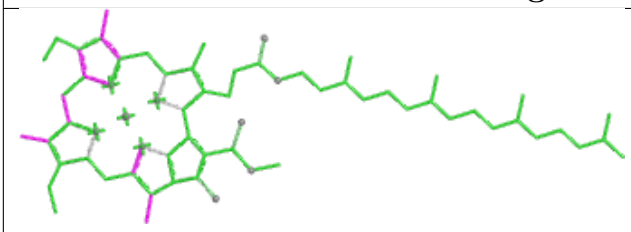


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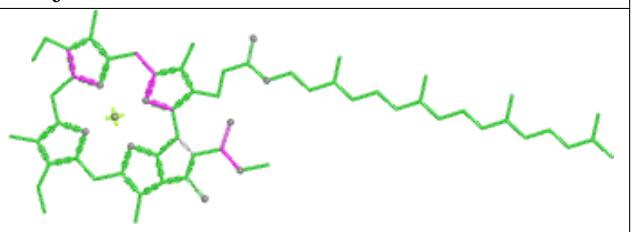


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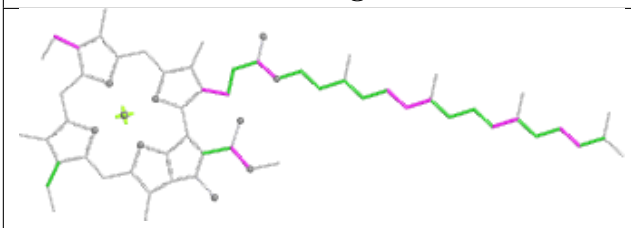
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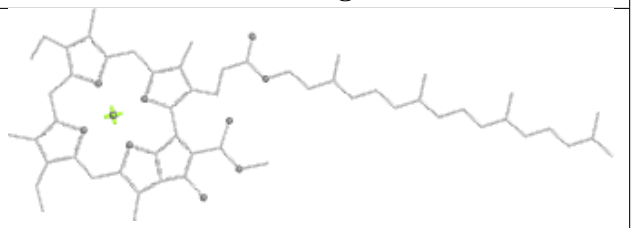
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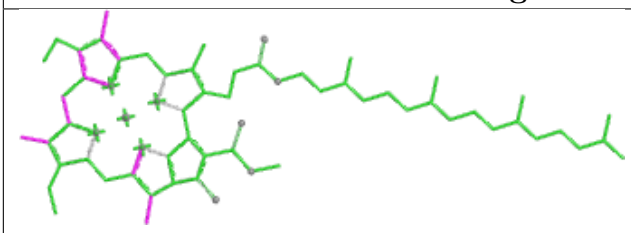


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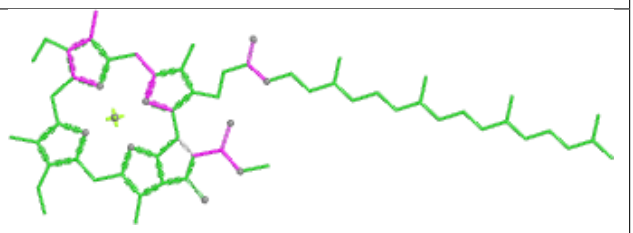


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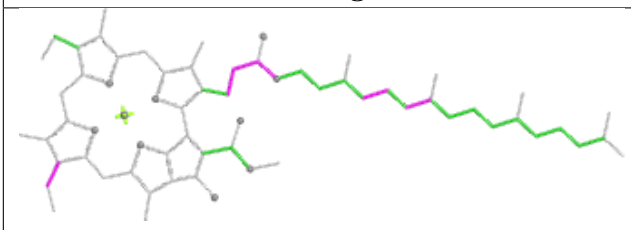
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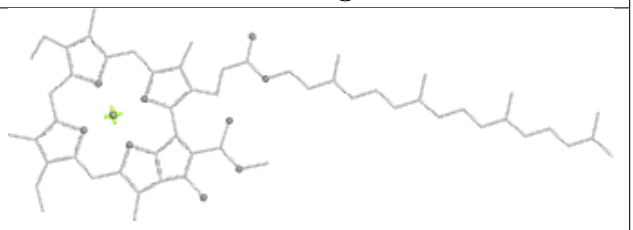
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Bond angles

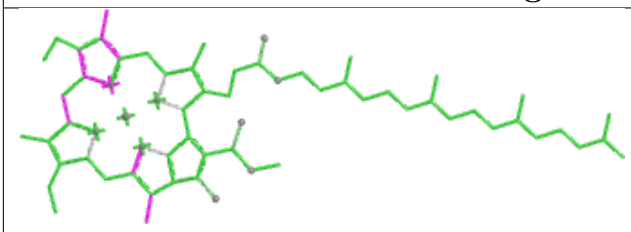


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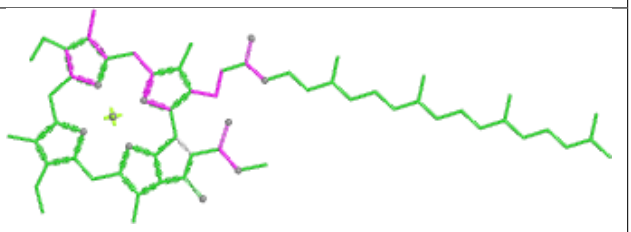


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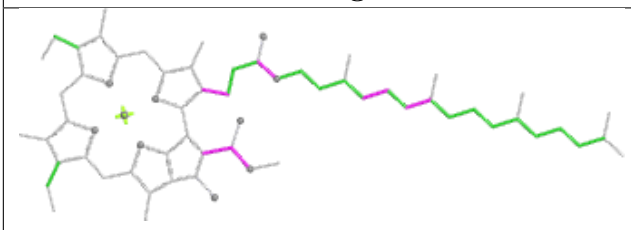
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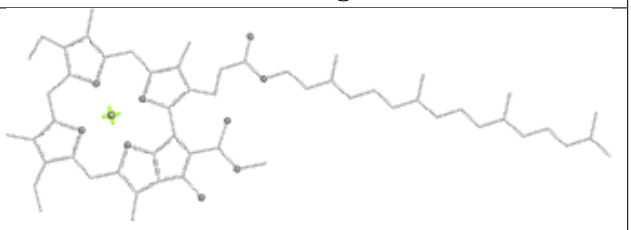
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Bond angles

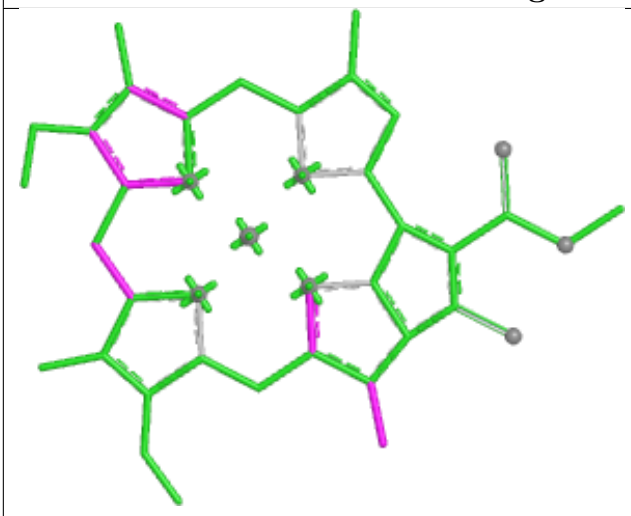


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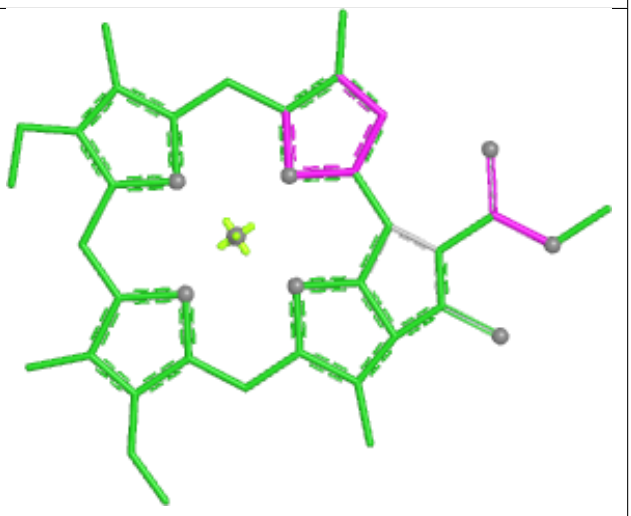


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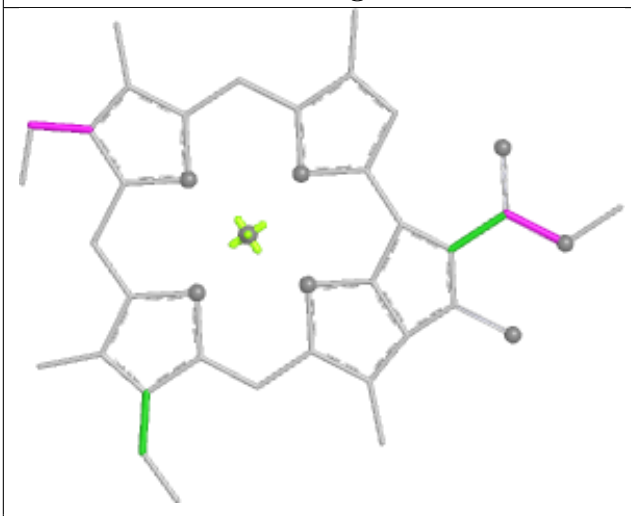
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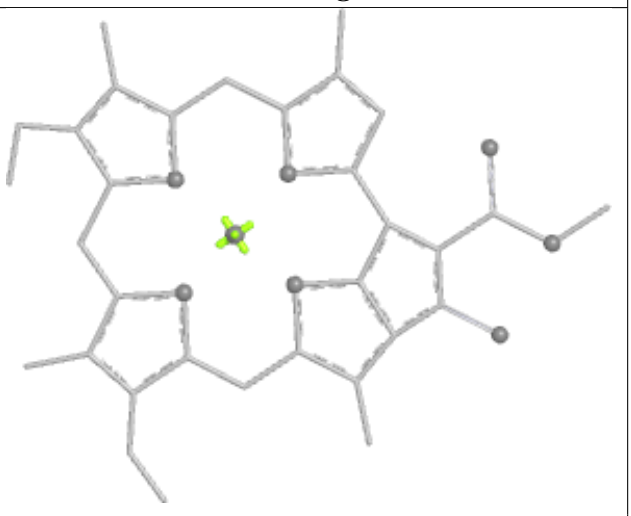
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Bond angles

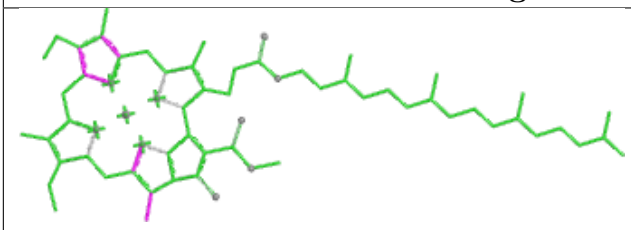


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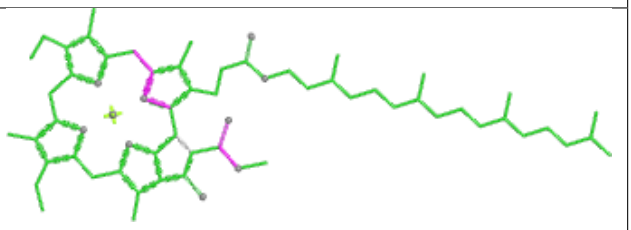


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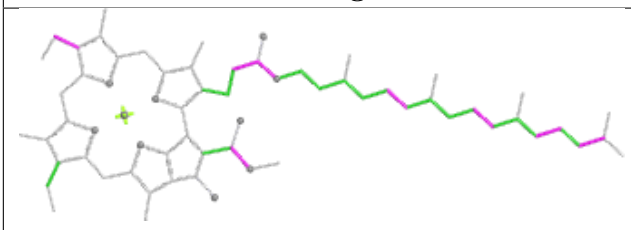
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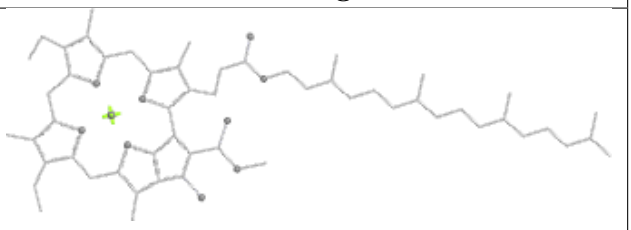
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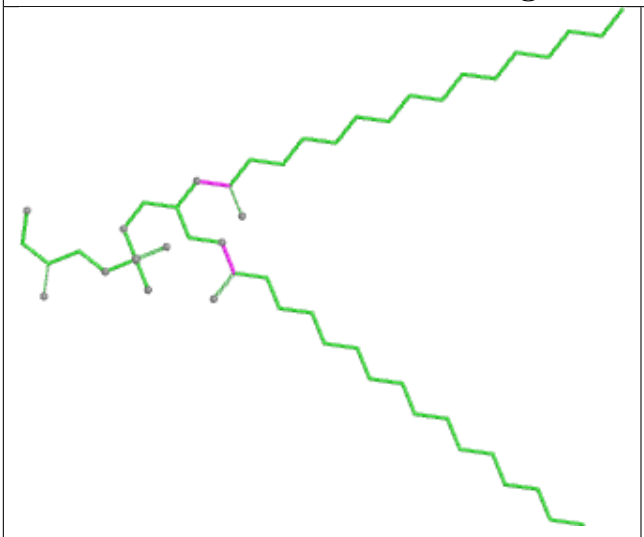


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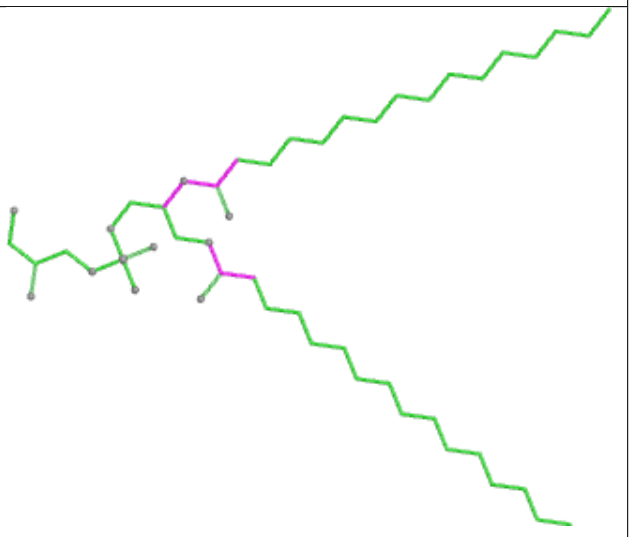


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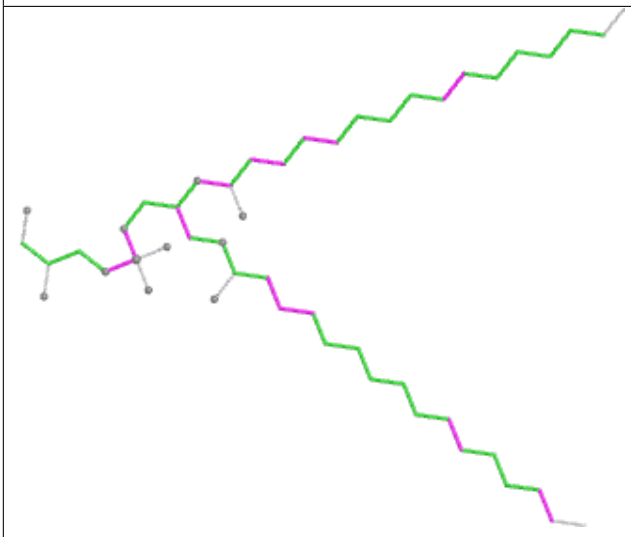
Ligand LHG Ll 102



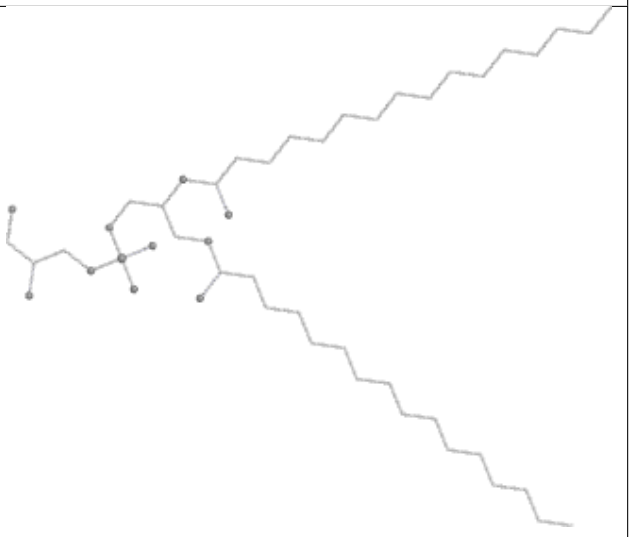
Bond lengths



Bond angles

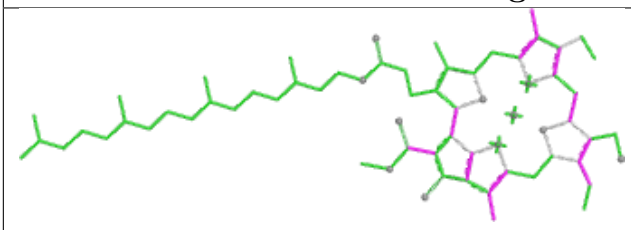


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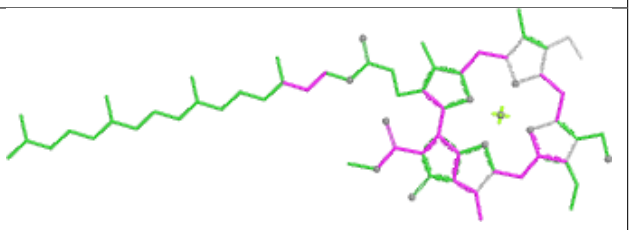


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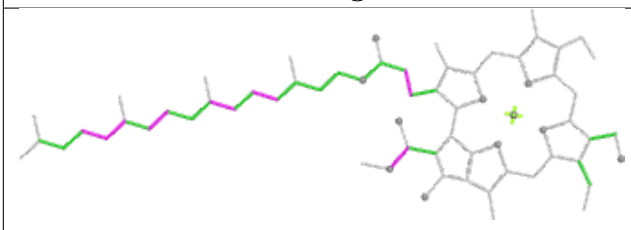
Ligand CHL NN 607



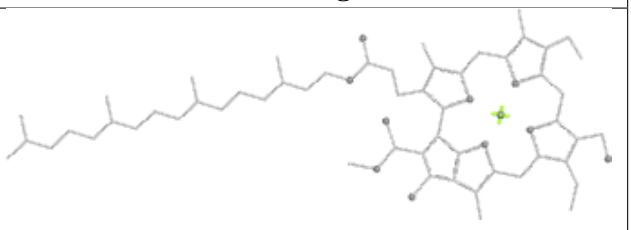
Bond lengths



Bond angles

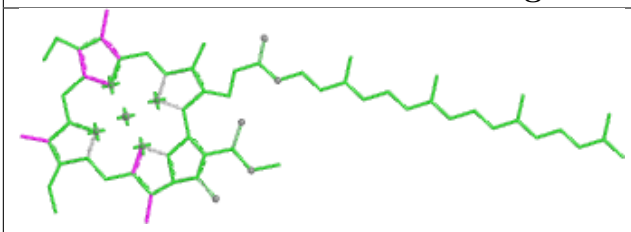


Torsions

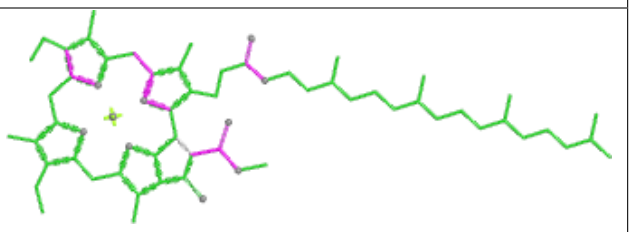


Rings

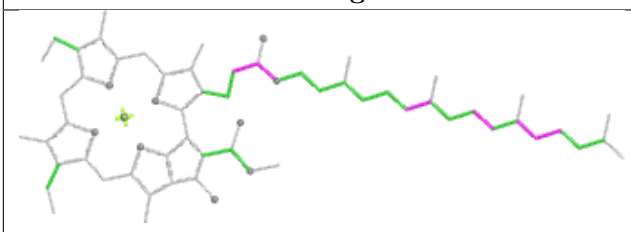
Ligand CLA B 618



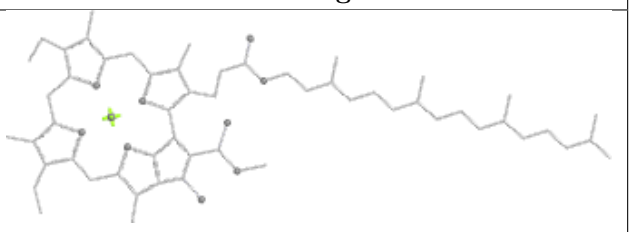
Bond lengths



Bond angles

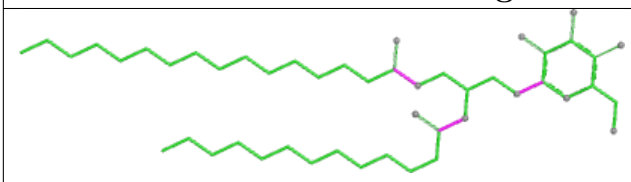


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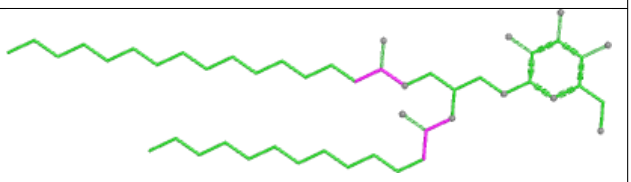


Rings

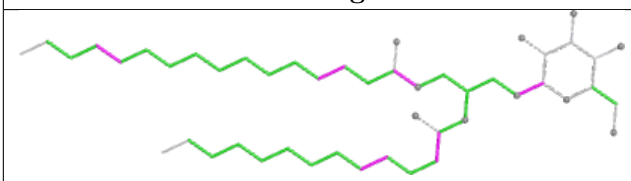
Ligand LMG WW 201



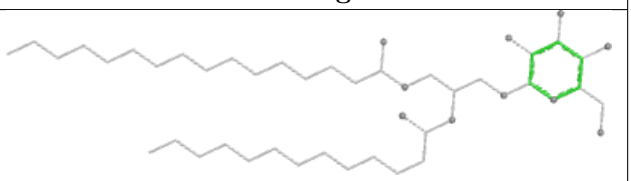
Bond lengths



Bond angles

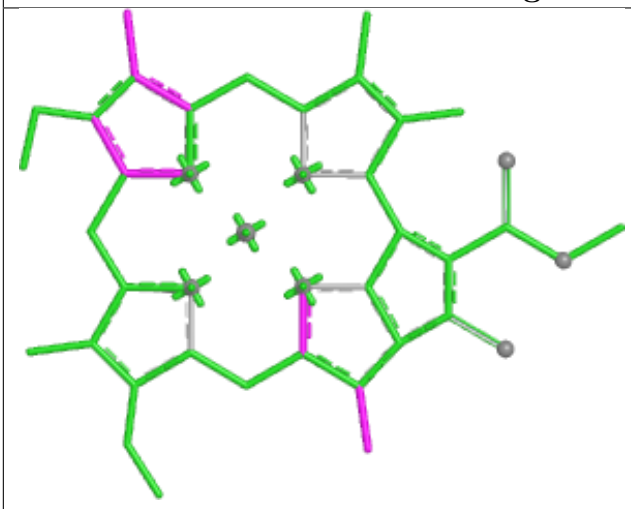


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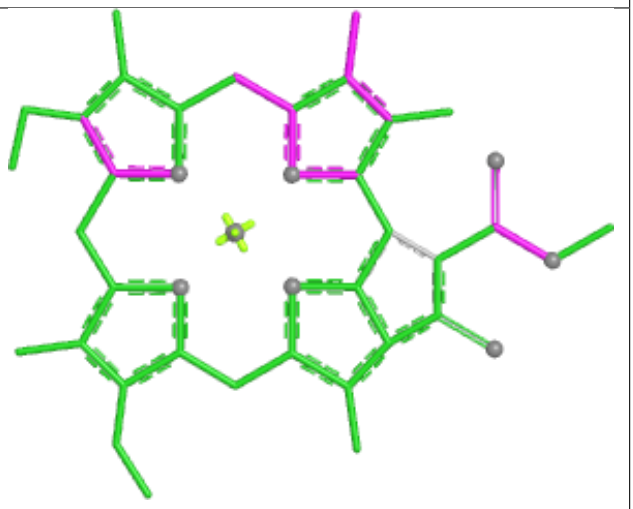


Rings

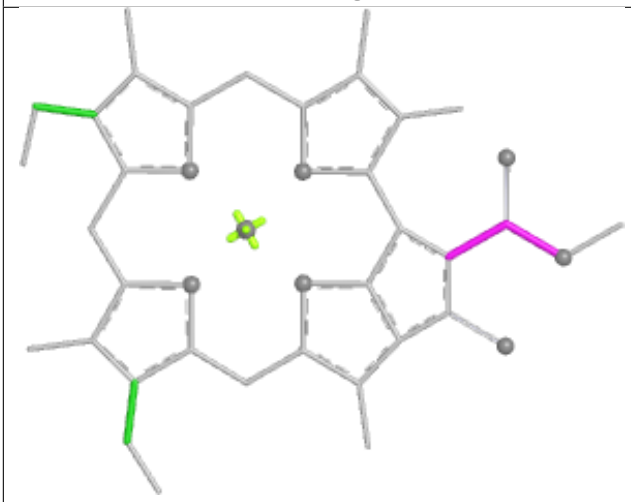
Ligand CLA N 604



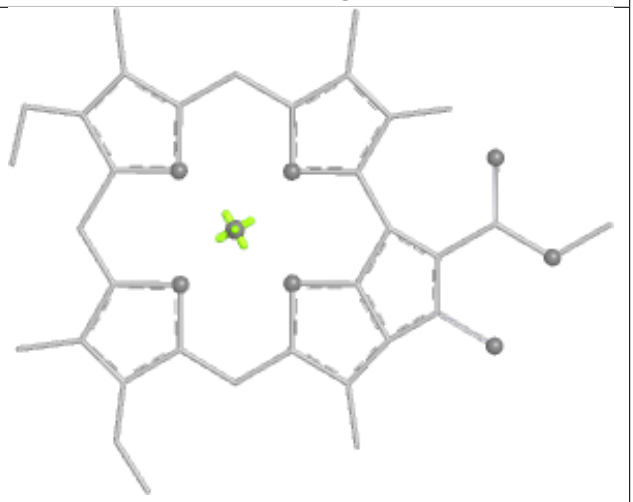
Bond lengths



Bond angles

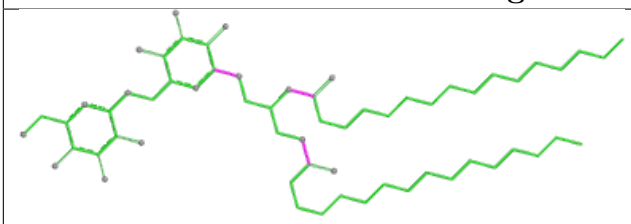


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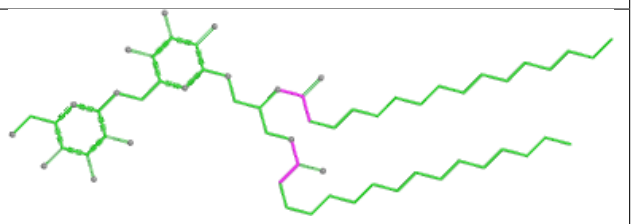


Rings

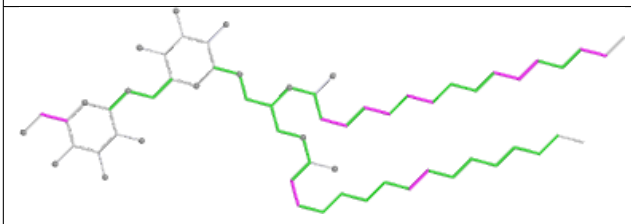
Ligand DGD BB 623



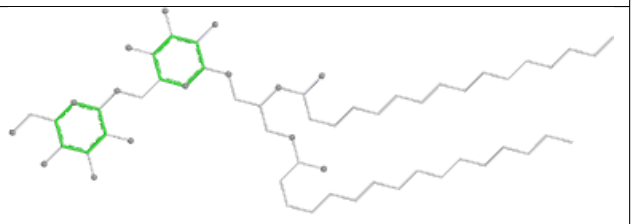
Bond lengths



Bond angles

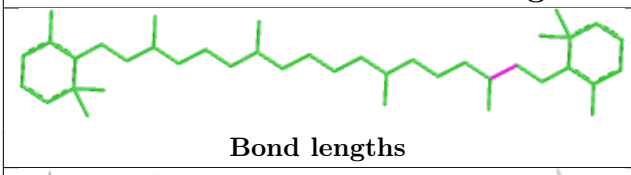


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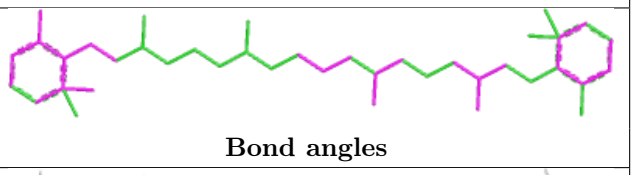


Rings

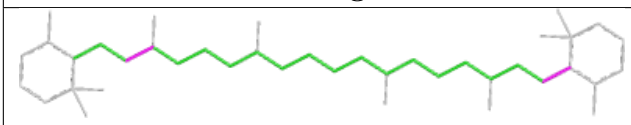
Ligand BCR c 516



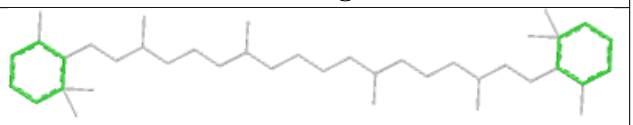
Bond lengths



Bond angles

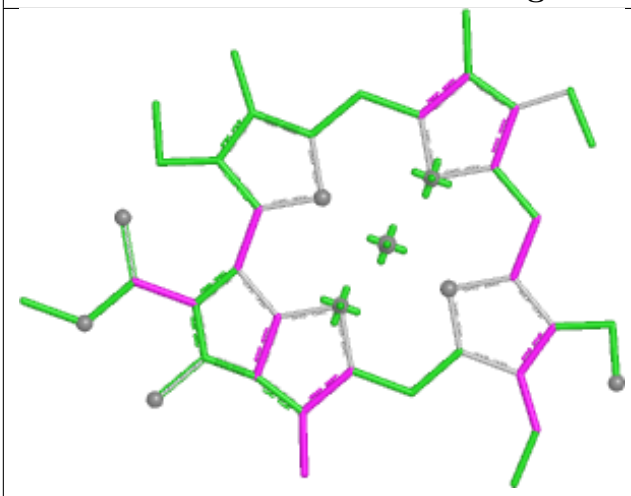


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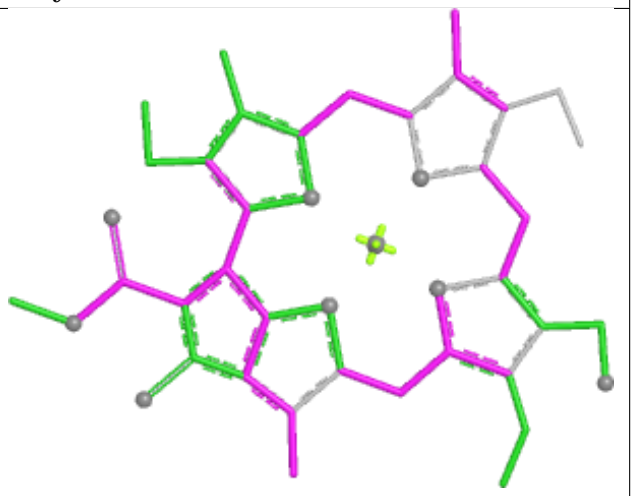


Rings

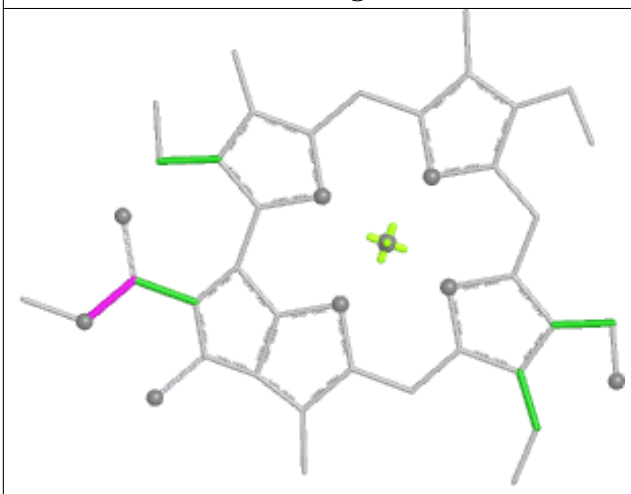
Ligand CHL y 309



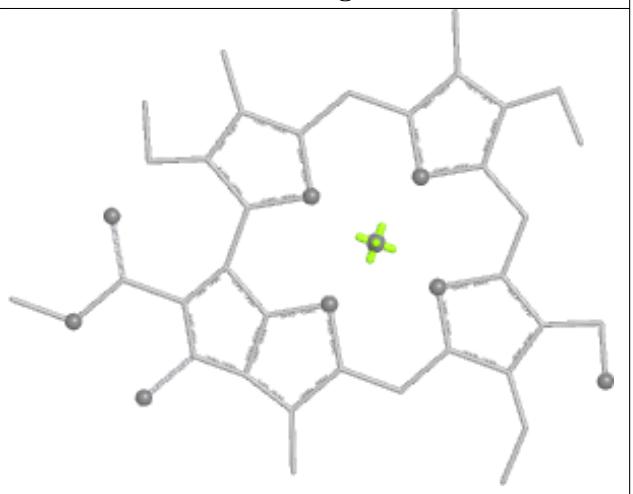
Bond lengths



Bond angles

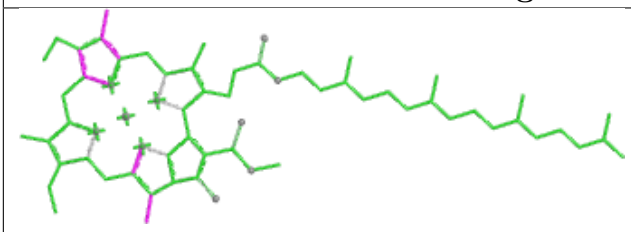


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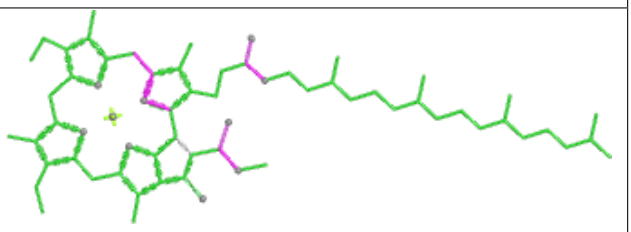


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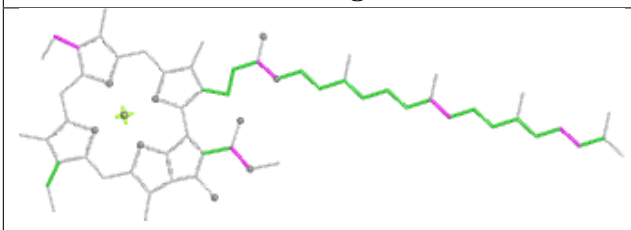
Ligand CLA Cc 514



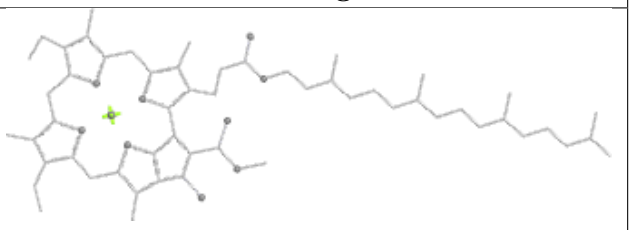
Bond lengths



Bond angles

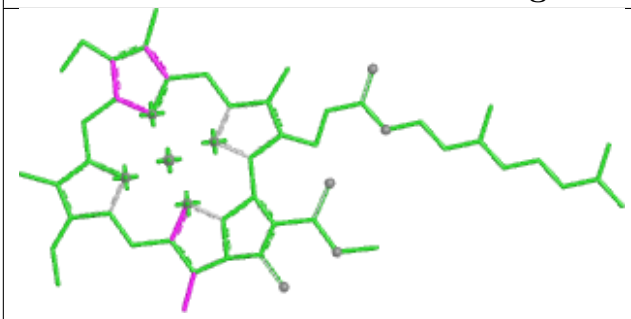


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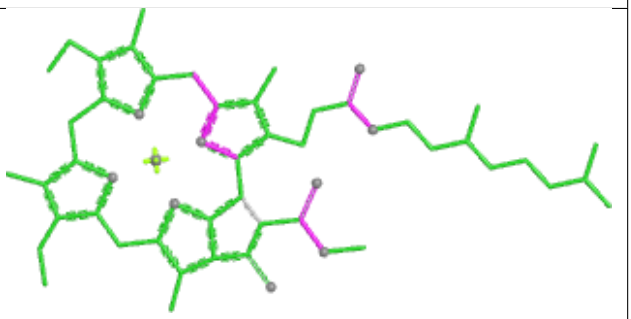


Rings

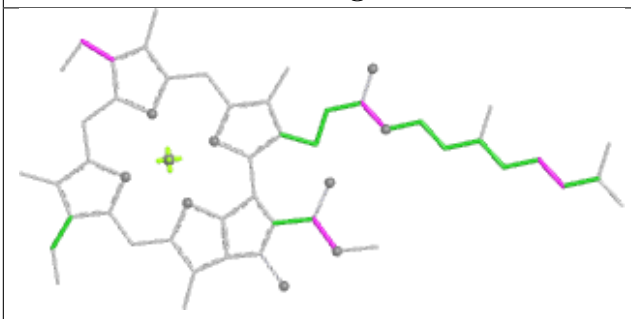
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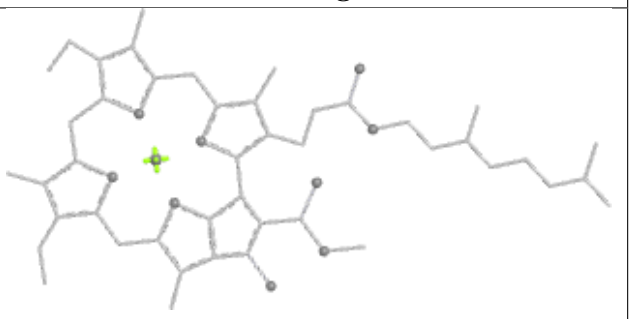
Bond lengths



Bond angles

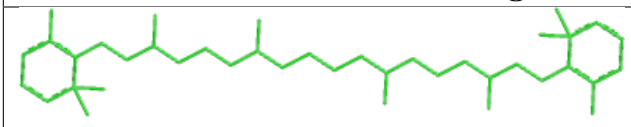


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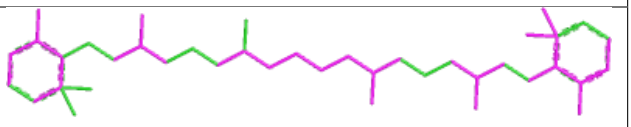


Rings

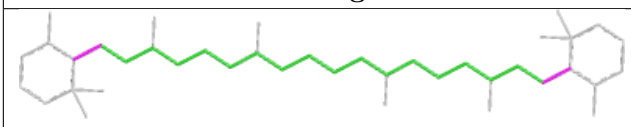
Ligand BCR KK 103



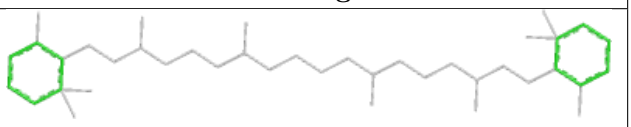
Bond lengths



Bond angles

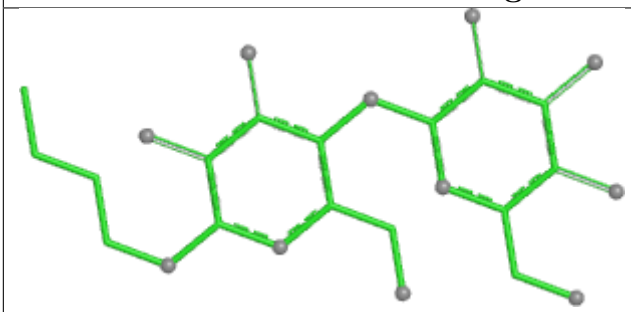


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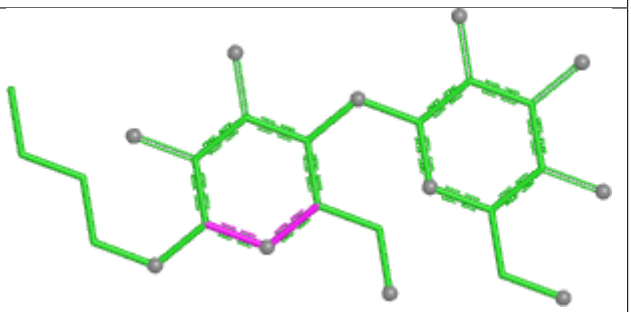


Rings

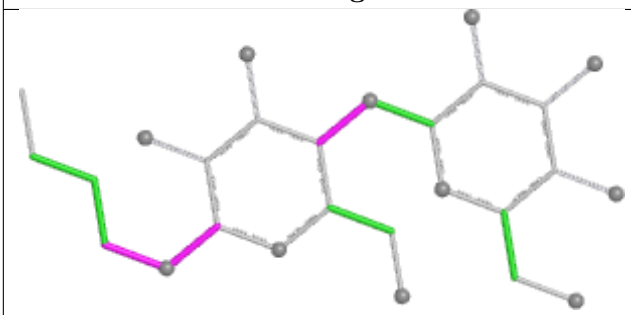
Ligand LMU KK 102



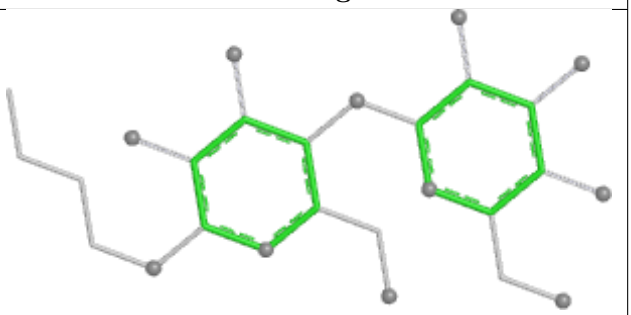
Bond lengths



Bond angles

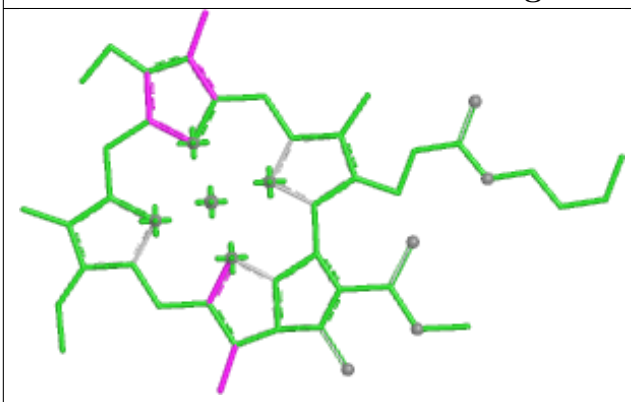


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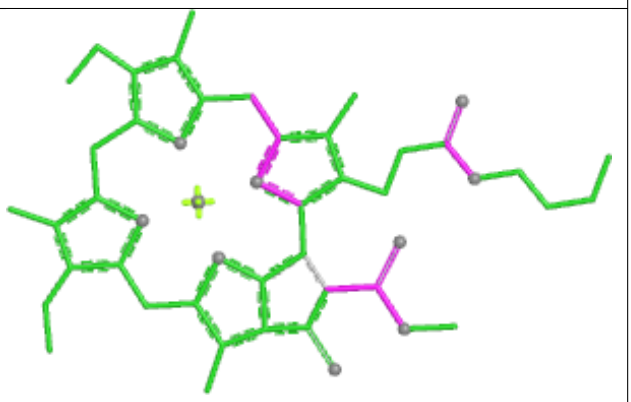


Rings

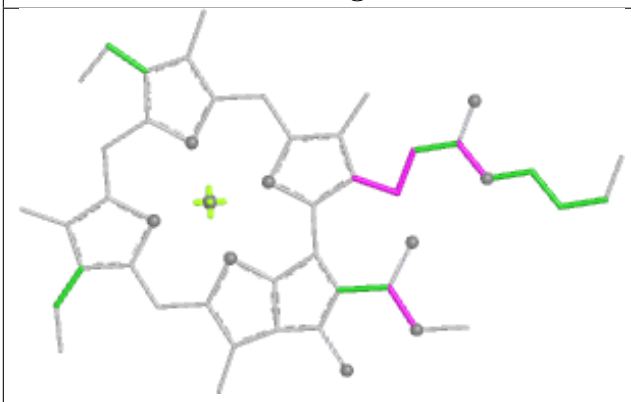
Ligand CLA C 515



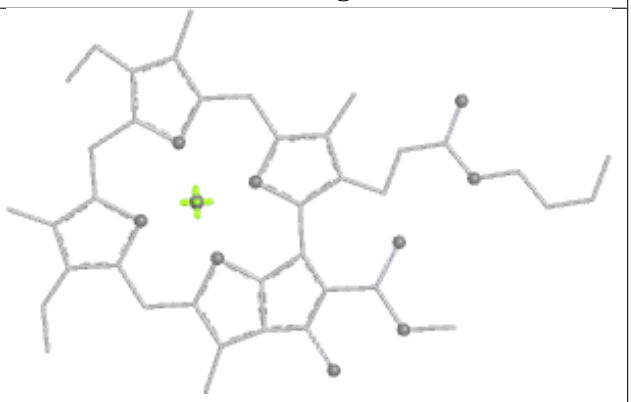
Bond lengths



Bond angles

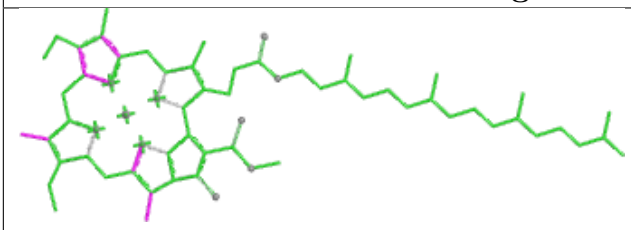


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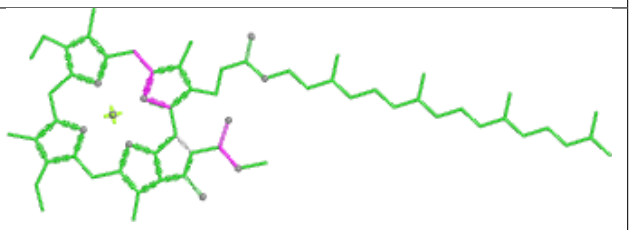


Rings

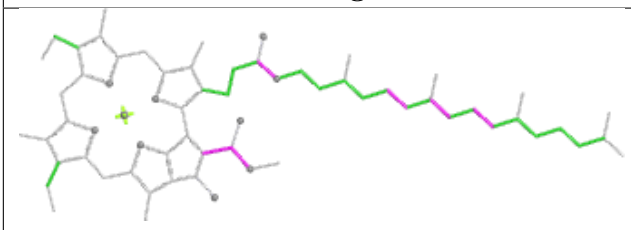
Ligand CLA BB 606



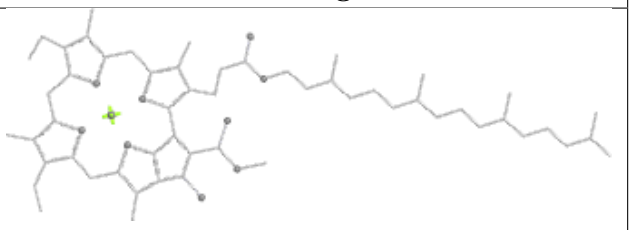
Bond lengths



Bond angles

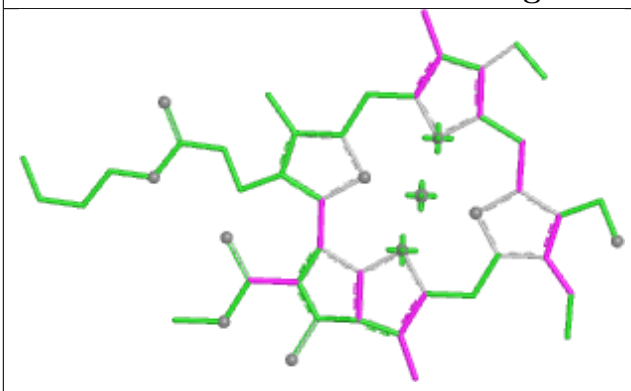


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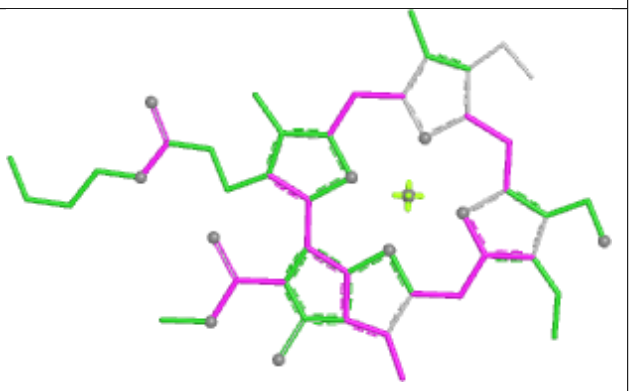


Rings

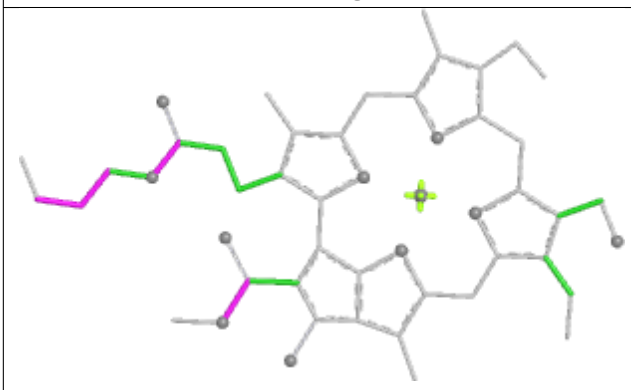
Ligand CHL Y 608



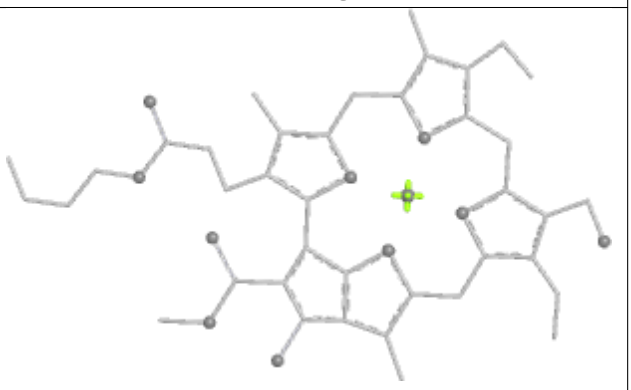
Bond lengths



Bond angles

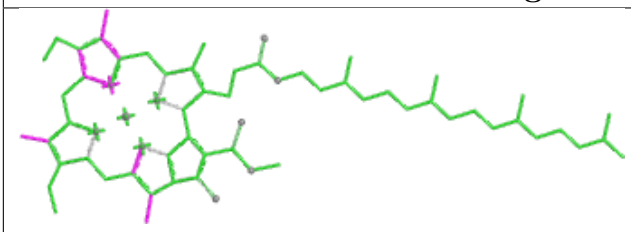


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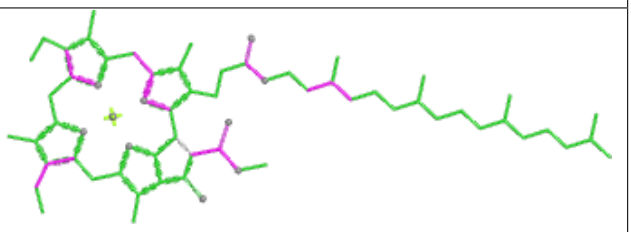


Rings

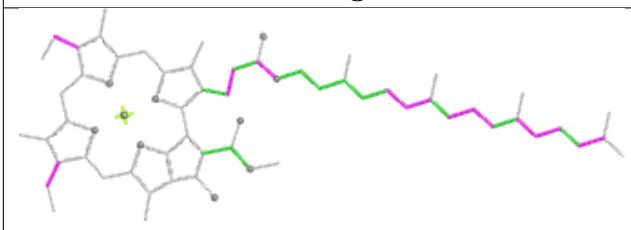
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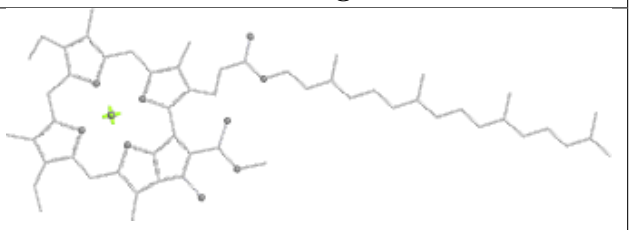
Bond lengths



Bond angles



Torsions



Rings

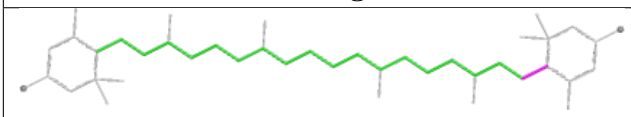
Ligand LUT Ss 614



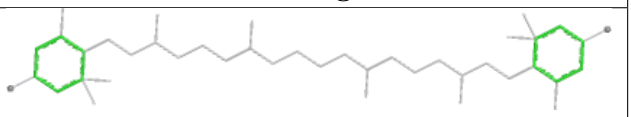
Bond lengths



Bond angles

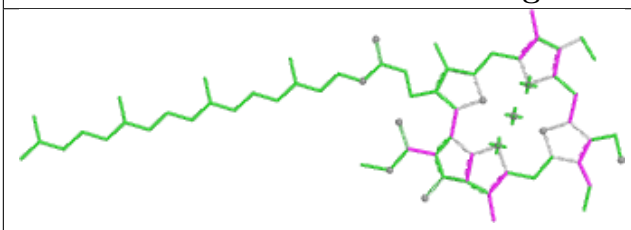


Torsions

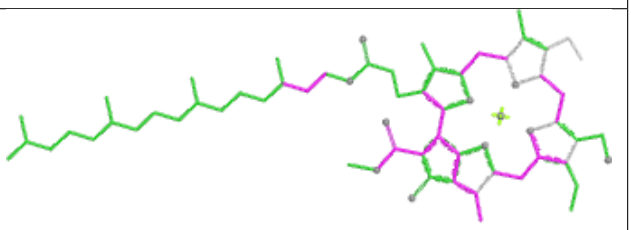


Rings

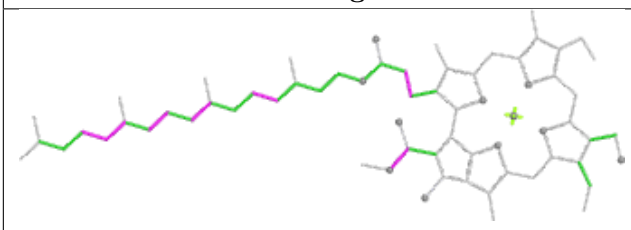
Ligand CHL N 607



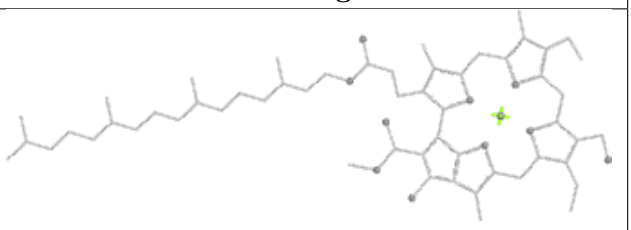
Bond lengths



Bond angles

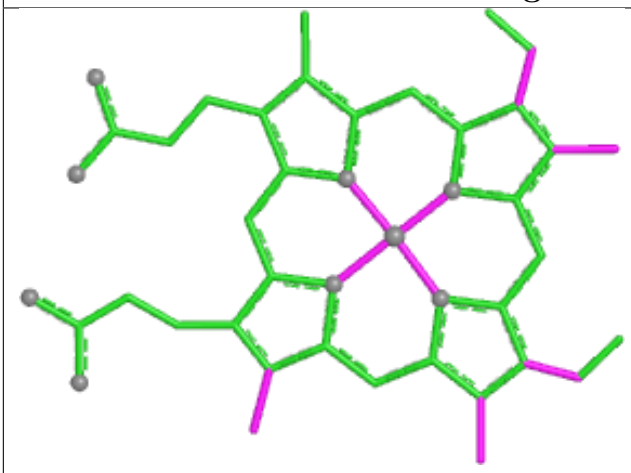


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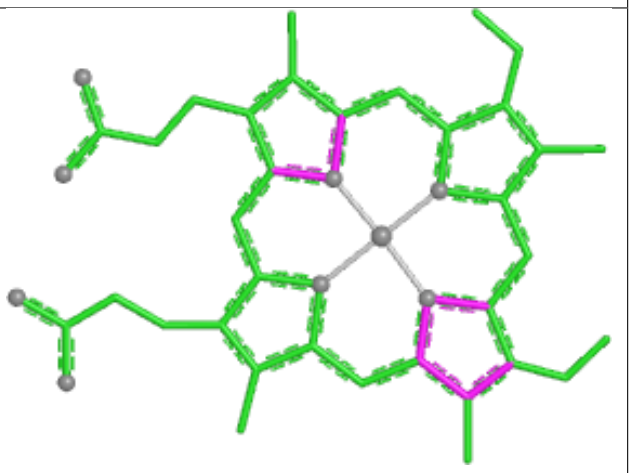


Rings

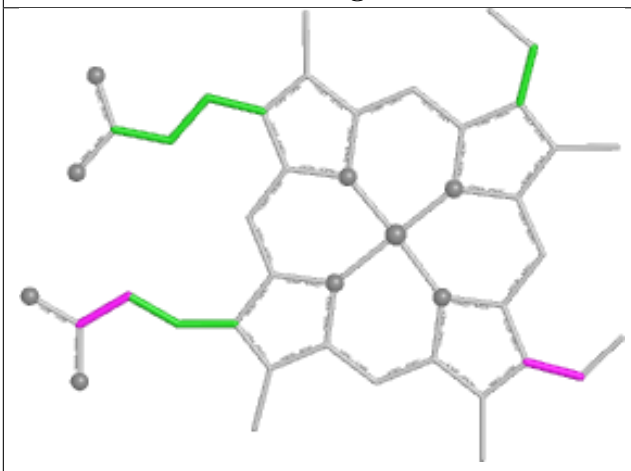
Ligand HEM e 101



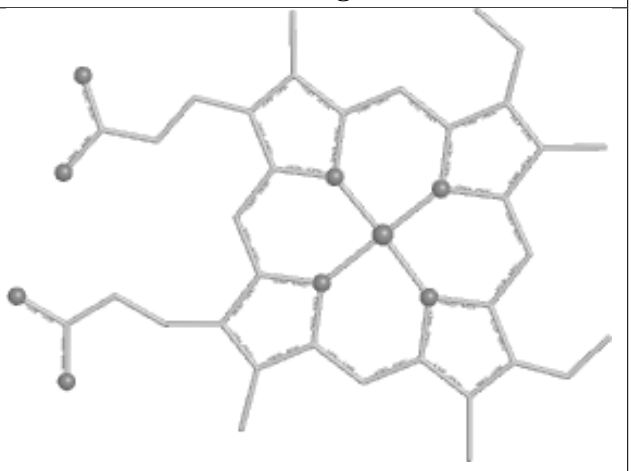
Bond lengths



Bond angles

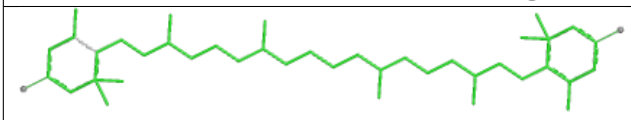


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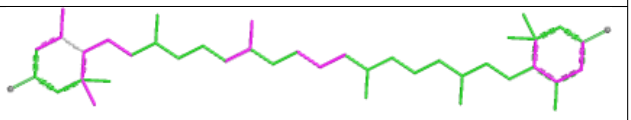


Rings

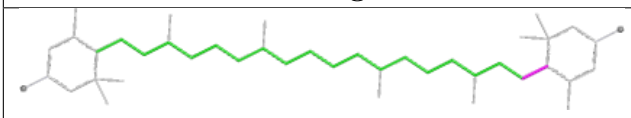
Ligand LUT G 615



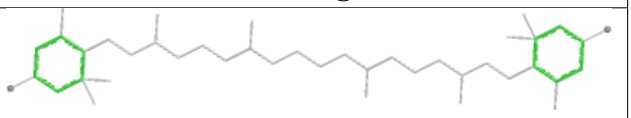
Bond lengths



Bond angles

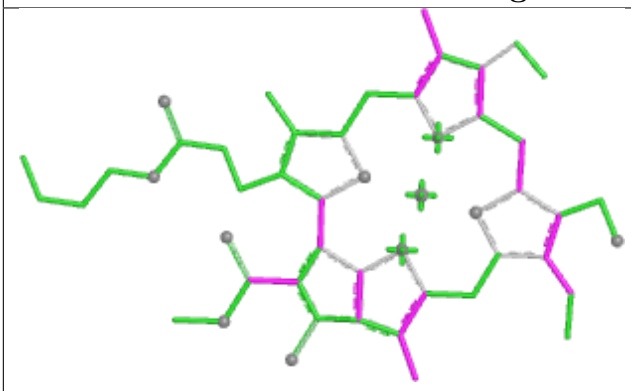


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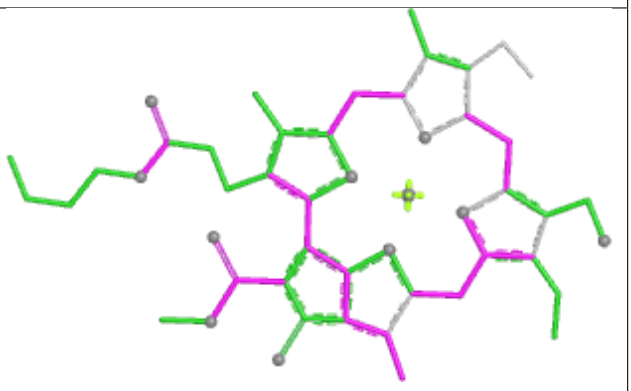


Rings

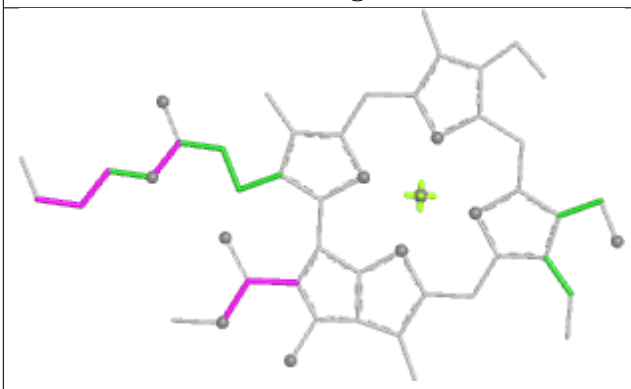
Ligand CHL YY 608



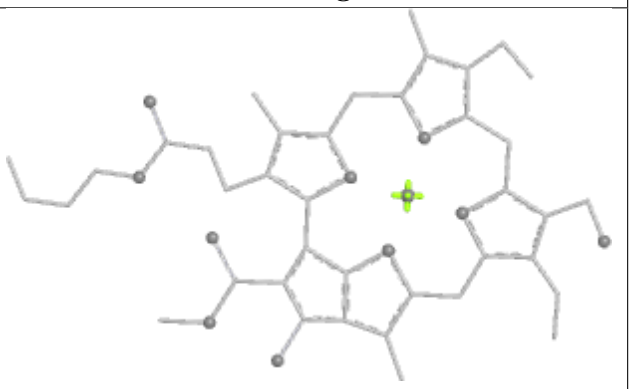
Bond lengths



Bond angles

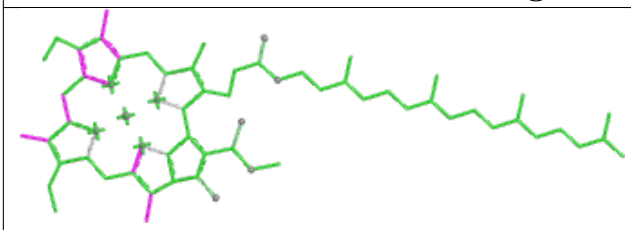


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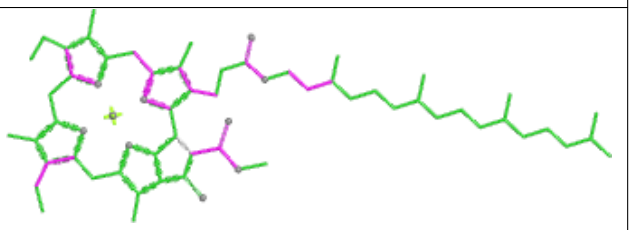


Rings

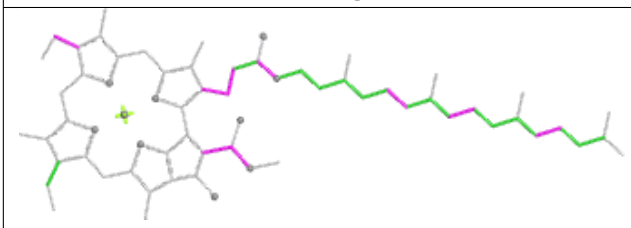
Ligand CLA n 602



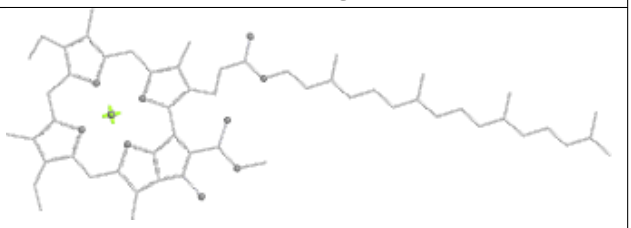
Bond lengths



Bond angles

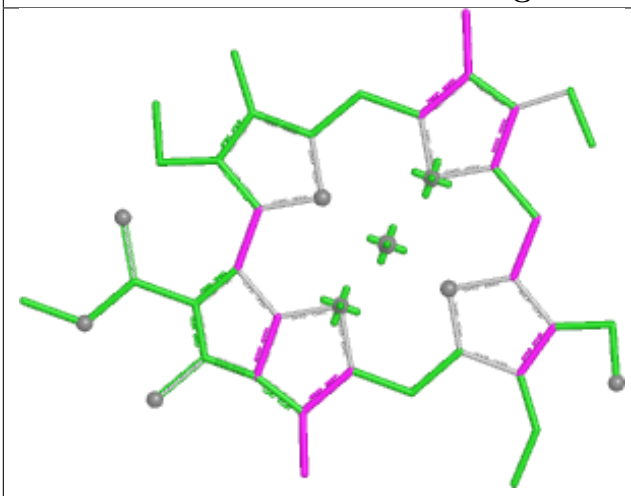


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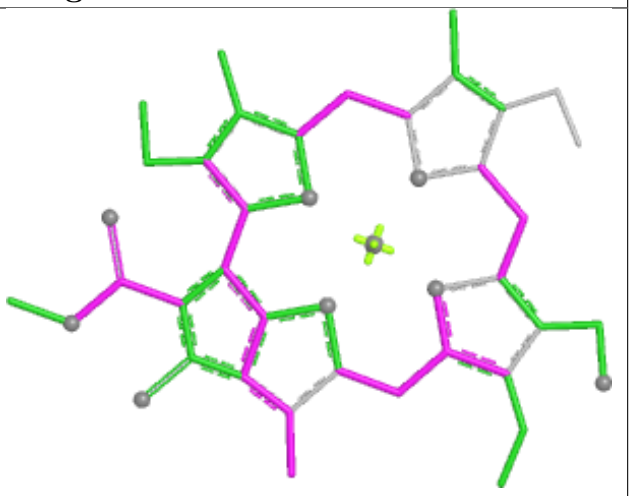


Rings

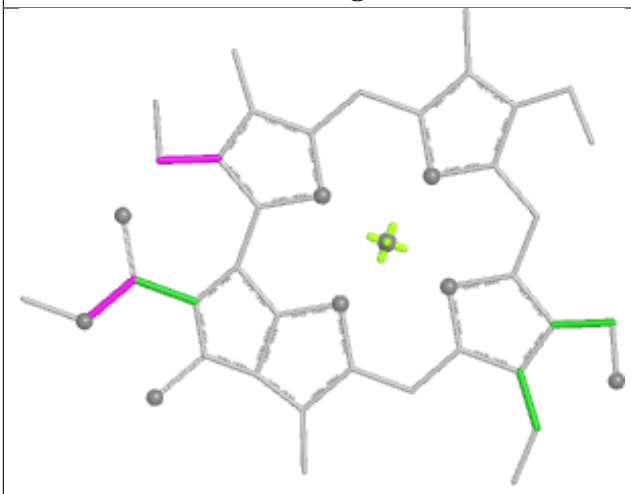
Ligand CHL Gg 307



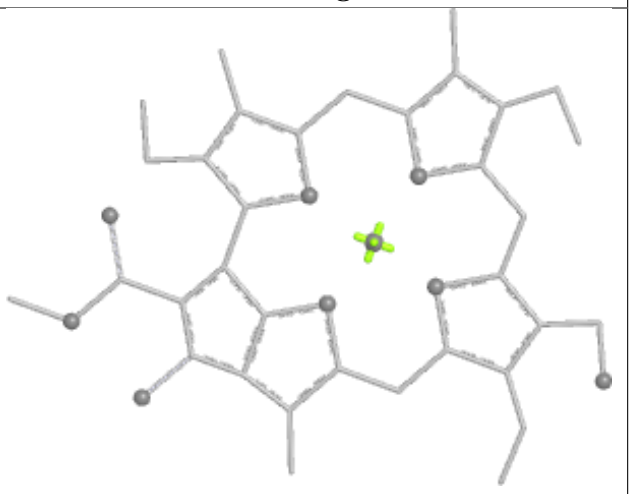
Bond lengths



Bond angles

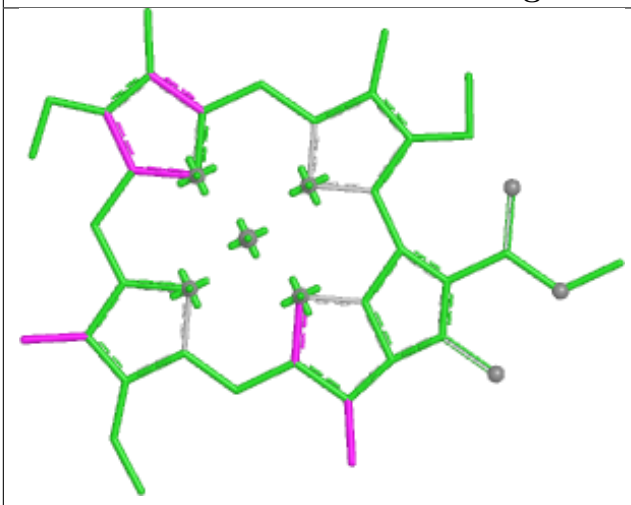


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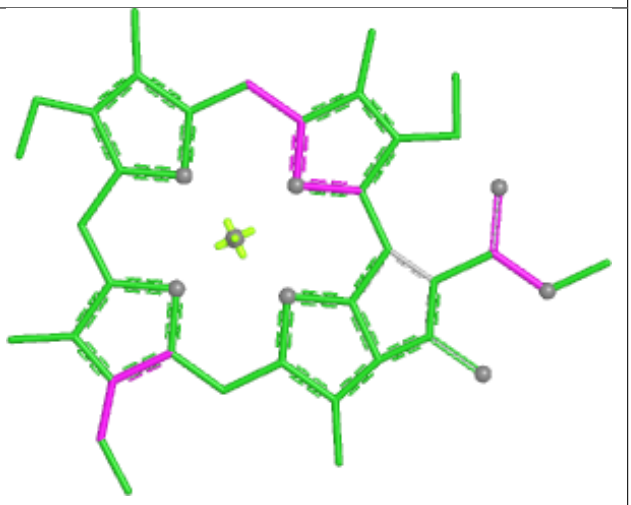


Rings

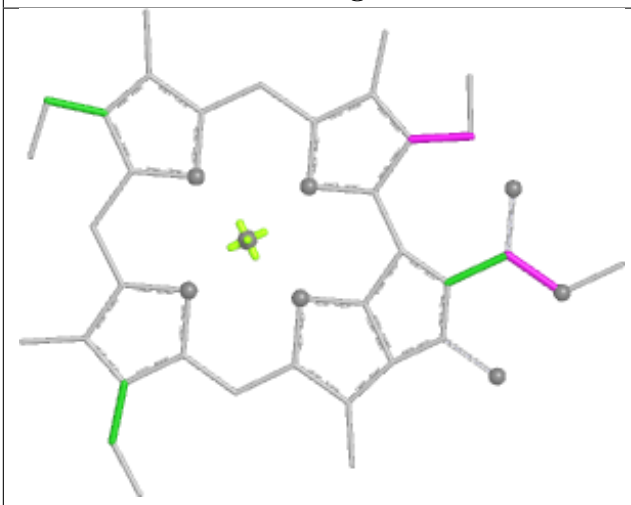
Ligand CLA N 612



Bond lengths



Bond angles

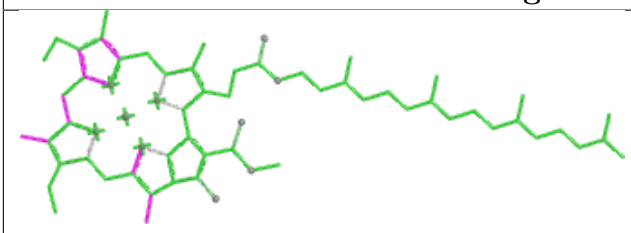


Torsions

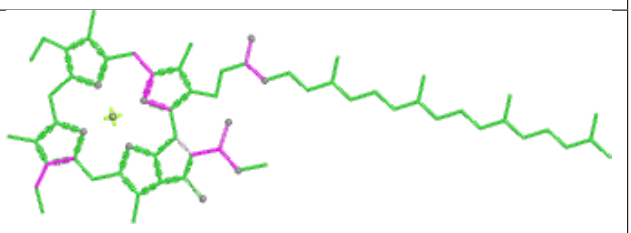


Rings

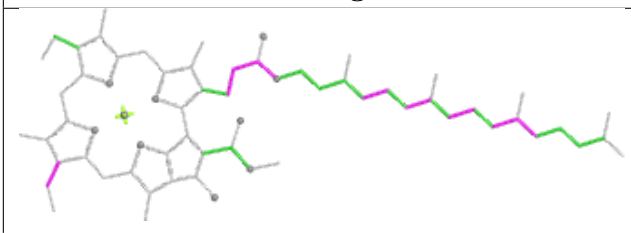
Ligand CLA D 404



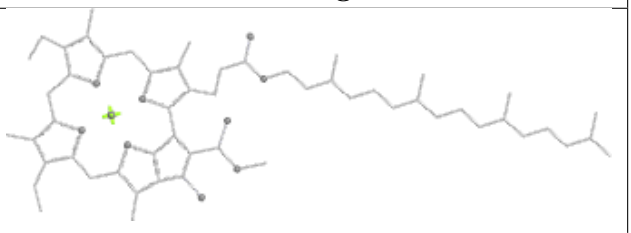
Bond lengths



Bond angles

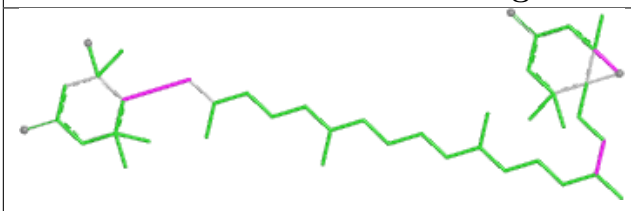


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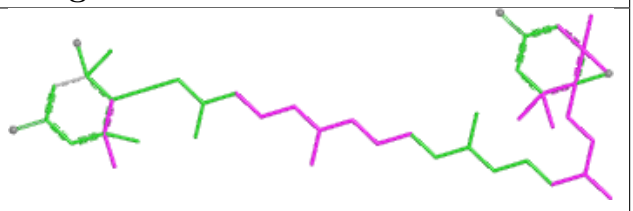


Rings

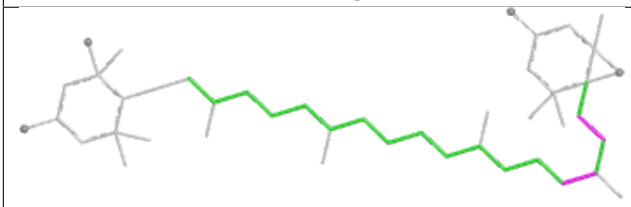
Ligand NEX Gg 318



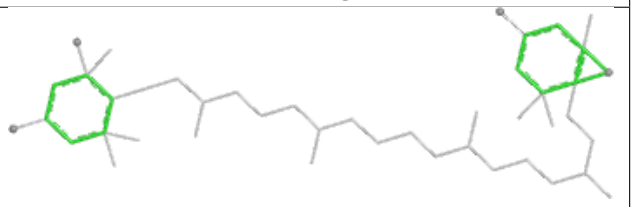
Bond lengths



Bond angles

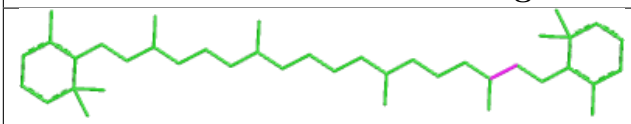


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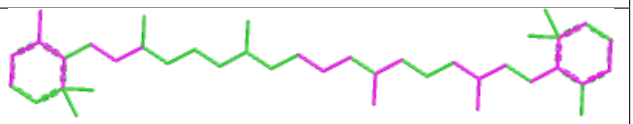


Rings

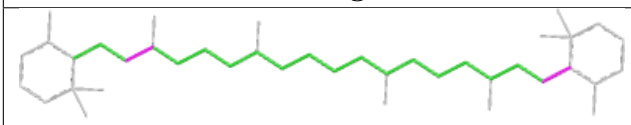
Ligand BCR Cc 518



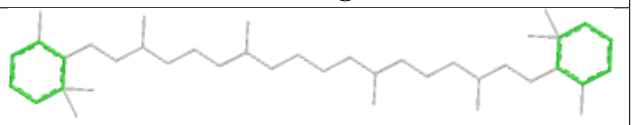
Bond lengths



Bond angles

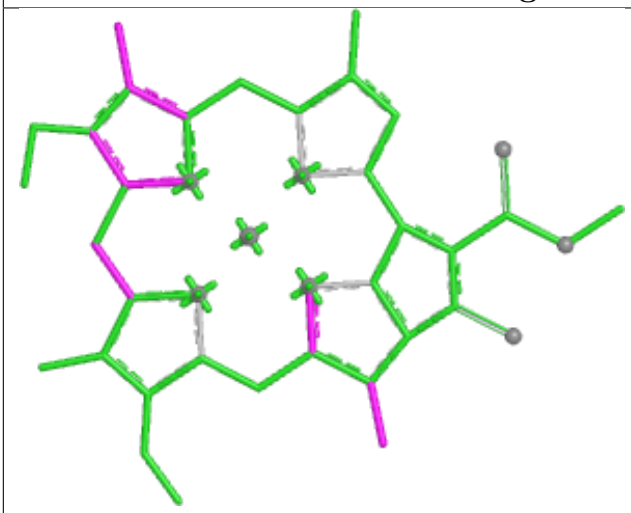


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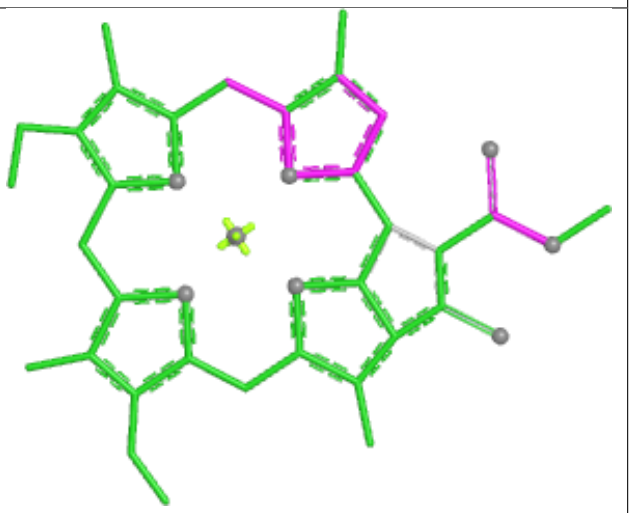


Rings

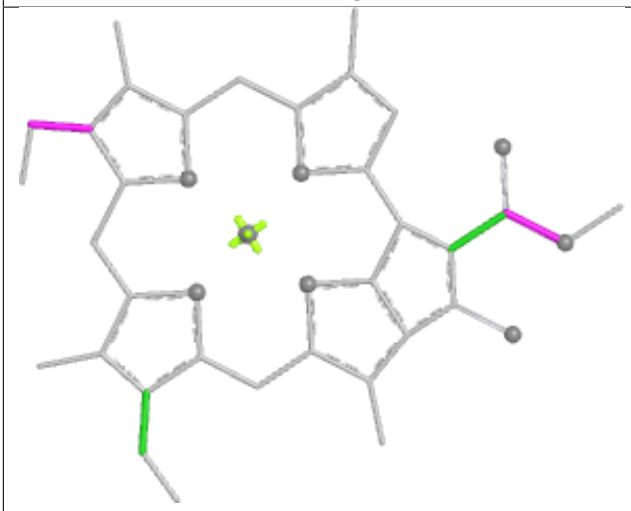
Ligand CLA 33 602



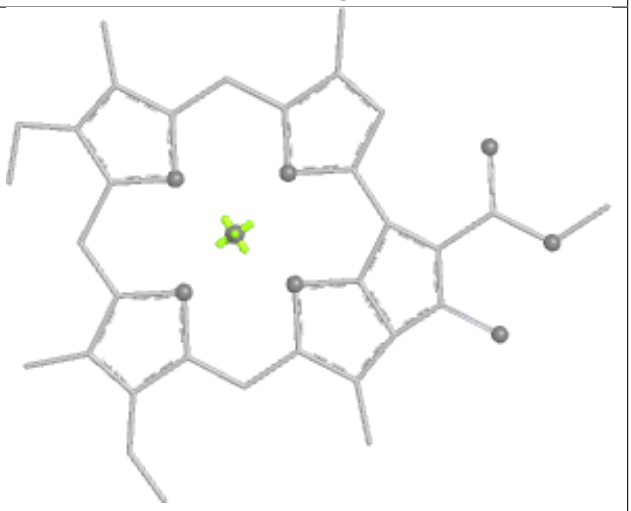
Bond lengths



Bond angles

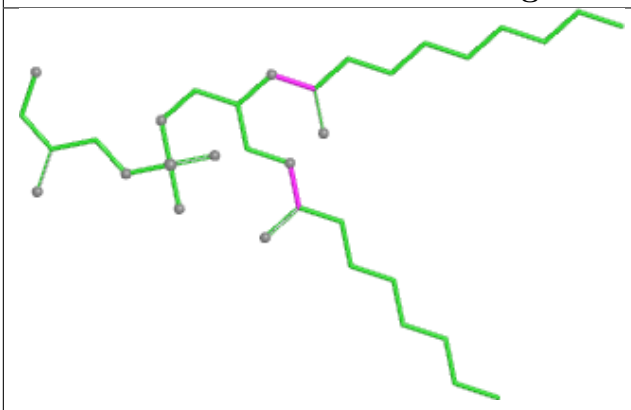


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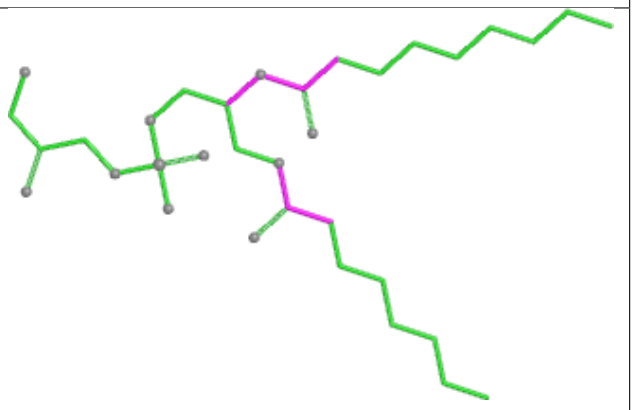


Rings

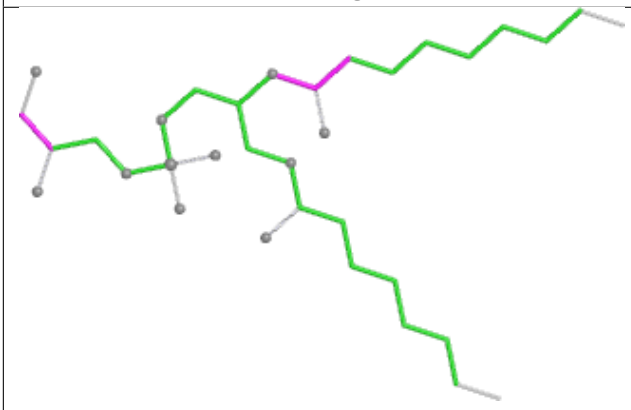
Ligand LHG G 618



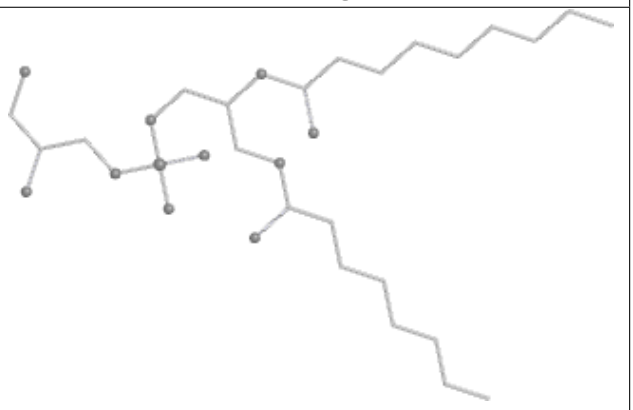
Bond lengths



Bond angles

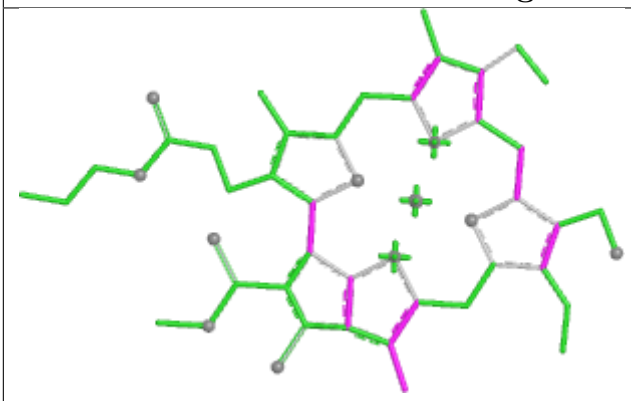


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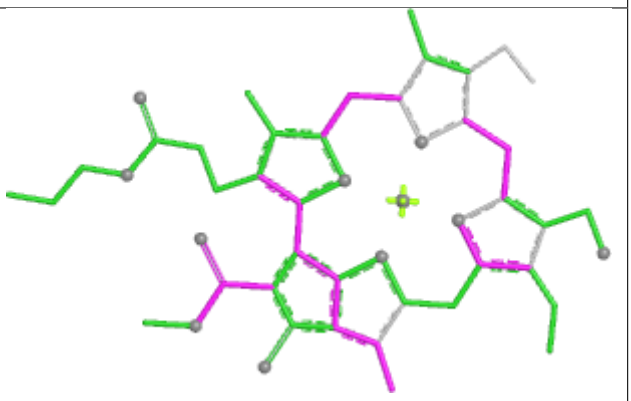


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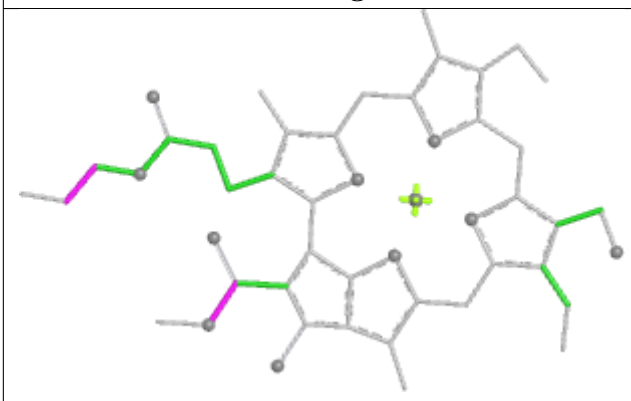
Ligand CHL SS 308



Bond lengths



Bond angles

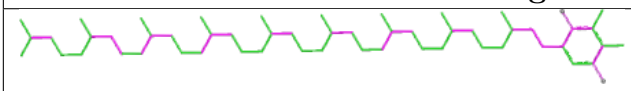


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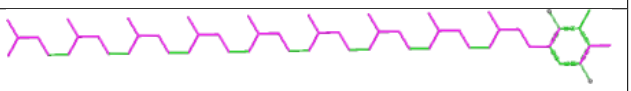


Rings

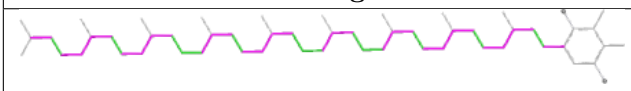
Ligand PL9 D 407



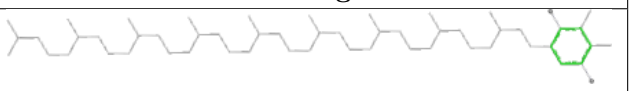
Bond lengths



Bond angles

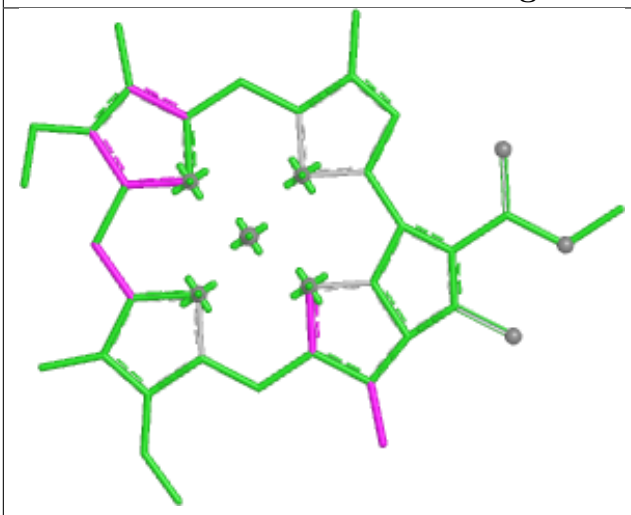


Torsions

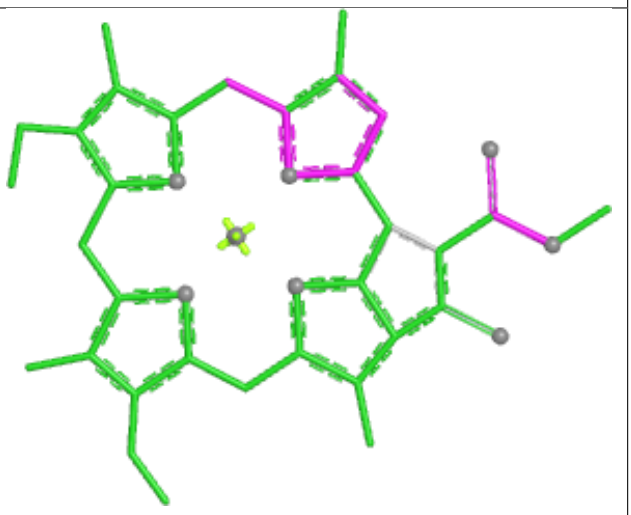


Rings

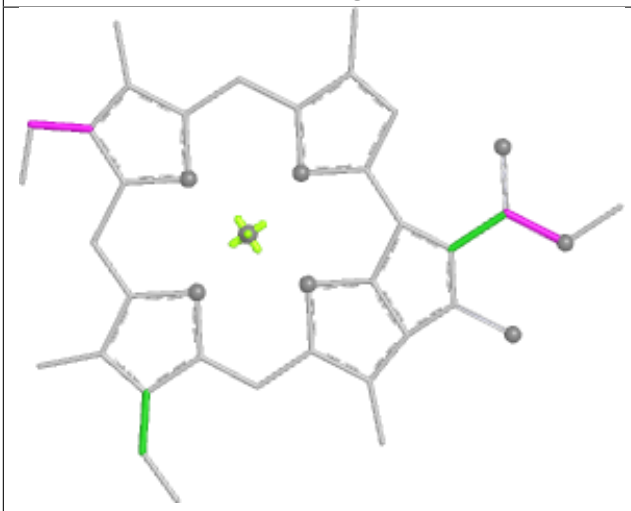
Ligand CLA 11 610



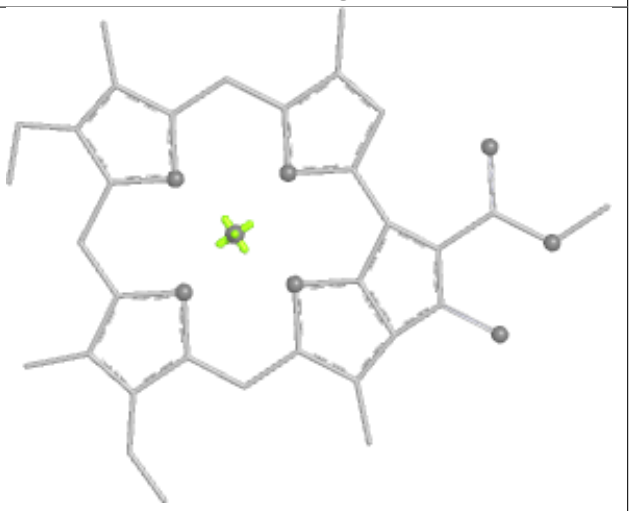
Bond lengths



Bond angles

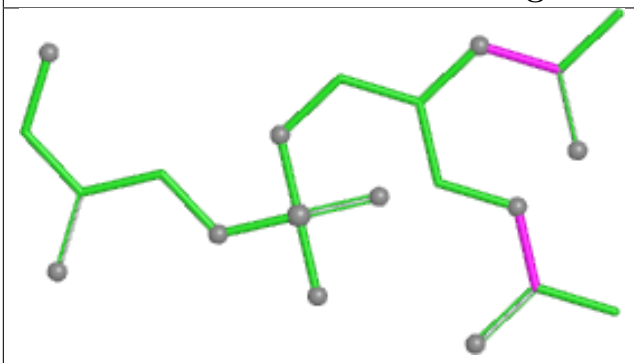


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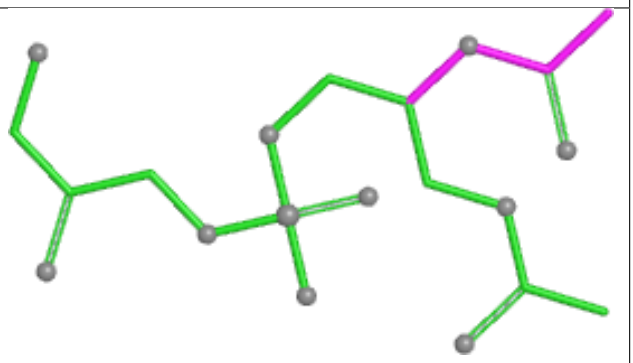


Rings

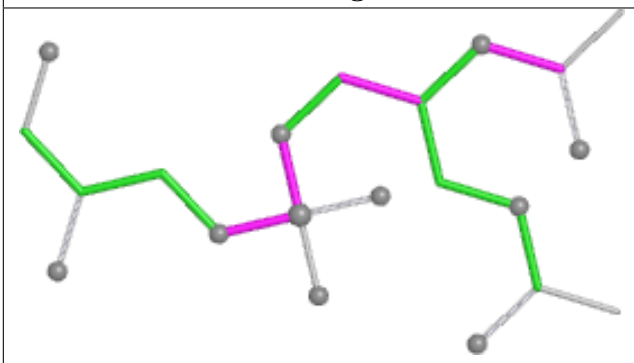
Ligand LHG 4 315



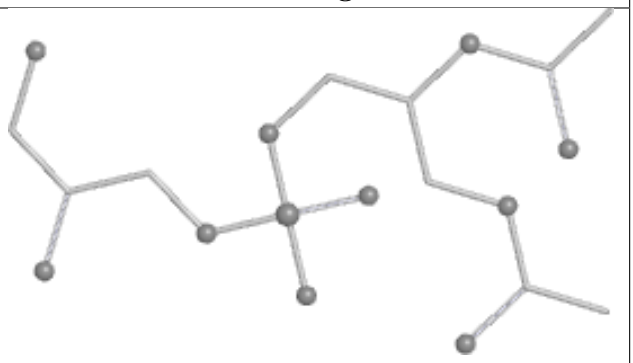
Bond lengths



Bond angles

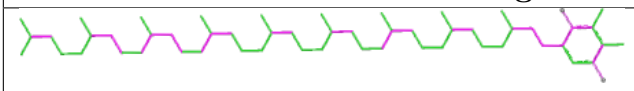


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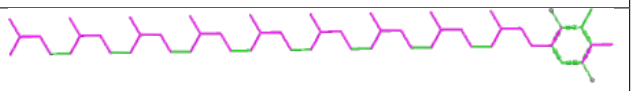


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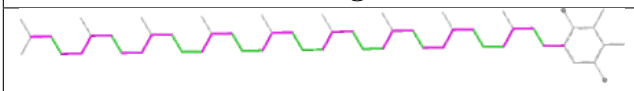
Ligand PL9 DD 406



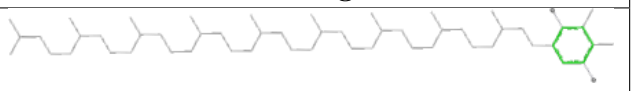
Bond lengths



Bond angles

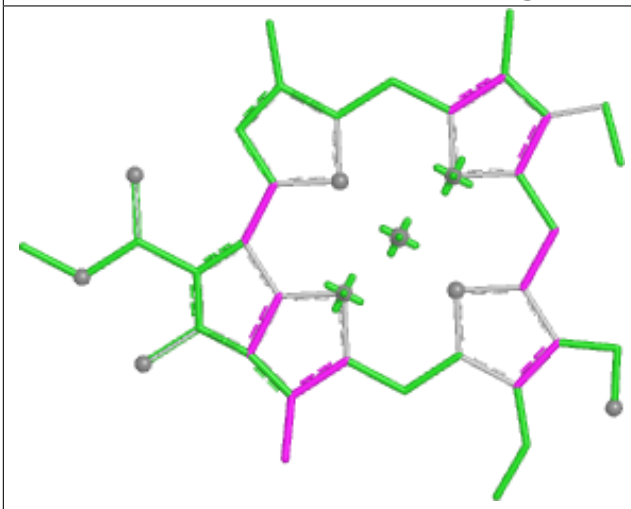


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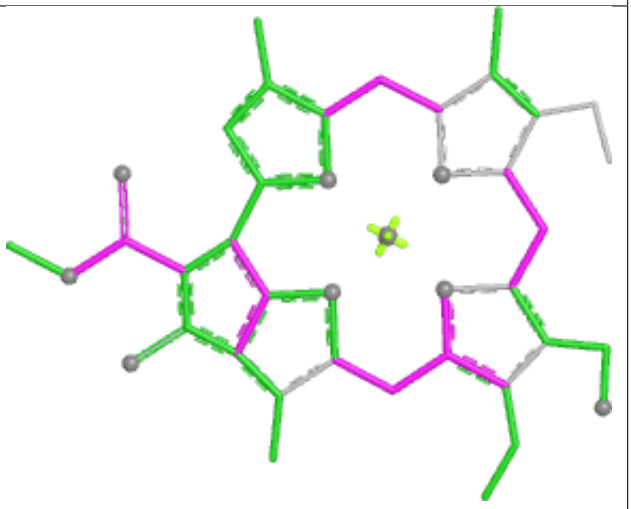


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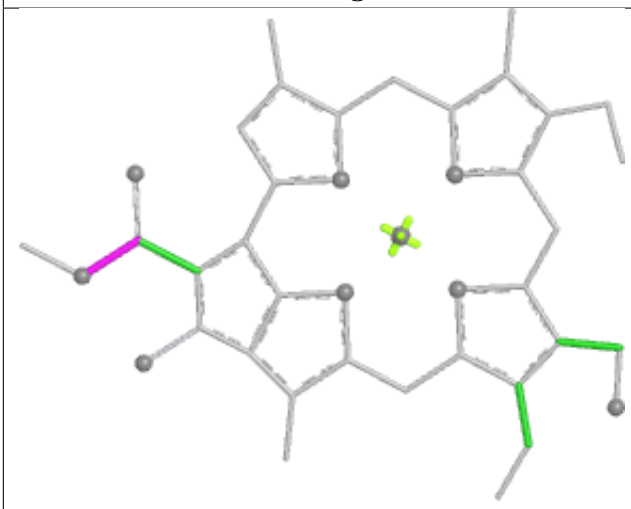
Ligand CHL 22 607



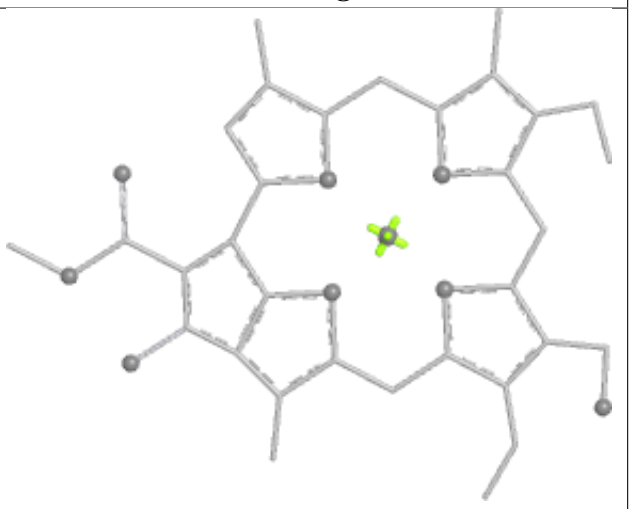
Bond lengths



Bond angles

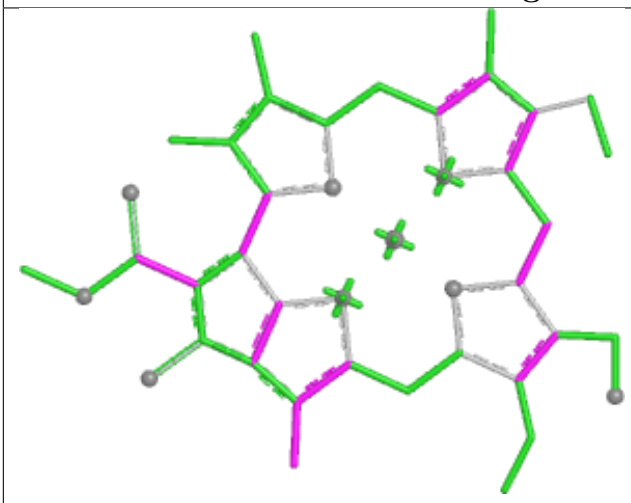


Torsions



Rings

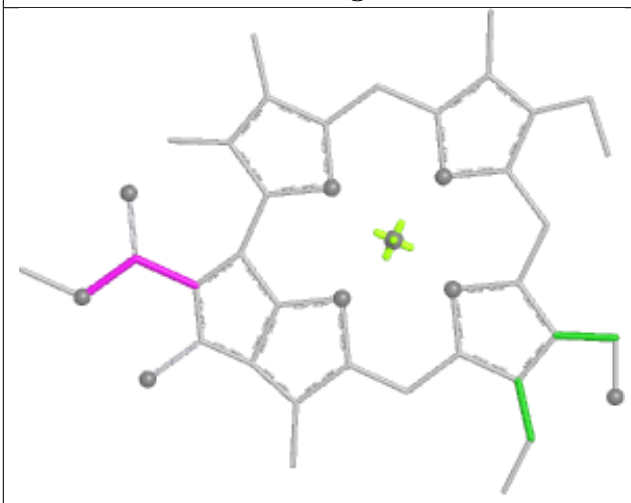
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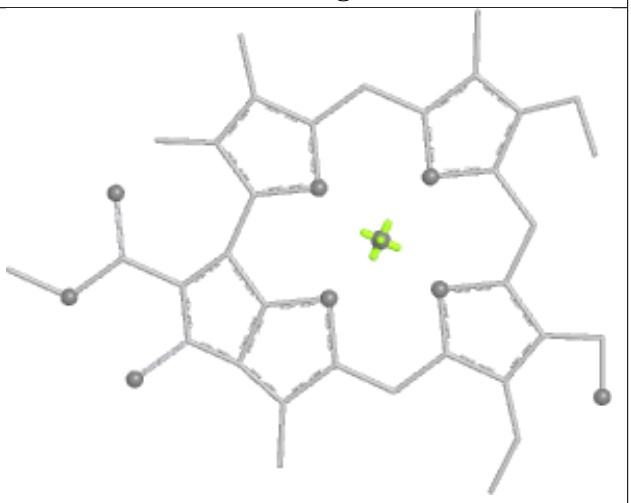
Bond lengths



Bond angles

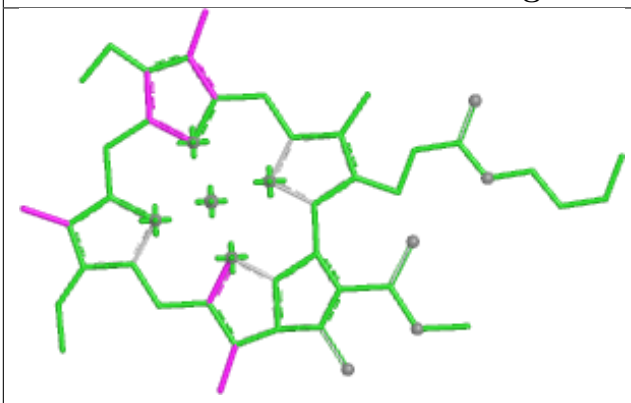


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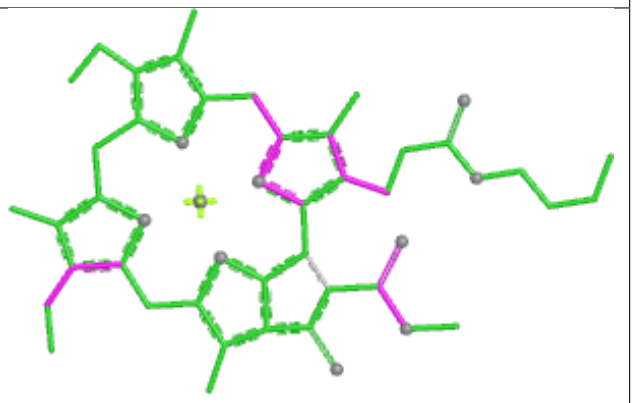


Rings

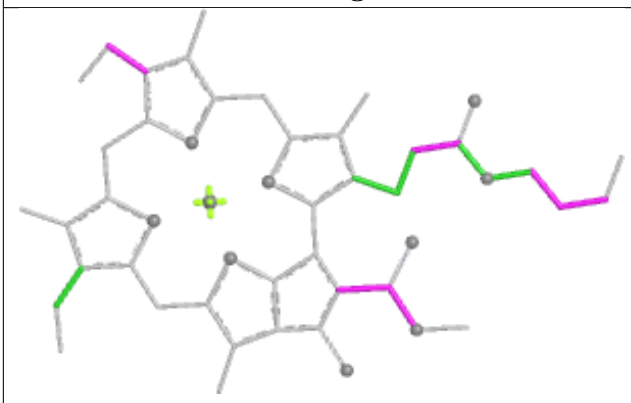
Ligand CLA G 612



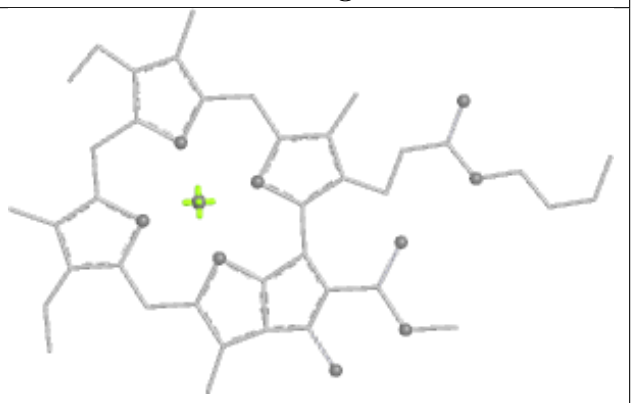
Bond lengths



Bond angles

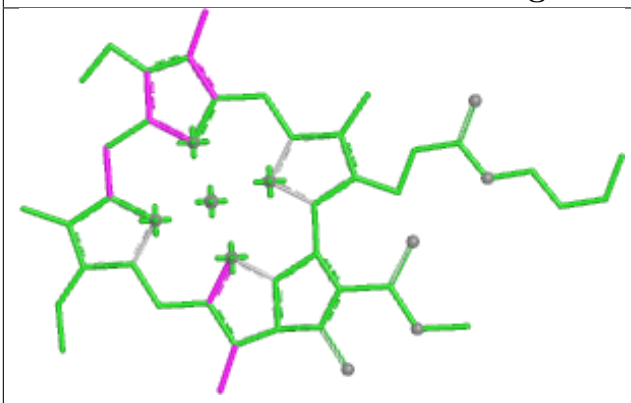


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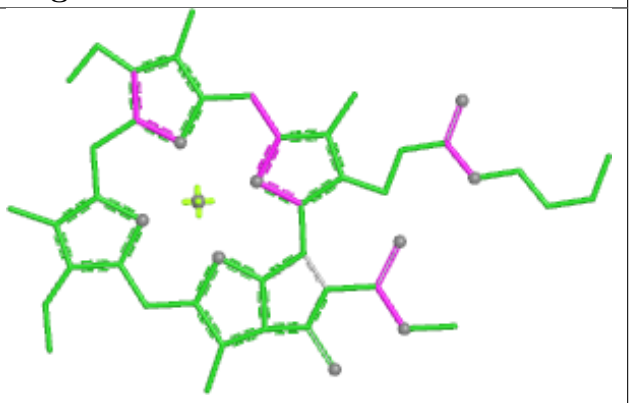


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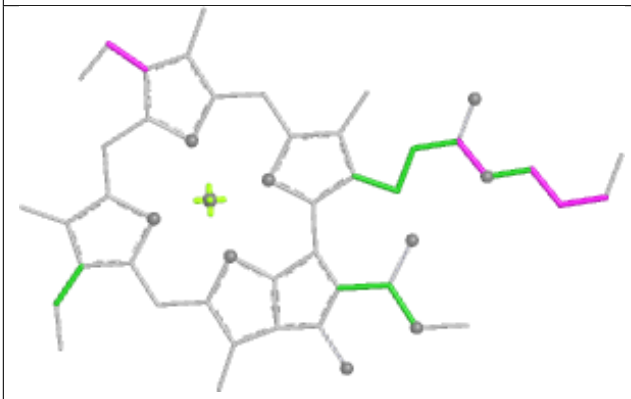
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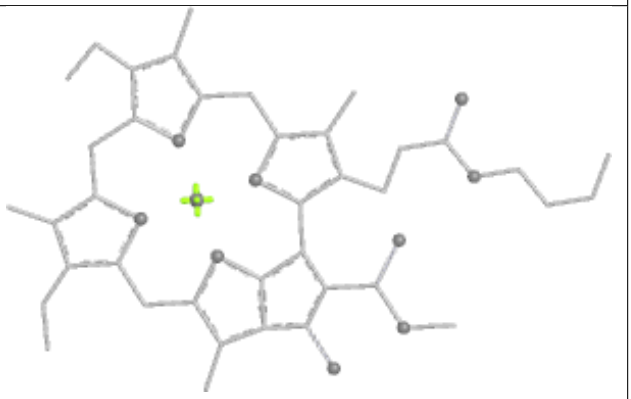
Bond lengths



Bond angles



Torsions

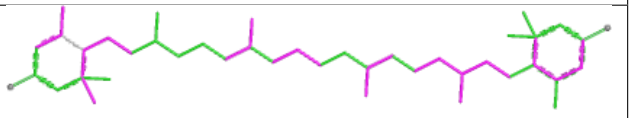


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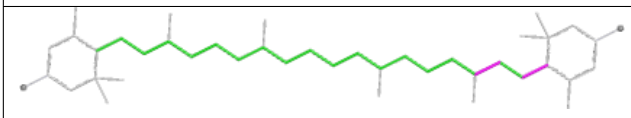
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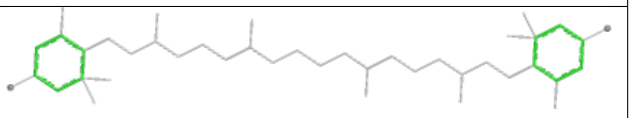
Bond lengths



Bond angles

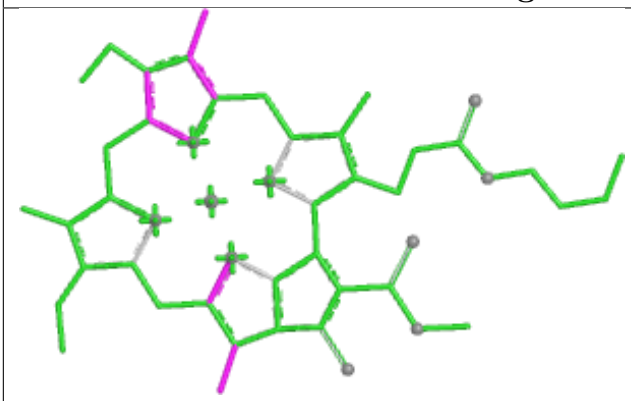


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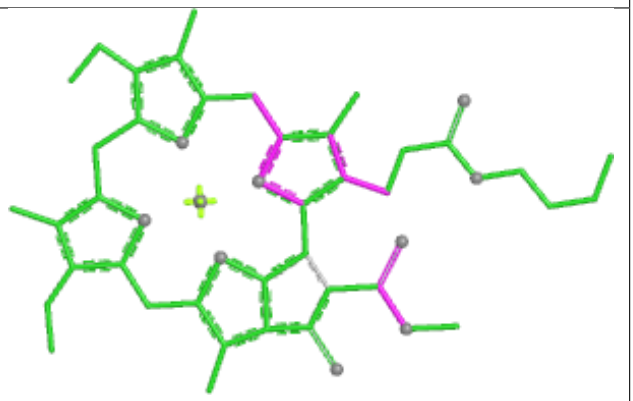


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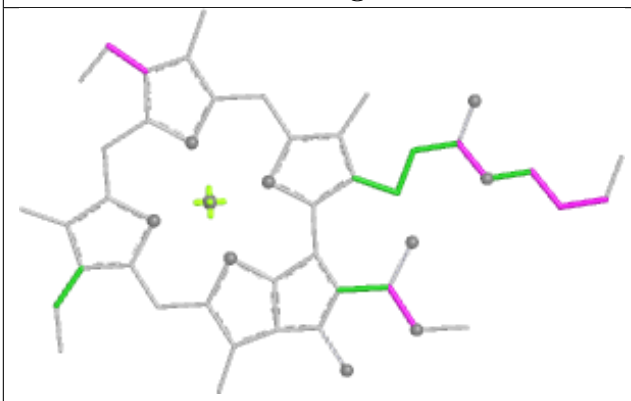
Ligand CLA SS 311



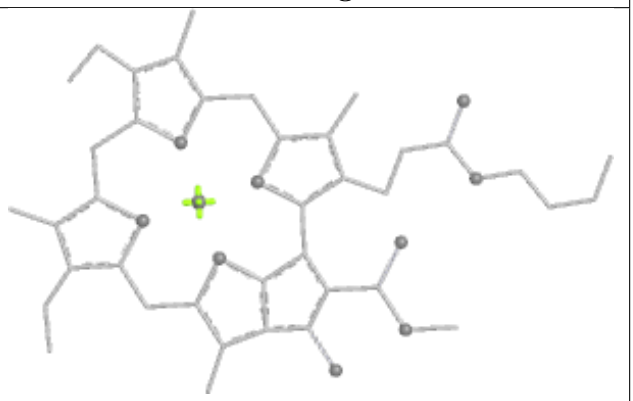
Bond lengths



Bond angles

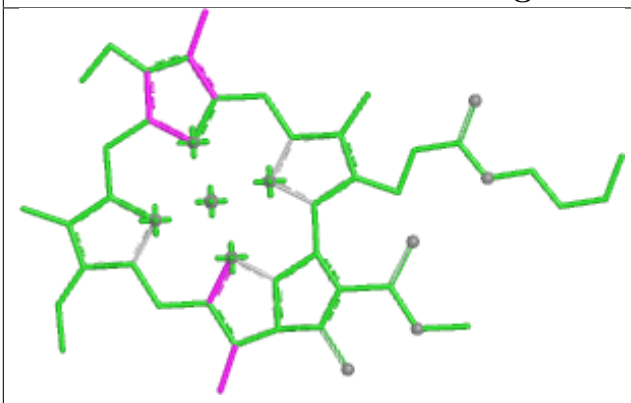


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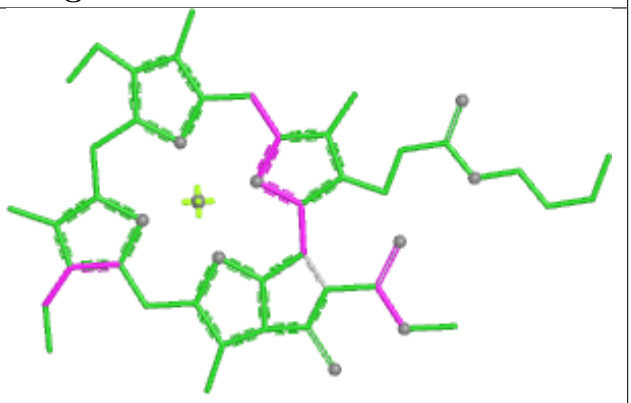


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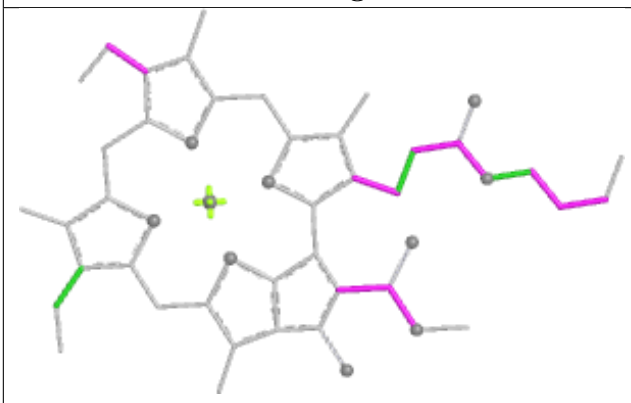
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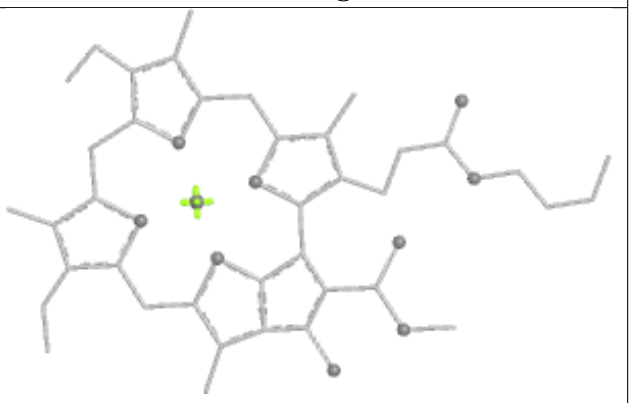
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Bond angles

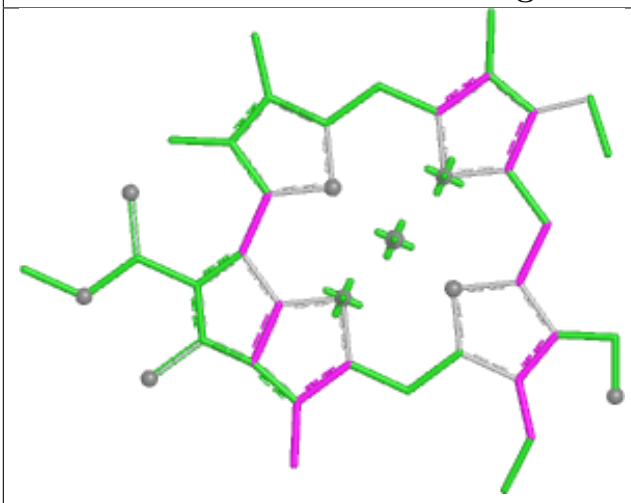


Torsions



Rings

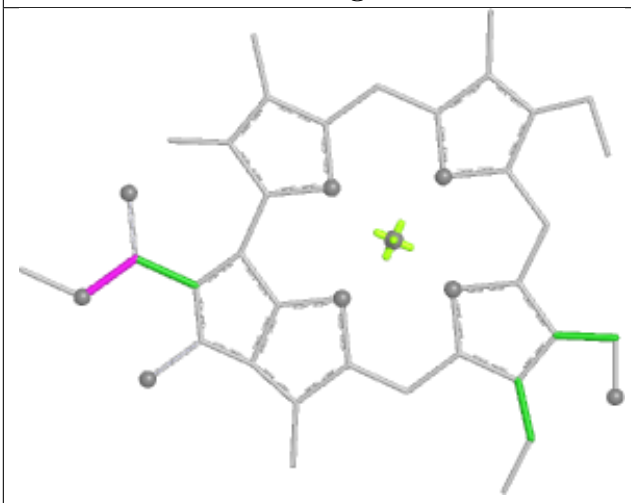
Ligand CHL SS 306



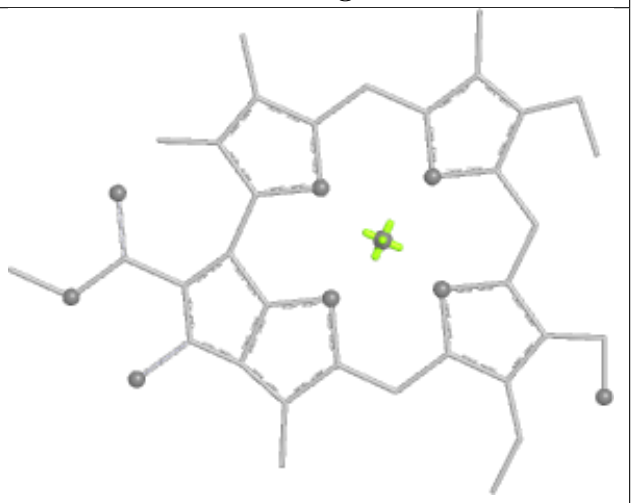
Bond lengths



Bond angles

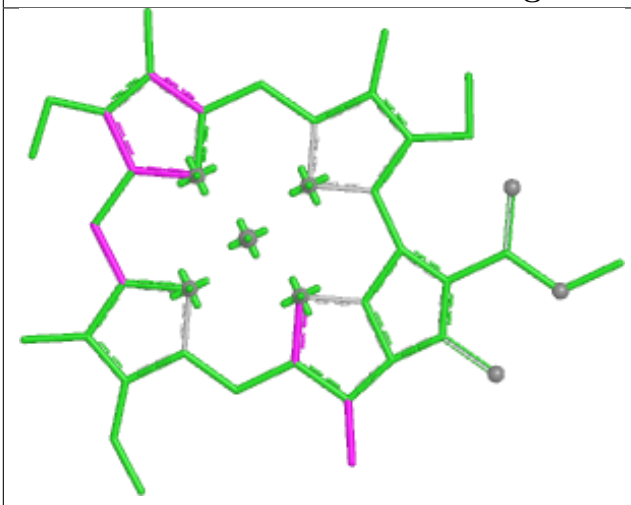


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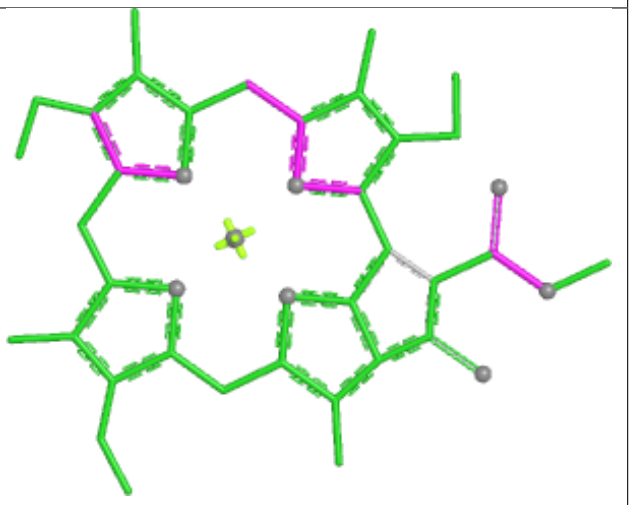


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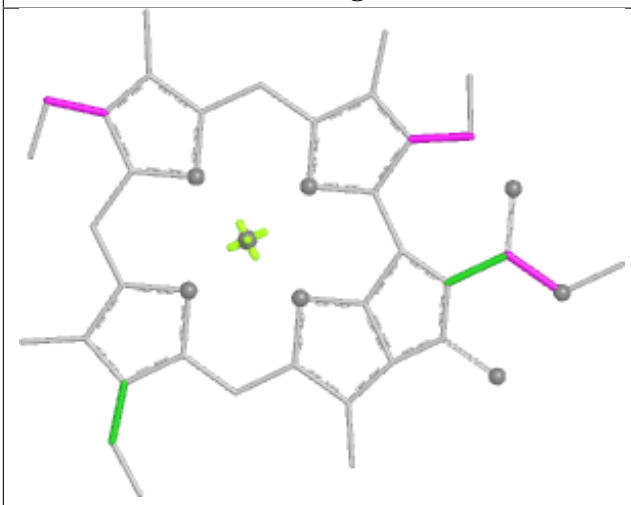
Ligand CLA Y 611



Bond lengths



Bond angles

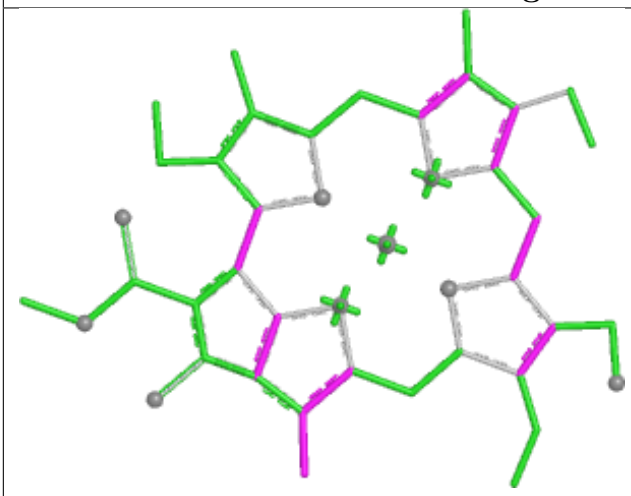


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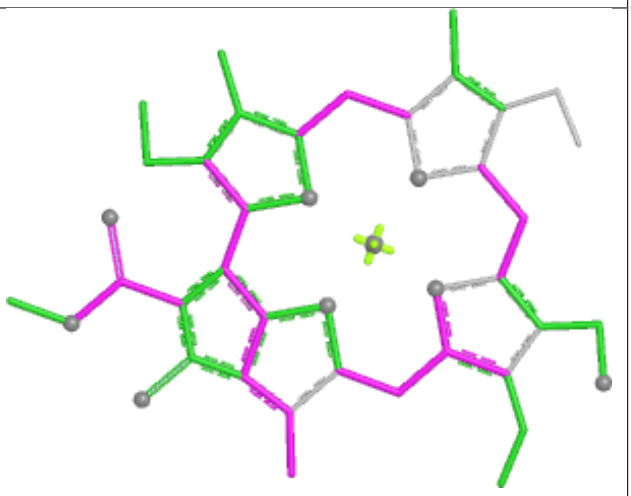


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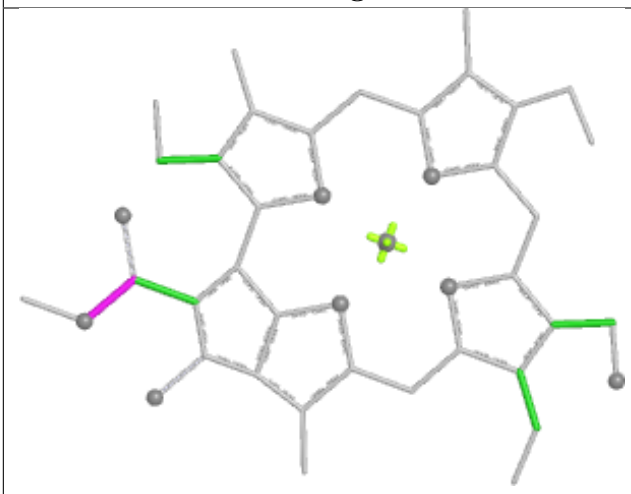
Ligand CHL G 605



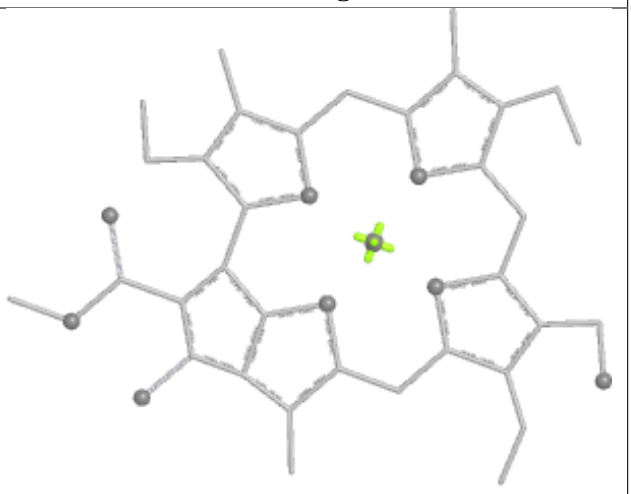
Bond lengths



Bond angles

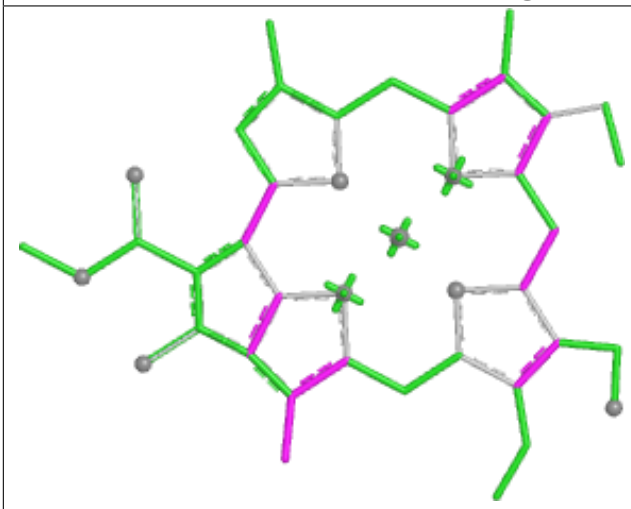


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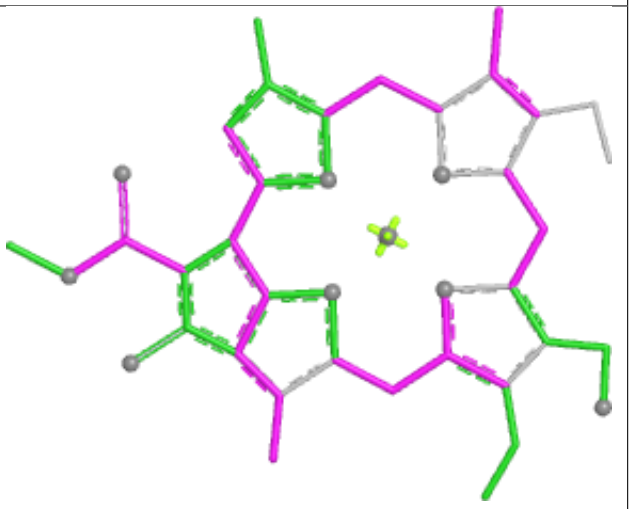


Rings

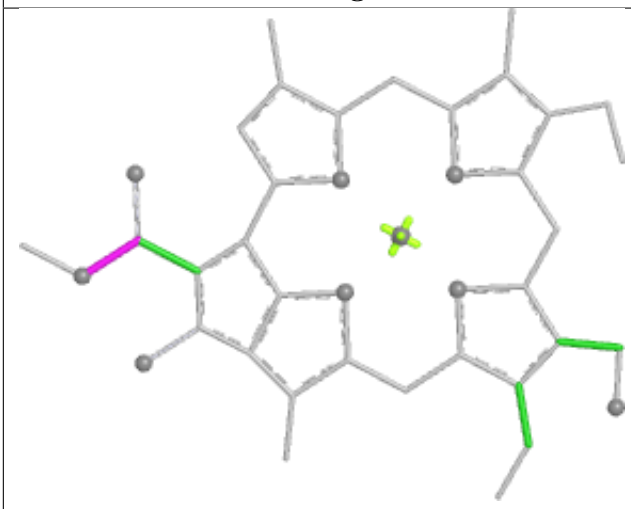
Ligand CHL 22 605



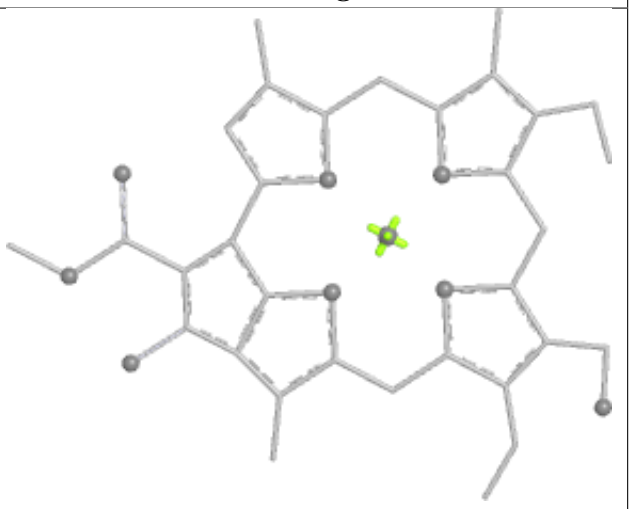
Bond lengths



Bond angles

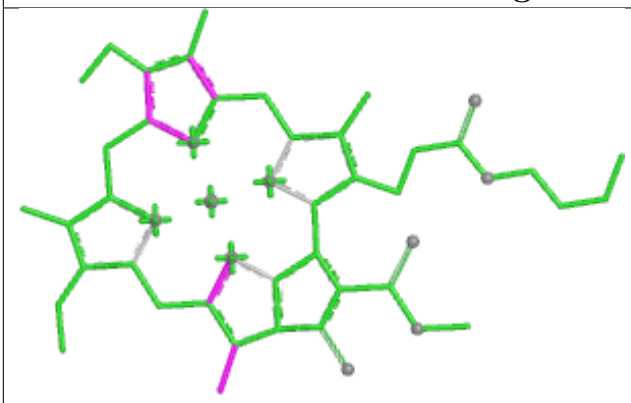


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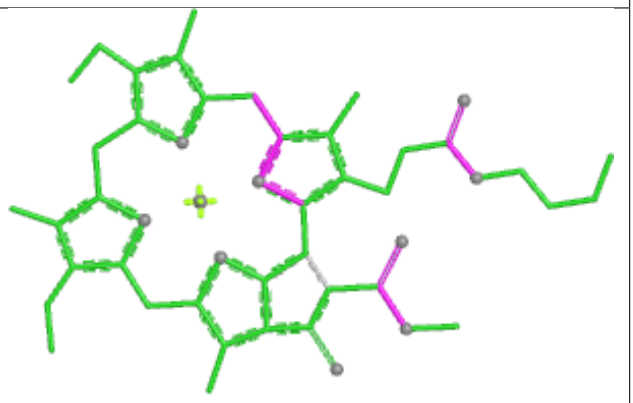


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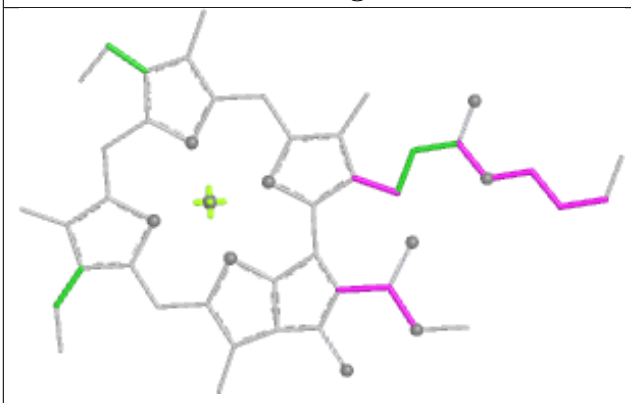
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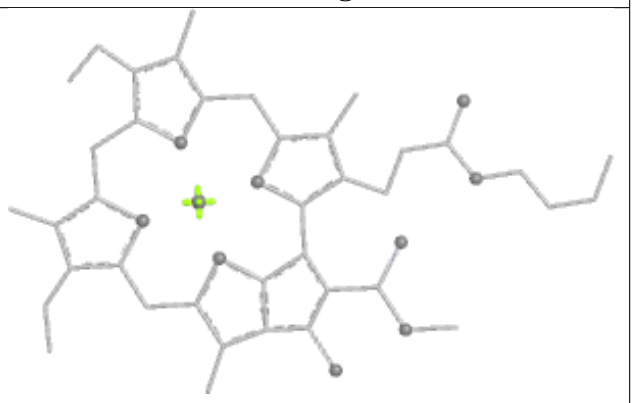
Bond lengths



Bond angles

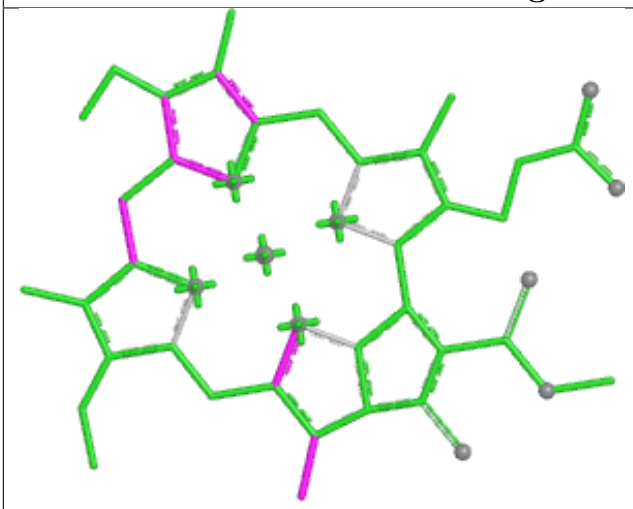


Torsions

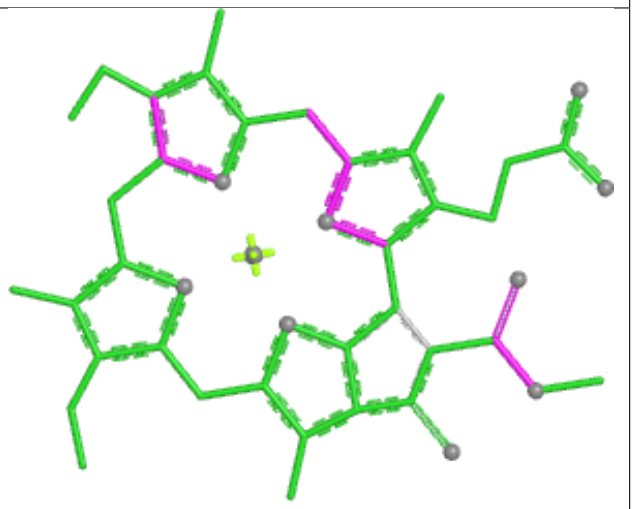


Rings

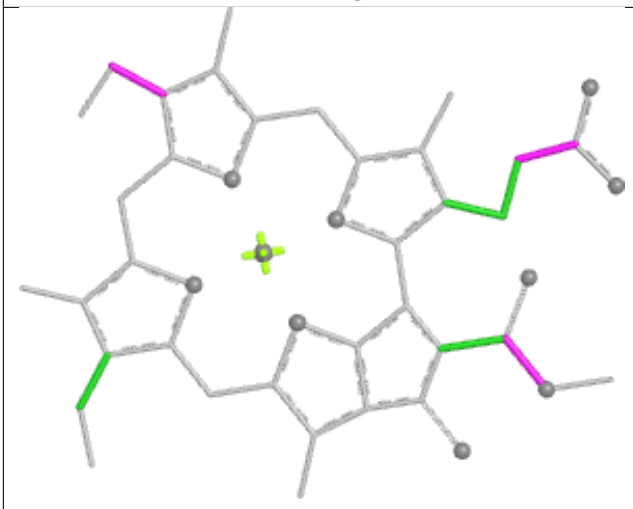
Ligand CLA 4 311



Bond lengths



Bond angles

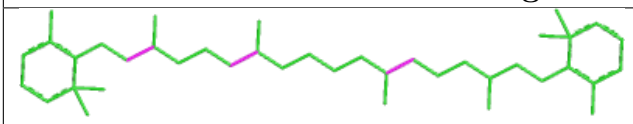


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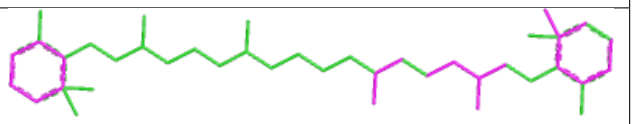


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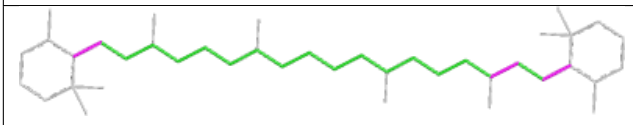
Ligand BCR A 409



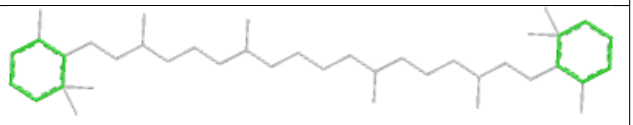
Bond lengths



Bond angles

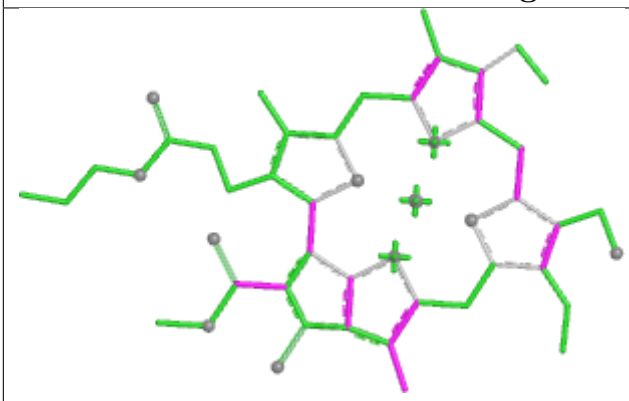


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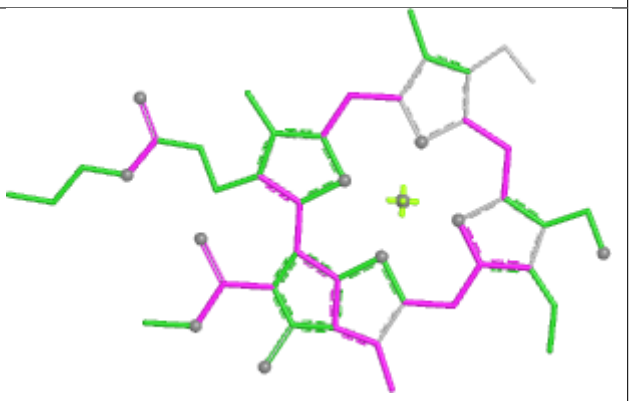


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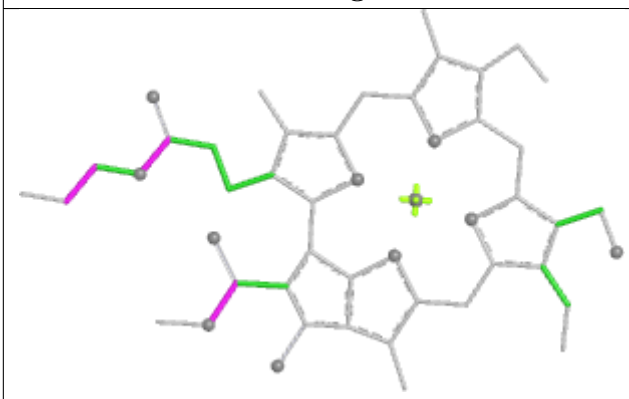
Ligand CHL Ss 607



Bond lengths



Bond angles

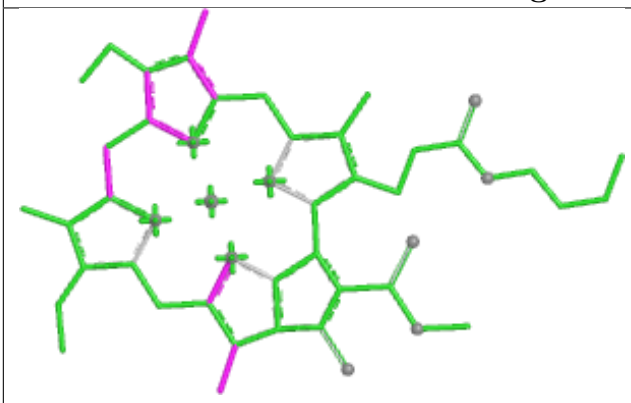


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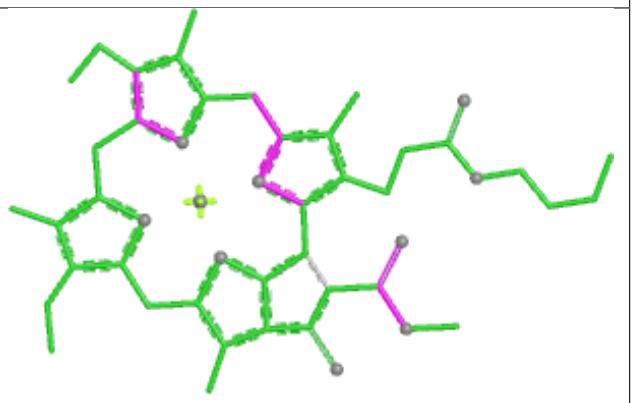


Rings

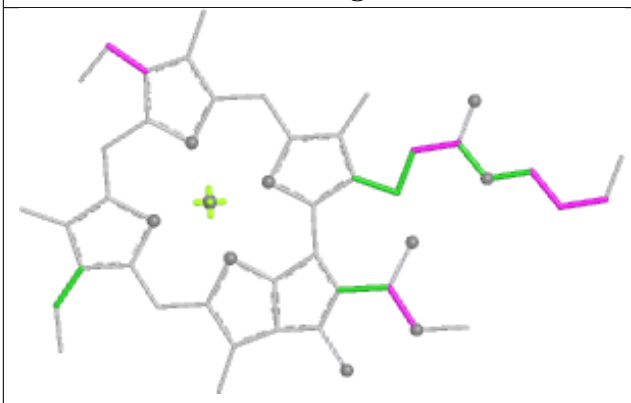
Ligand CLA r 603



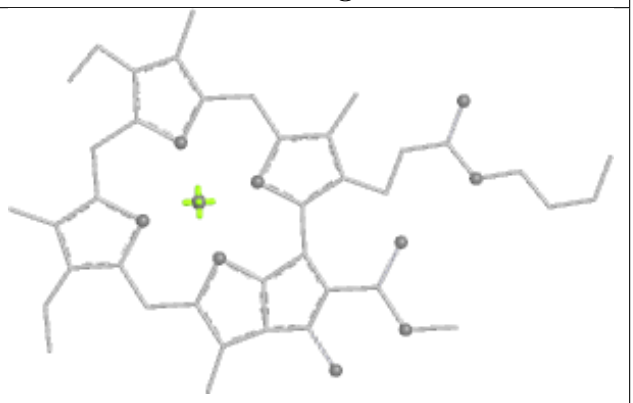
Bond lengths



Bond angles

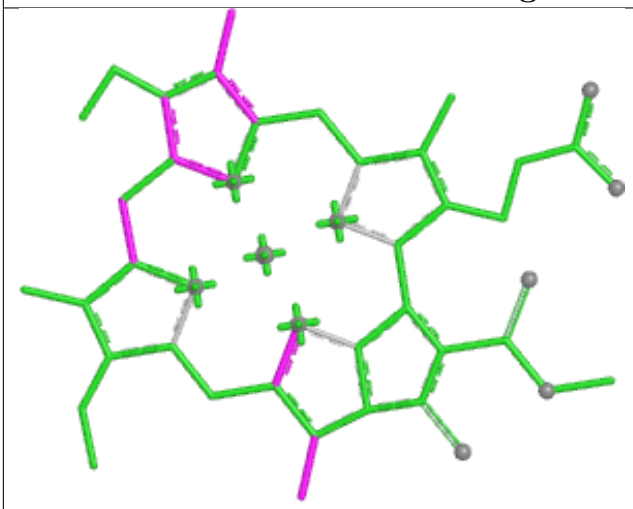


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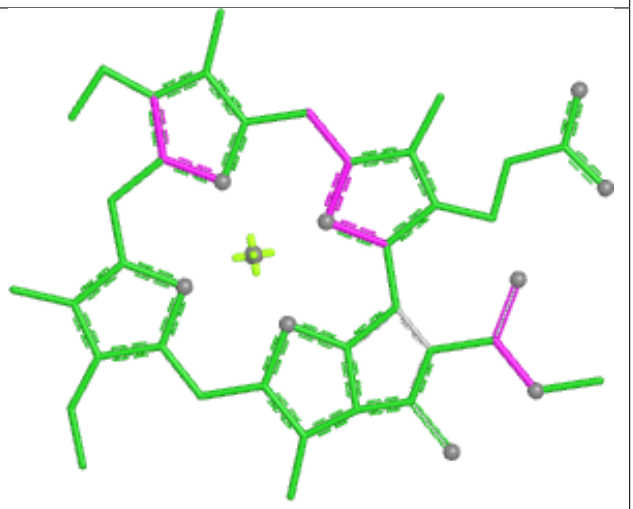


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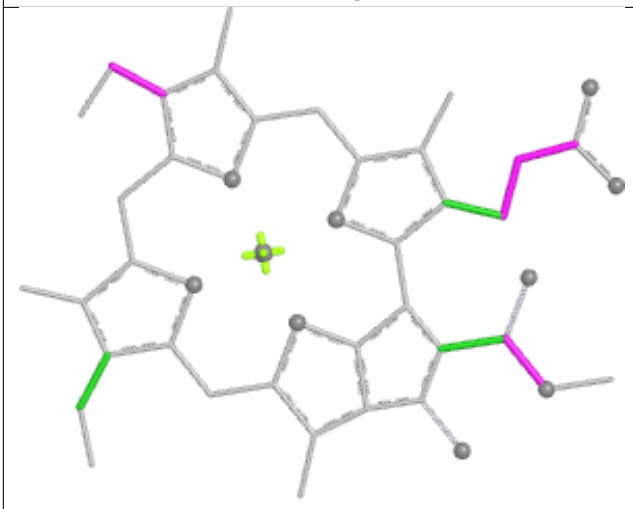
Ligand CLA 44 604



Bond lengths



Bond angles

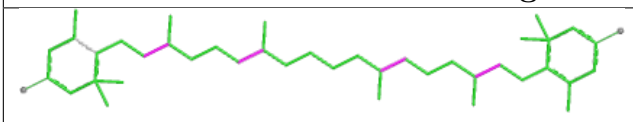


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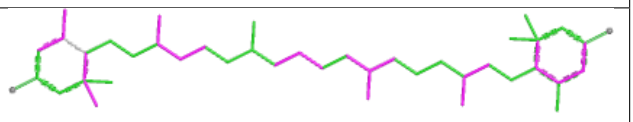


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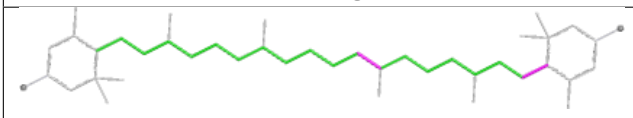
Ligand LUT 22 614



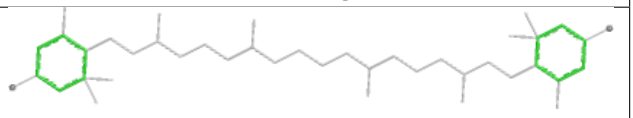
Bond lengths



Bond angles

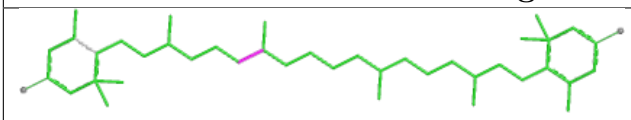


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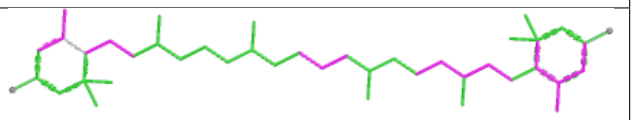


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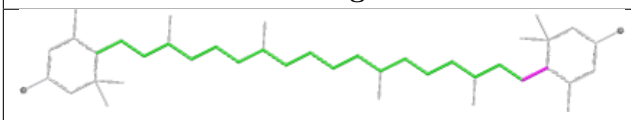
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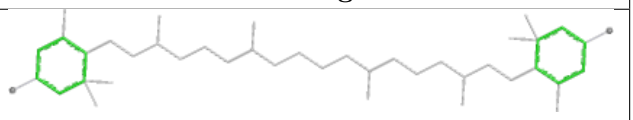
Bond lengths



Bond angles

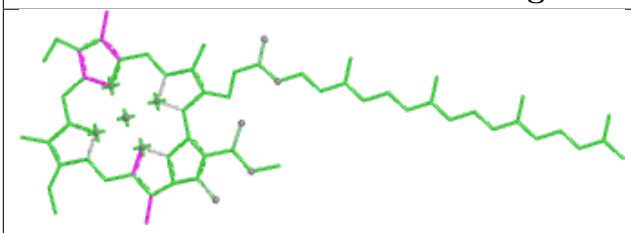


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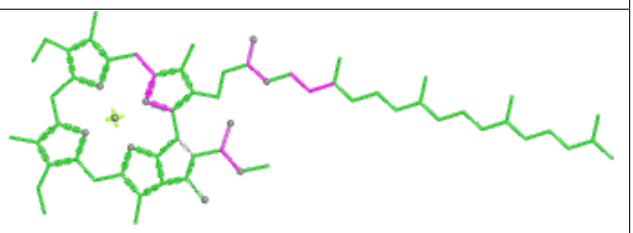


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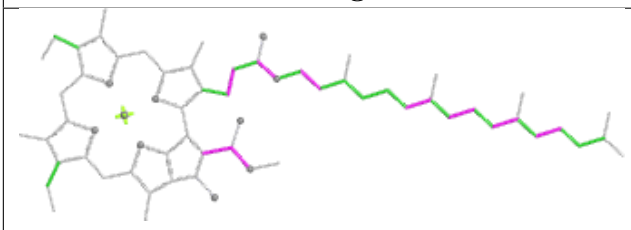
Ligand CLA b 612



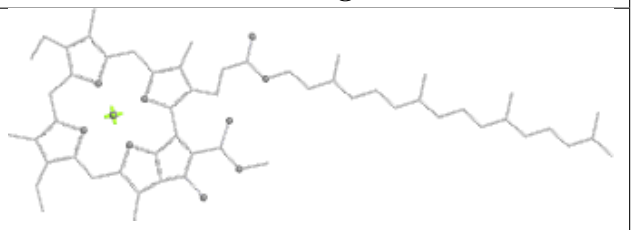
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Bond angles

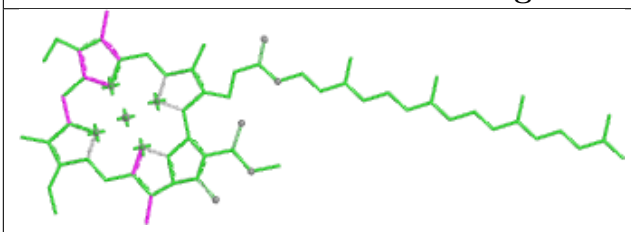


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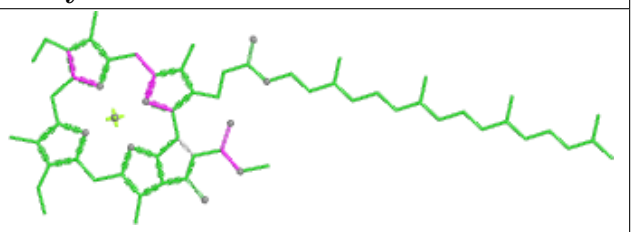


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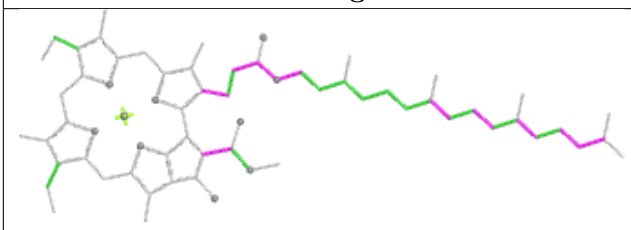
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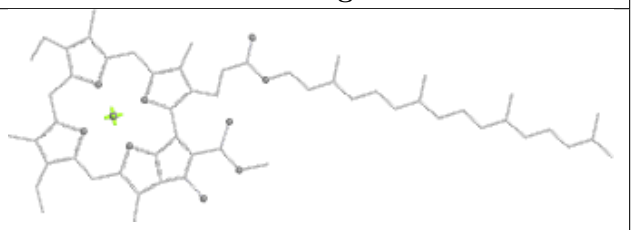
Bond lengths



Bond angles

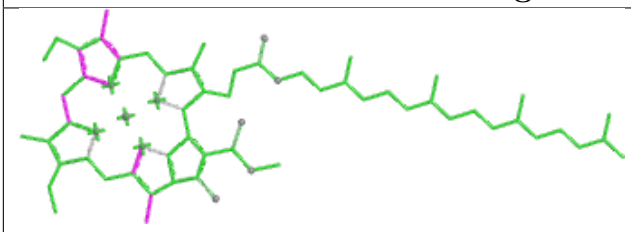


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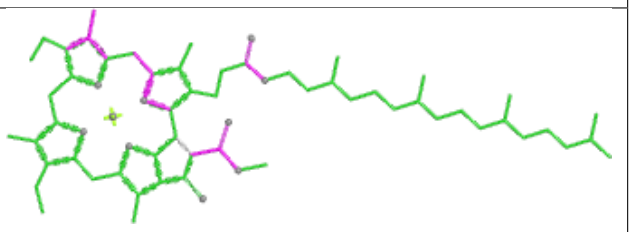


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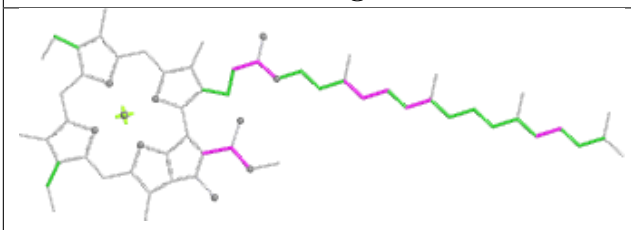
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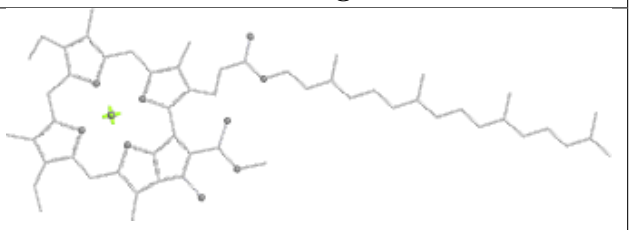
Bond lengths



Bond angles

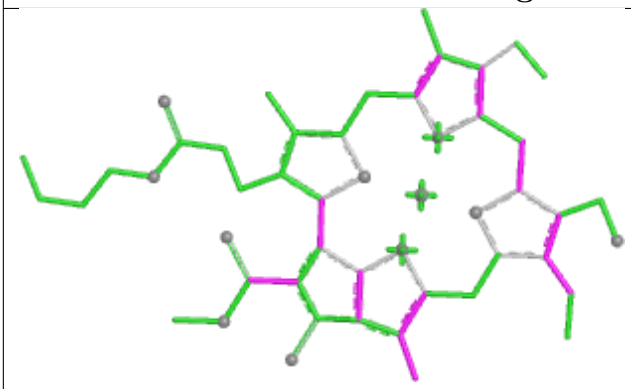


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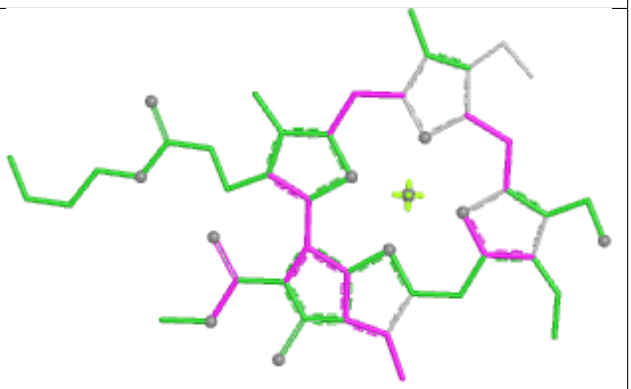


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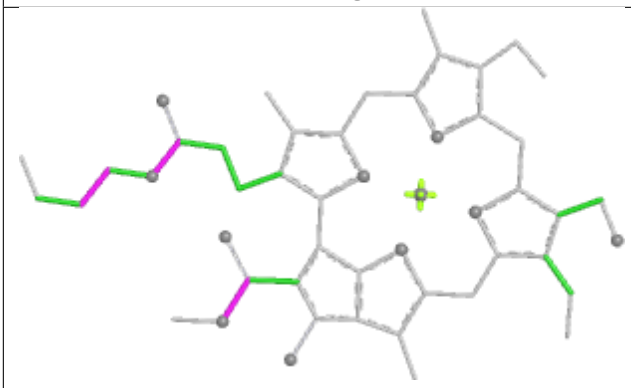
Ligand CHL Rr 606



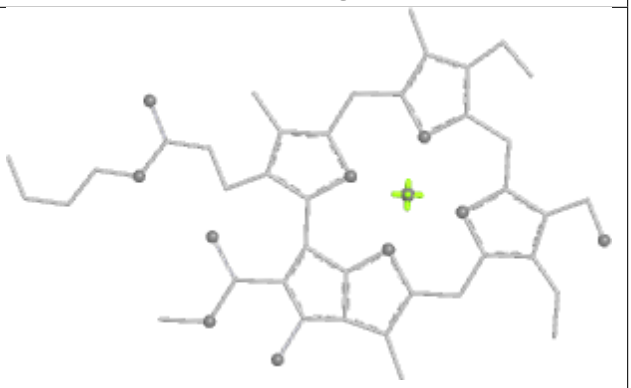
Bond lengths



Bond angles

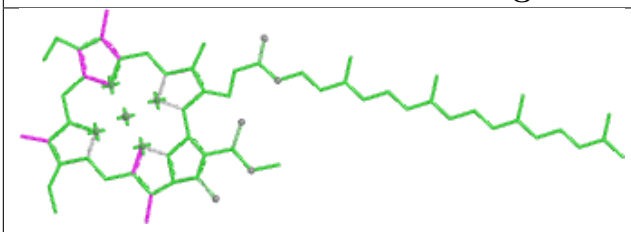


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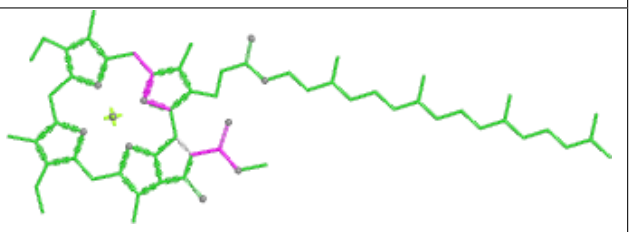


Rings

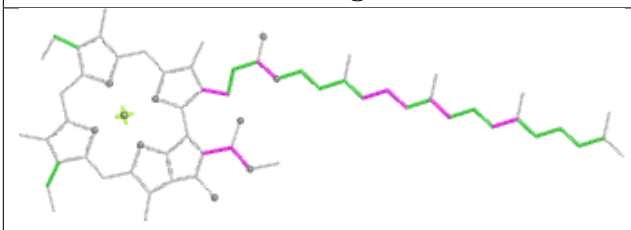
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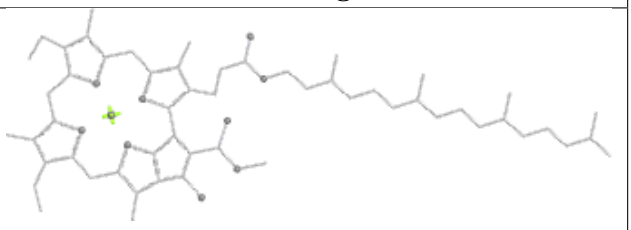
Bond lengths



Bond angles

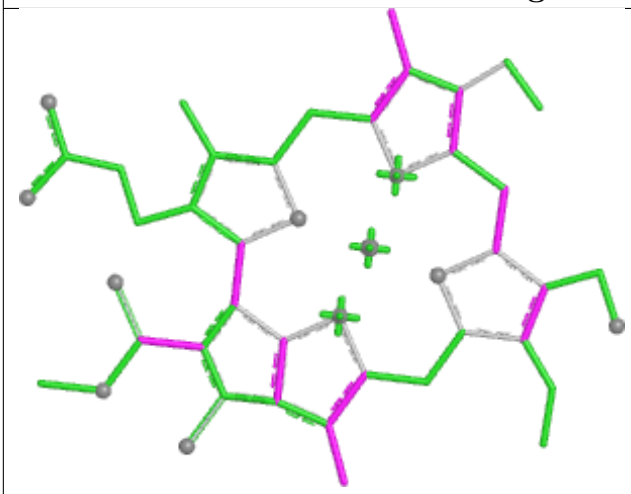


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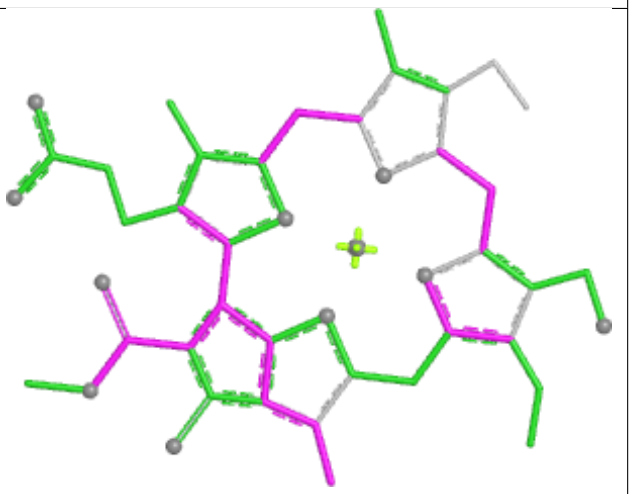


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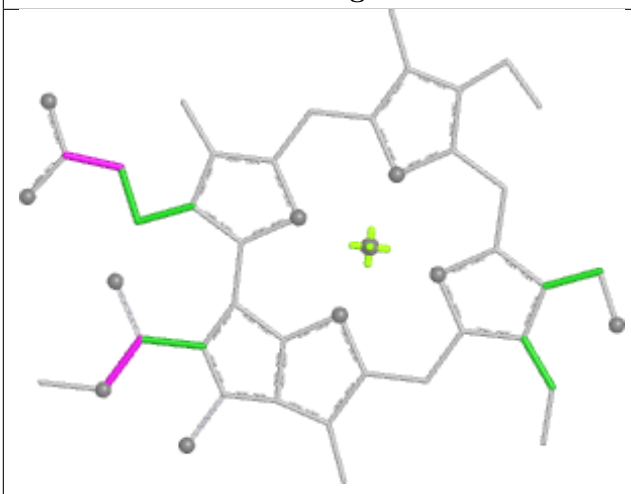
Ligand CHL 4 307



Bond lengths



Bond angles

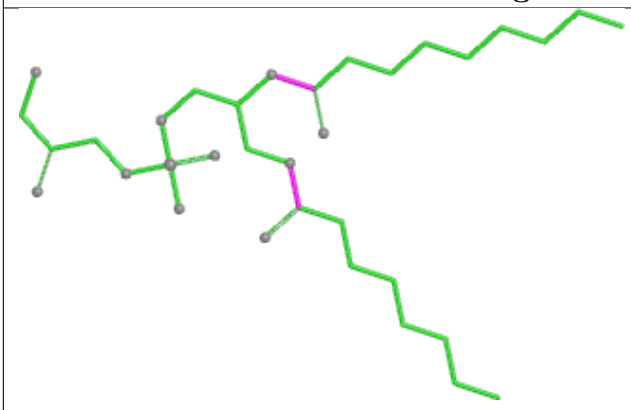


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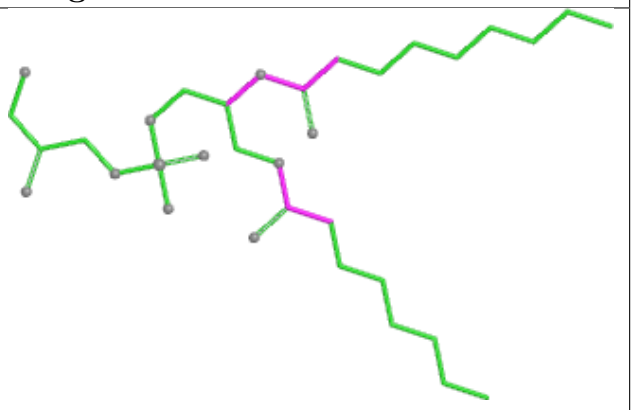


Rings

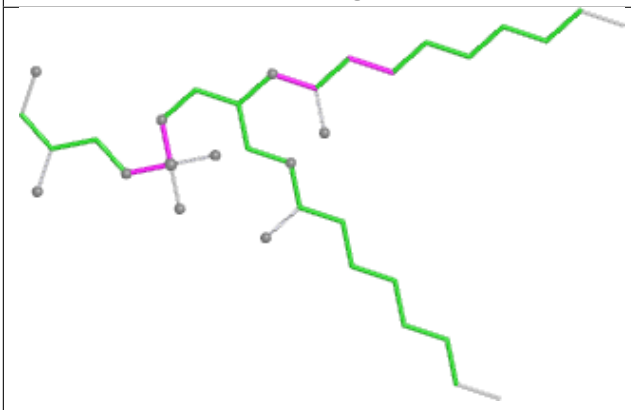
Ligand LHG Gg 319



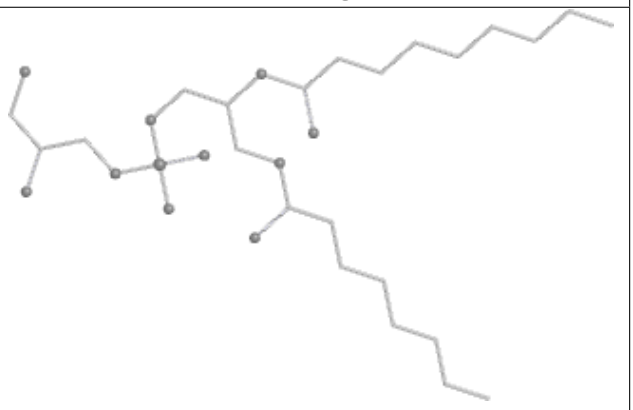
Bond lengths



Bond angles

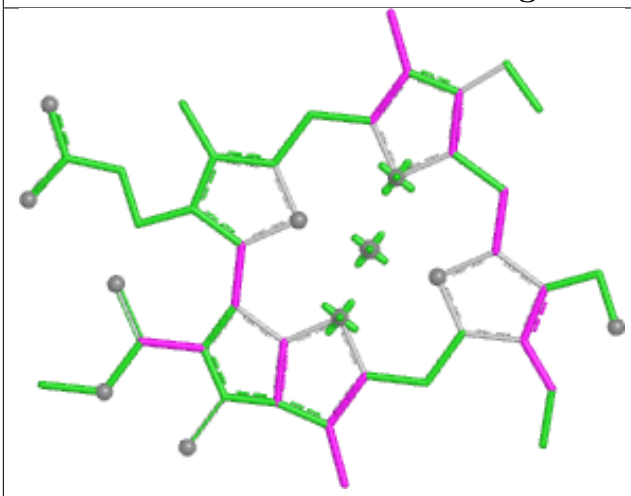


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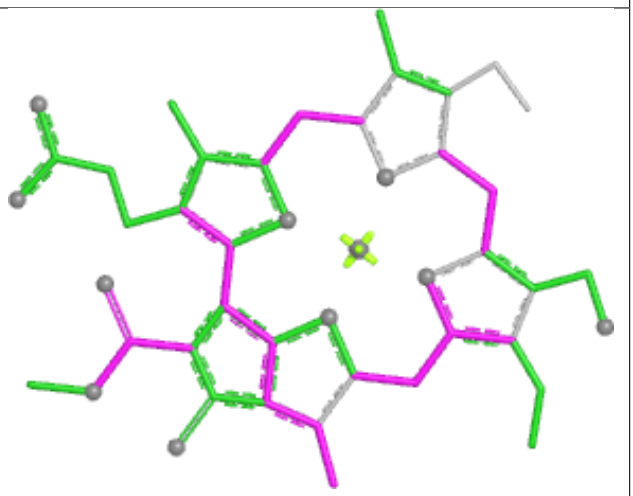


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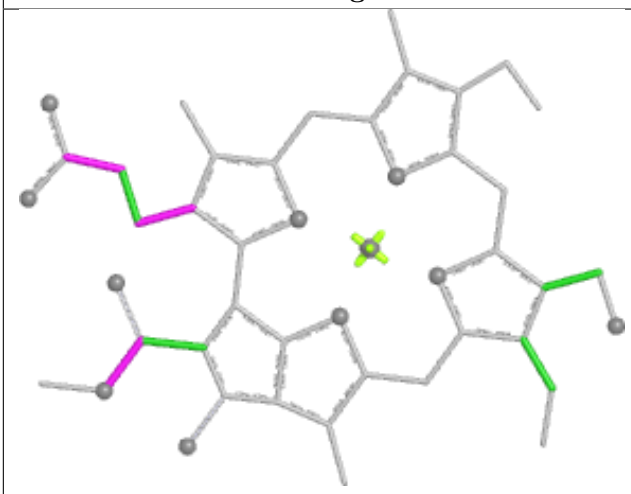
Ligand CHL 44 607



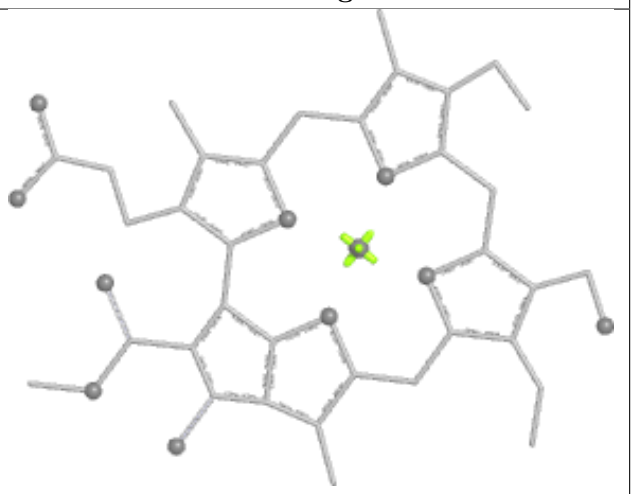
Bond lengths



Bond angles

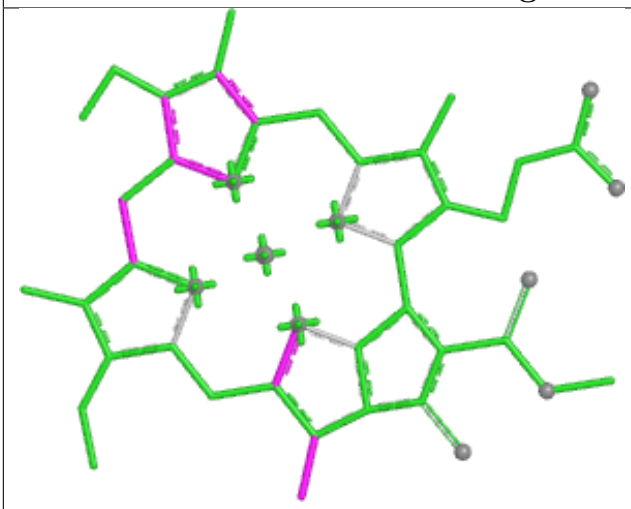


Torsions

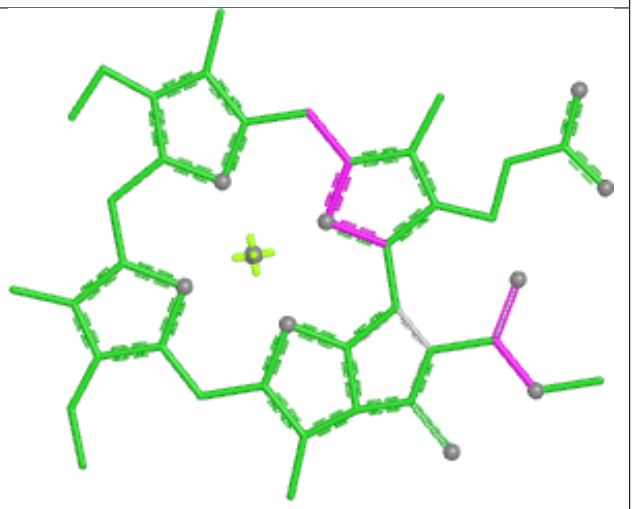


Rings

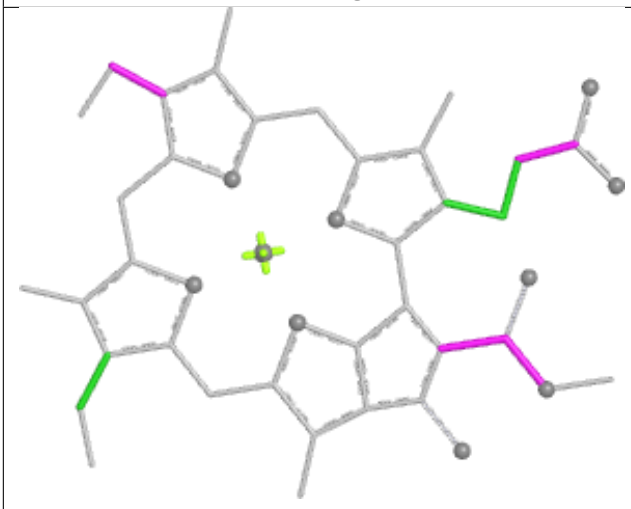
Ligand CLA 44 610



Bond lengths



Bond angles

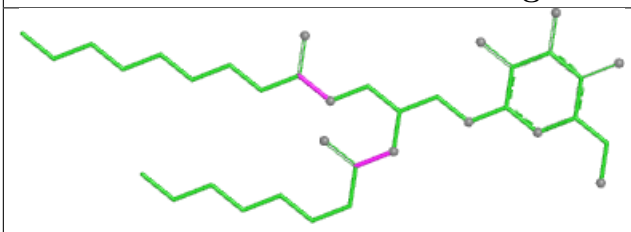


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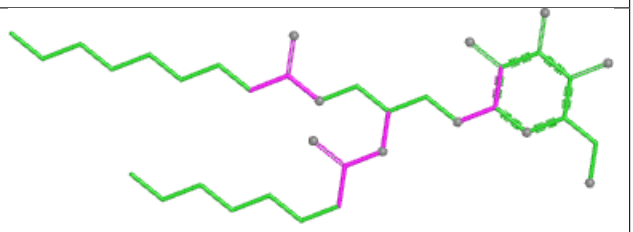


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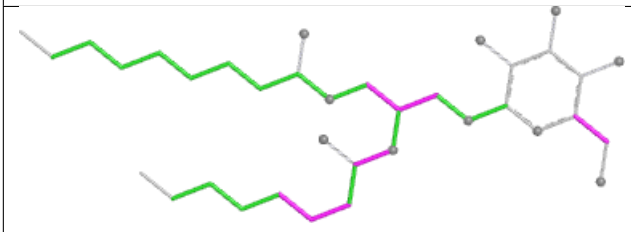
Ligand LMG b 621



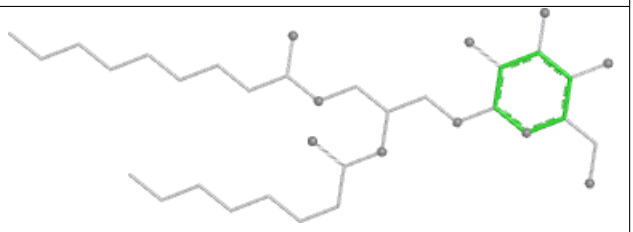
Bond lengths



Bond angles

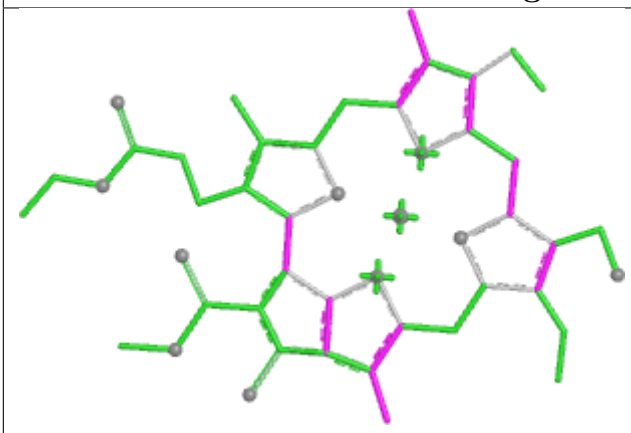


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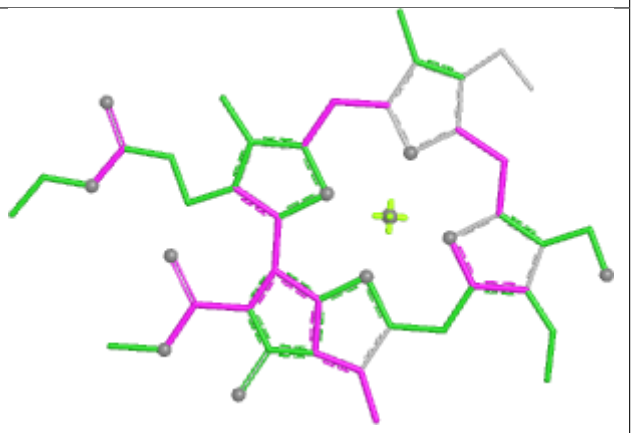


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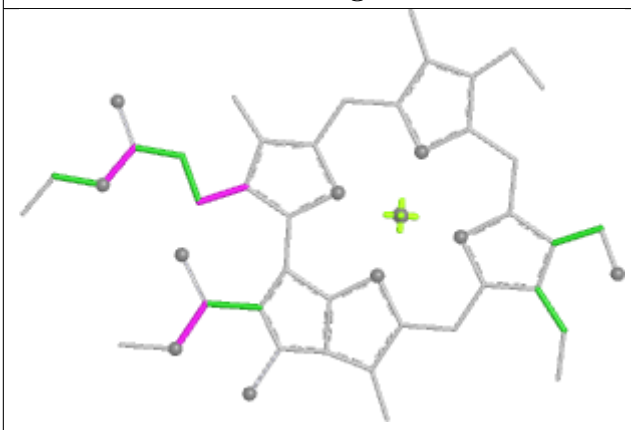
Ligand CHL Y 605



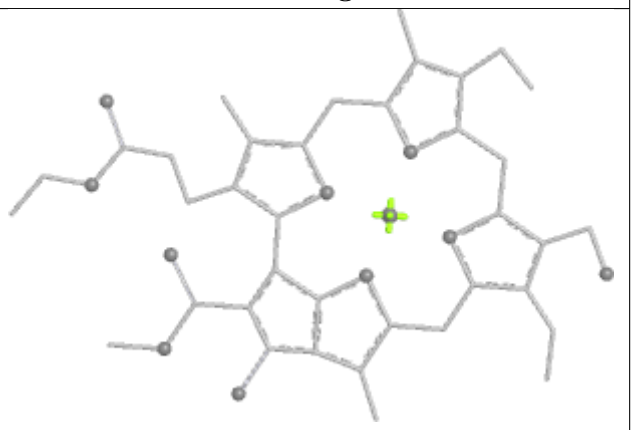
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Bond angles

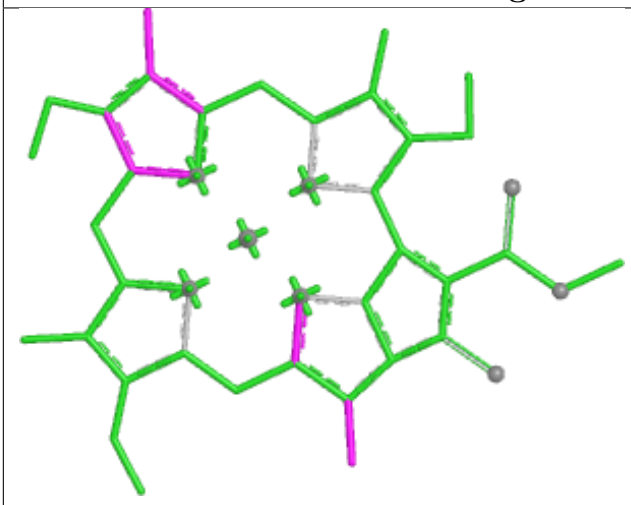


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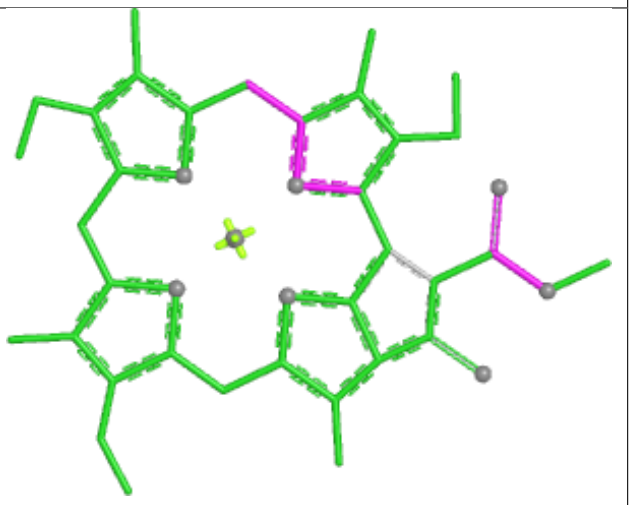


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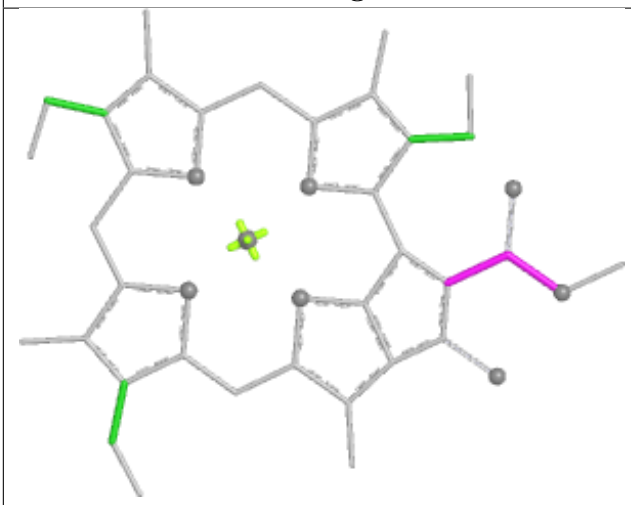
Ligand CLA NN 603



Bond lengths



Bond angles

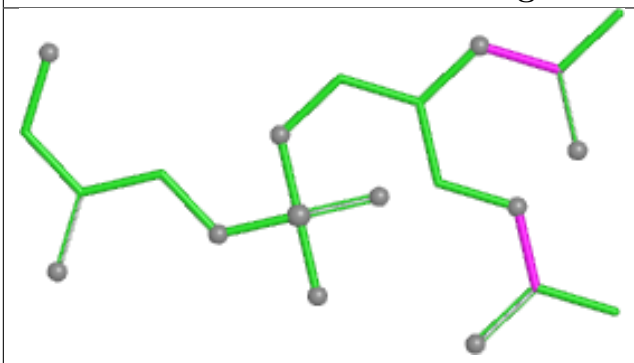


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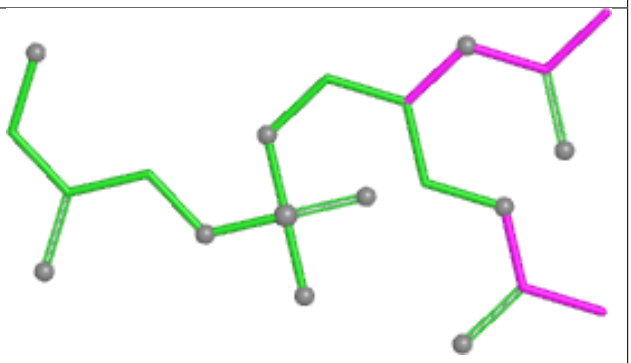


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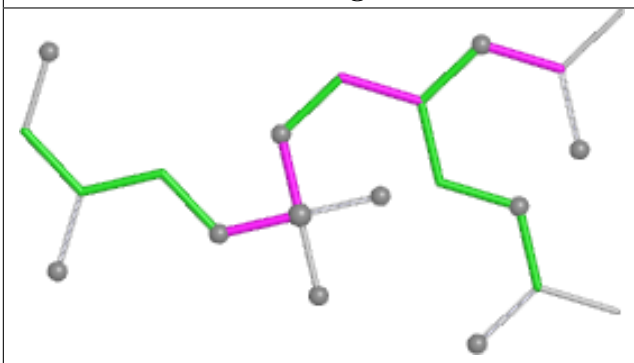
Ligand LHG 44 614



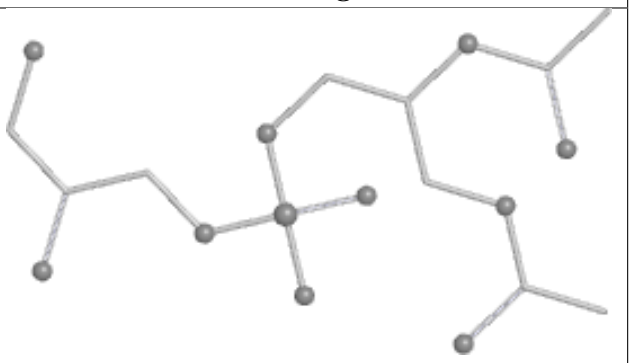
Bond lengths



Bond angles

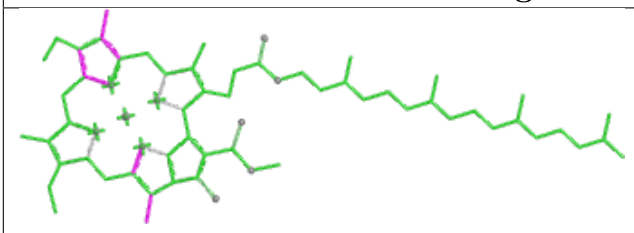


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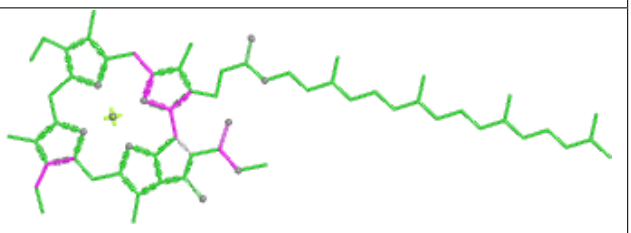


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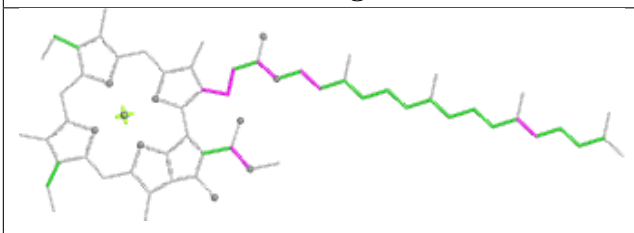
Ligand CLA Aa 405



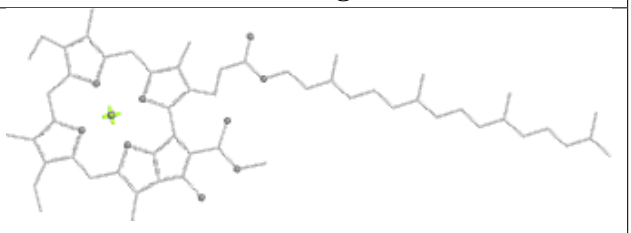
Bond lengths



Bond angles

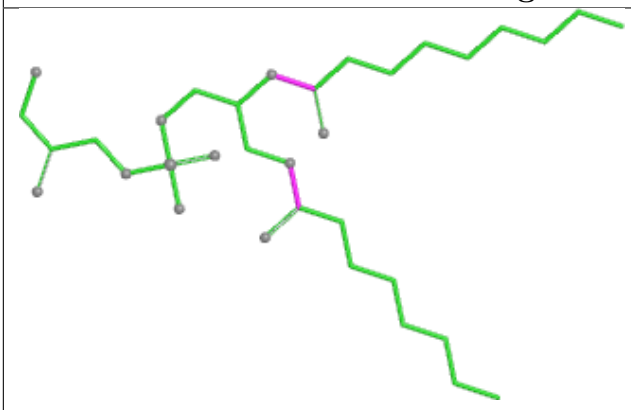


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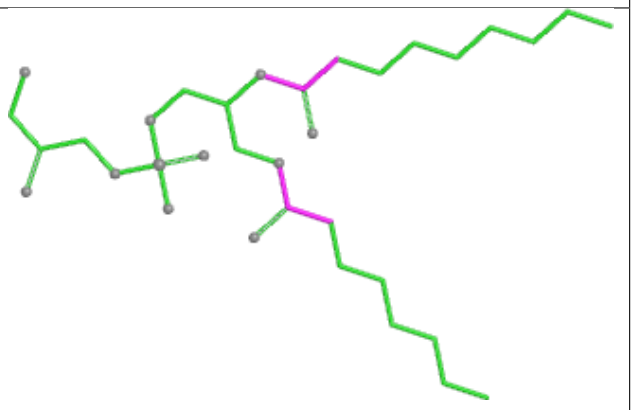


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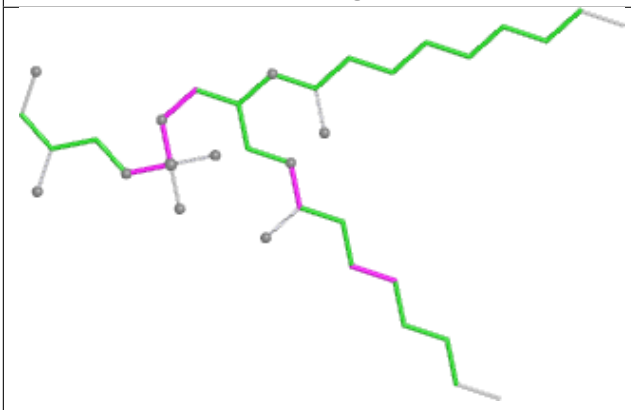
Ligand LHG 22 615



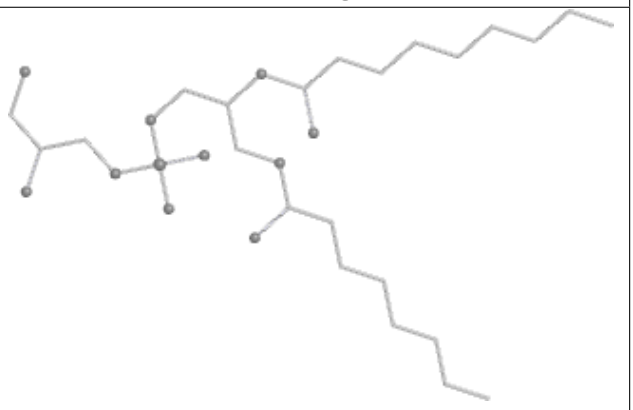
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Bond angles

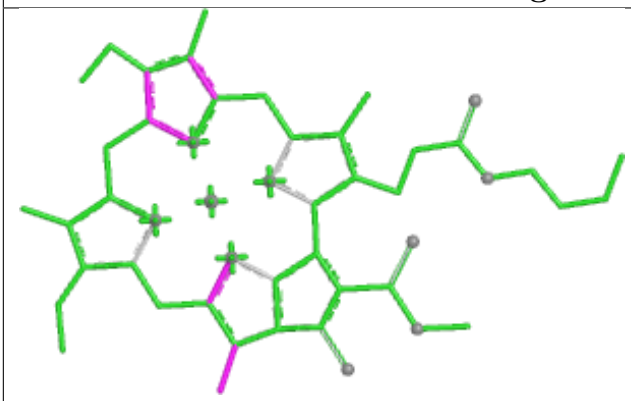


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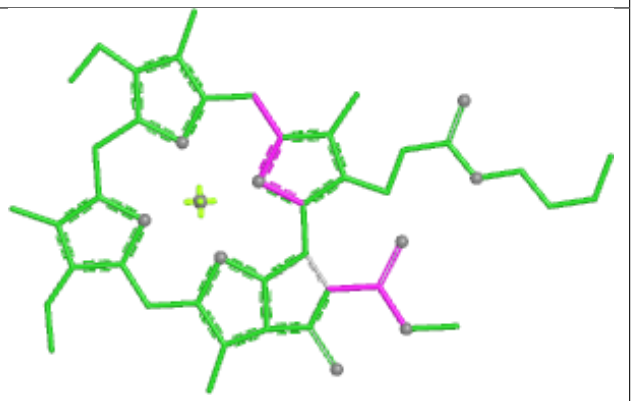


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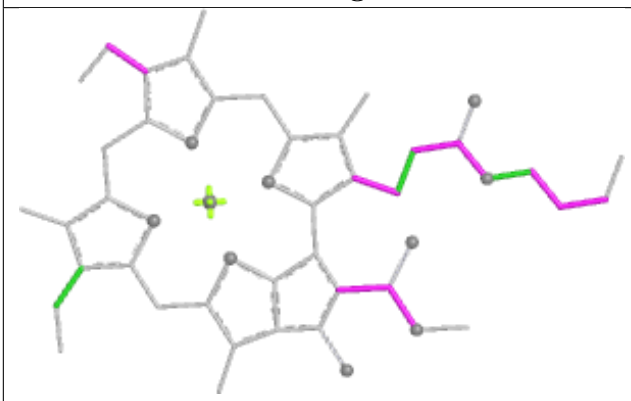
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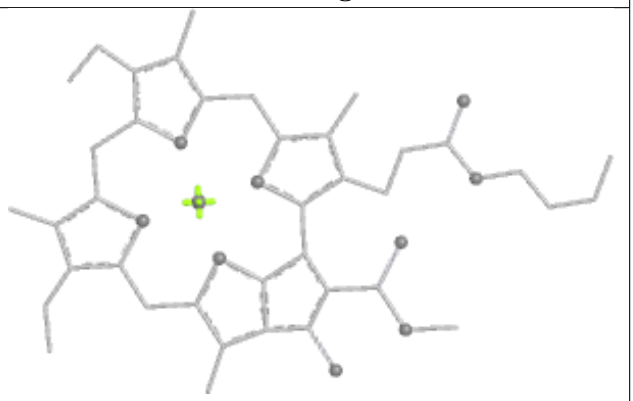
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Bond angles

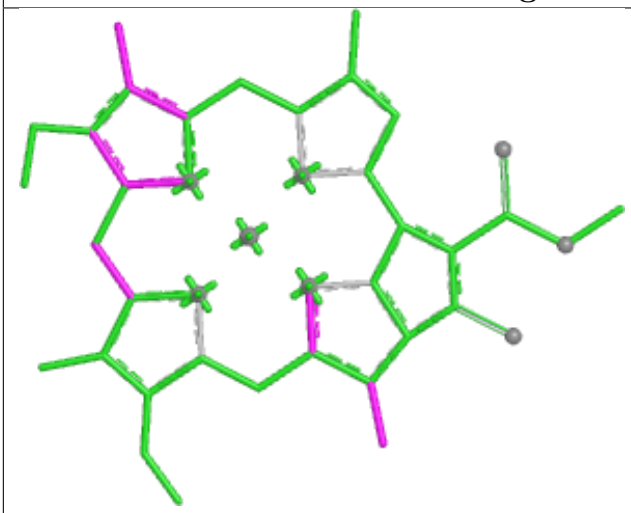


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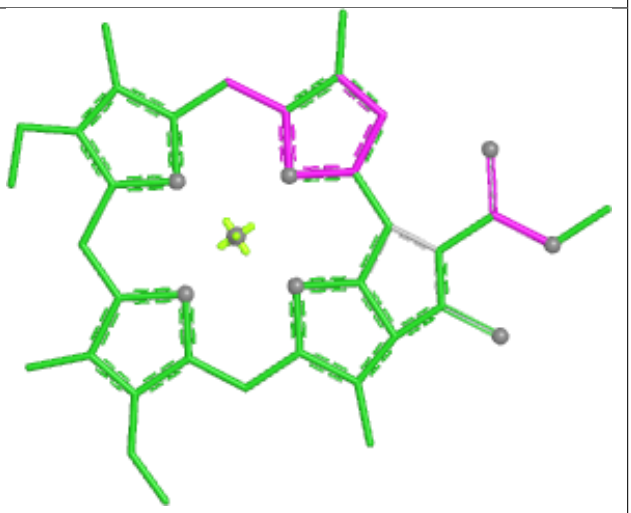


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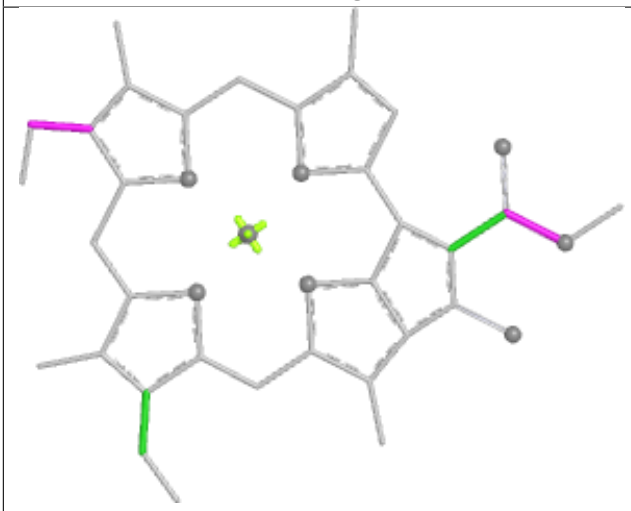
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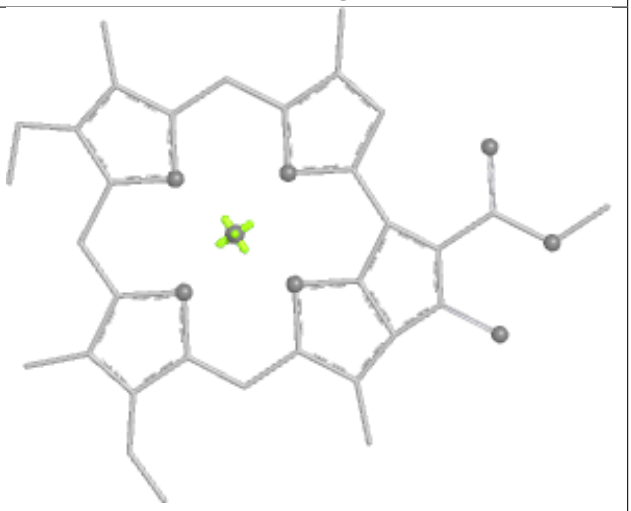
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Bond angles

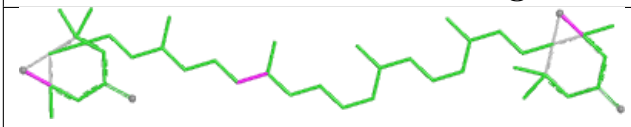


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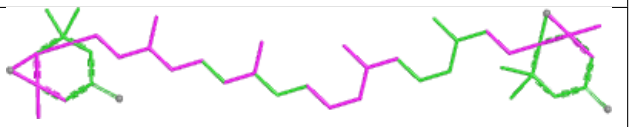


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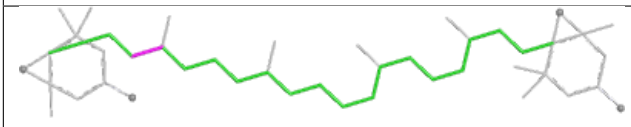
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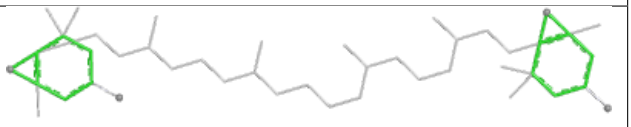
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Bond angles

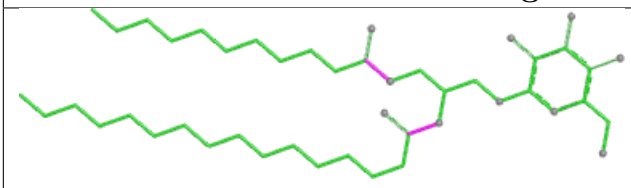


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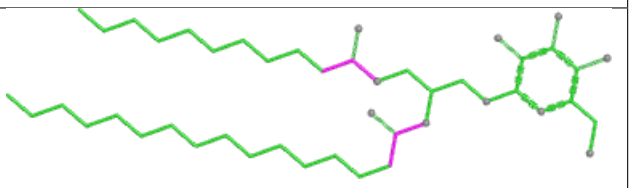


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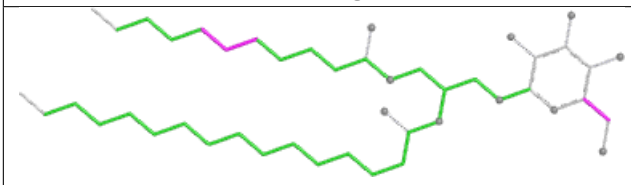
Ligand LMG F 101



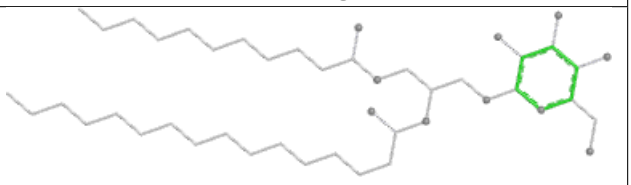
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Bond angles

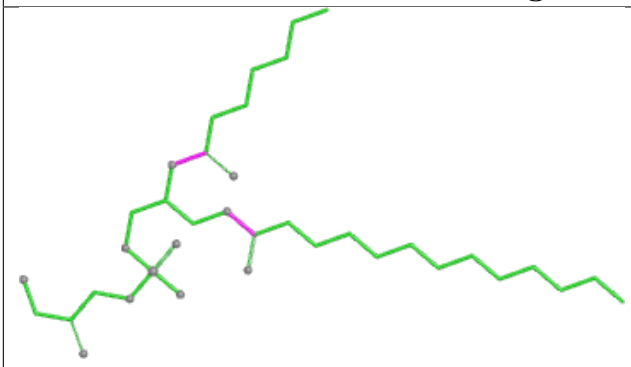


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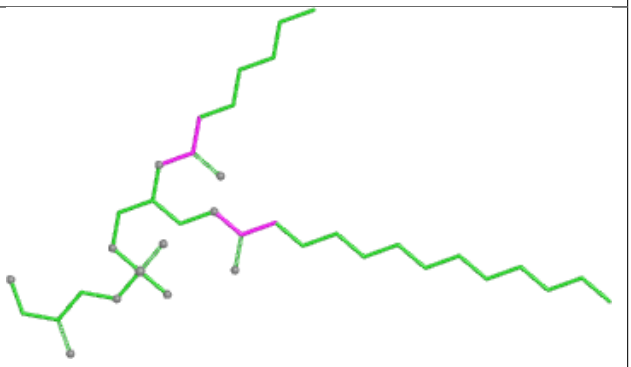


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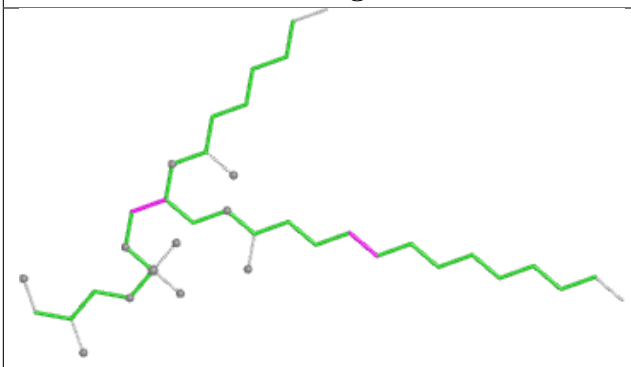
Ligand LHG a 414



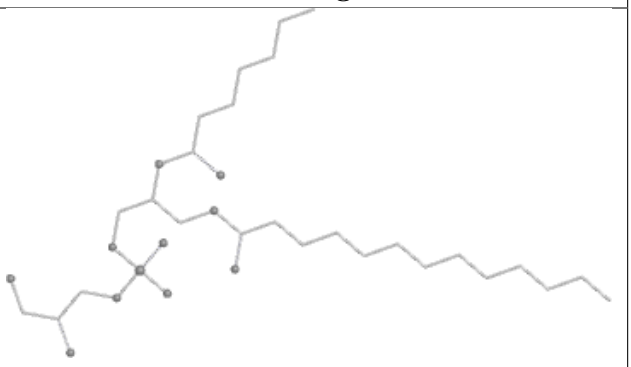
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Bond angles

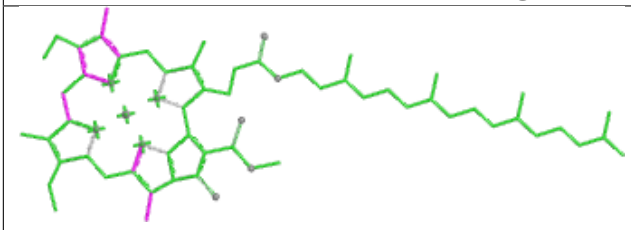


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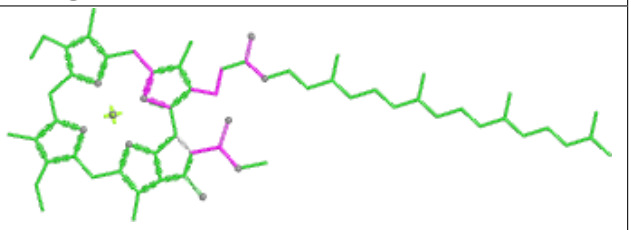


Rings

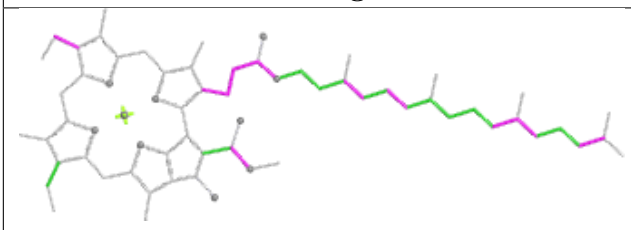
Ligand CLA Gg 312



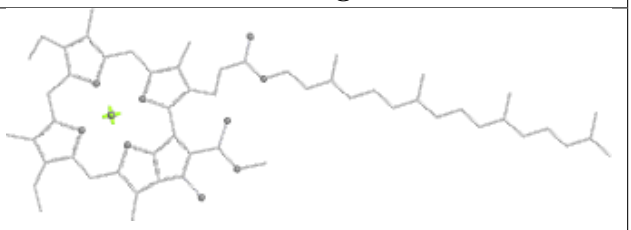
Bond lengths



Bond angles

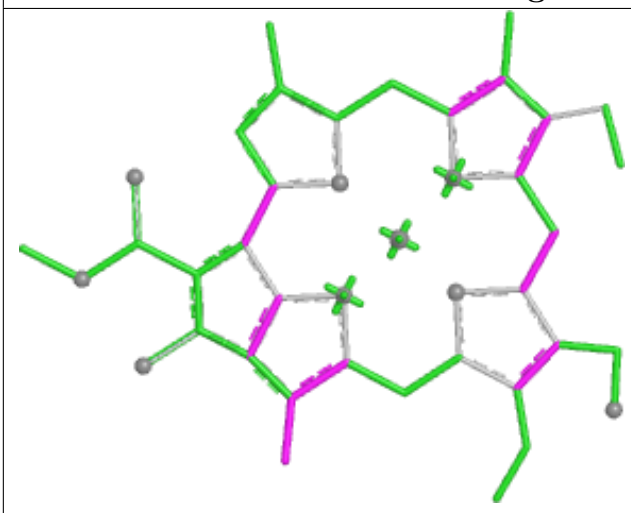


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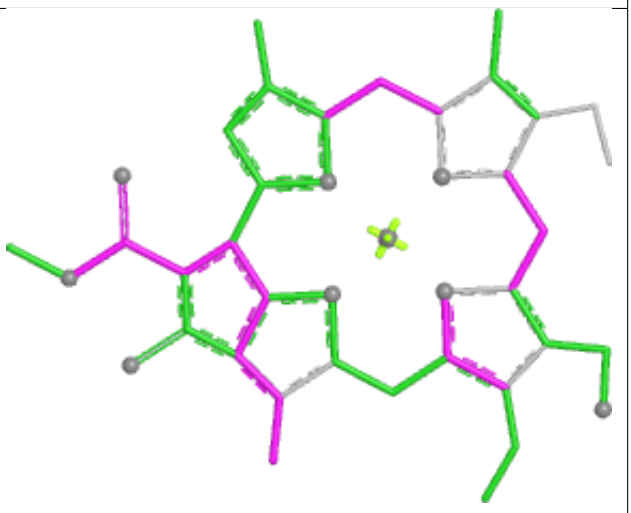


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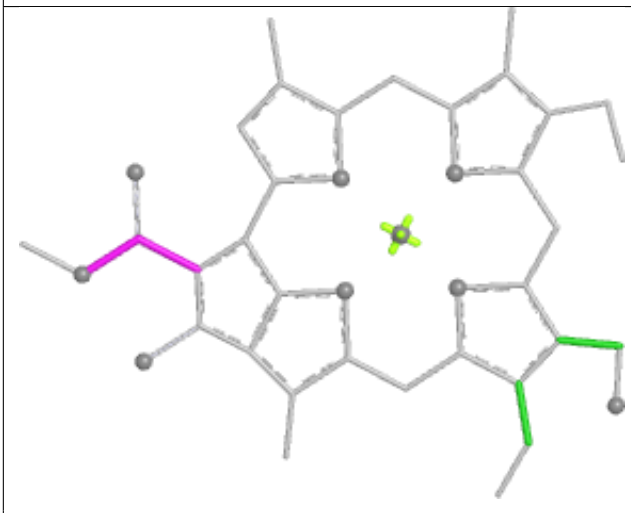
Ligand CHL 3 601



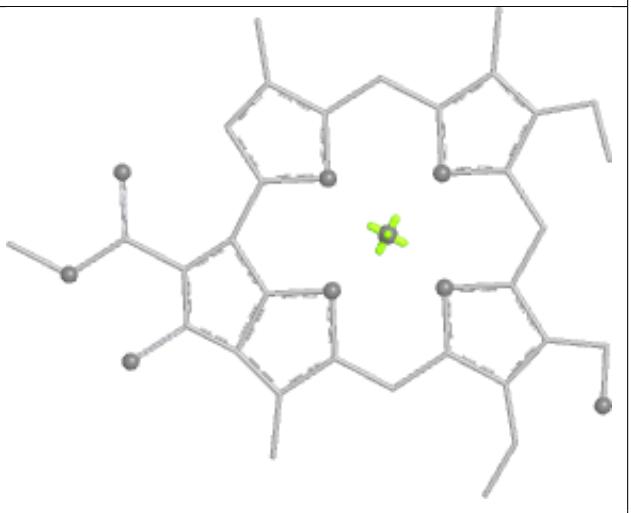
Bond lengths



Bond angles

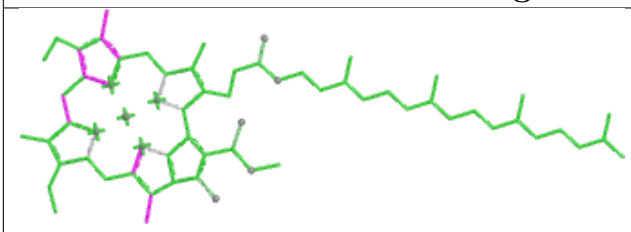


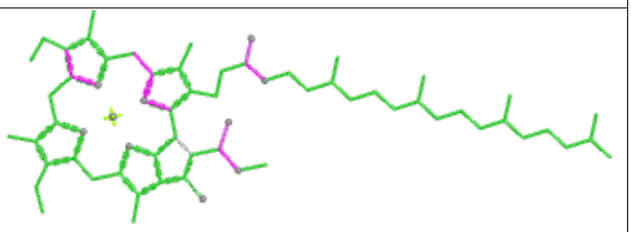
Torsions

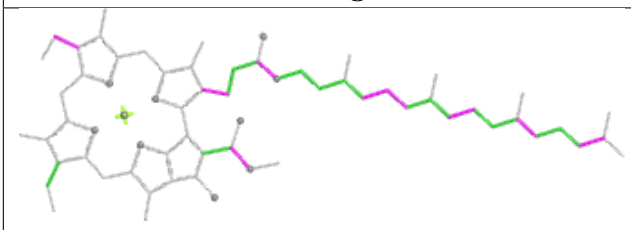


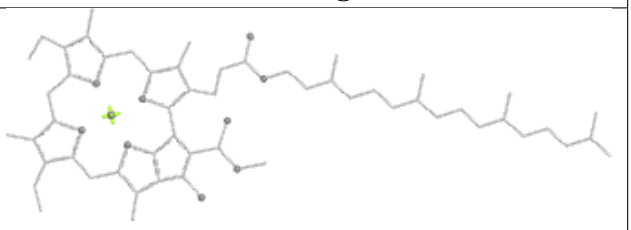
Rings

Ligand CLA Dd 402


Bond lengths

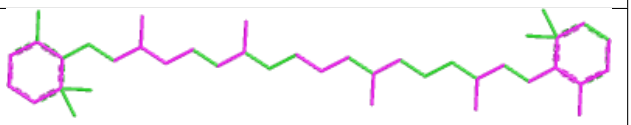

Bond angles

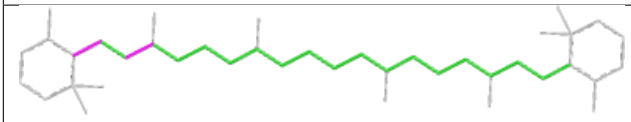

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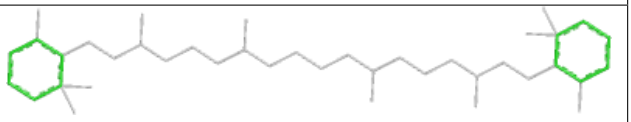

Rings

Ligand BCR c 514

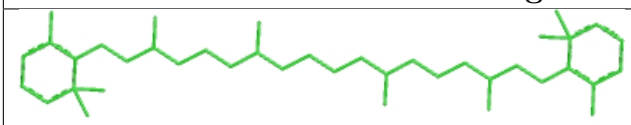

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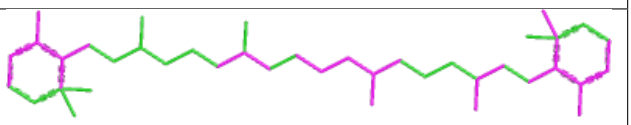

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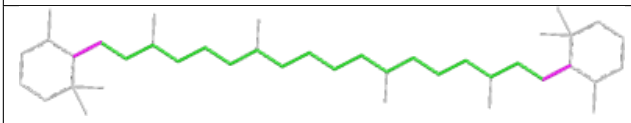

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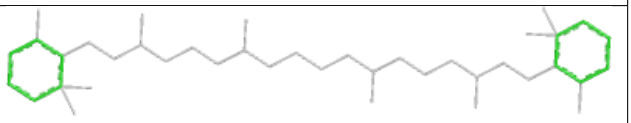

Rings

Ligand BCR d 403


Bond lengths

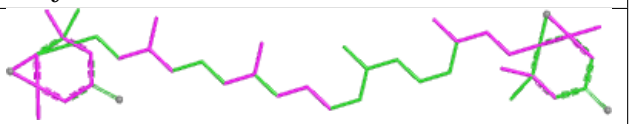

Bond angles

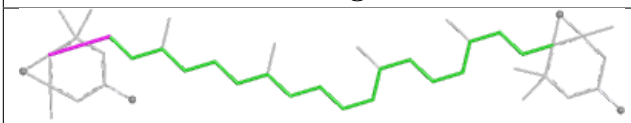

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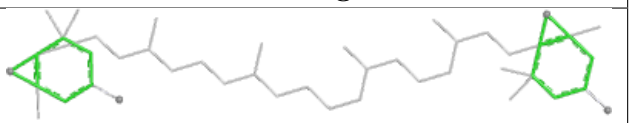

Rings

Ligand XAT y 301

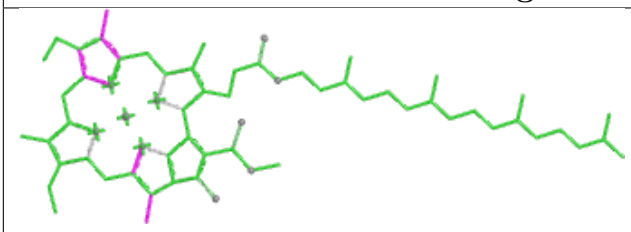

Bond lengths


Bond angles

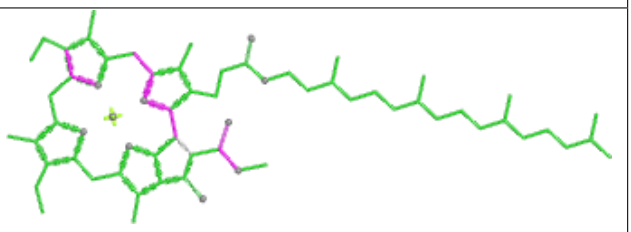

Torsions


Rings

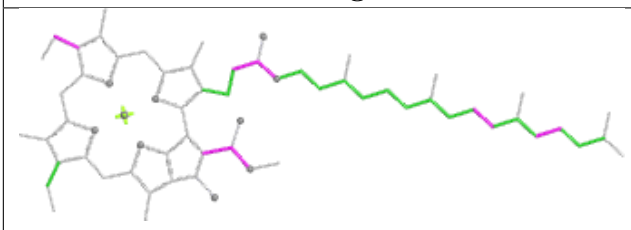
Ligand CLA Cc 509



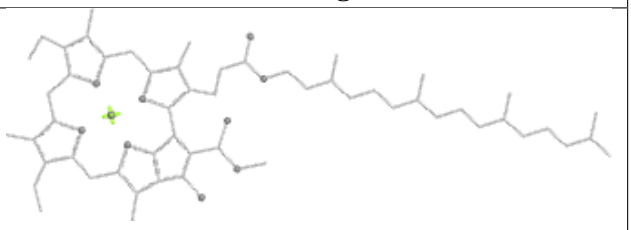
Bond lengths



Bond angles

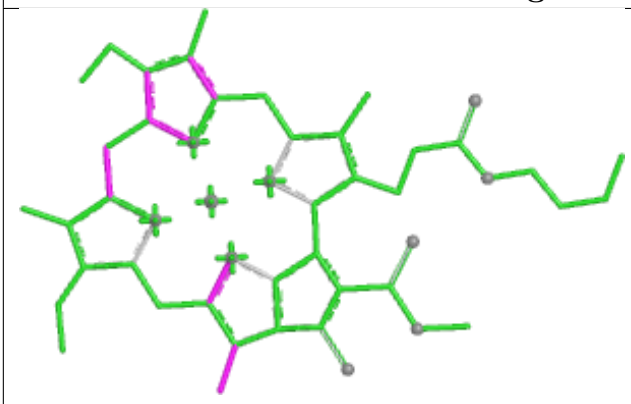


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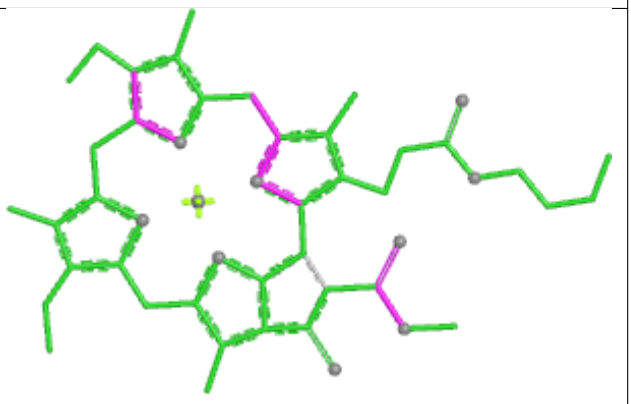


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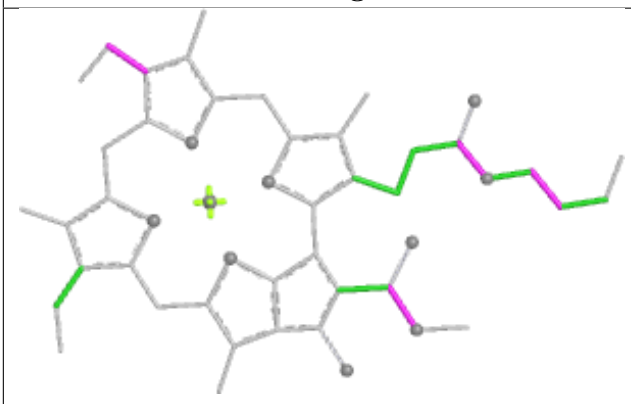
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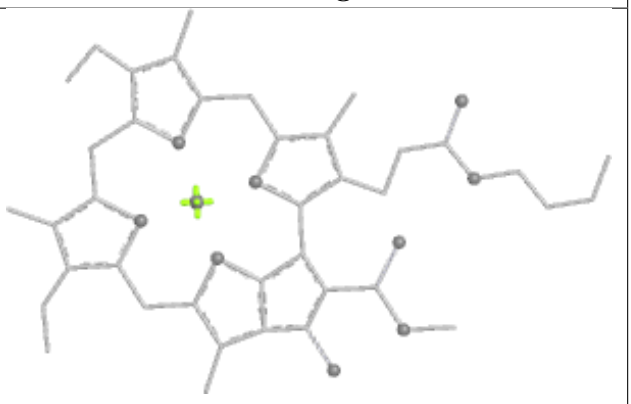
Bond lengths



Bond angles

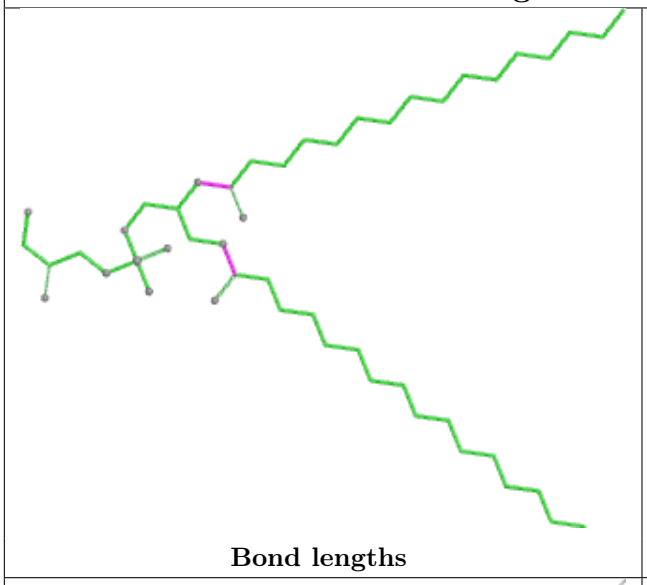


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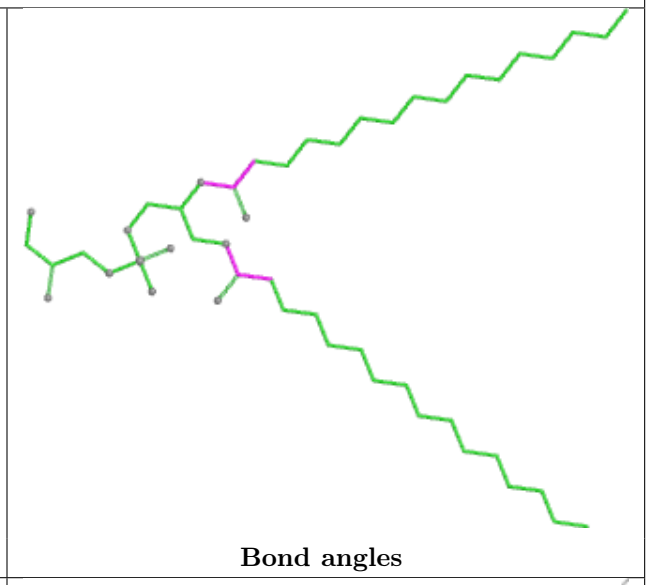


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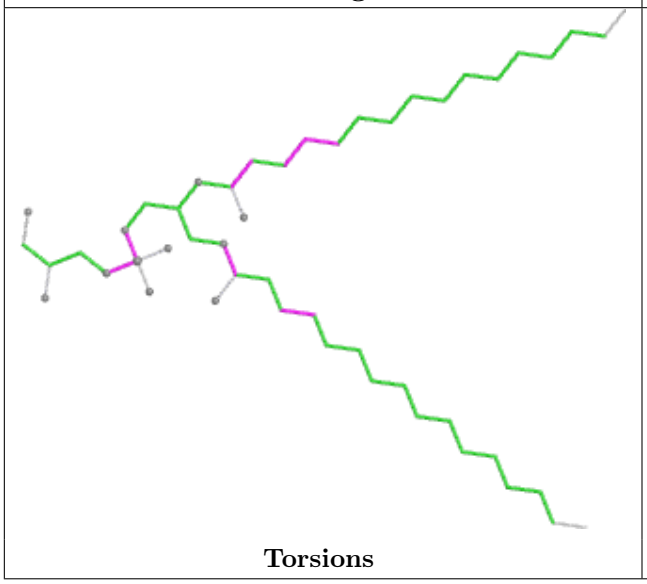
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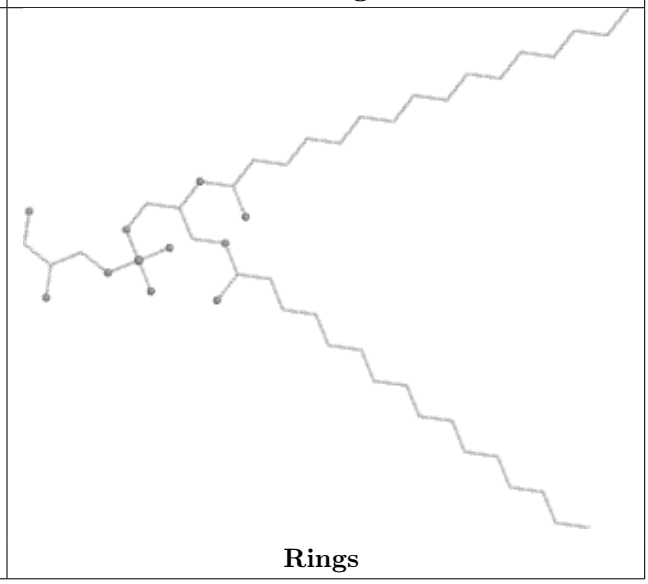
Bond lengths



Bond angles

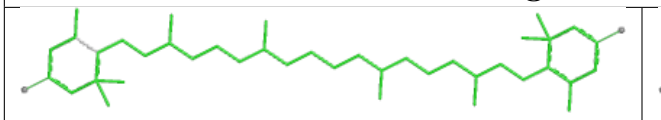


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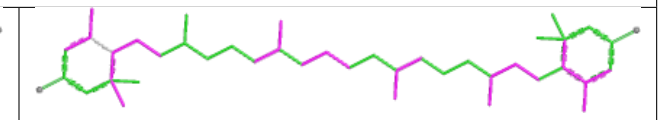


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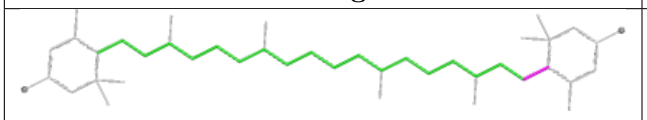
Ligand LUT Y 616



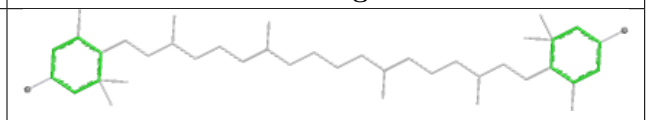
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Bond angles

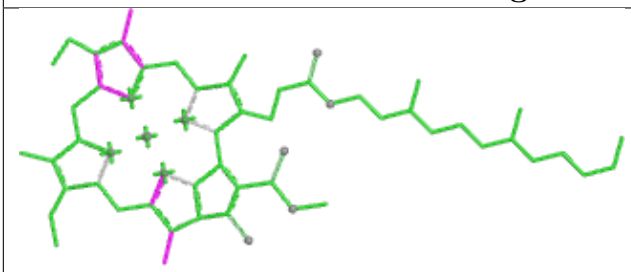


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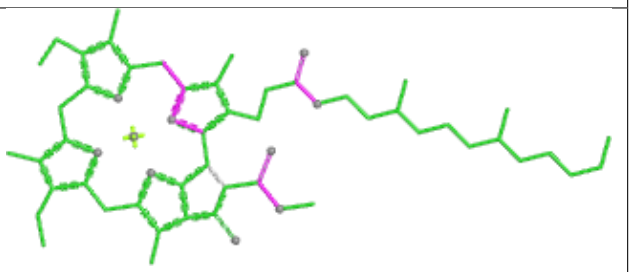


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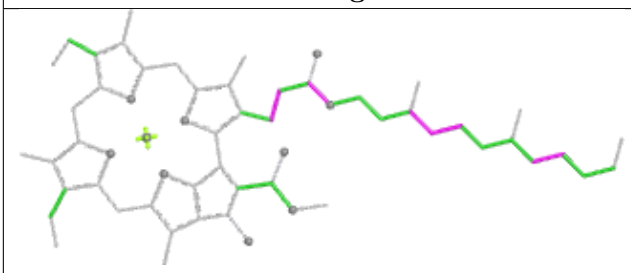
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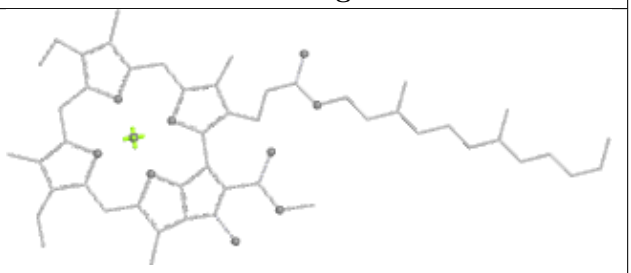
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Bond angles

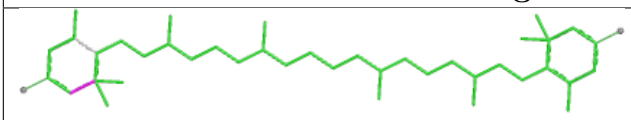


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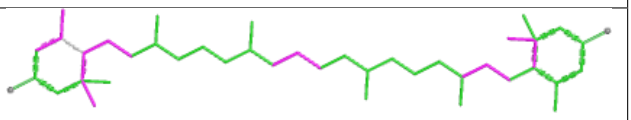


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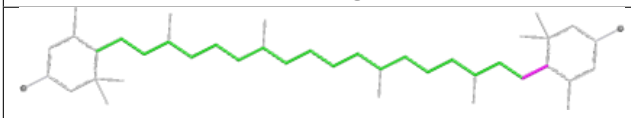
Ligand LUT Nn 306



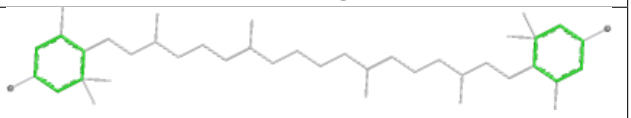
Bond lengths



Bond angles

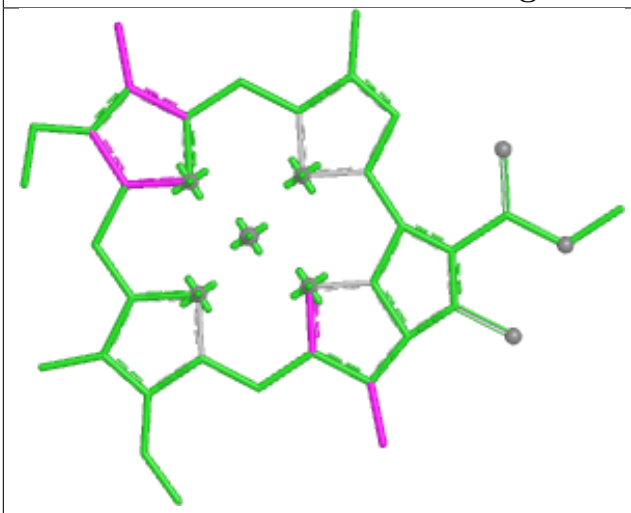


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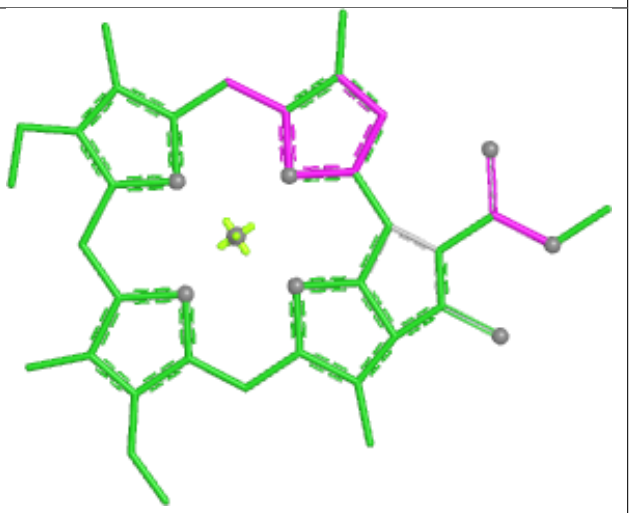


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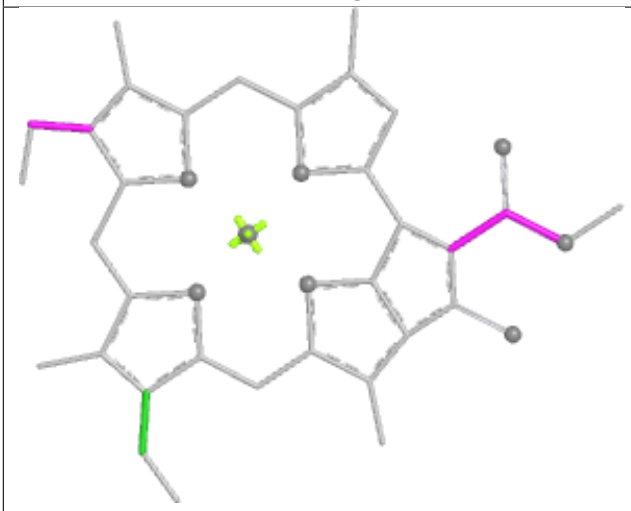
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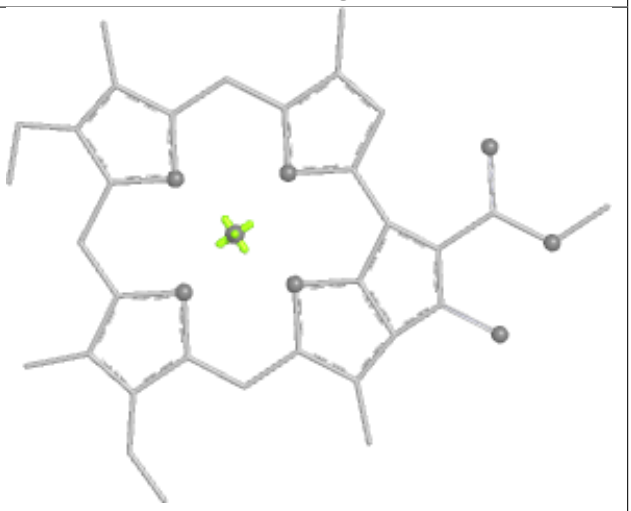
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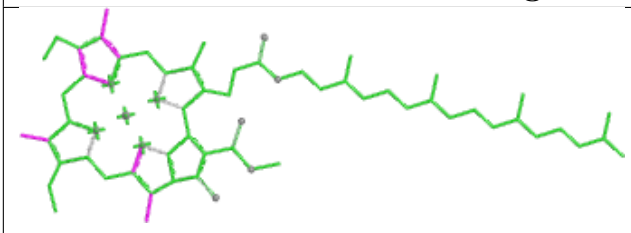


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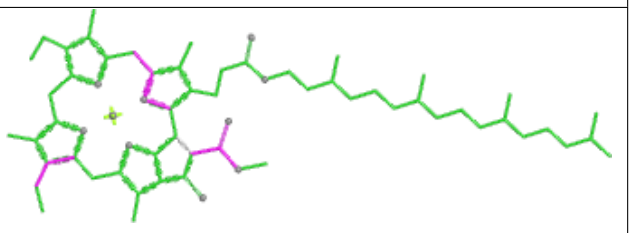


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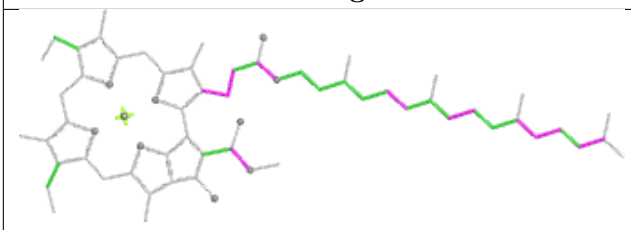
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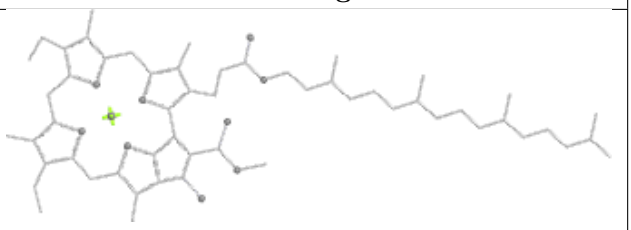
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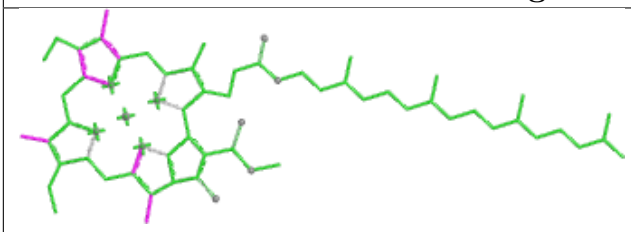


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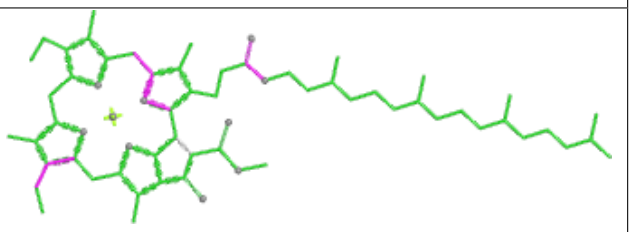


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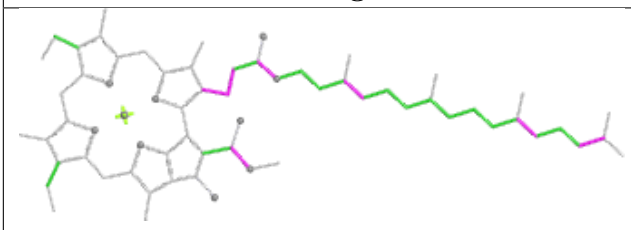
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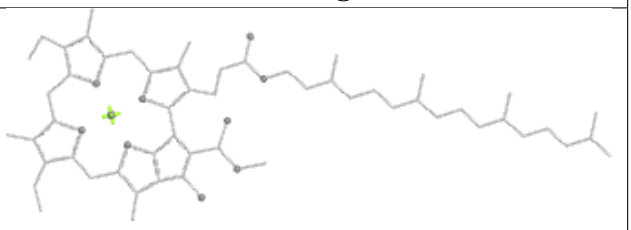
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Bond angles

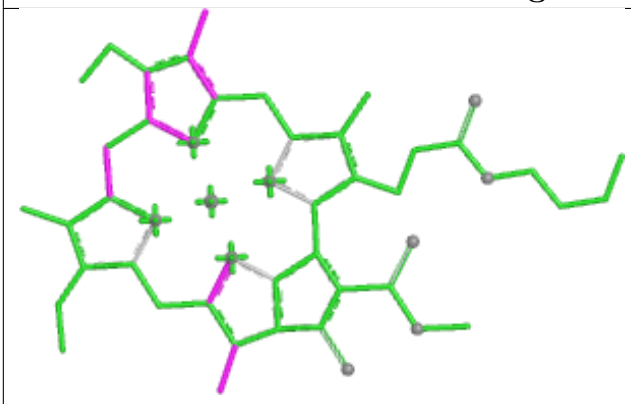


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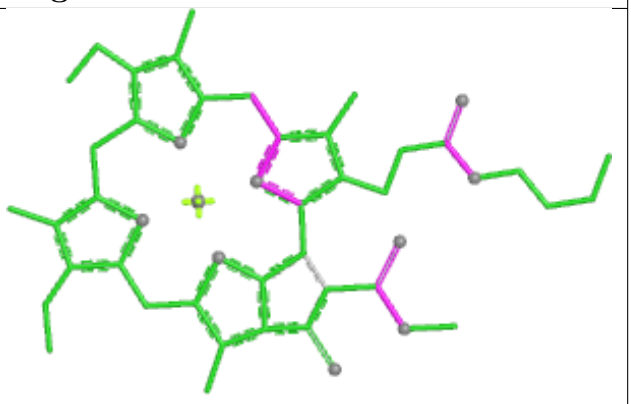


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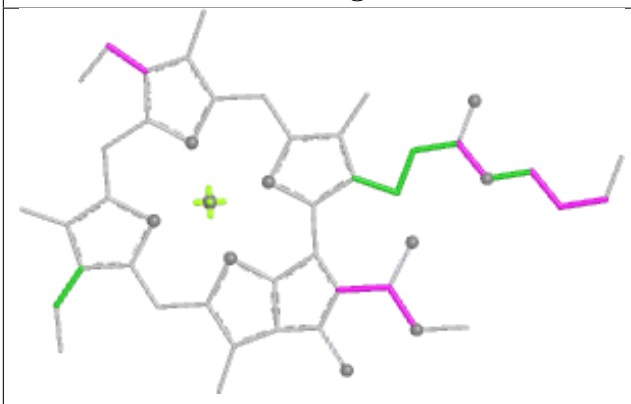
Ligand CLA g 614



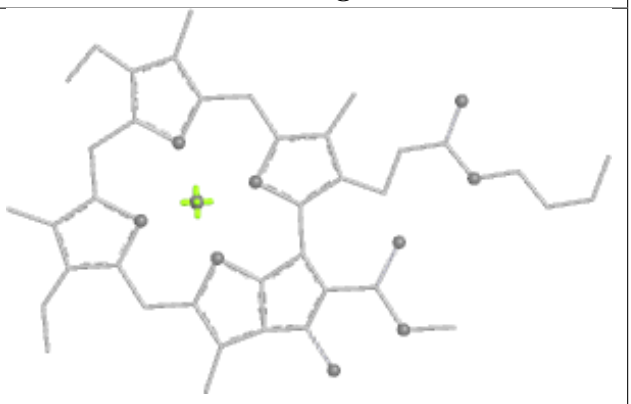
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Bond angles

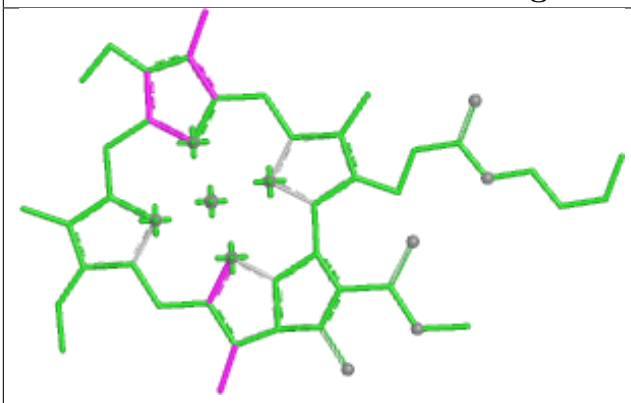


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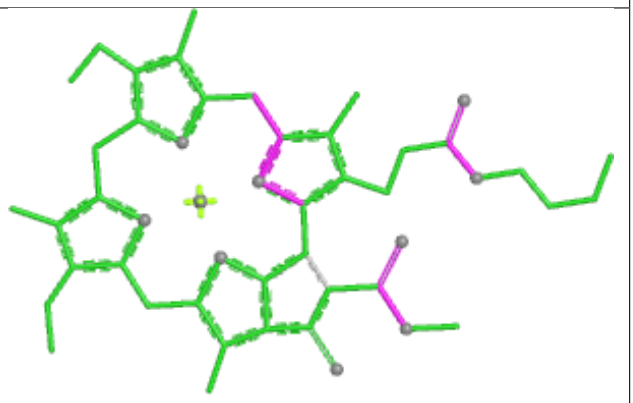


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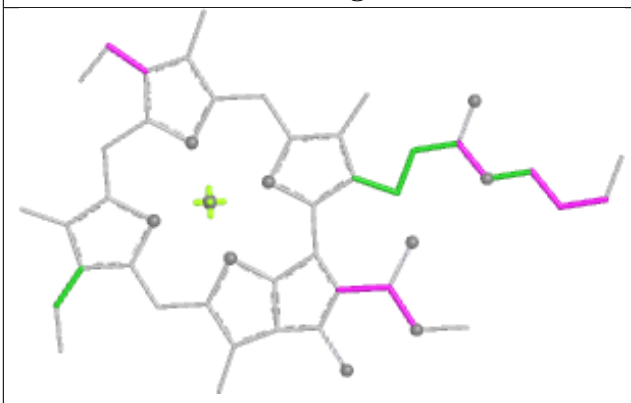
Ligand CLA s 604



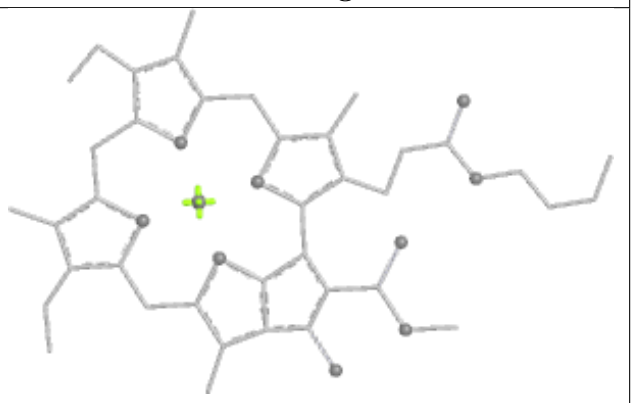
Bond lengths



Bond angles

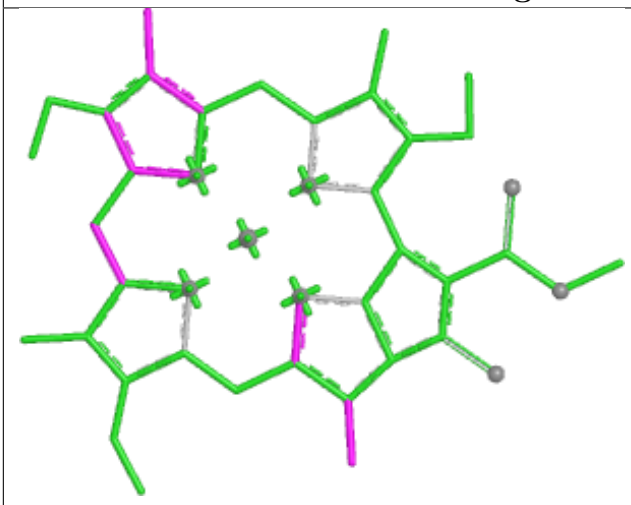


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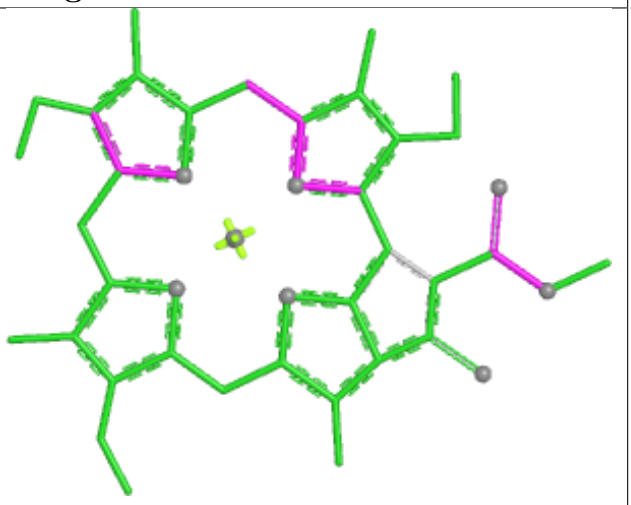


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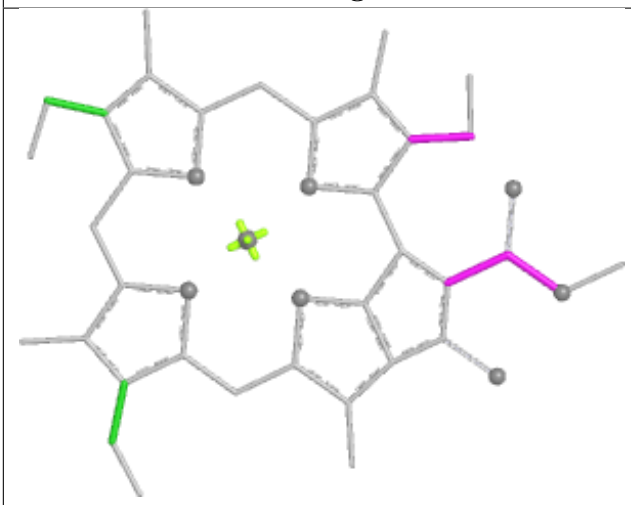
Ligand CLA Gg 305



Bond lengths



Bond angles

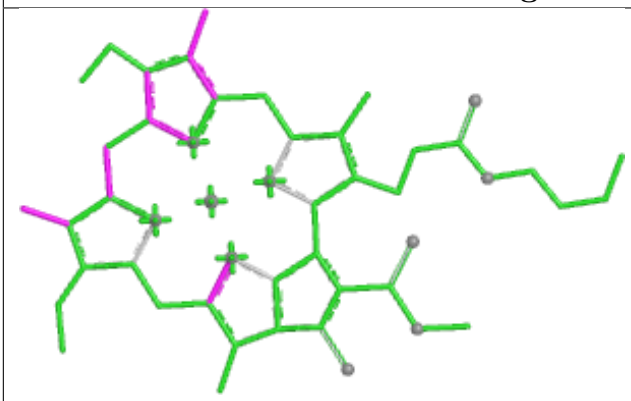


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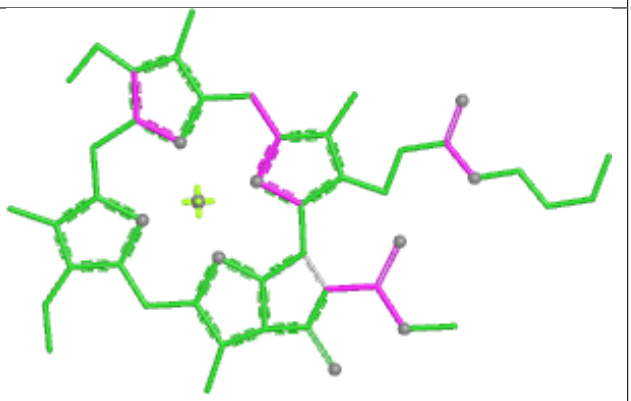


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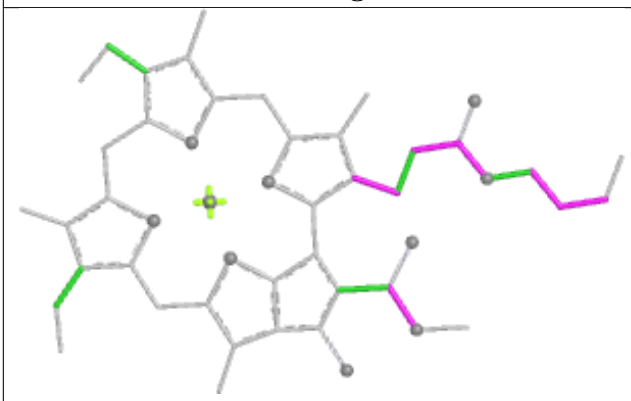
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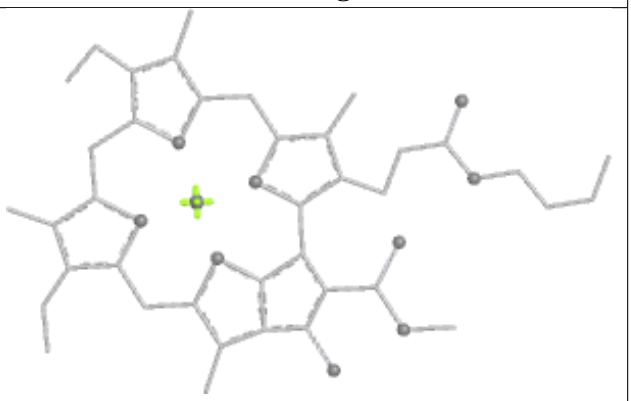
Bond lengths



Bond angles

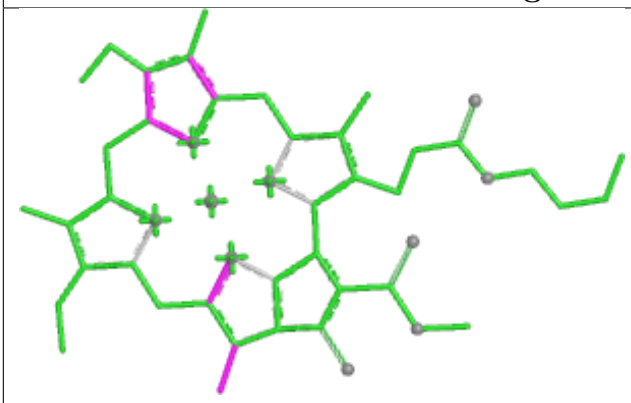


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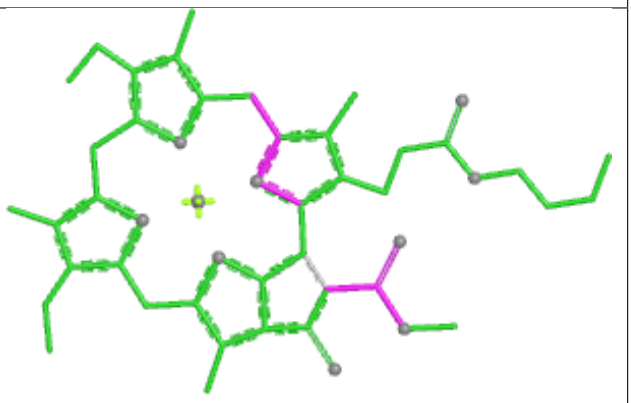


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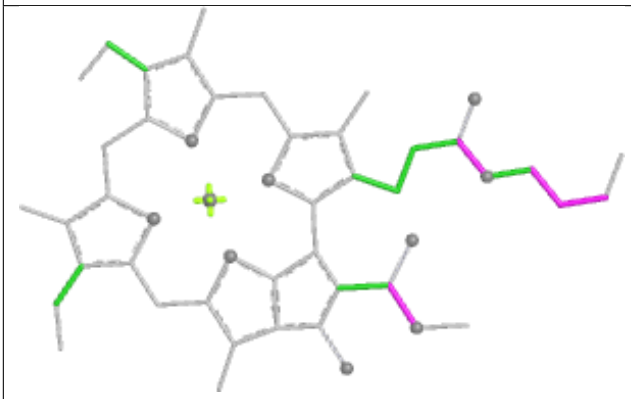
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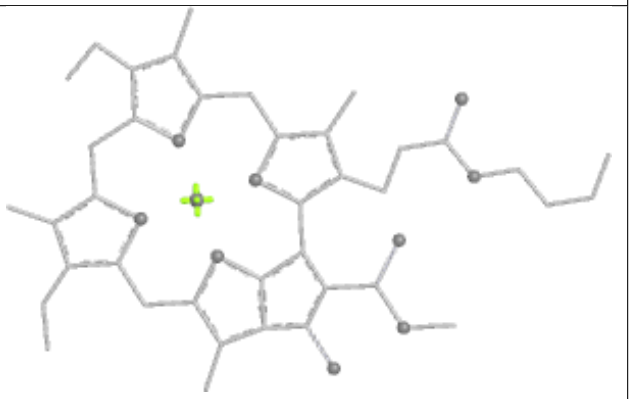
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Bond angles

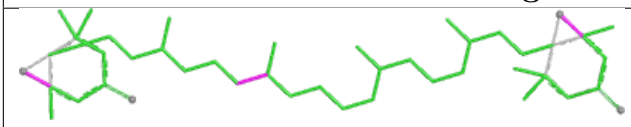


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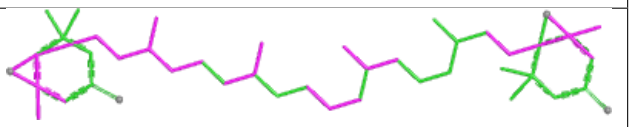


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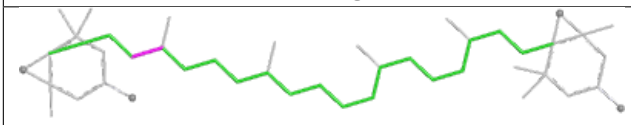
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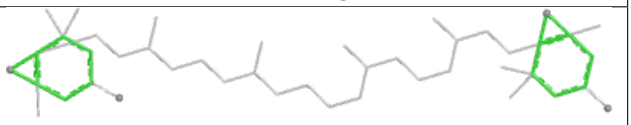
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Bond angles

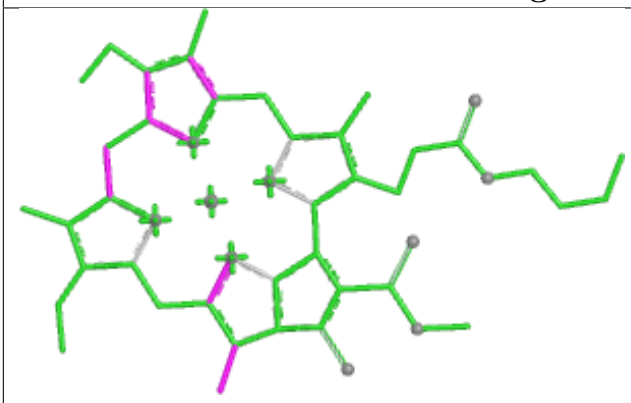


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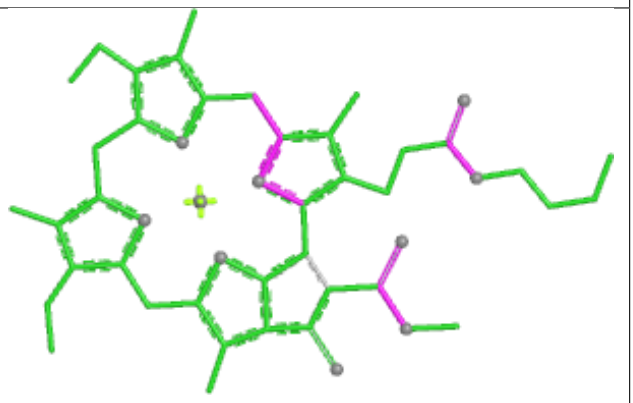


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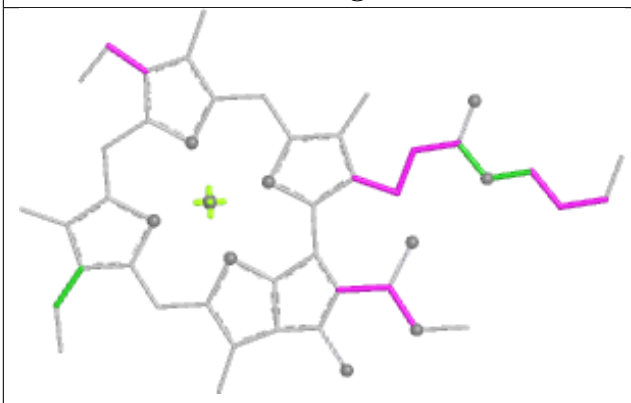
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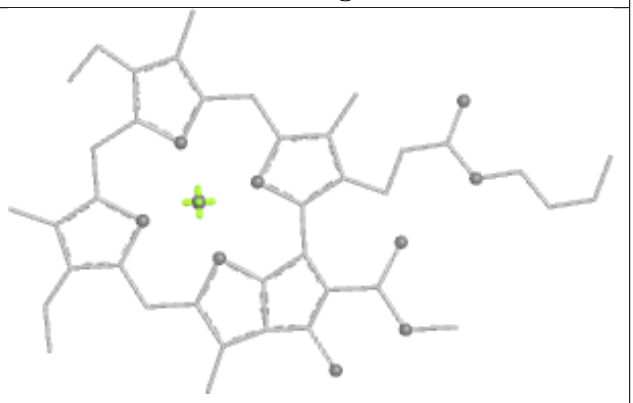
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Bond angles

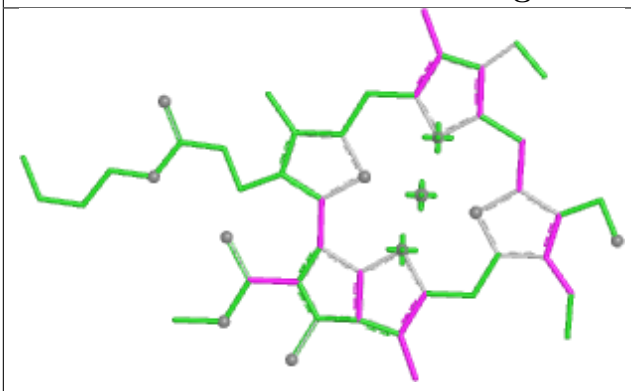


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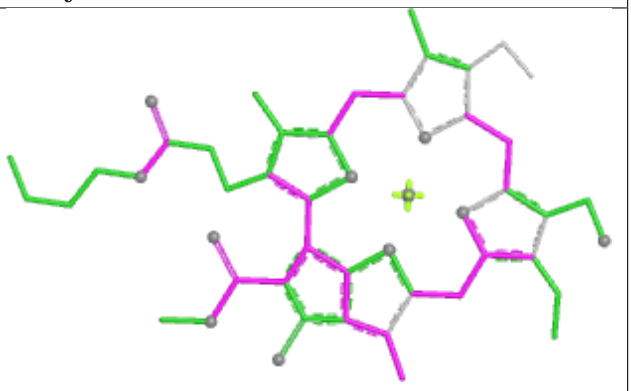


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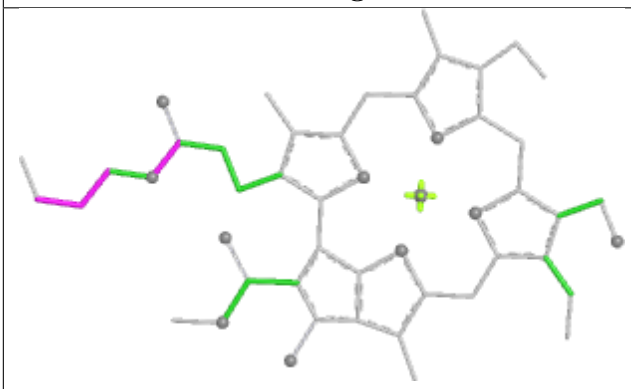
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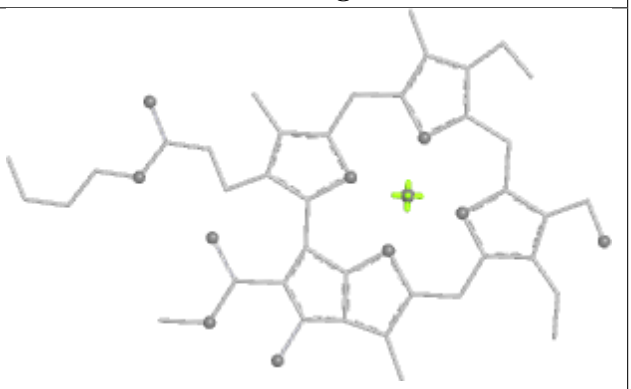
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Bond angles

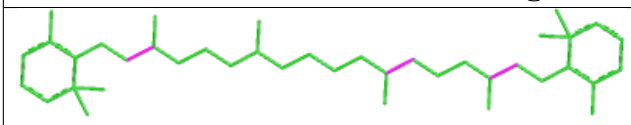


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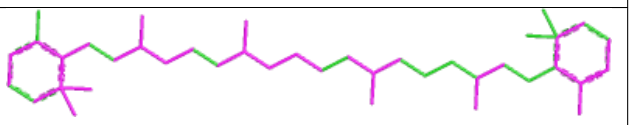


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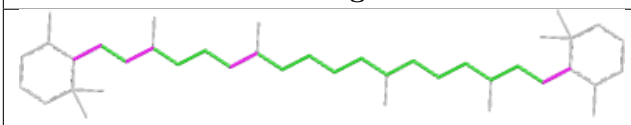
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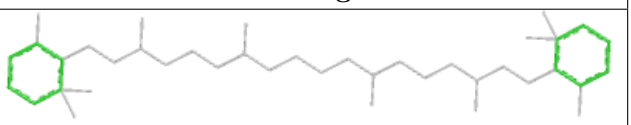
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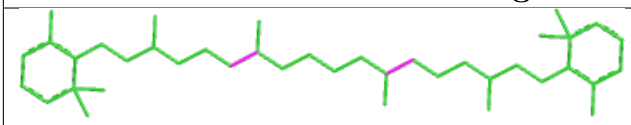


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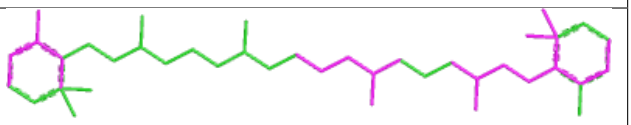


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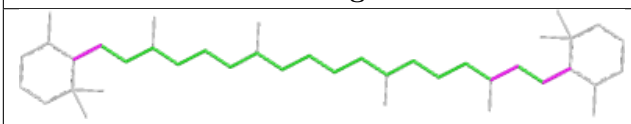
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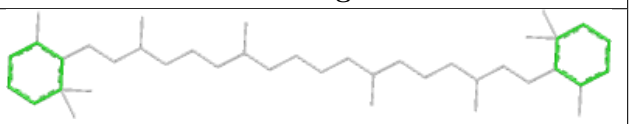
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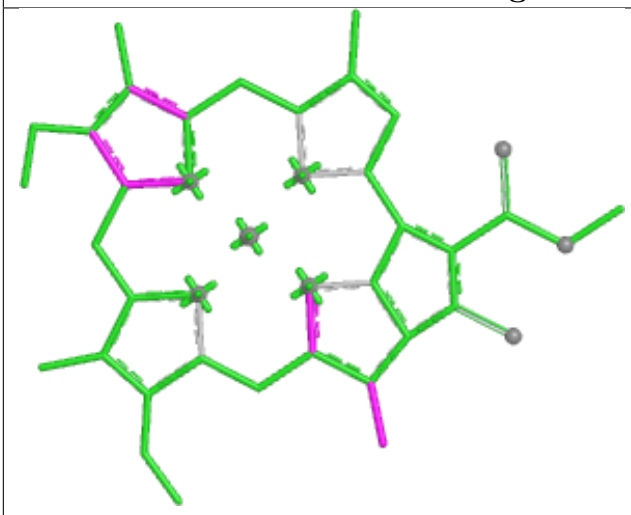


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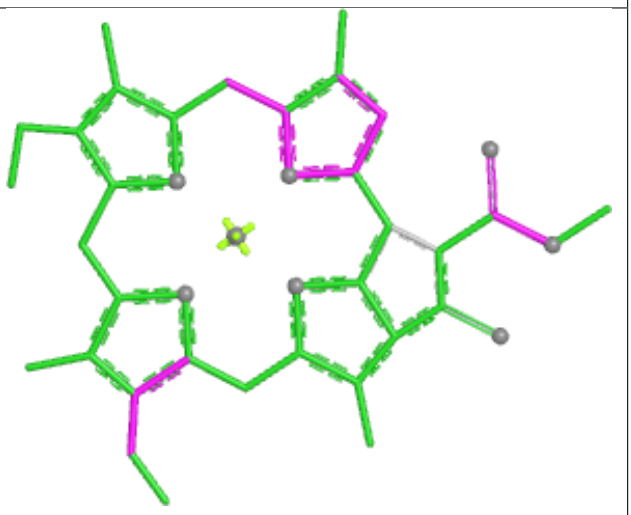


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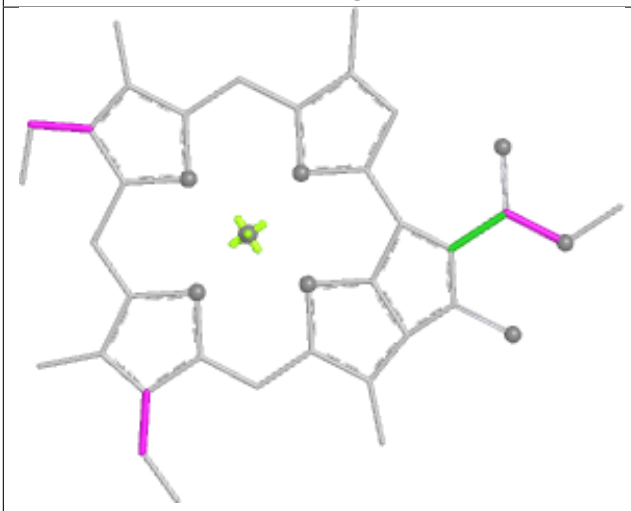
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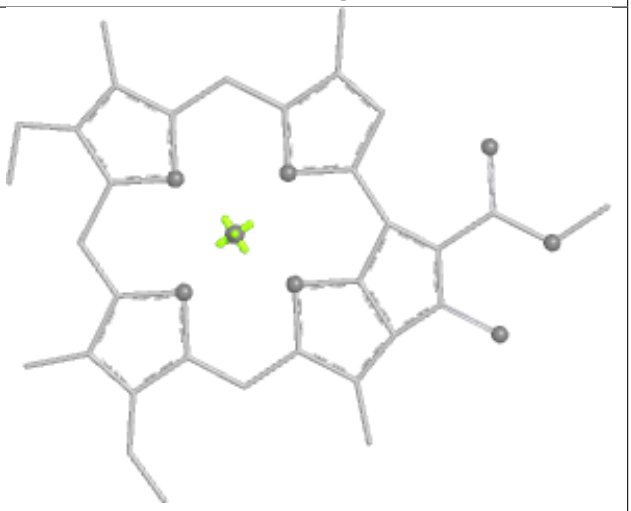
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Bond angles

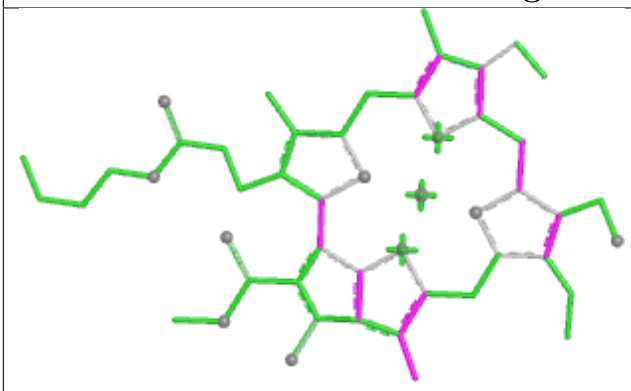


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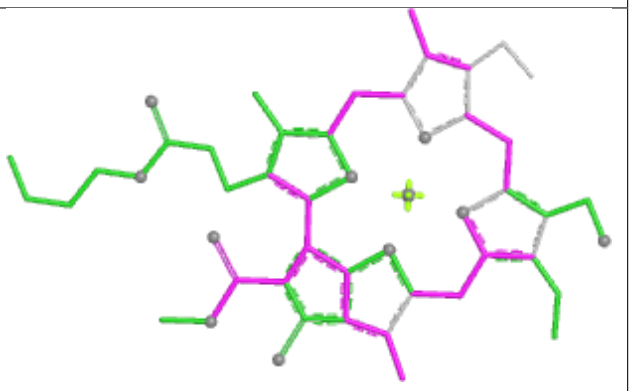


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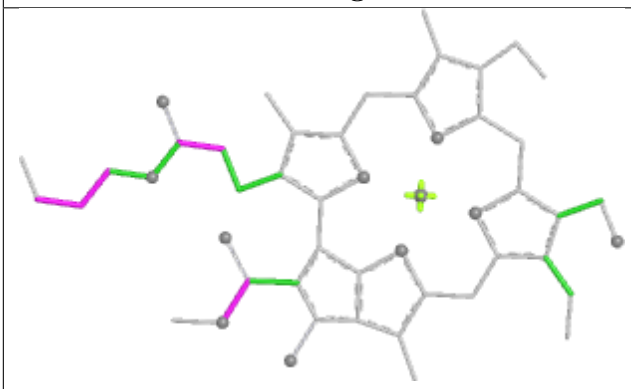
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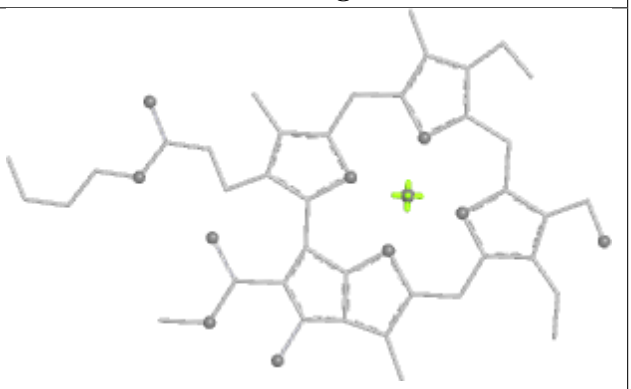
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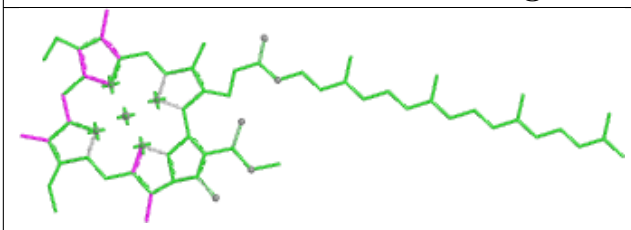


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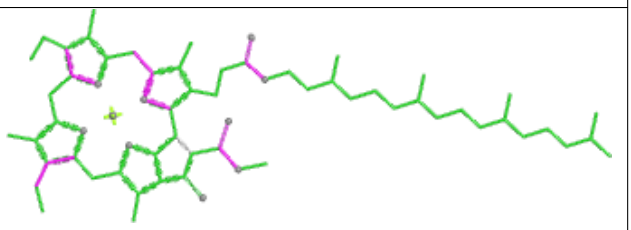


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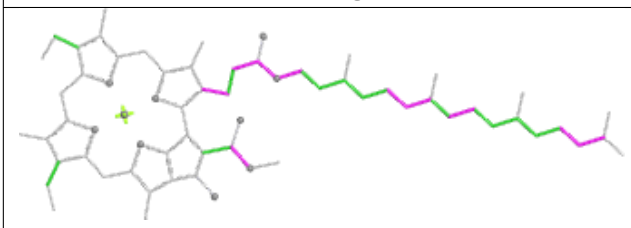
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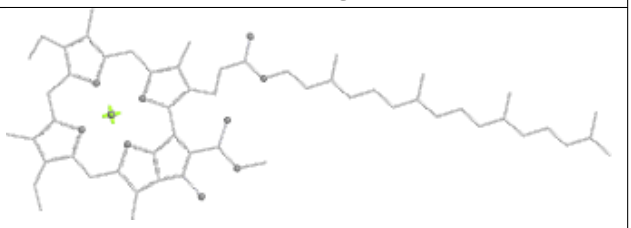
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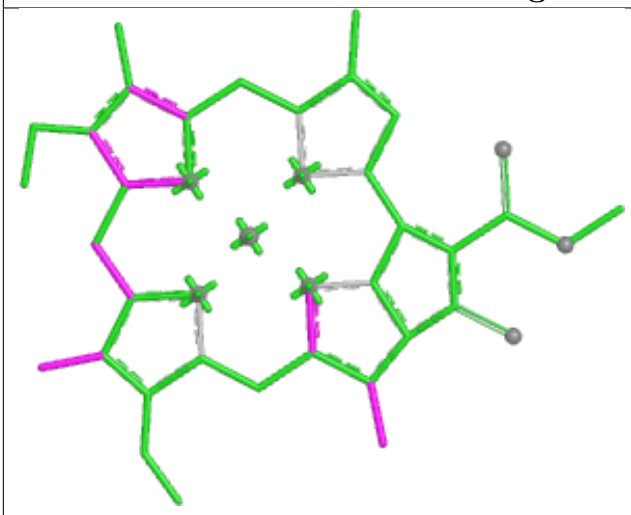


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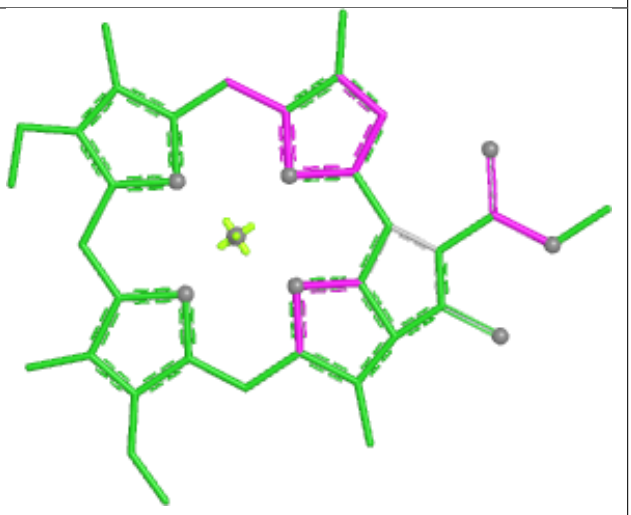


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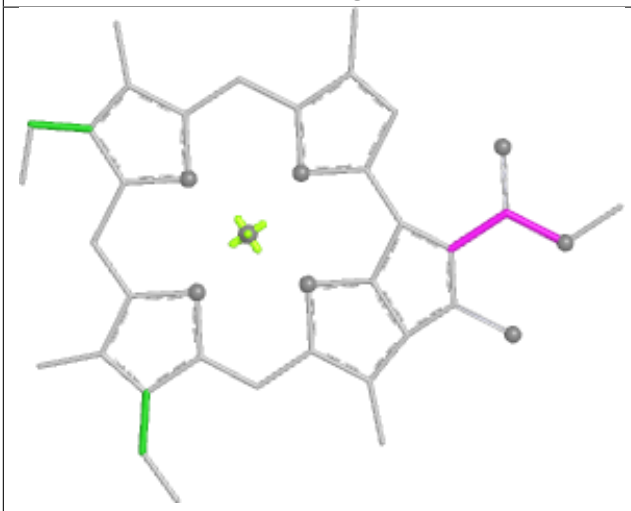
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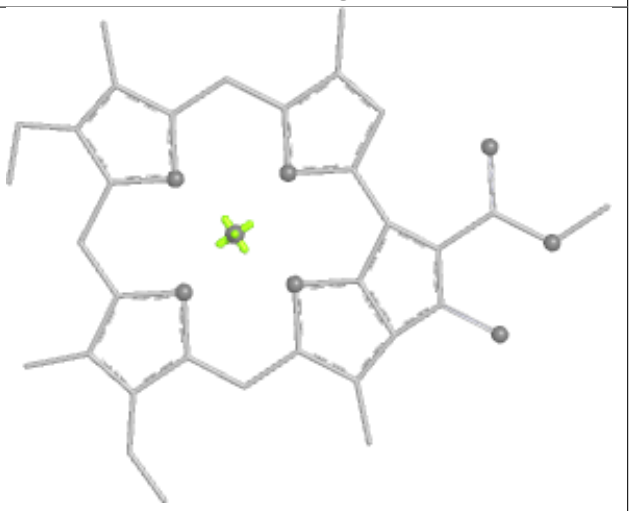
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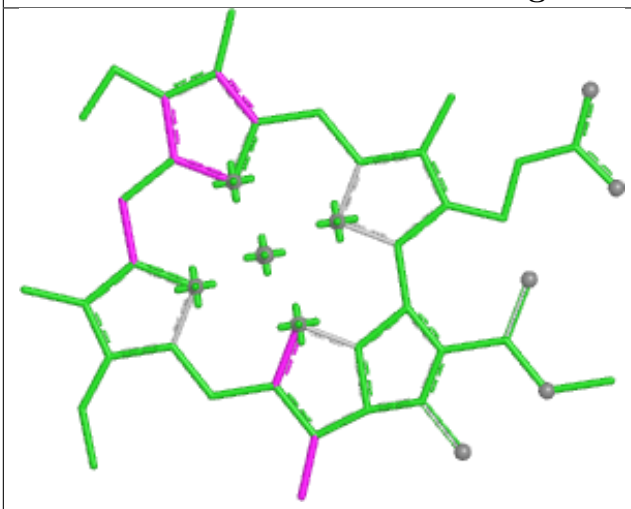


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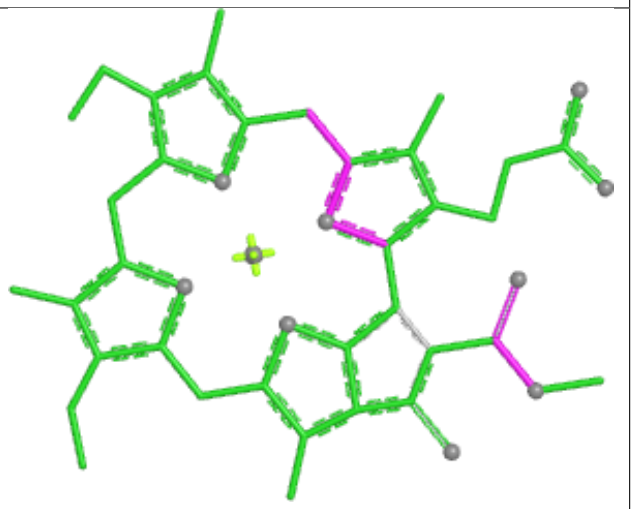


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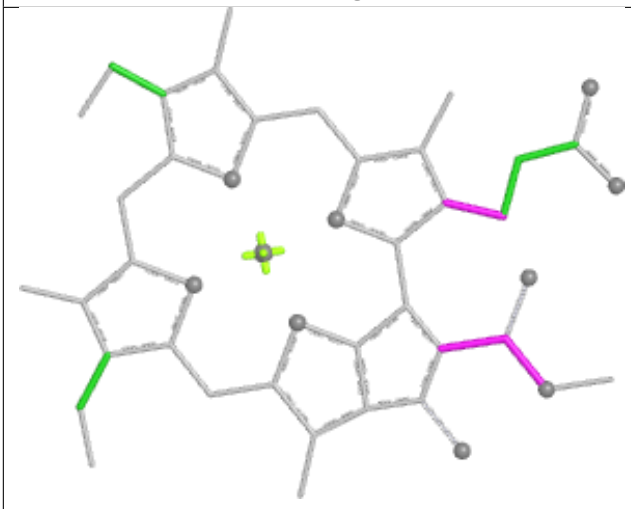
Ligand CLA 4 310



Bond lengths



Bond angles

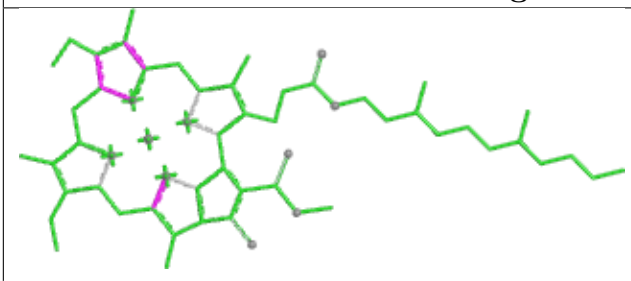


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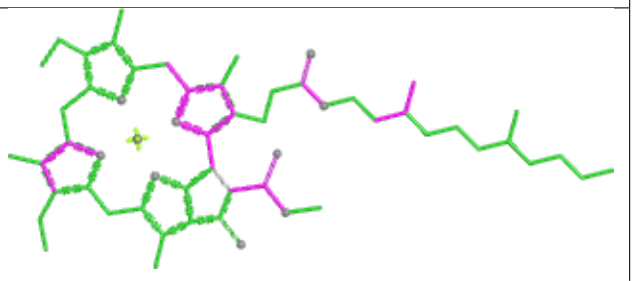


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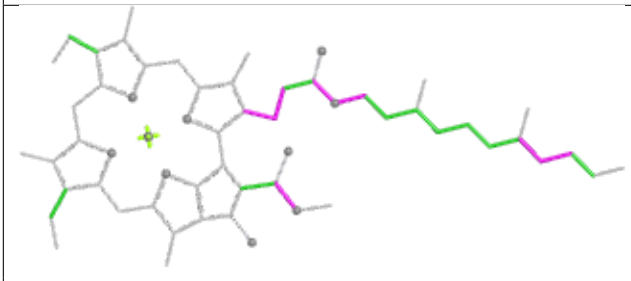
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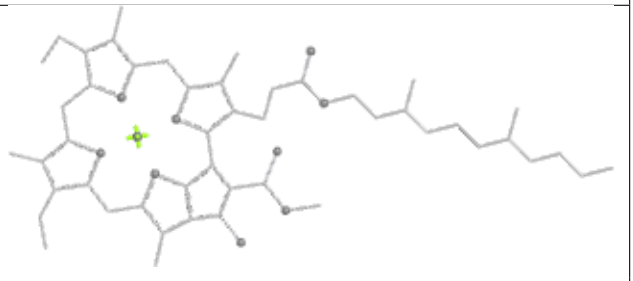
Bond lengths



Bond angles

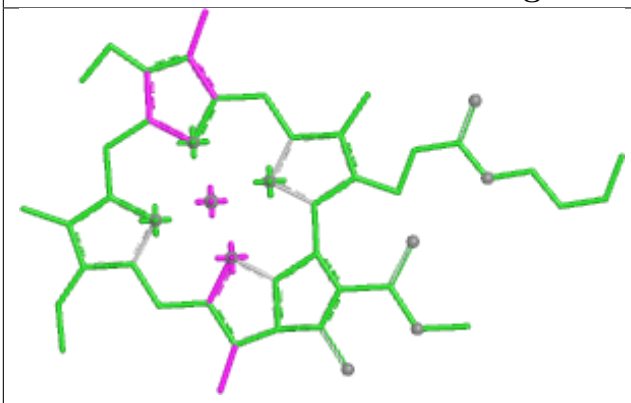


Torsions

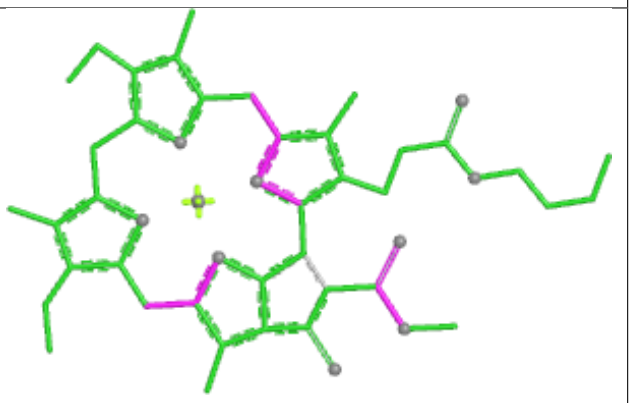


Rings

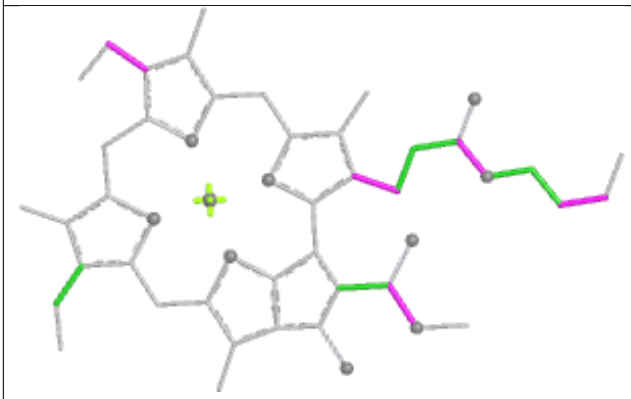
Ligand CLA N 613



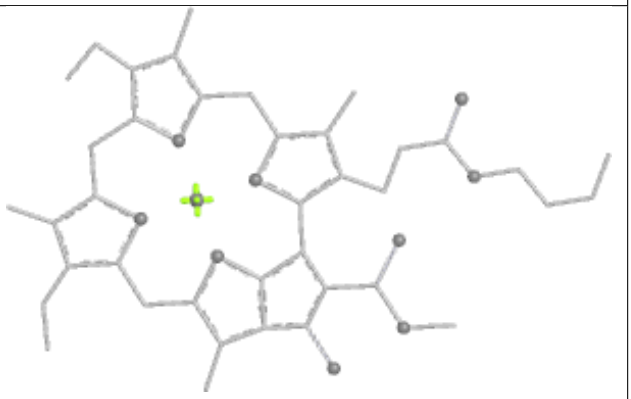
Bond lengths



Bond angles

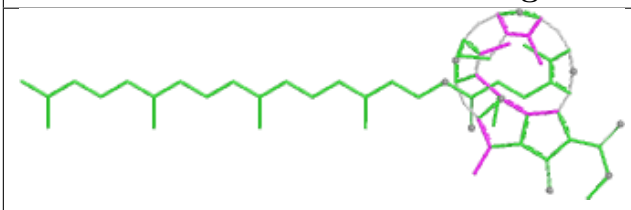


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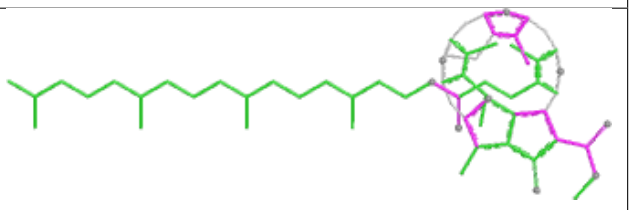


Rings

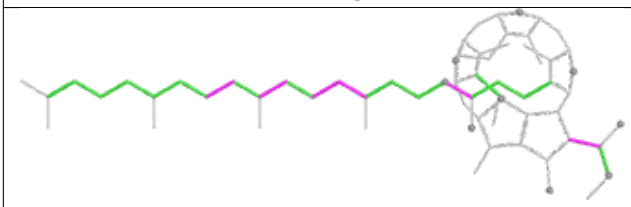
Ligand PHO D 402



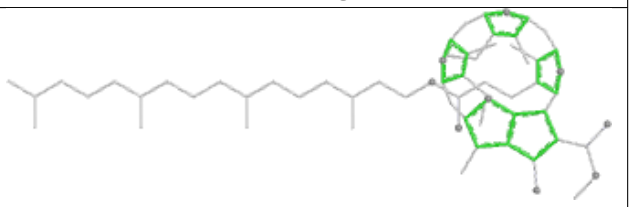
Bond lengths



Bond angles

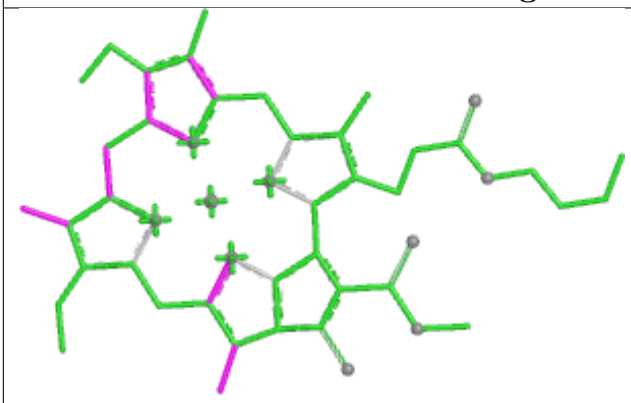


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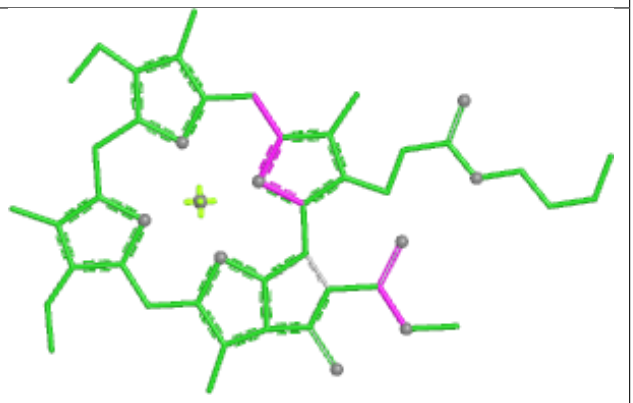


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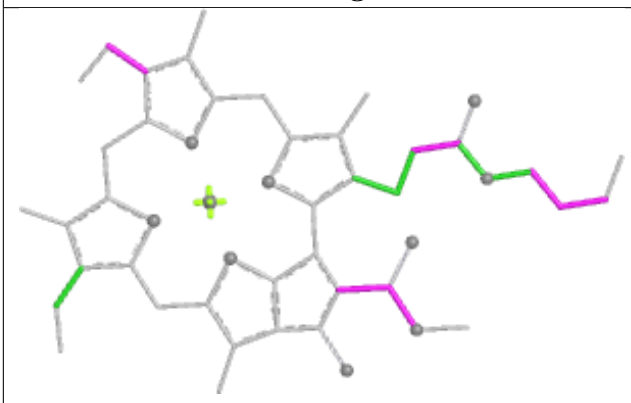
Ligand CLA 44 615



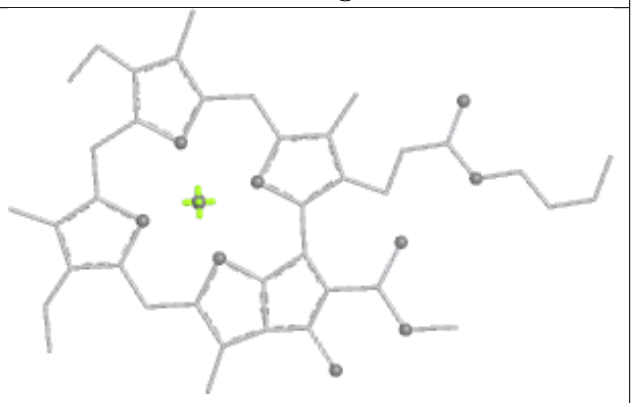
Bond lengths



Bond angles



Torsions

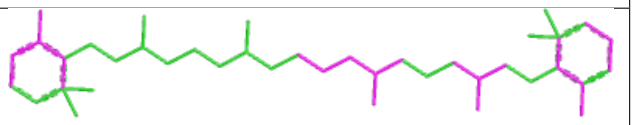


Rings

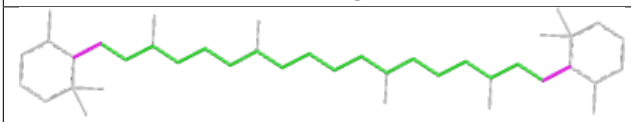
Ligand BCR B 613



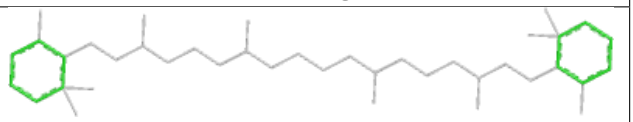
Bond lengths



Bond angles

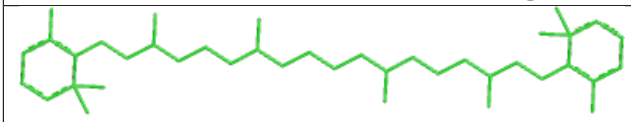


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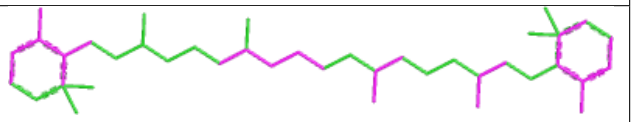


Rings

Ligand BCR D 406



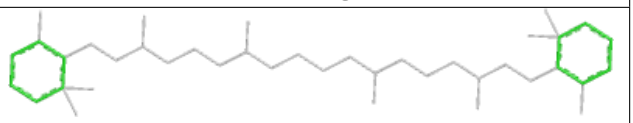
Bond lengths



Bond angles

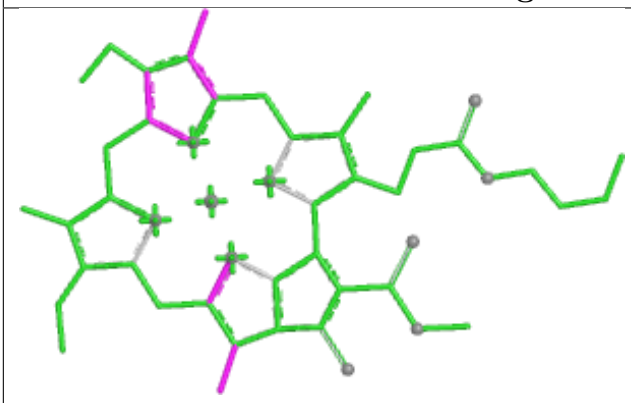


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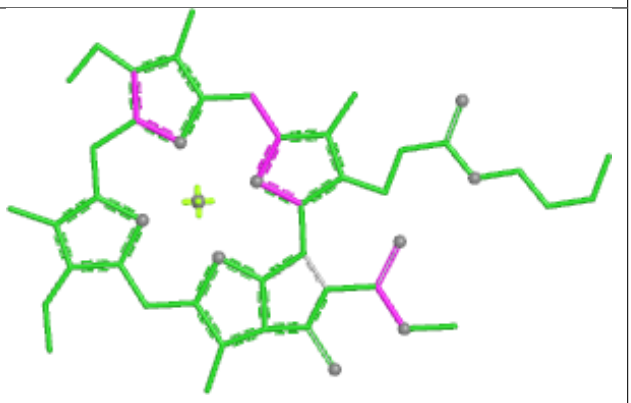


Rings

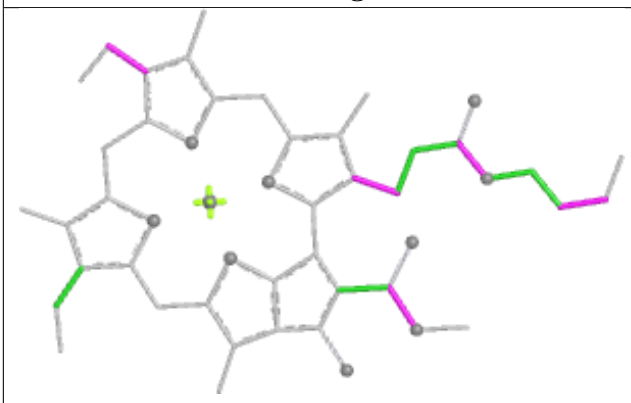
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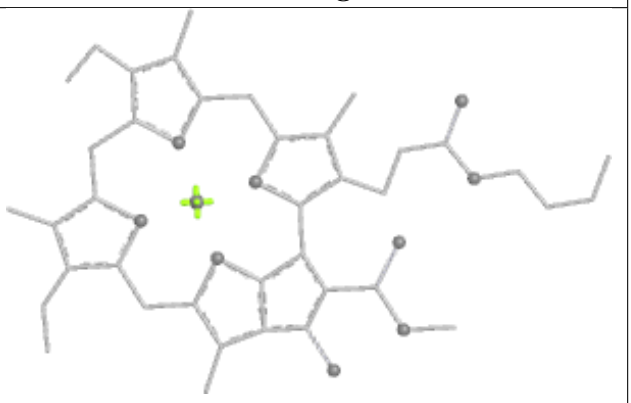
Bond lengths



Bond angles

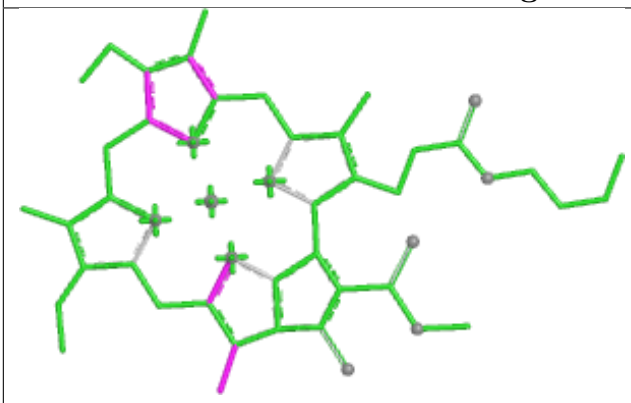


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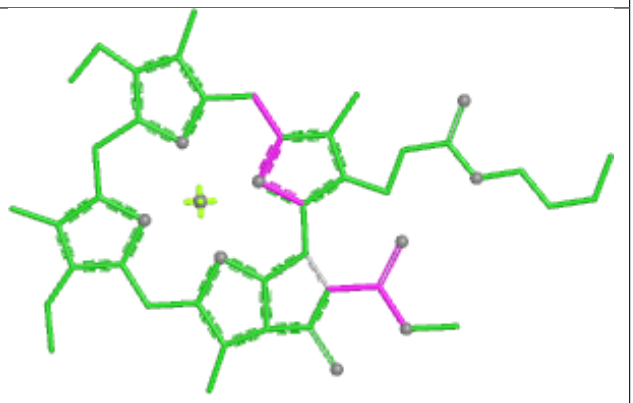


Rings

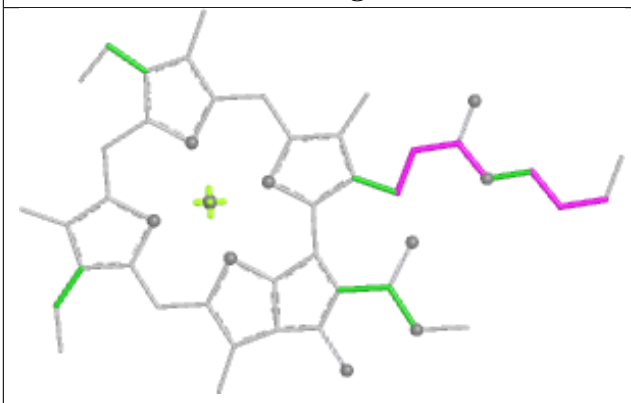
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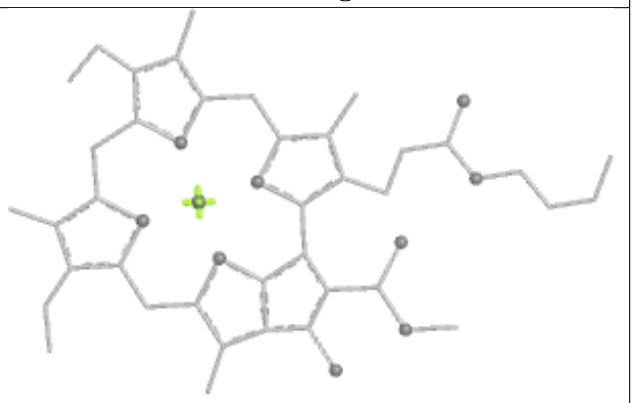
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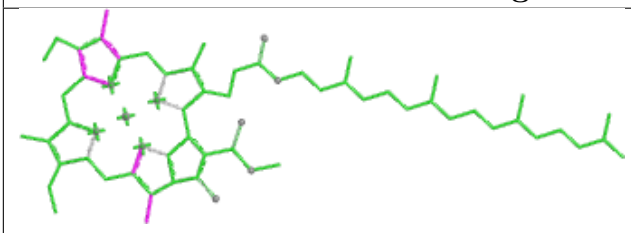


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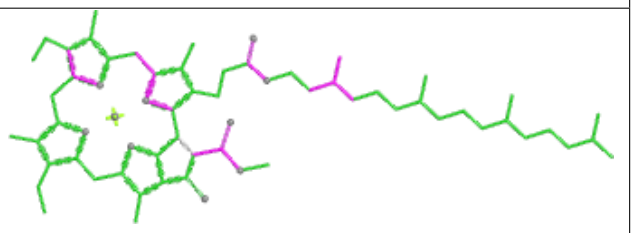


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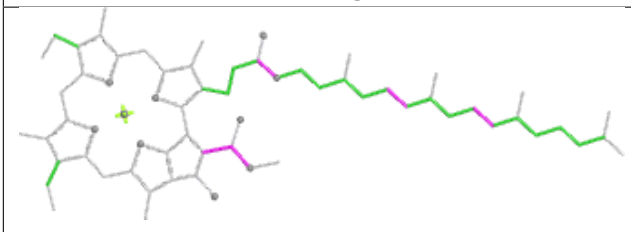
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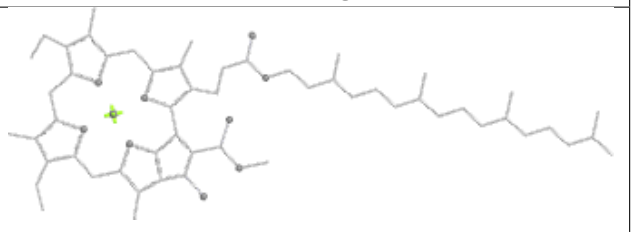
Bond lengths



Bond angles

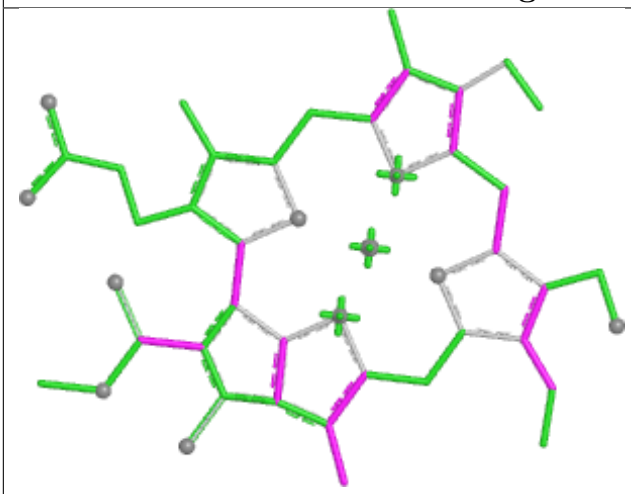


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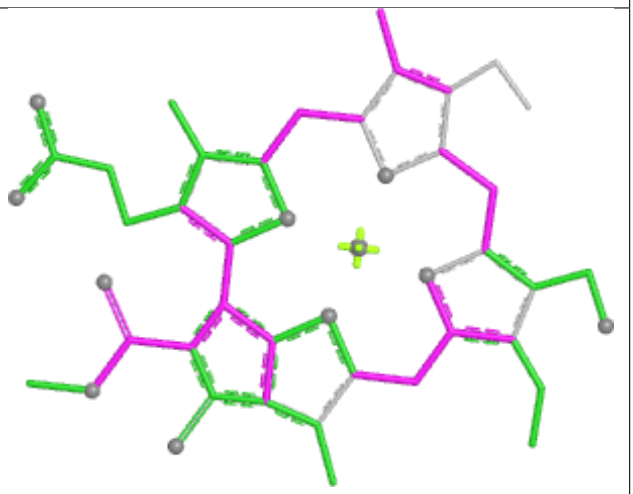


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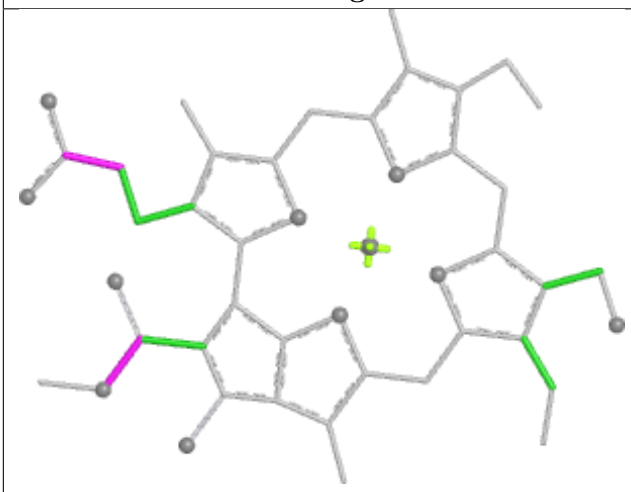
Ligand CHL 44 605



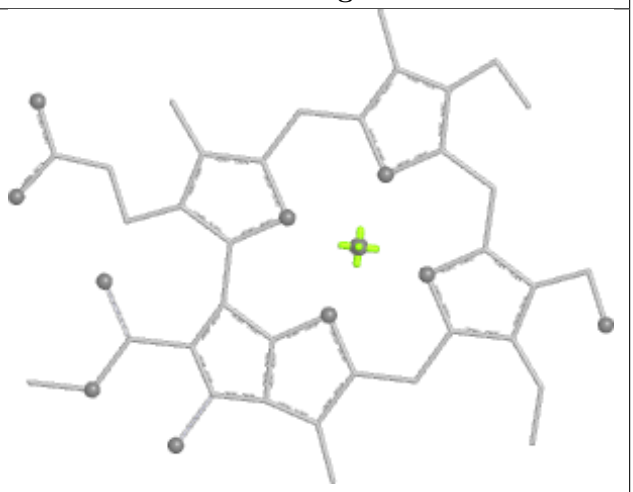
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Bond angles

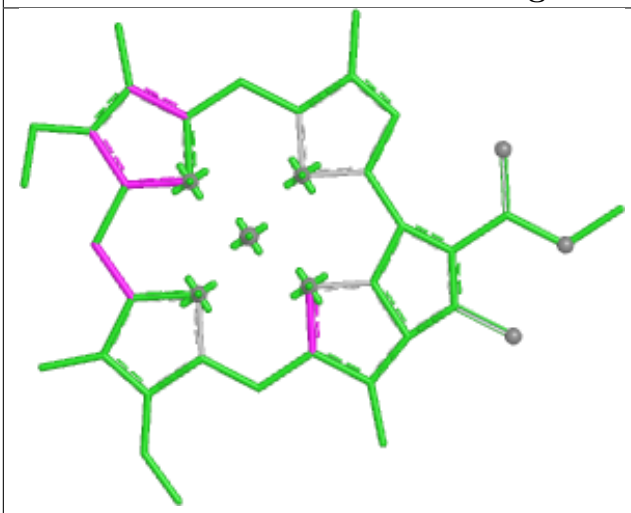


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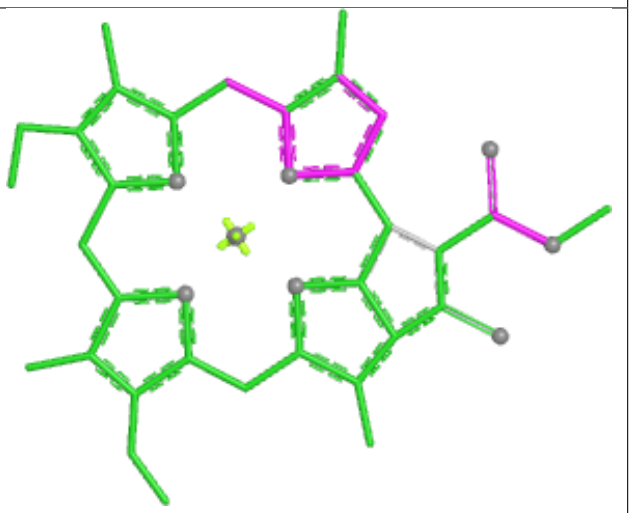


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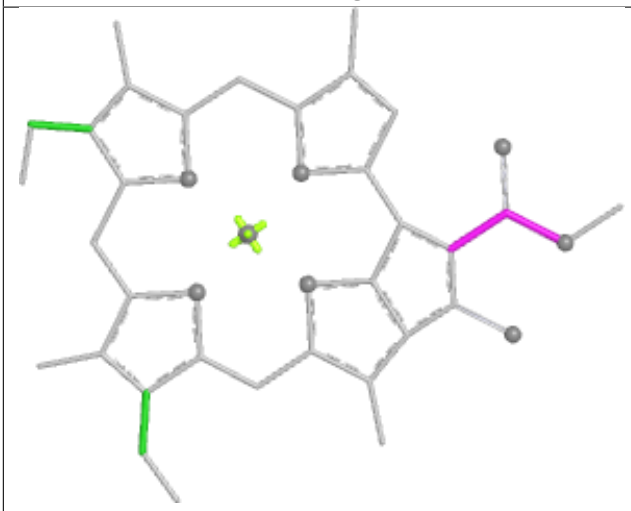
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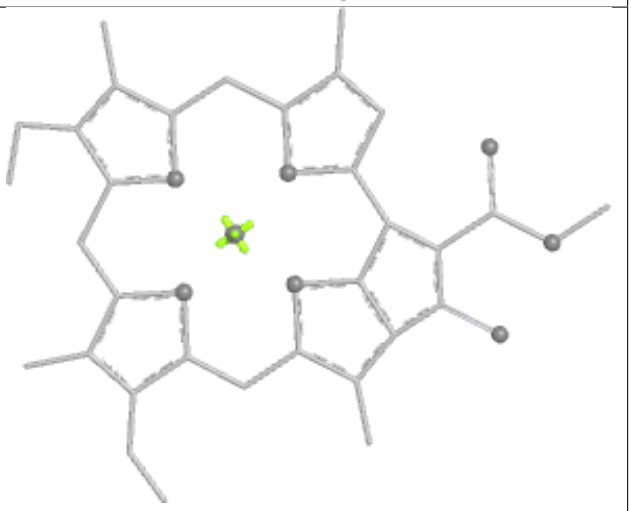
Bond lengths



Bond angles

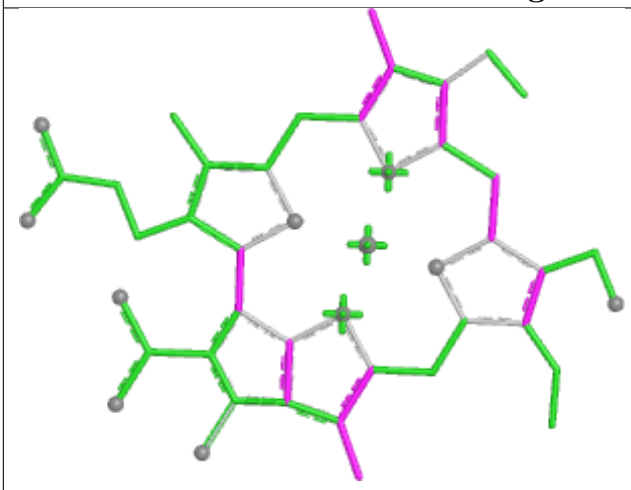


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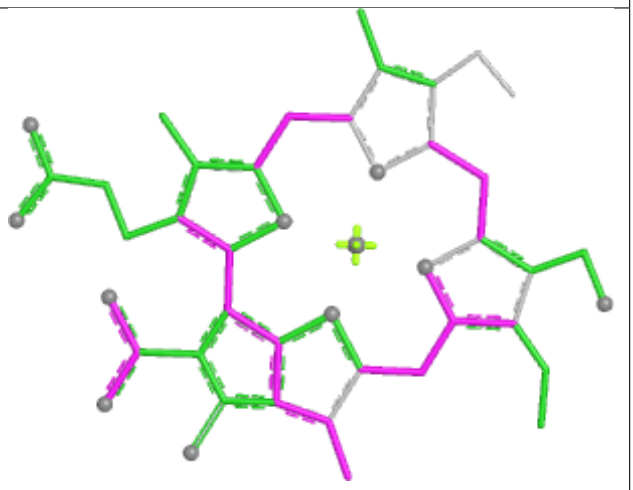


Rings

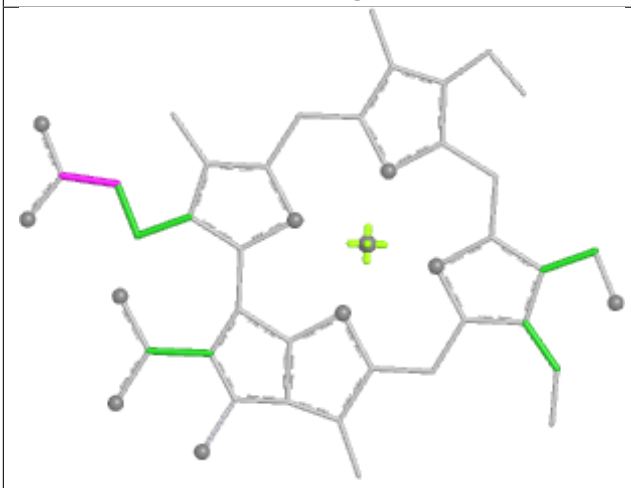
Ligand CHL 4 302



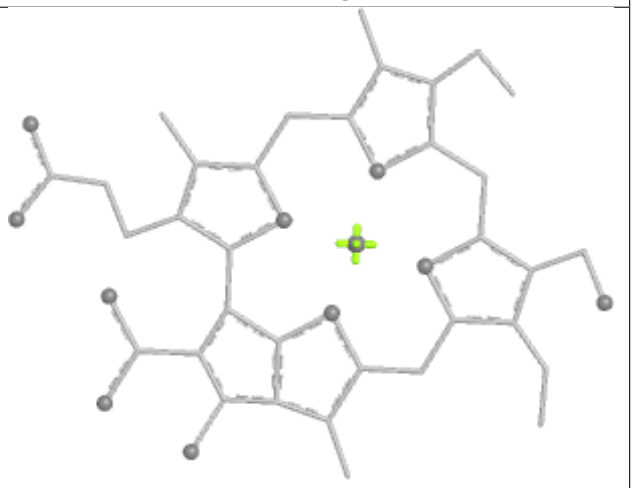
Bond lengths



Bond angles

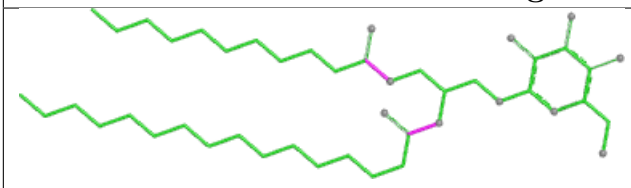


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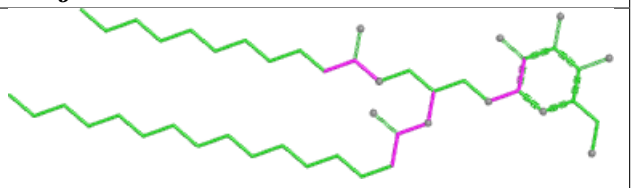


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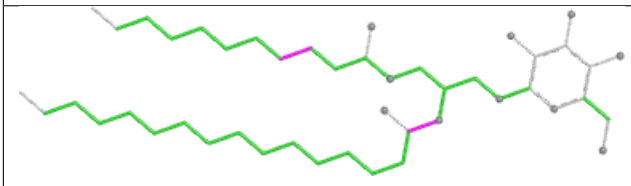
Ligand LMG j 101



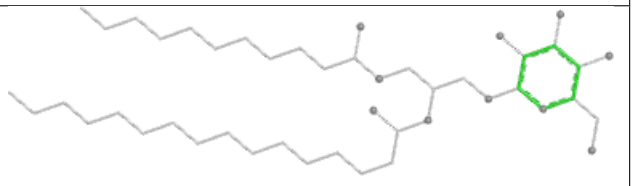
Bond lengths



Bond angles

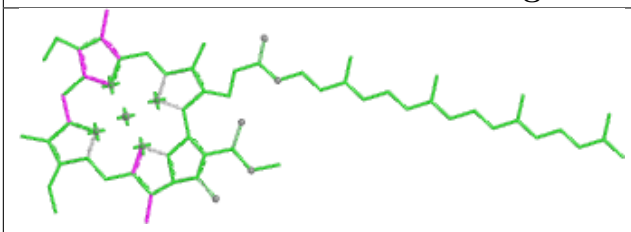


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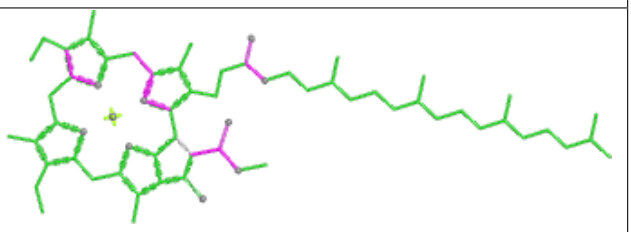


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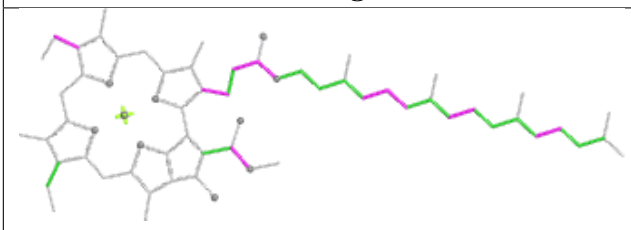
Ligand CLA N 602



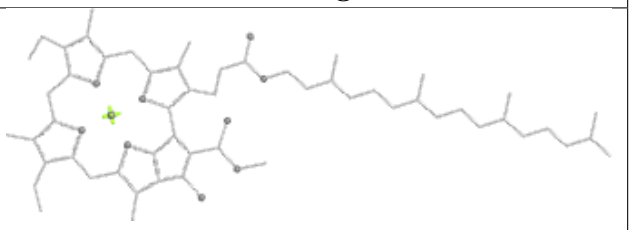
Bond lengths



Bond angles

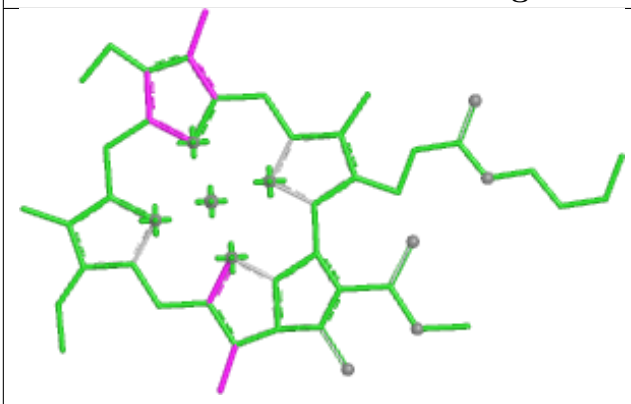


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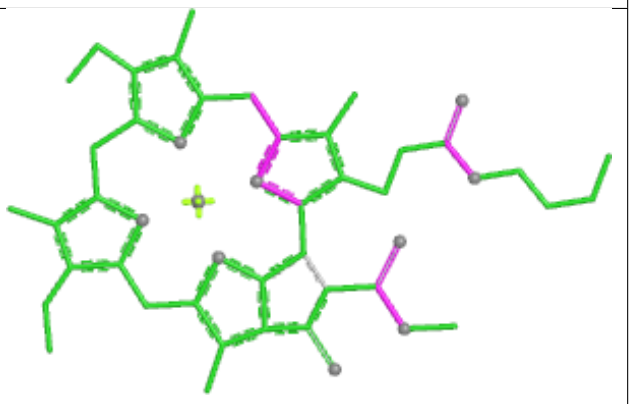


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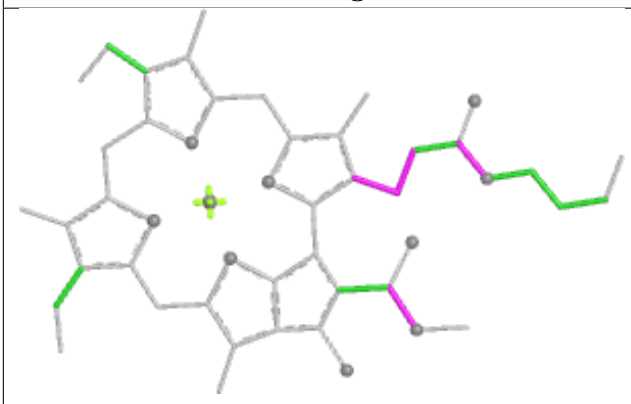
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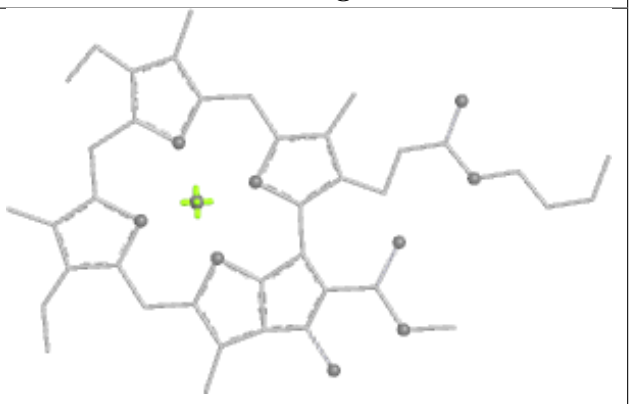
Bond lengths



Bond angles

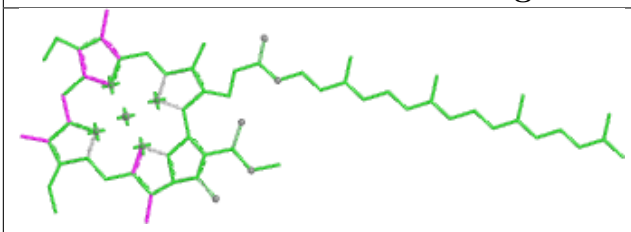


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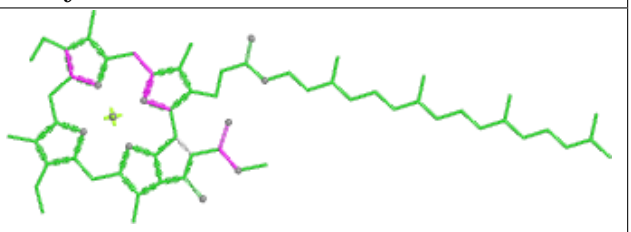


Rings

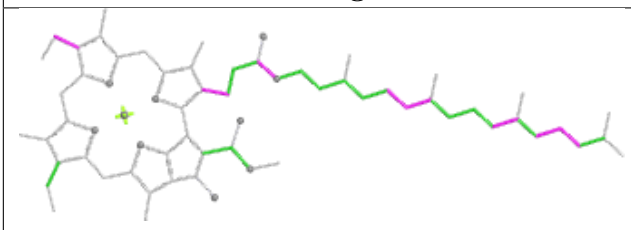
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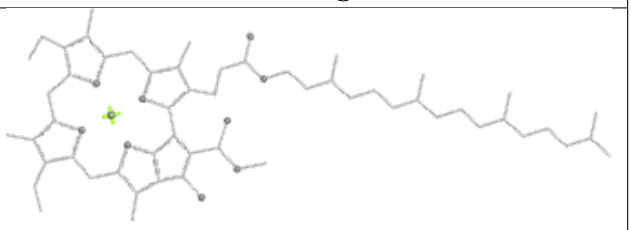
Bond lengths



Bond angles

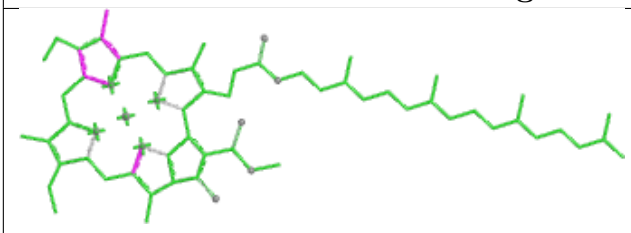


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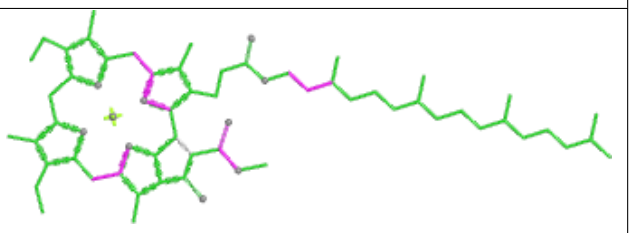


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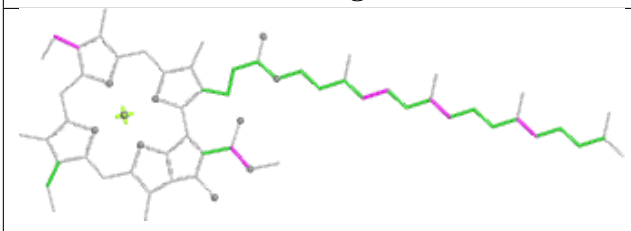
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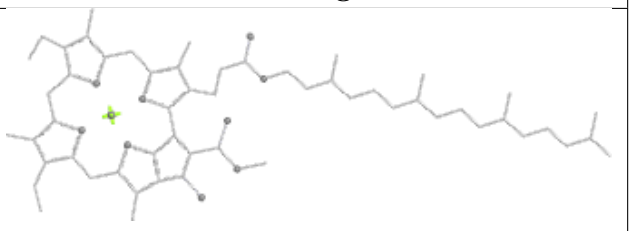
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Bond angles

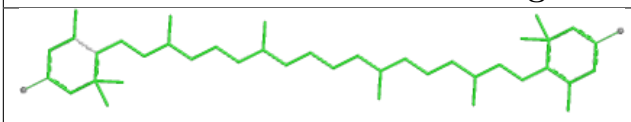


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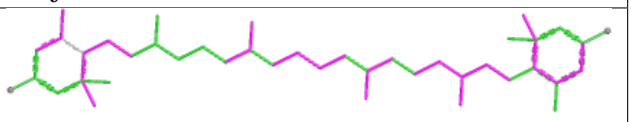


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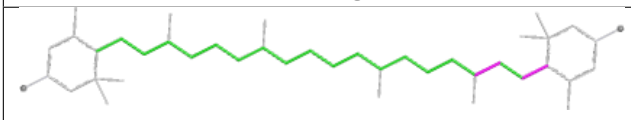
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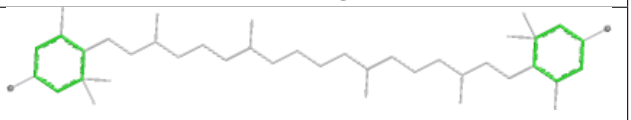
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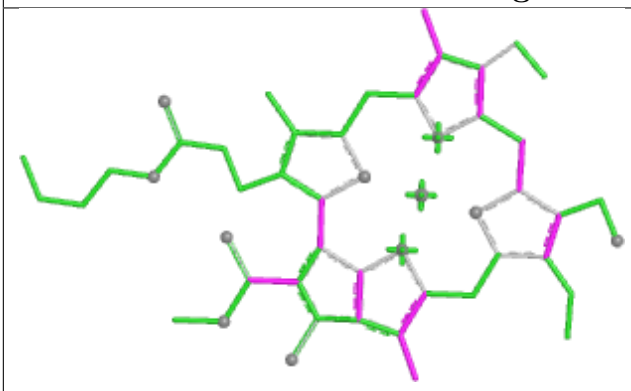


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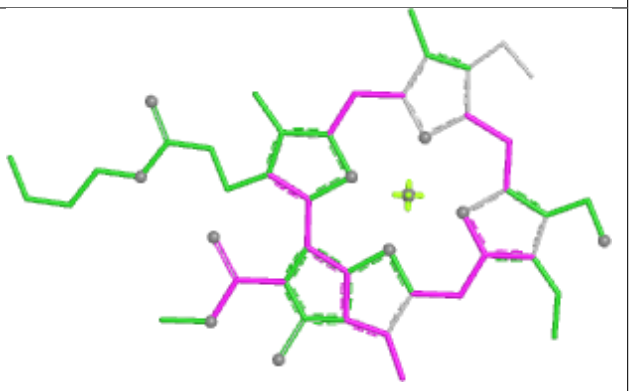


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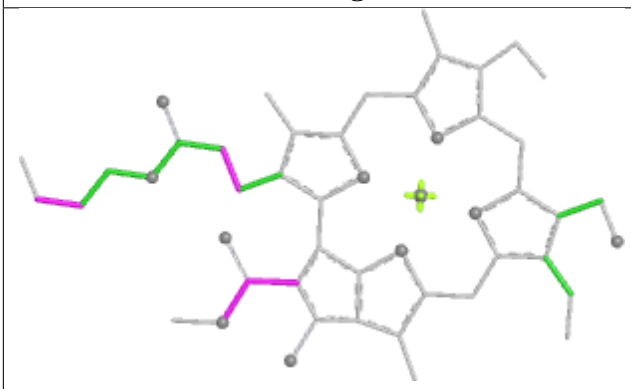
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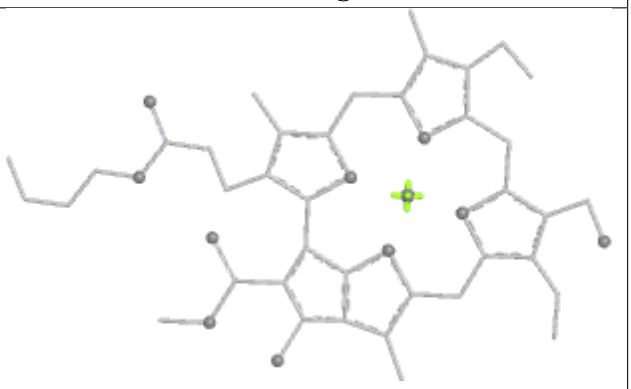
Bond lengths



Bond angles

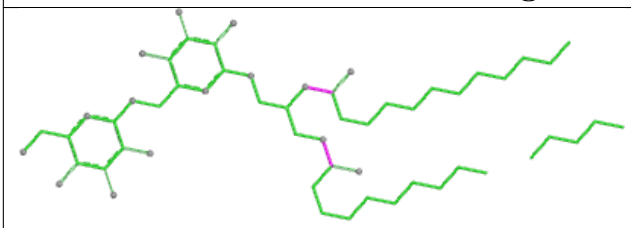


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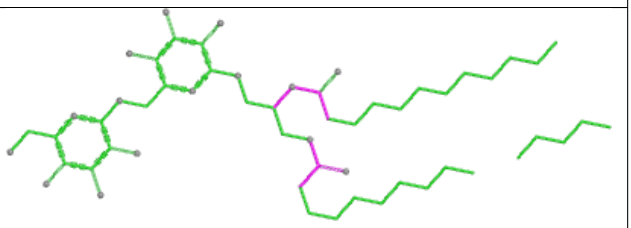


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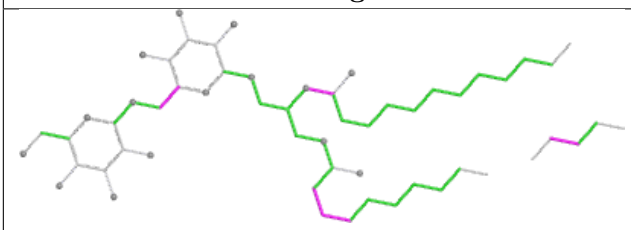
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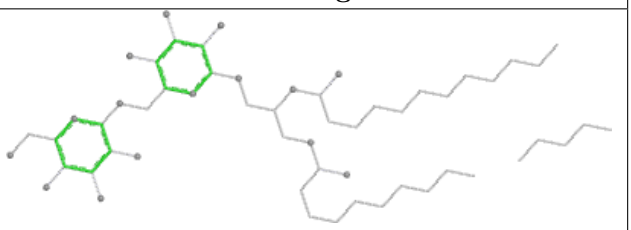
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Bond angles

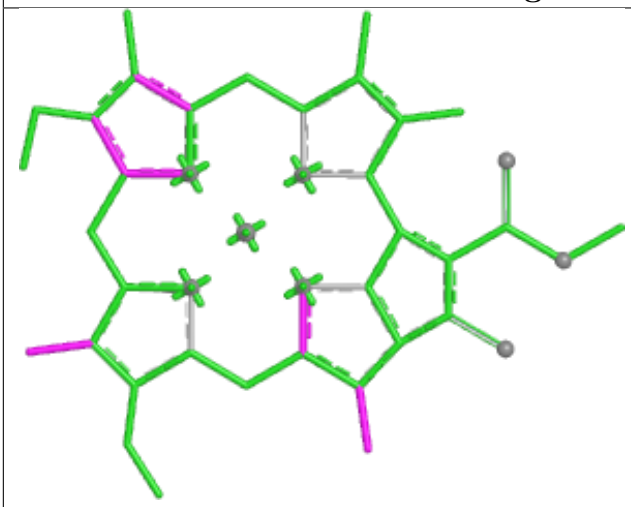


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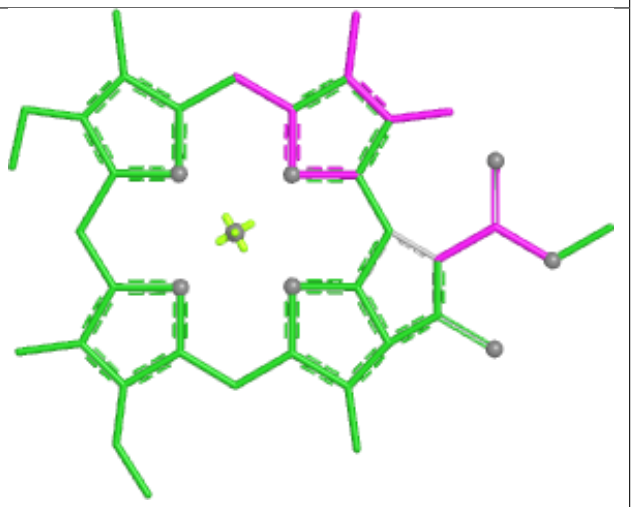


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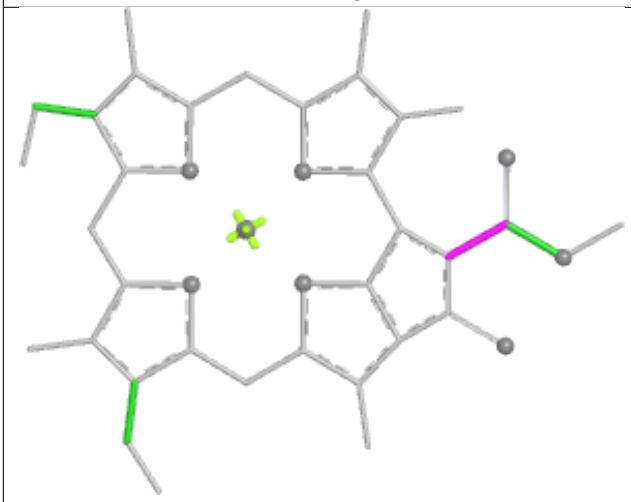
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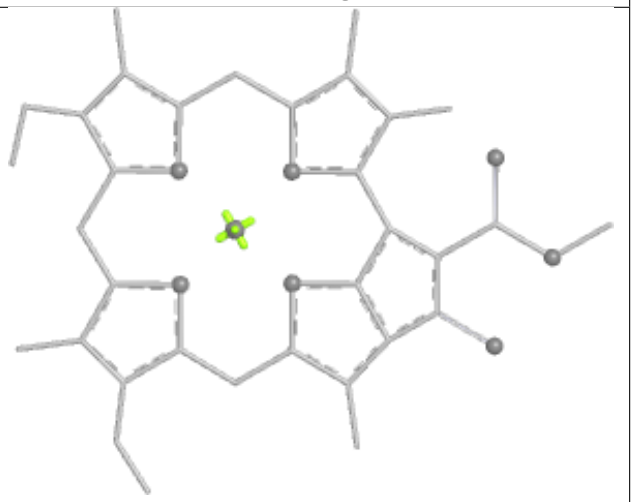
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Bond angles

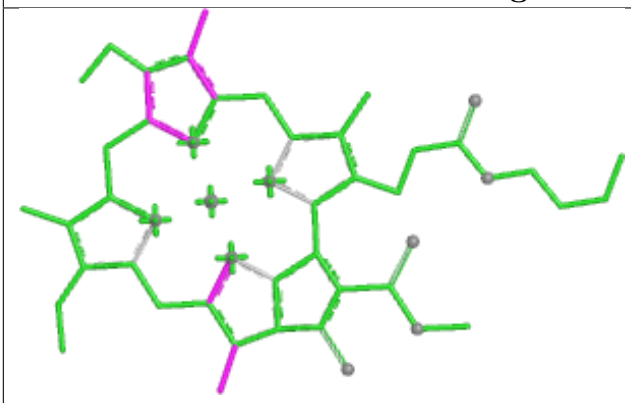


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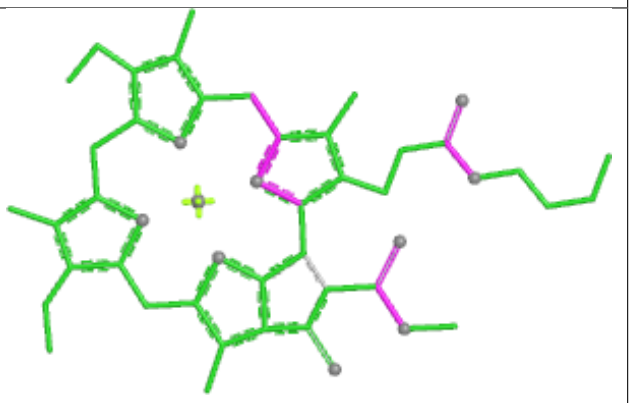


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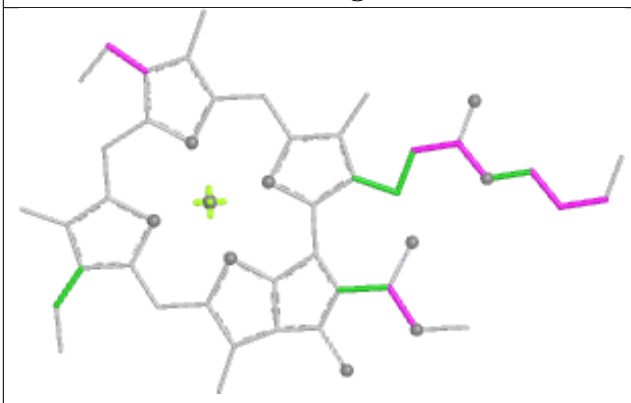
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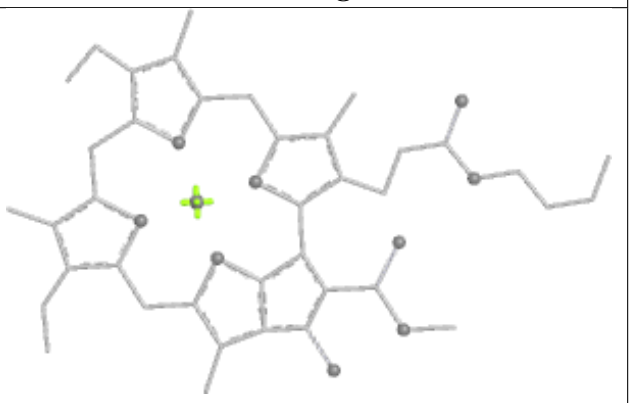
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Bond angles

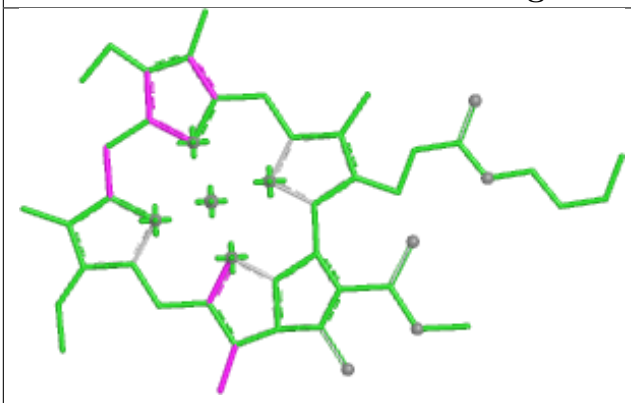


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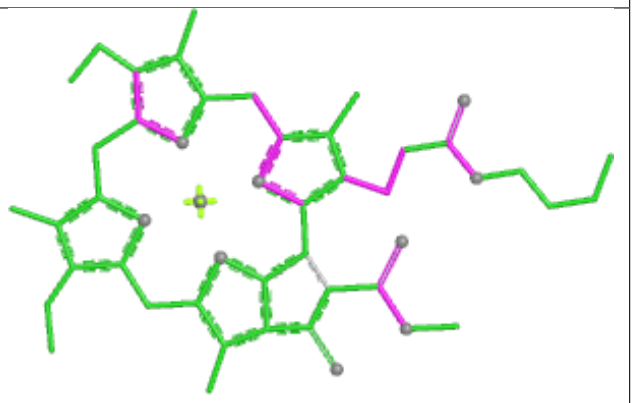


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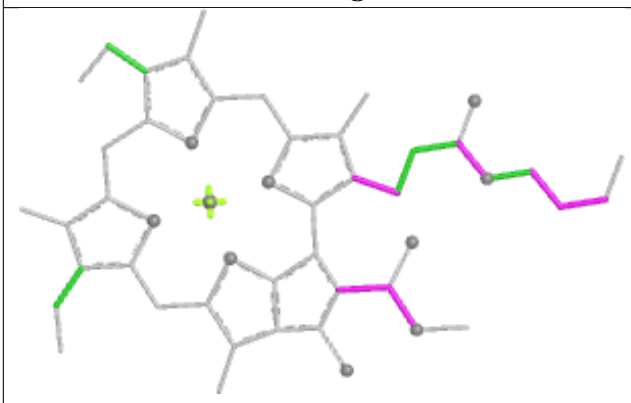
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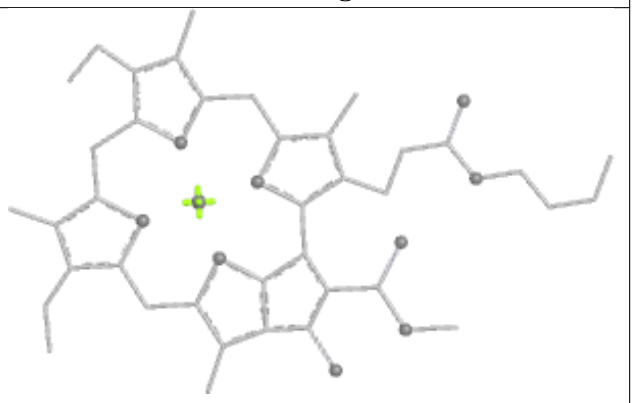
Bond lengths



Bond angles



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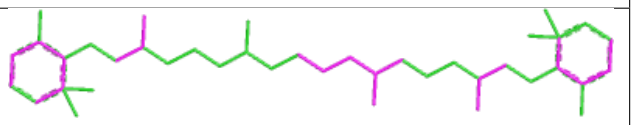


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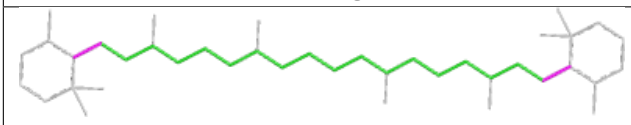
Ligand BCR B 612



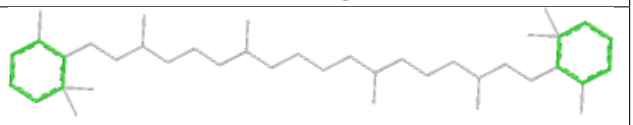
Bond lengths



Bond angles

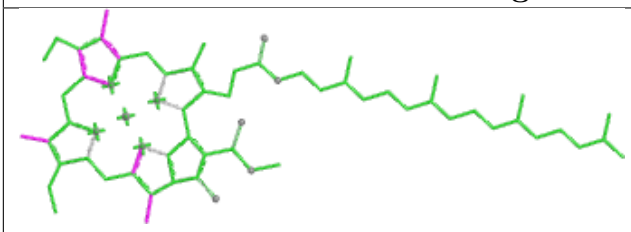


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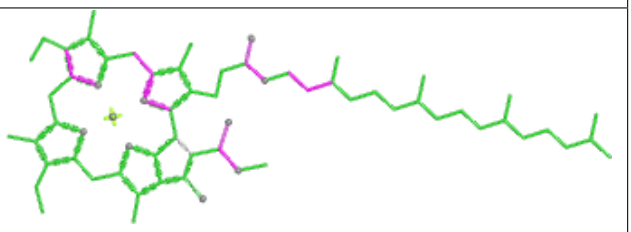


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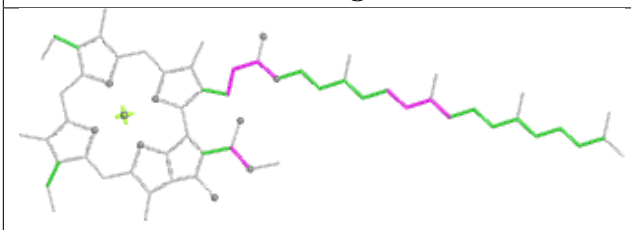
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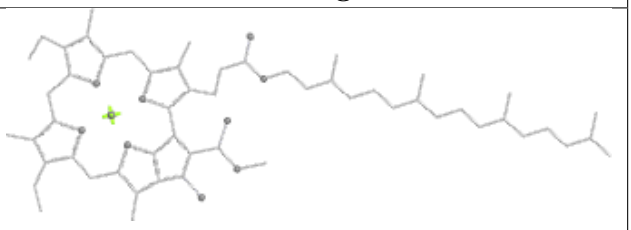
Bond lengths



Bond angles

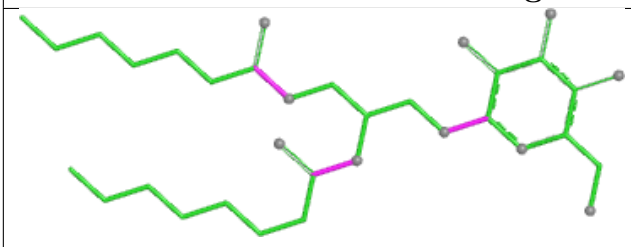


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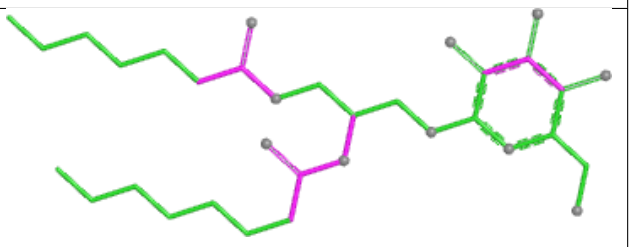


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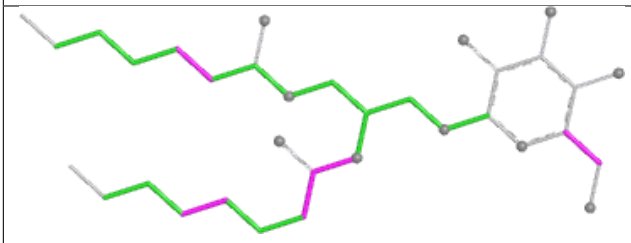
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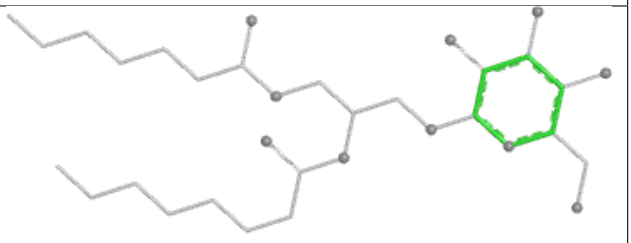
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Bond angles

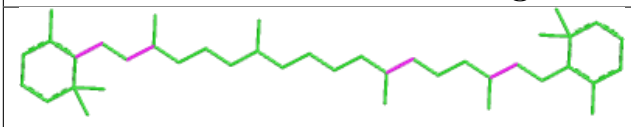


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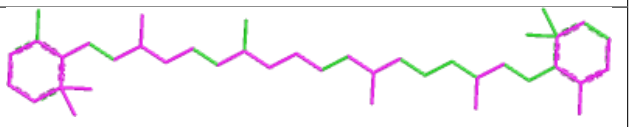


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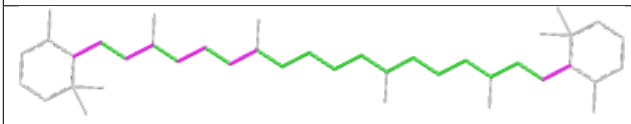
Ligand BCR Hh 101



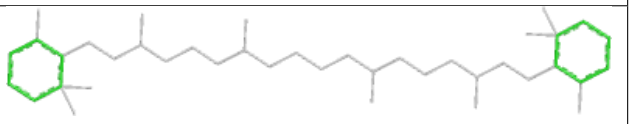
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Bond angles

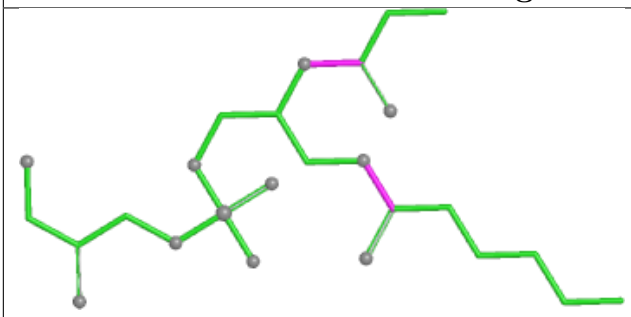


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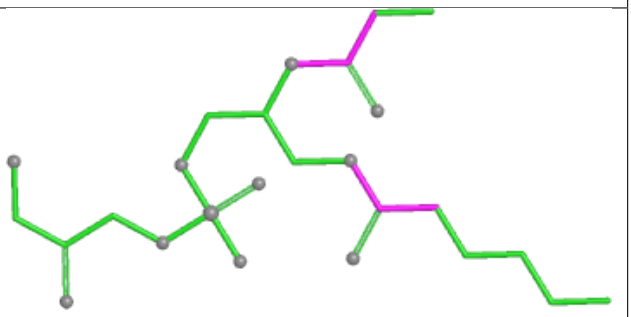


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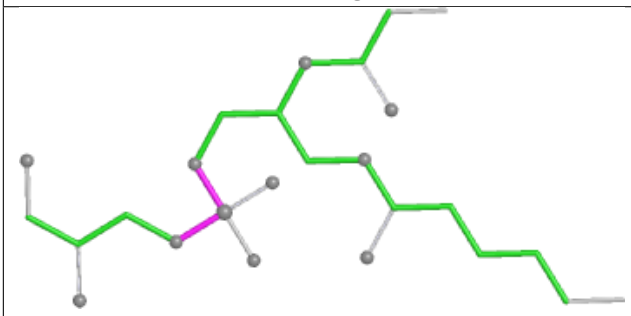
Ligand LHG SS 301



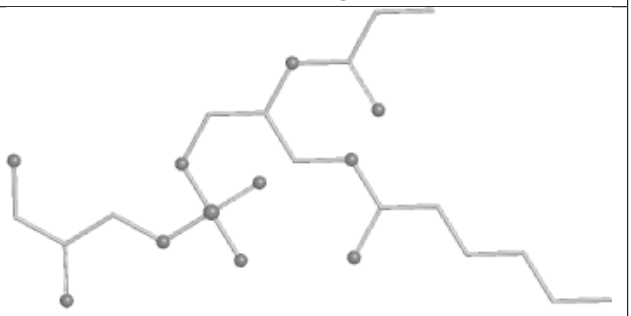
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Bond angles

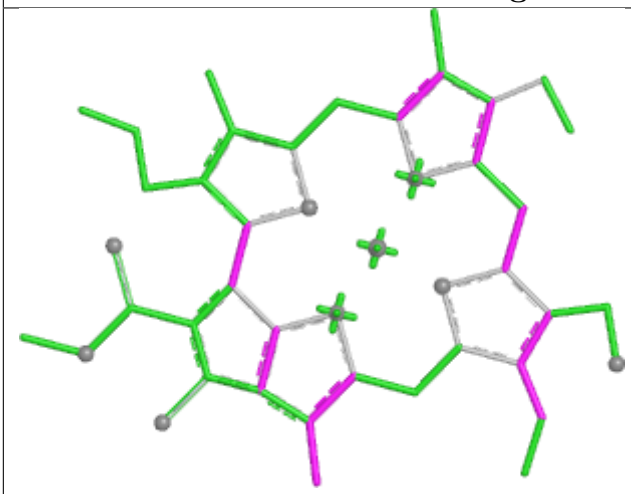


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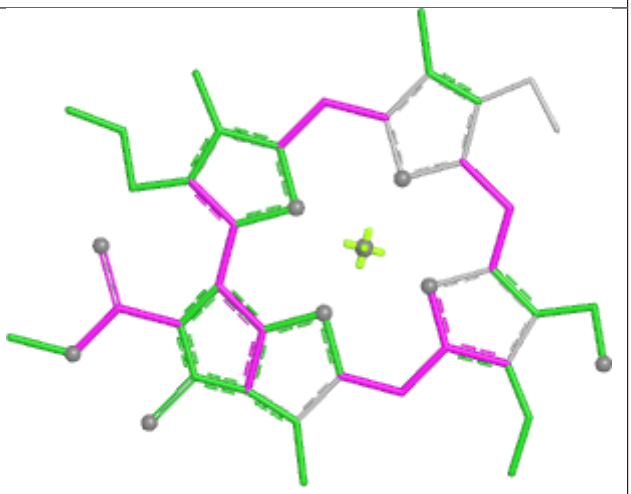


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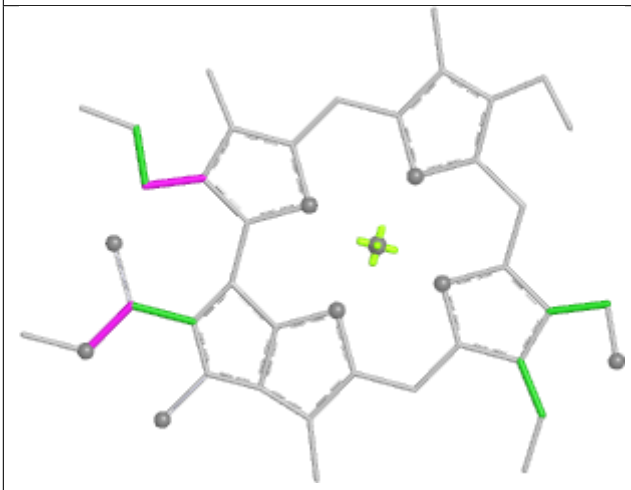
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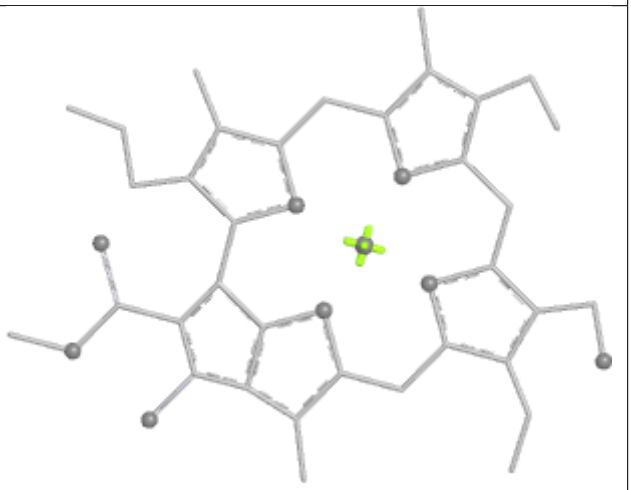
Bond lengths



Bond angles

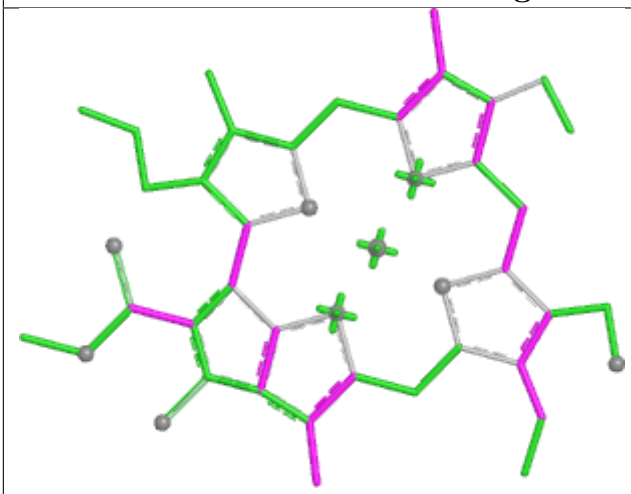


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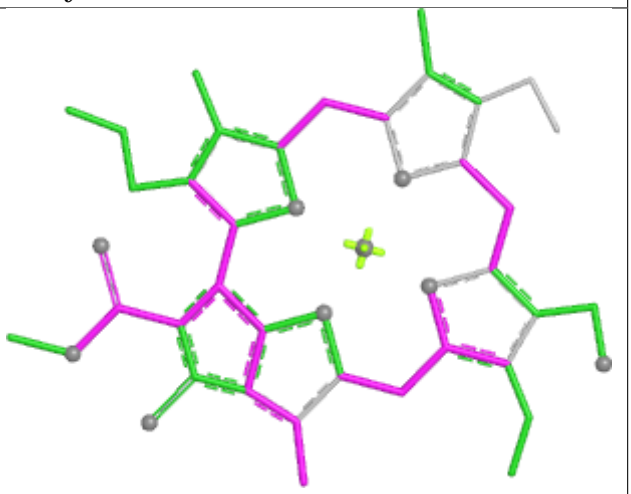


Rings

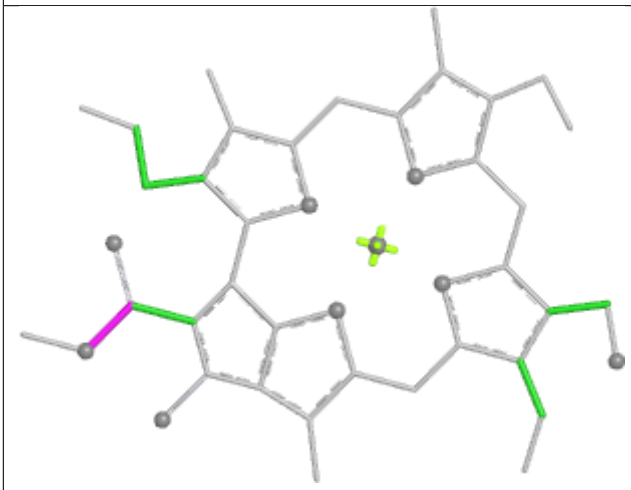
Ligand CHL Yy 606



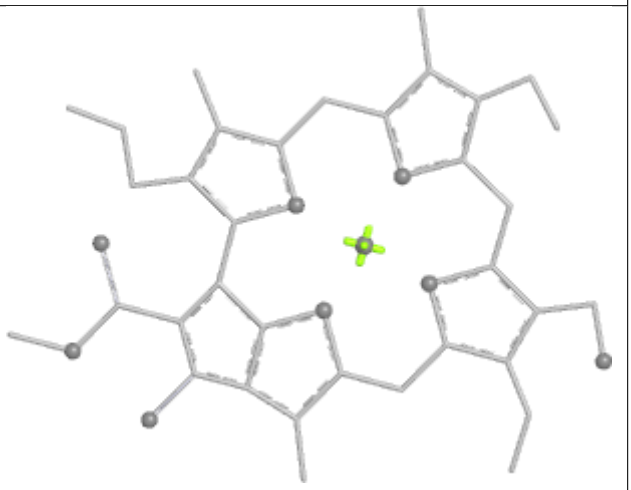
Bond lengths



Bond angles

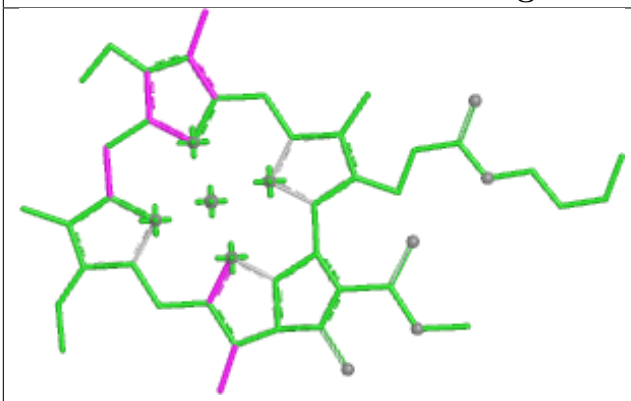


Torsions

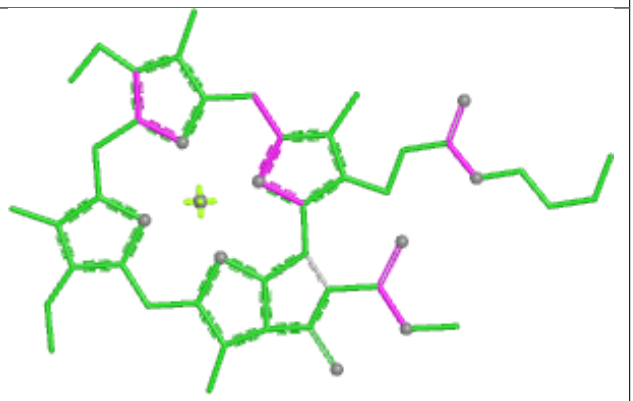


Rings

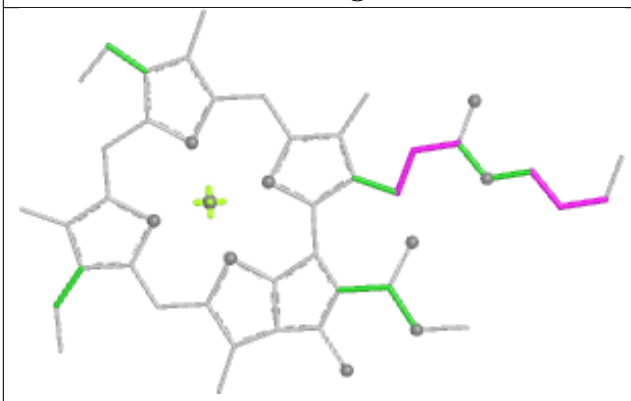
Ligand CLA SS 314



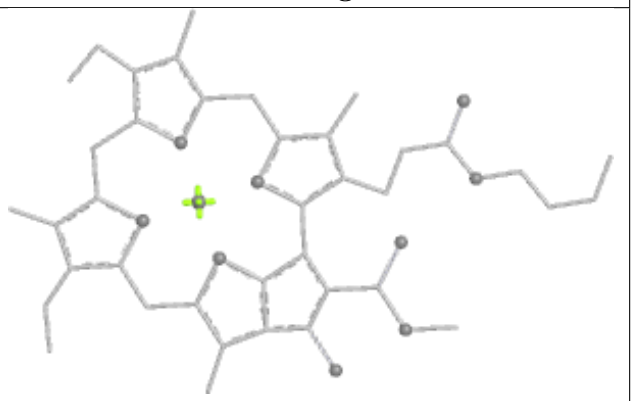
Bond lengths



Bond angles

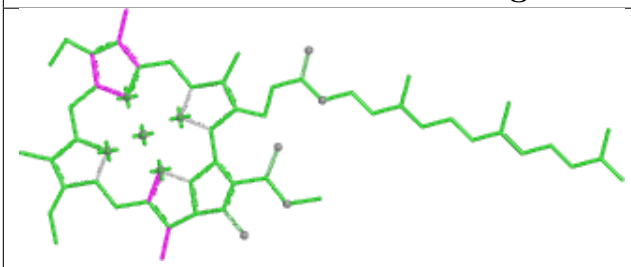


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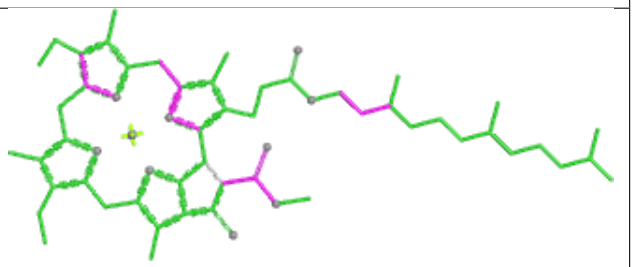


Rings

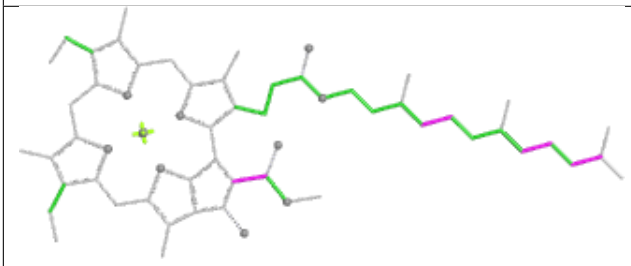
Ligand CLA AA 408



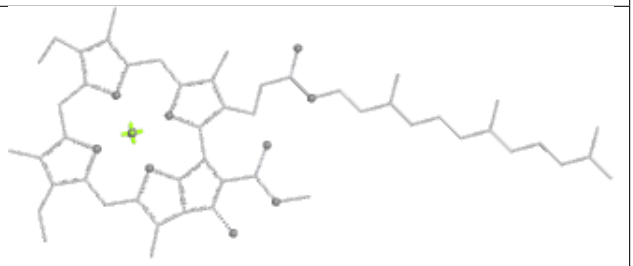
Bond lengths



Bond angles

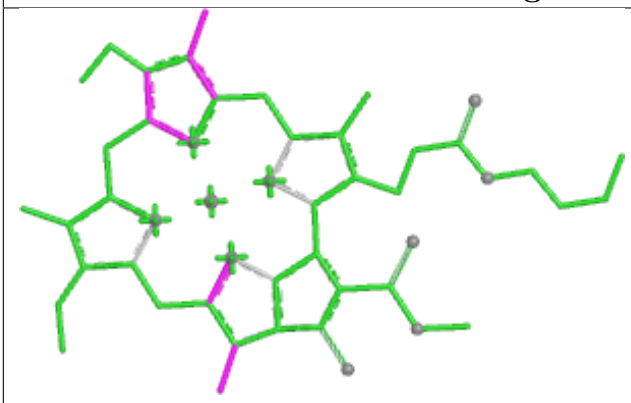


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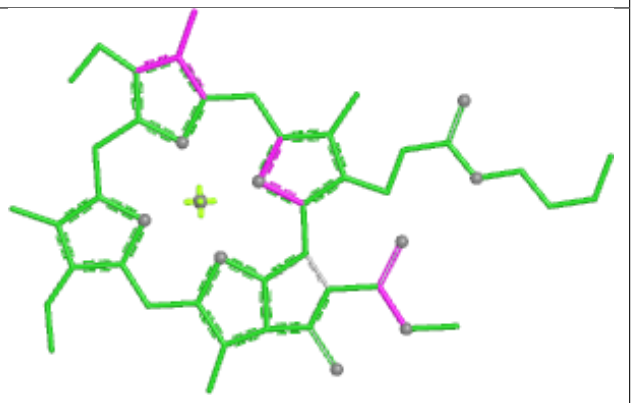


Rings

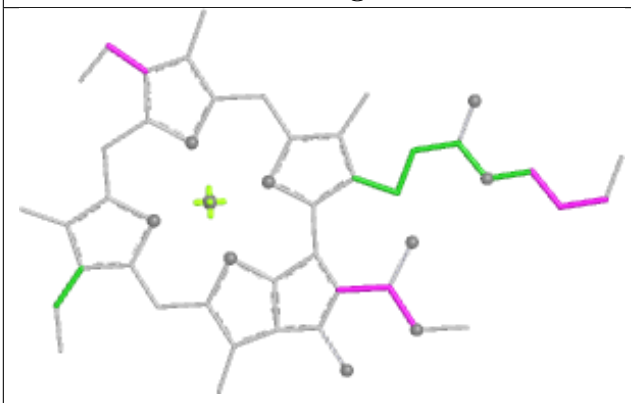
Ligand CLA R 601



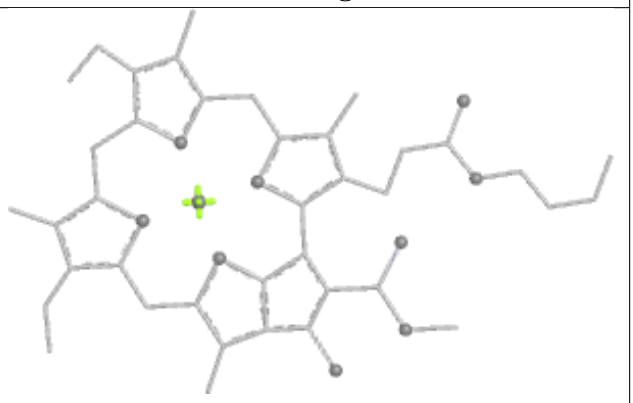
Bond lengths



Bond angles

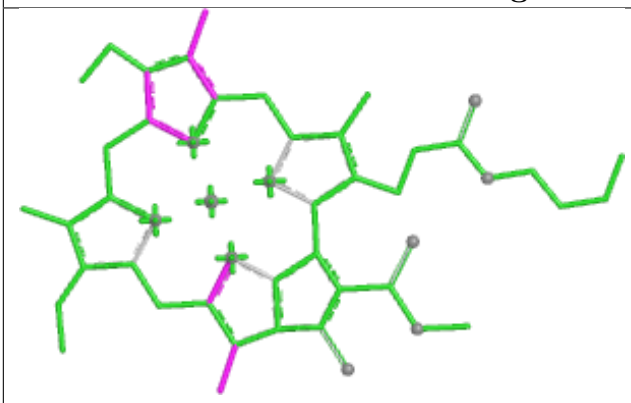


Torsions

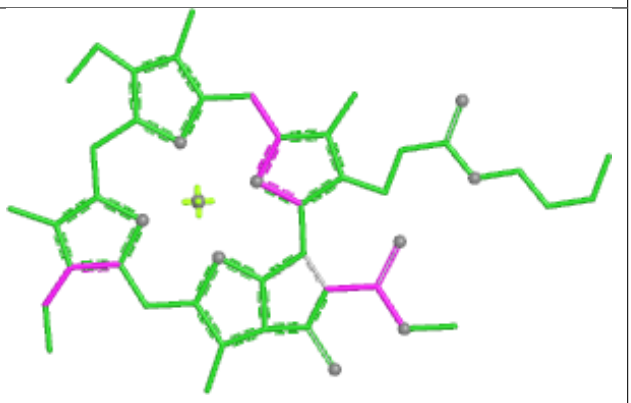


Rings

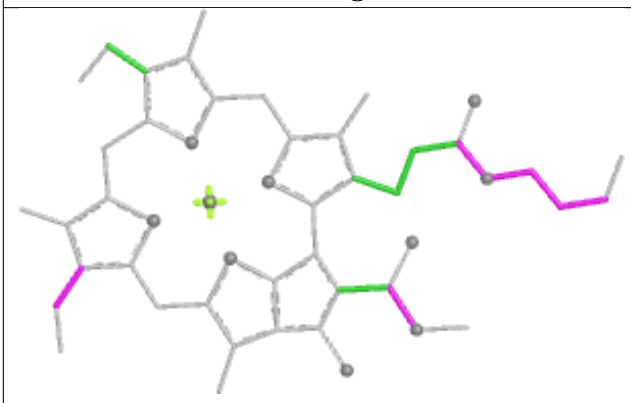
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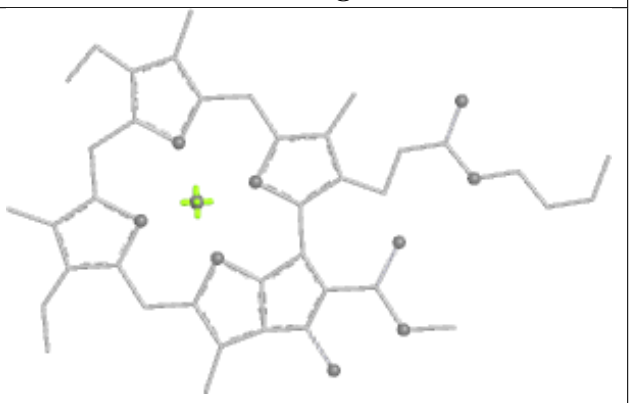
Bond lengths



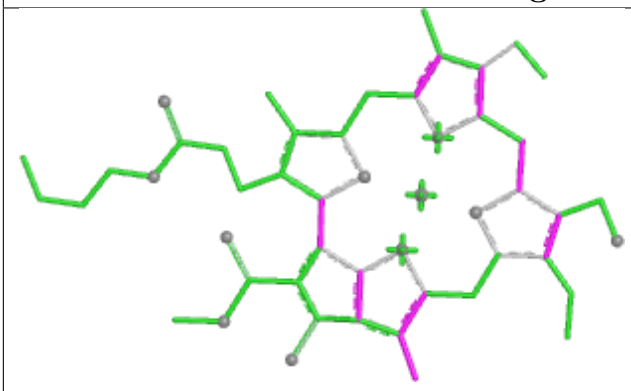
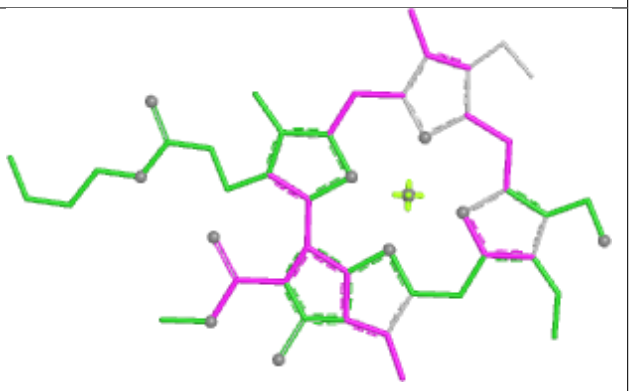
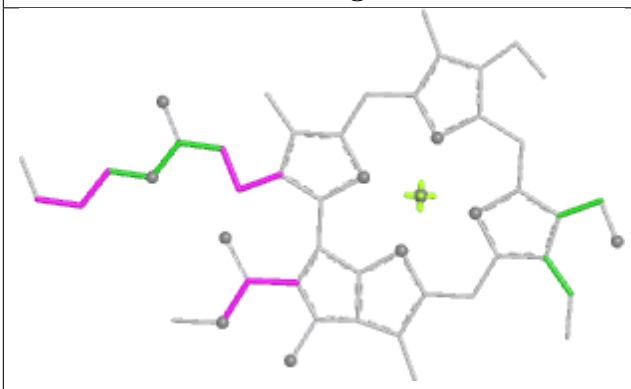
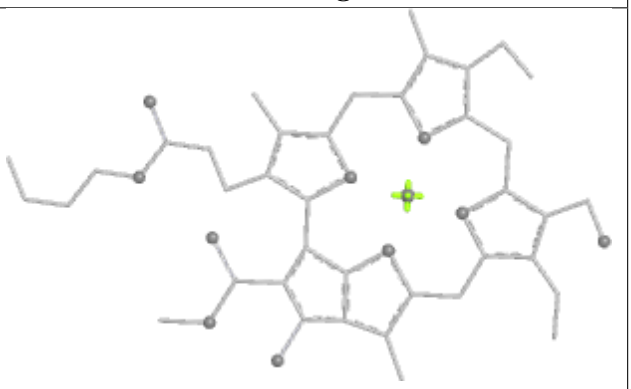
Bond angles

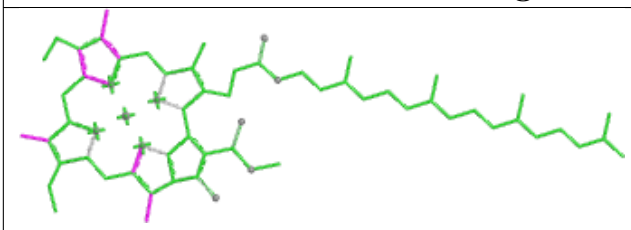
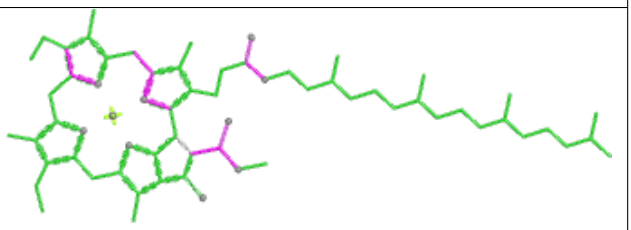
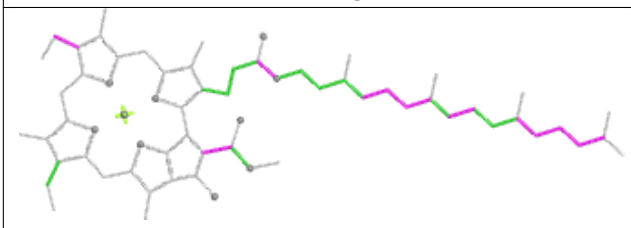
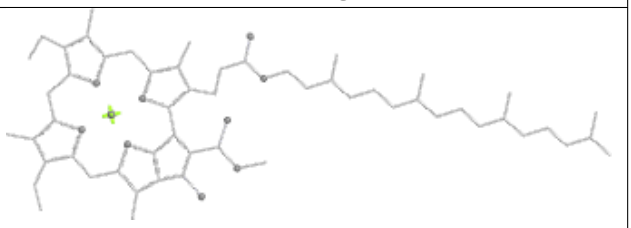


Torsions

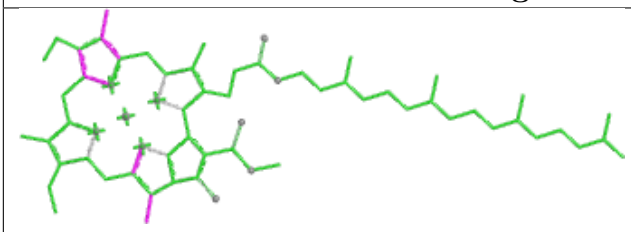


Rings

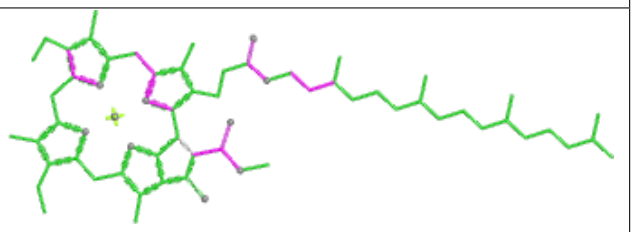
Ligand CHL s 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Bb 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

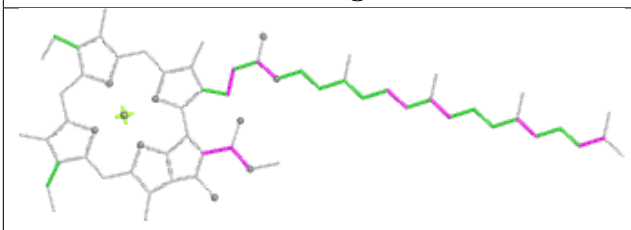
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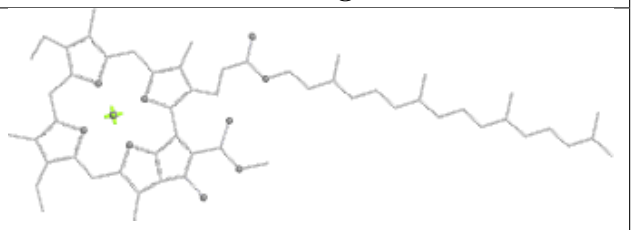
Bond lengths



Bond angles

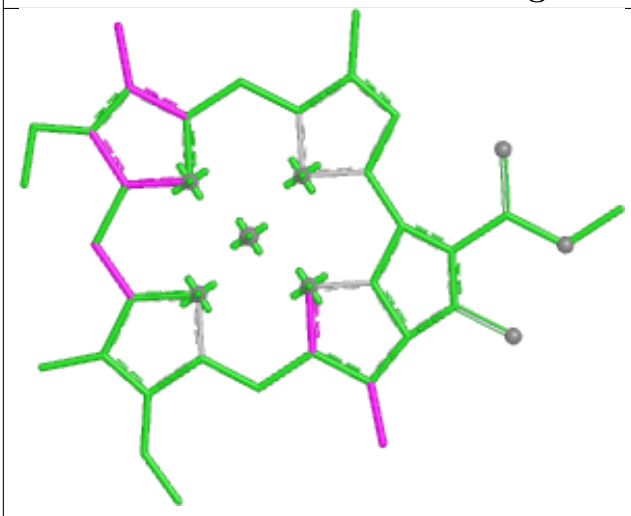


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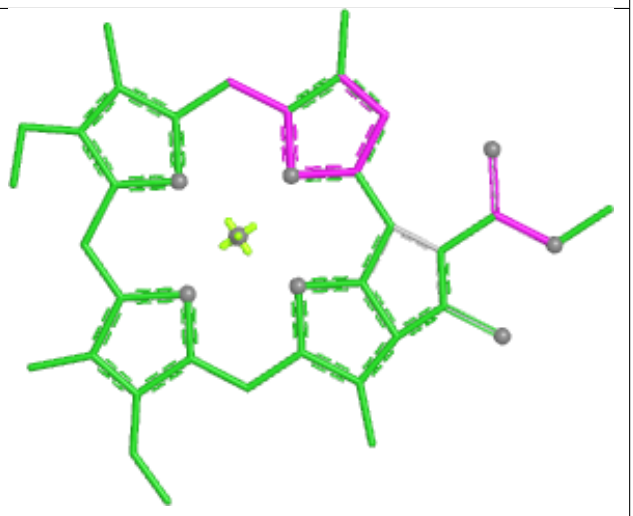


Rings

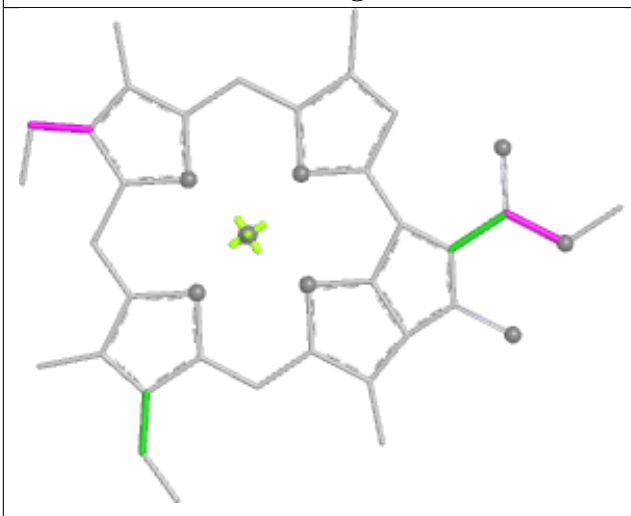
Ligand CLA 2 603



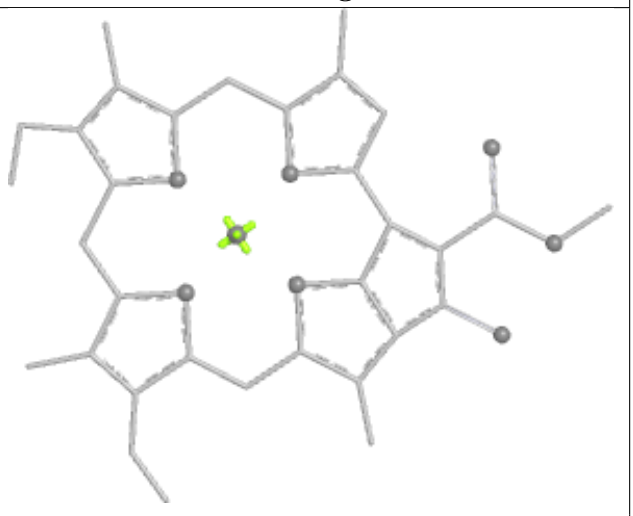
Bond lengths



Bond angles

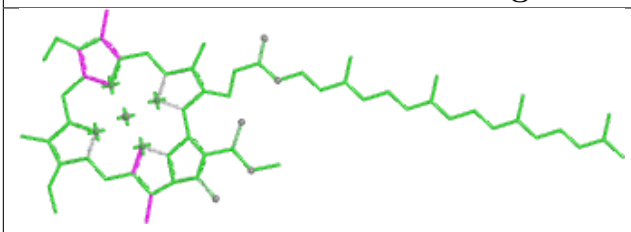


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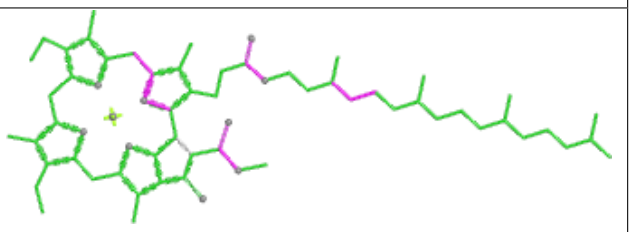


Rings

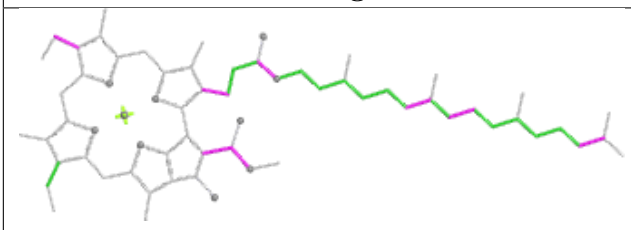
Ligand CLA CC 504



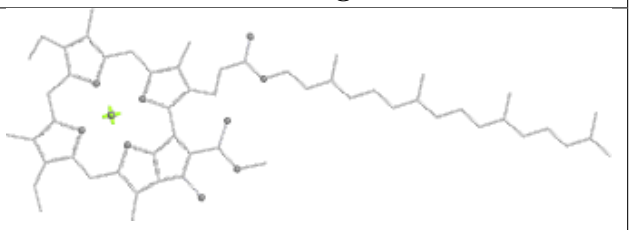
Bond lengths



Bond angles

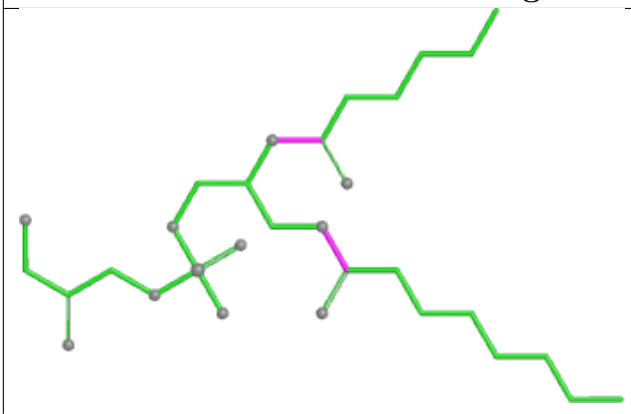


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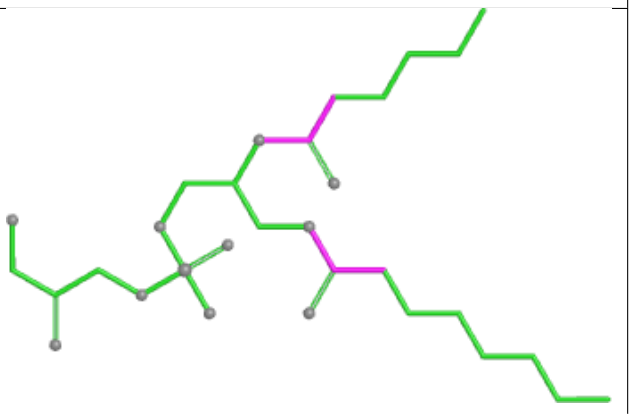


Rings

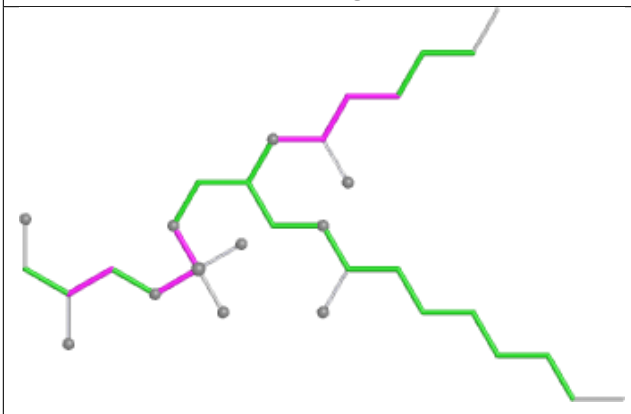
Ligand LHG C 522



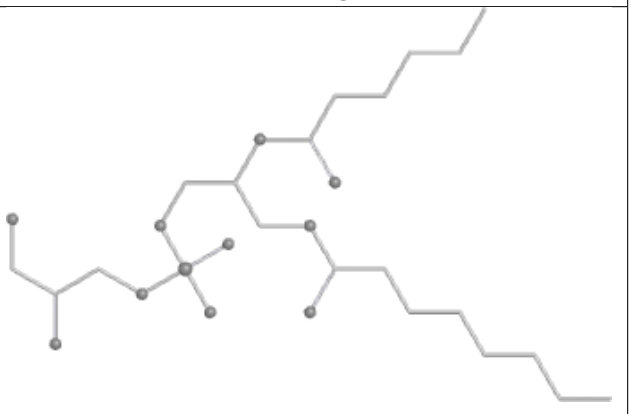
Bond lengths



Bond angles

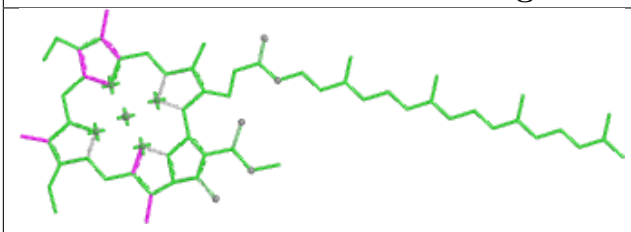


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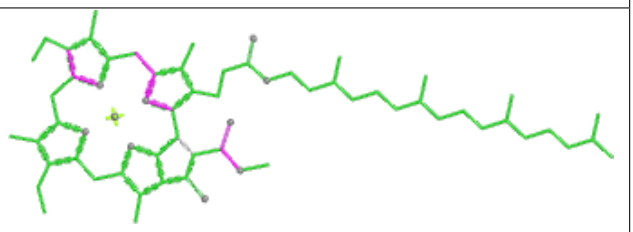


Rings

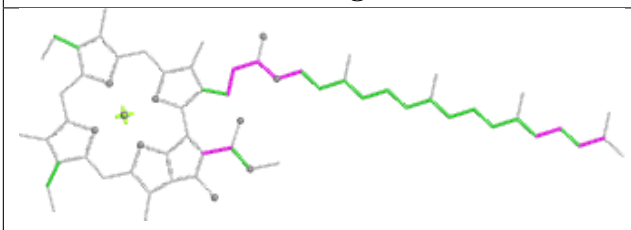
Ligand CLA Cc 507



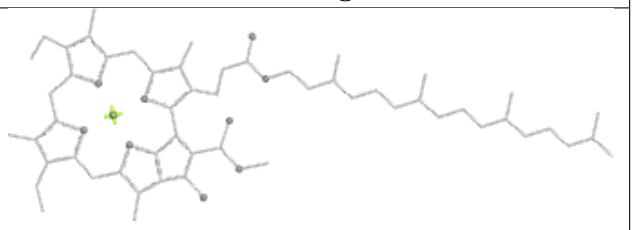
Bond lengths



Bond angles

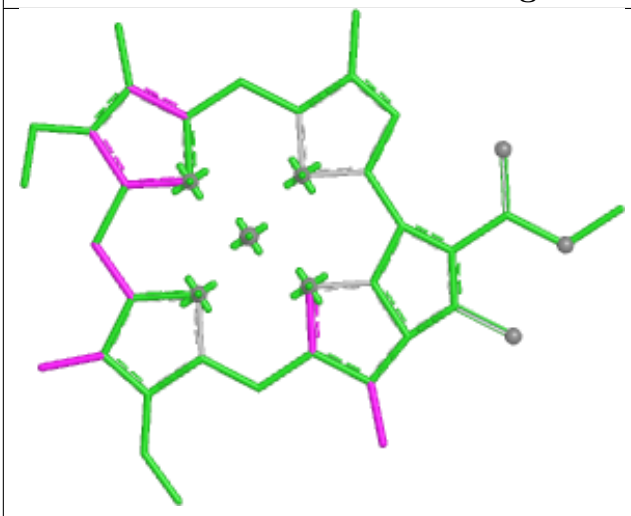


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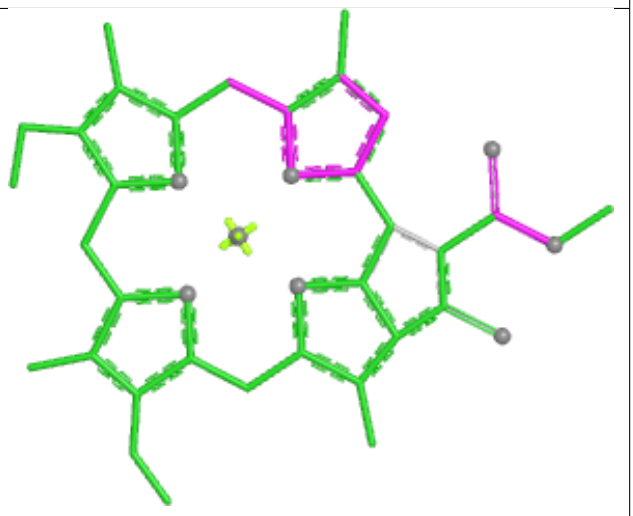


Rings

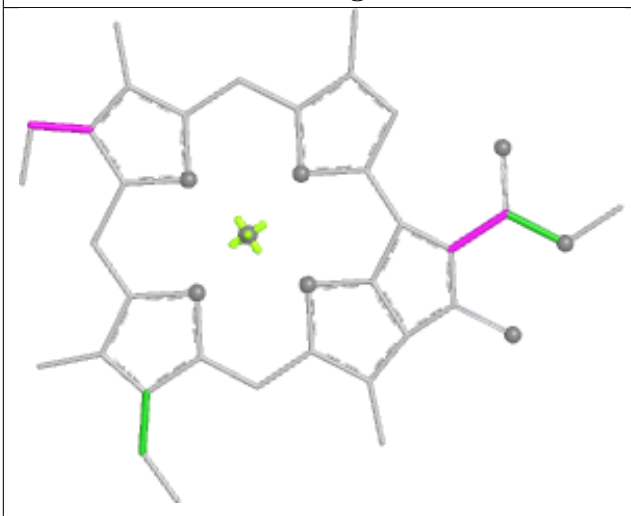
Ligand CLA 22 602



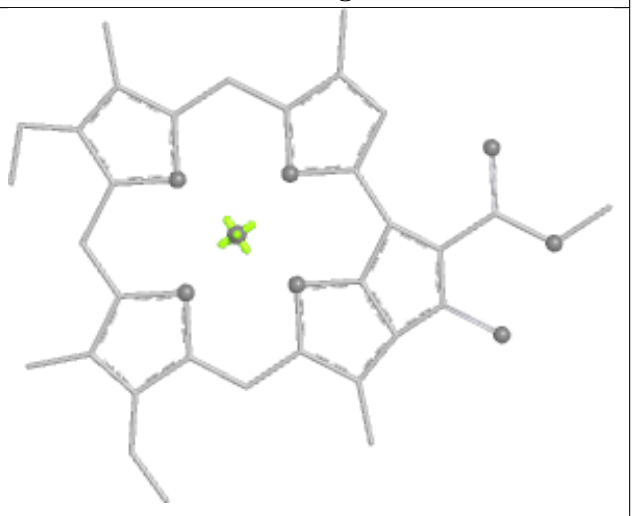
Bond lengths



Bond angles

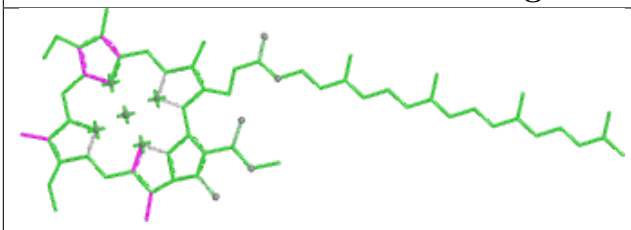


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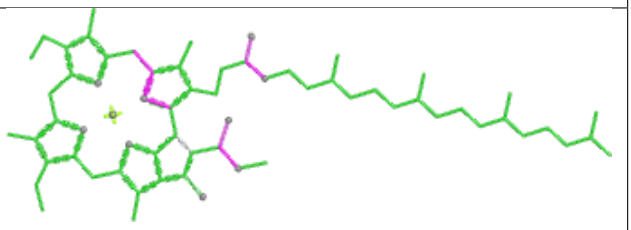


Rings

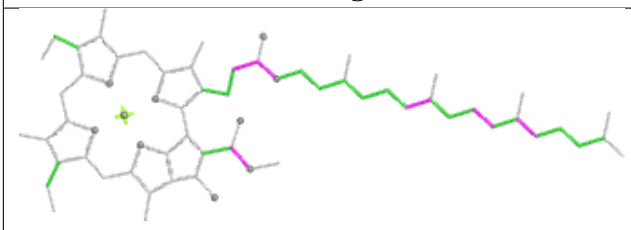
Ligand CLA B 608



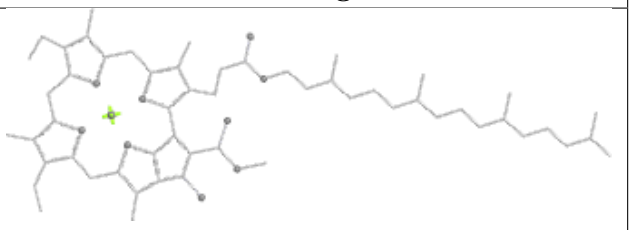
Bond lengths



Bond angles

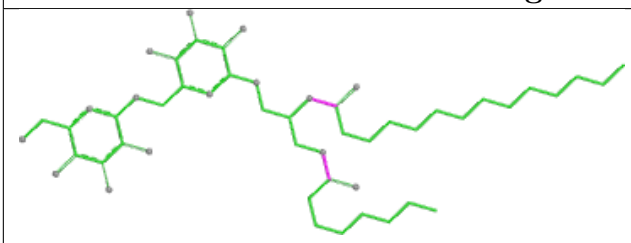


Torsions

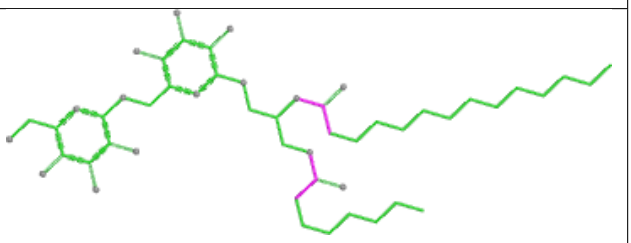


Rings

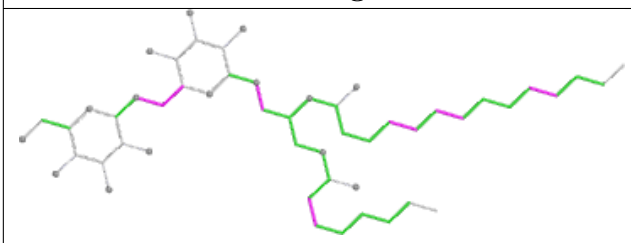
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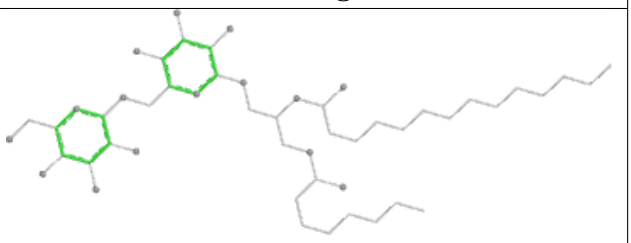
Bond lengths



Bond angles

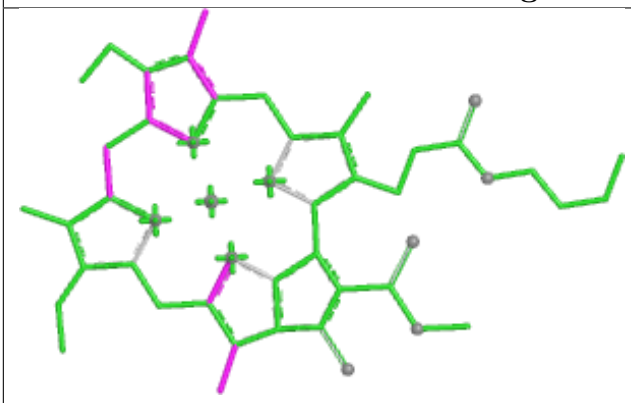


Torsions

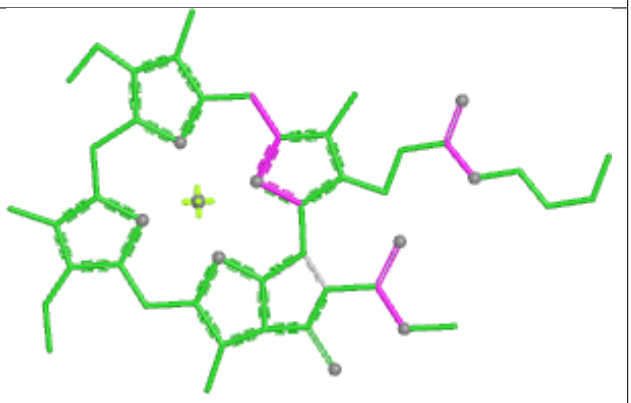


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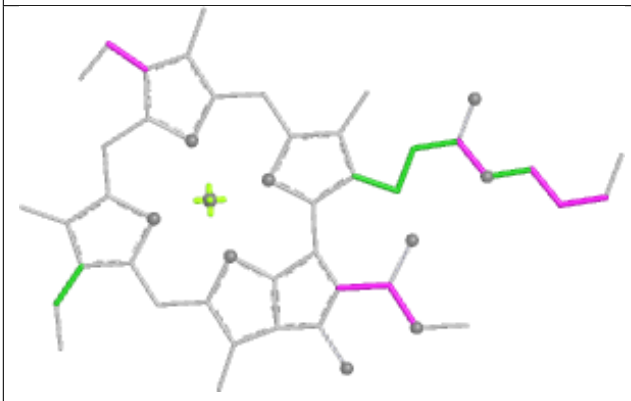
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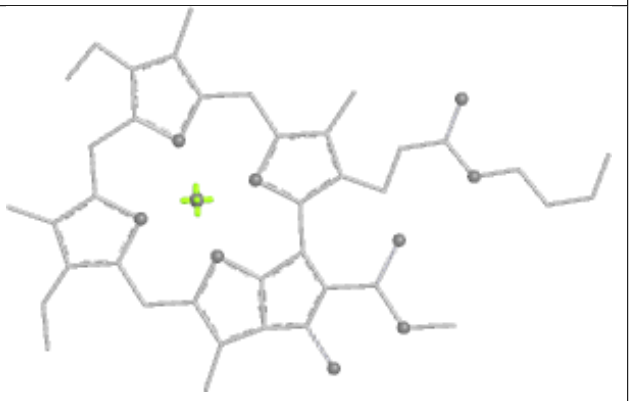
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Bond angles

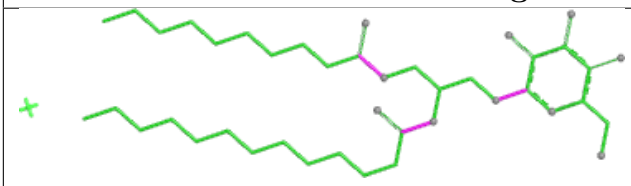


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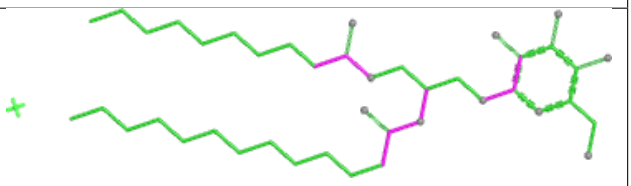


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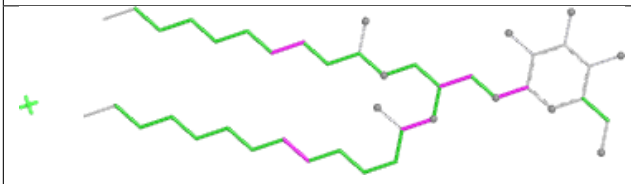
Ligand LMG Aa 412



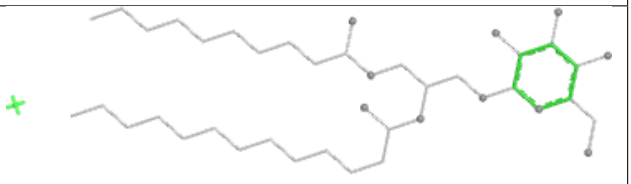
Bond lengths



Bond angles

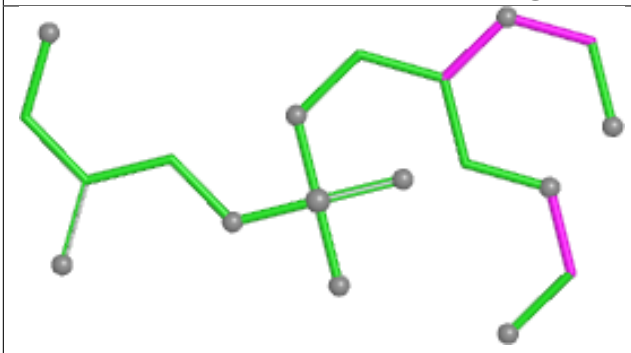


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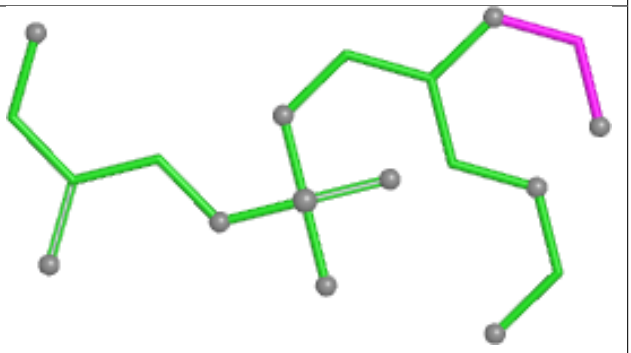


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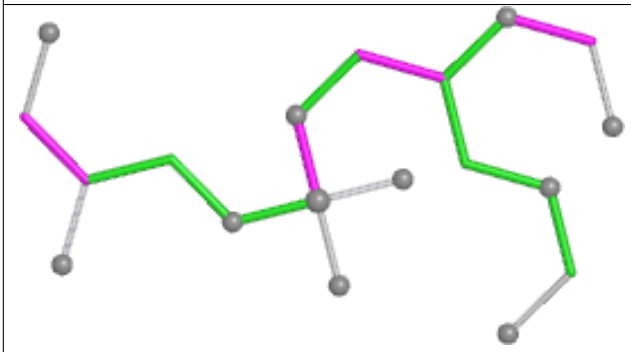
Ligand LHG 4 301



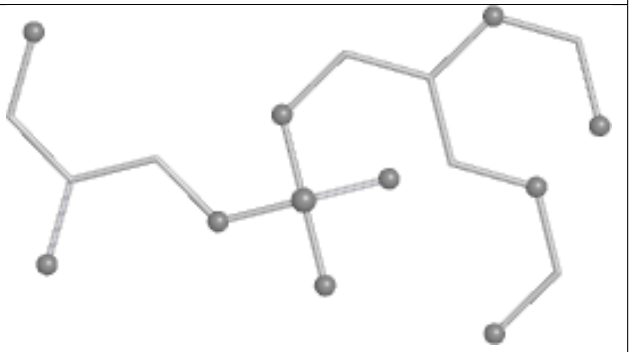
Bond lengths



Bond angles

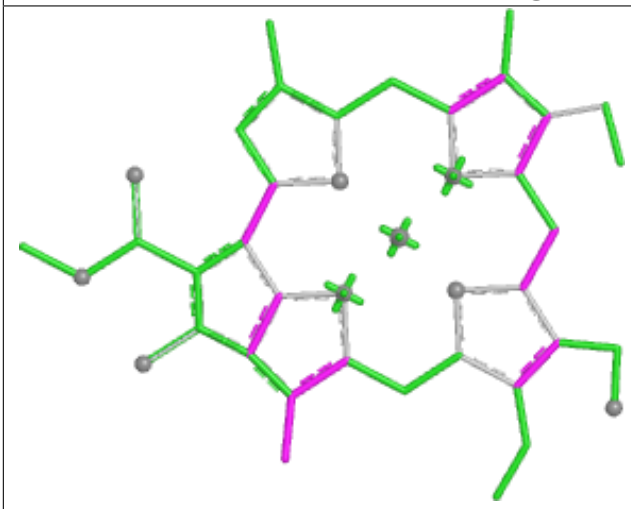


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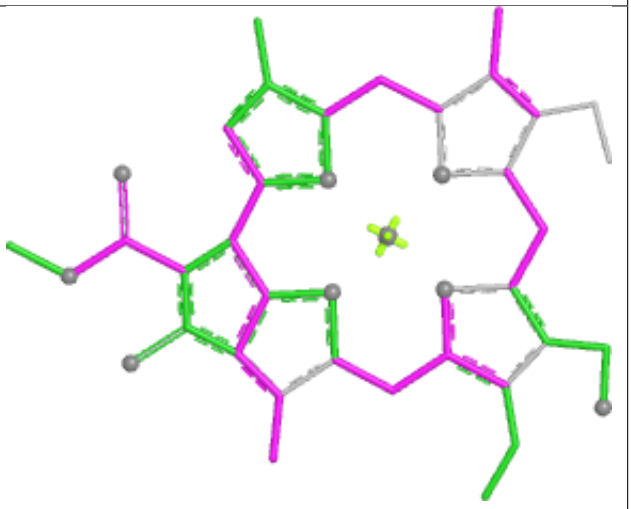


Rings

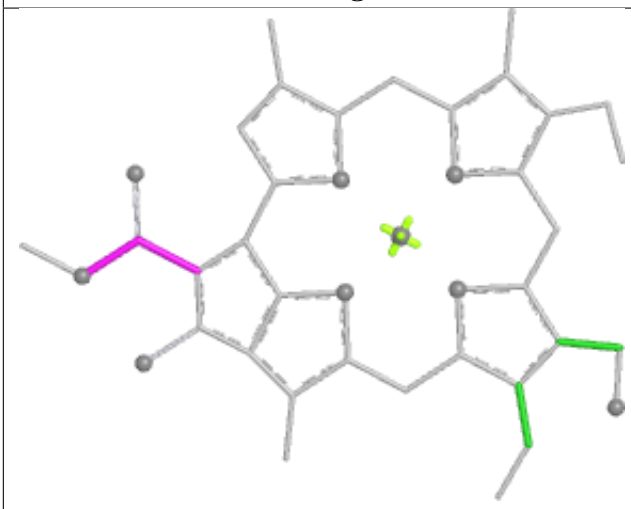
Ligand CHL 1 607



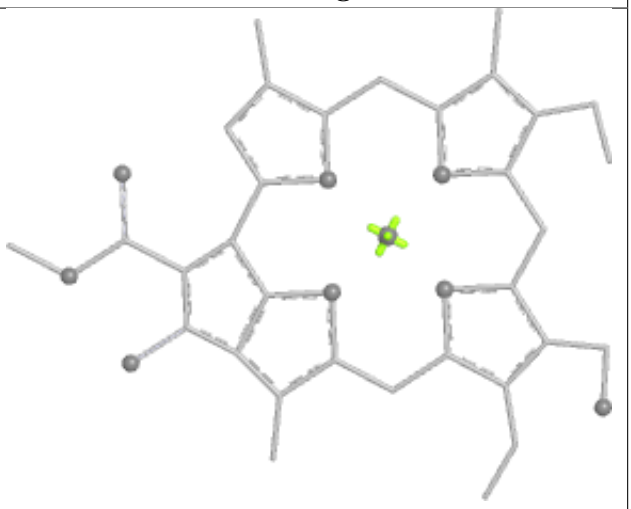
Bond lengths



Bond angles

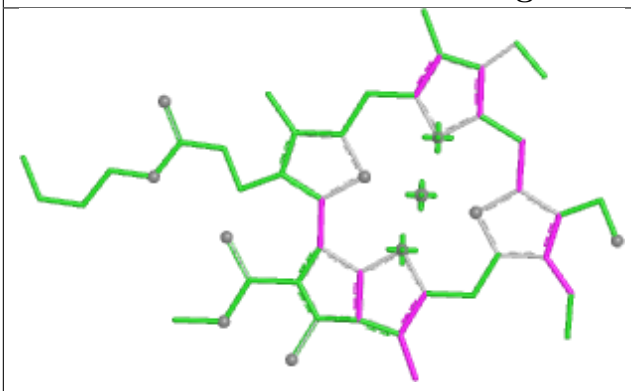


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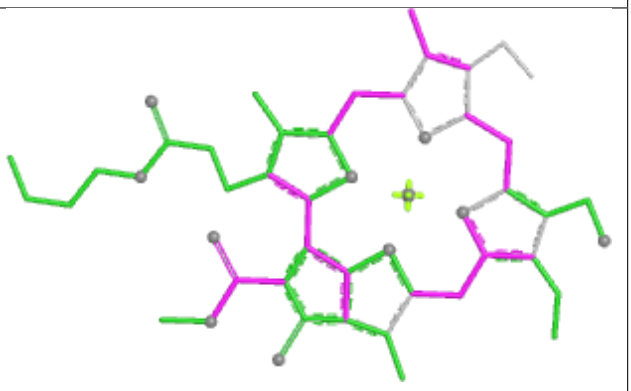


Rings

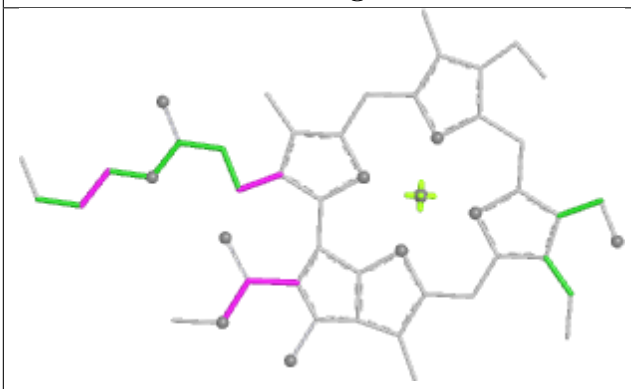
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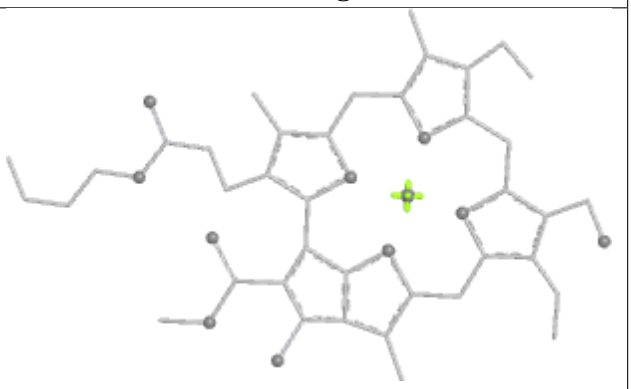
Bond lengths



Bond angles

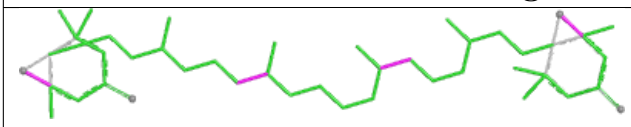


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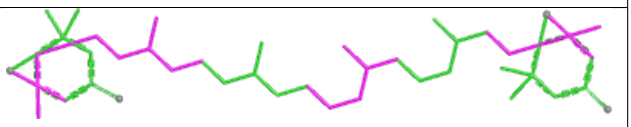


Rings

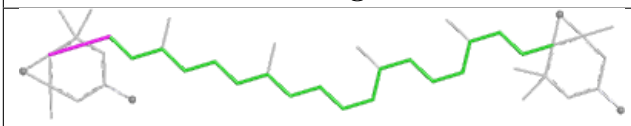
Ligand XAT G 619



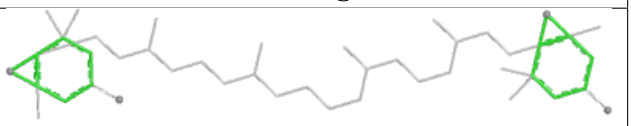
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Bond angles

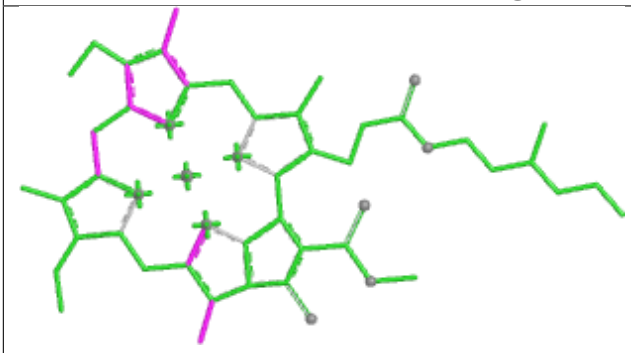


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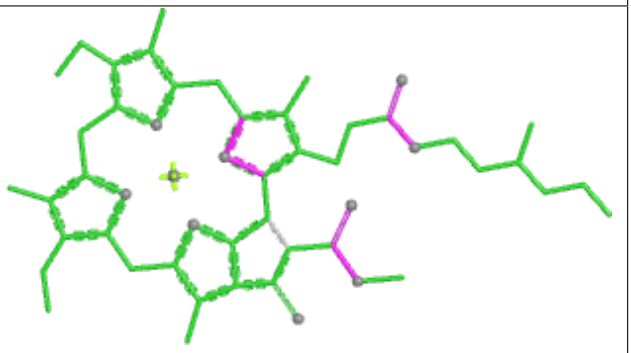


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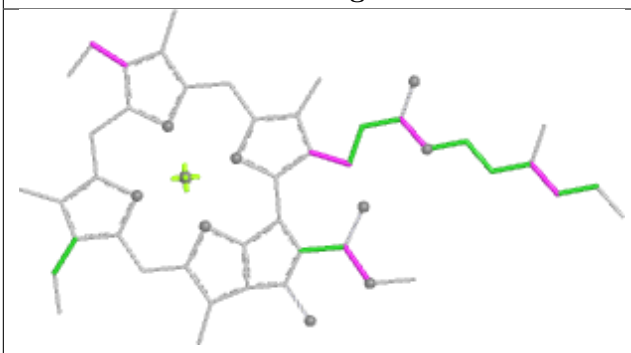
Ligand CLA GG 611



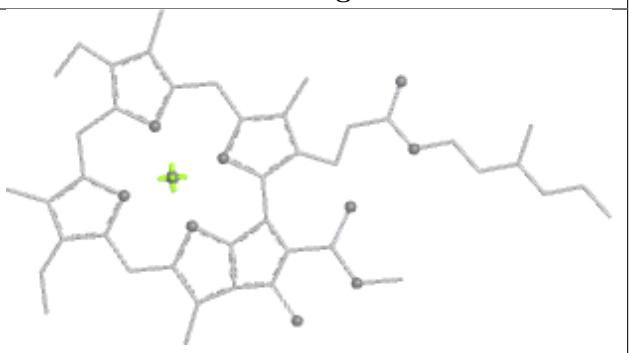
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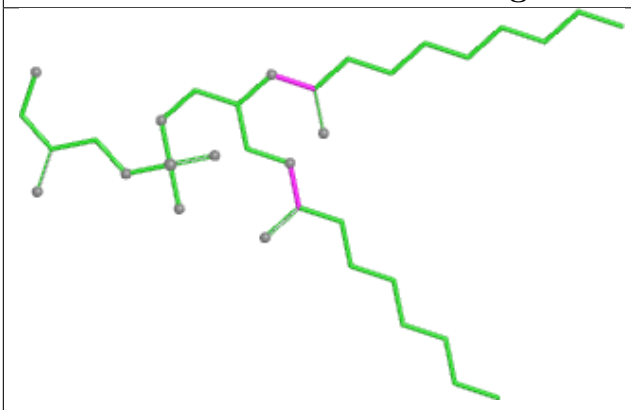


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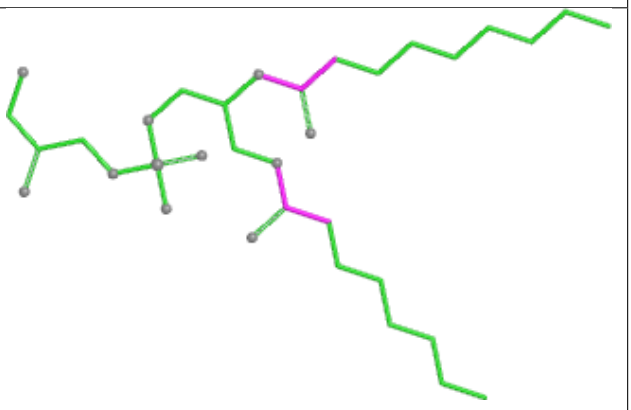


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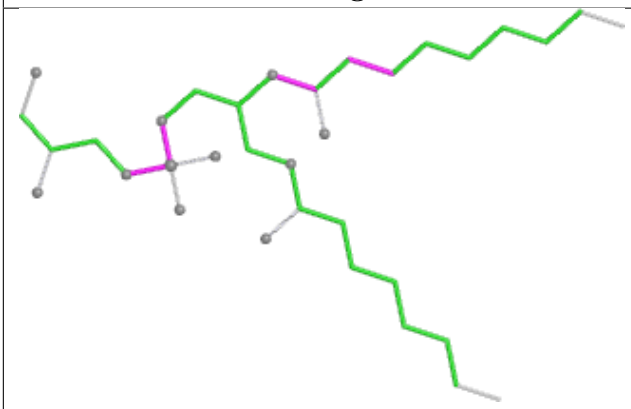
Ligand LHG CC 521



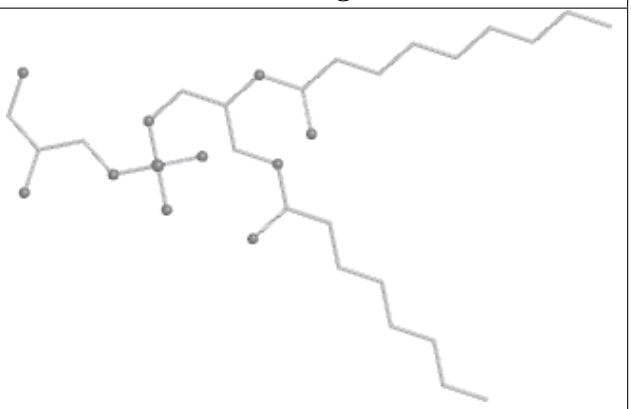
Bond lengths



Bond angles

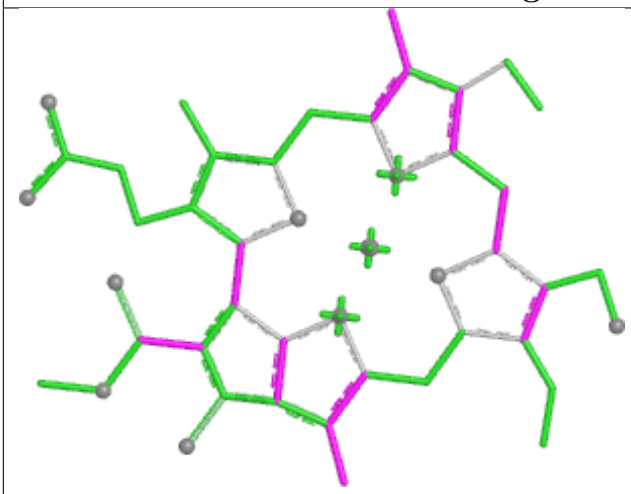


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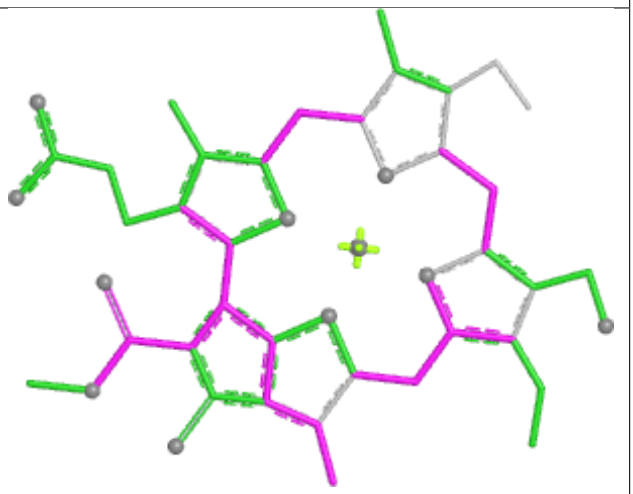


Rings

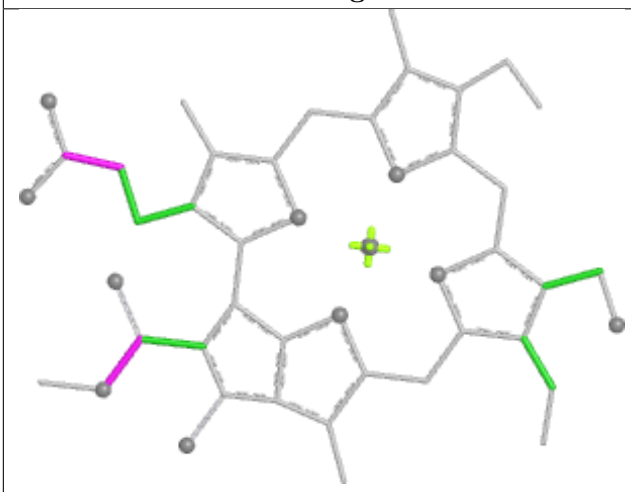
Ligand CHL G 607



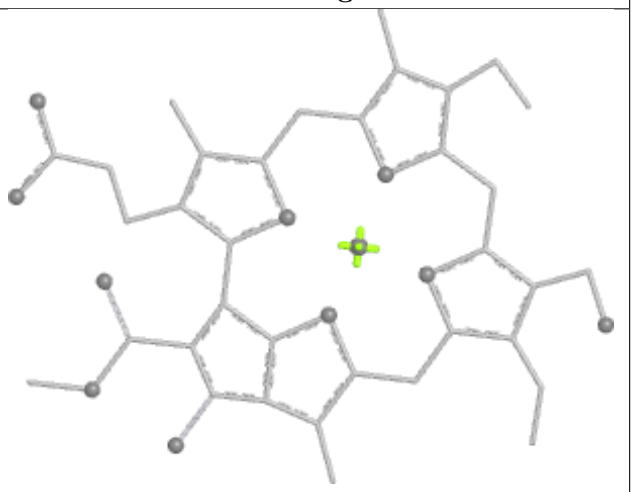
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Bond angles

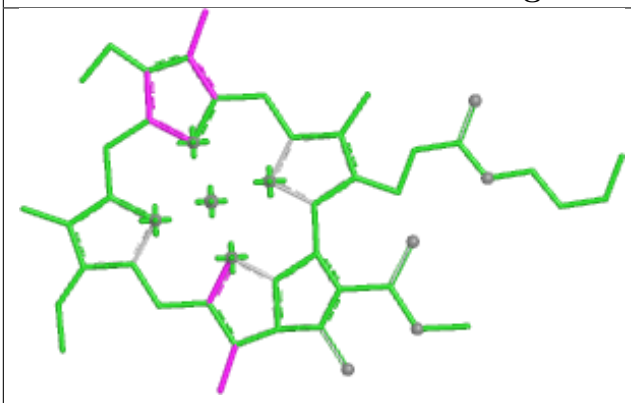


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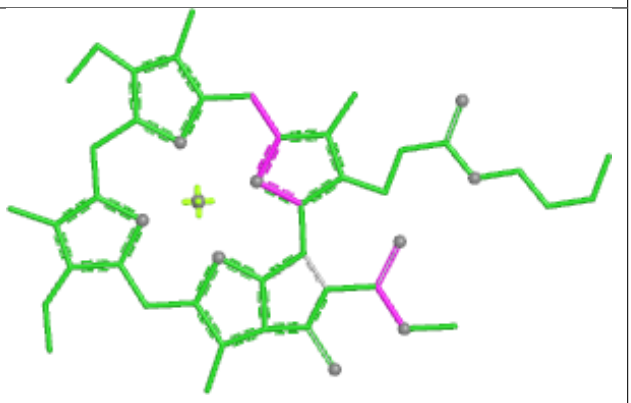


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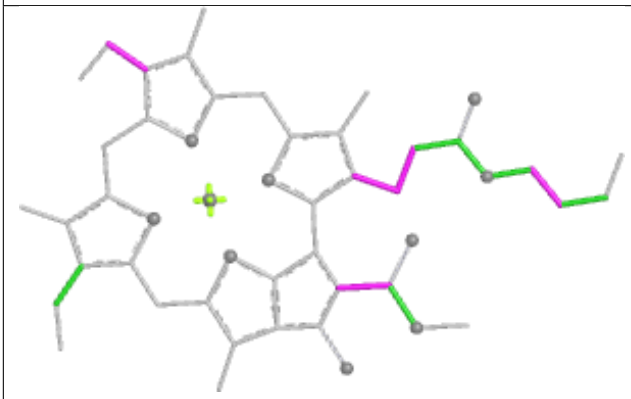
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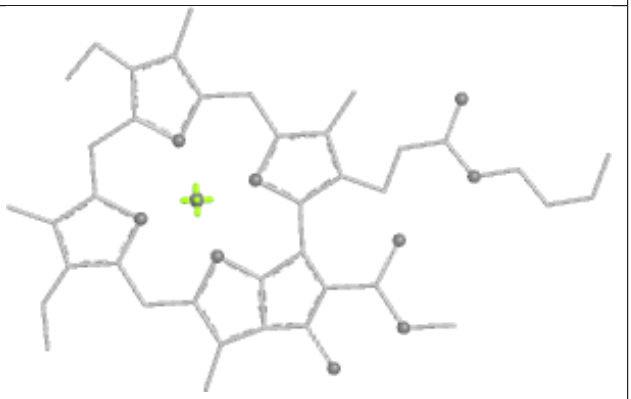
Bond lengths



Bond angles



Torsions

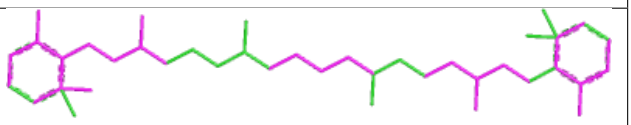


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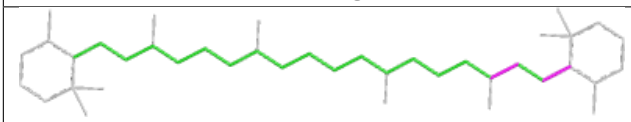
Ligand BCR H 101



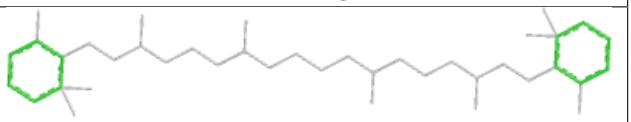
Bond lengths



Bond angles

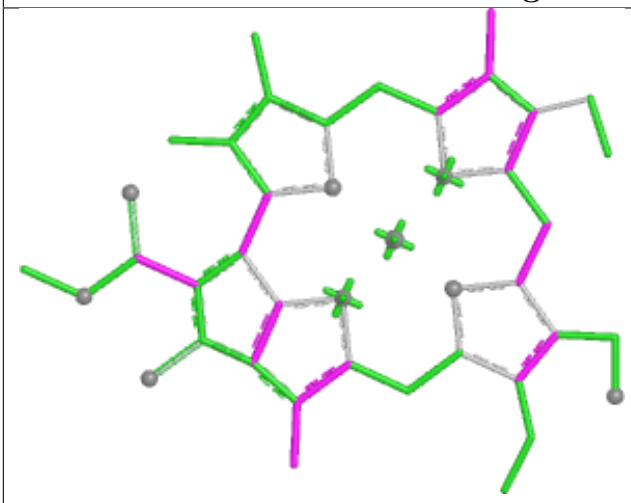


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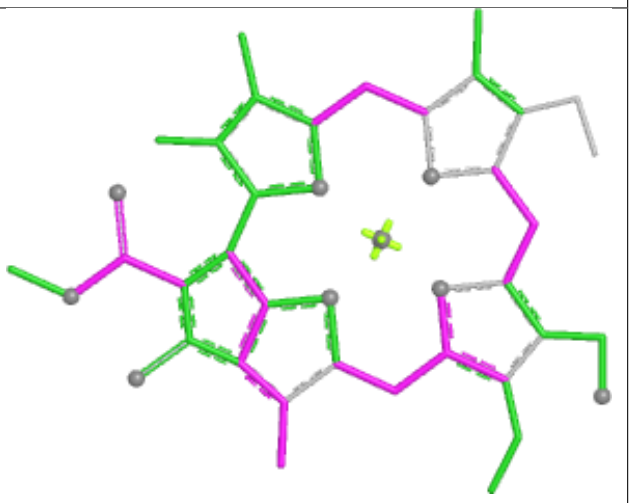


Rings

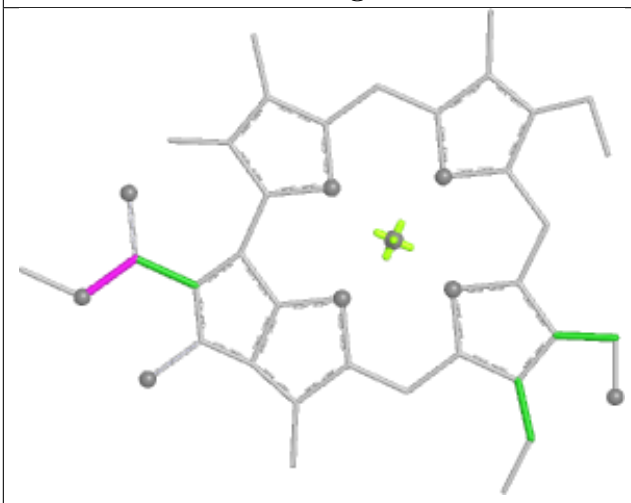
Ligand CHL N 608



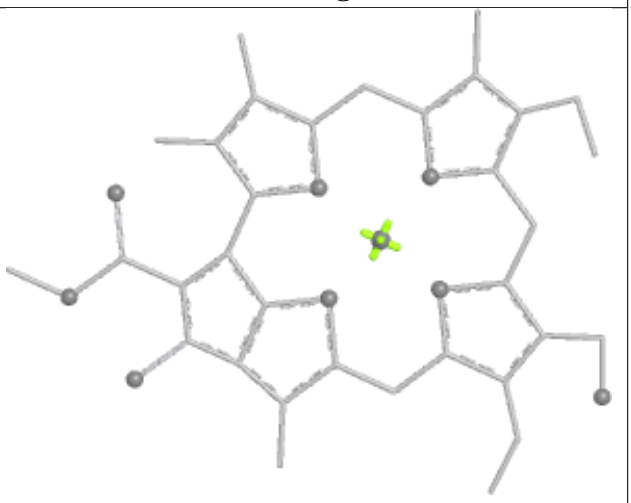
Bond lengths



Bond angles

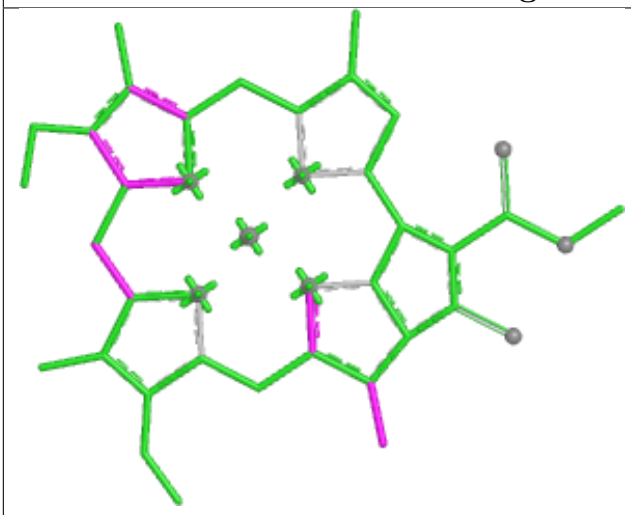


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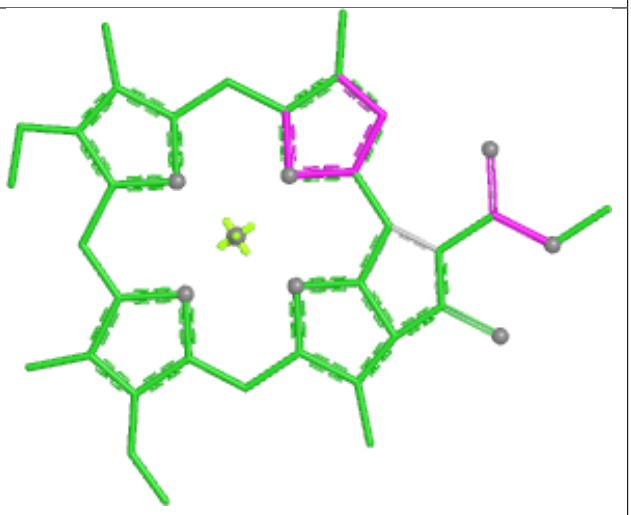


Rings

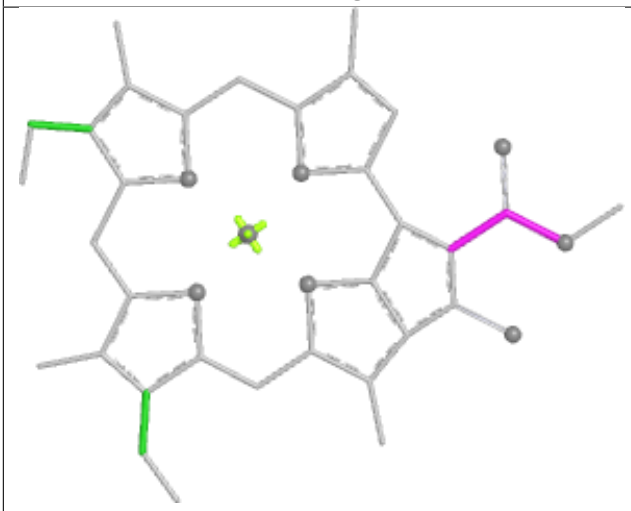
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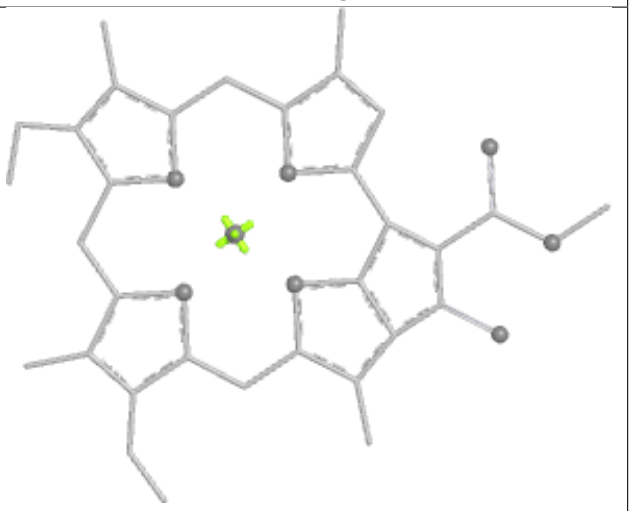
Bond lengths



Bond angles

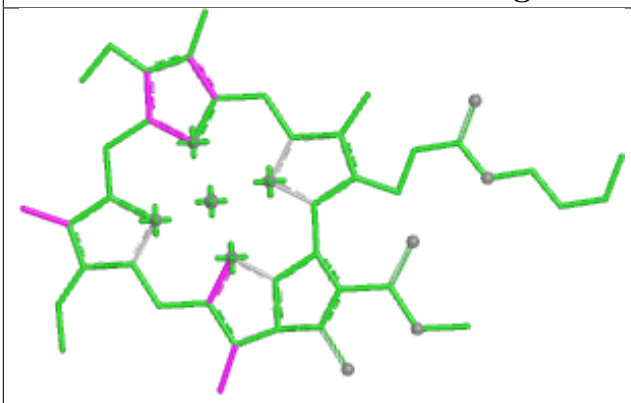


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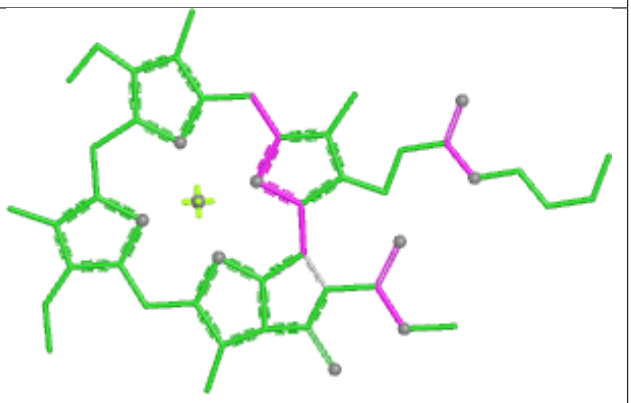


Rings

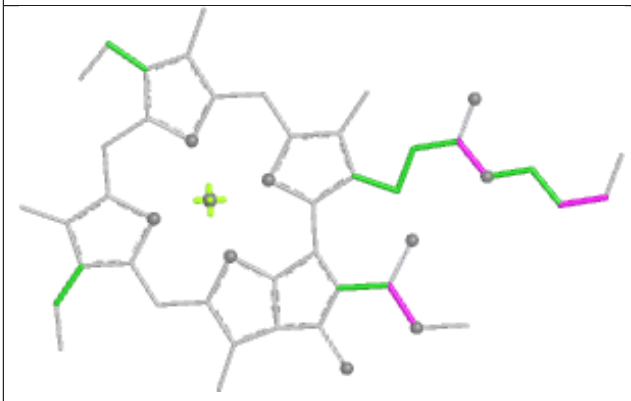
Ligand CLA Nn 303



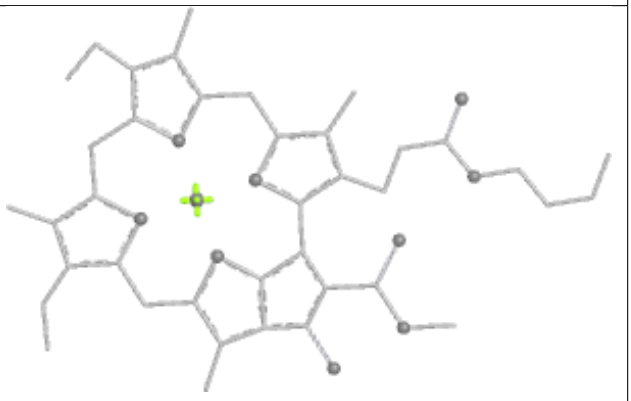
Bond lengths



Bond angles



Torsions

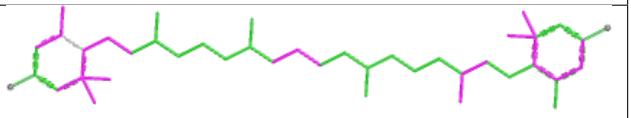


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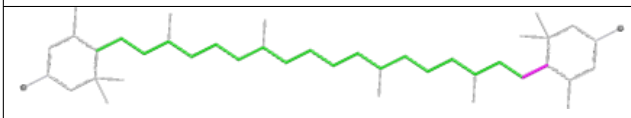
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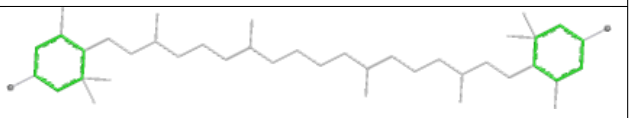
Bond lengths



Bond angles

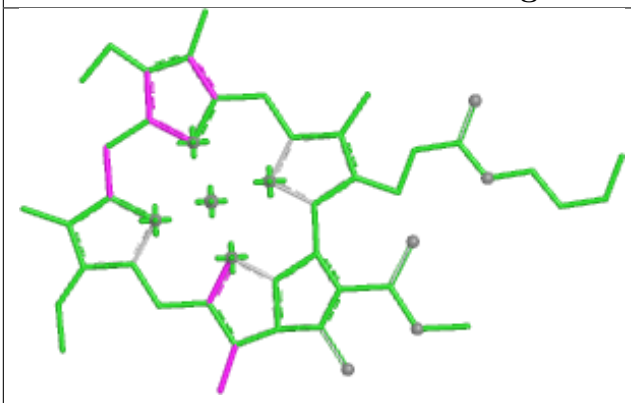


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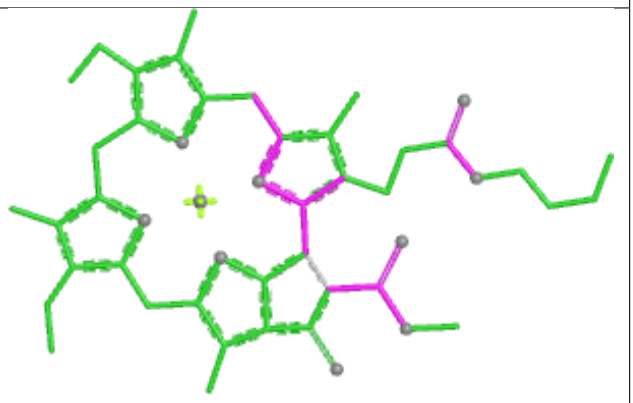


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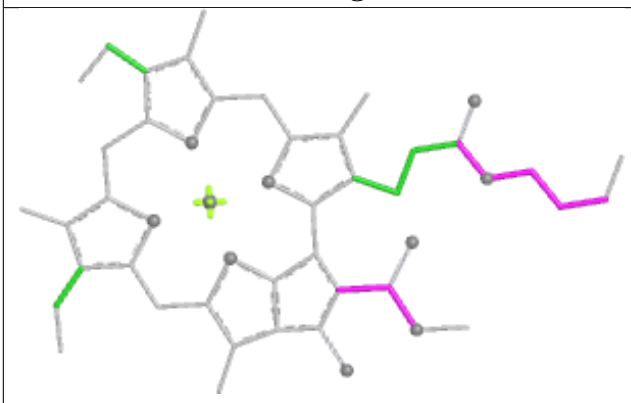
Ligand CLA Ss 611



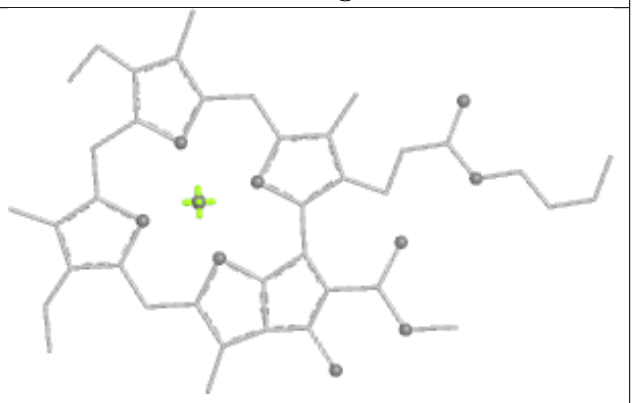
Bond lengths



Bond angles

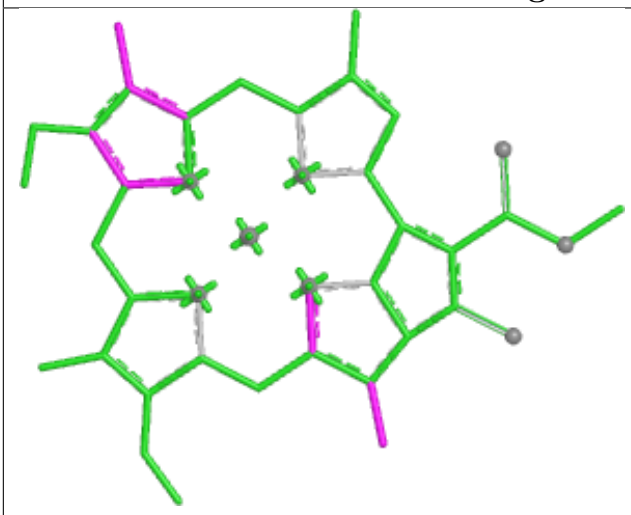


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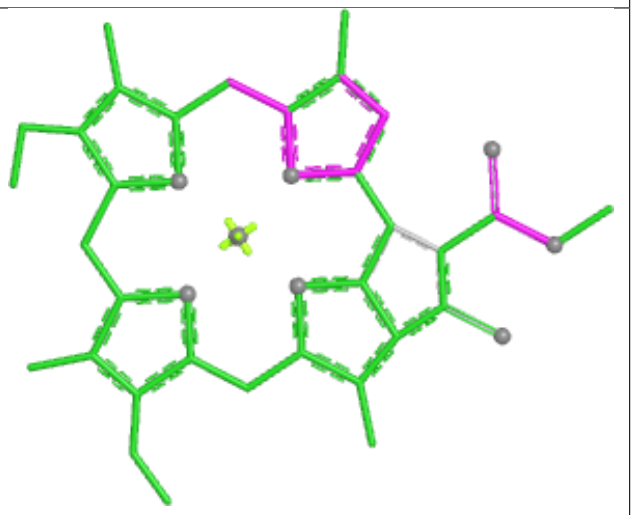


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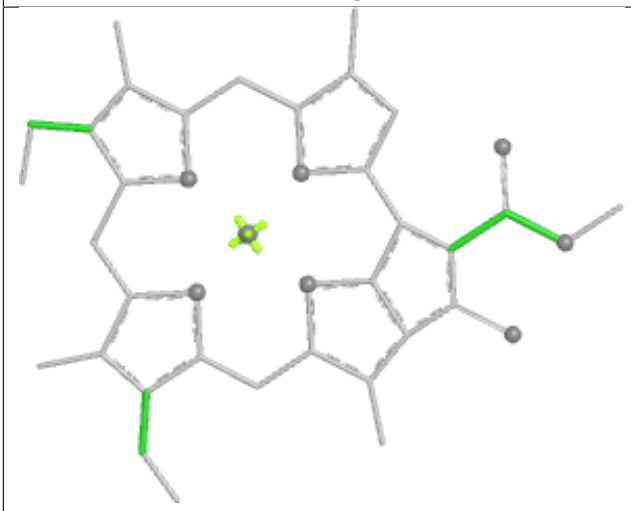
Ligand CLA 1 612



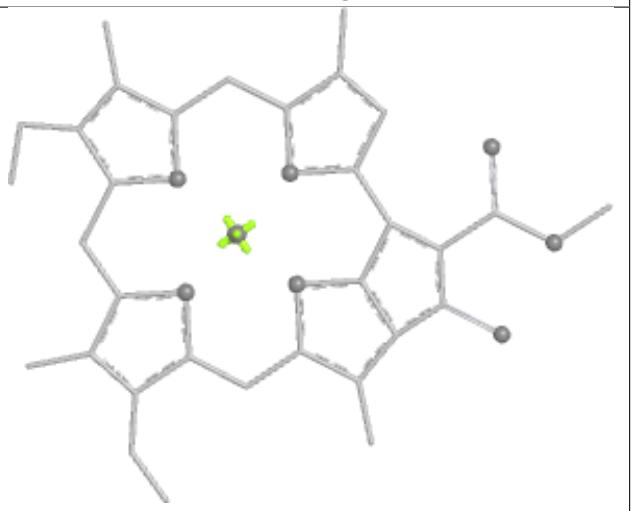
Bond lengths



Bond angles

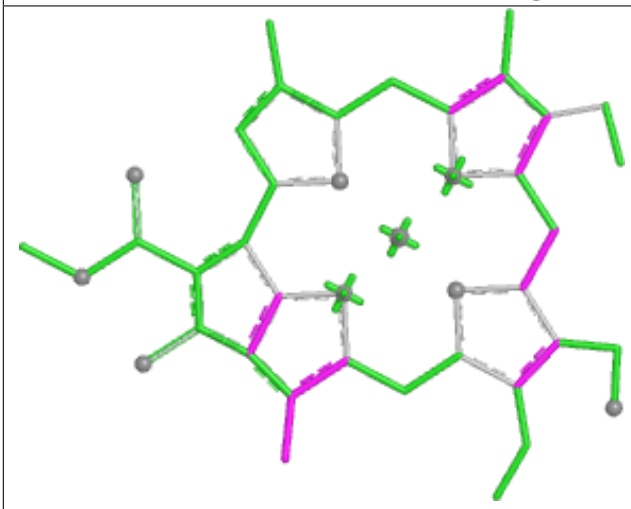


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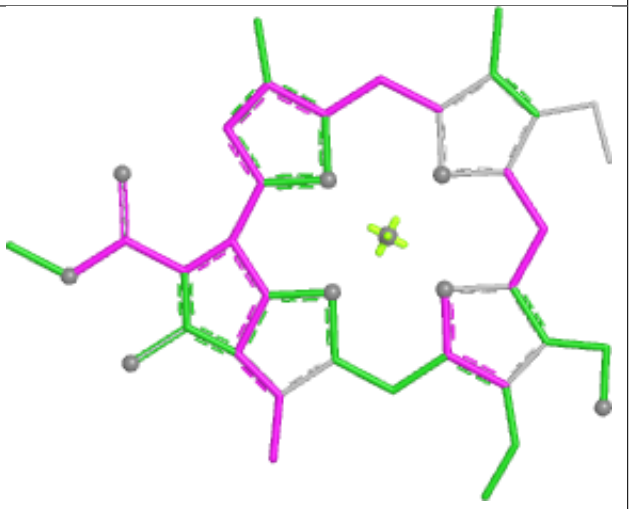


Rings

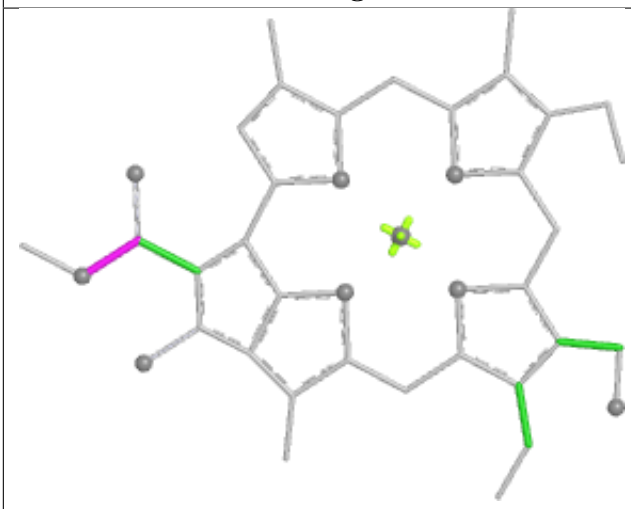
Ligand CHL 1 605



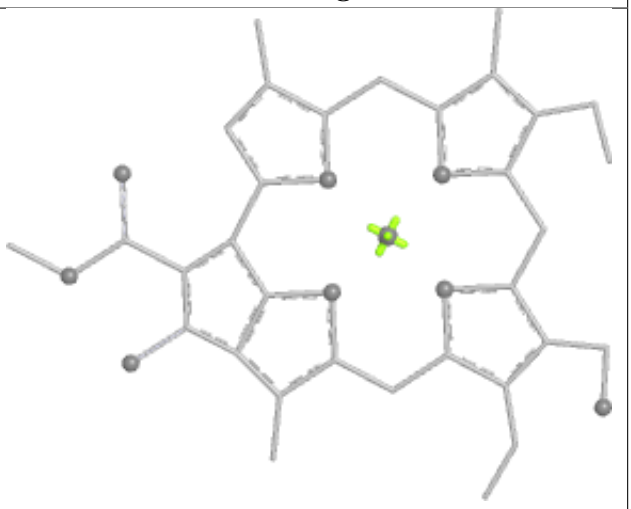
Bond lengths



Bond angles

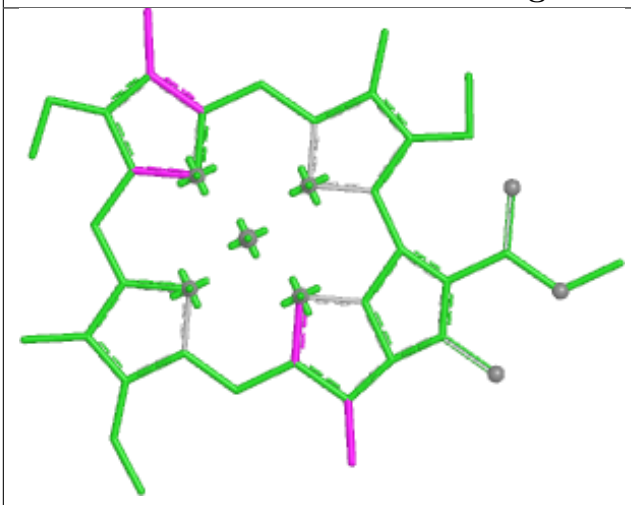


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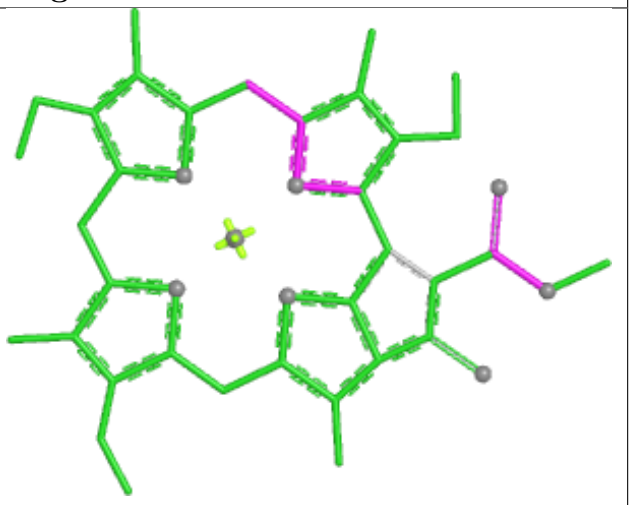


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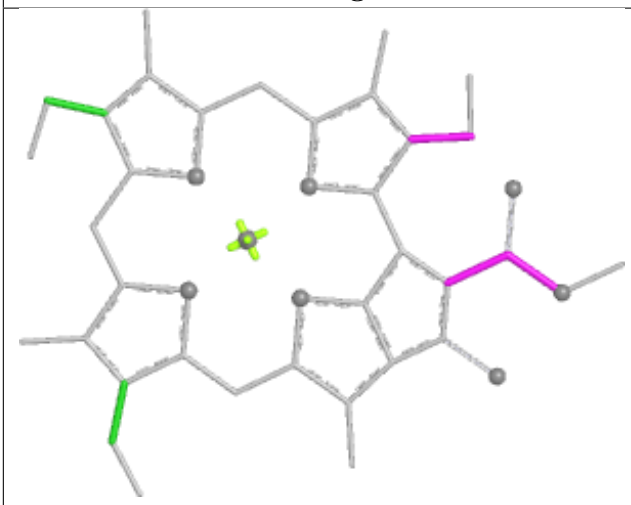
Ligand CLA g 604



Bond lengths



Bond angles

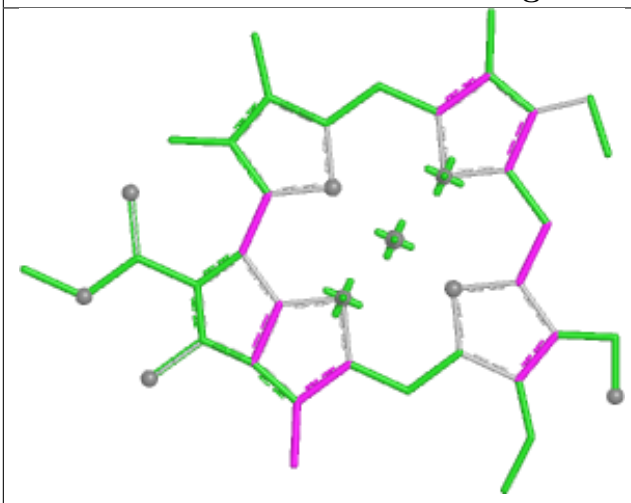


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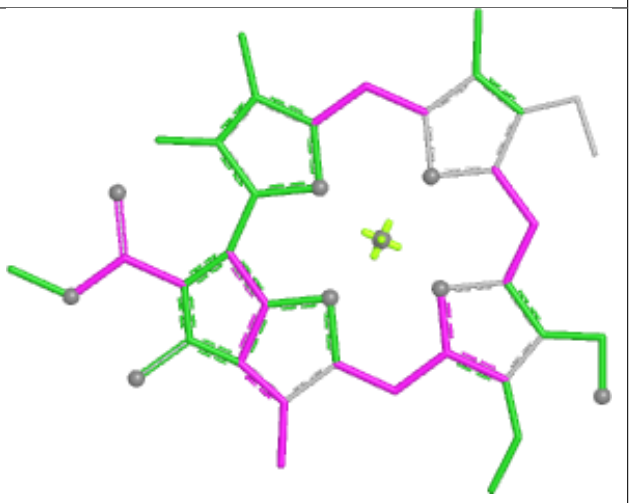


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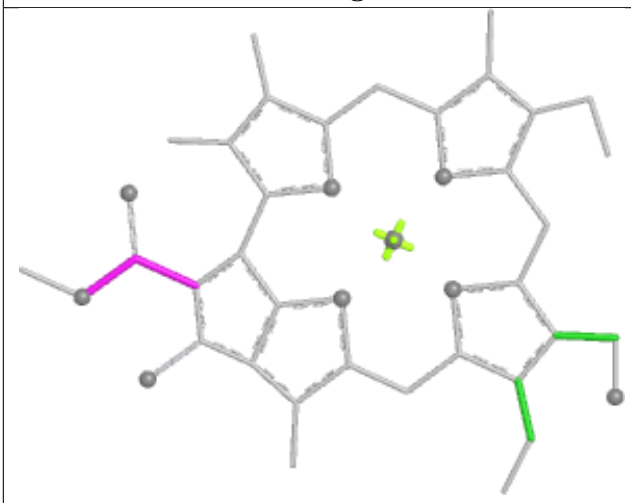
Ligand CHL G 608



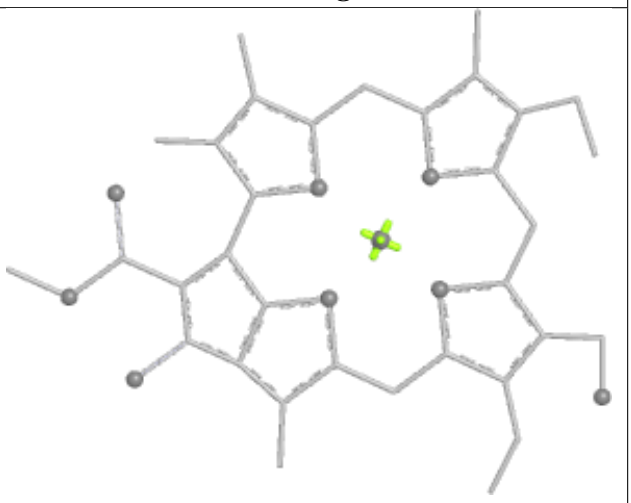
Bond lengths



Bond angles

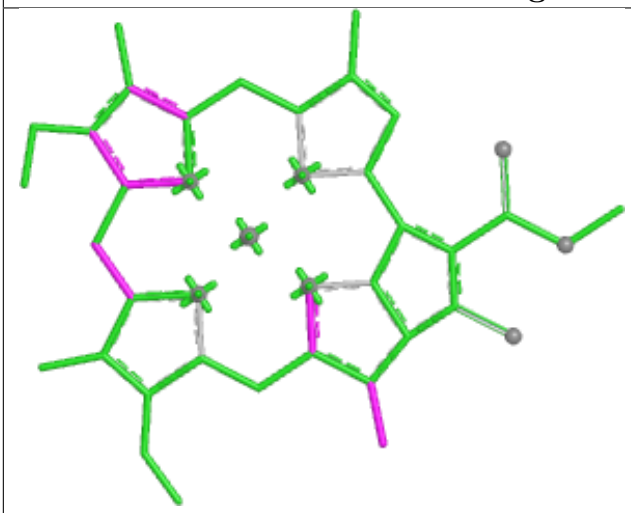


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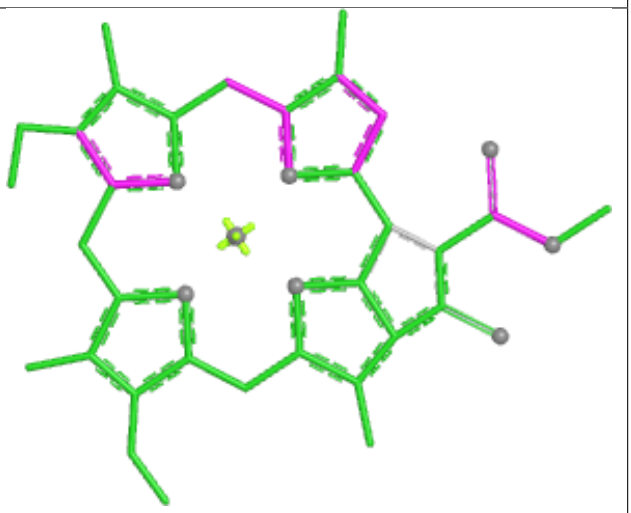


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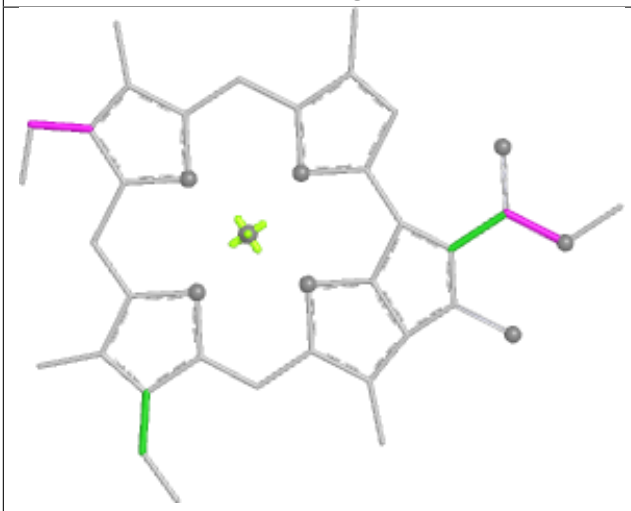
Ligand CLA 2 613



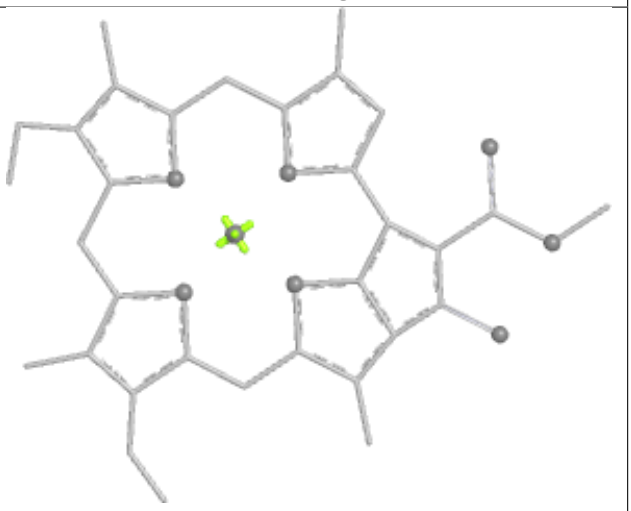
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Bond angles

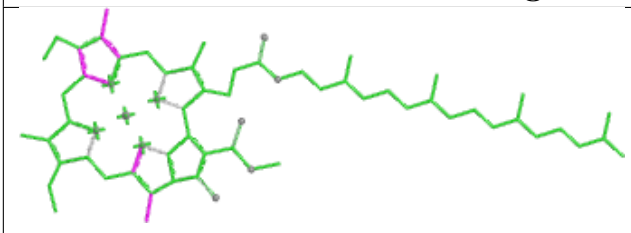


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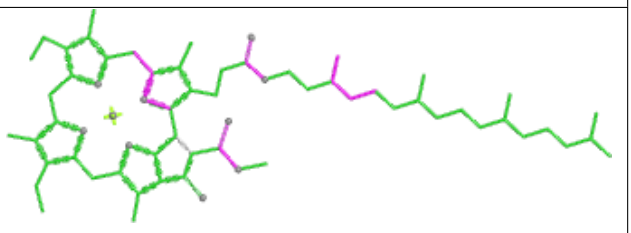


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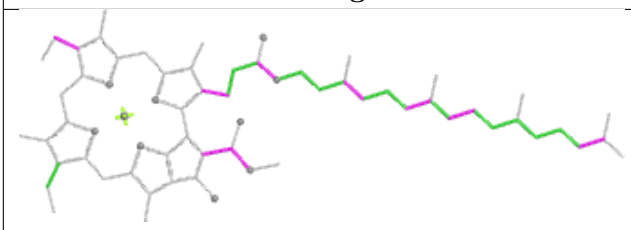
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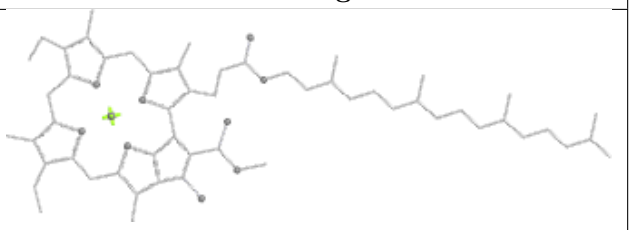
Bond lengths



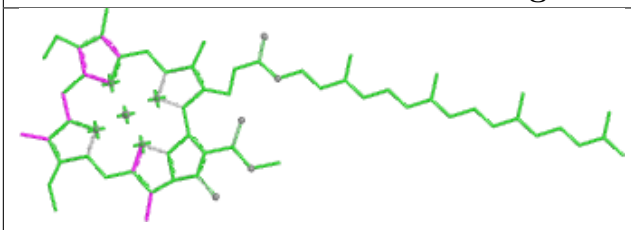
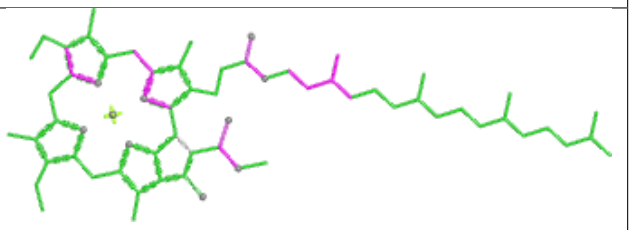
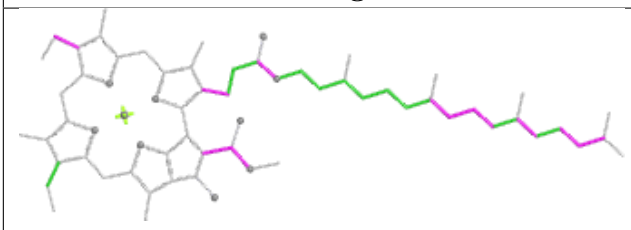
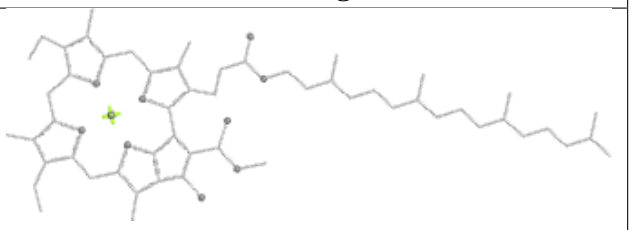
Bond angles

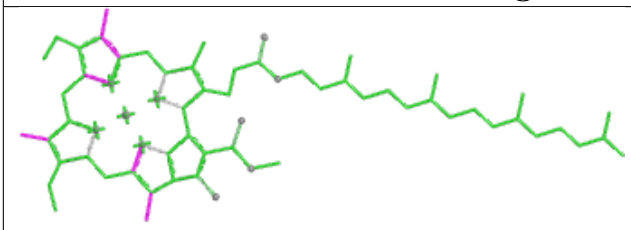
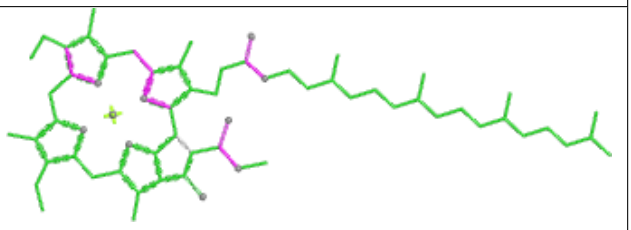
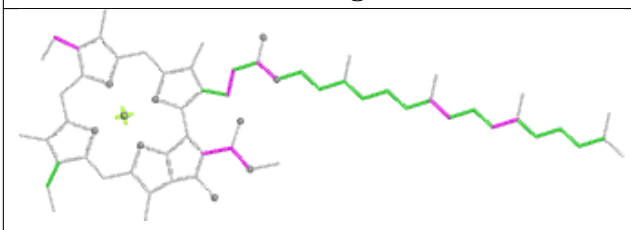
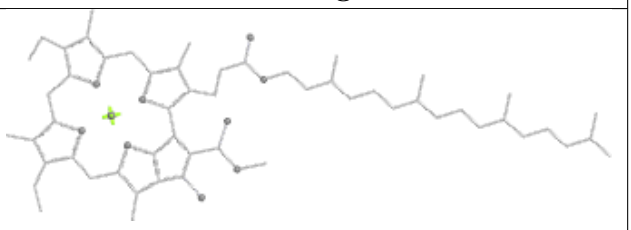


Torsions

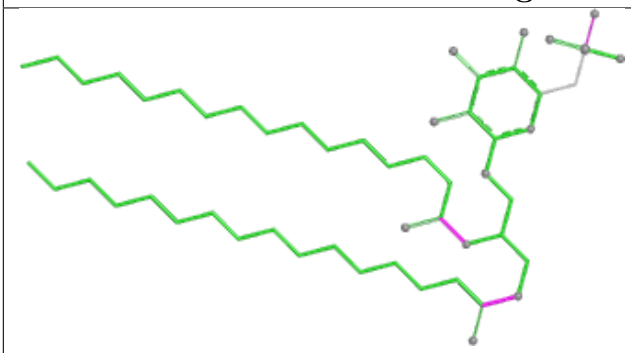


Rings

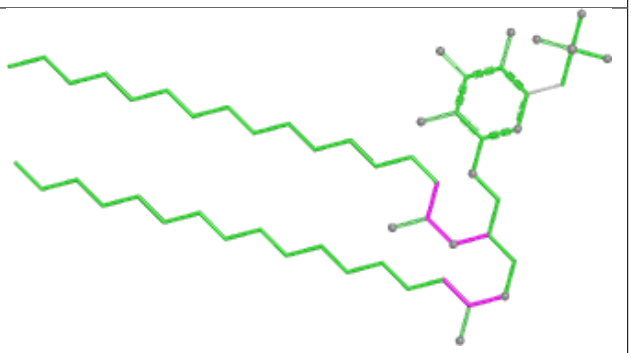
Ligand CLA c 506	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA Bb 608	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

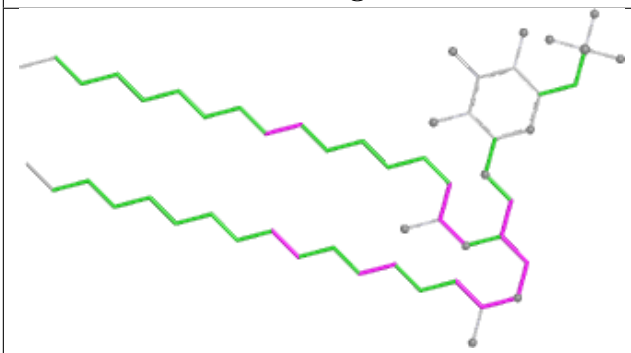
Ligand SQD LL 102



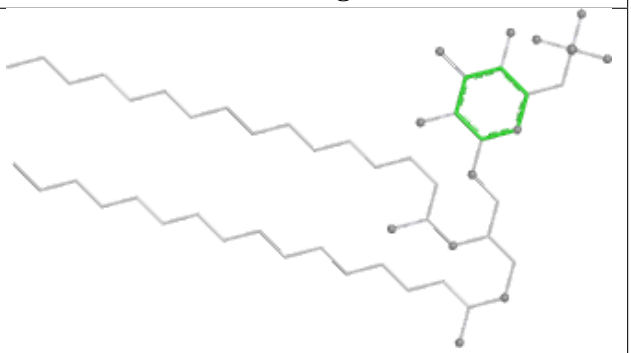
Bond lengths



Bond angles

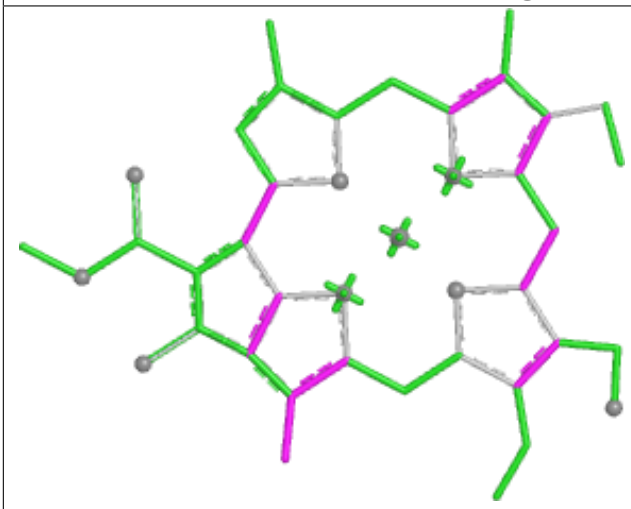


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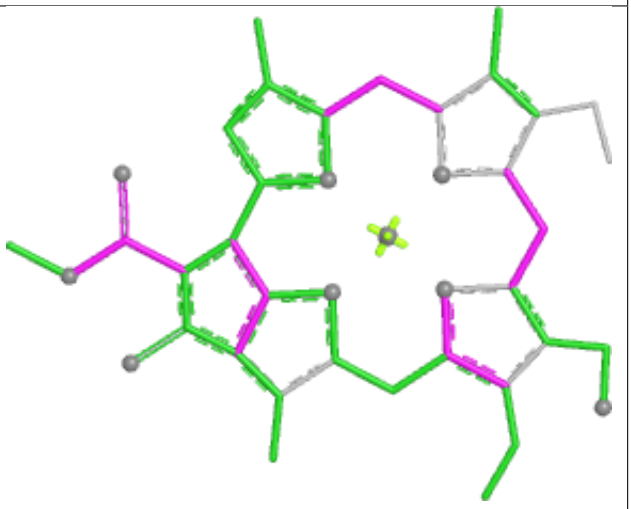


Rings

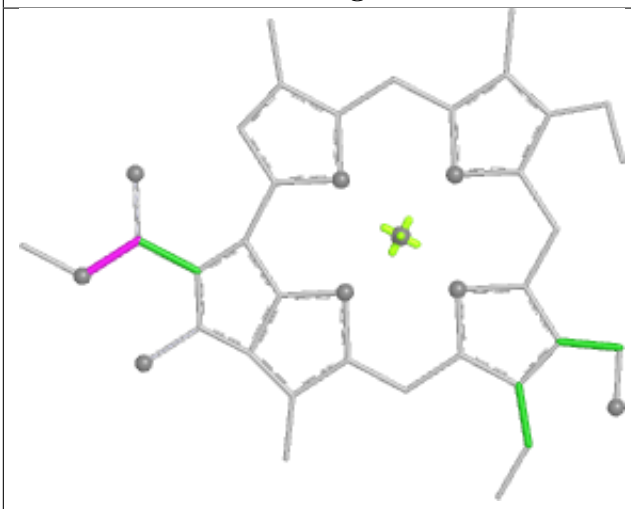
Ligand CHL 22 608



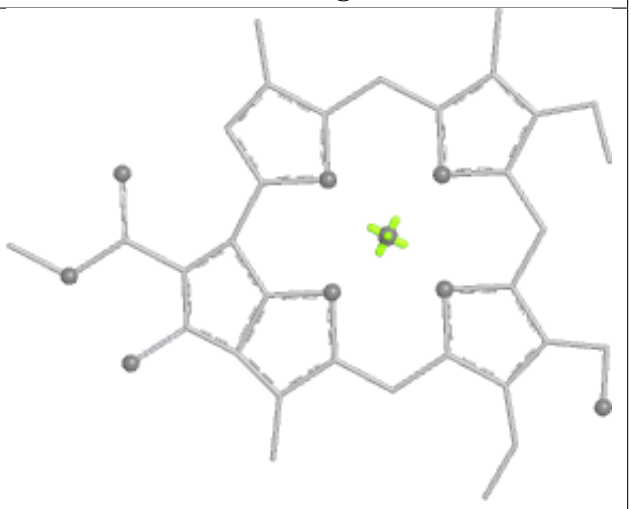
Bond lengths



Bond angles

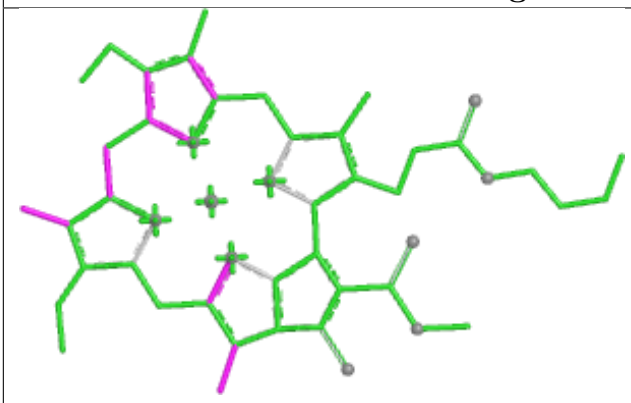


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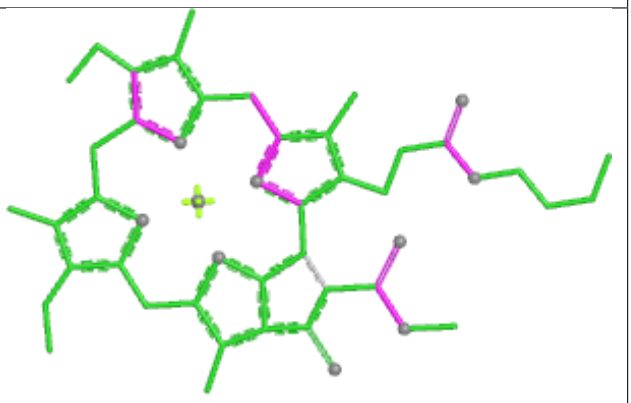


Rings

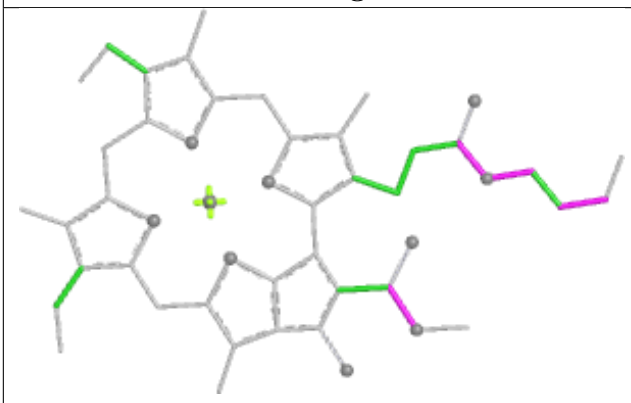
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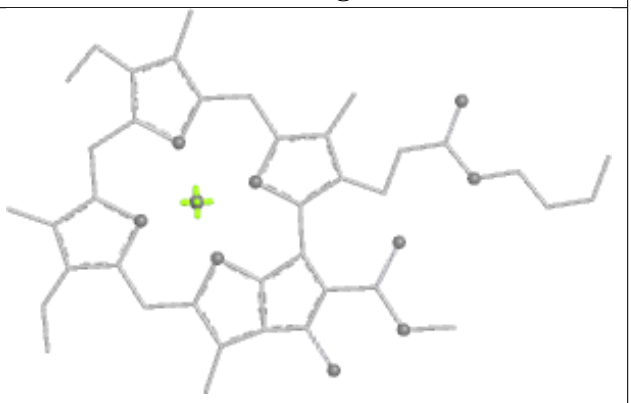
Bond lengths



Bond angles

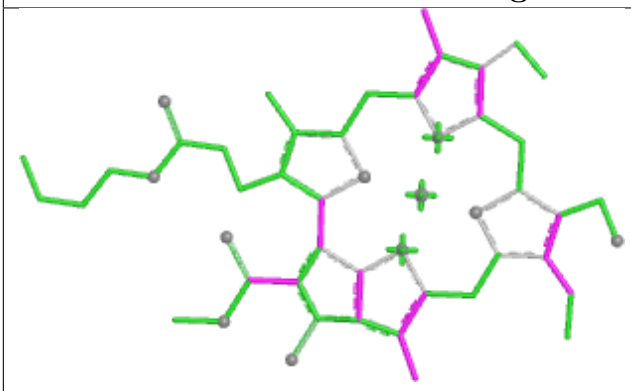


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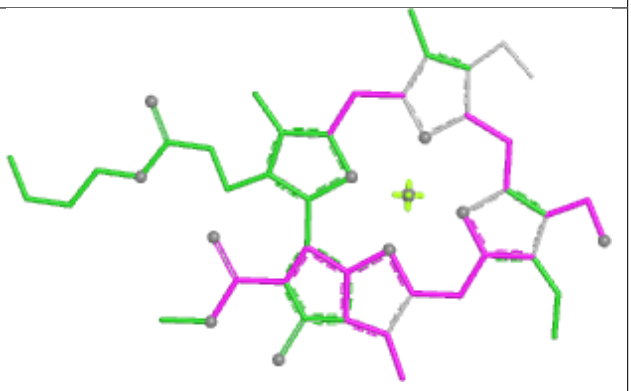


Rings

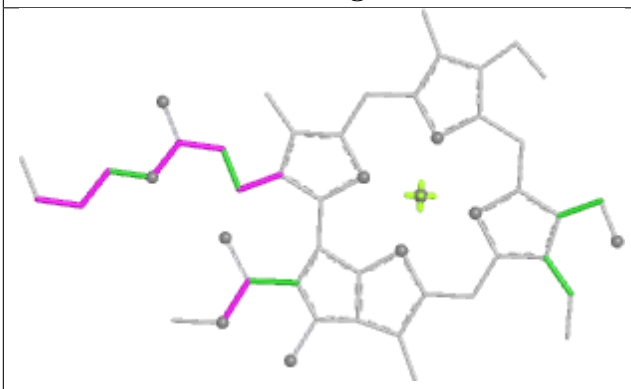
Ligand CHL RR 306



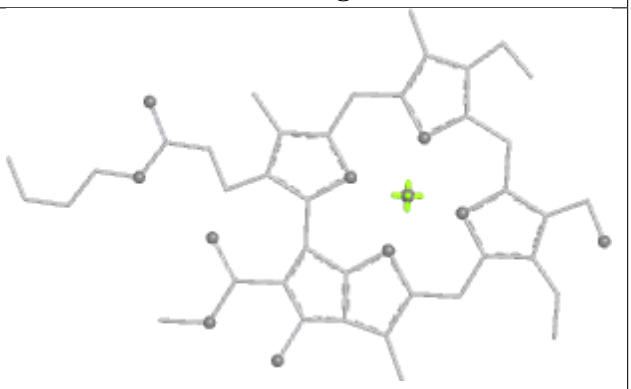
Bond lengths



Bond angles

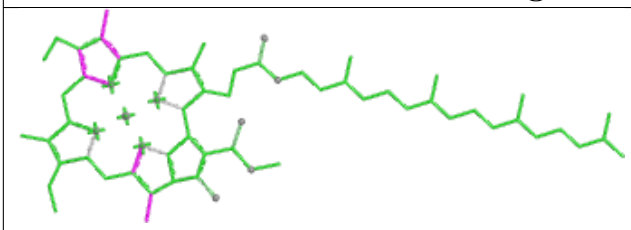


Torsions

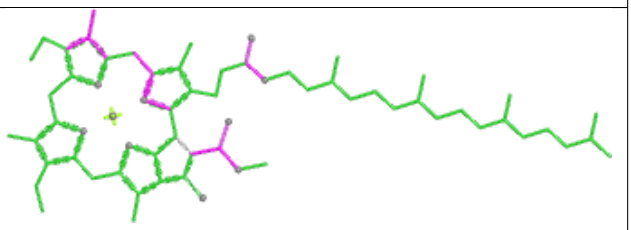


Rings

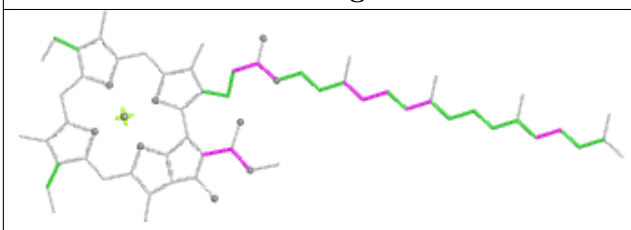
Ligand CLA b 613



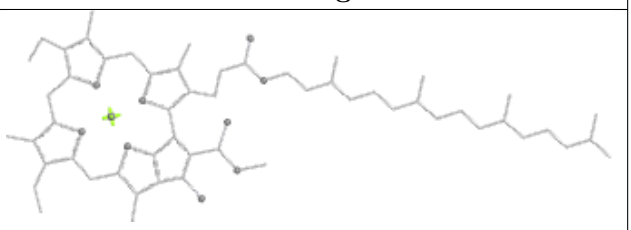
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Bond angles

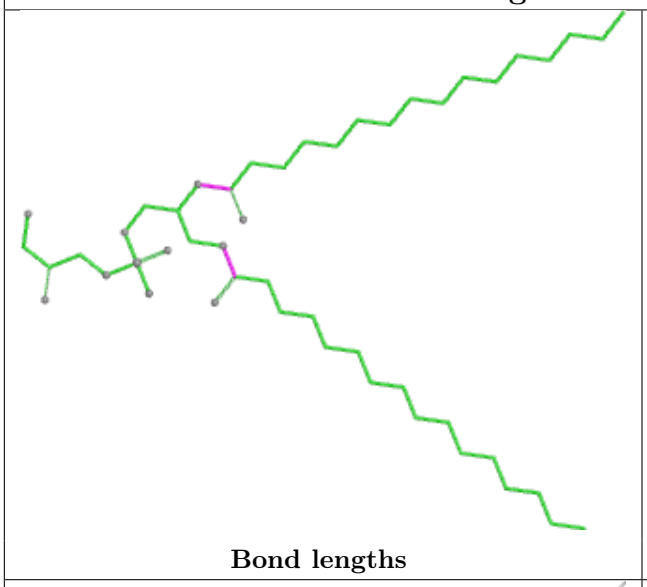


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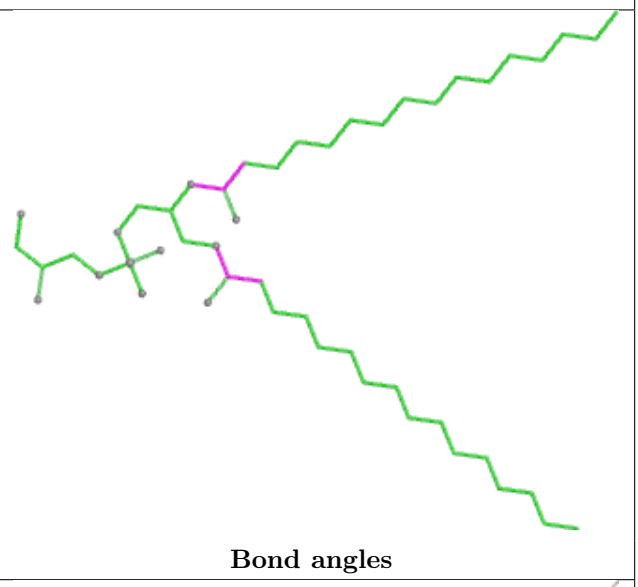


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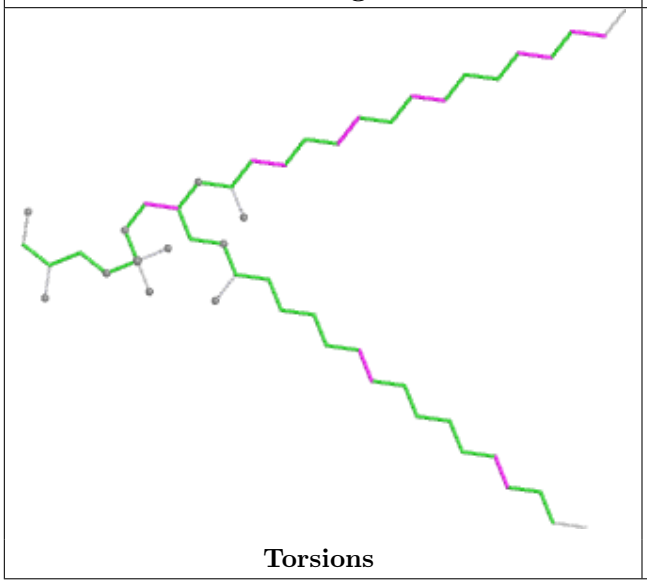
Ligand LHG DD 408



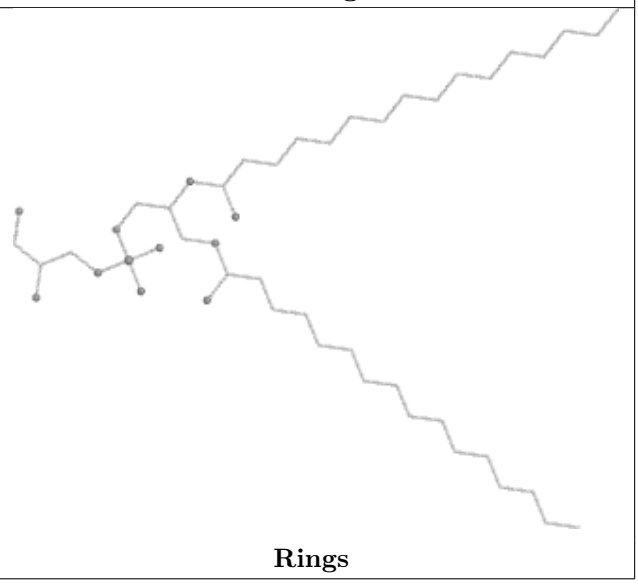
Bond lengths



Bond angles

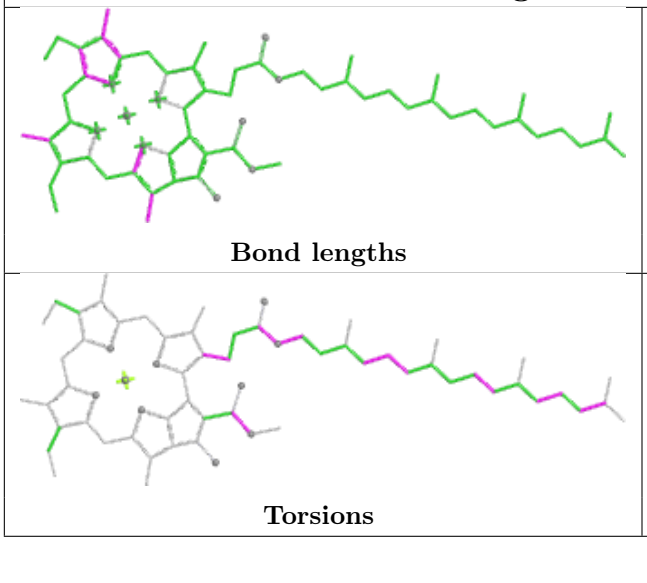


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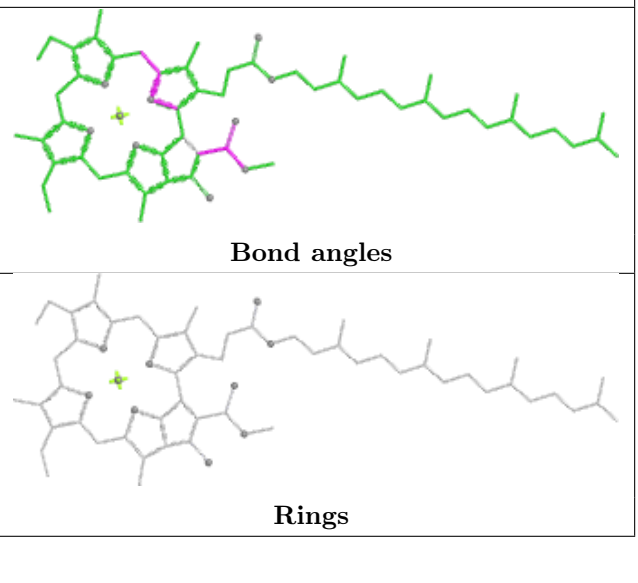


Rings

Ligand CLA CC 509



Bond lengths

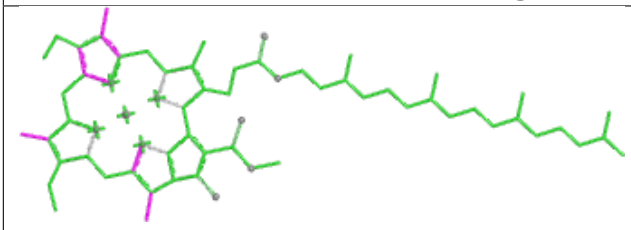


Bond angles

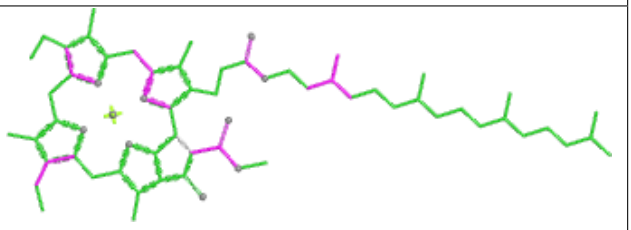
Torsions

Rings

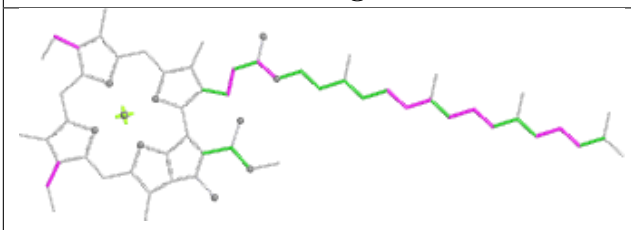
Ligand CLA BB 609



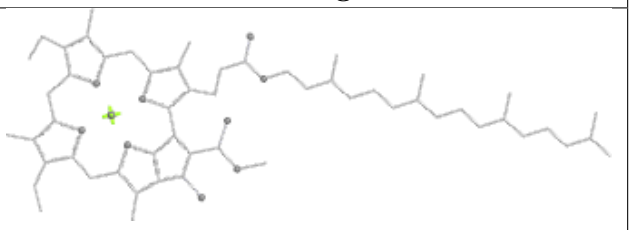
Bond lengths



Bond angles

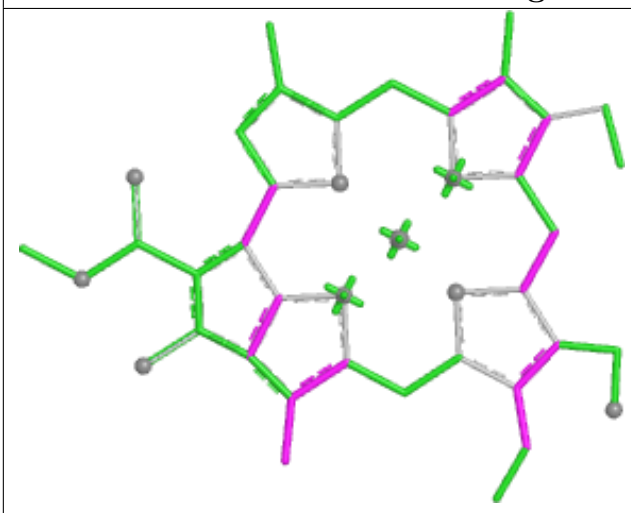


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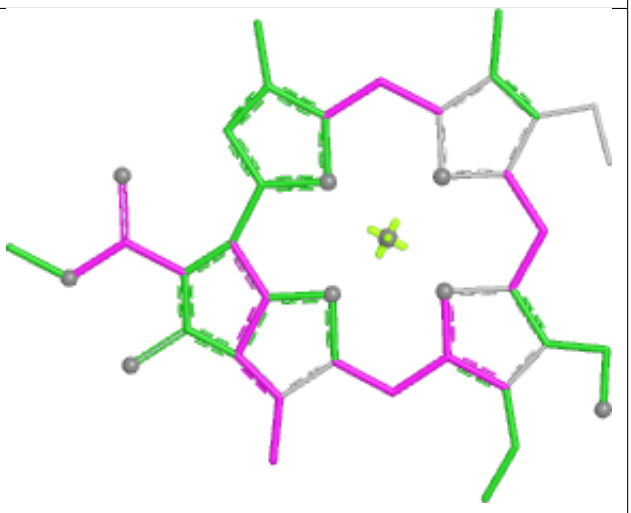


Rings

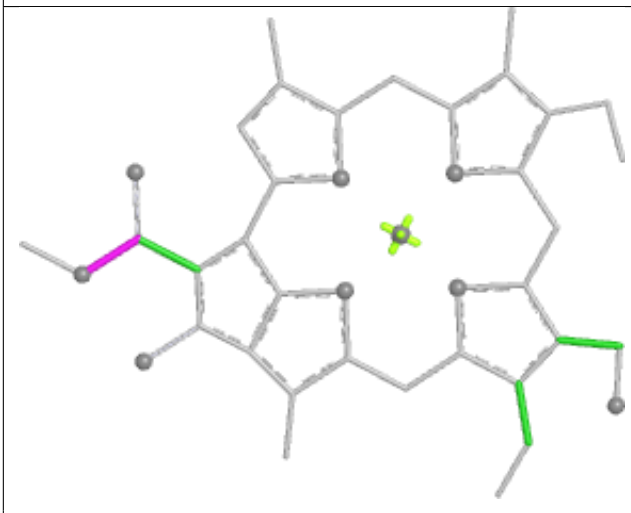
Ligand CHL 3 606



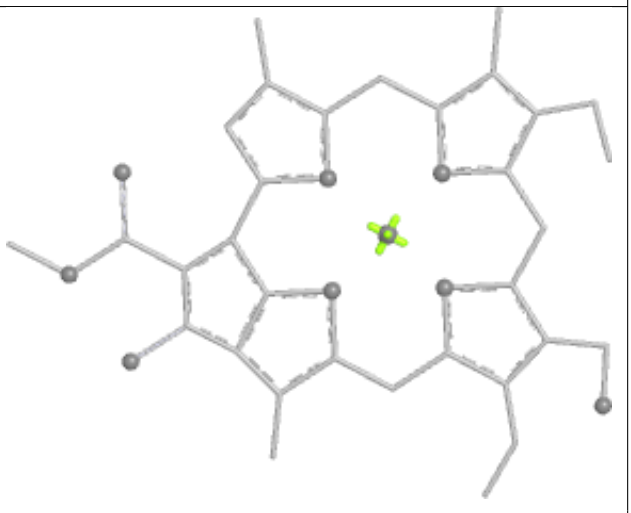
Bond lengths



Bond angles

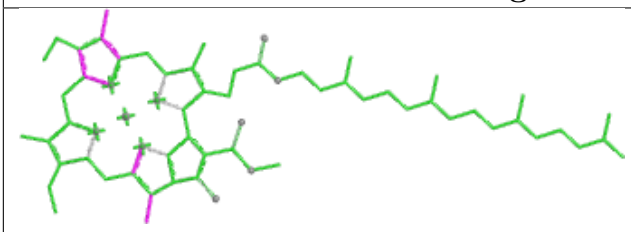


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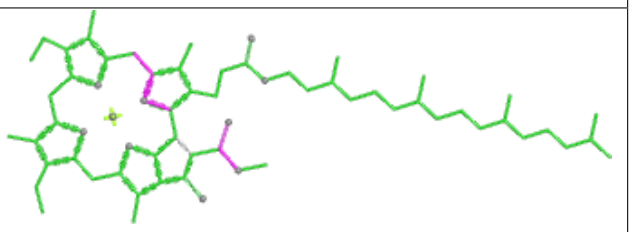


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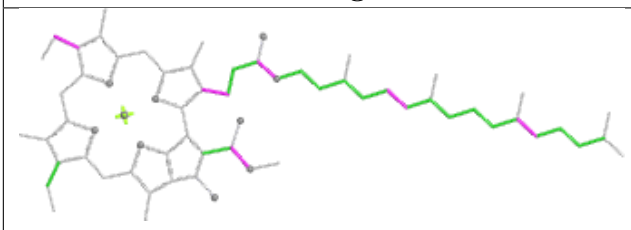
Ligand CLA DD 404



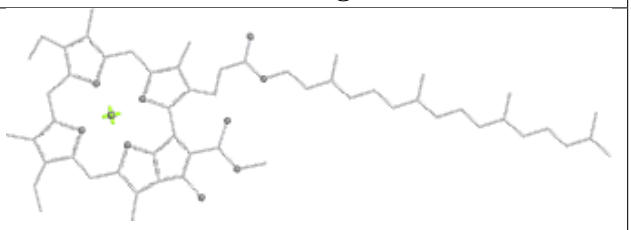
Bond lengths



Bond angles

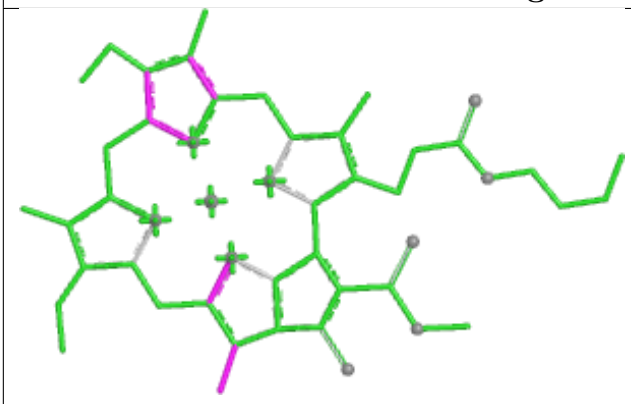


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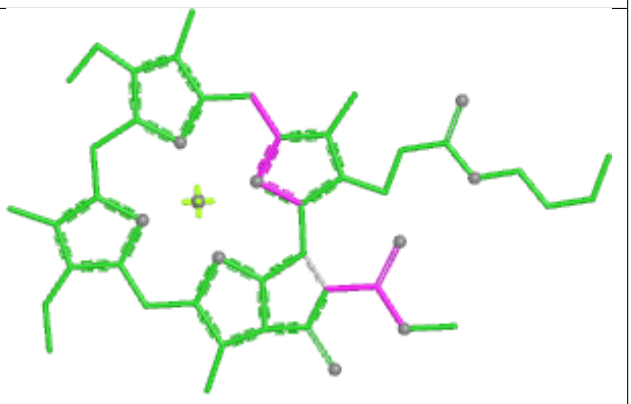


Rings

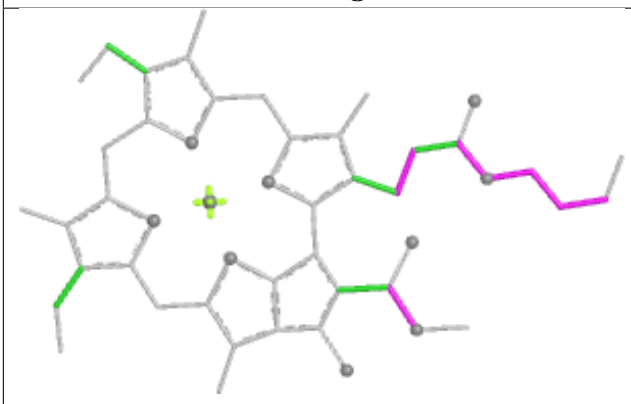
Ligand CLA n 614



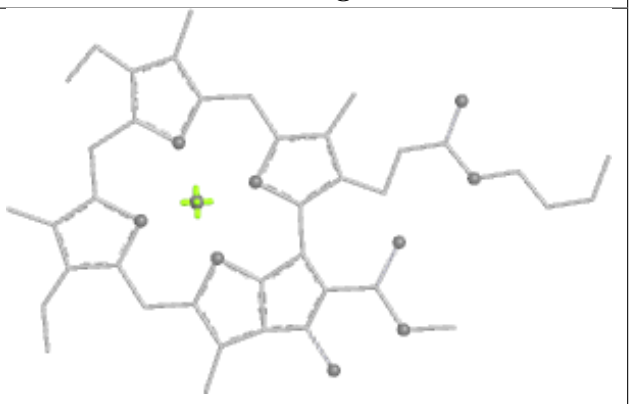
Bond lengths



Bond angles

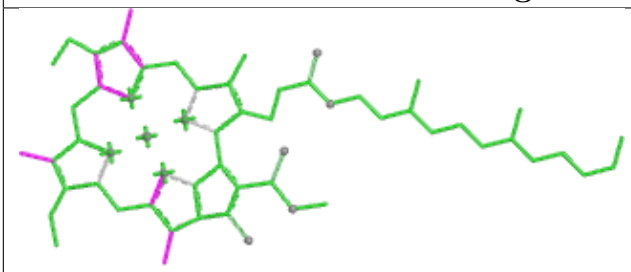


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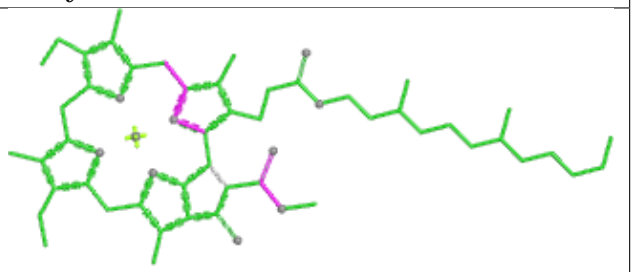


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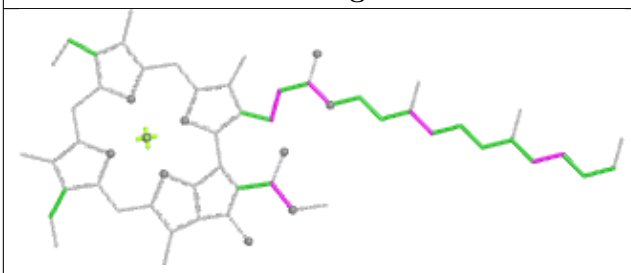
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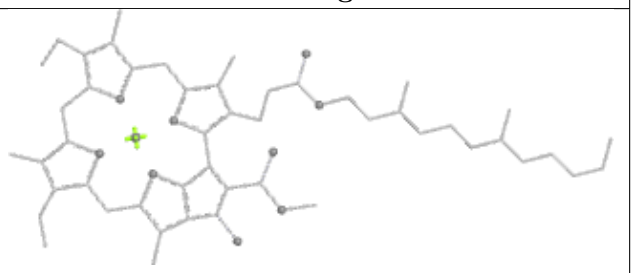
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Bond angles

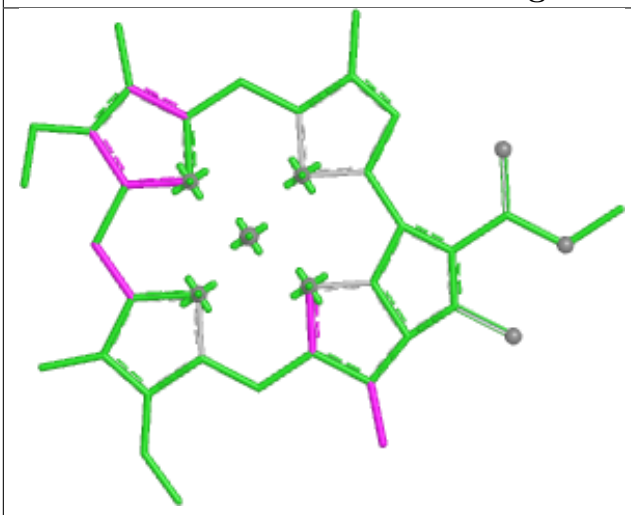


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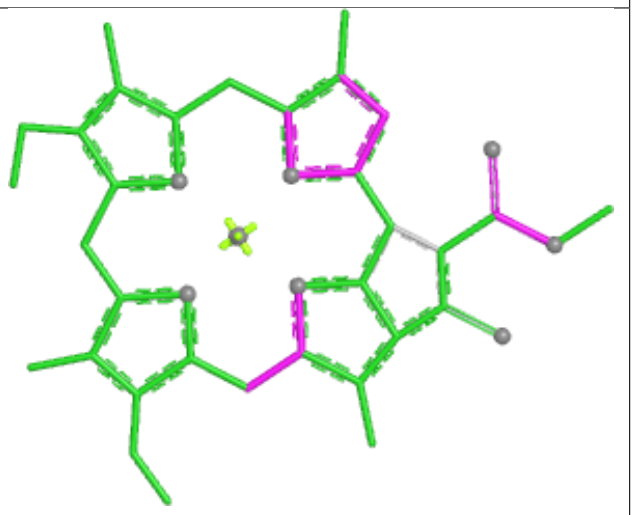


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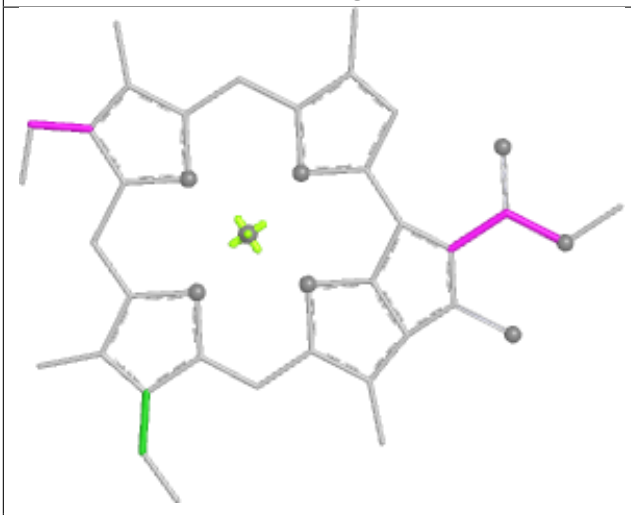
Ligand CLA 1 613



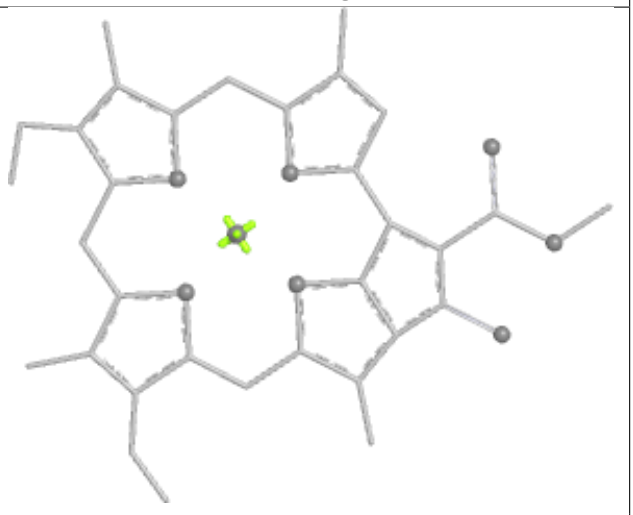
Bond lengths



Bond angles

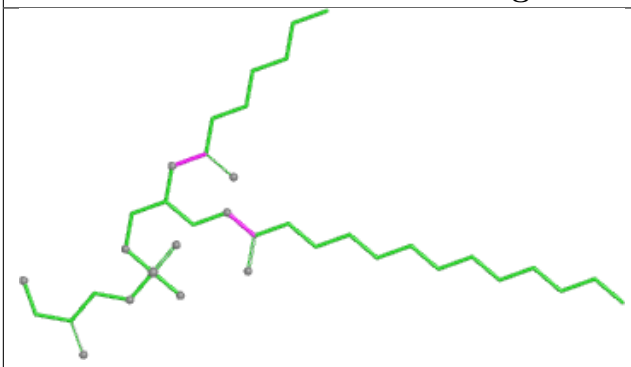


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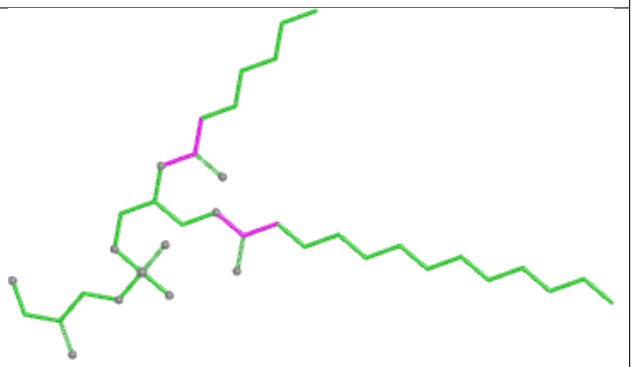


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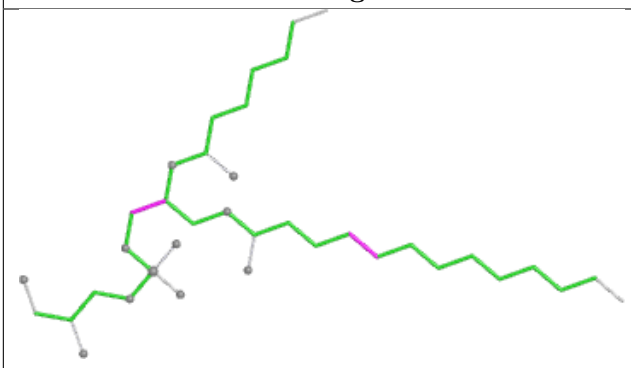
Ligand LHG Dd 407



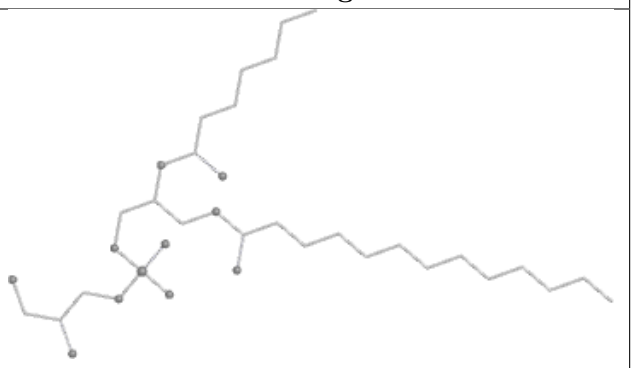
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Bond angles

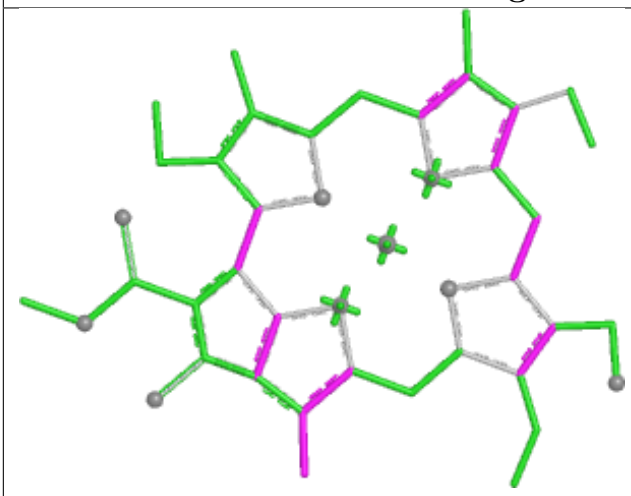


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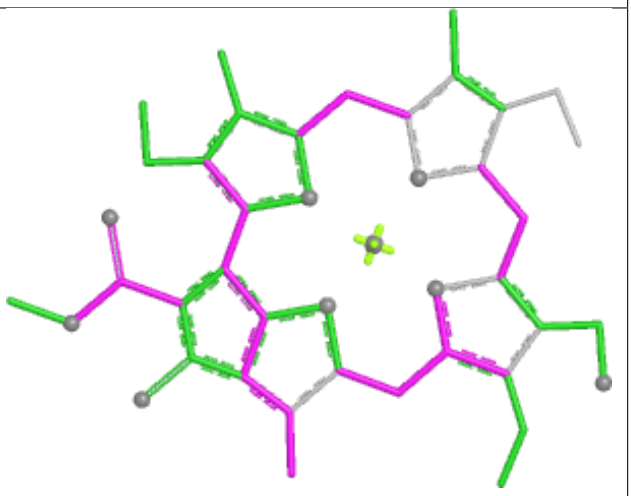


Rings

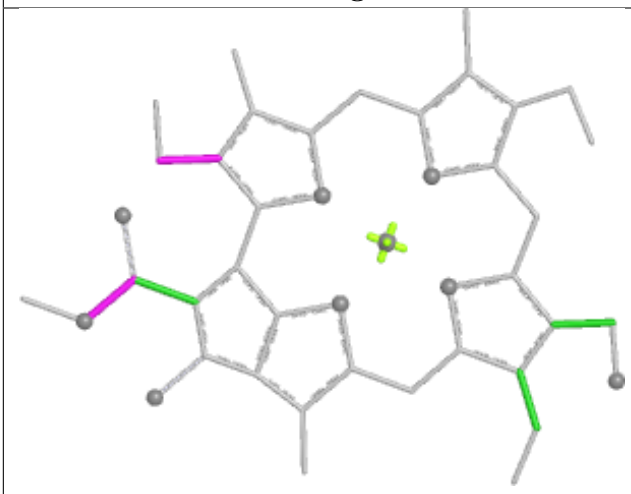
Ligand CHL GG 606



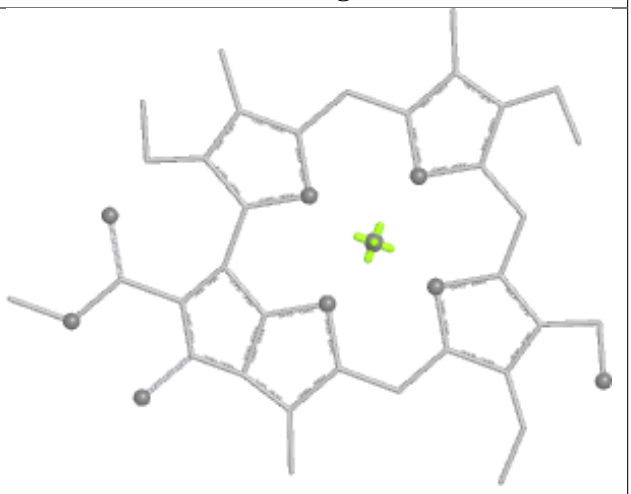
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Bond angles

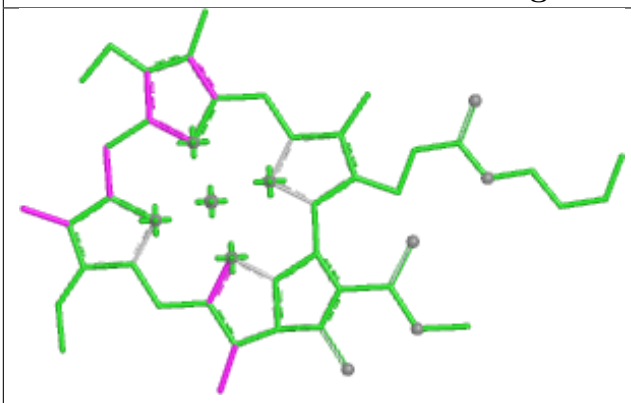


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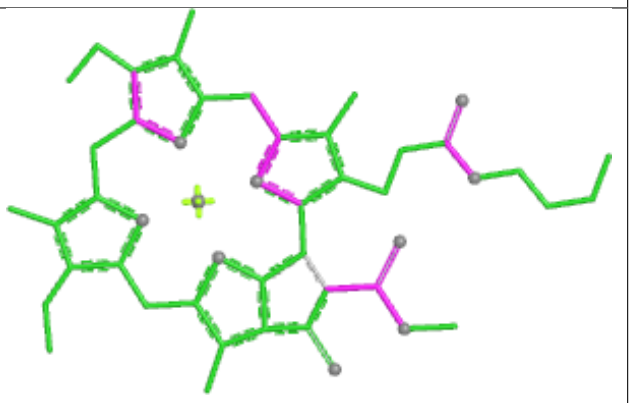


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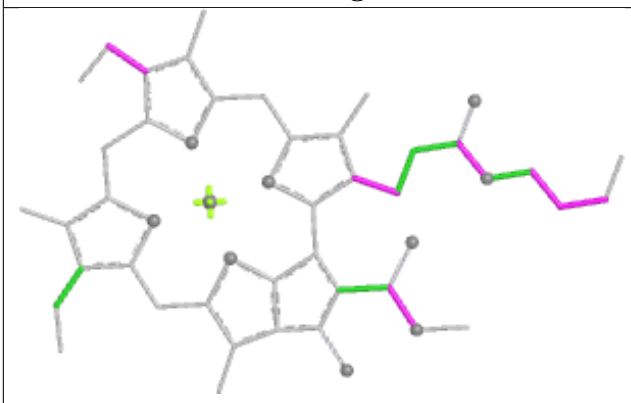
Ligand CLA s 609



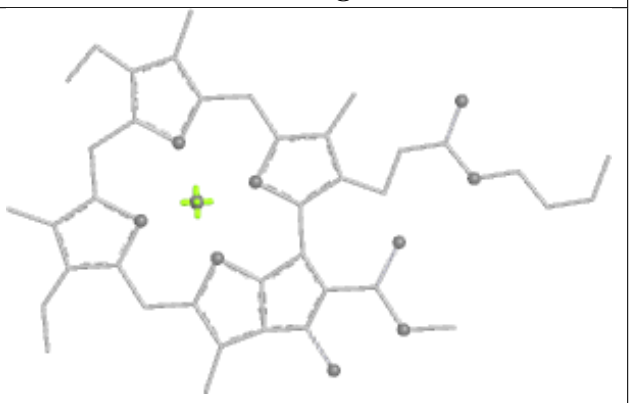
Bond lengths



Bond angles

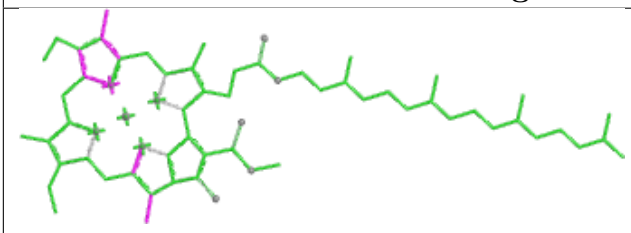


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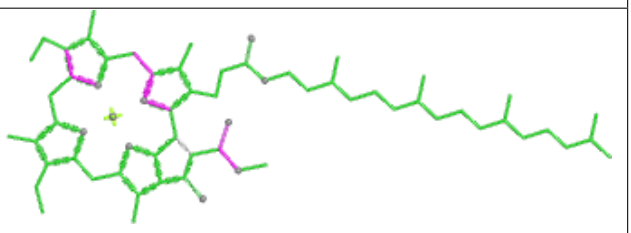


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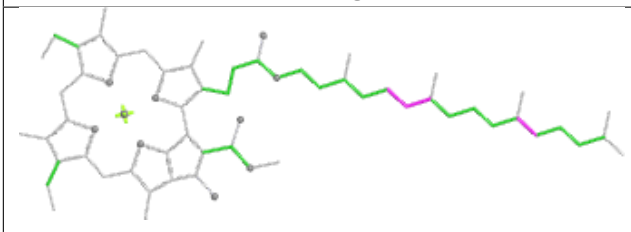
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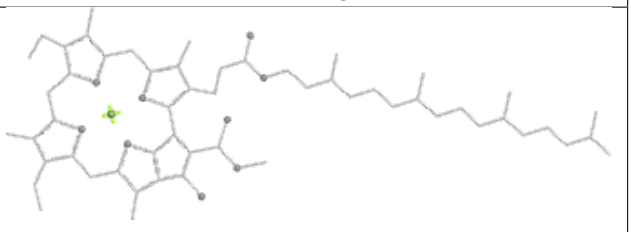
Bond lengths



Bond angles

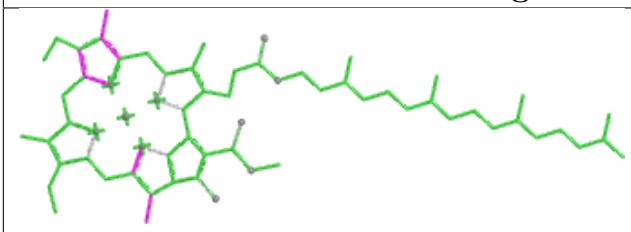


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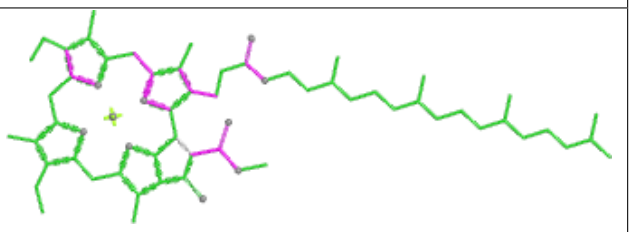


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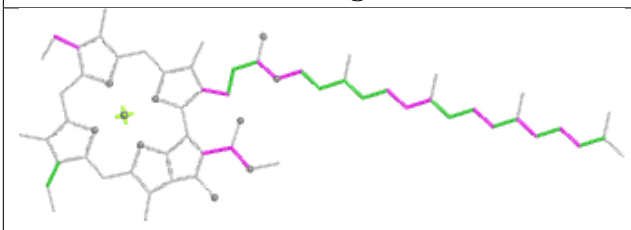
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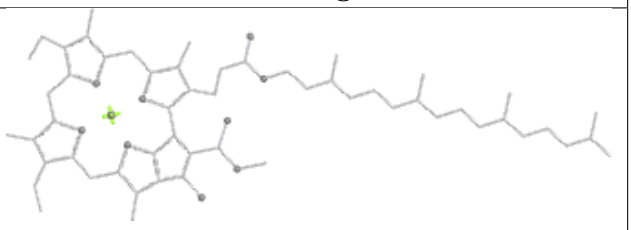
Bond lengths



Bond angles



Torsions

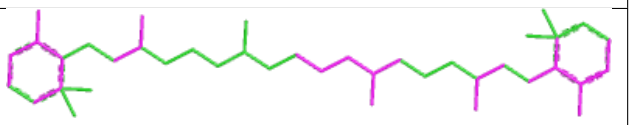


Rings

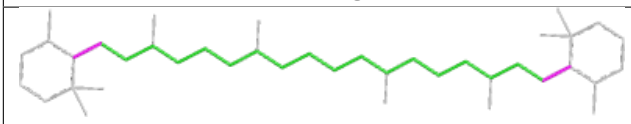
Ligand BCR BB 616



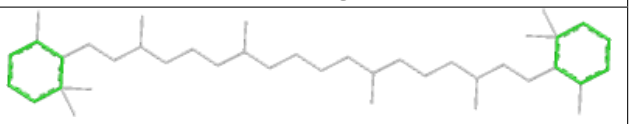
Bond lengths



Bond angles

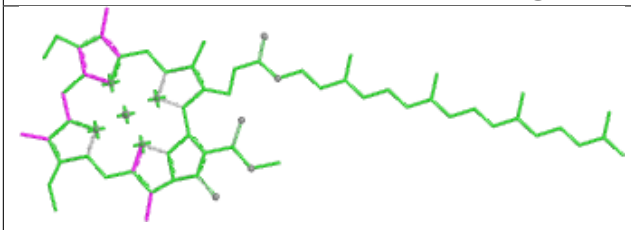


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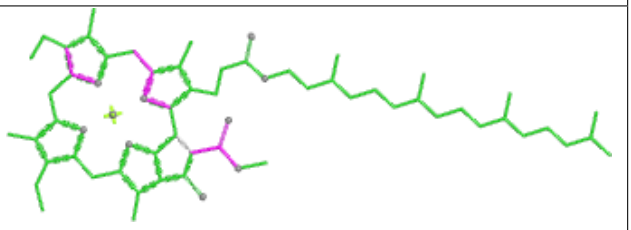


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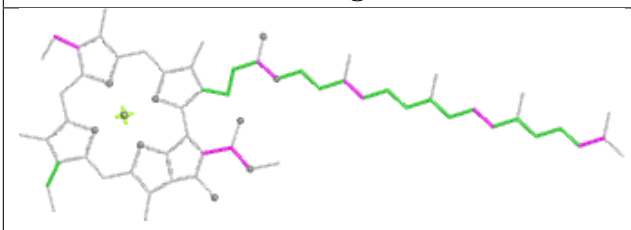
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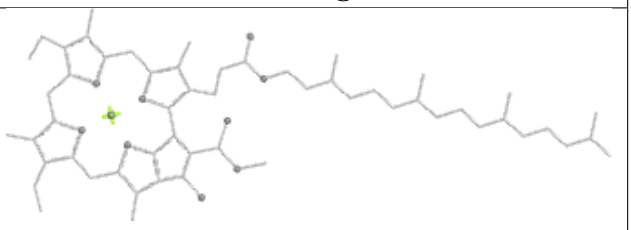
Bond lengths



Bond angles



Torsions

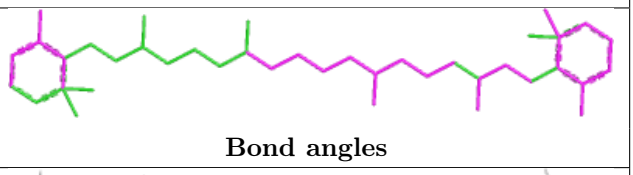


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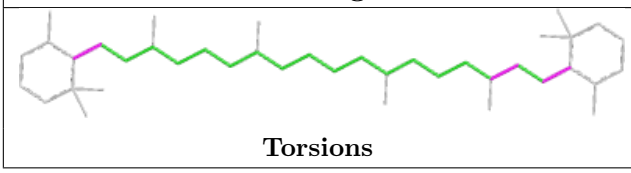
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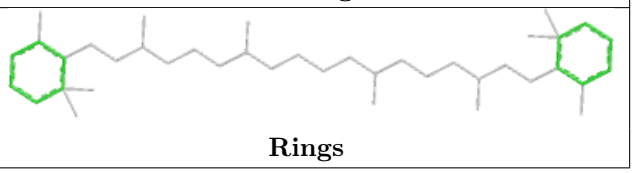
Bond lengths



Bond angles

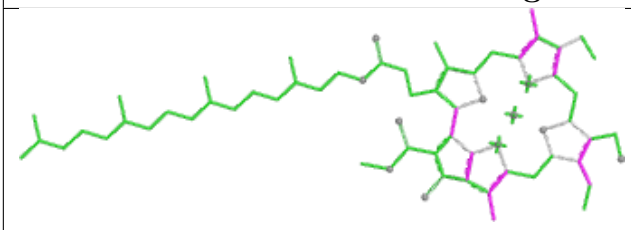


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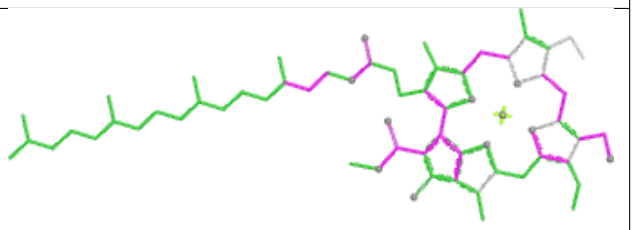


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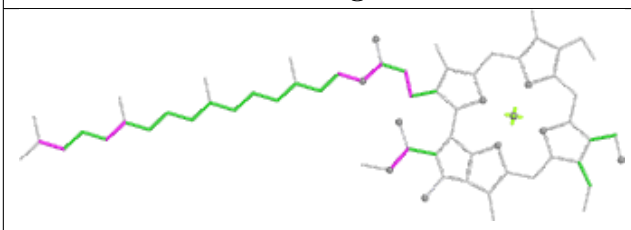
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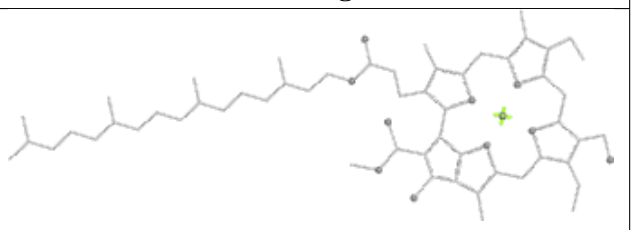
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Bond angles

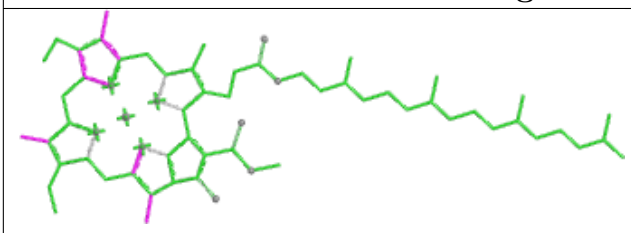


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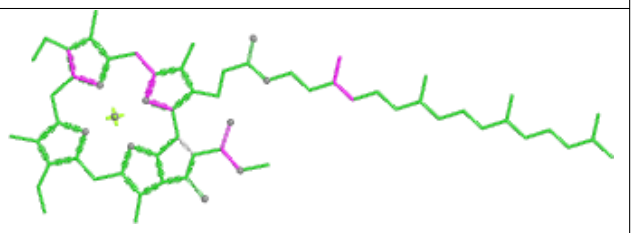


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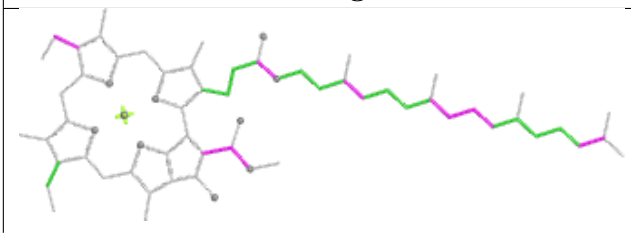
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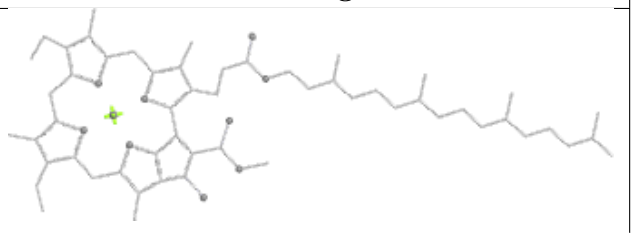
Bond lengths



Bond angles

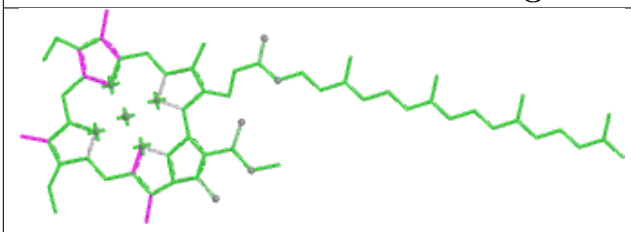


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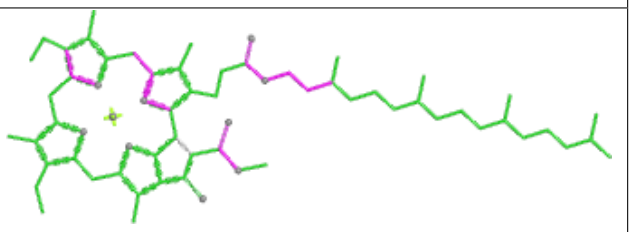


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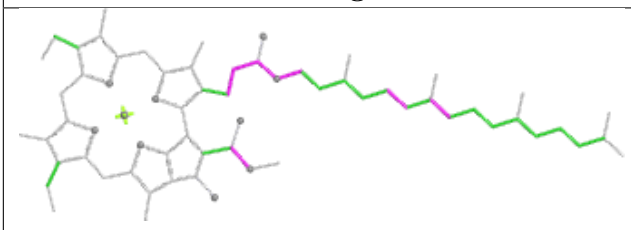
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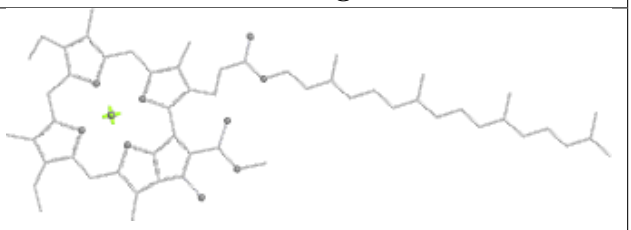
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Bond angles

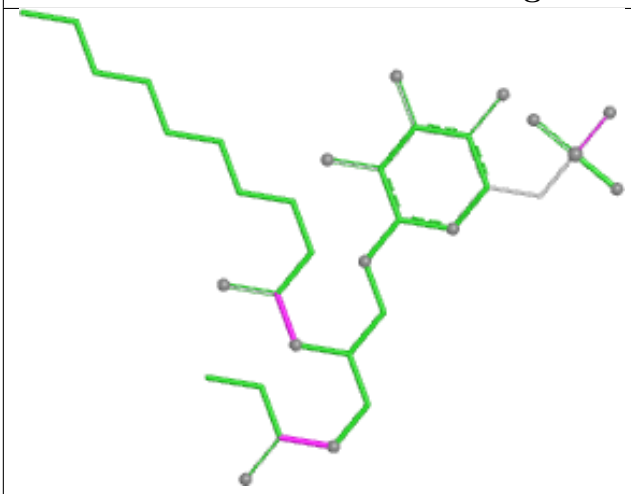


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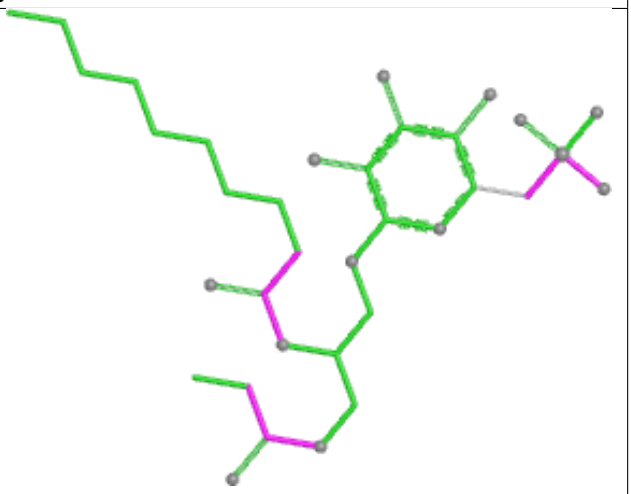


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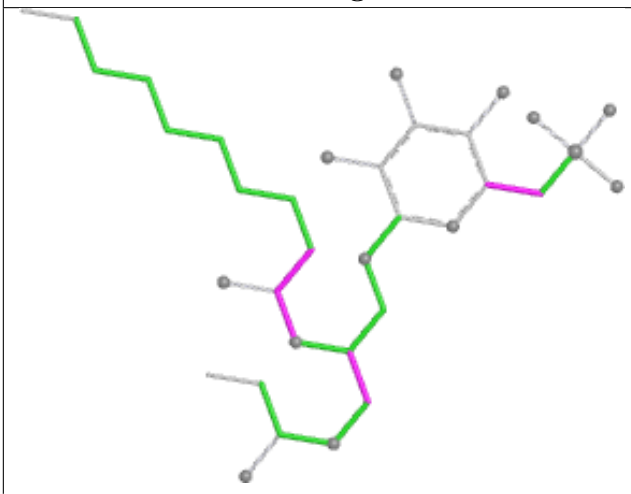
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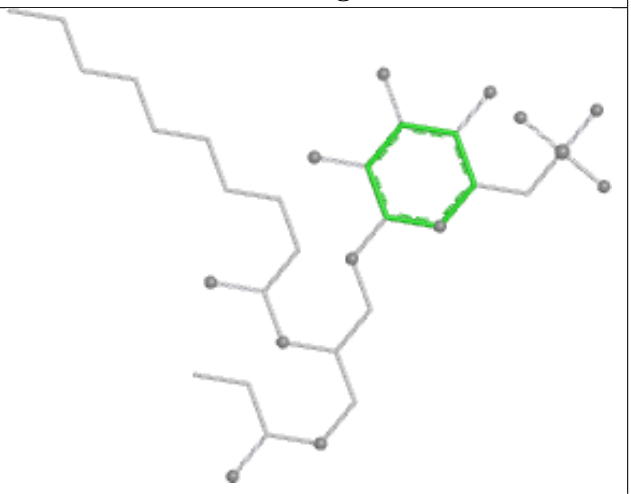
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Bond angles

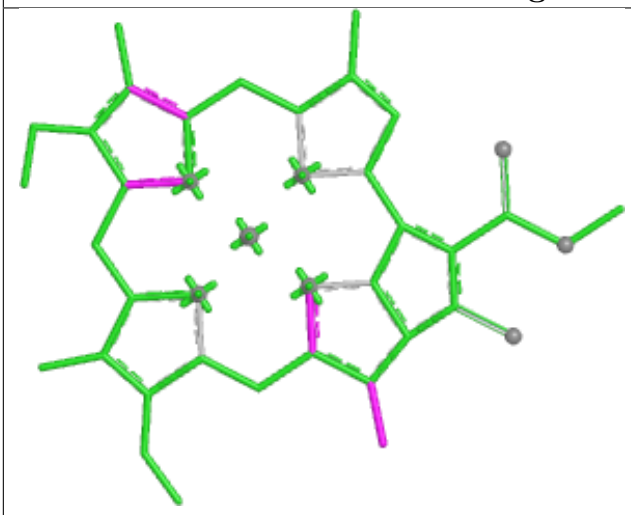


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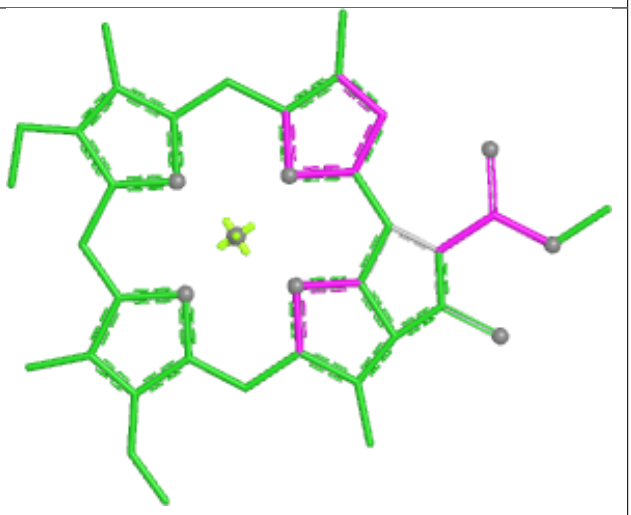


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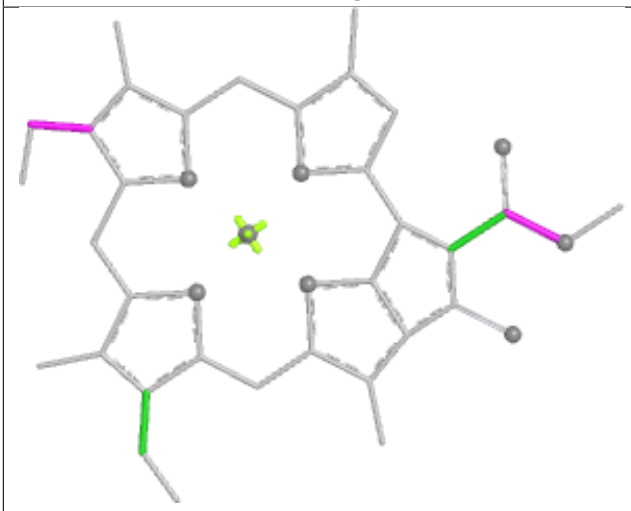
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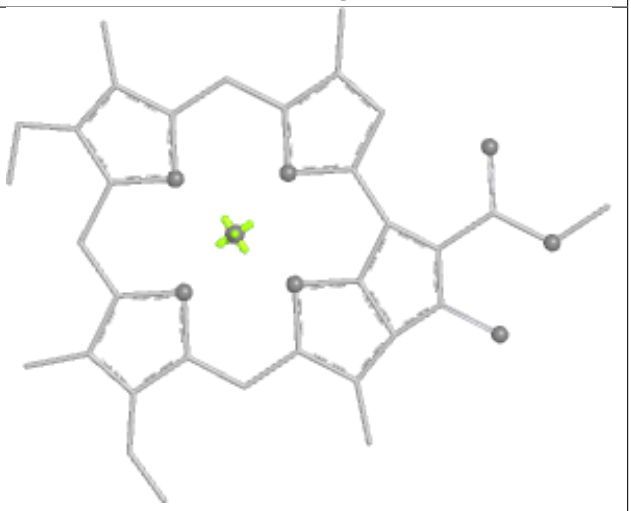
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Bond angles

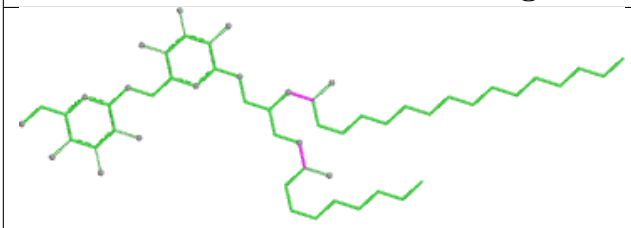


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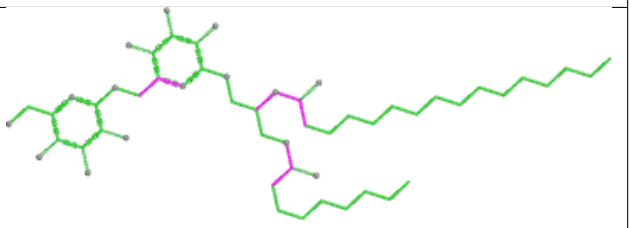


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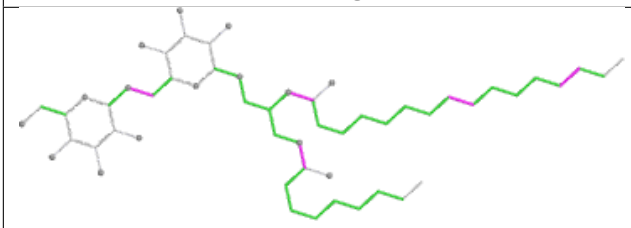
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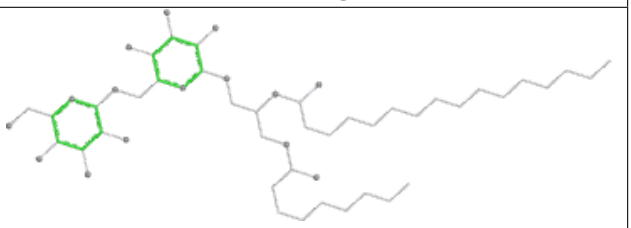
Bond lengths



Bond angles

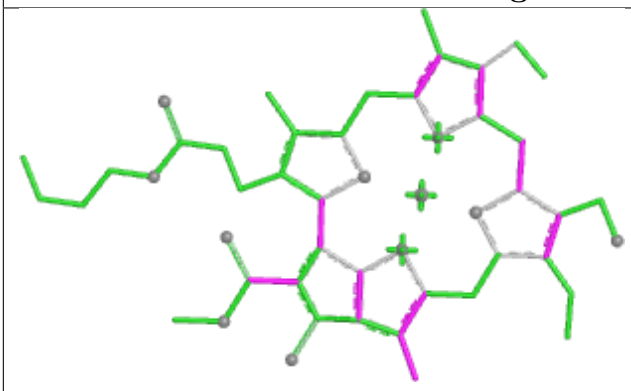


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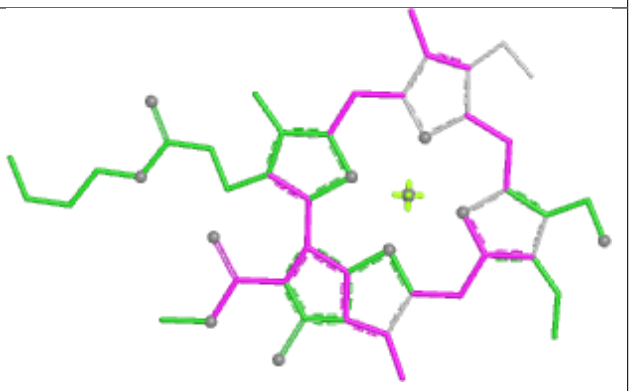


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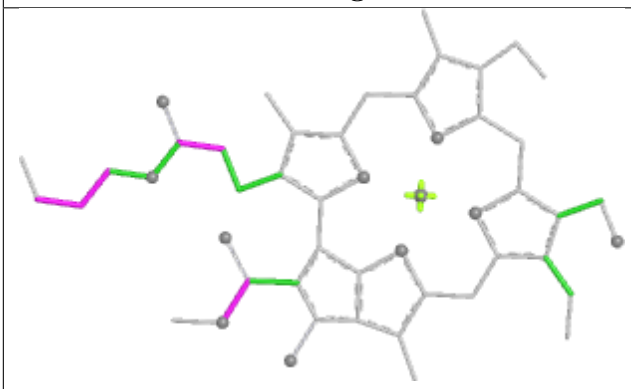
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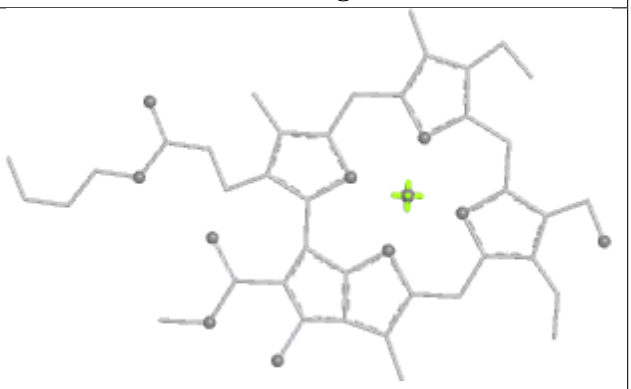
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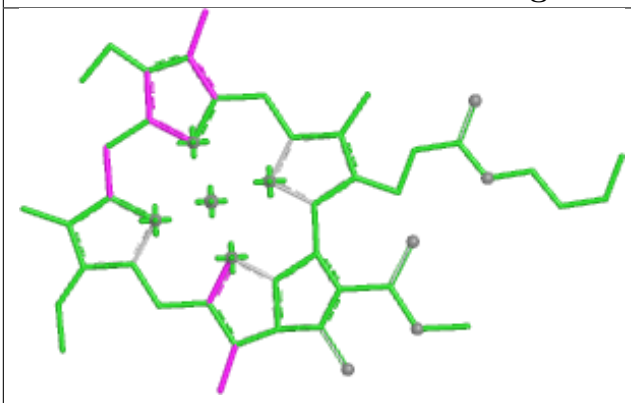


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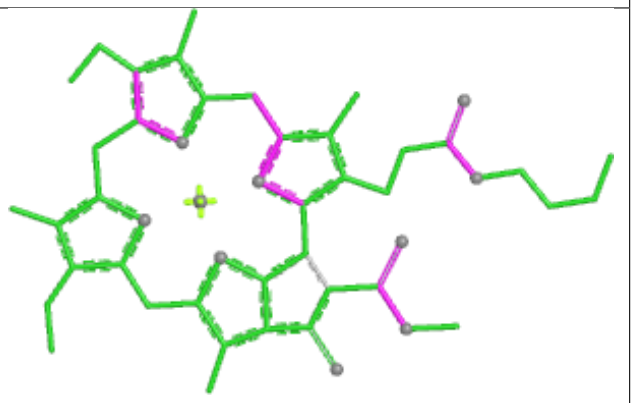


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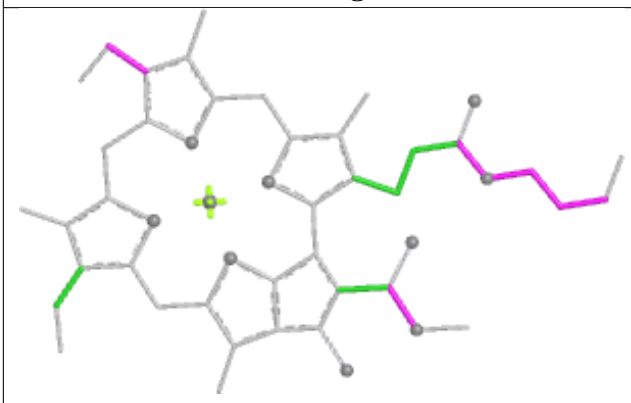
Ligand CLA r 613



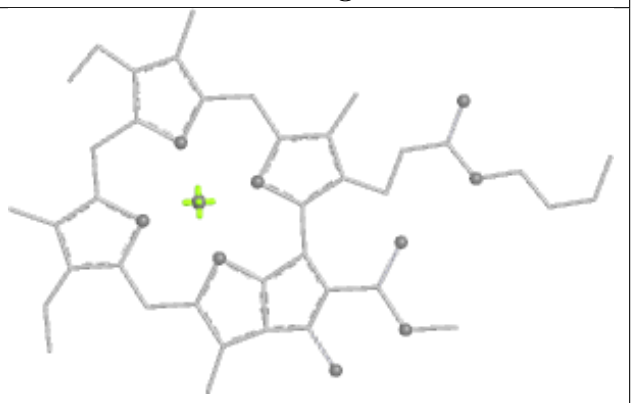
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Bond angles

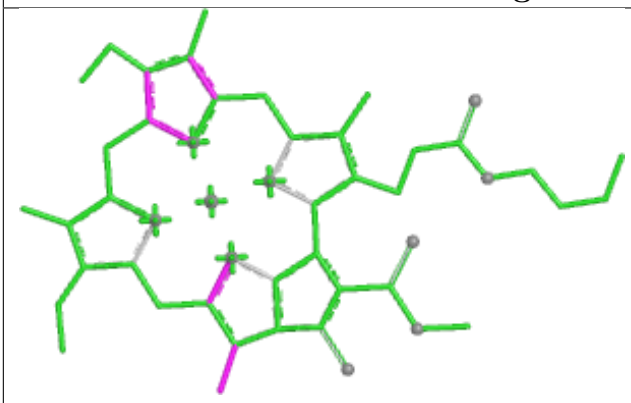


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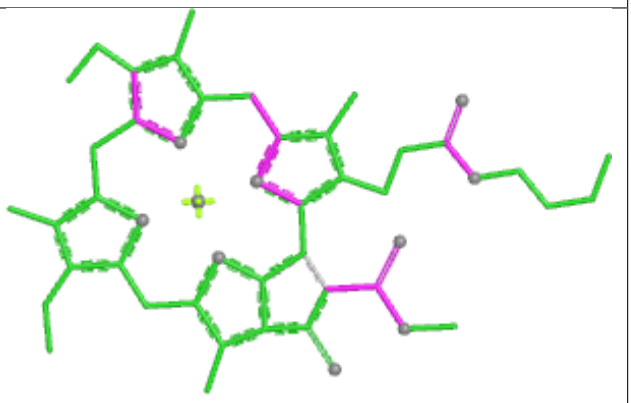


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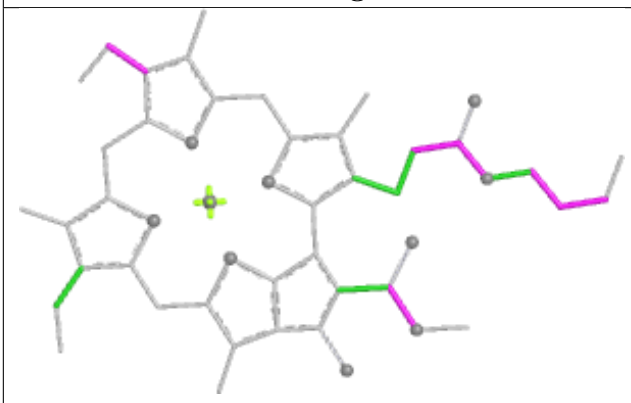
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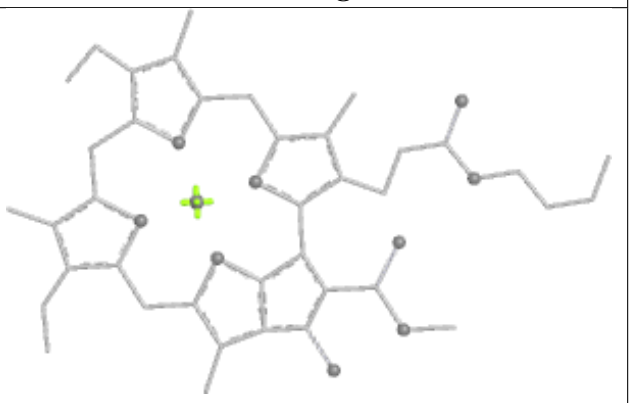
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Bond angles

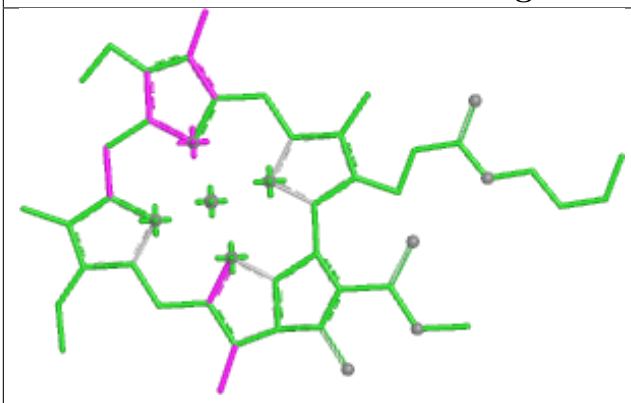


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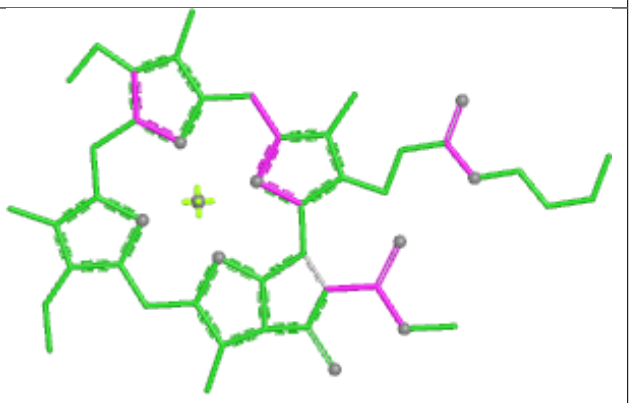


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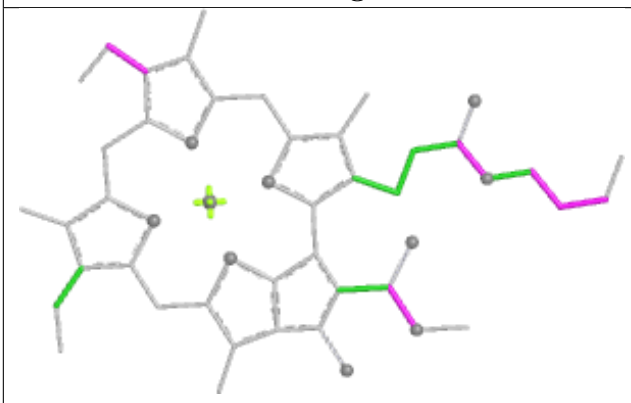
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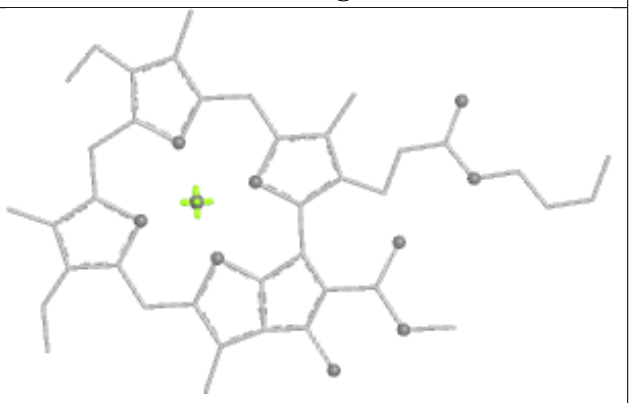
Bond lengths



Bond angles

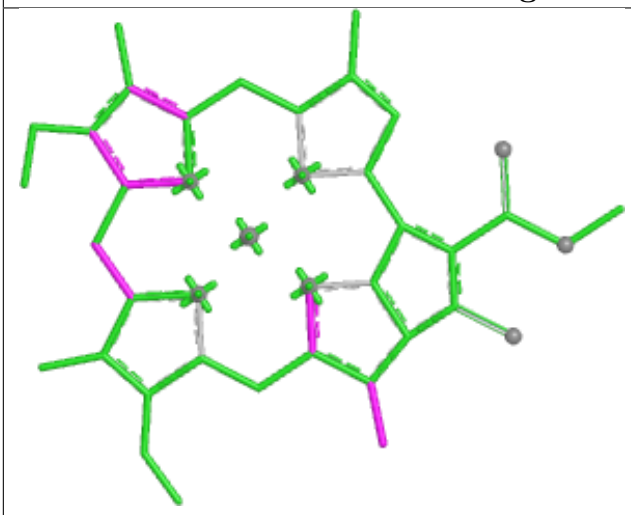


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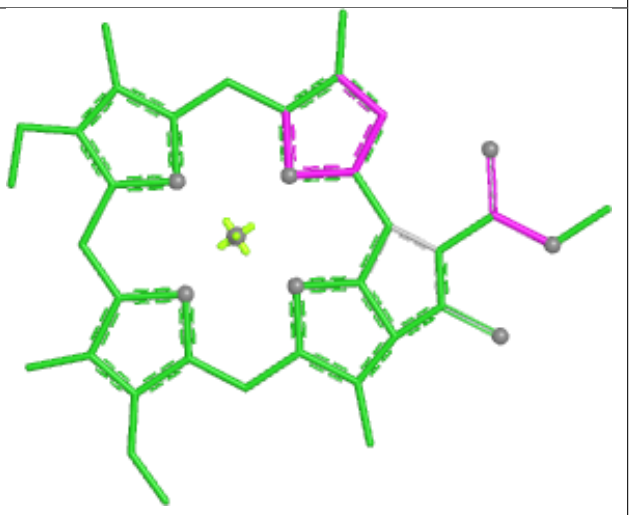


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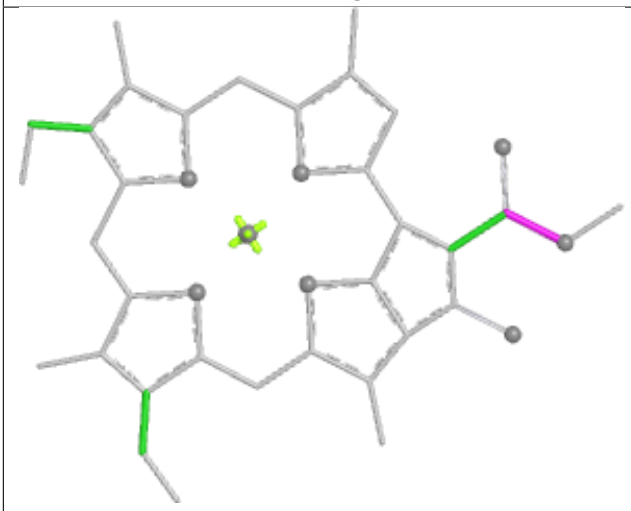
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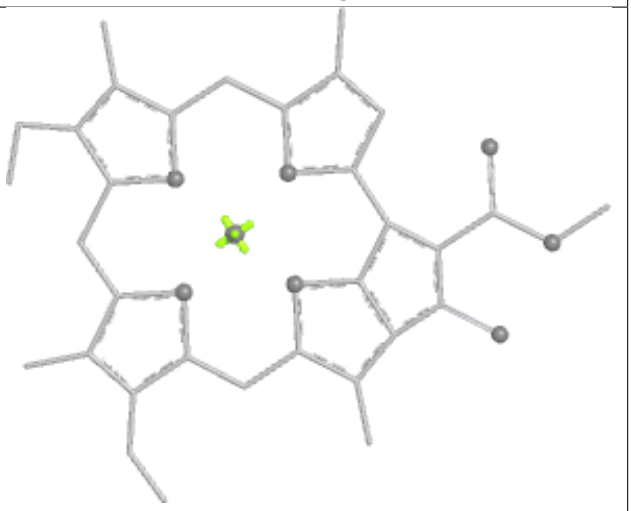
Bond lengths



Bond angles

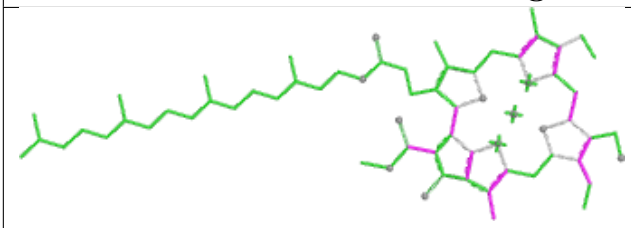


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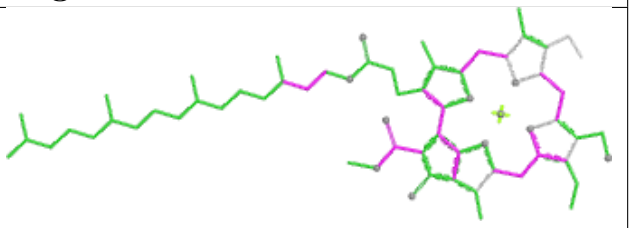


Rings

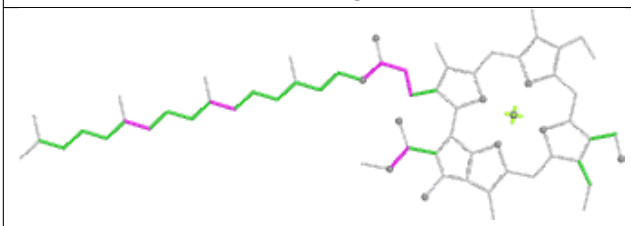
Ligand CHL g 601



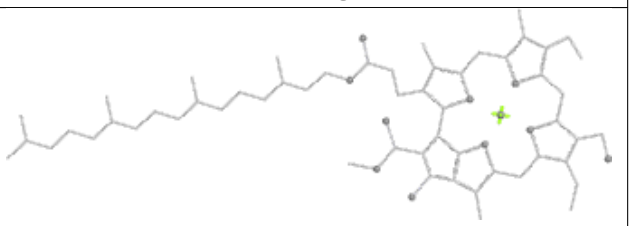
Bond lengths



Bond angles

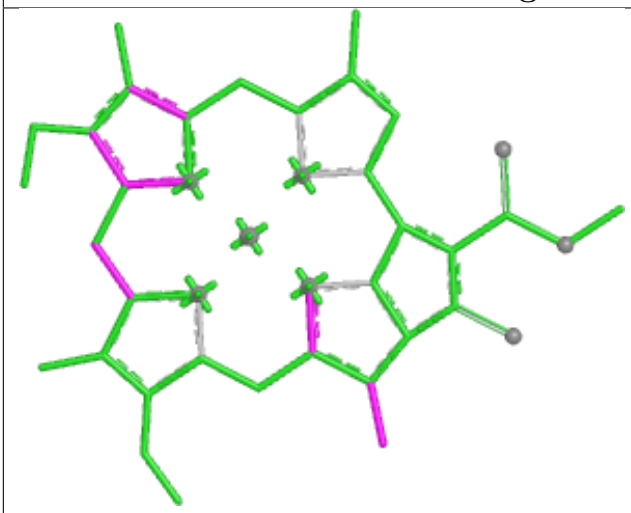


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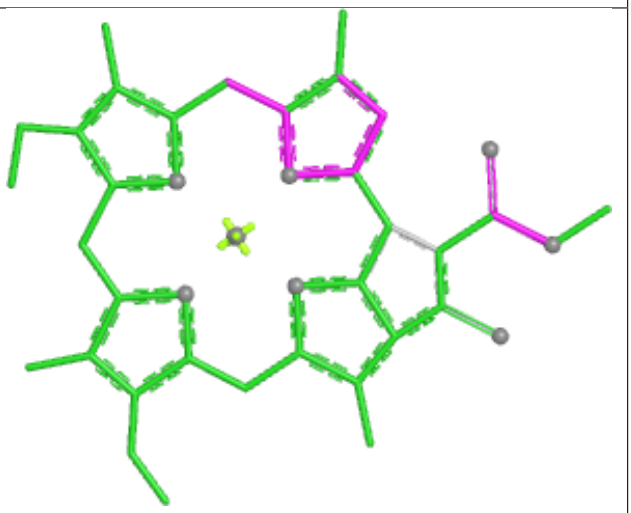


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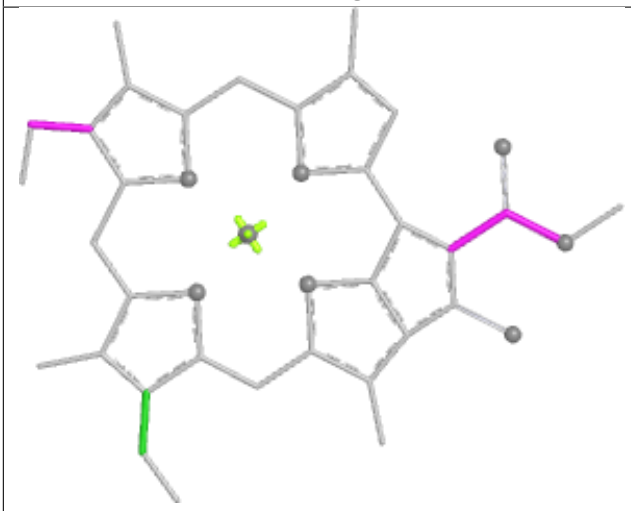
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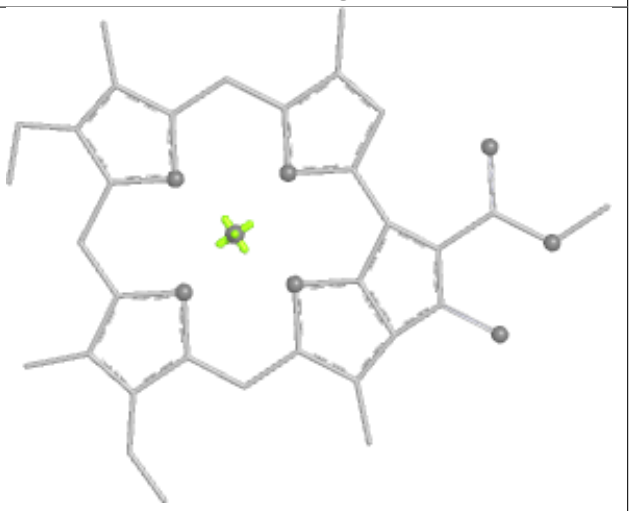
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Bond angles

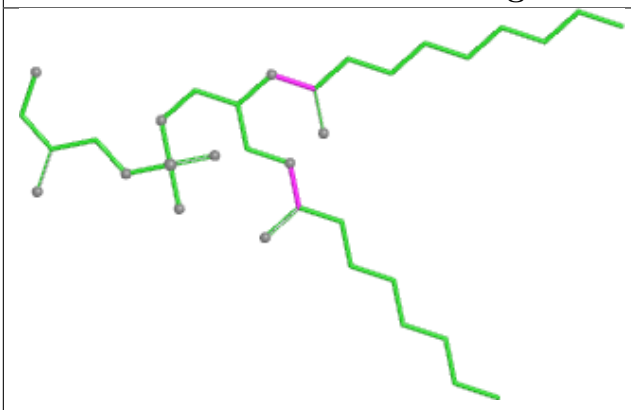


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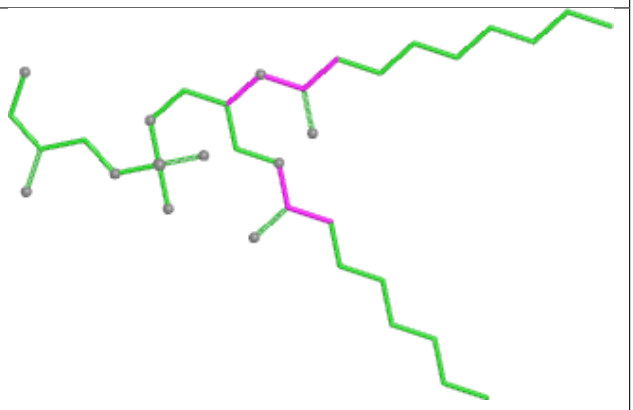


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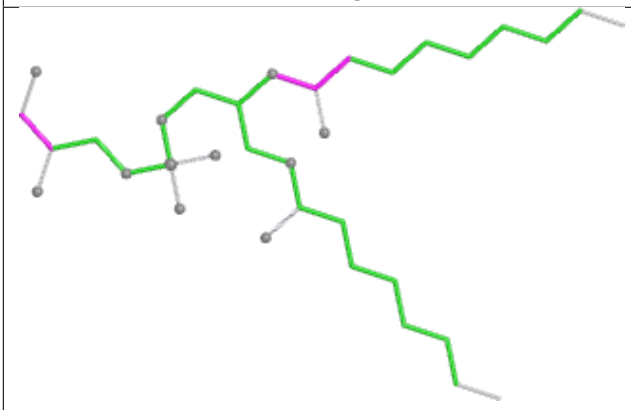
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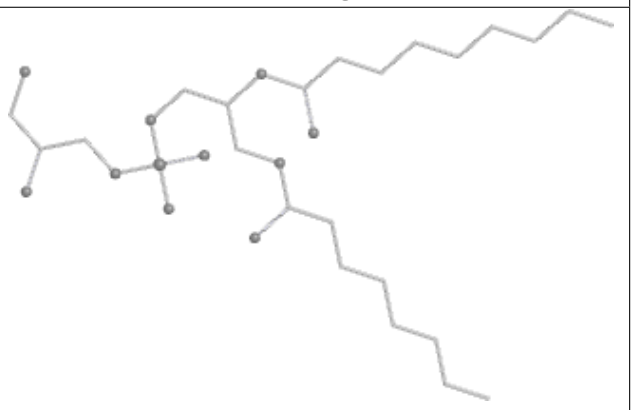
Bond lengths



Bond angles

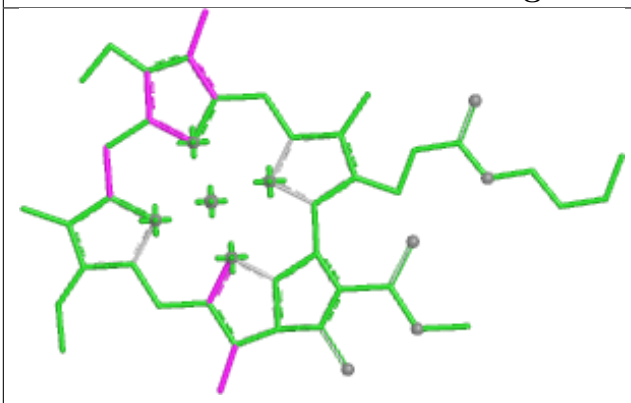


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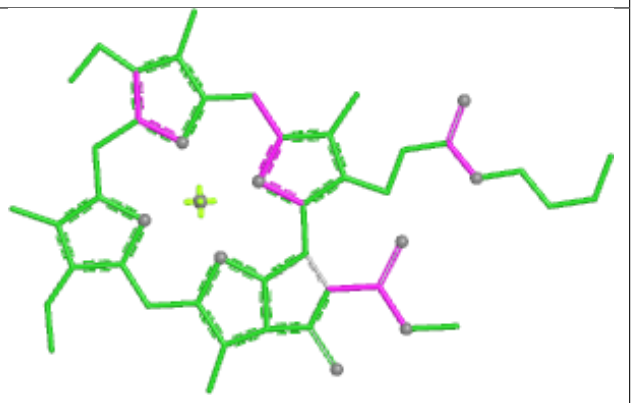


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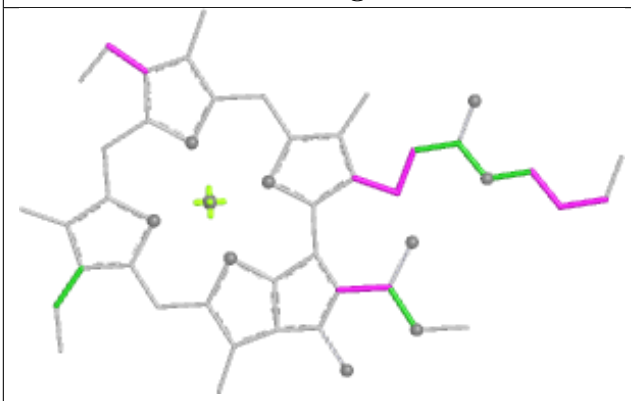
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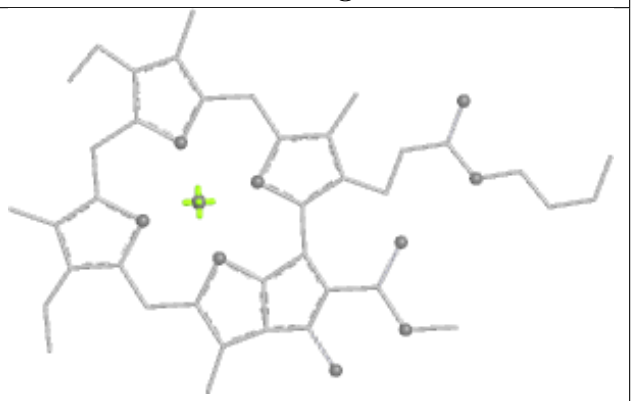
Bond lengths



Bond angles

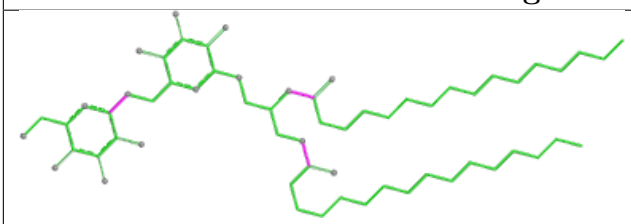


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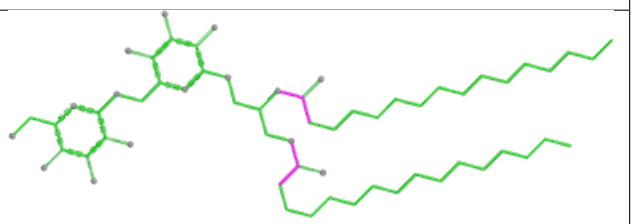


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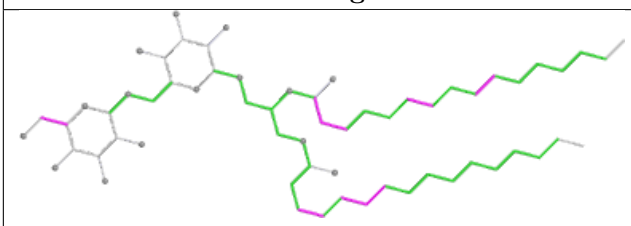
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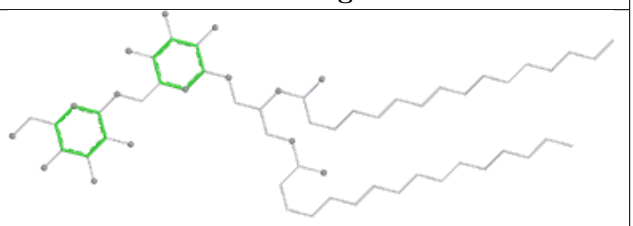
Bond lengths



Bond angles

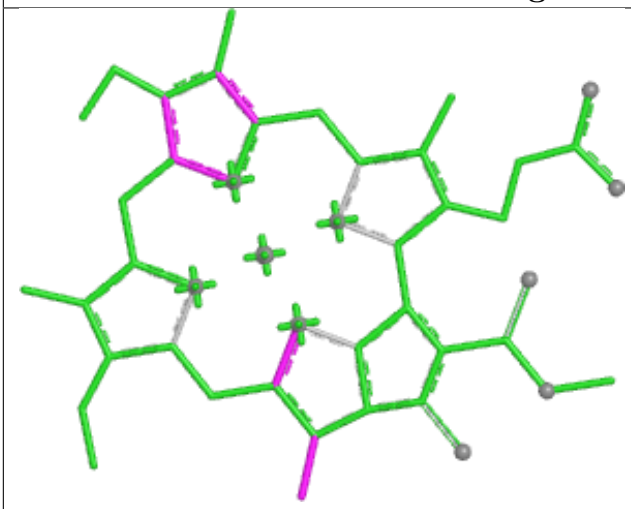


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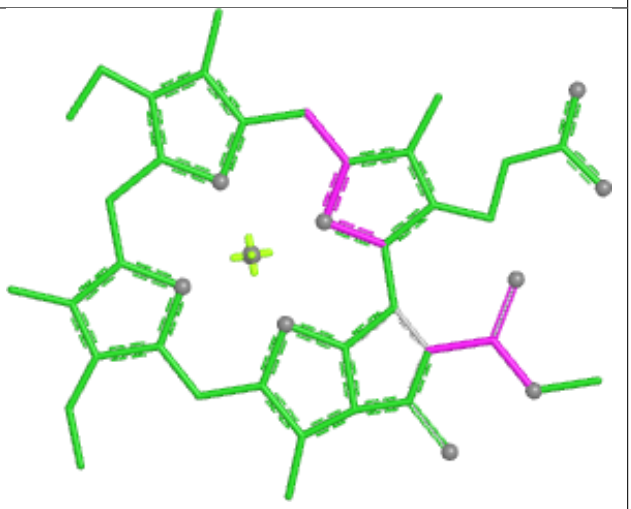


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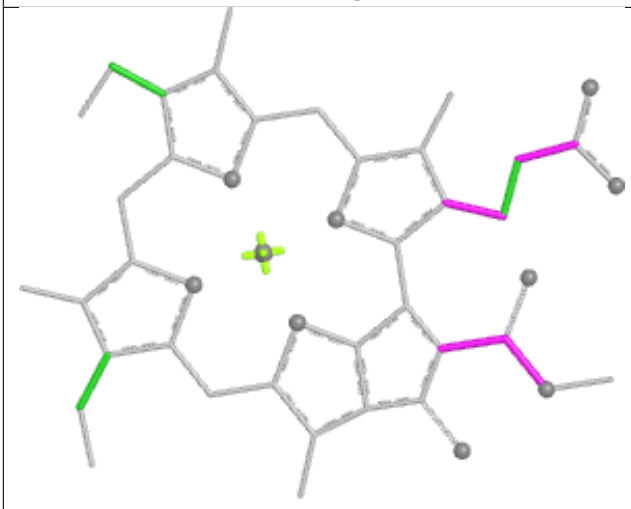
Ligand CLA 4 303



Bond lengths



Bond angles

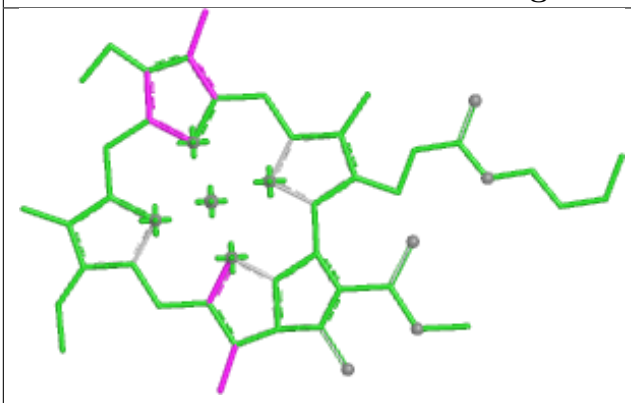


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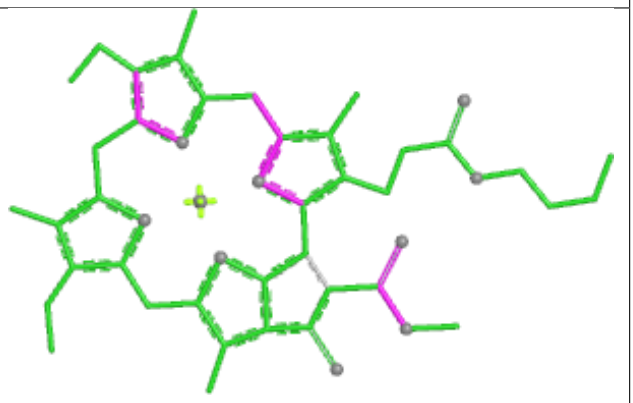


Rings

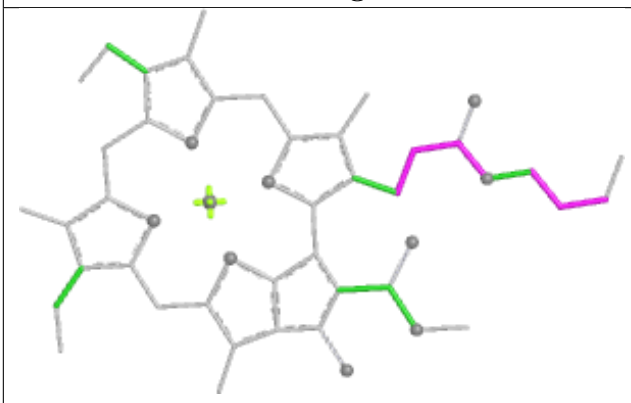
Ligand CLA s 612



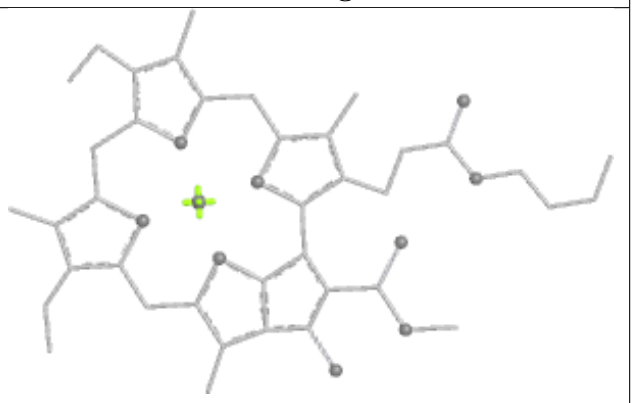
Bond lengths



Bond angles

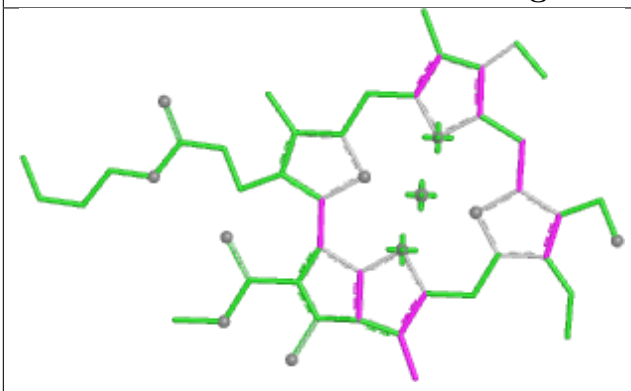


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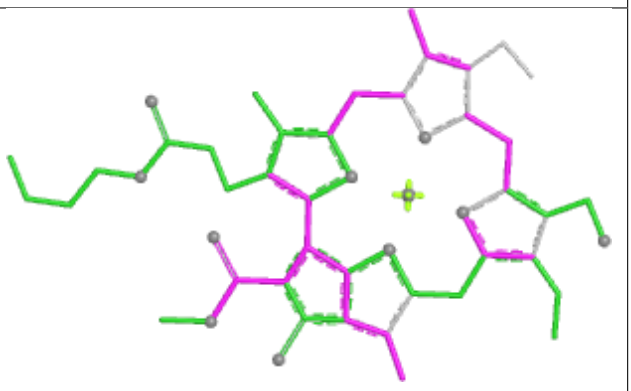


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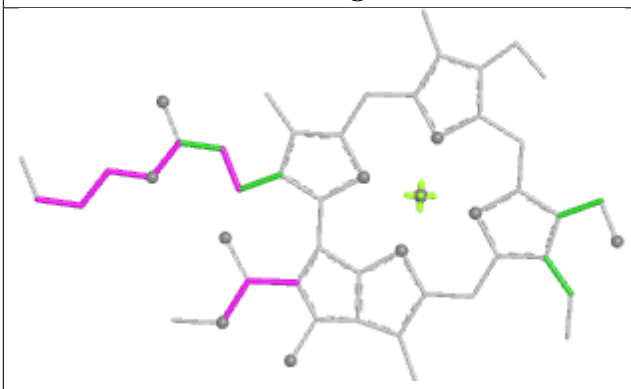
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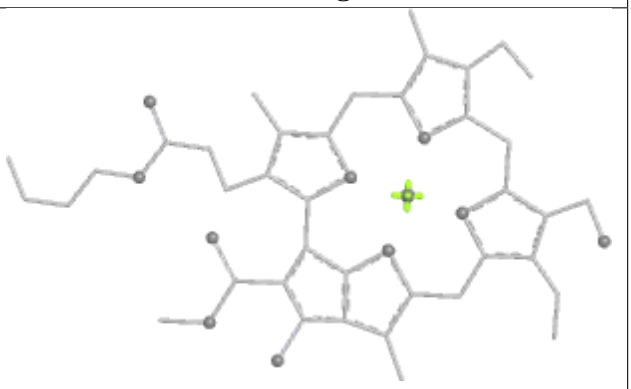
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Bond angles

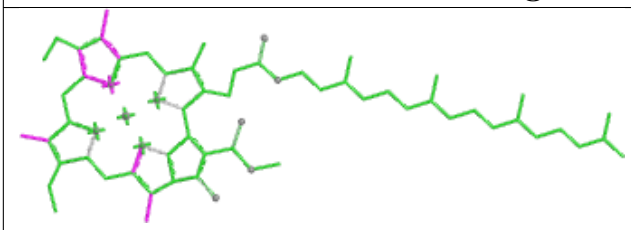


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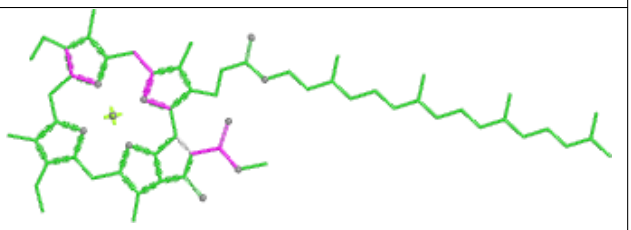


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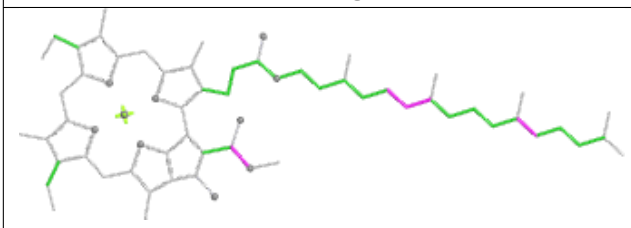
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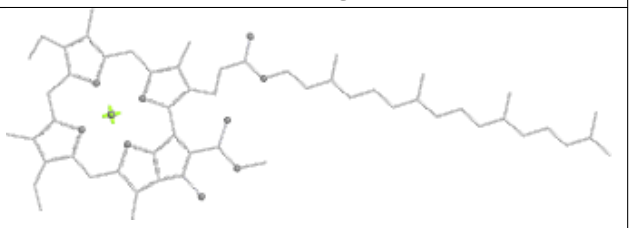
Bond lengths



Bond angles

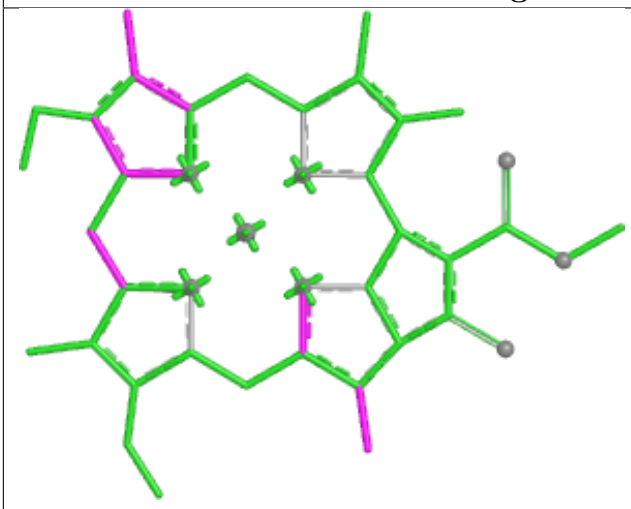


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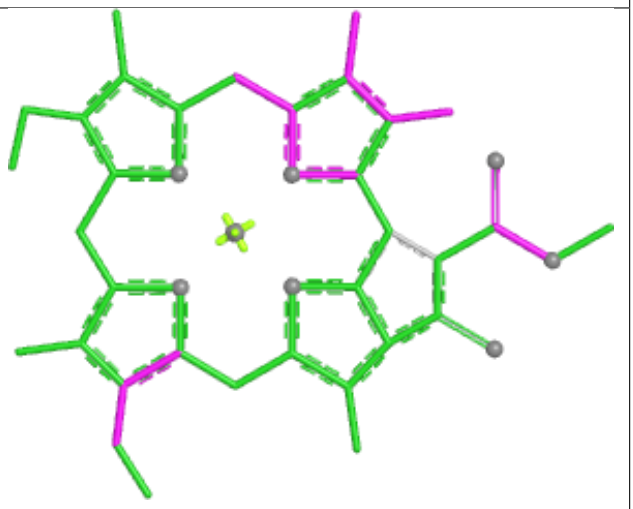


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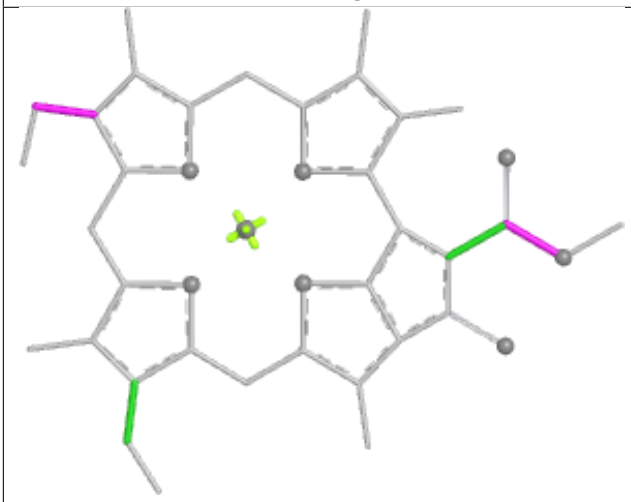
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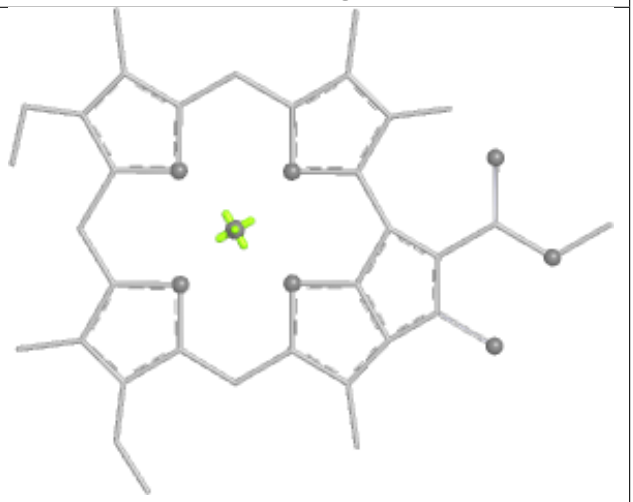
Bond lengths



Bond angles



Torsions

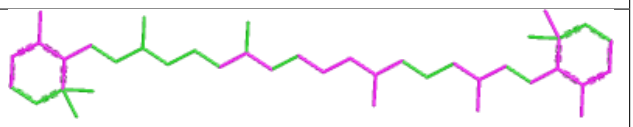


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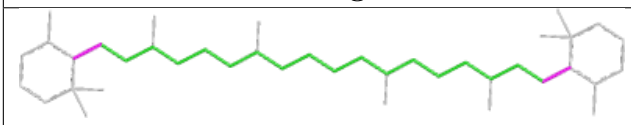
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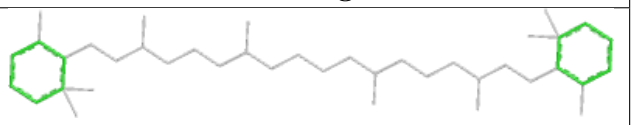
Bond lengths



Bond angles

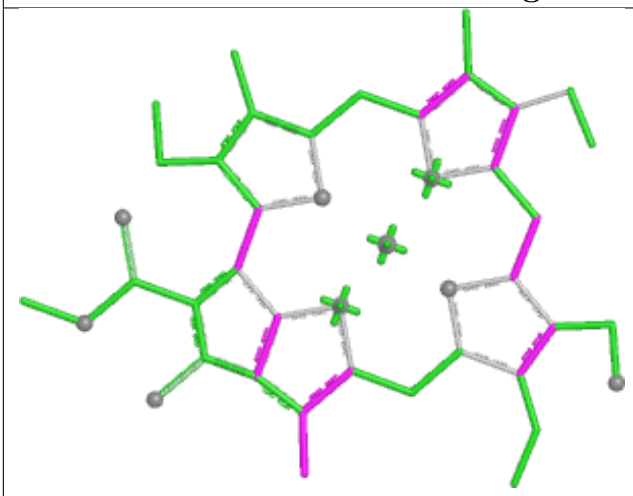


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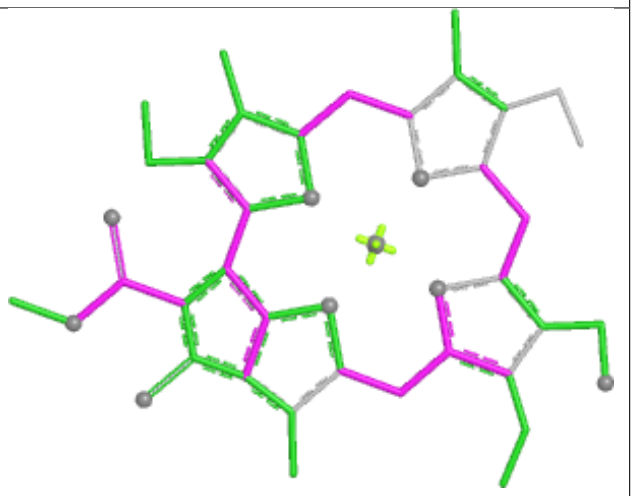


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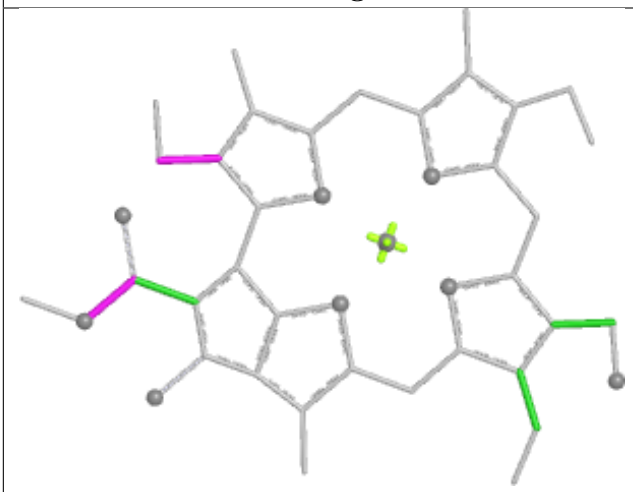
Ligand CHL G 606



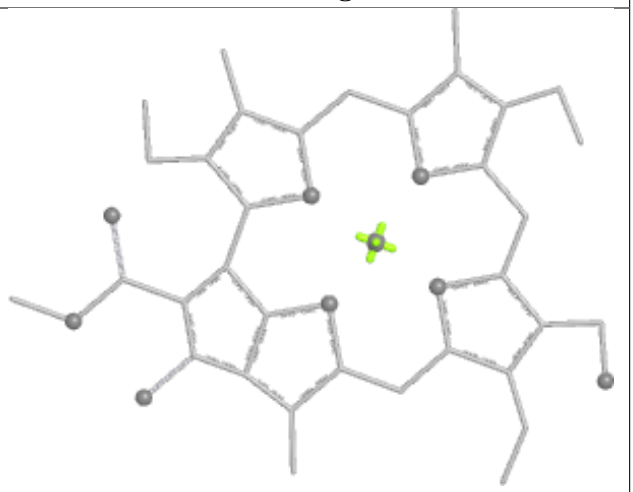
Bond lengths



Bond angles

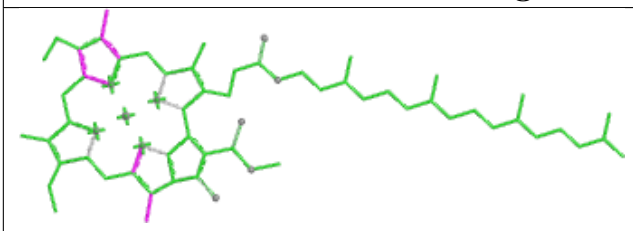


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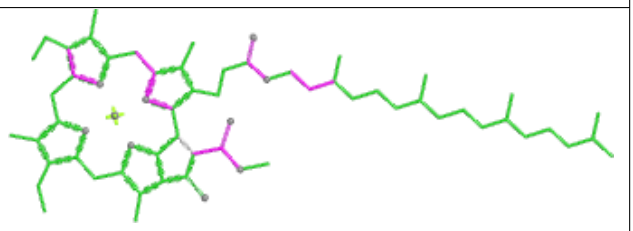


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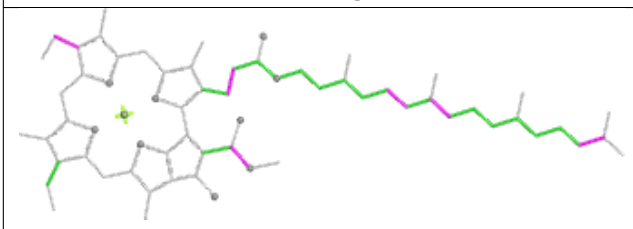
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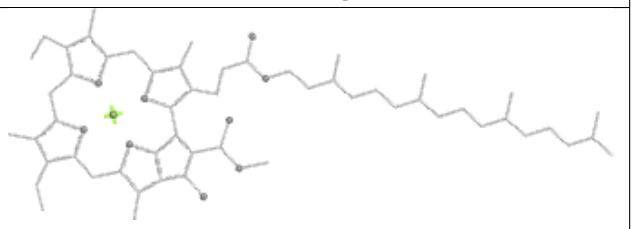
Bond lengths



Bond angles

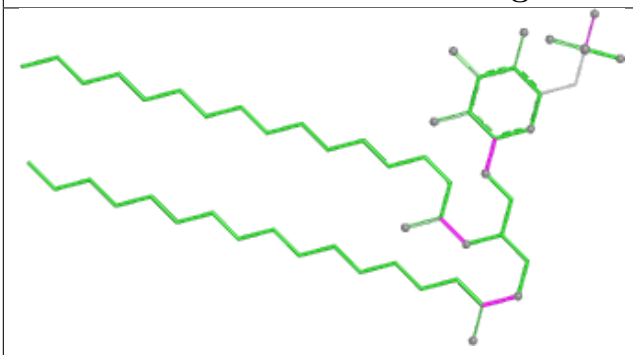


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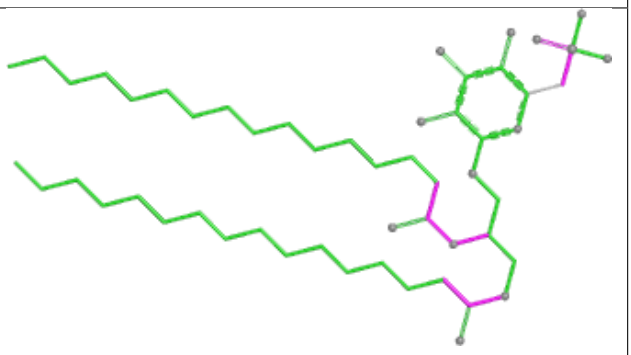


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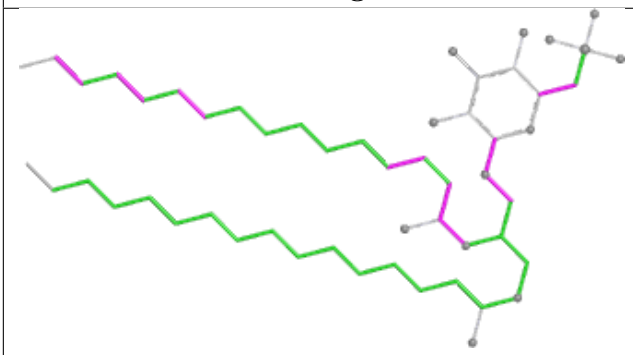
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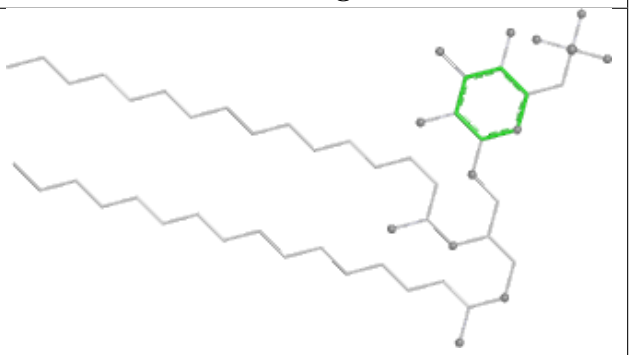
Bond lengths



Bond angles



Torsions

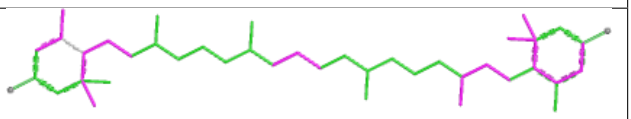


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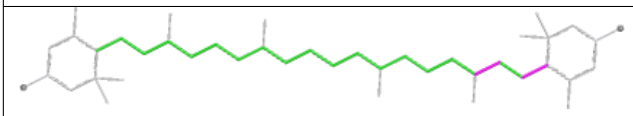
Ligand LUT N 616



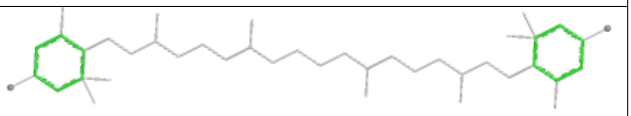
Bond lengths



Bond angles

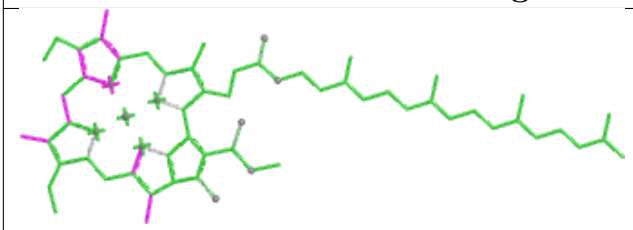


Torsions

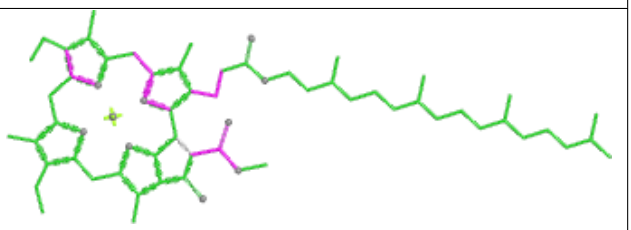


Rings

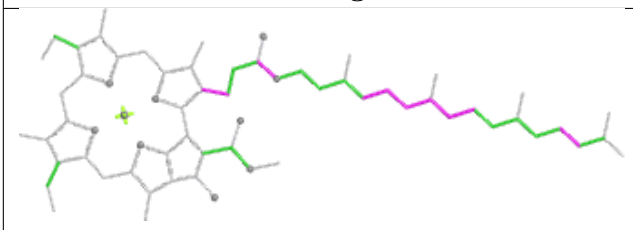
Ligand CLA CC 502



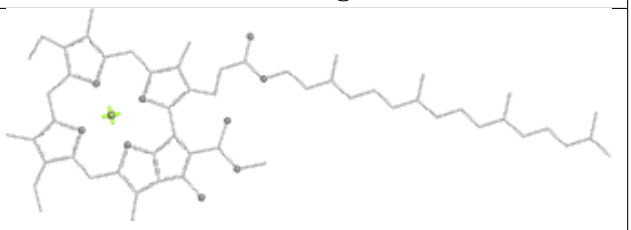
Bond lengths



Bond angles

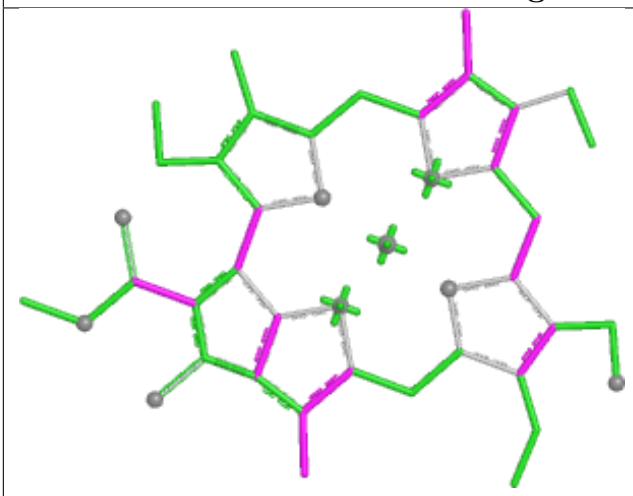


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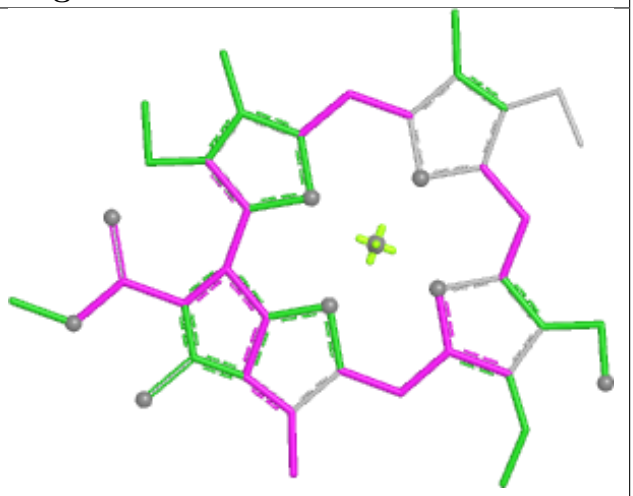


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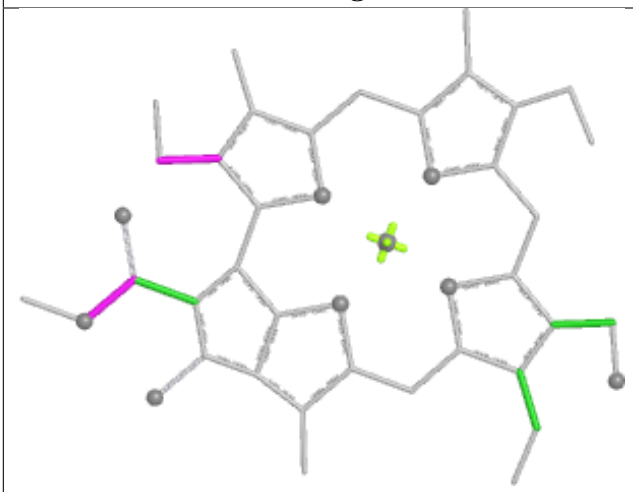
Ligand CHL g 606



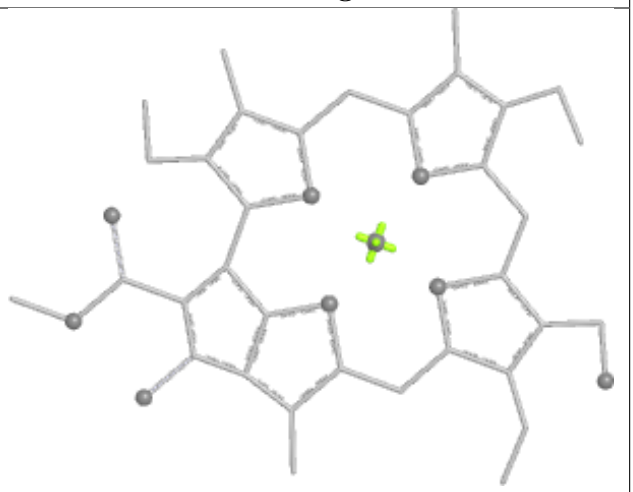
Bond lengths



Bond angles

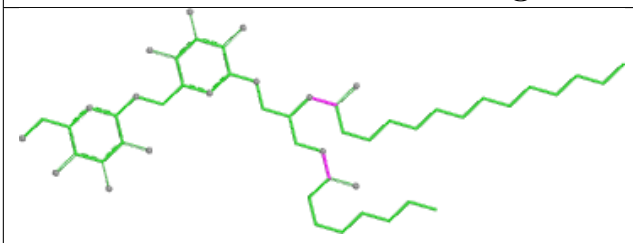


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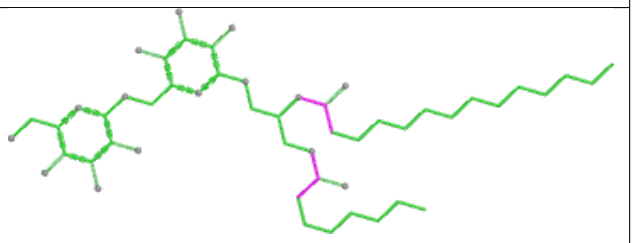


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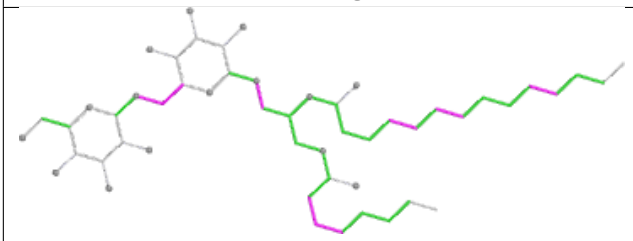
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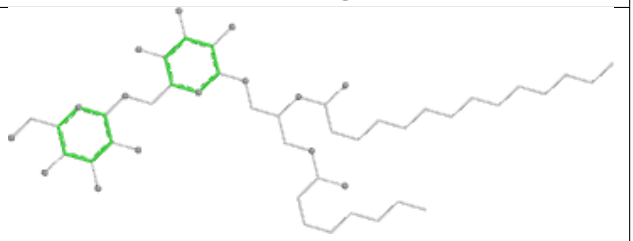
Bond lengths



Bond angles

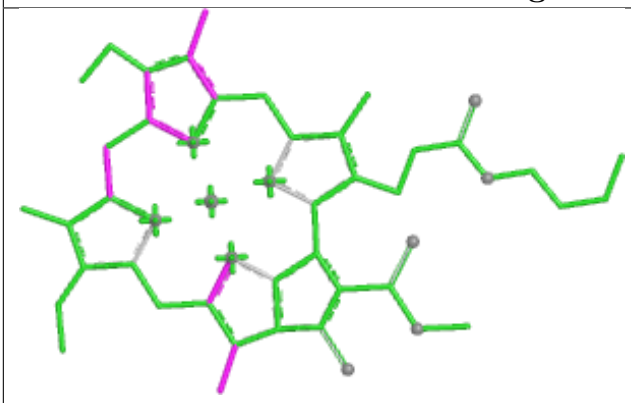


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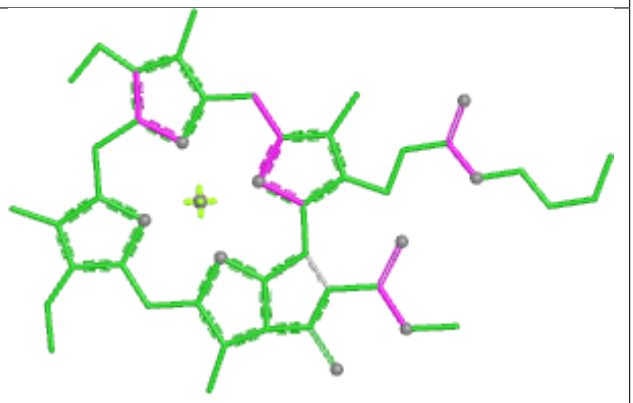


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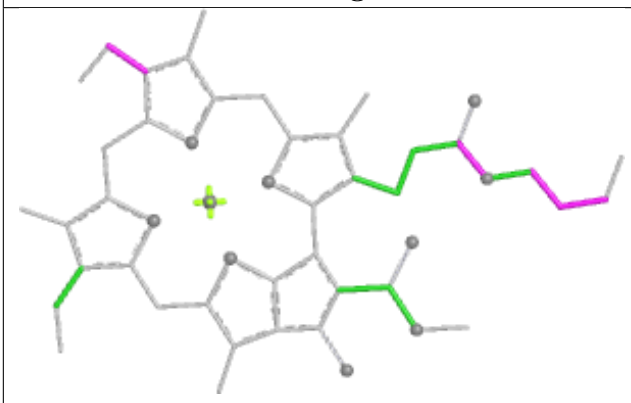
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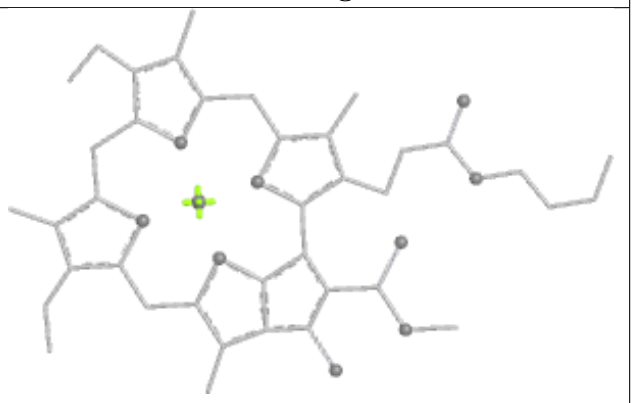
Bond lengths



Bond angles



Torsions

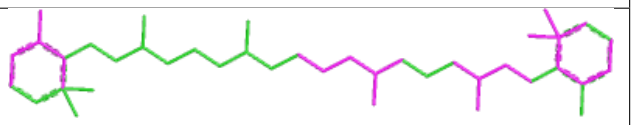


Rings

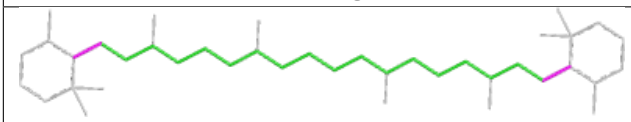
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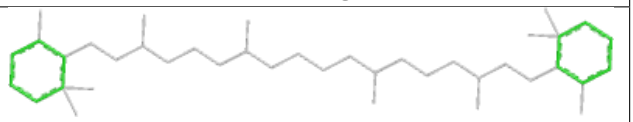
Bond lengths



Bond angles

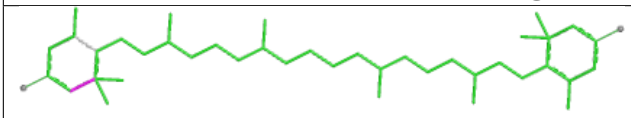


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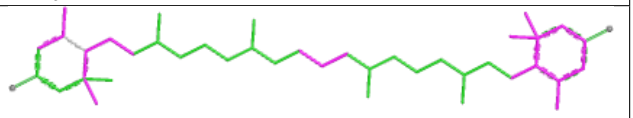


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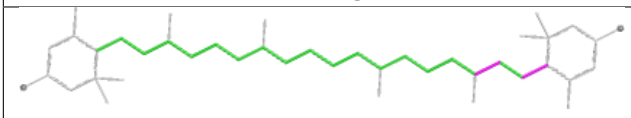
Ligand LUT y 317



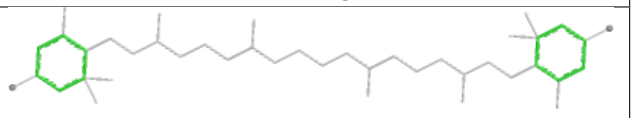
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Bond angles

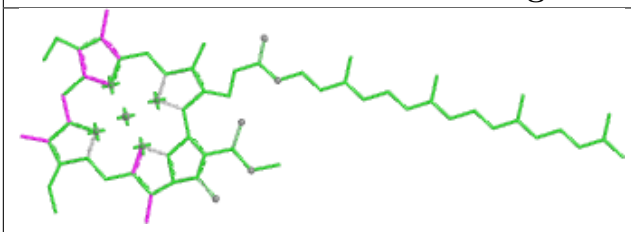


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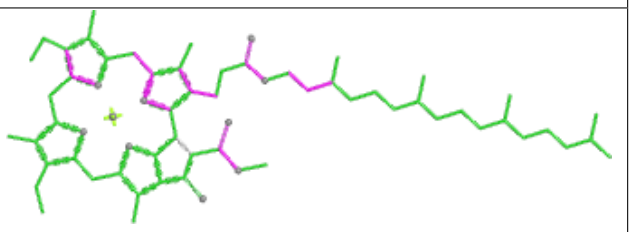


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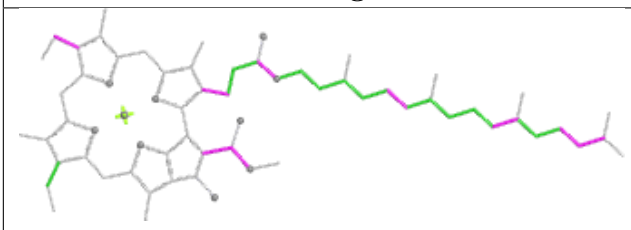
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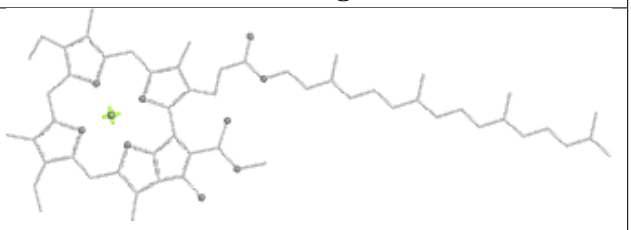
Bond lengths



Bond angles

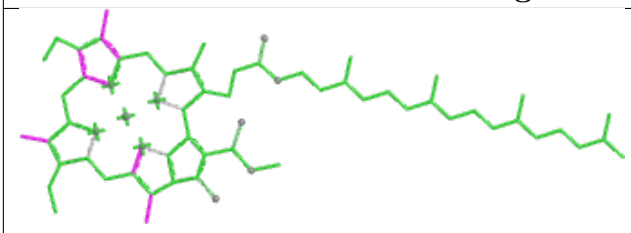


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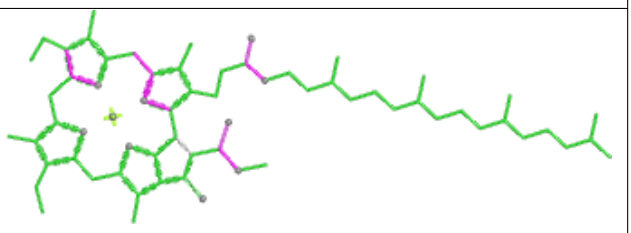


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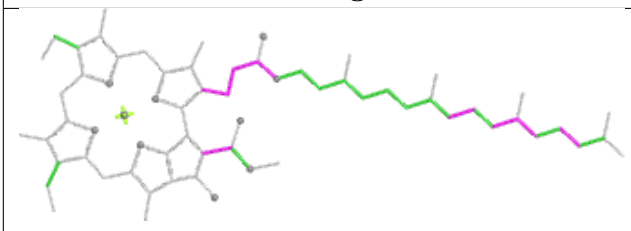
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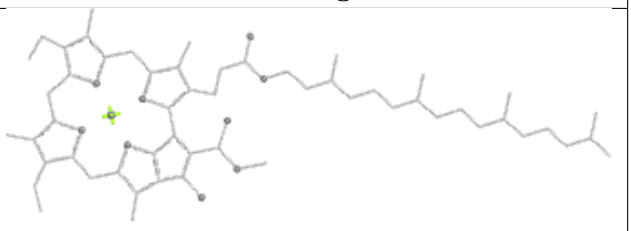
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Bond angles

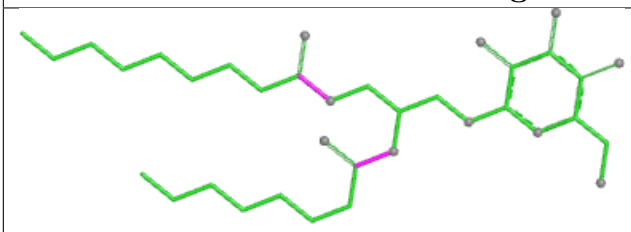


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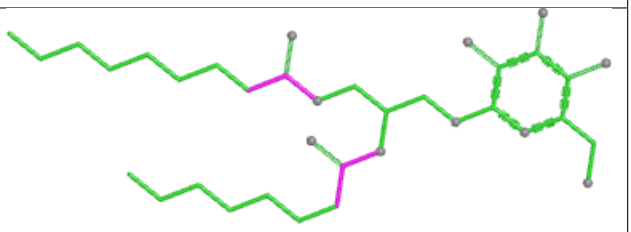


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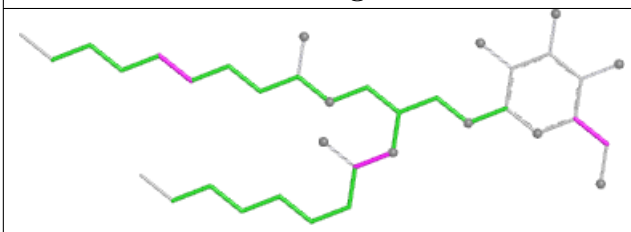
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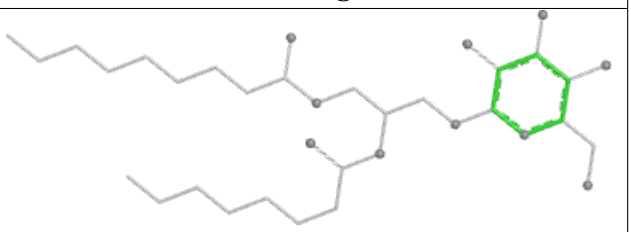
Bond lengths



Bond angles

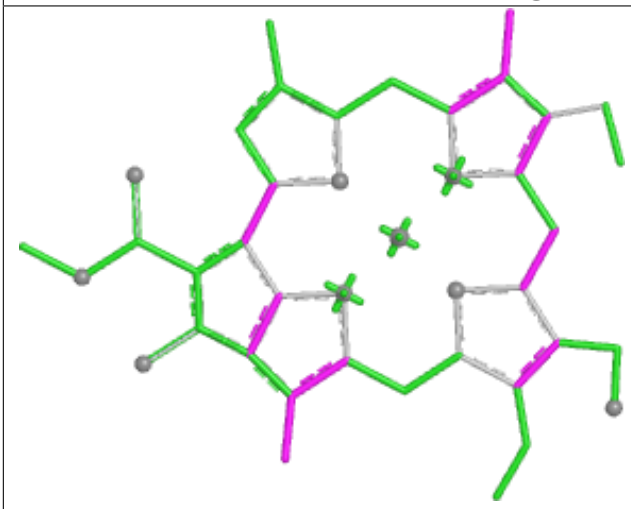


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Rings

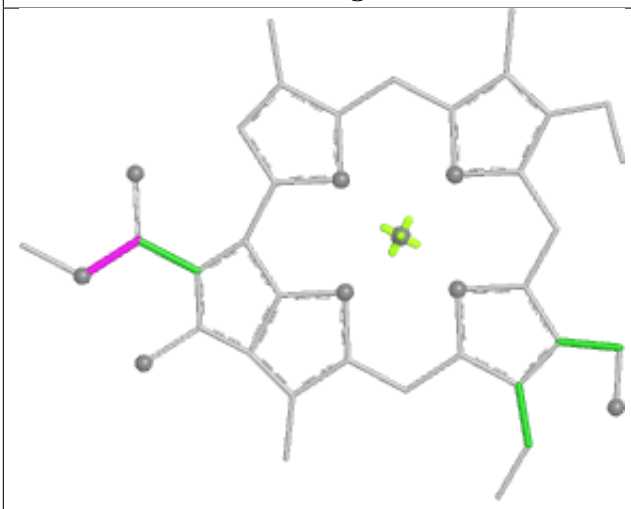
Ligand CHL 2 601



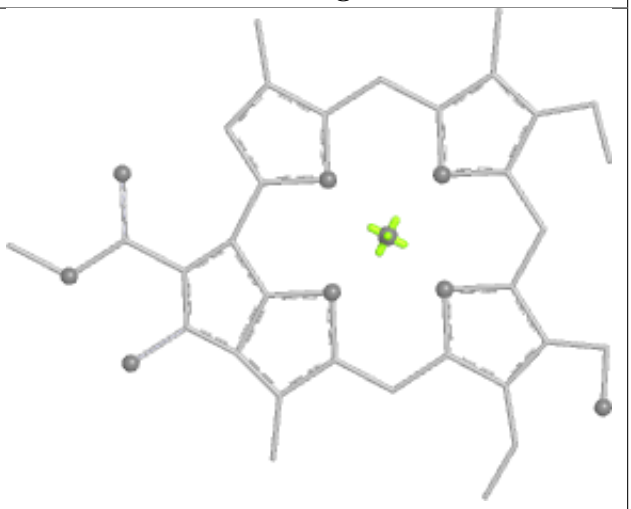
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Bond angles

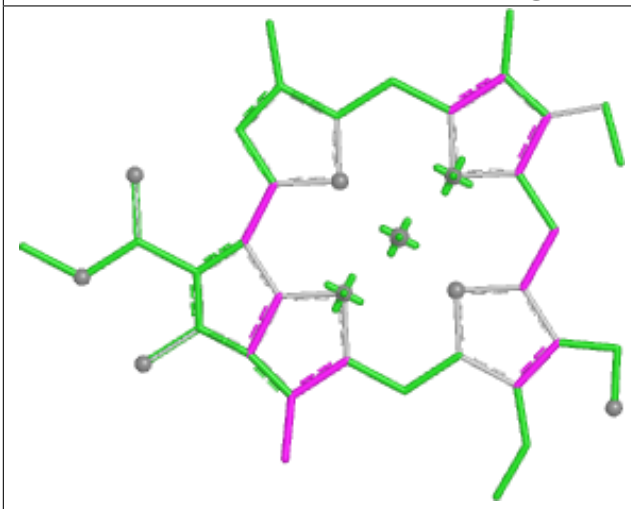


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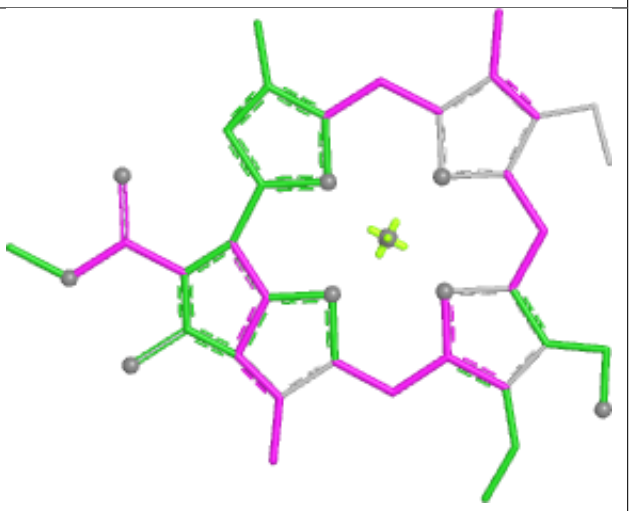


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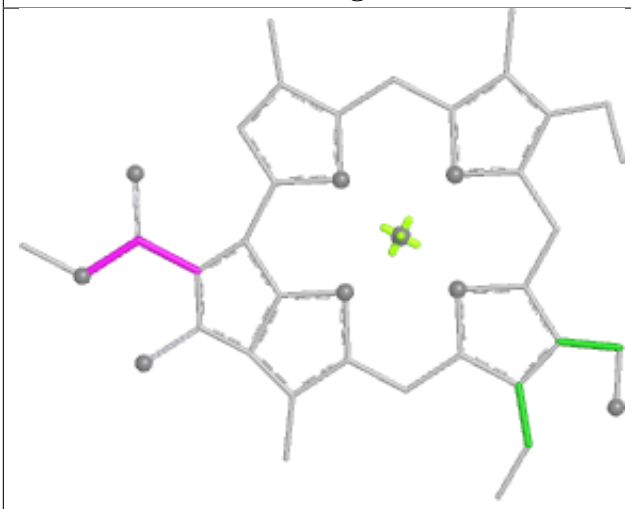
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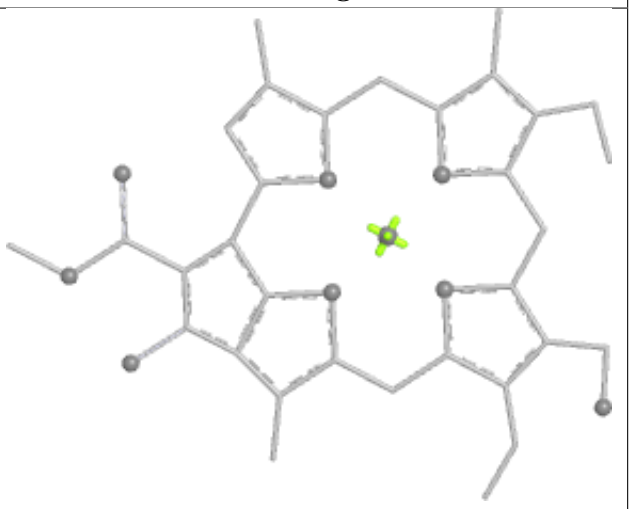
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Bond angles

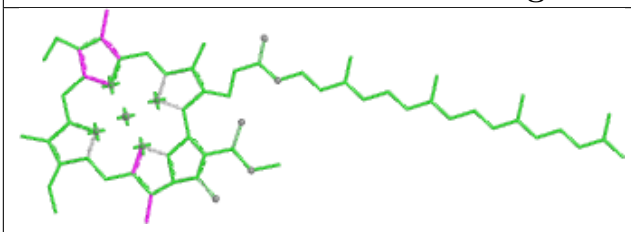


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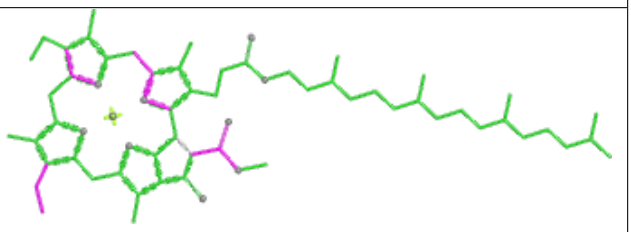


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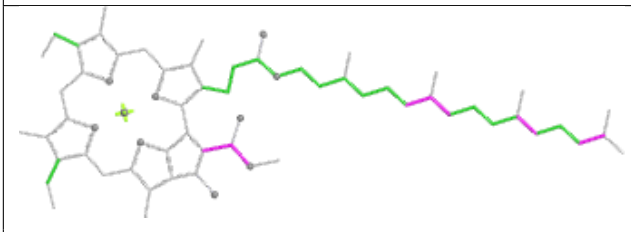
Ligand CLA b 602



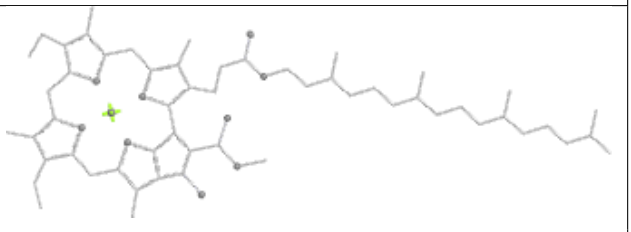
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Bond angles

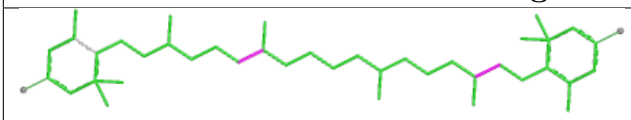


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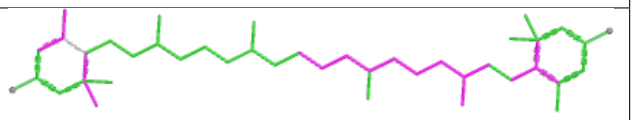


Rings

Ligand LUT s 614



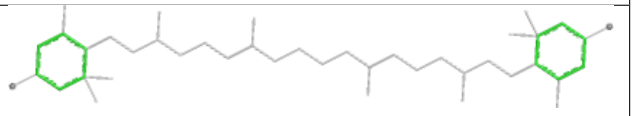
Bond lengths



Bond angles

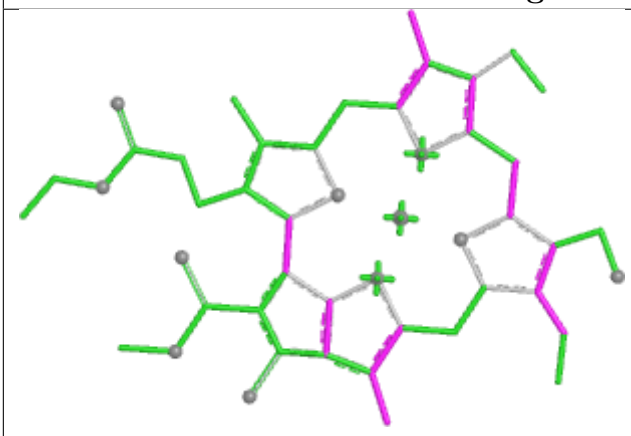


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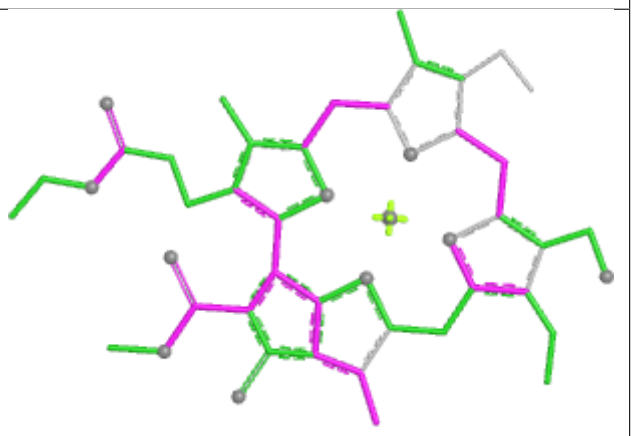


Rings

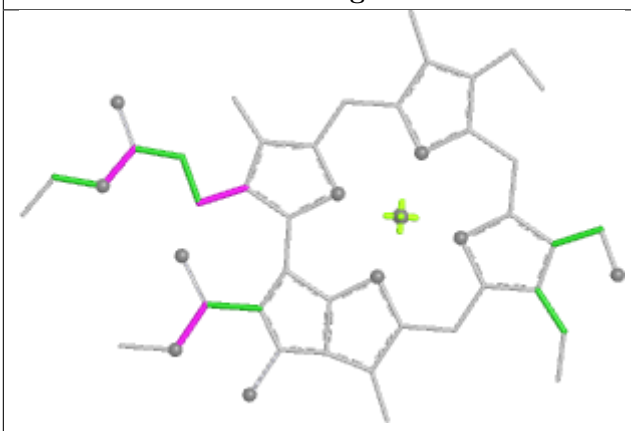
Ligand CHL n 605



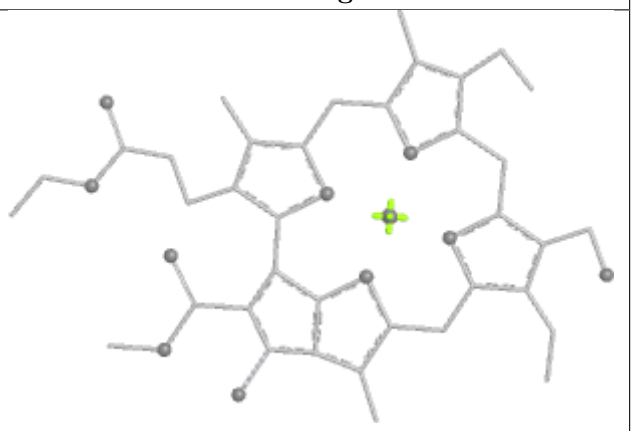
Bond lengths



Bond angles

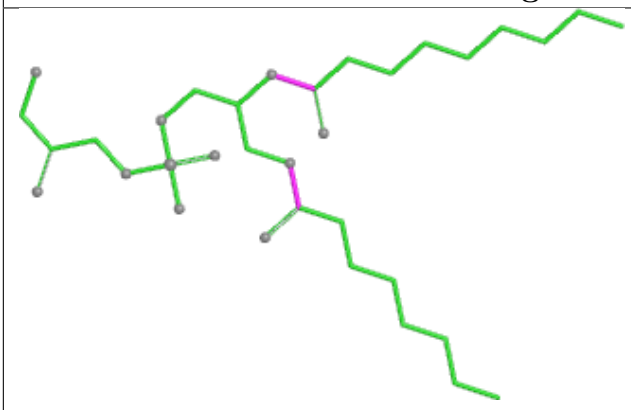


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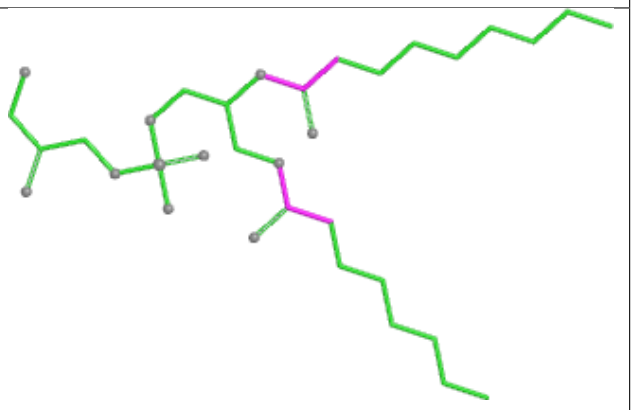


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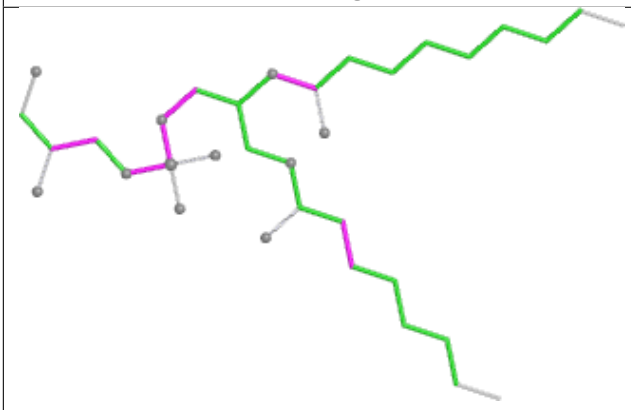
Ligand LHG K 101



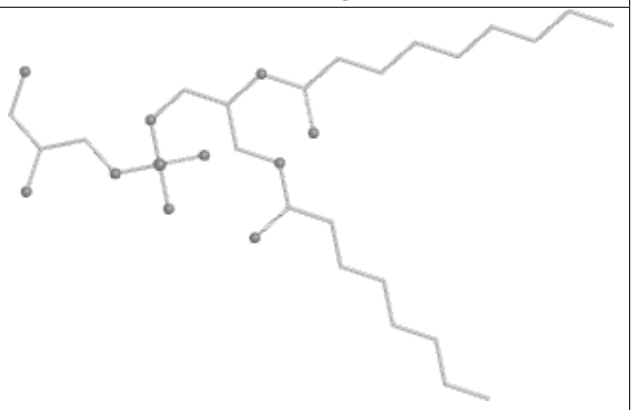
Bond lengths



Bond angles

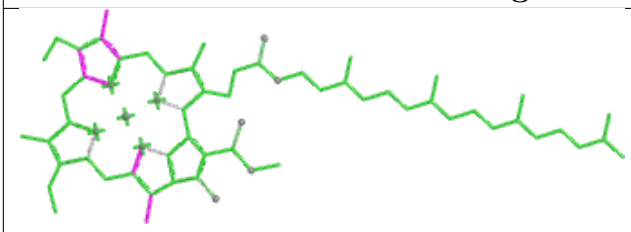


Torsions

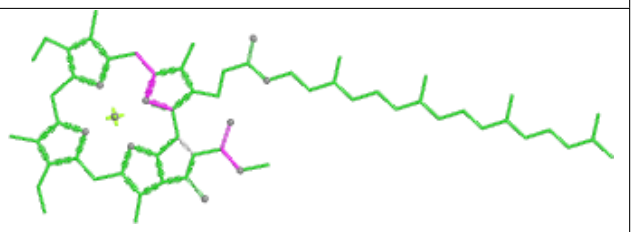


Rings

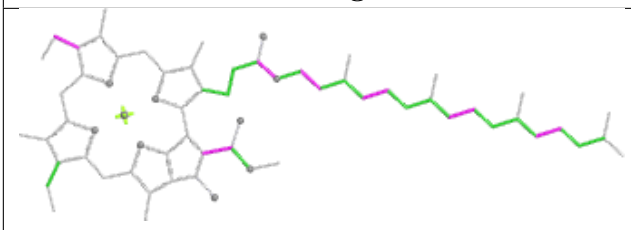
Ligand CLA CC 513



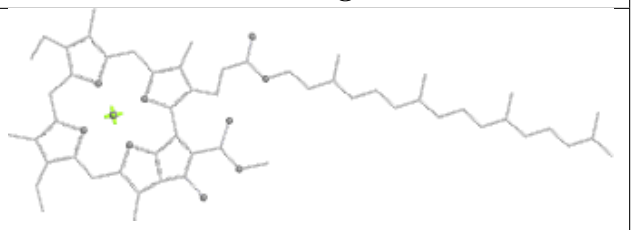
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Bond angles

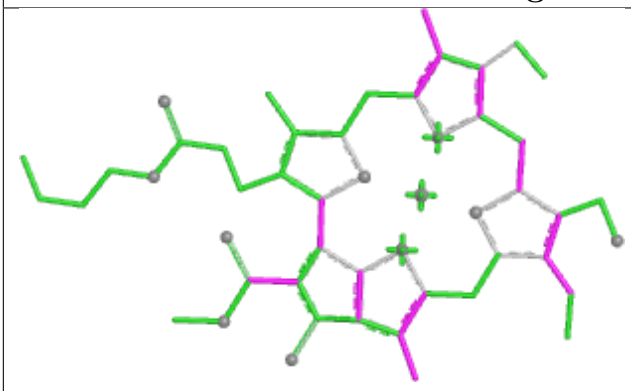


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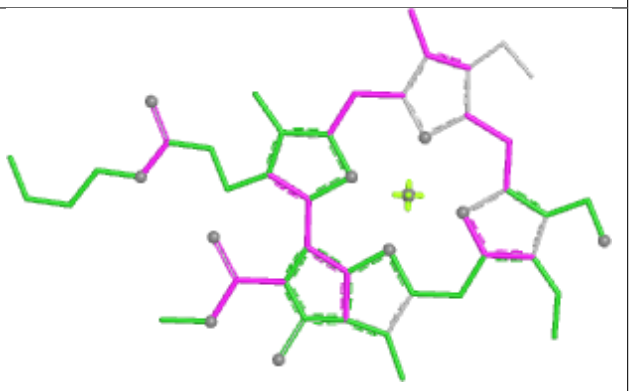


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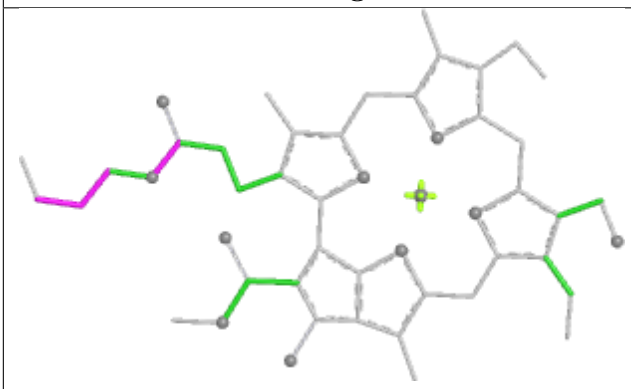
Ligand CHL n 609



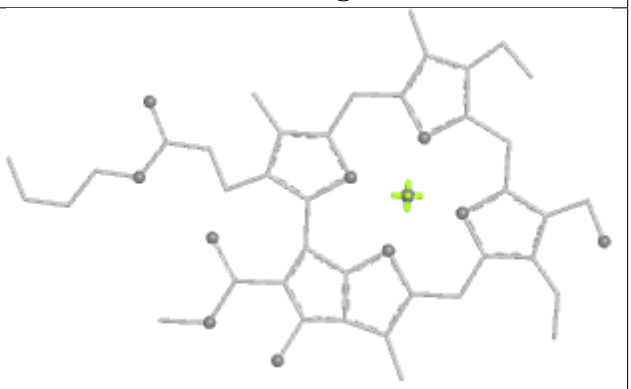
Bond lengths



Bond angles

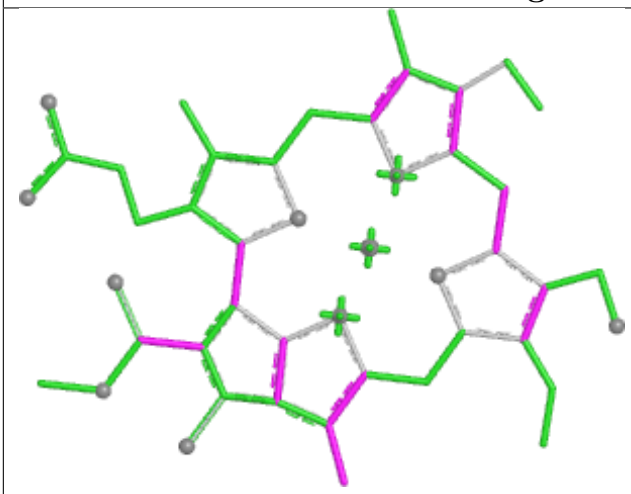


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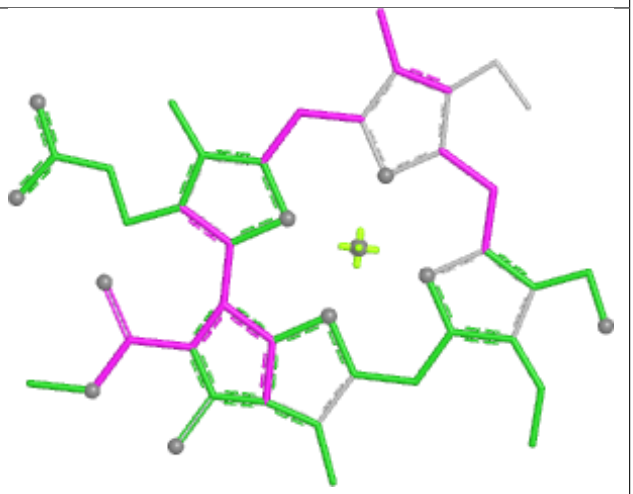


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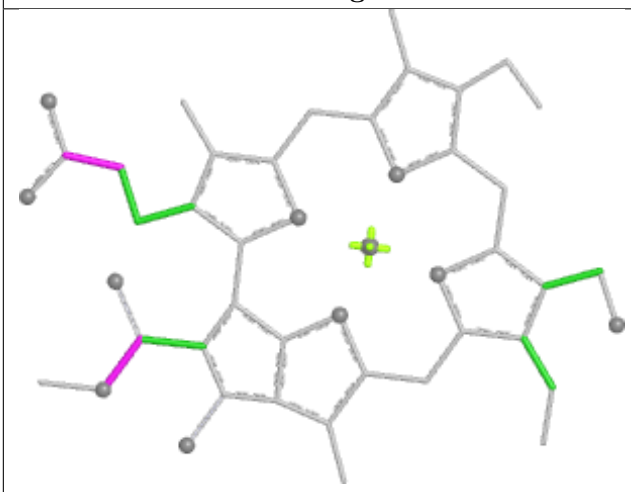
Ligand CHL 4 306



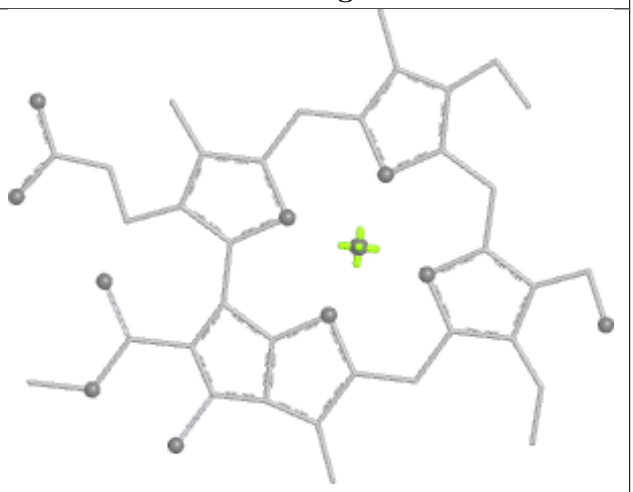
Bond lengths



Bond angles

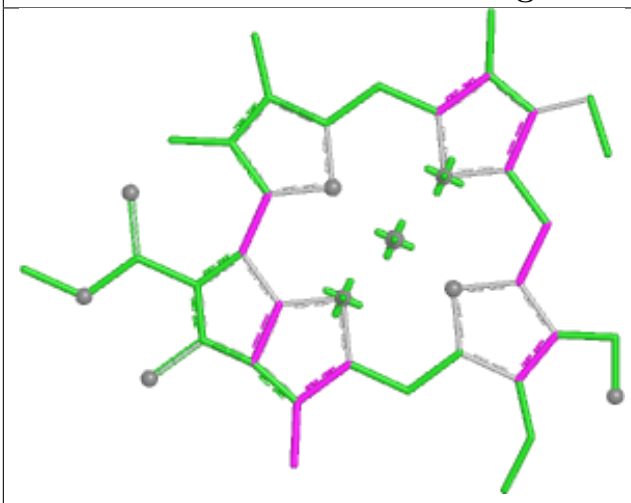


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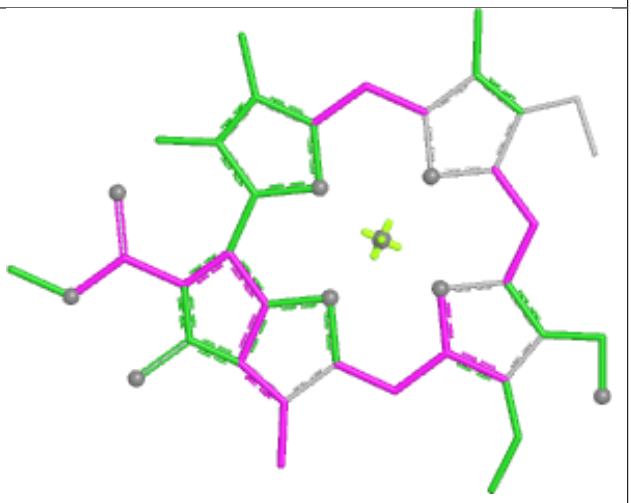


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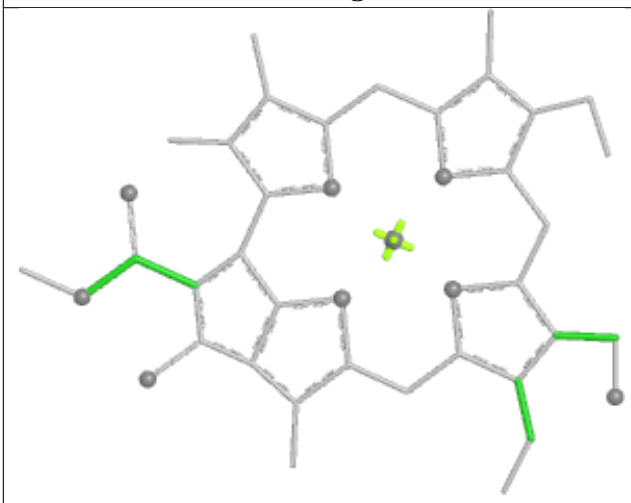
Ligand CHL SS 307



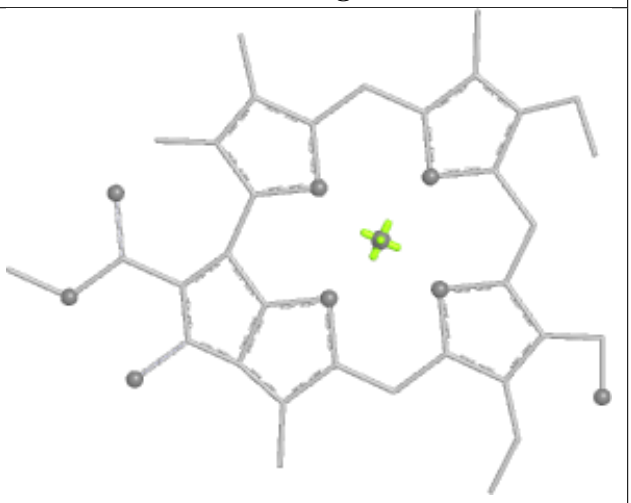
Bond lengths



Bond angles

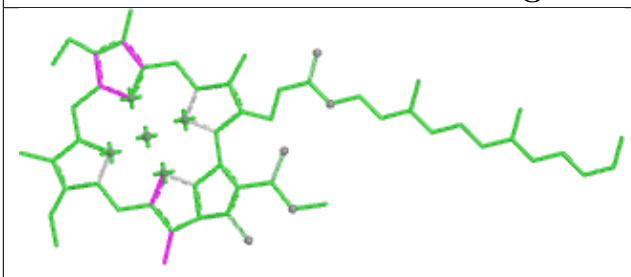


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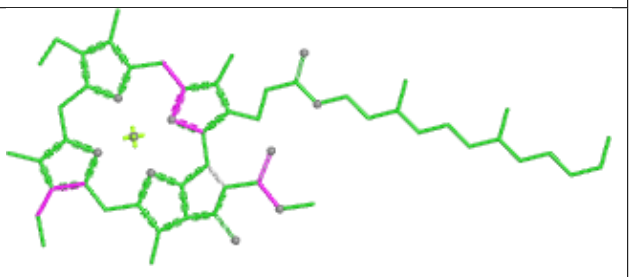


Rings

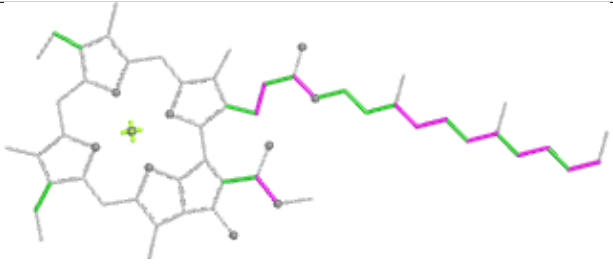
Ligand CLA Y 613



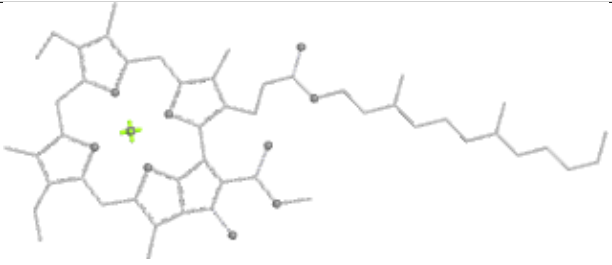
Bond lengths



Bond angles

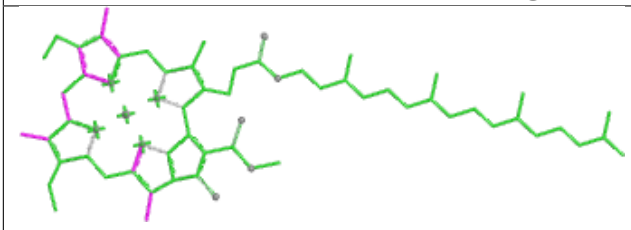


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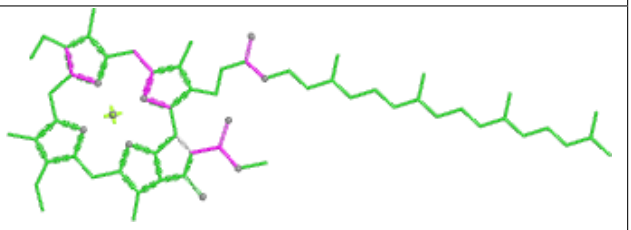


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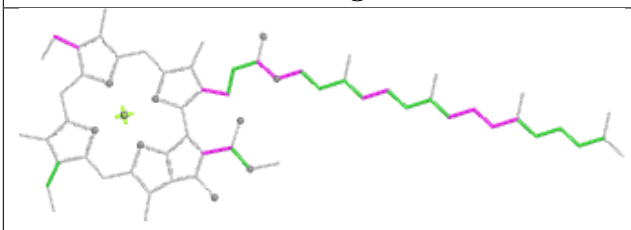
Ligand CLA C 511



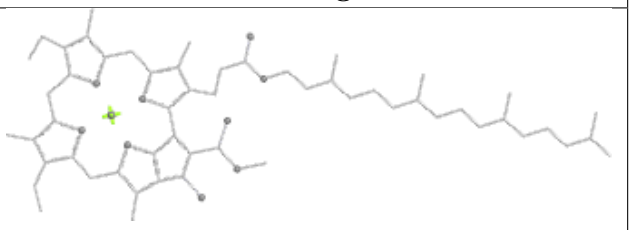
Bond lengths



Bond angles

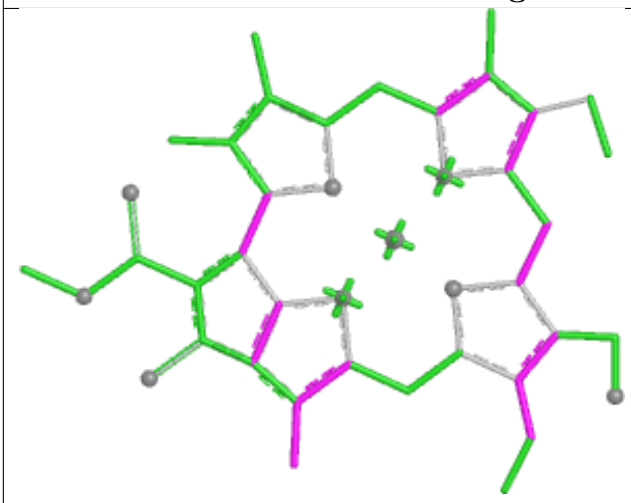


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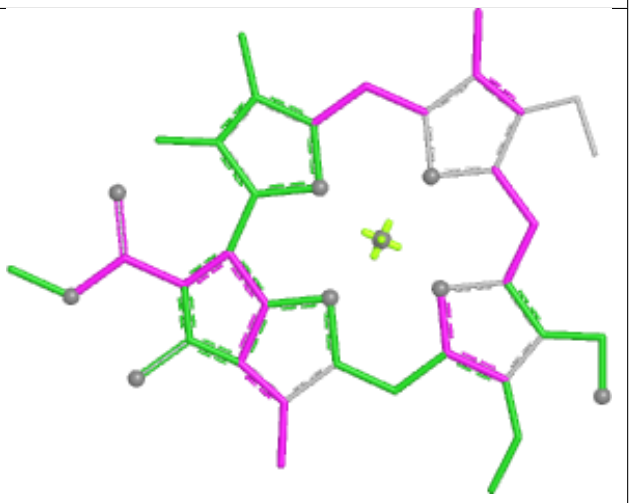


Rings

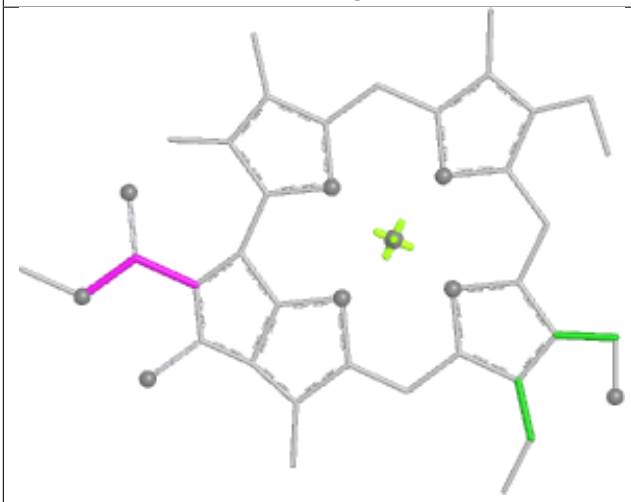
Ligand CHL NN 605



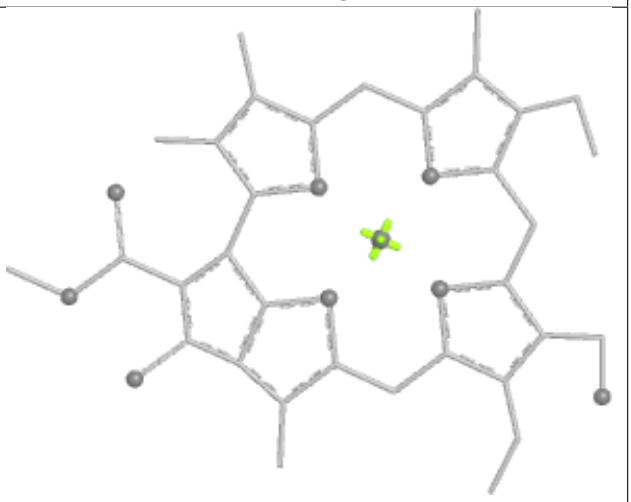
Bond lengths



Bond angles

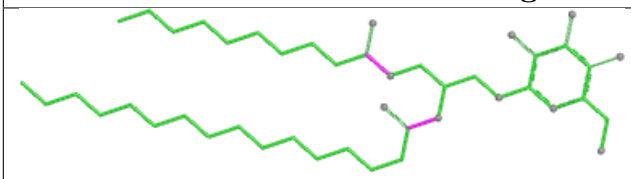


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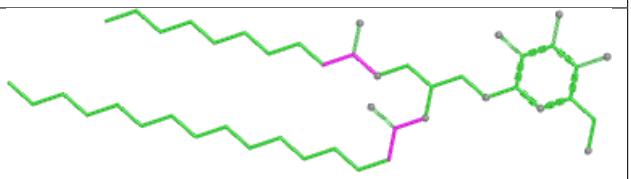


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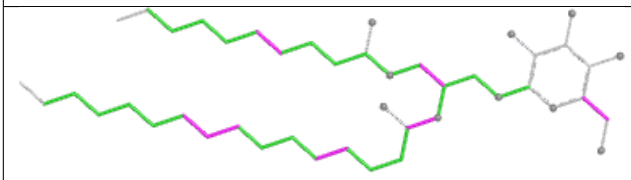
Ligand LMG B 615



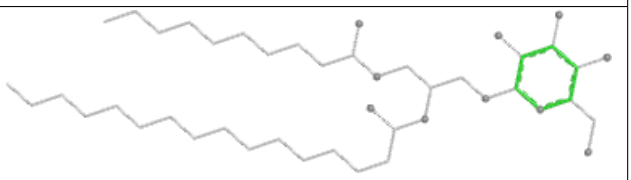
Bond lengths



Bond angles

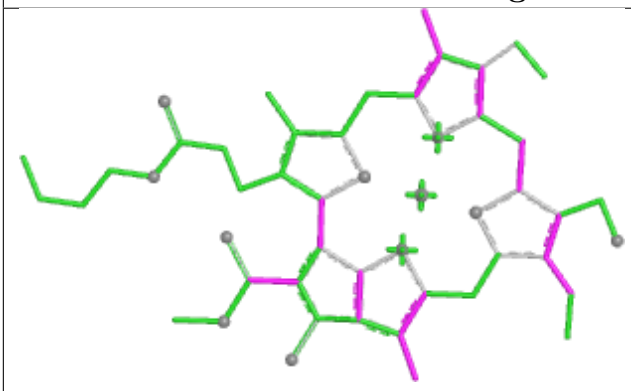


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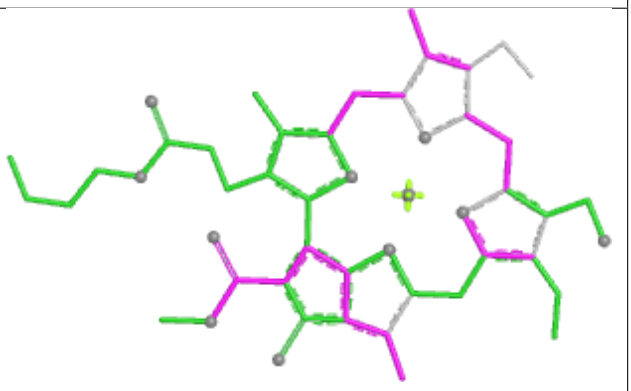


Rings

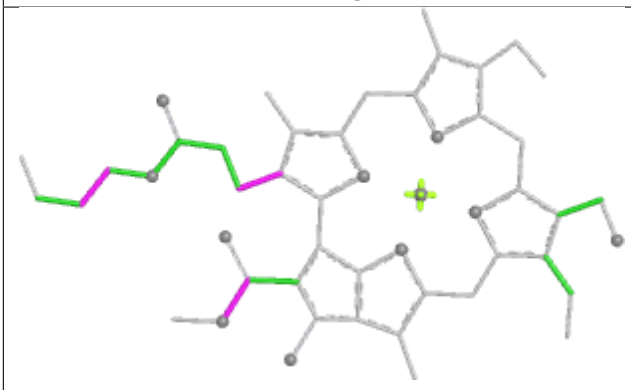
Ligand CHL NN 609



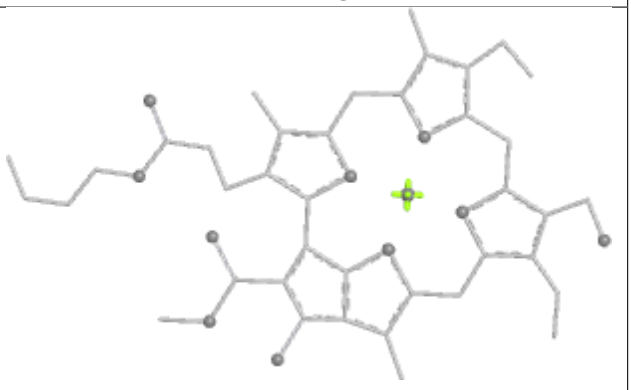
Bond lengths



Bond angles

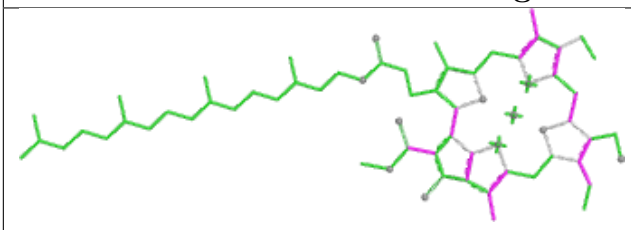


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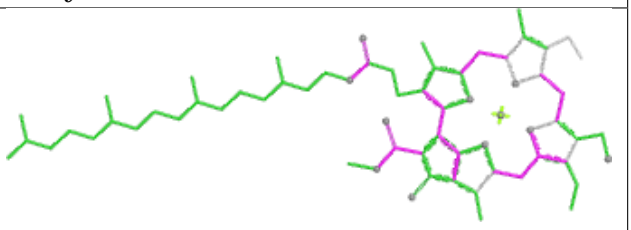


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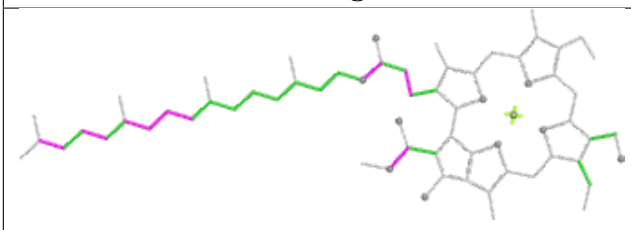
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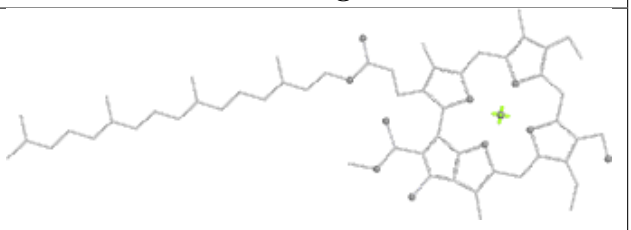
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Bond angles

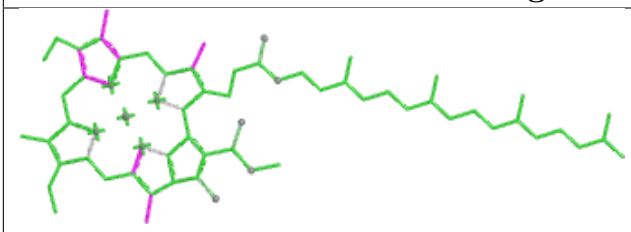


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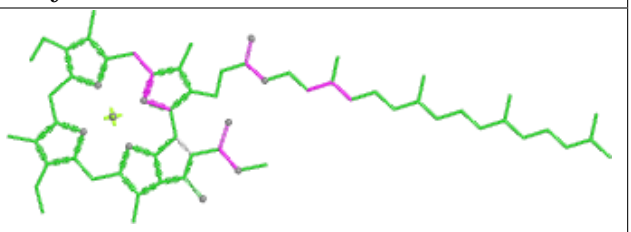


Rings

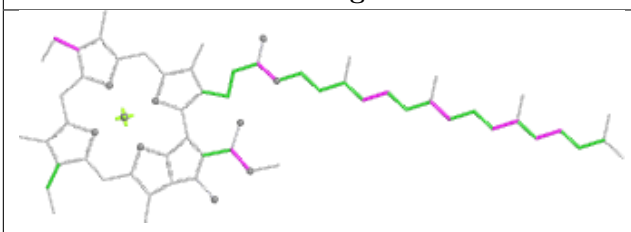
Ligand CLA y 314



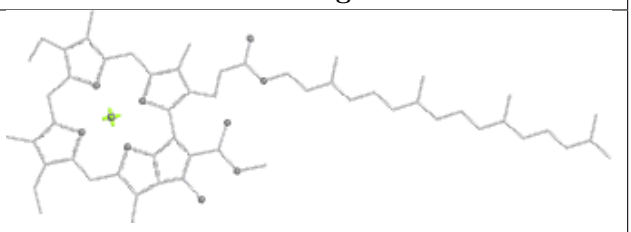
Bond lengths



Bond angles

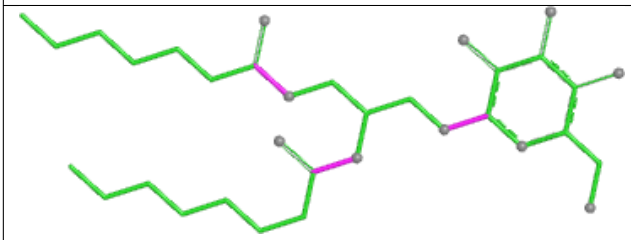


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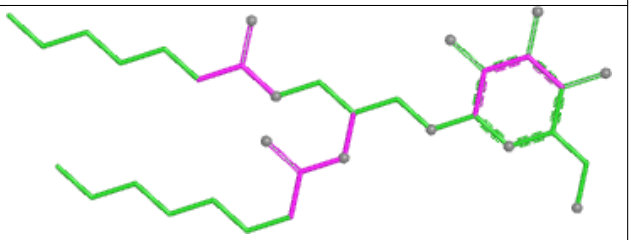


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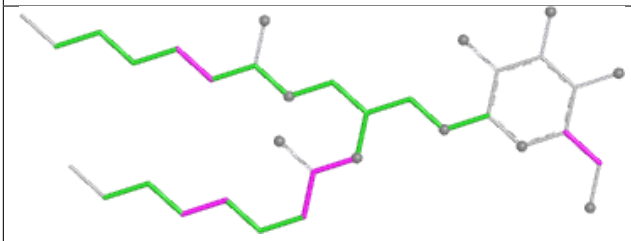
Ligand LMG Cc 501



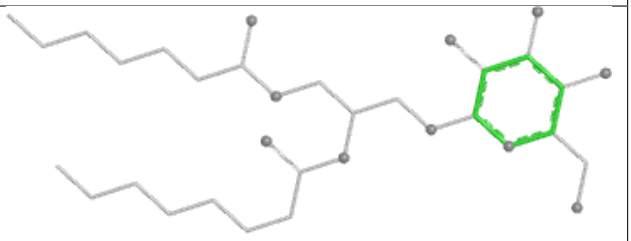
Bond lengths



Bond angles

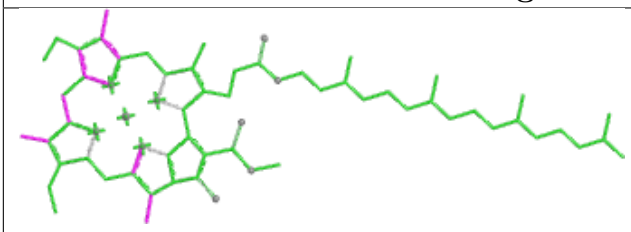


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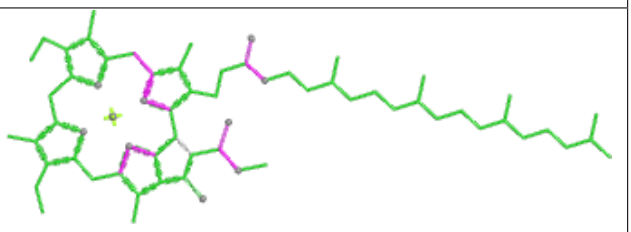


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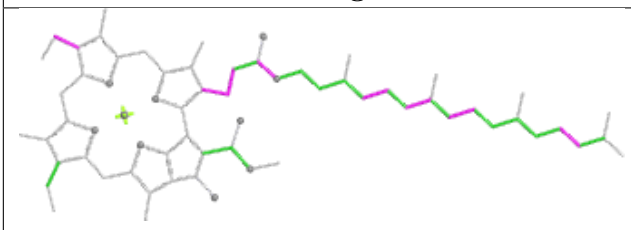
Ligand CLA Rr 602



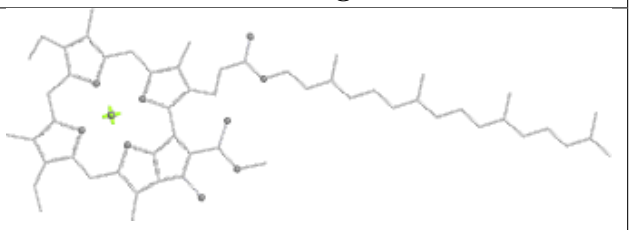
Bond lengths



Bond angles

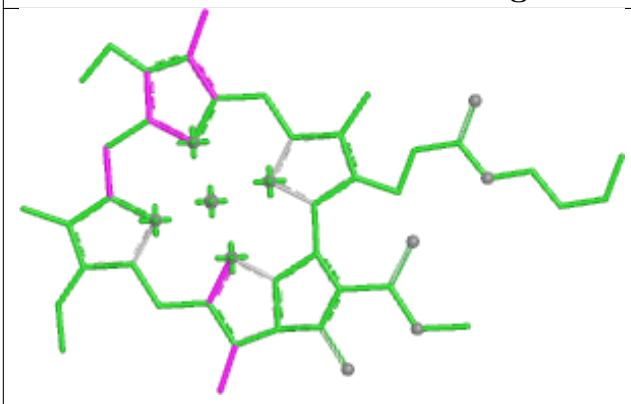


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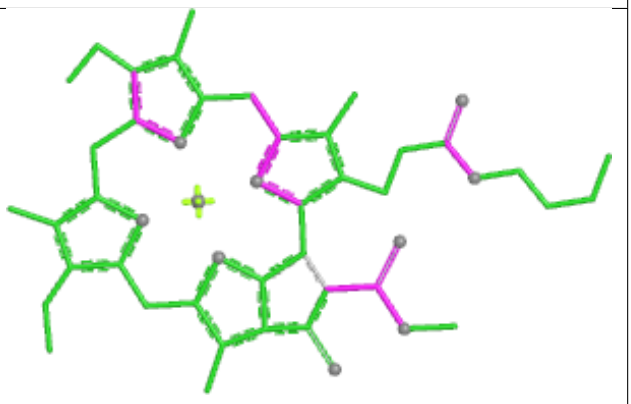


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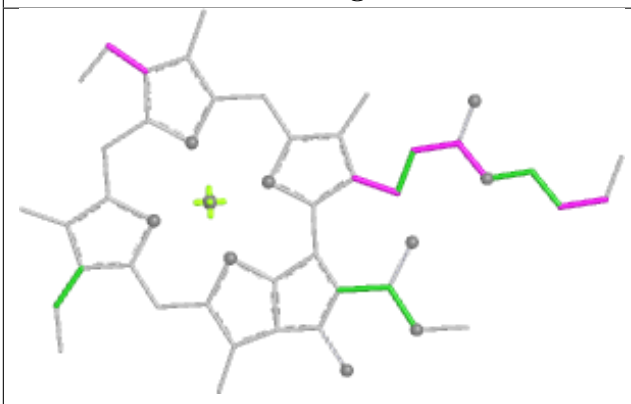
Ligand CLA AA 406



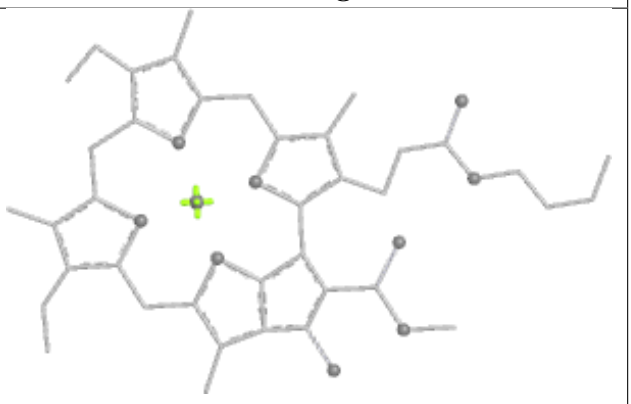
Bond lengths



Bond angles

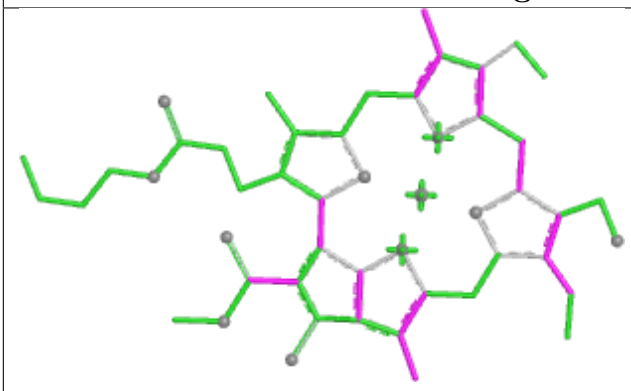


Torsions

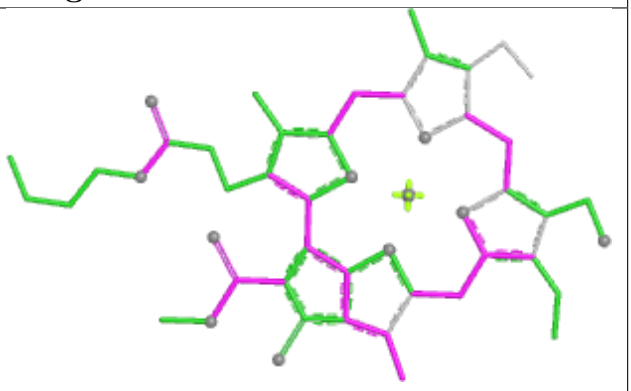


Rings

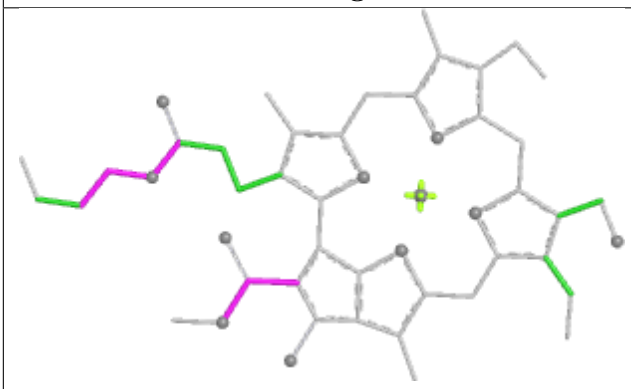
Ligand CHL Gg 308



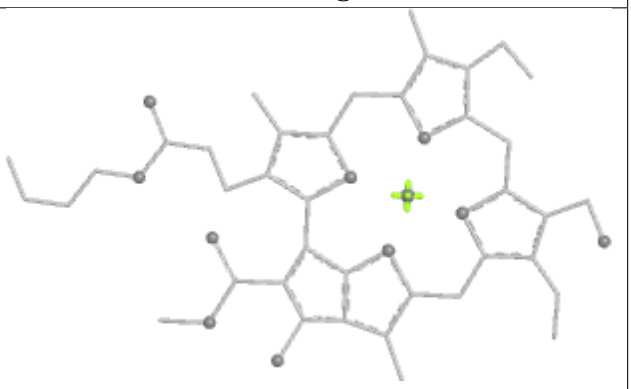
Bond lengths



Bond angles

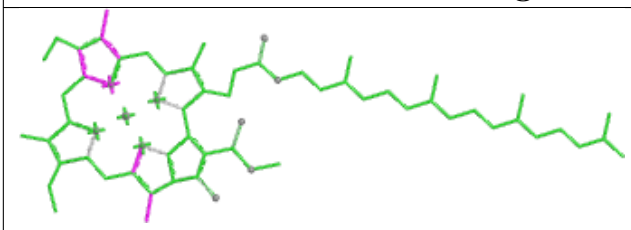


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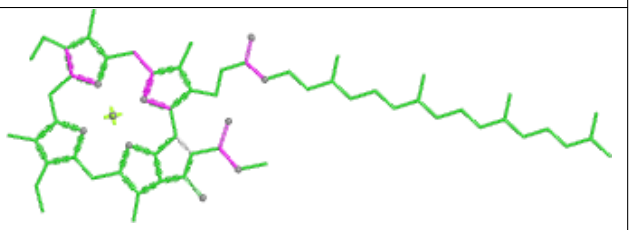


Rings

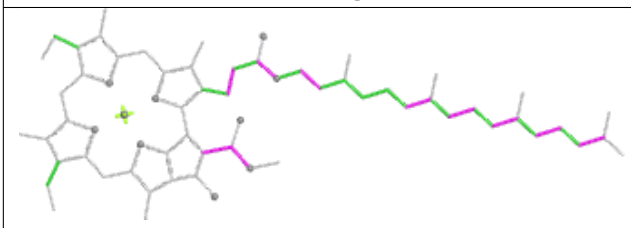
Ligand CLA Bb 612



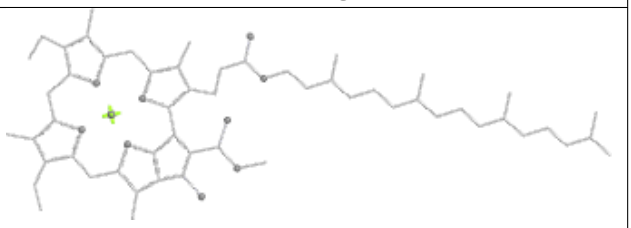
Bond lengths



Bond angles

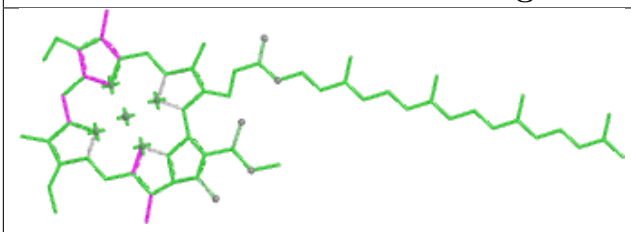


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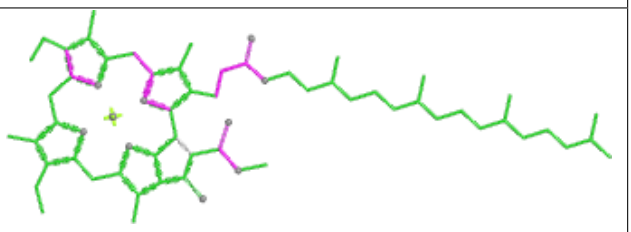


Rings

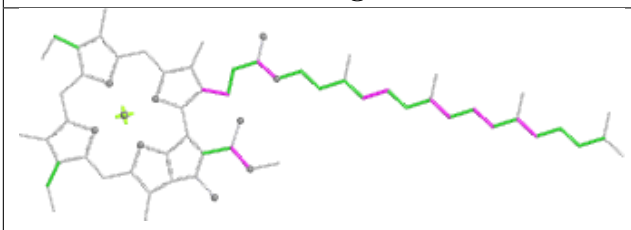
Ligand CLA Cc 505



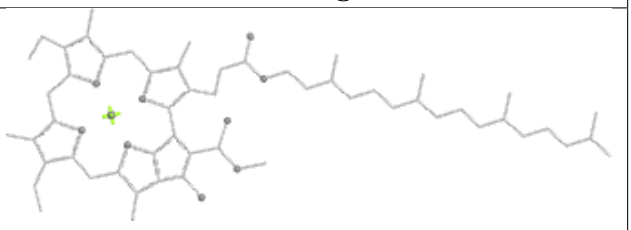
Bond lengths



Bond angles

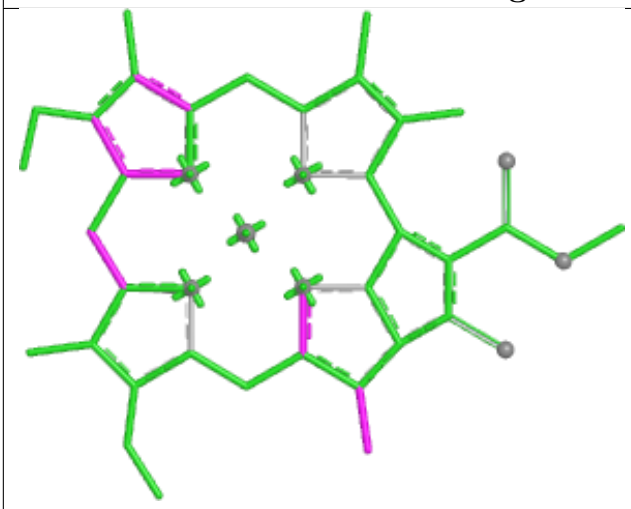


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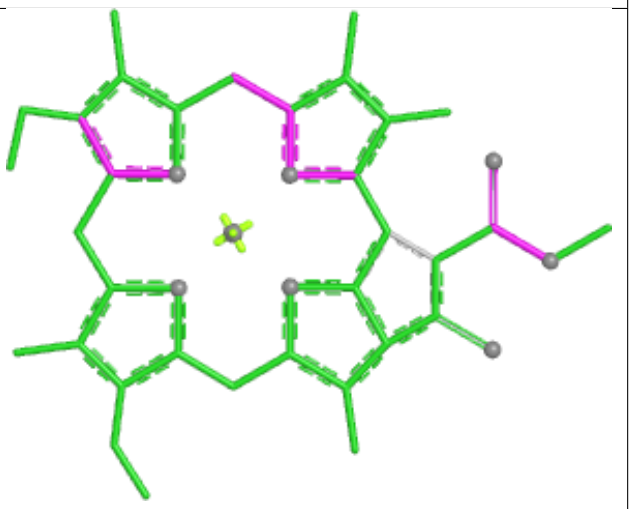


Rings

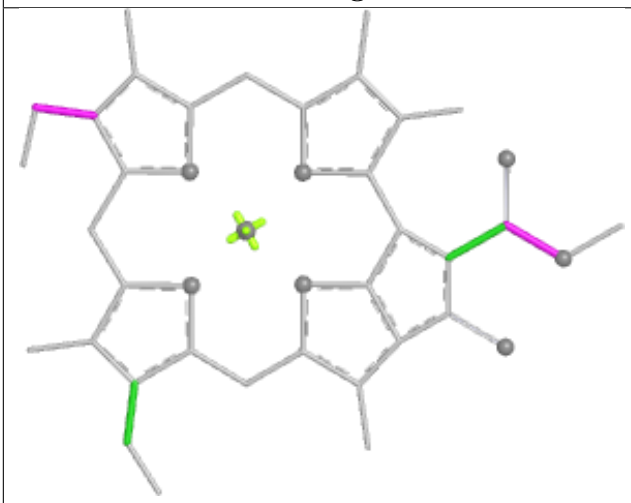
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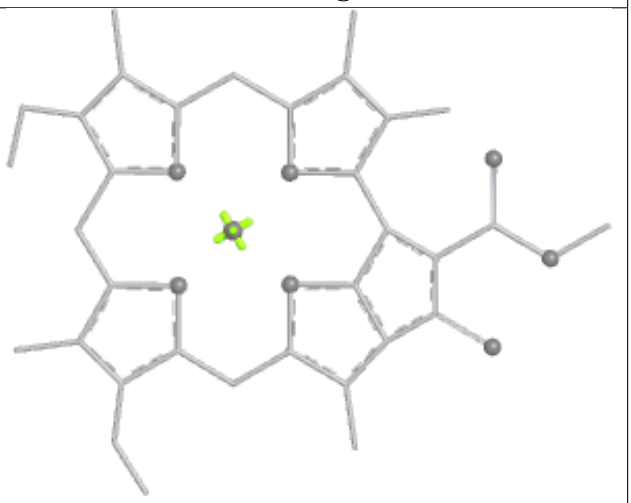
Bond lengths



Bond angles

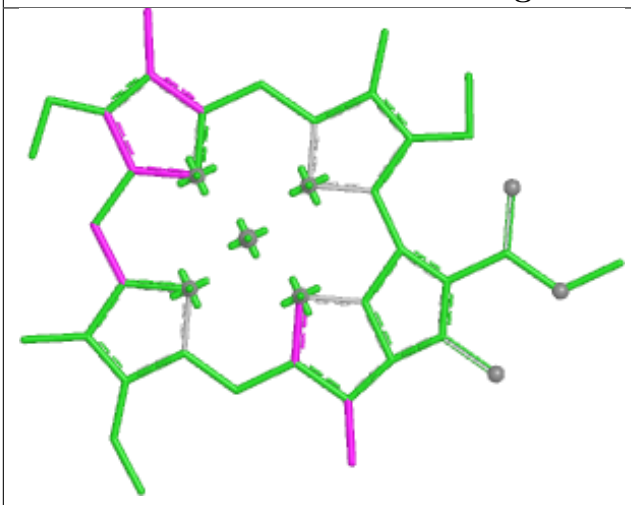


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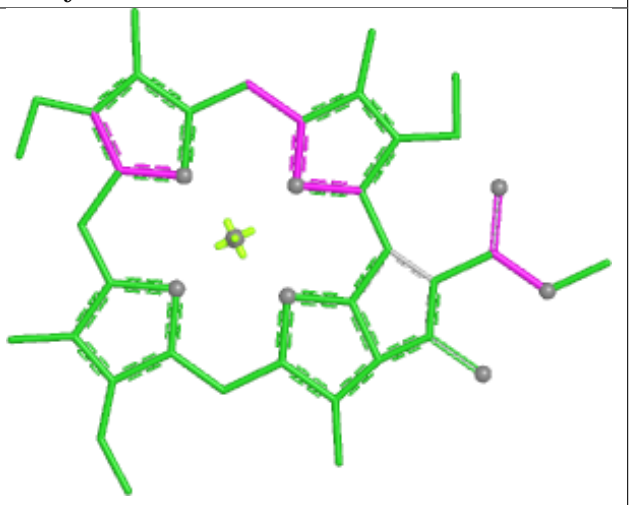


Rings

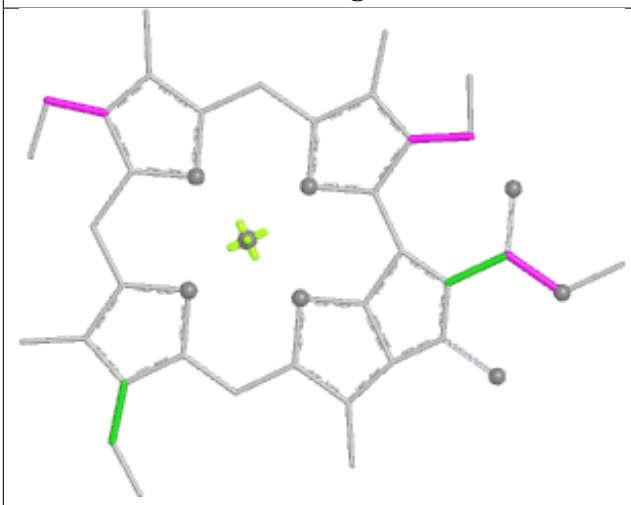
Ligand CLA Yy 611



Bond lengths



Bond angles

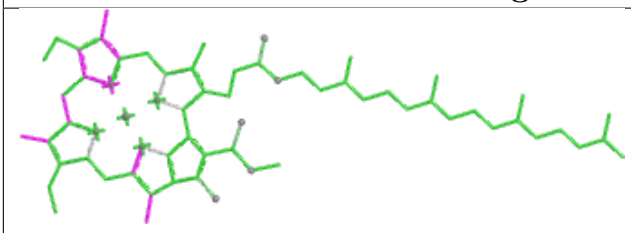


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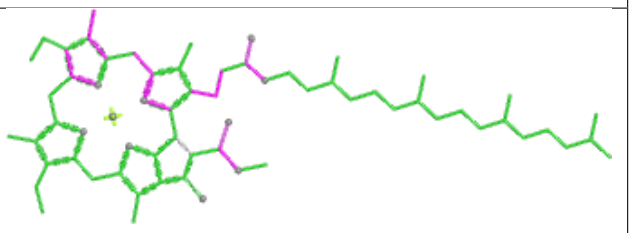


Rings

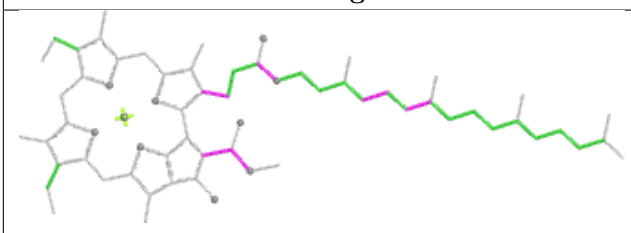
Ligand CLA CC 507



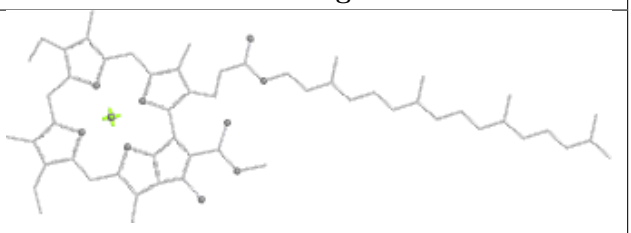
Bond lengths



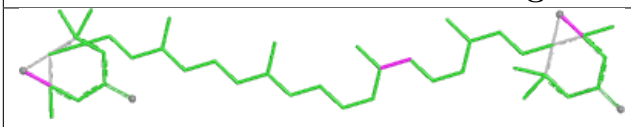
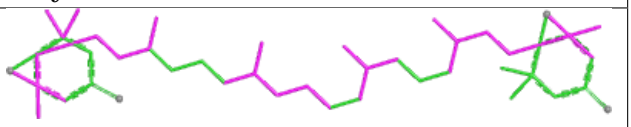
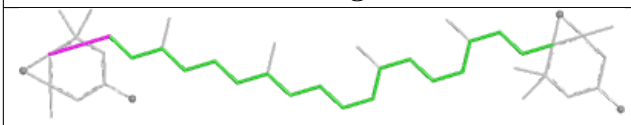
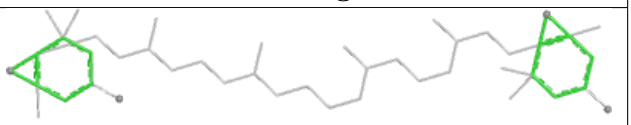
Bond angles

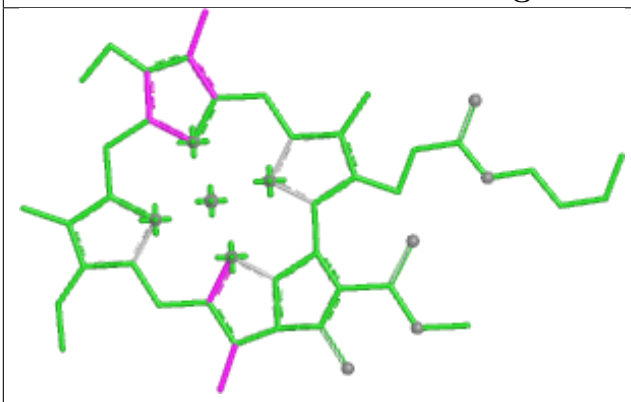
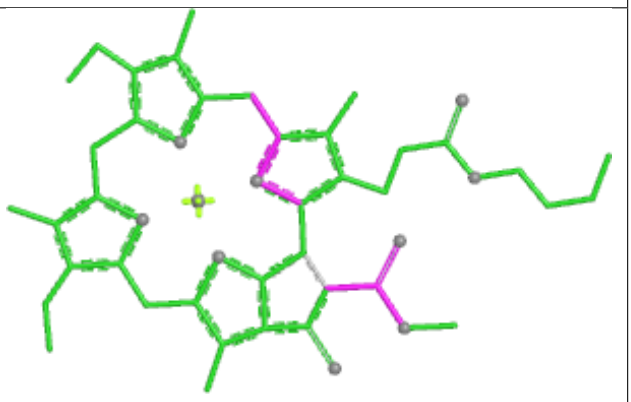
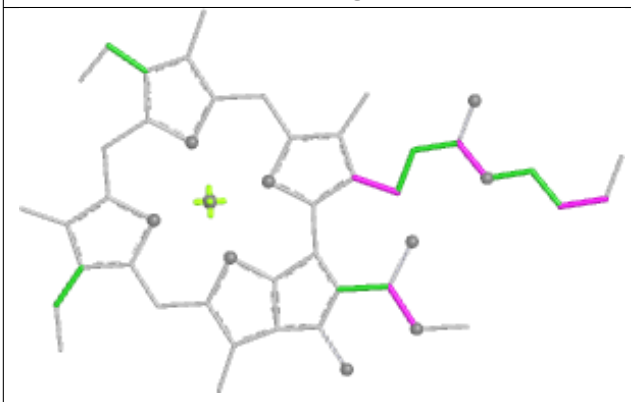
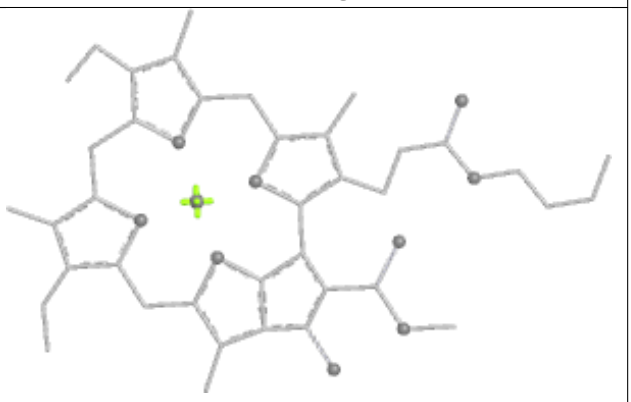


Torsions

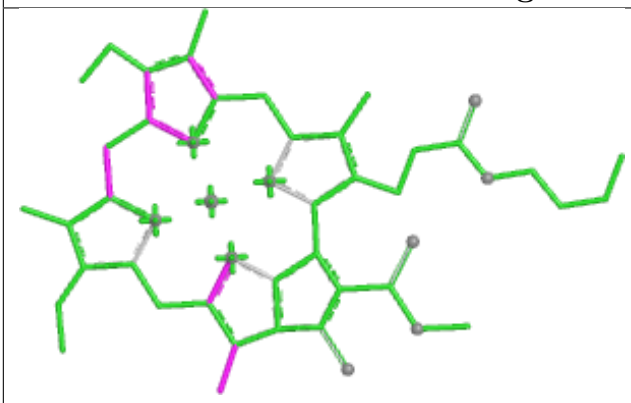


Rings

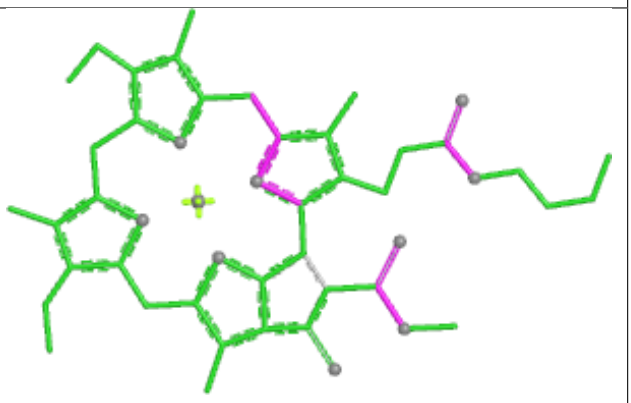
Ligand XAT y 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Nn 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

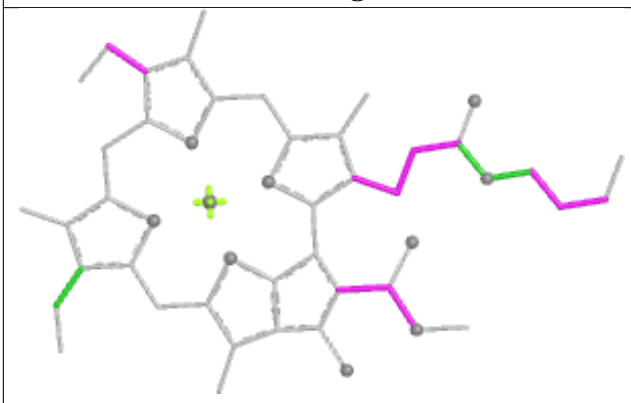
Ligand CLA Rr 601



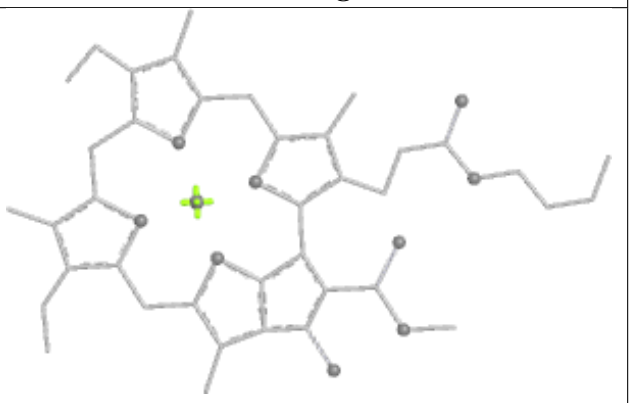
Bond lengths



Bond angles



Torsions



Rings

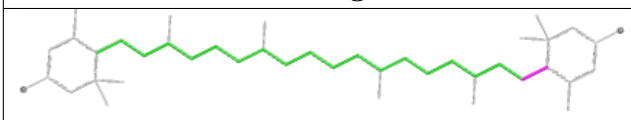
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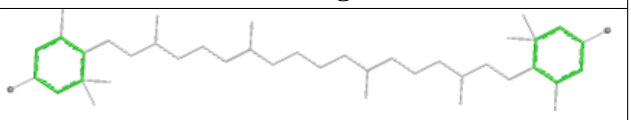
Bond lengths



Bond angles

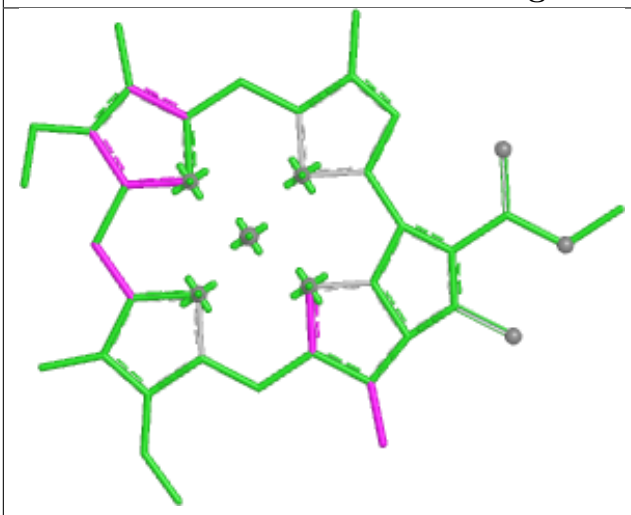


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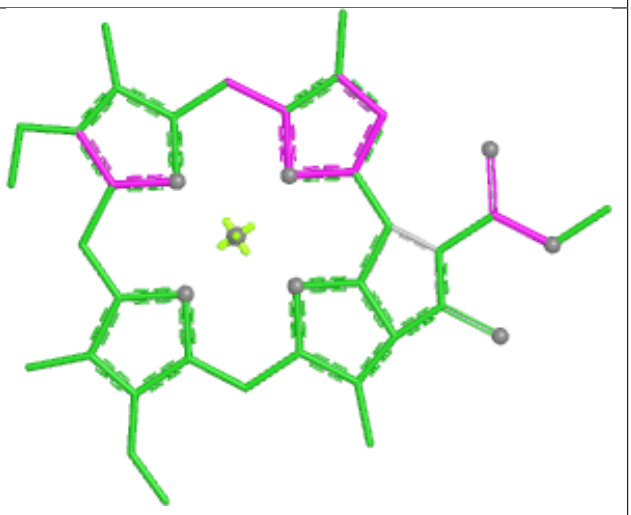


Rings

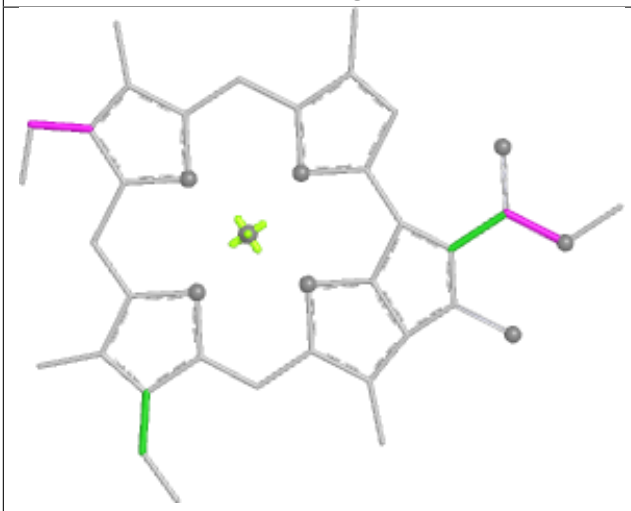
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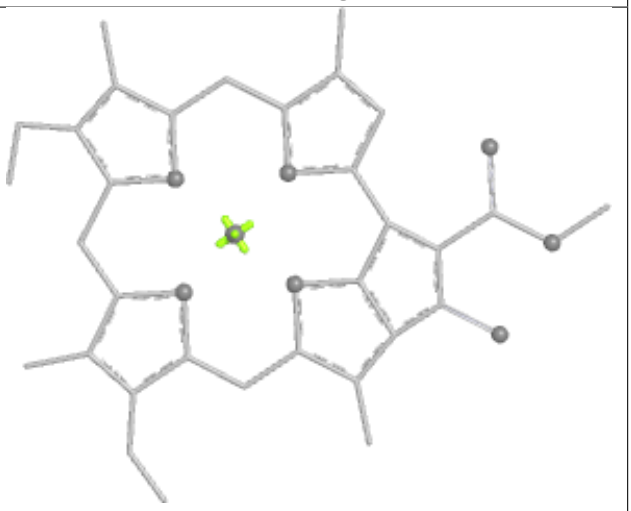
Bond lengths



Bond angles

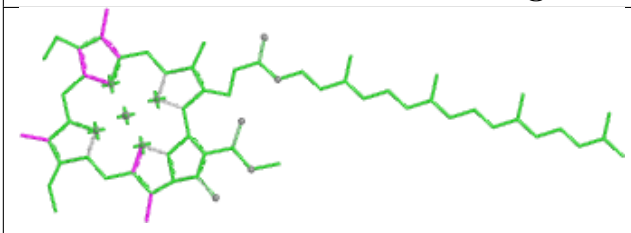


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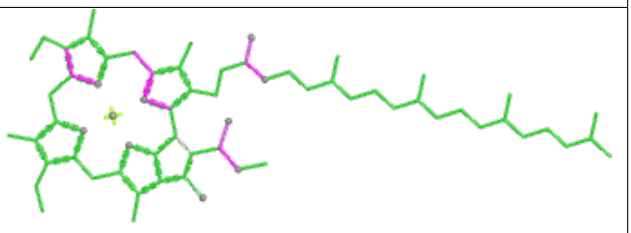


Rings

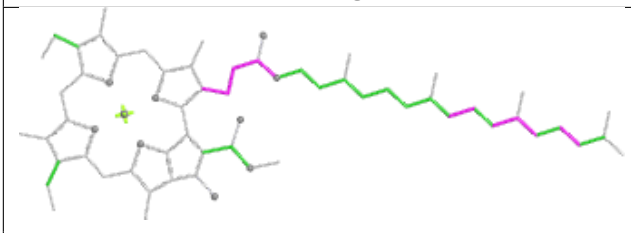
Ligand CLA b 616



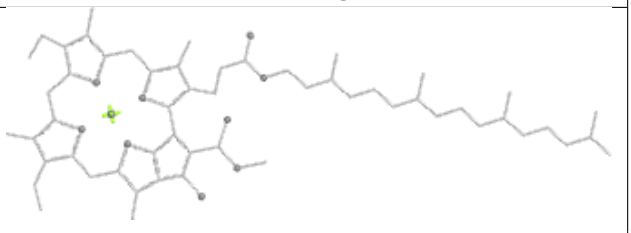
Bond lengths



Bond angles

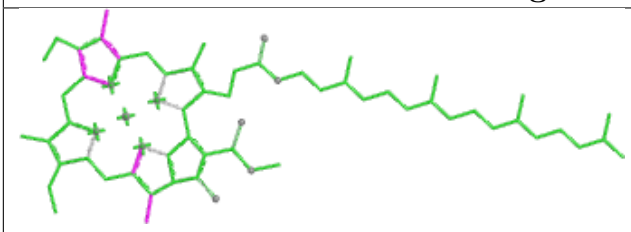


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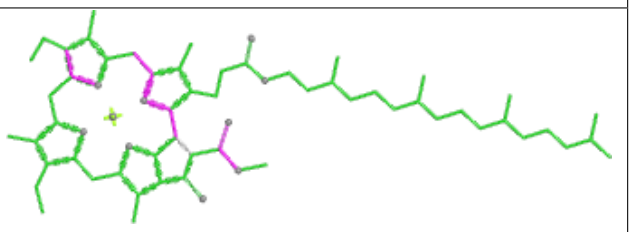


Rings

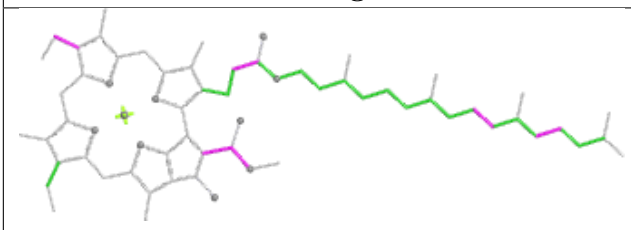
Ligand CLA c 507



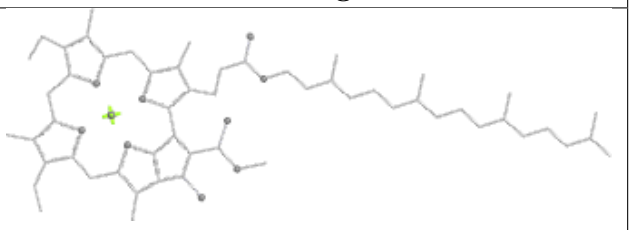
Bond lengths



Bond angles

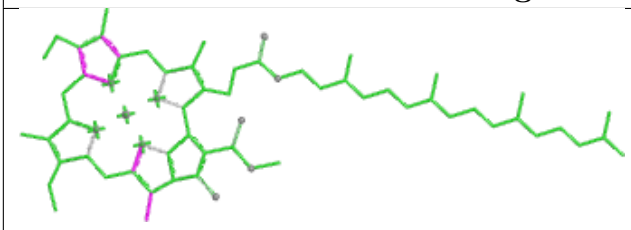


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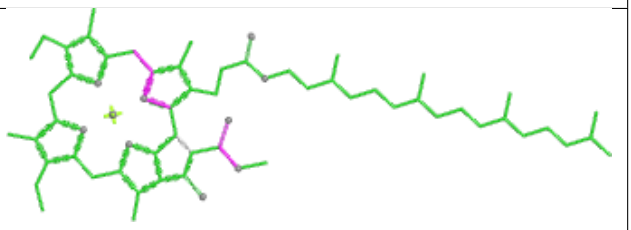


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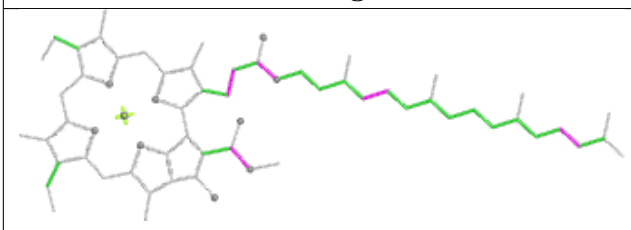
Ligand CLA Bb 614



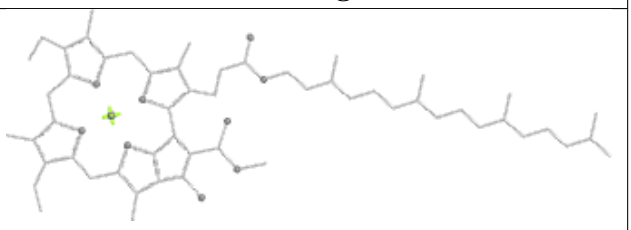
Bond lengths



Bond angles



Torsions

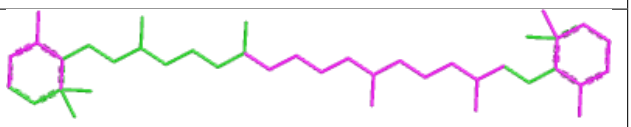


Rings

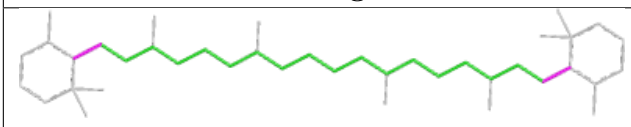
Ligand BCR T 101



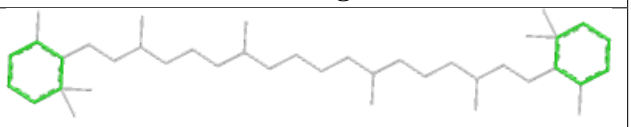
Bond lengths



Bond angles

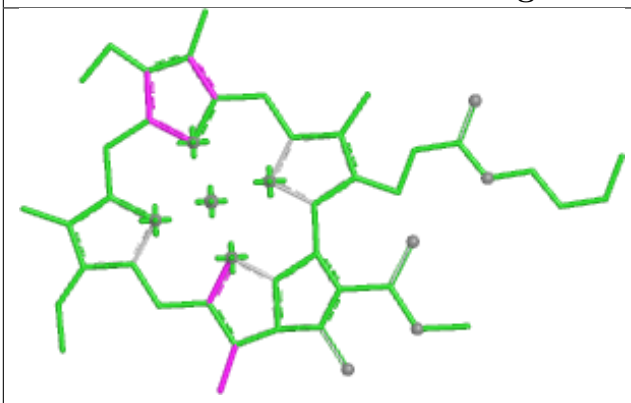


Torsions

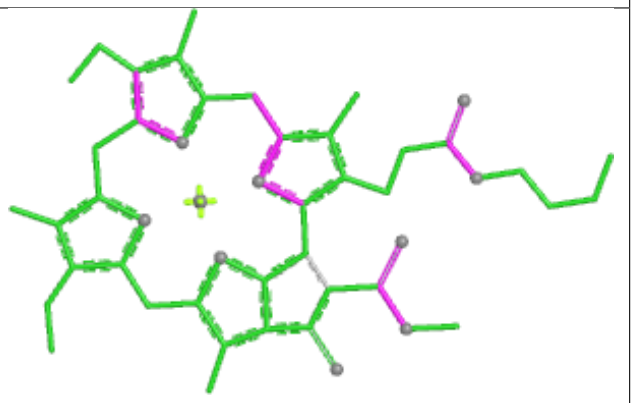


Rings

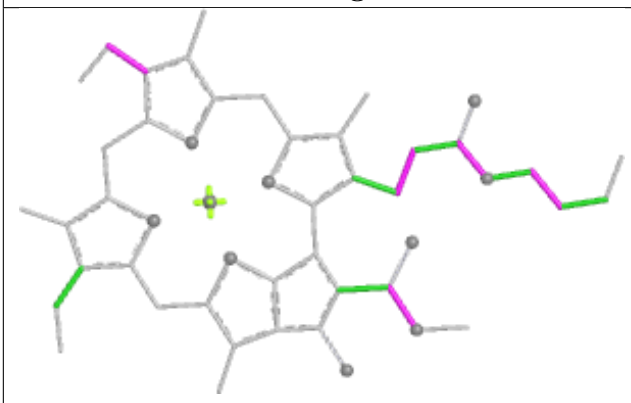
Ligand CLA SS 313



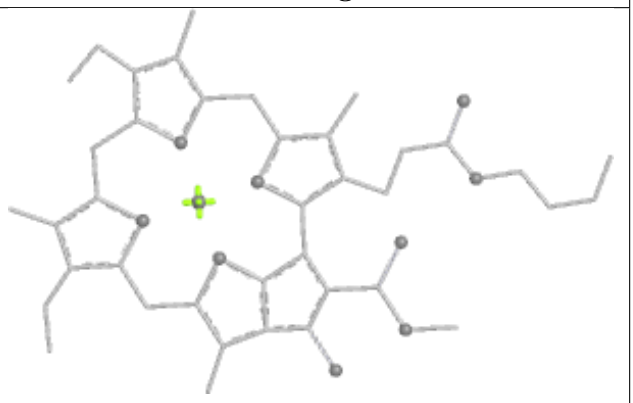
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Bond angles

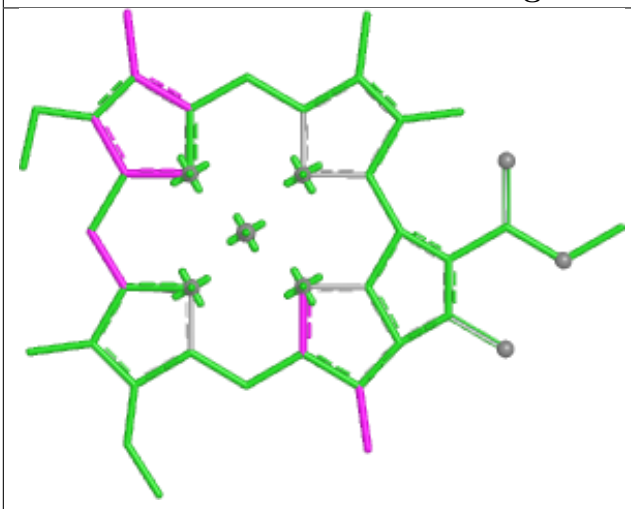


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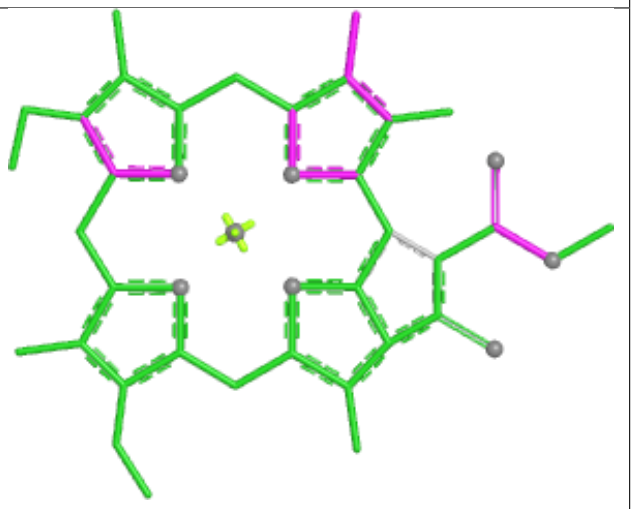


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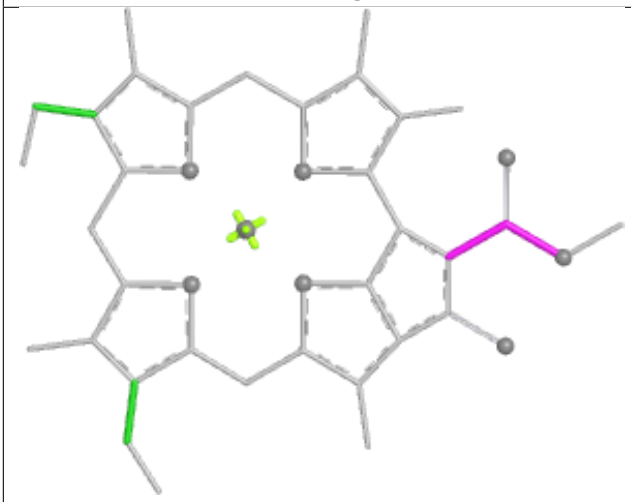
Ligand CLA X 201



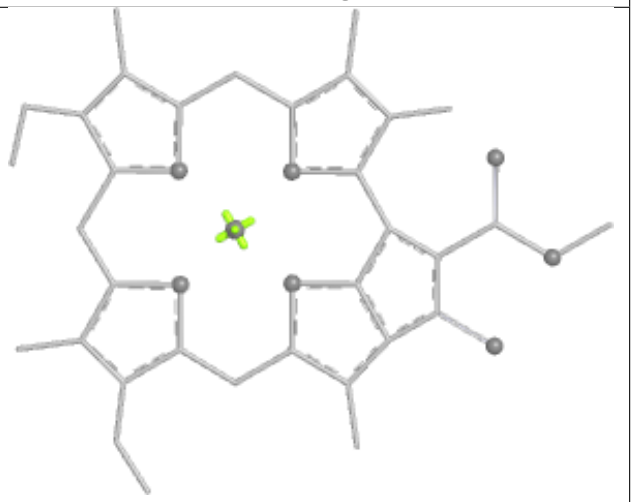
Bond lengths



Bond angles

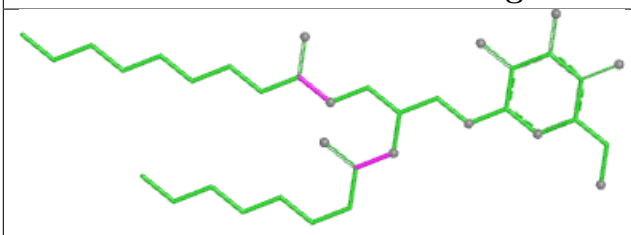


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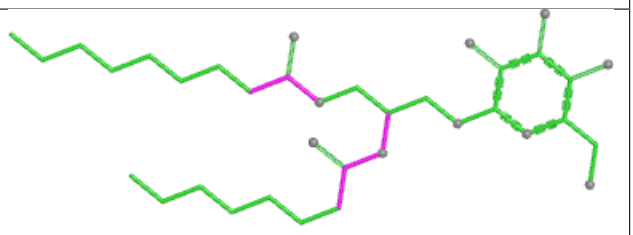


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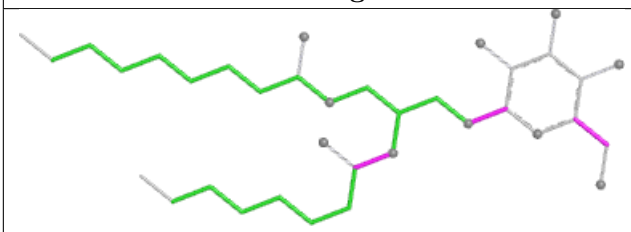
Ligand LMG AA 415



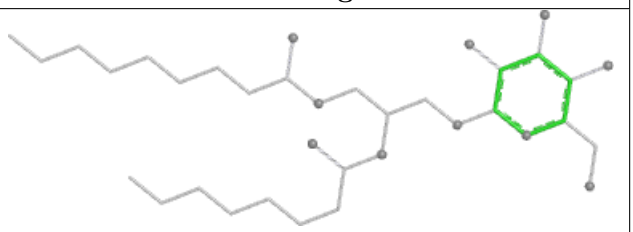
Bond lengths



Bond angles

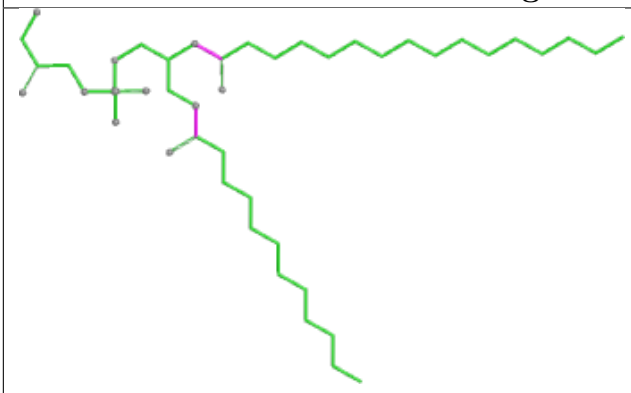


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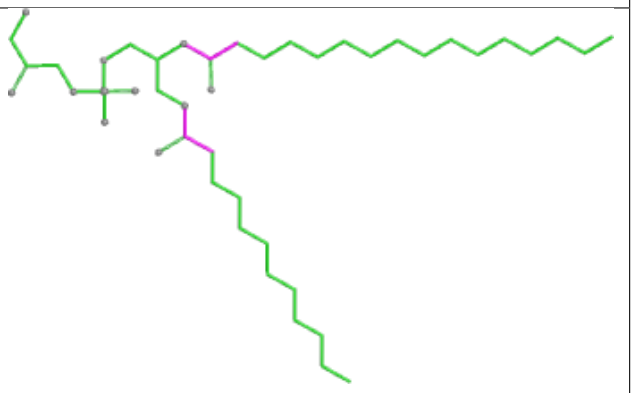


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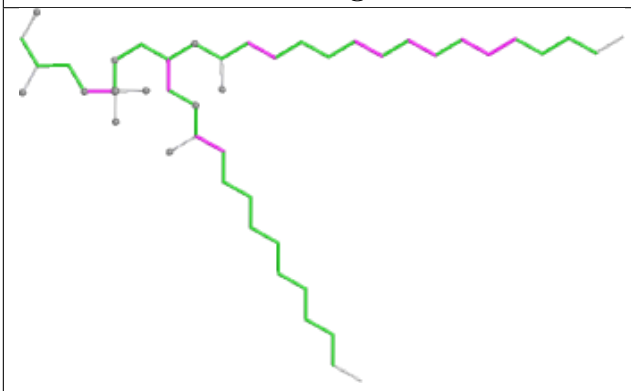
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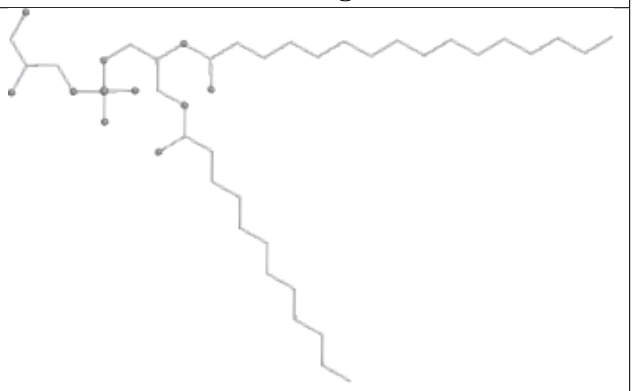
Bond lengths



Bond angles

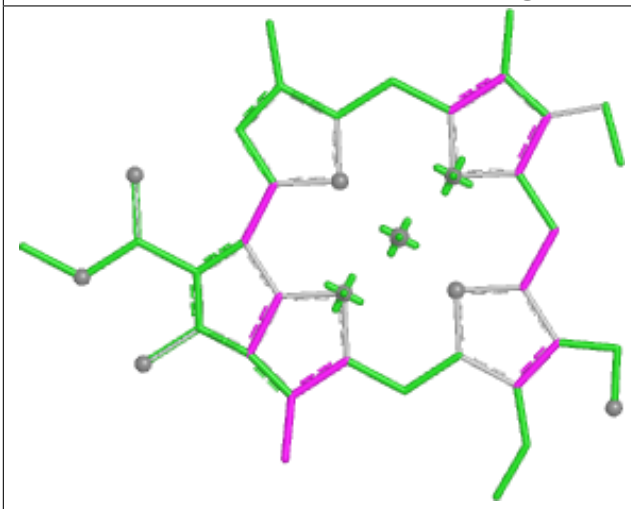


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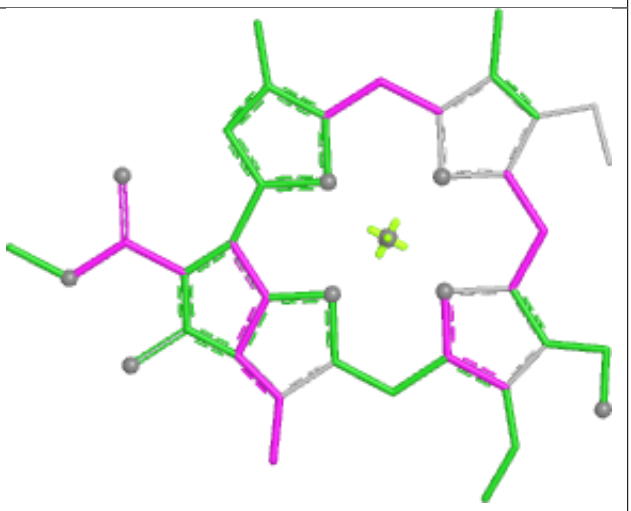


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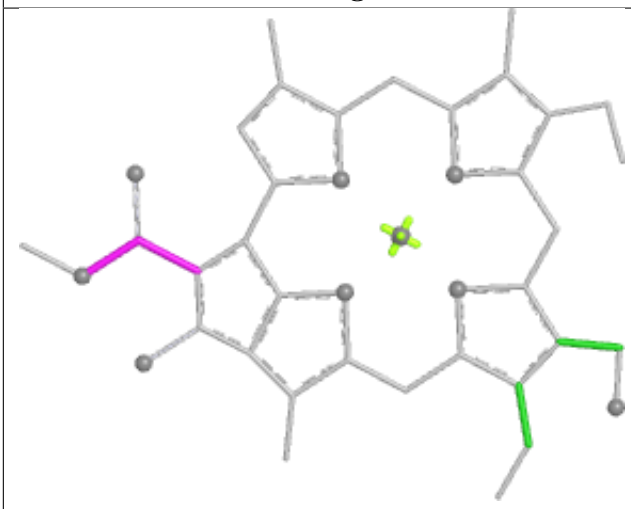
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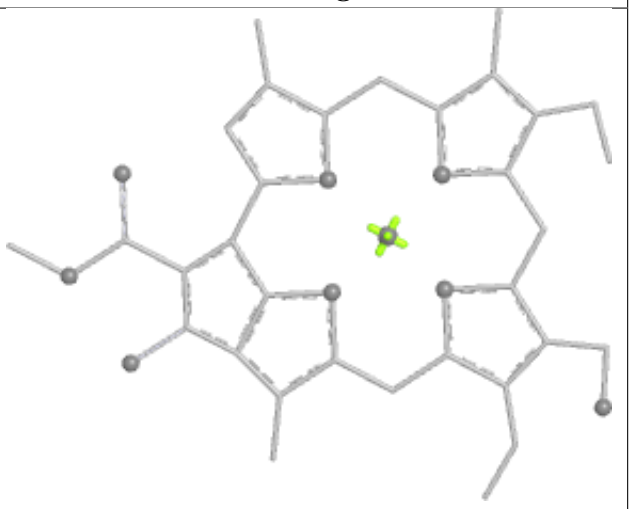
Bond lengths



Bond angles

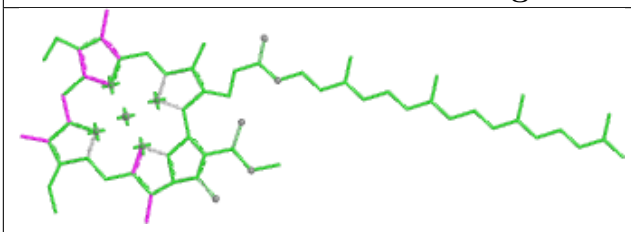


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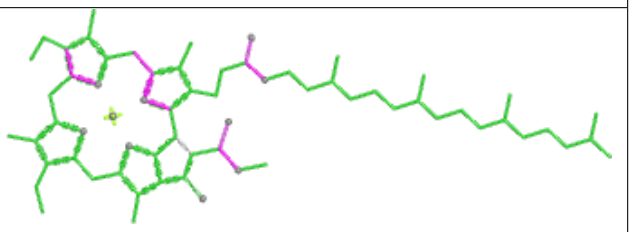


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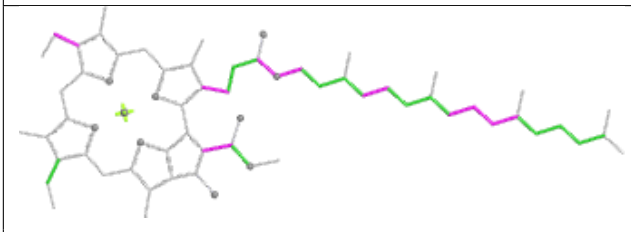
Ligand CLA CC 510



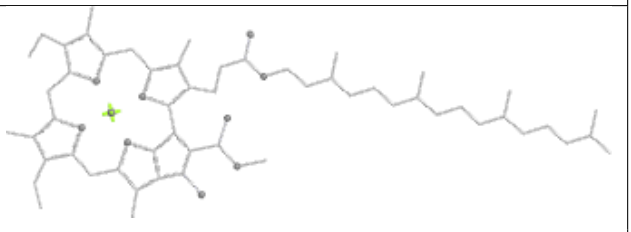
Bond lengths



Bond angles

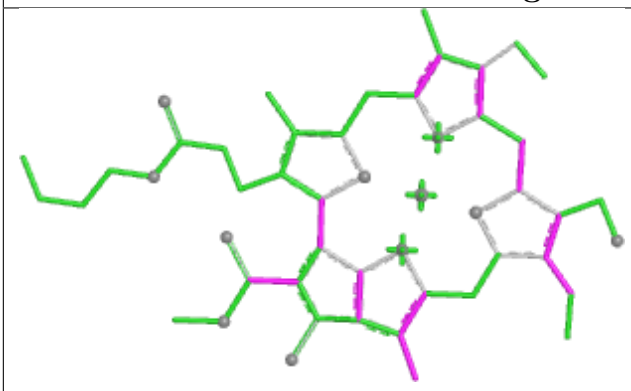


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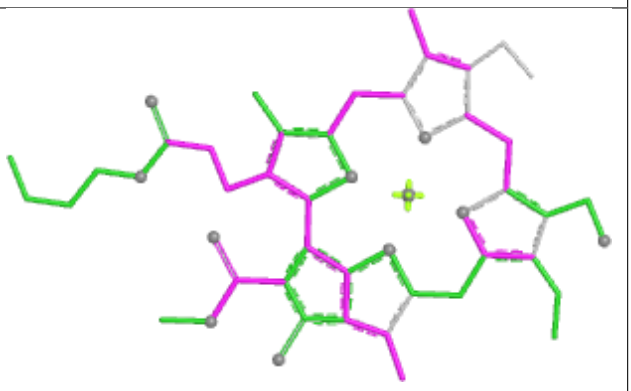


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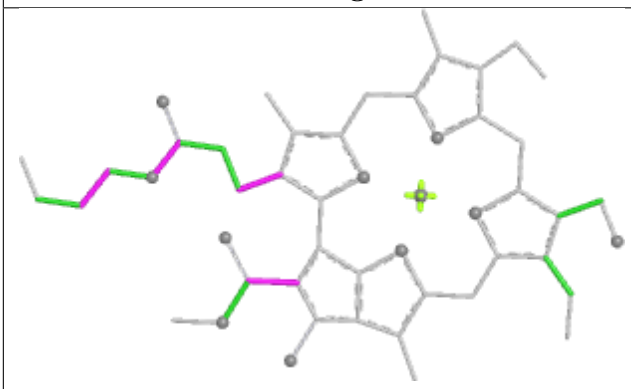
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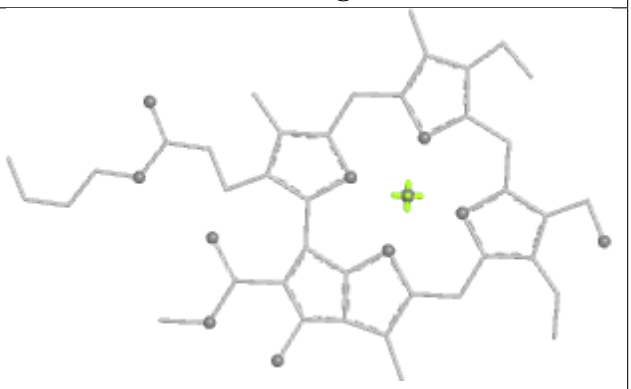
Bond lengths



Bond angles

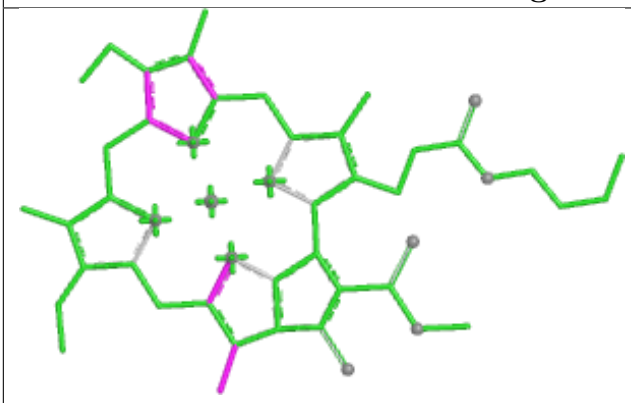


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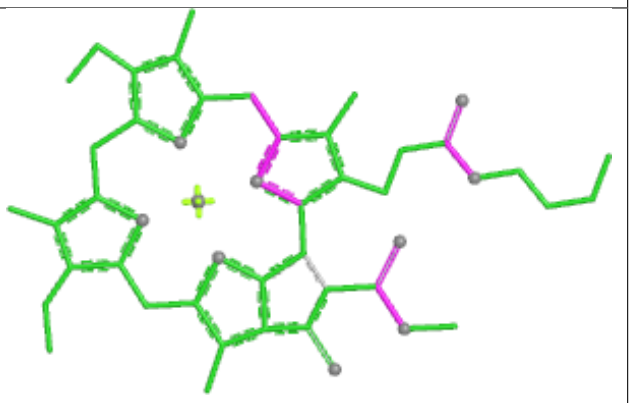


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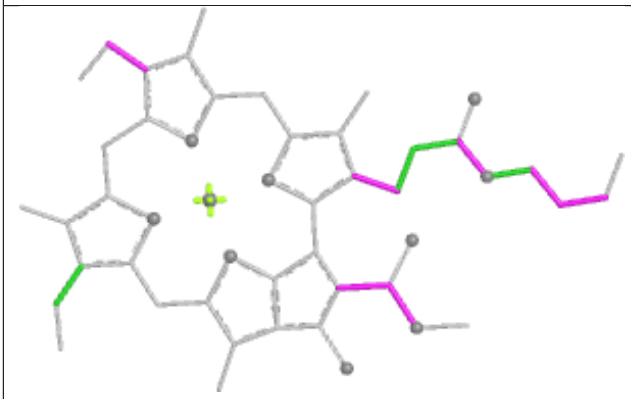
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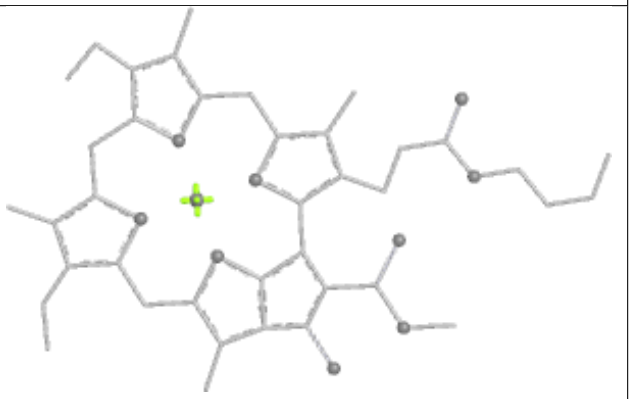
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Bond angles



Torsions

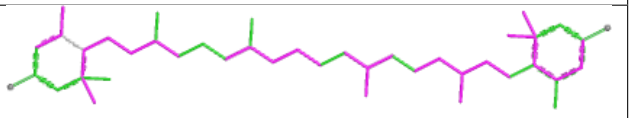


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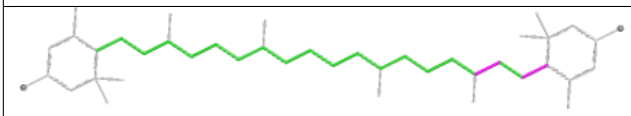
Ligand LUT RR 315



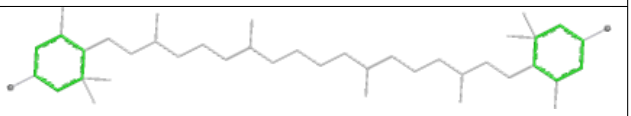
Bond lengths



Bond angles

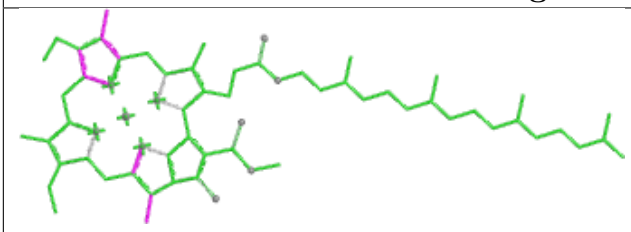


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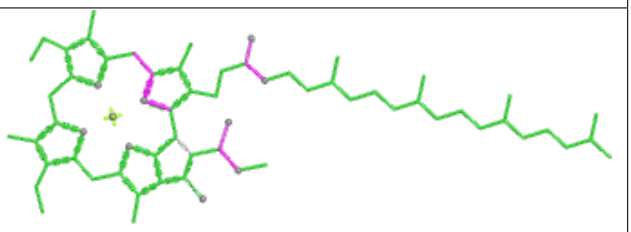


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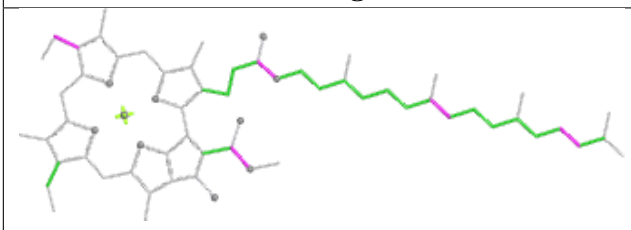
Ligand CLA c 512



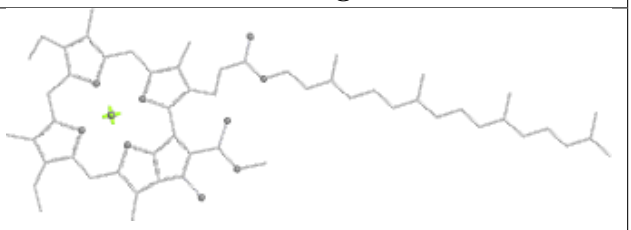
Bond lengths



Bond angles



Torsions

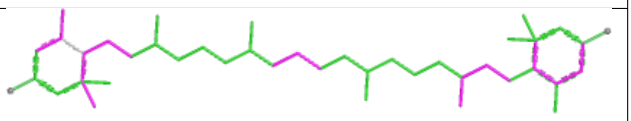


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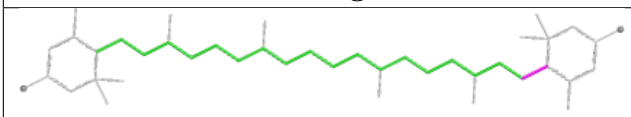
Ligand LUT Nn 307



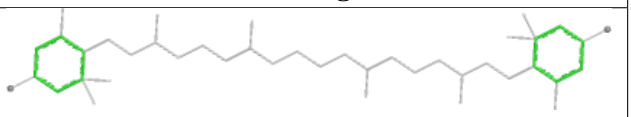
Bond lengths



Bond angles

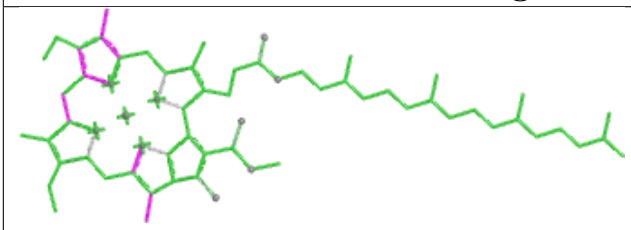


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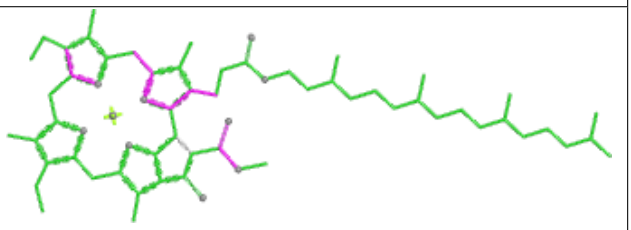


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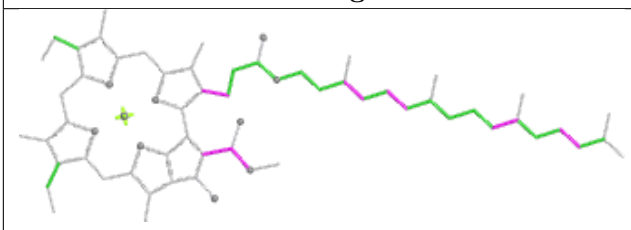
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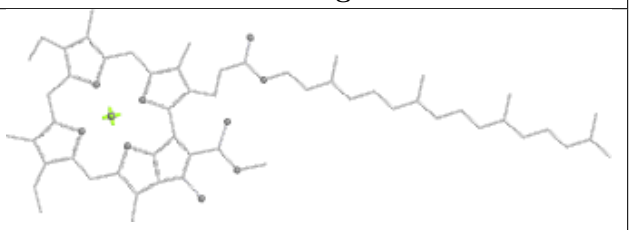
Bond lengths



Bond angles

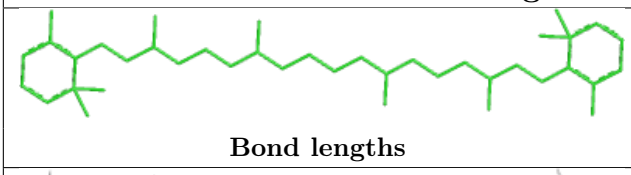


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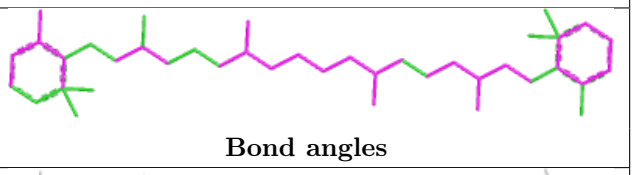


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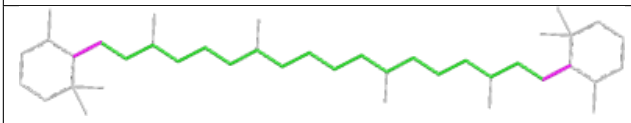
Ligand BCR B 616



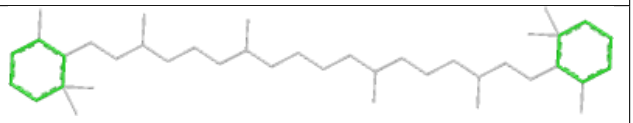
Bond lengths



Bond angles

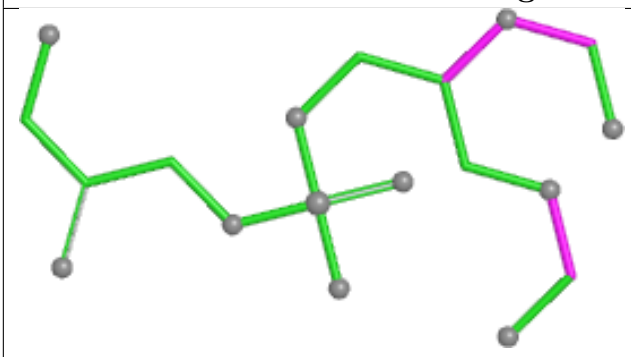


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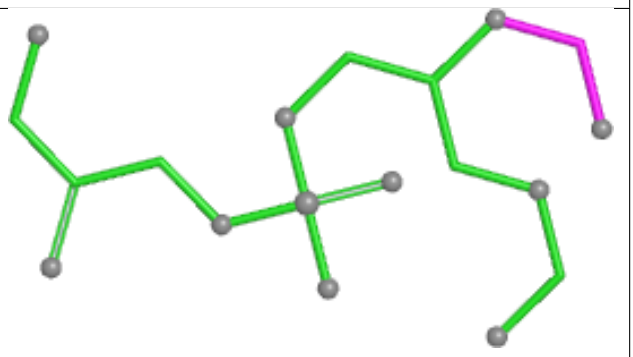


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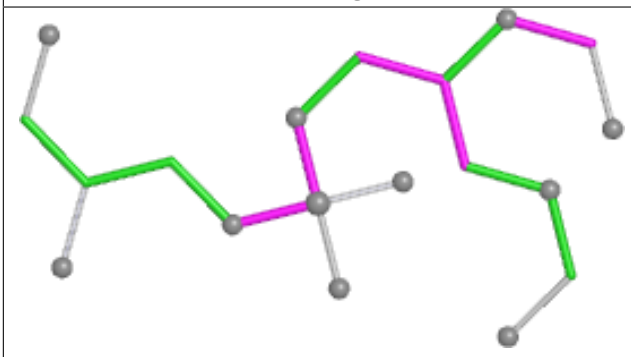
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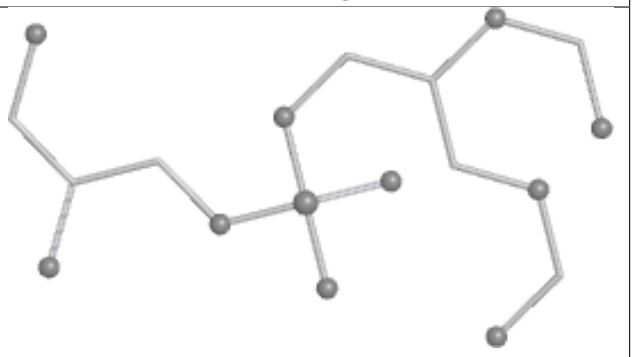
Bond lengths



Bond angles

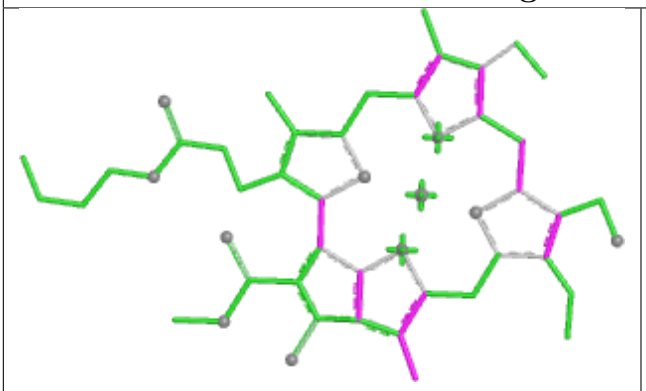


Torsions

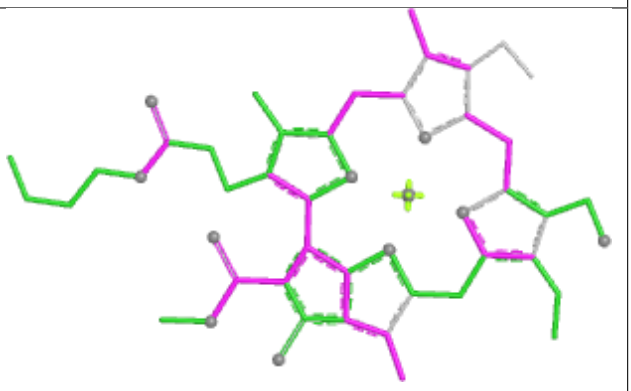


Rings

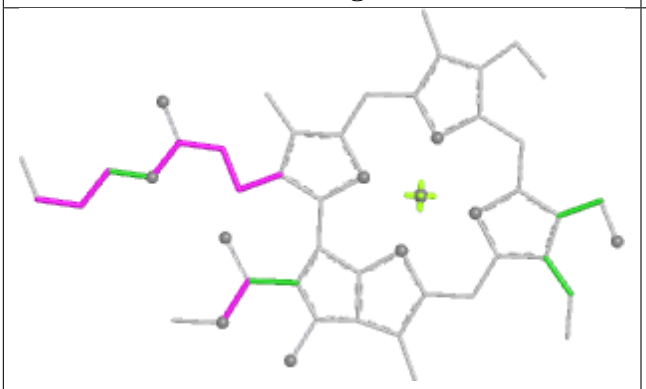
Ligand CHL Ss 605



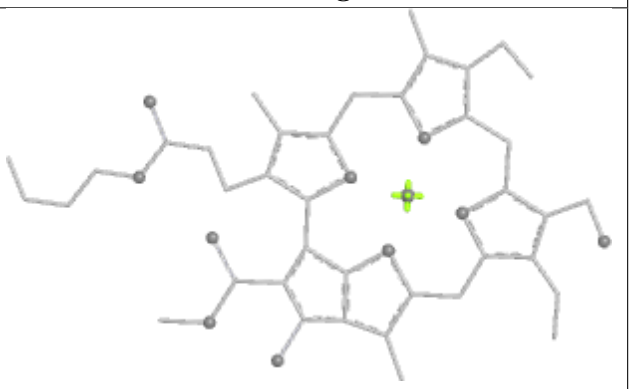
Bond lengths



Bond angles

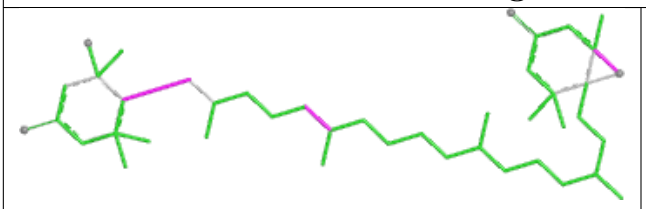


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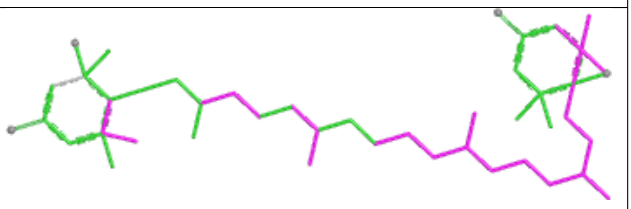


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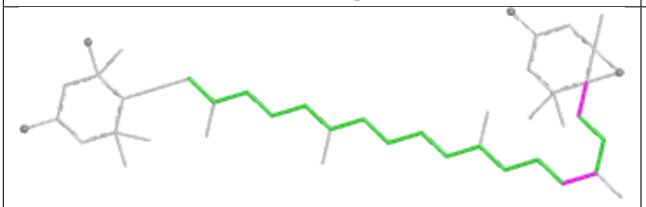
Ligand NEX RR 317



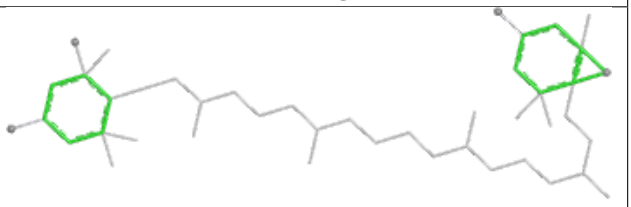
Bond lengths



Bond angles

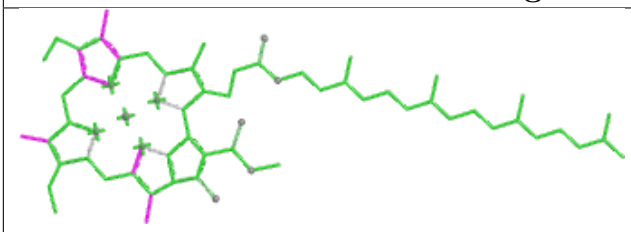


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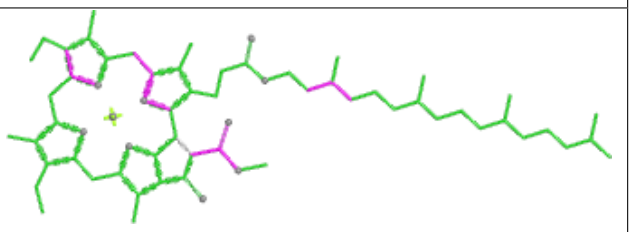


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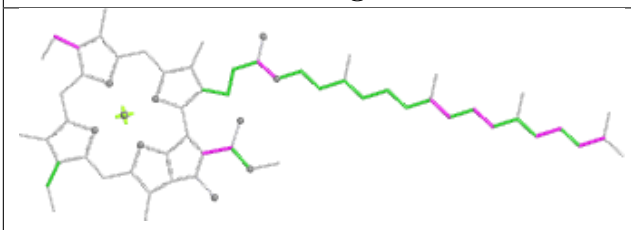
Ligand CLA C 509



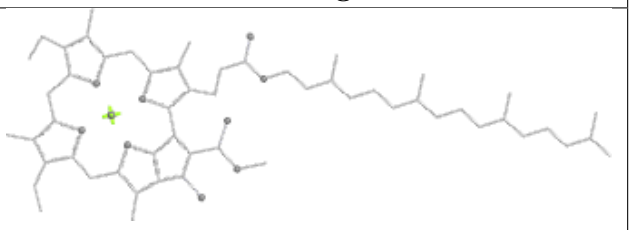
Bond lengths



Bond angles

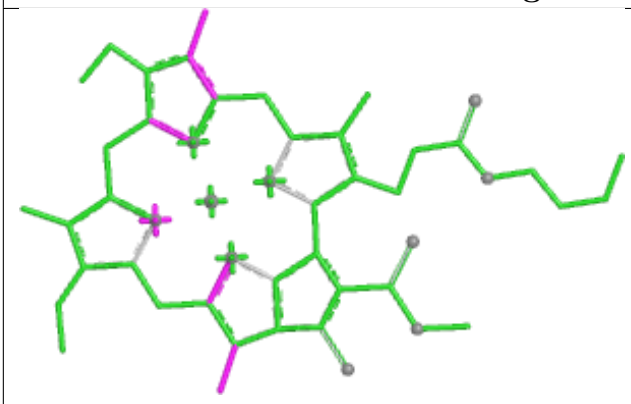


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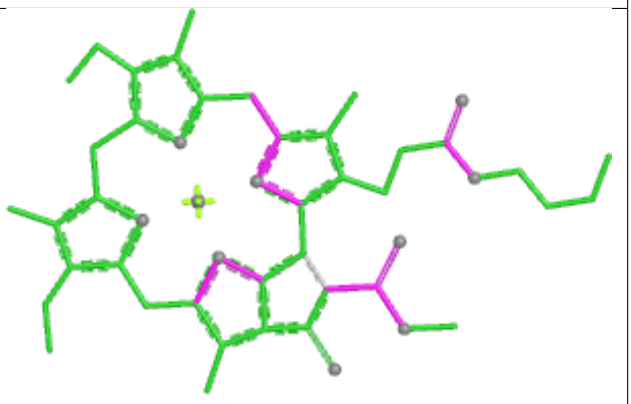


Rings

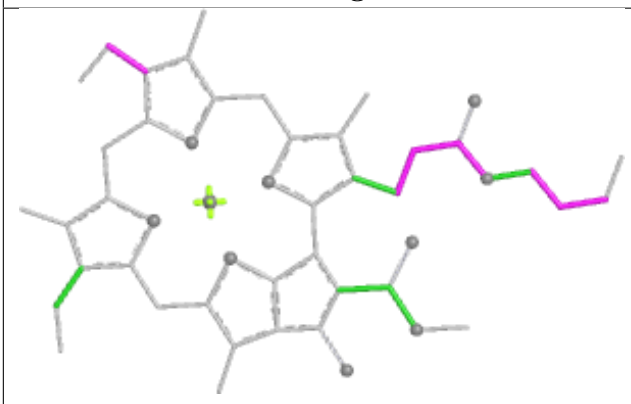
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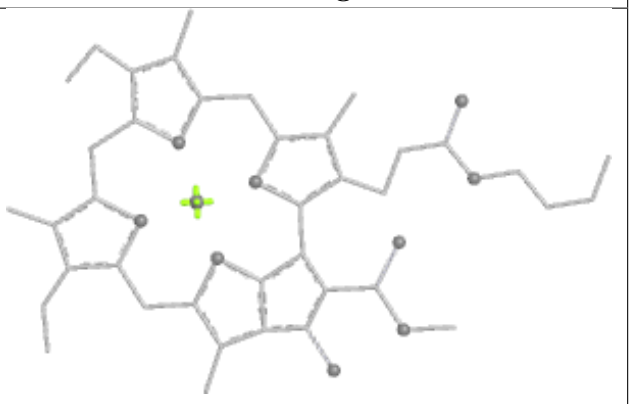
Bond lengths



Bond angles

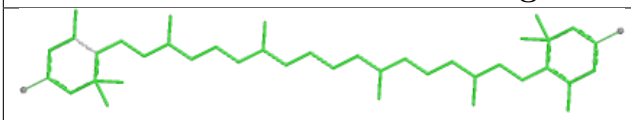


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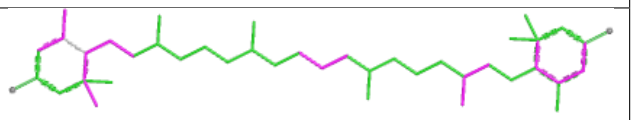


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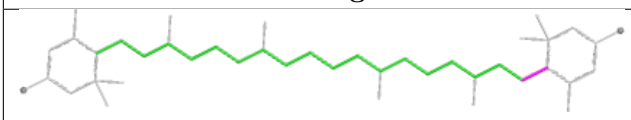
Ligand LUT 44 612



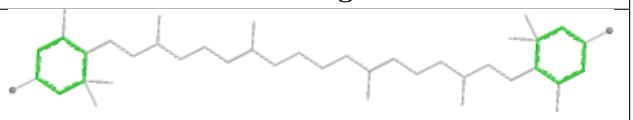
Bond lengths



Bond angles

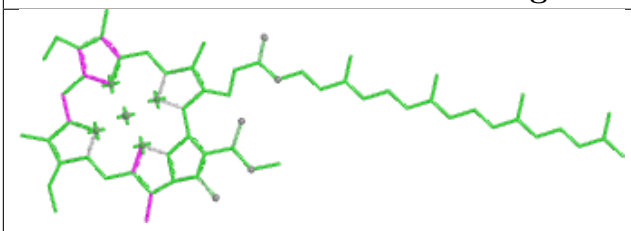


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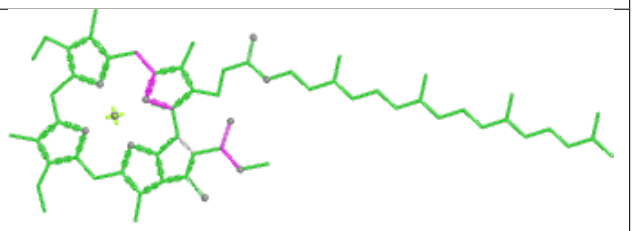


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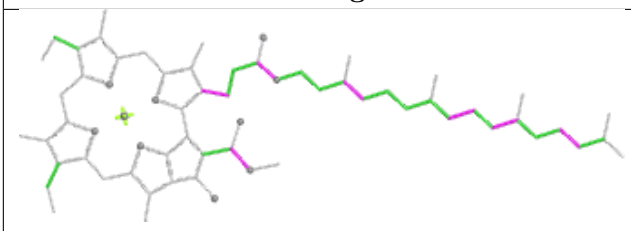
Ligand CLA r 609



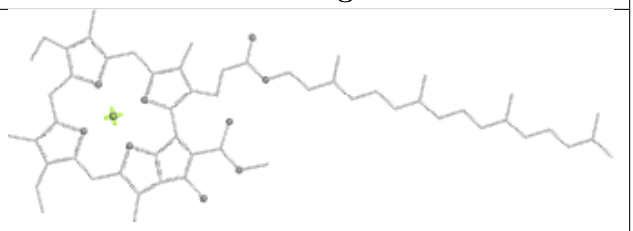
Bond lengths



Bond angles

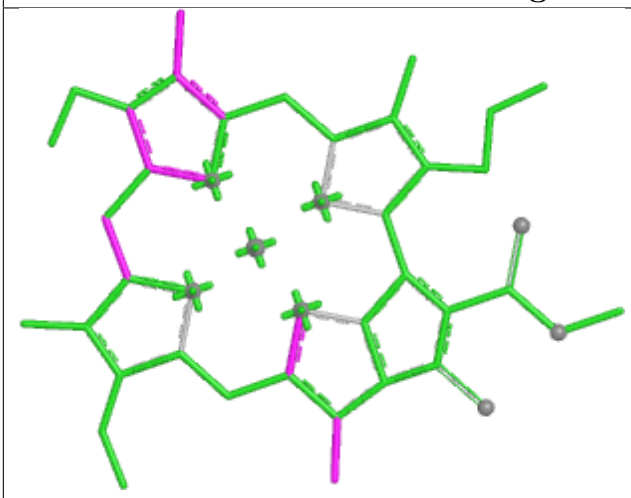


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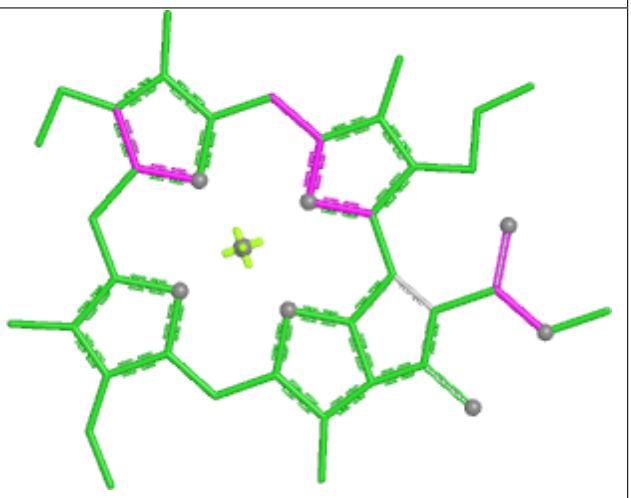


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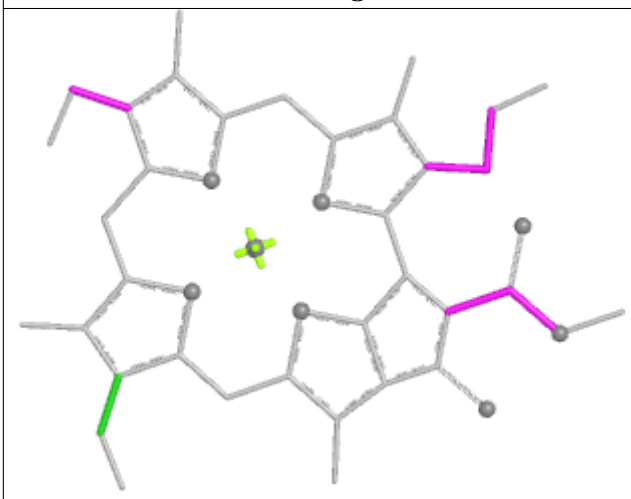
Ligand CLA c 513



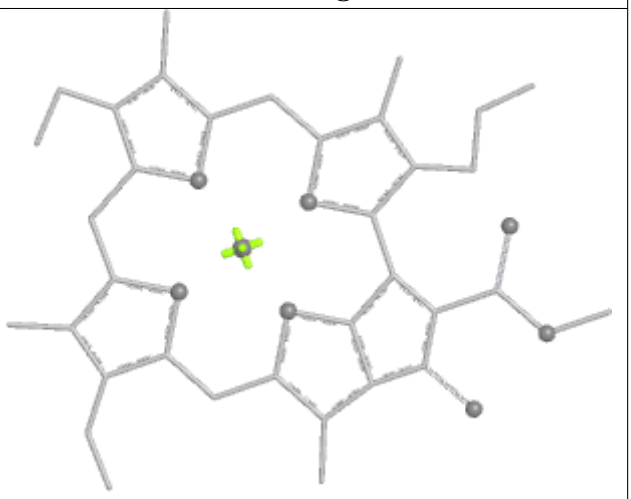
Bond lengths



Bond angles

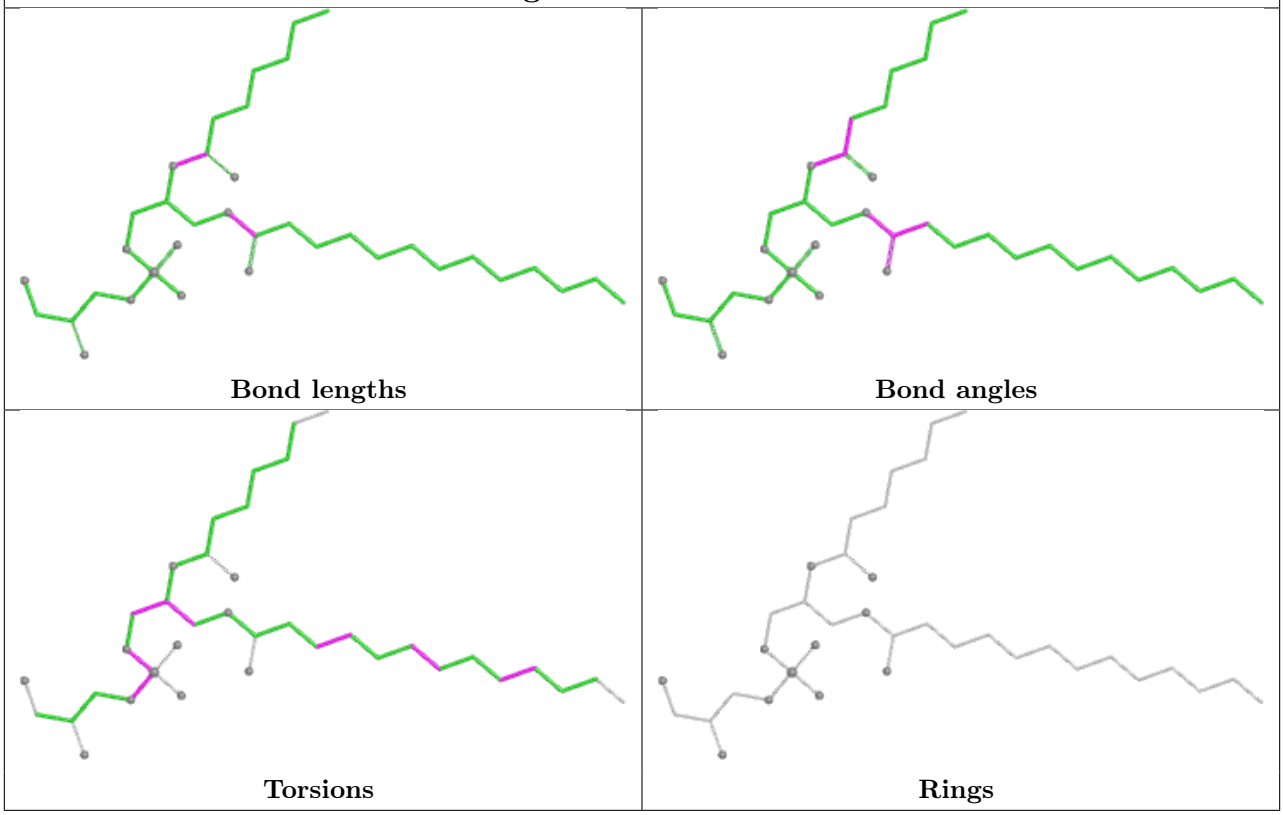


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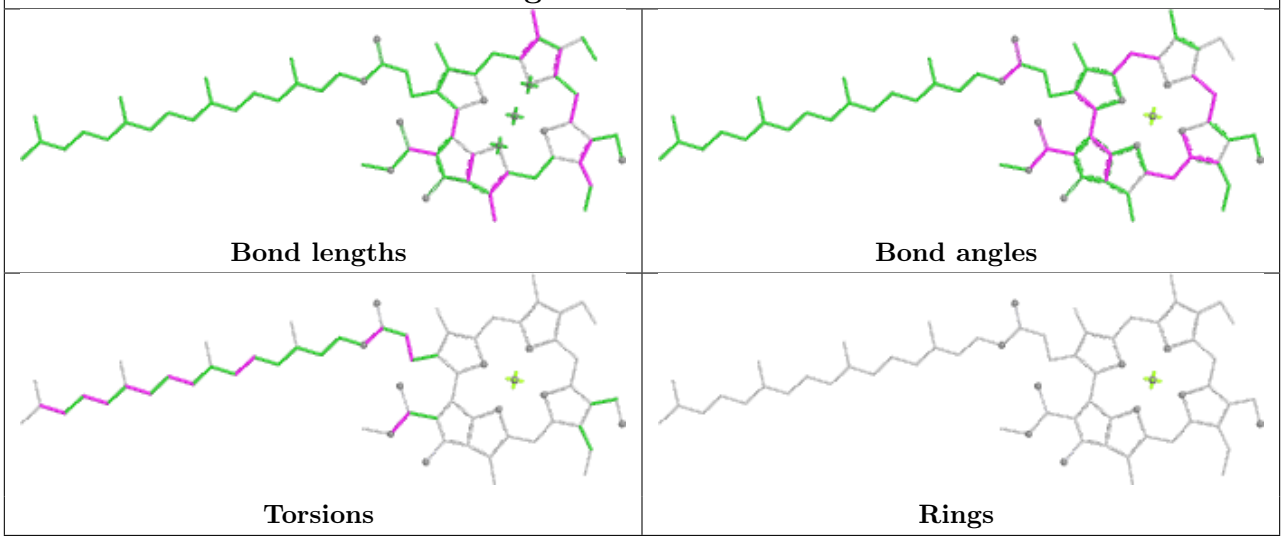


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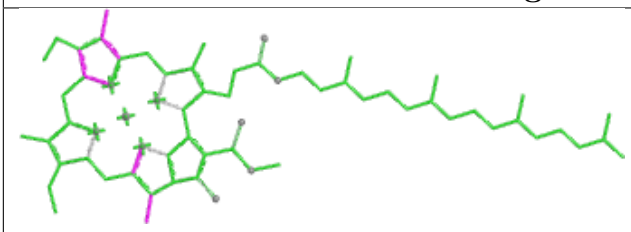
Ligand LHG A 413



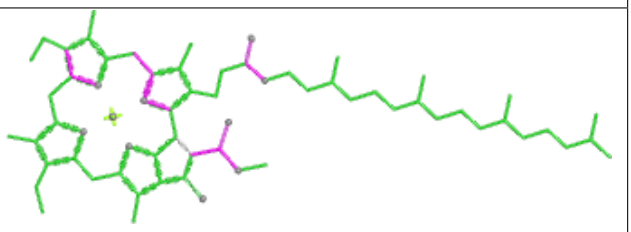
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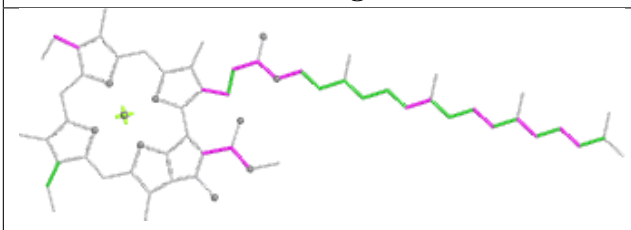
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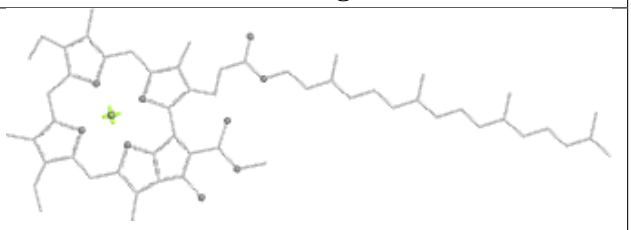
Bond lengths



Bond angles

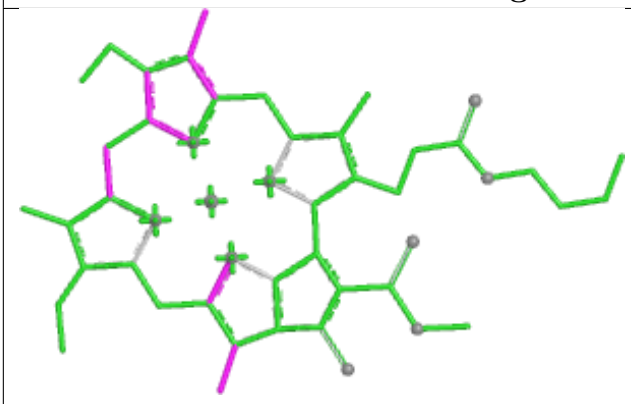


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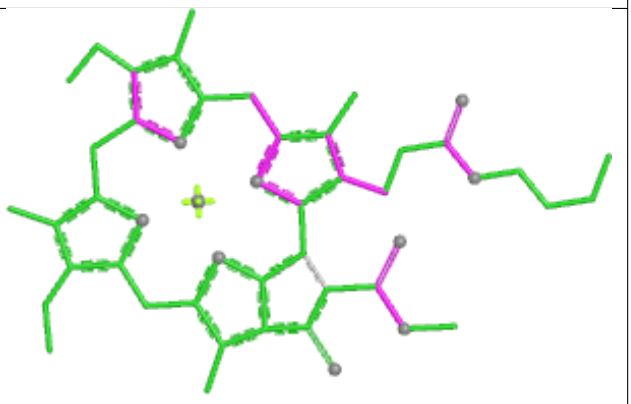


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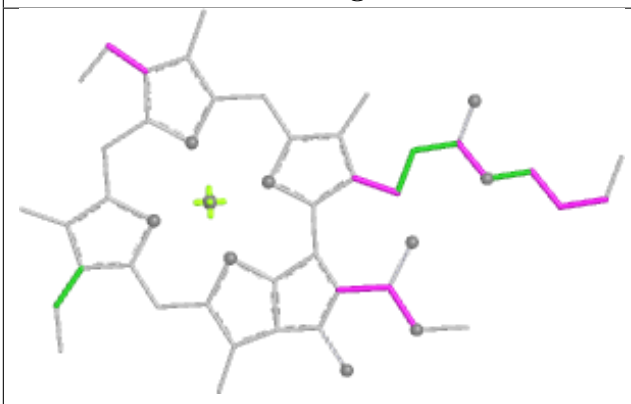
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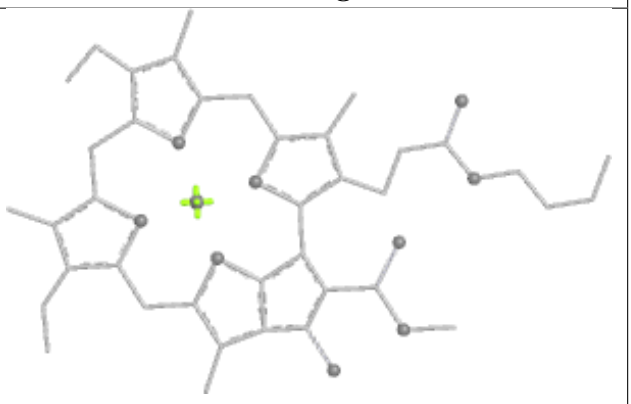
Bond lengths



Bond angles

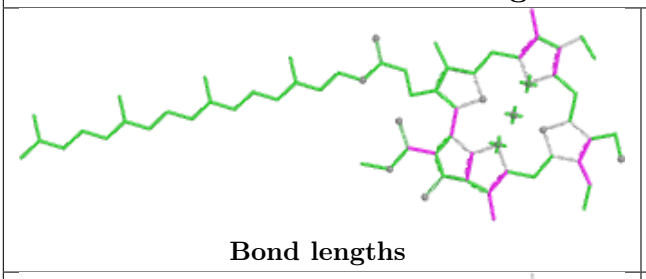


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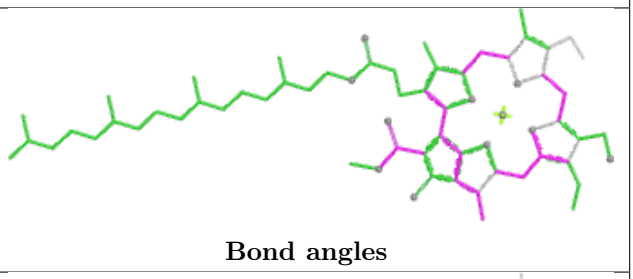


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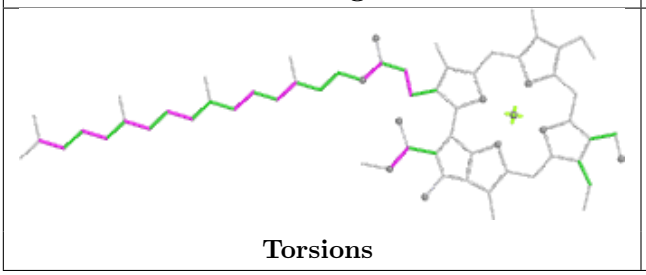
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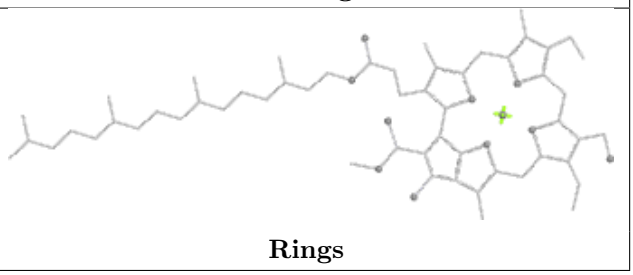
Bond lengths



Bond angles

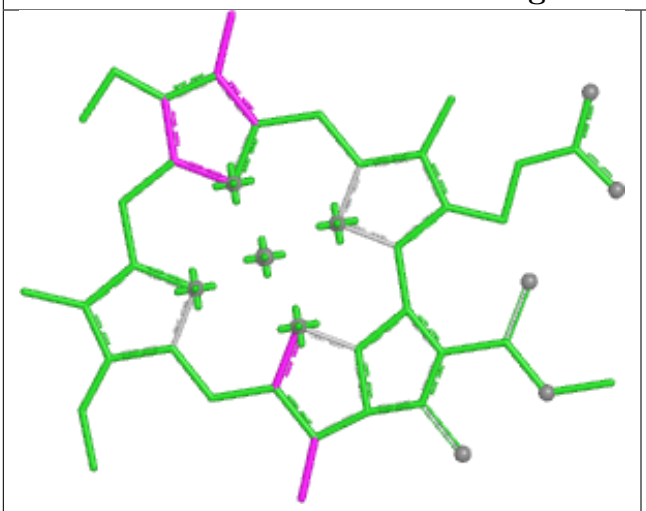


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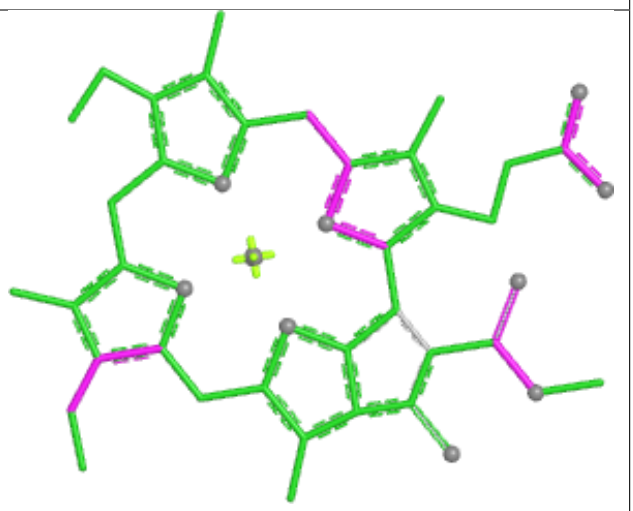


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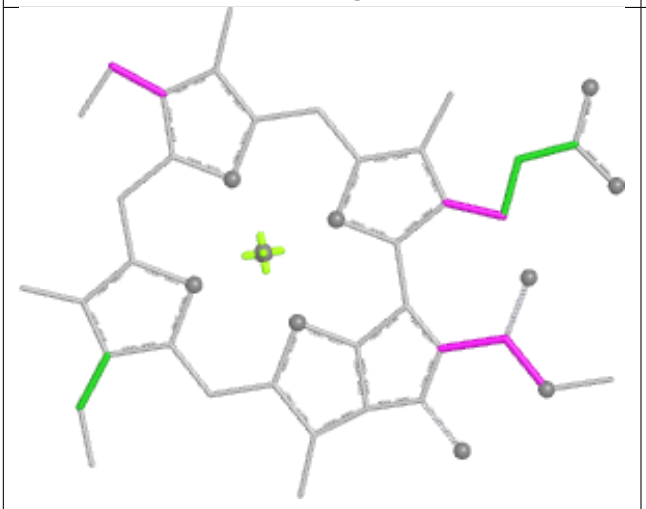
Ligand CLA 4 304



Bond lengths



Bond angles

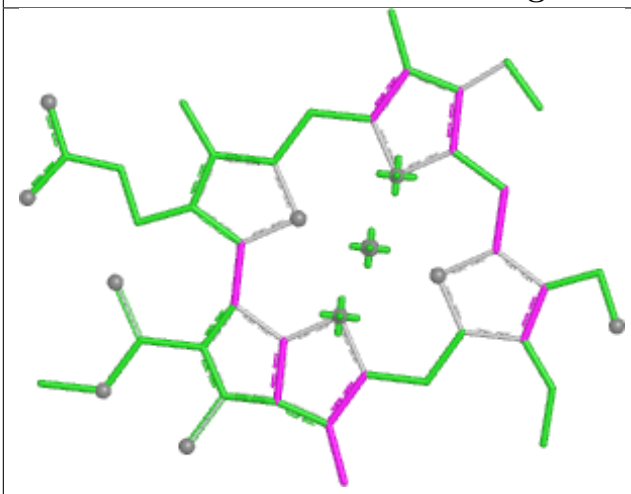


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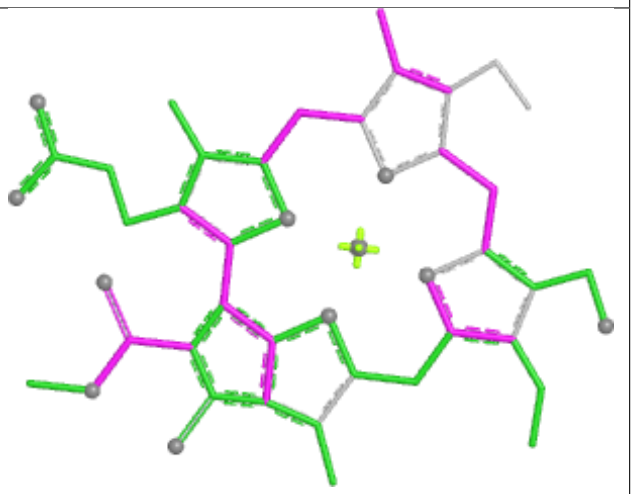


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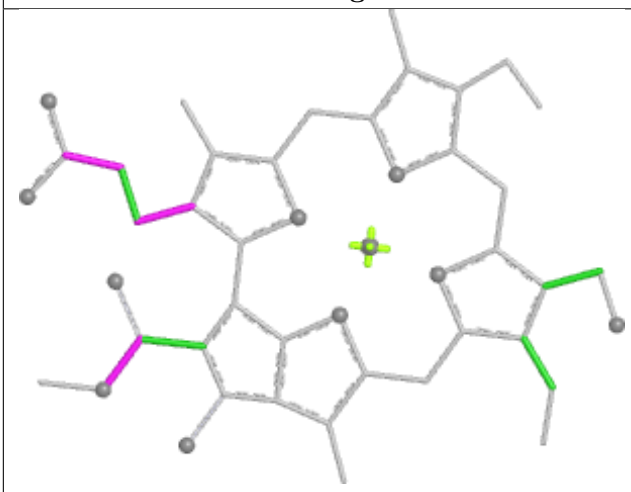
Ligand CHL 4 309



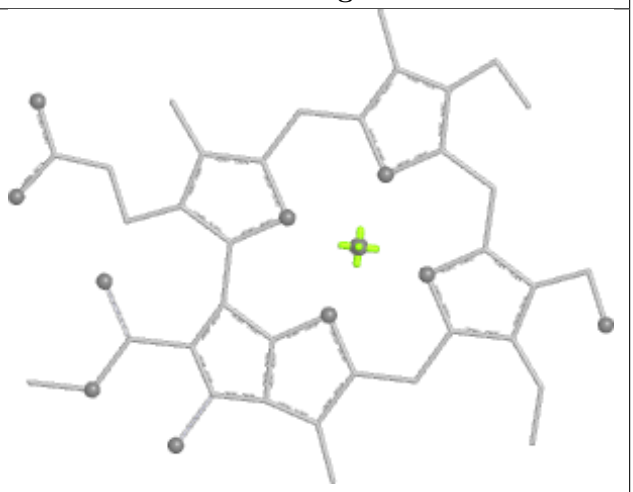
Bond lengths



Bond angles



Torsions

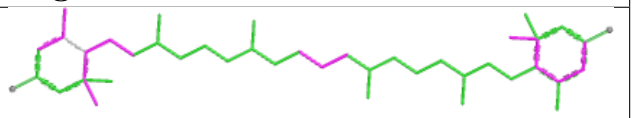


Rings

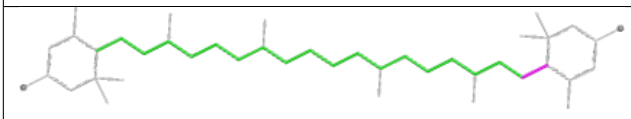
Ligand LUT g 615



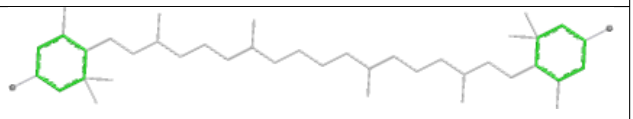
Bond lengths



Bond angles

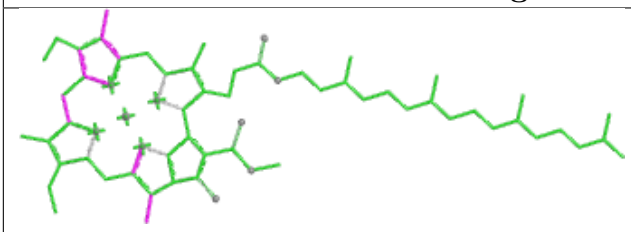


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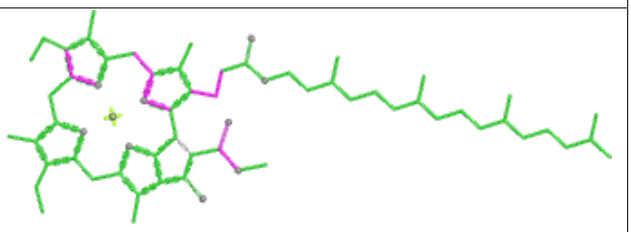


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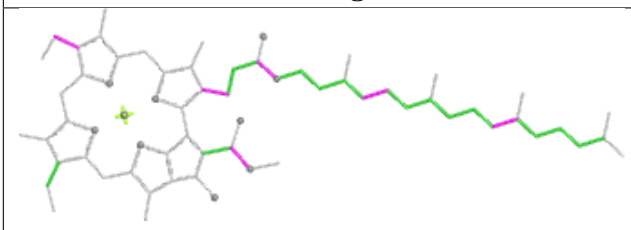
Ligand CLA RR 309



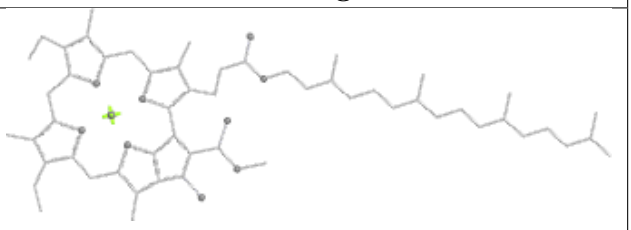
Bond lengths



Bond angles

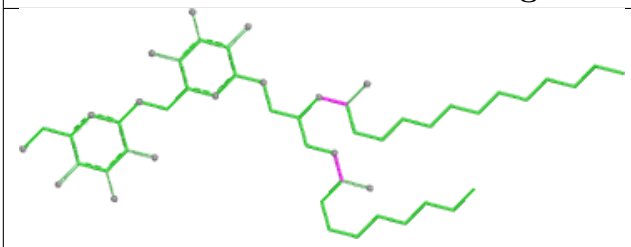


Torsions

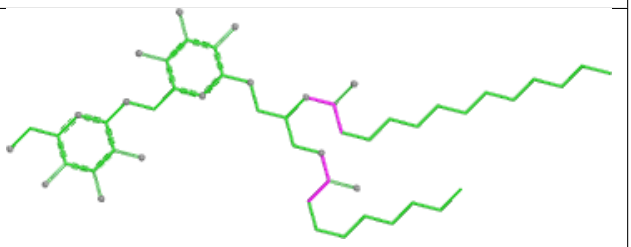


Rings

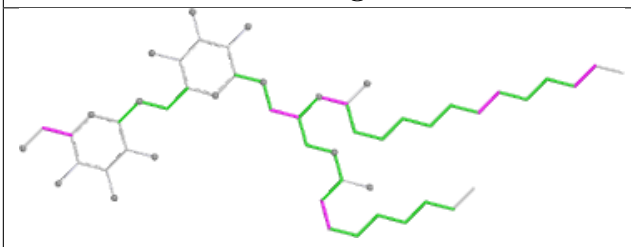
Ligand DGD C 523



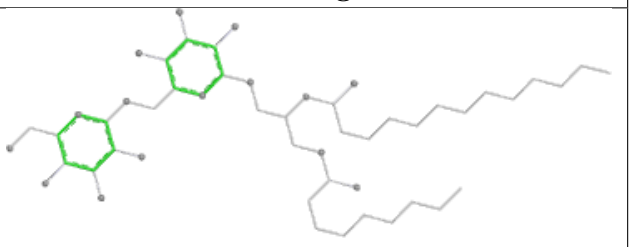
Bond lengths



Bond angles

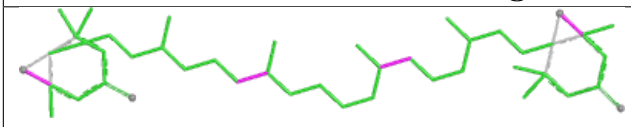


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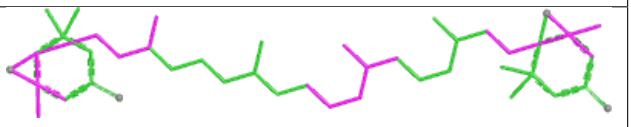


Rings

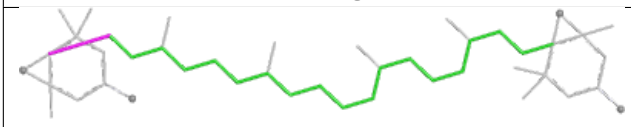
Ligand XAT GG 619



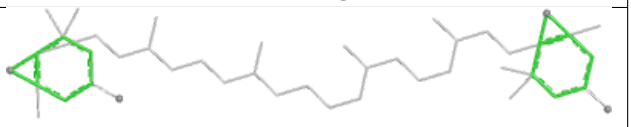
Bond lengths



Bond angles

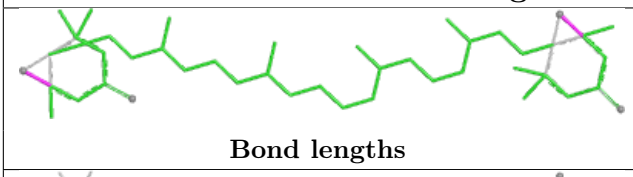


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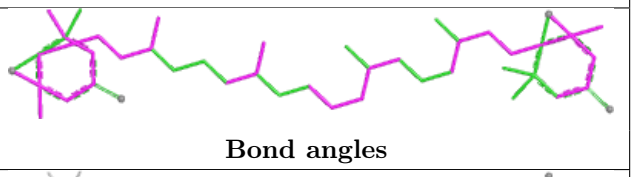


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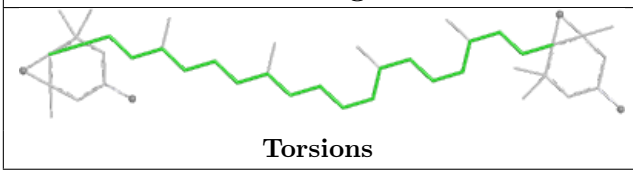
Ligand XAT RR 316



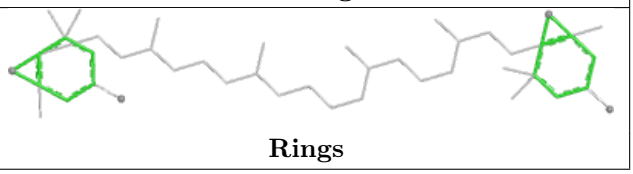
Bond lengths



Bond angles

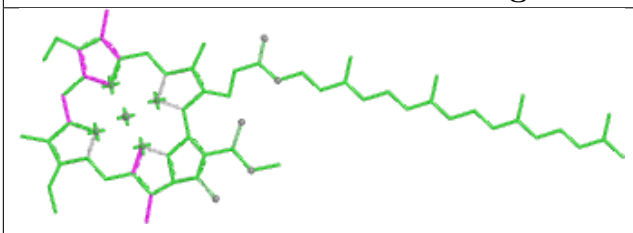


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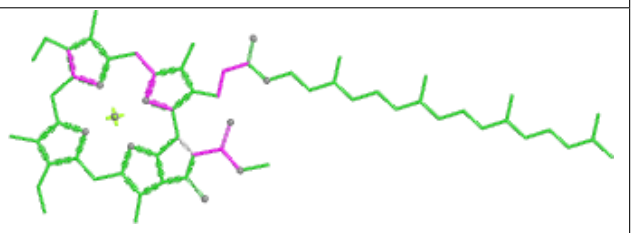


Rings

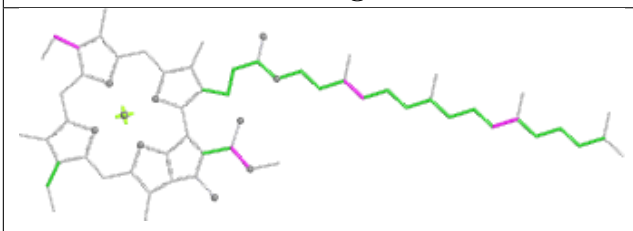
Ligand CLA DD 401



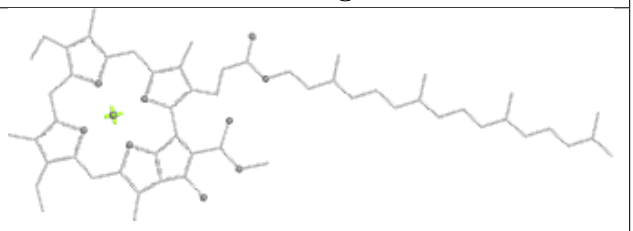
Bond lengths



Bond angles

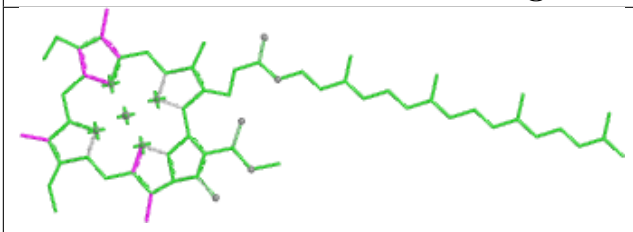


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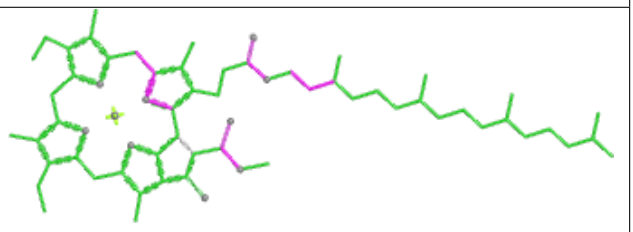


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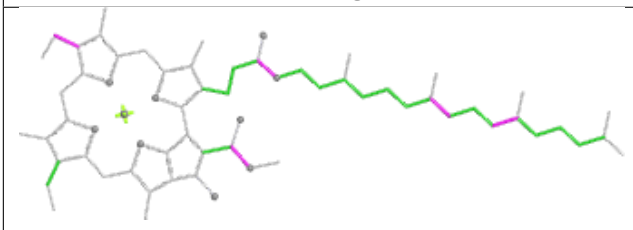
Ligand CLA b 608



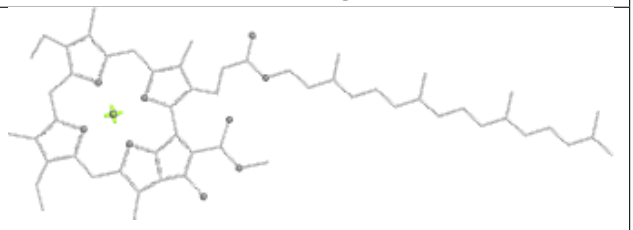
Bond lengths



Bond angles

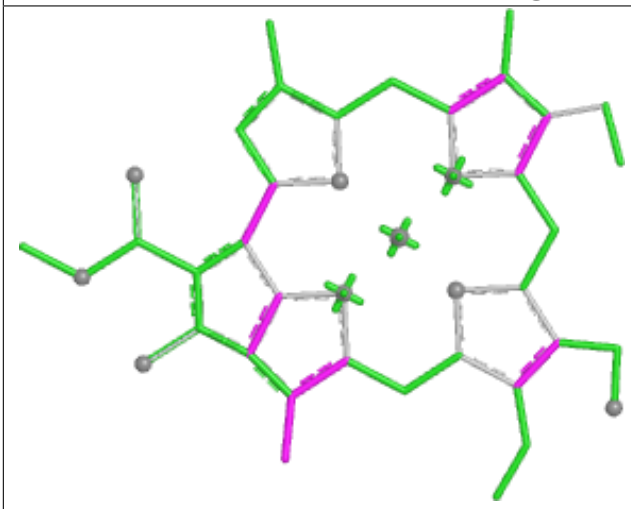


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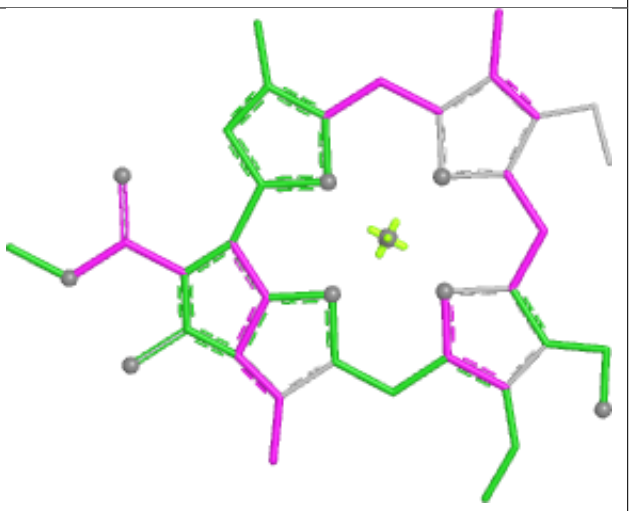


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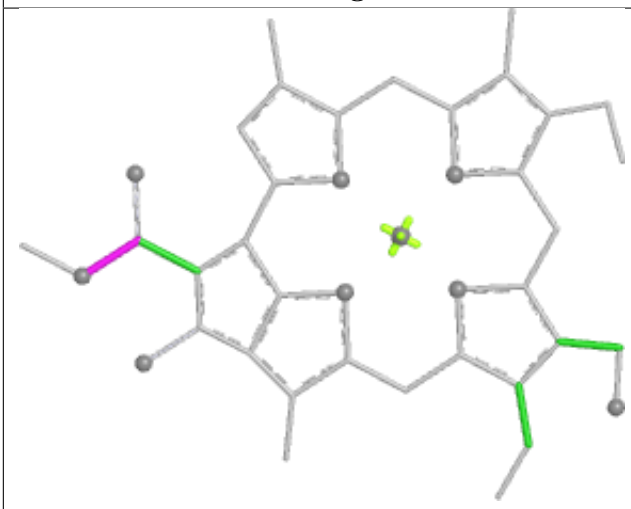
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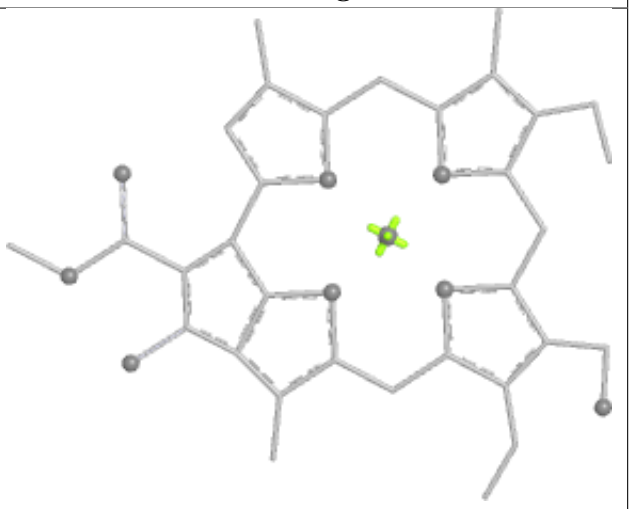
Bond lengths



Bond angles

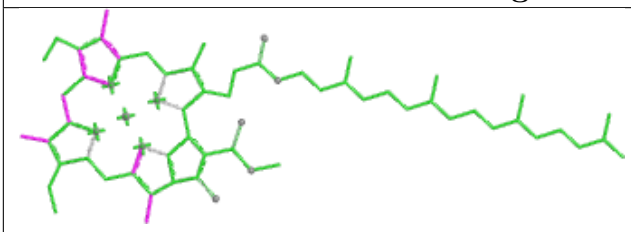


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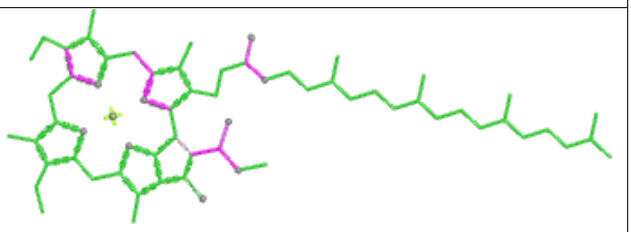


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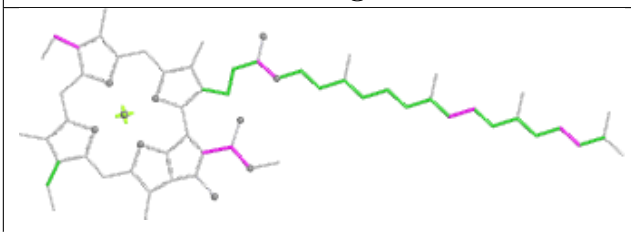
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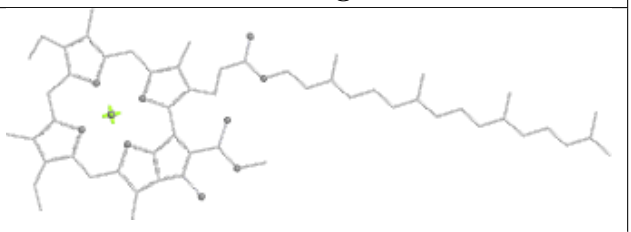
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Bond angles

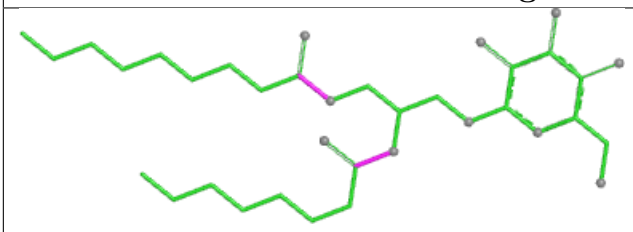


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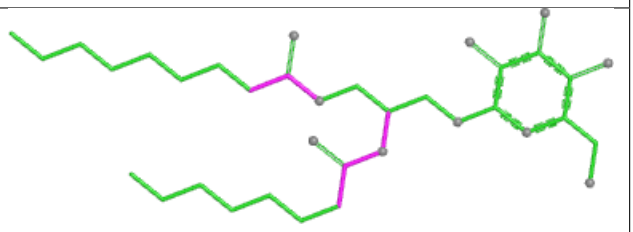


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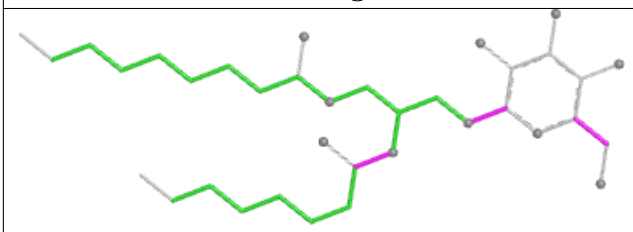
Ligand LMG A 415



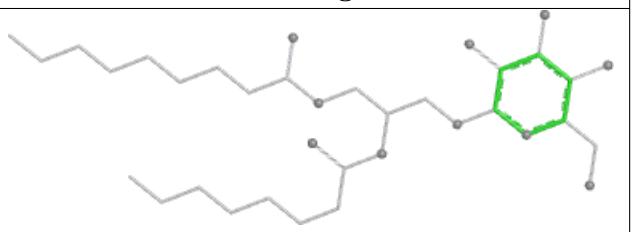
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Bond angles

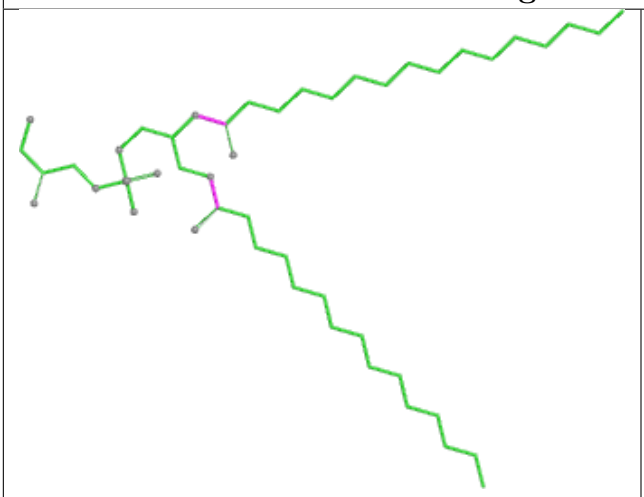


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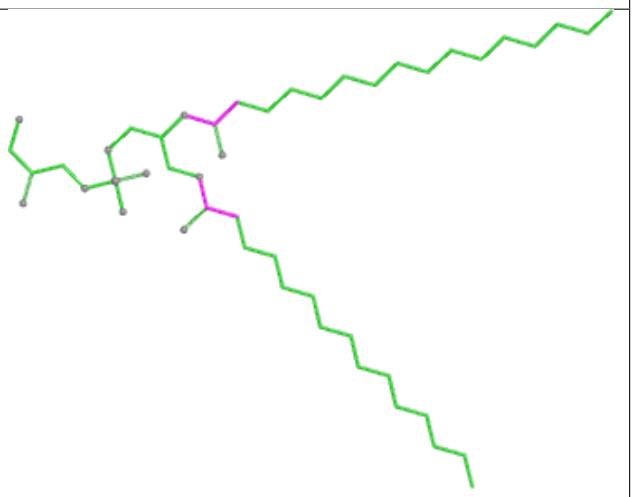


Rings

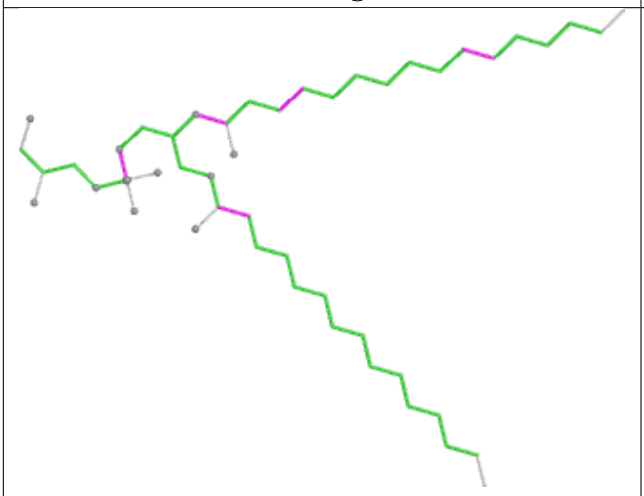
Ligand LHG Ss 616



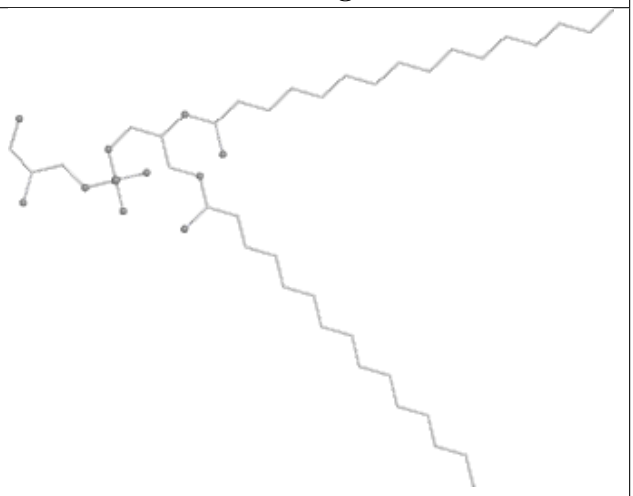
Bond lengths



Bond angles

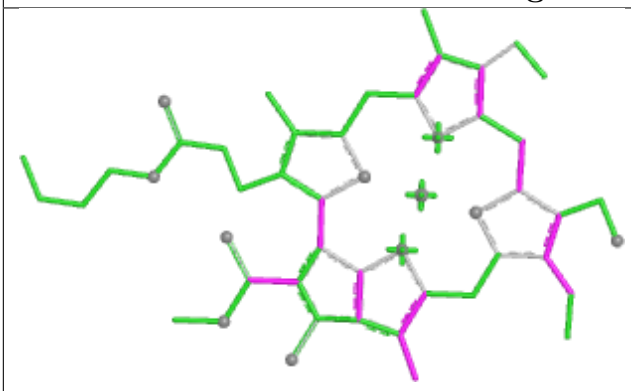


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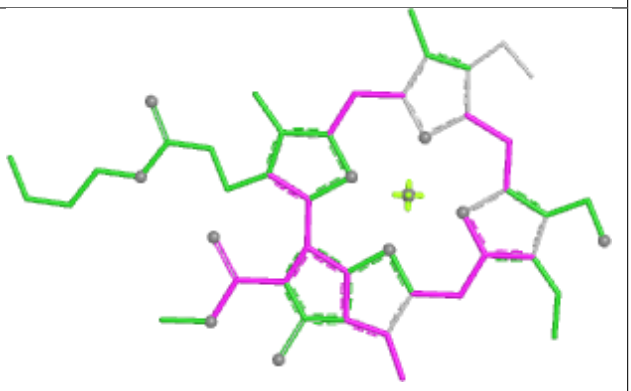


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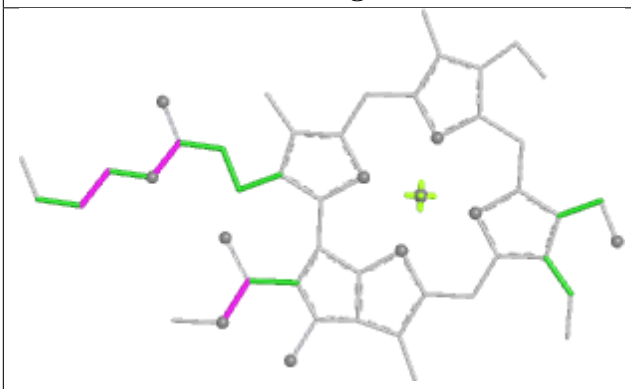
Ligand CHL n 601



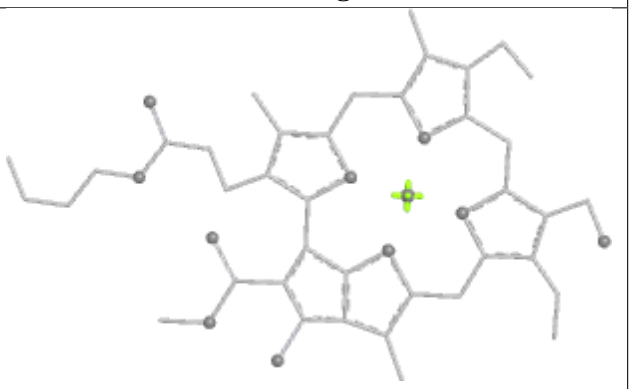
Bond lengths



Bond angles

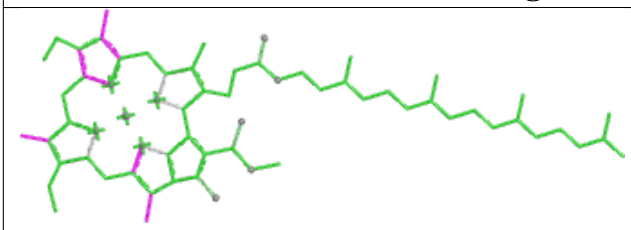


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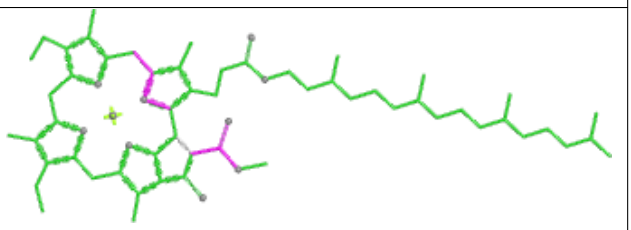


Rings

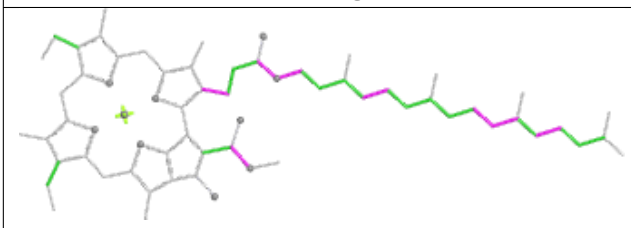
Ligand CLA C 510



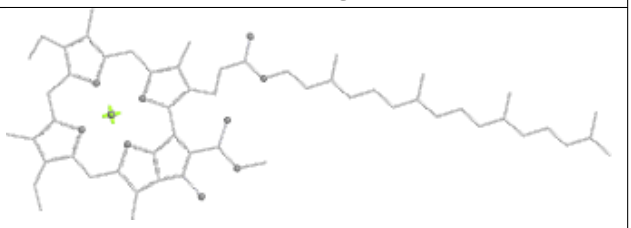
Bond lengths



Bond angles

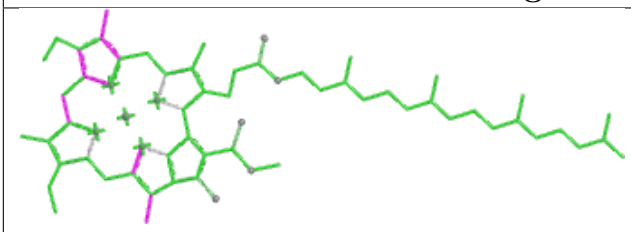


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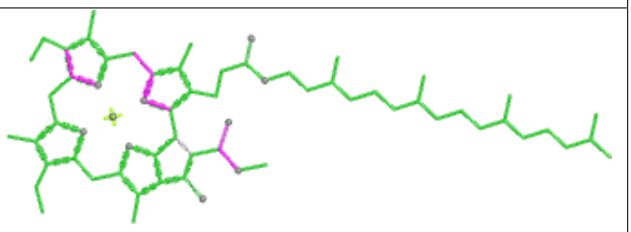


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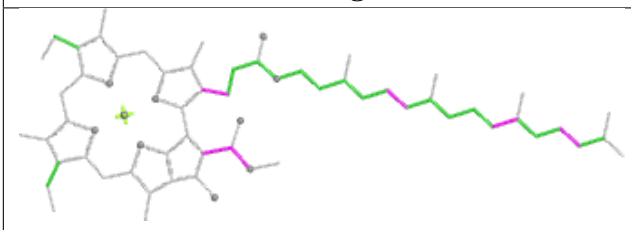
Ligand CLA B 604



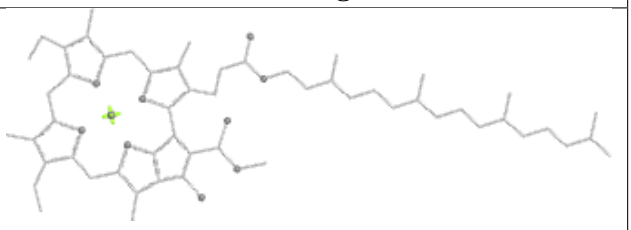
Bond lengths



Bond angles

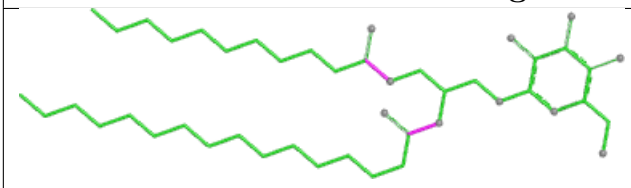


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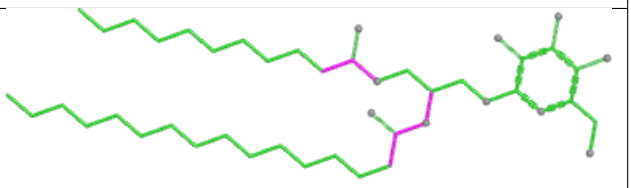


Rings

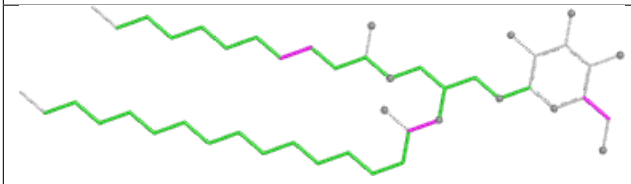
Ligand LMG Dd 408



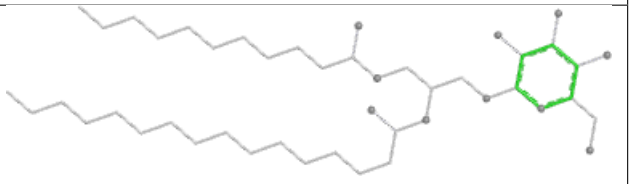
Bond lengths



Bond angles



Torsions



Rings

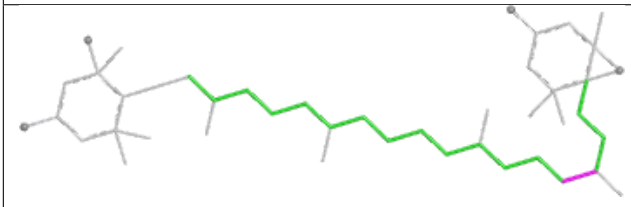
Ligand NEX NN 618



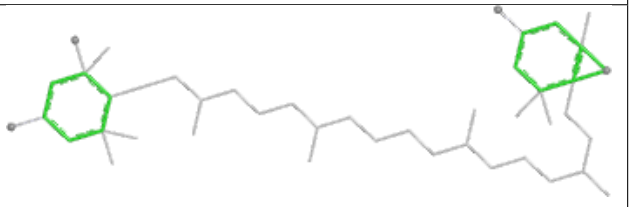
Bond lengths



Bond angles

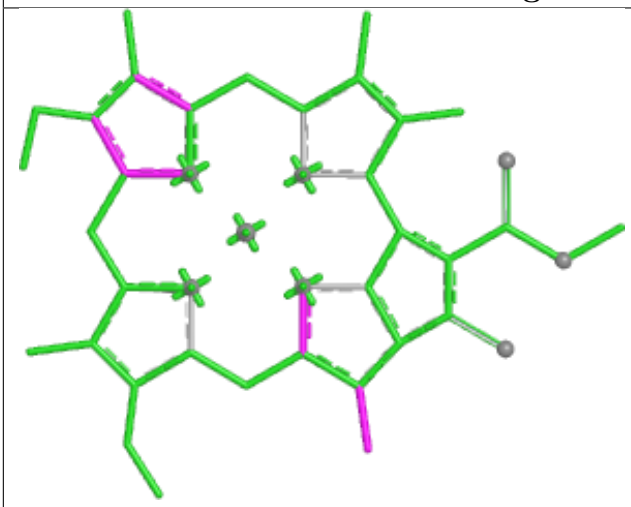


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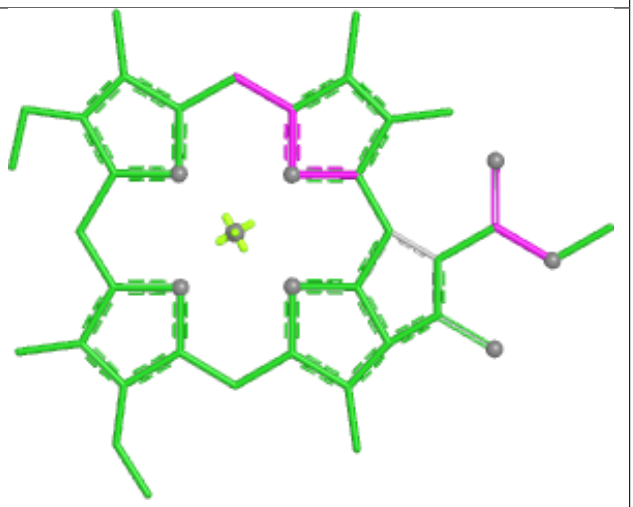


Rings

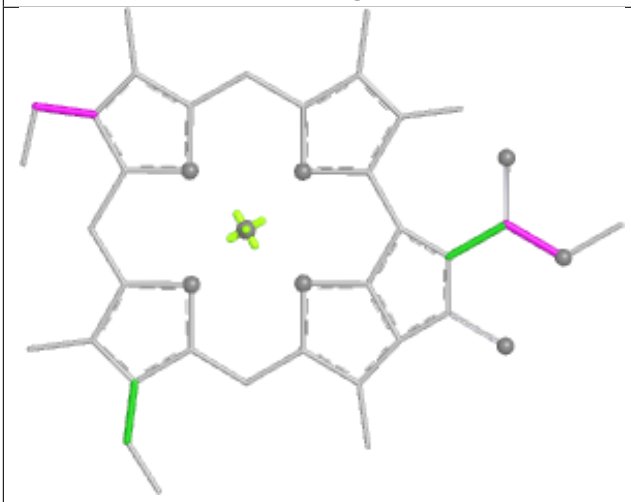
Ligand CLA G 614



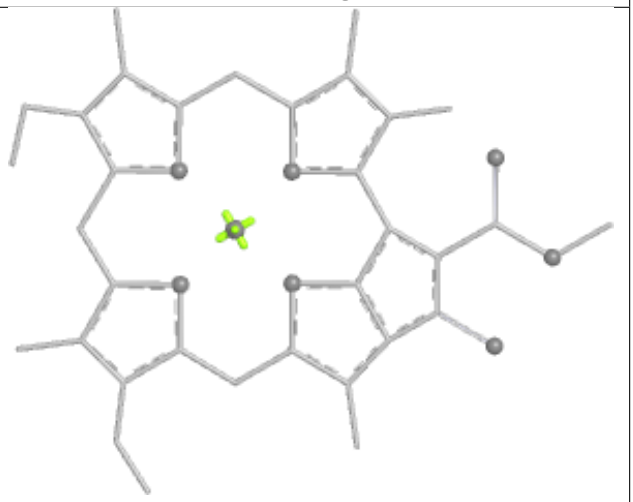
Bond lengths



Bond angles

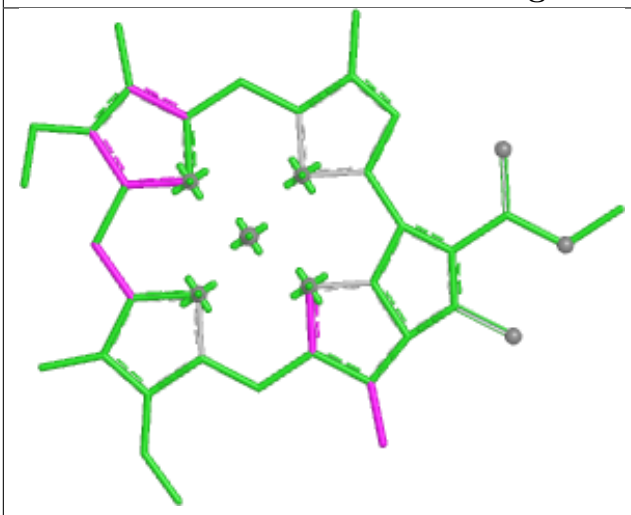


Torsions

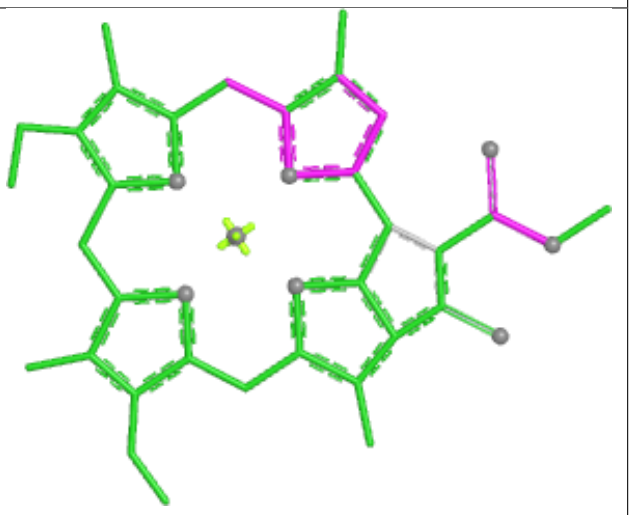


Rings

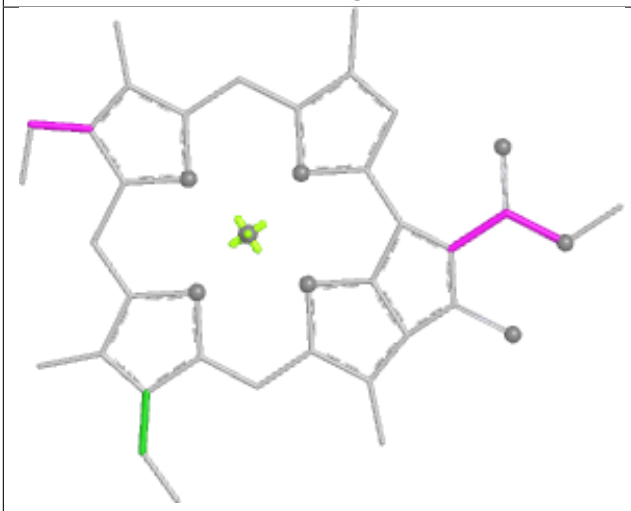
Ligand CLA 3 603



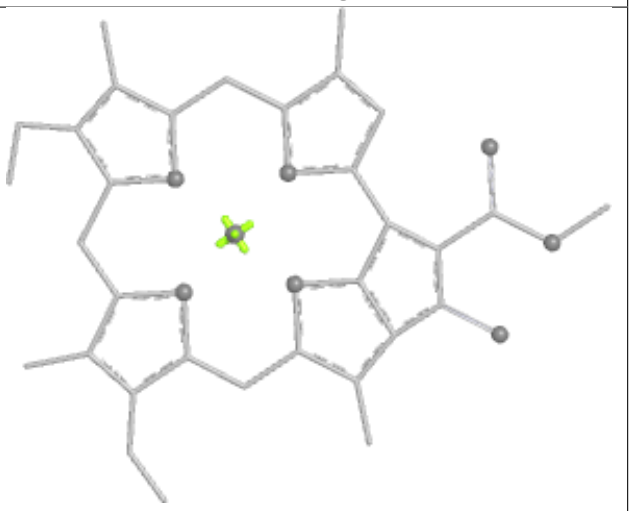
Bond lengths



Bond angles

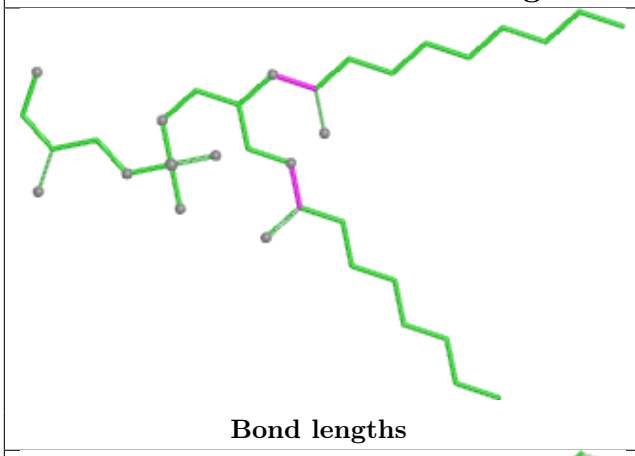


Torsions

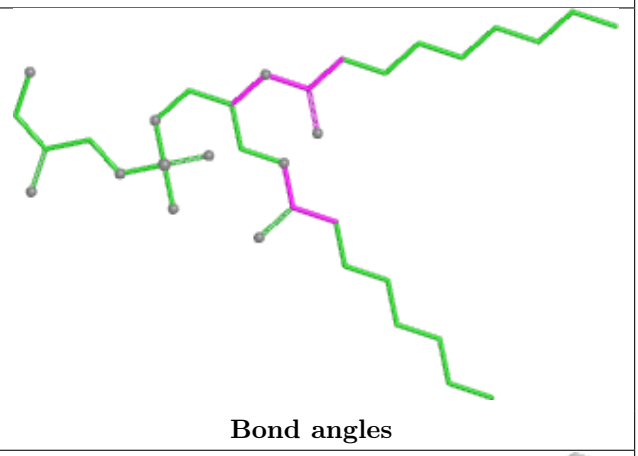


Rings

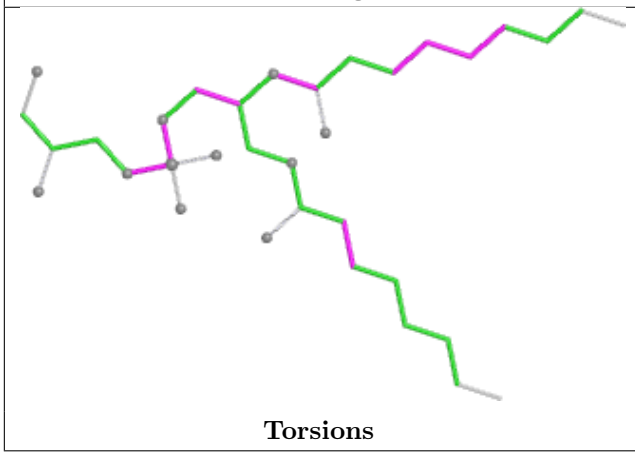
Ligand LHG A 411



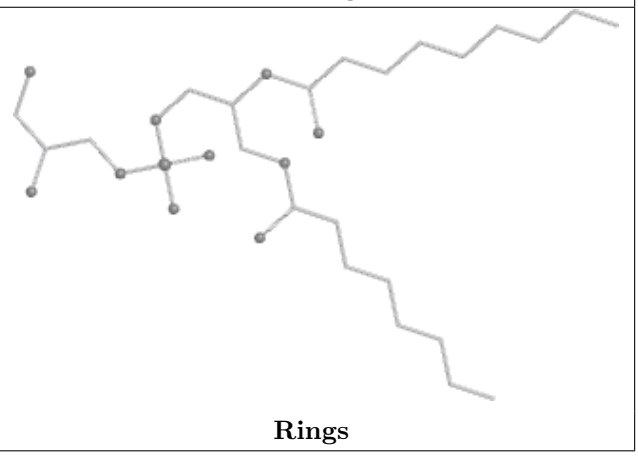
Bond lengths



Bond angles

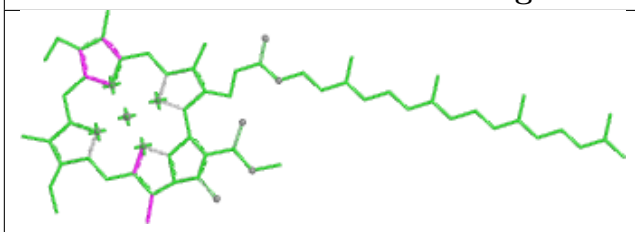


Torsions

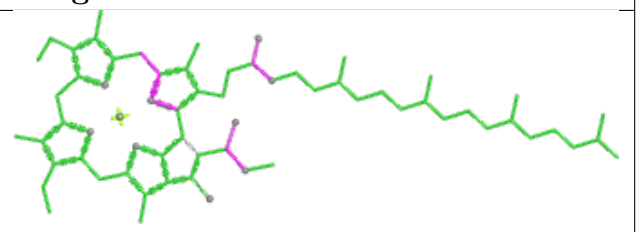


Rings

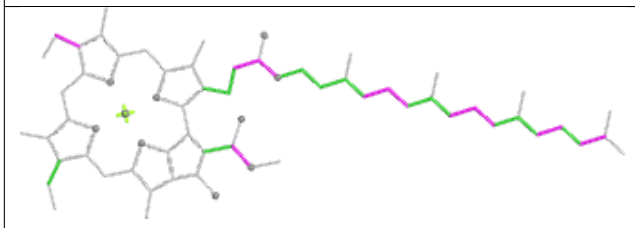
Ligand CLA Gg 304



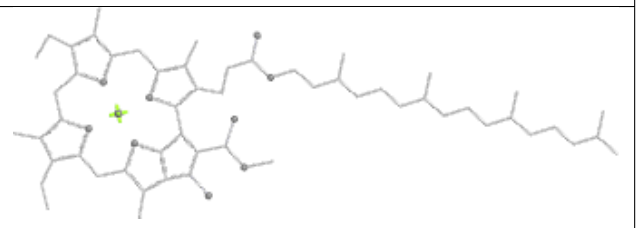
Bond lengths



Bond angles

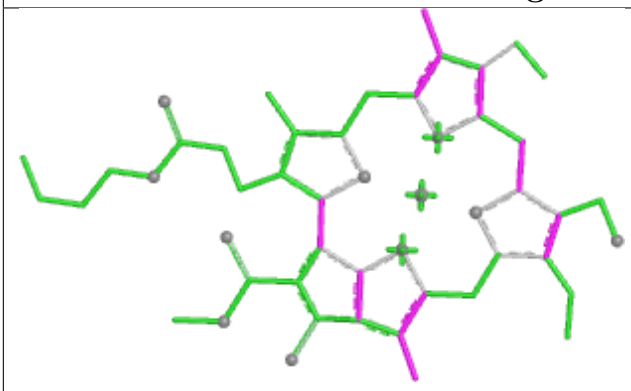


Torsions

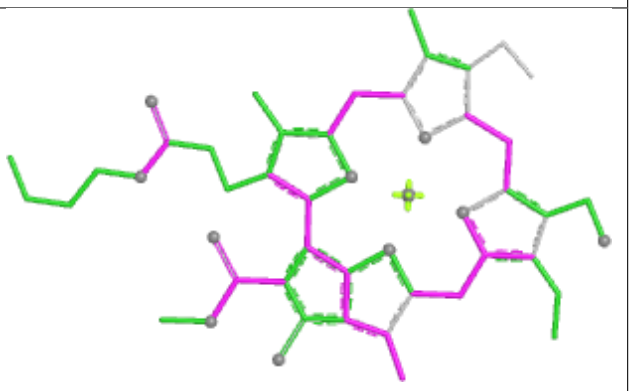


Rings

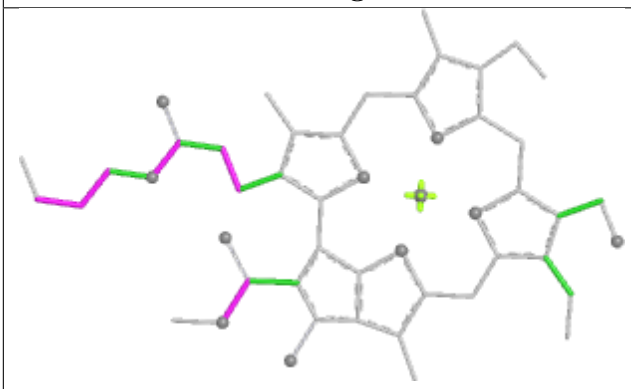
Ligand CHL n 608



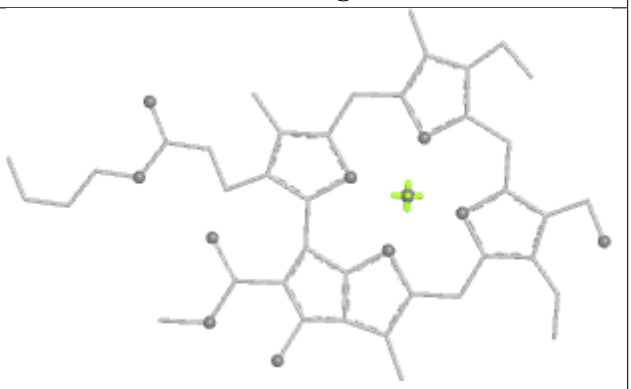
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

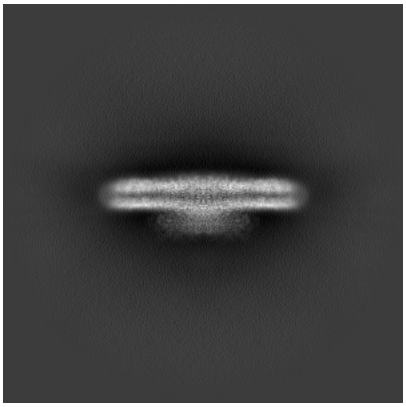
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-39860. These allow visual inspection of the internal detail of the map and identification of artifacts.

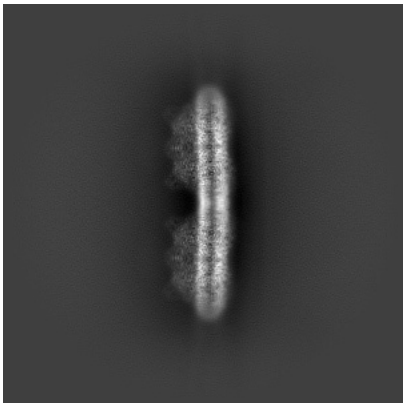
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

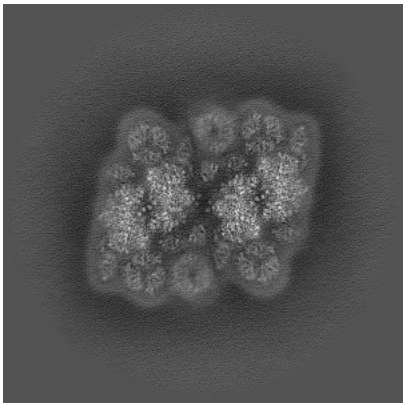
5.1.1 Primary map



X



Y

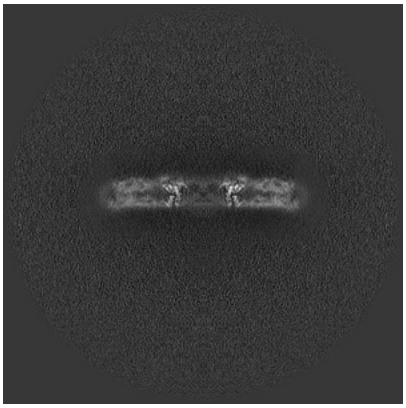


Z

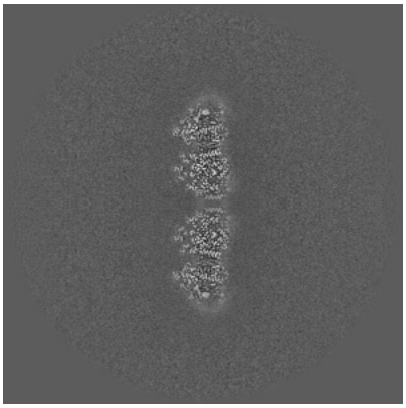
The images above show the map projected in three orthogonal directions.

5.2 Central slices

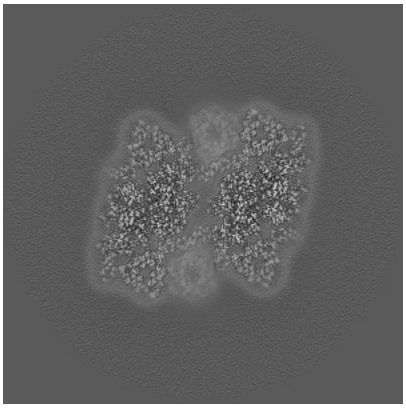
5.2.1 Primary map



X Index: 240



Y Index: 240

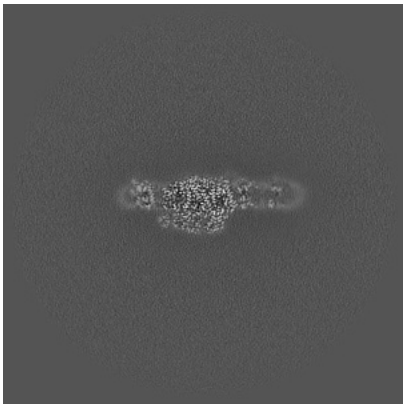


Z Index: 240

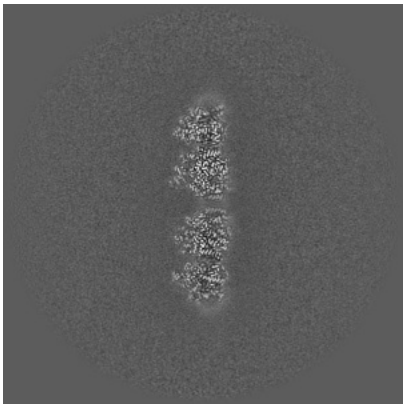
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

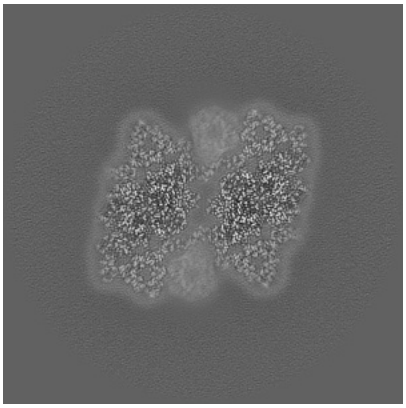
5.3.1 Primary map



X Index: 286



Y Index: 239

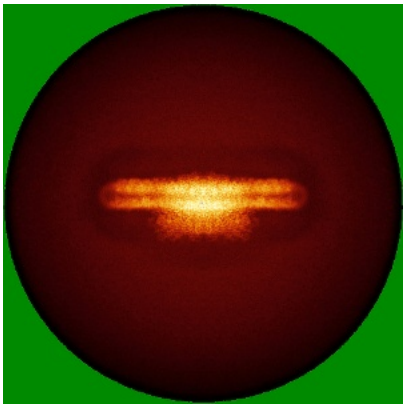


Z Index: 239

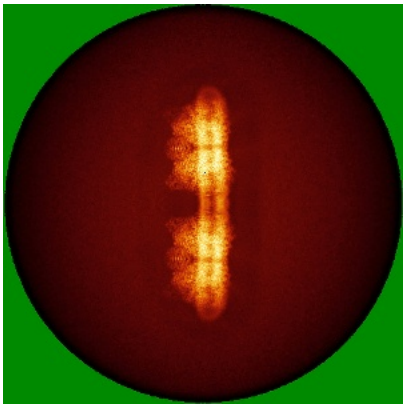
The images above show the largest variance slices of the map in three orthogonal directions.

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

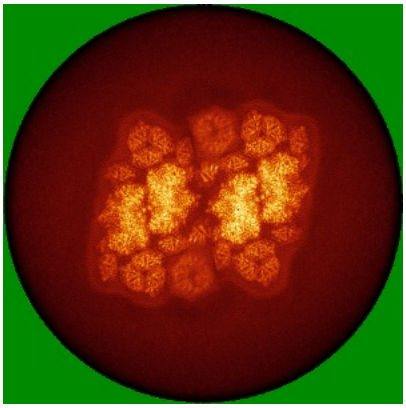
5.4.1 Primary map



X



Y

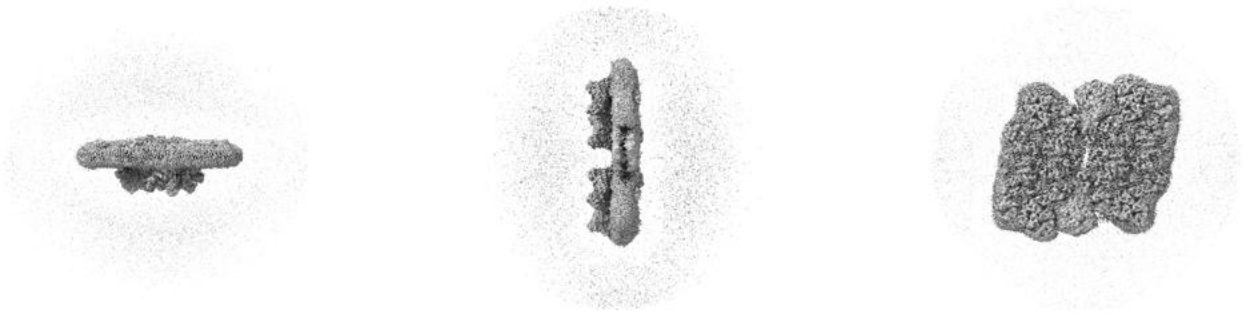


Z

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

5.5 Orthogonal surface views (i)

5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

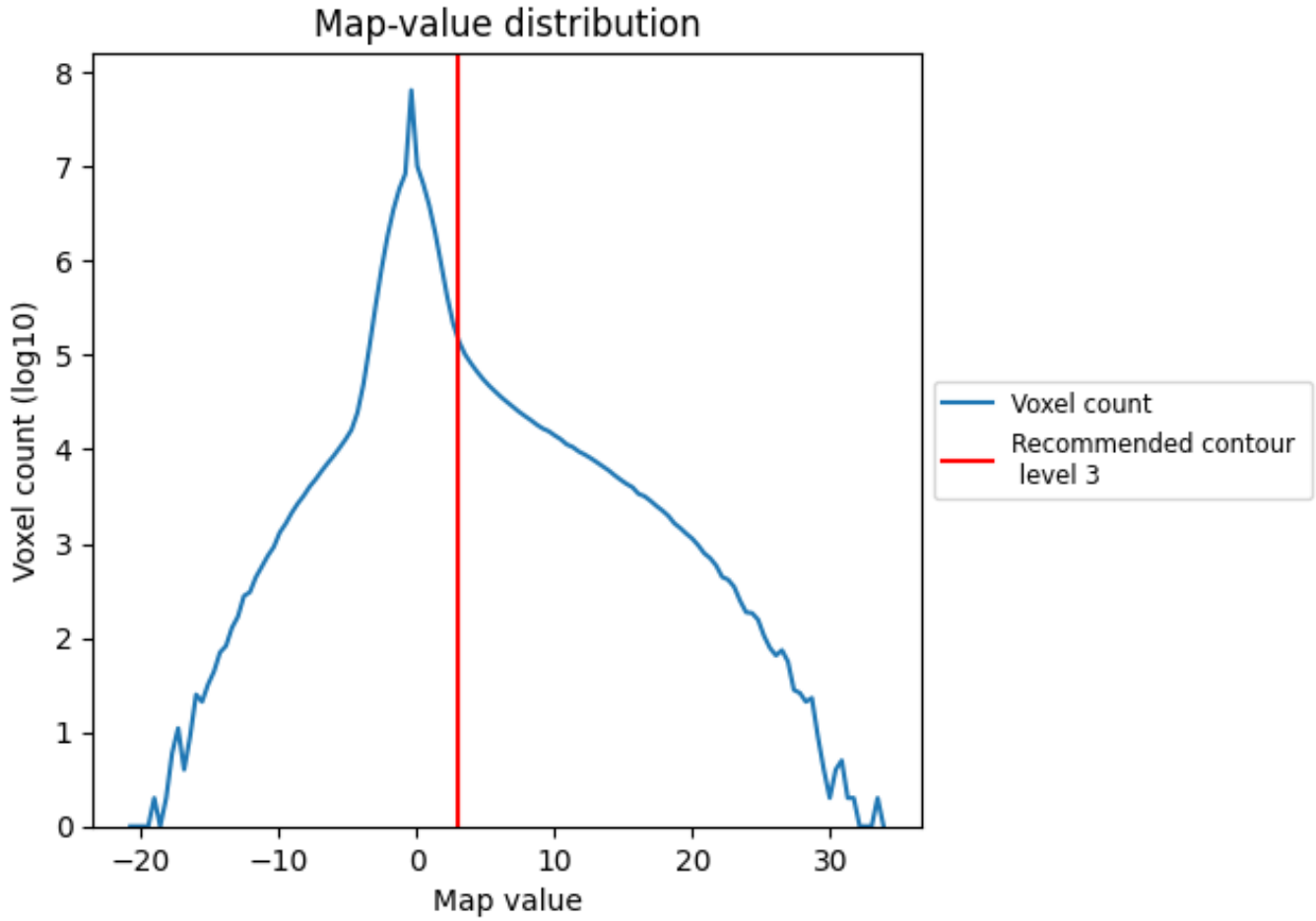
5.6 Mask visualisation (i)

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

6 Map analysis

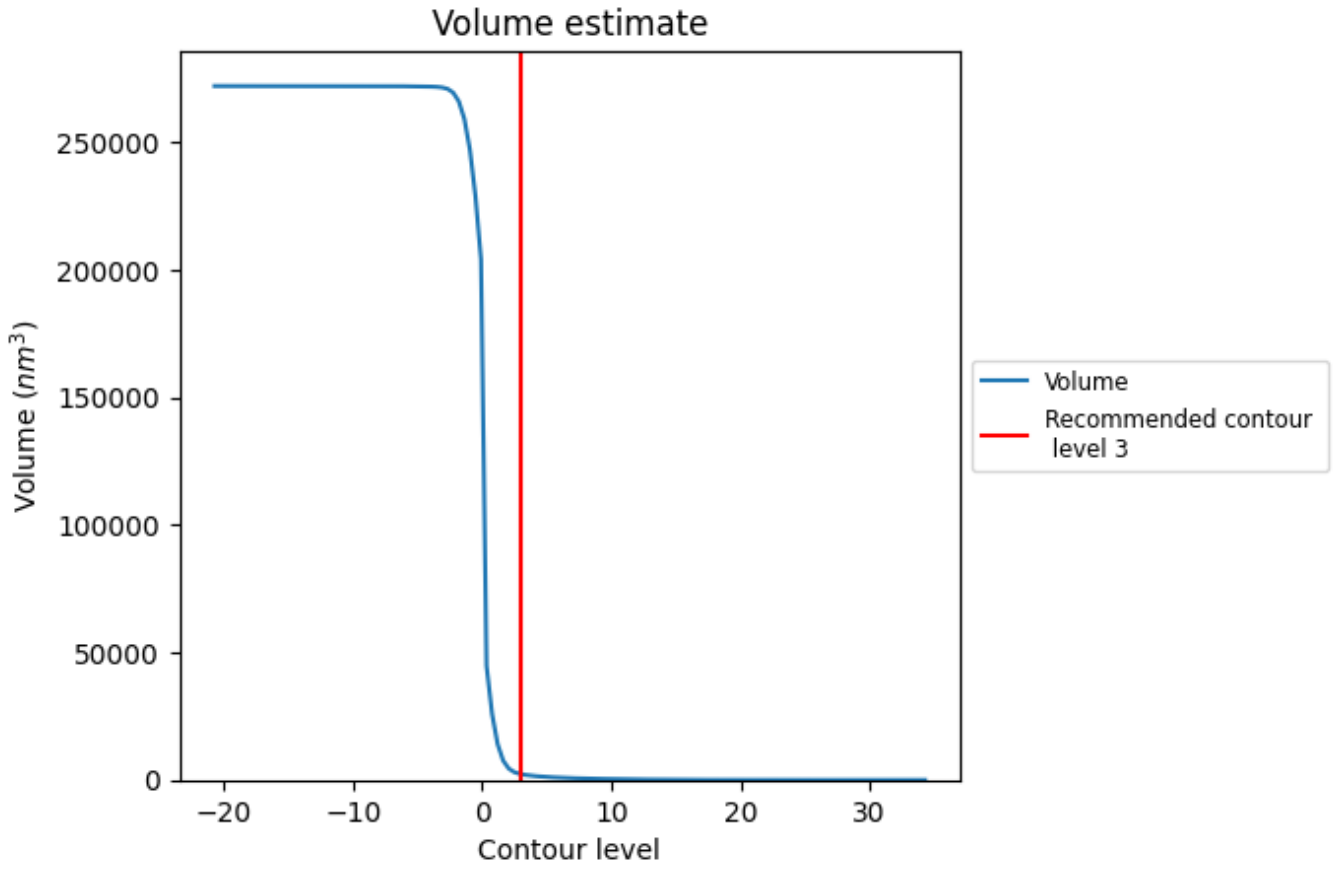
This section contains the results of statistical analysis of the map.

6.1 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.

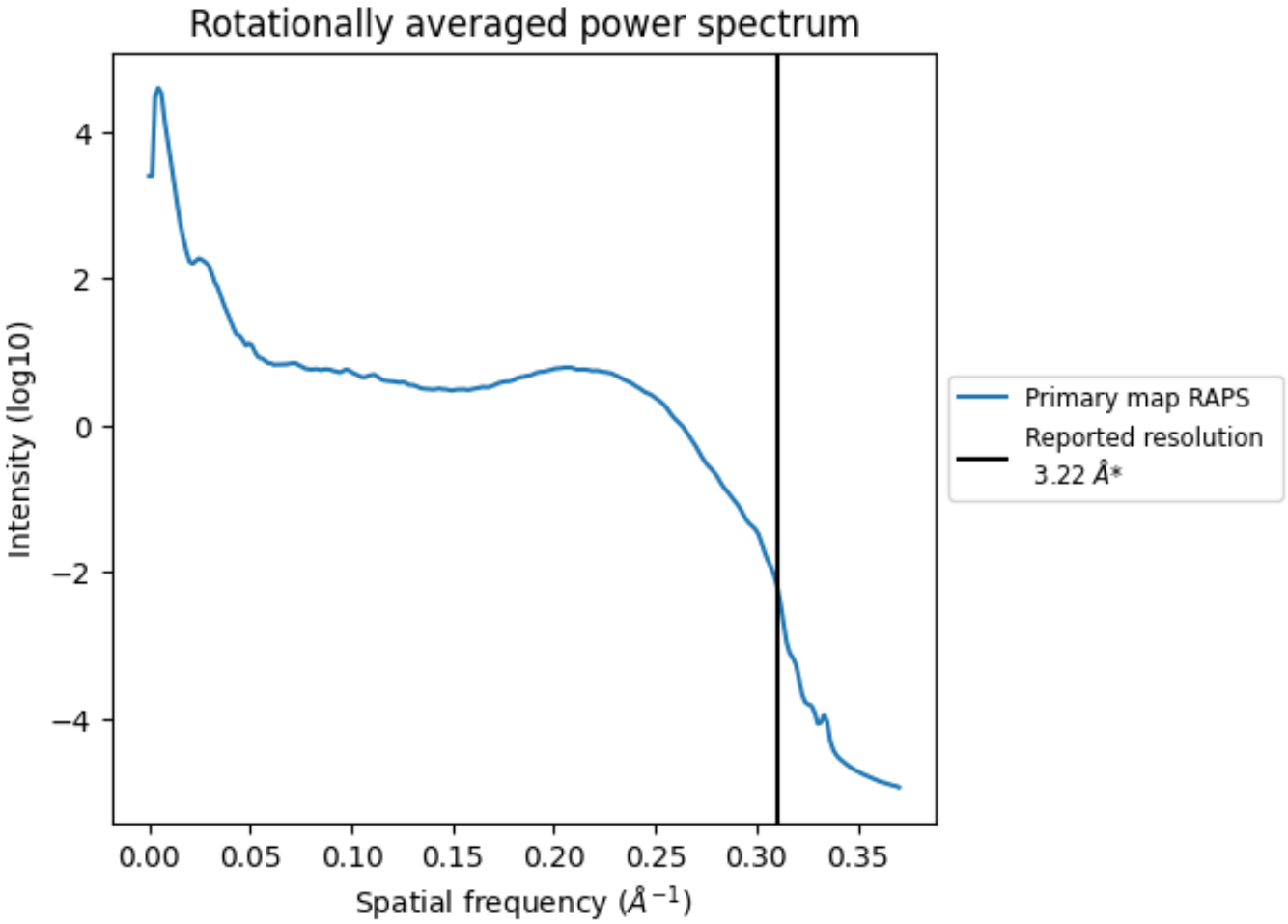
6.2 Volume estimate



The volume at the recommended contour level is 2290 nm^3; this corresponds to an approximate mass of 2069 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.

6.3 Rotationally averaged power spectrum (i)

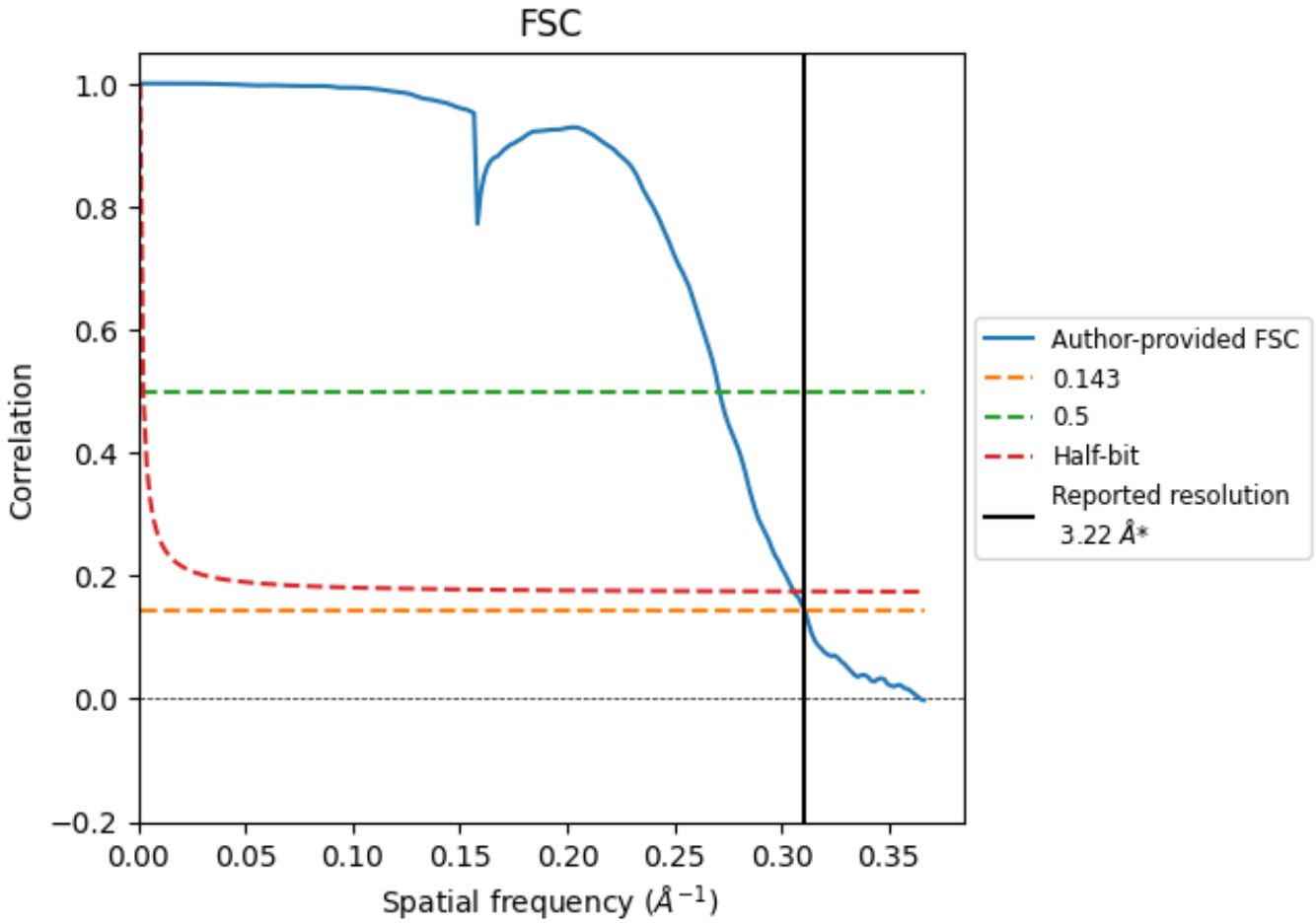


*Reported resolution corresponds to spatial frequency of 0.311 Å^{-1}

7 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.

7.1 FSC



*Reported resolution corresponds to spatial frequency of 0.311 Å^{-1}

7.2 Resolution estimates (i)

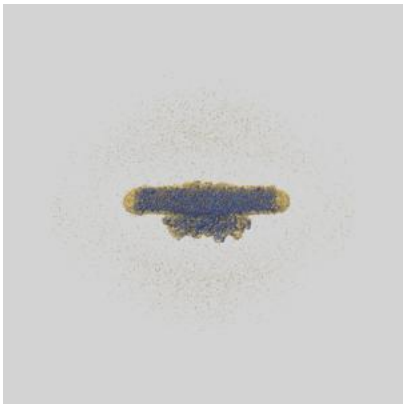
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.69	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

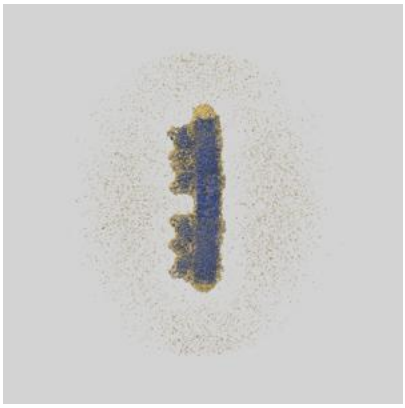
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39860 and PDB model 8Z9D. Per-residue inclusion information can be found in section **??** on page **??**.

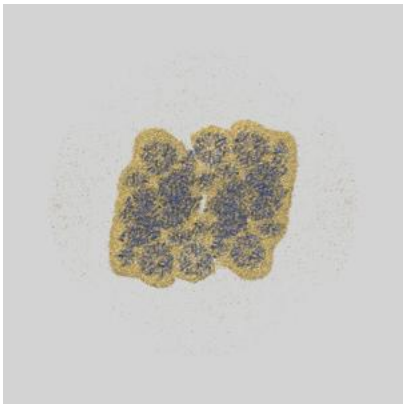
8.1 Map-model overlay



X



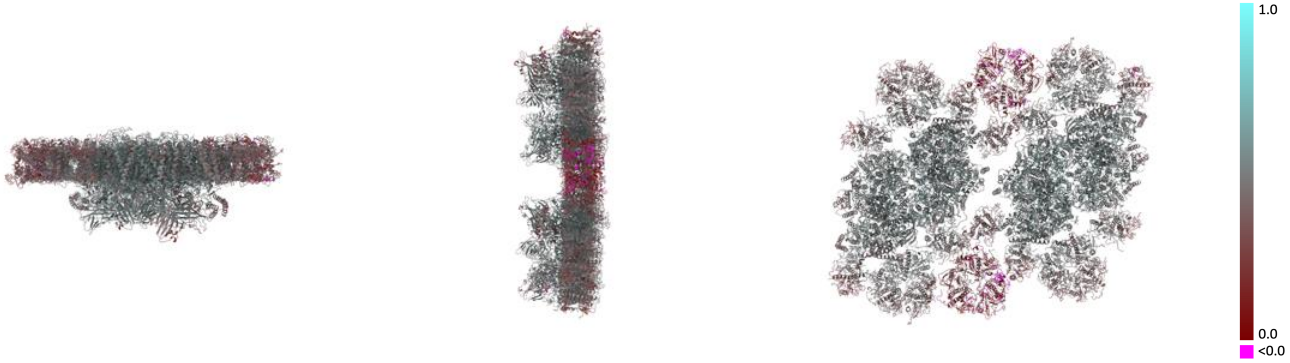
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

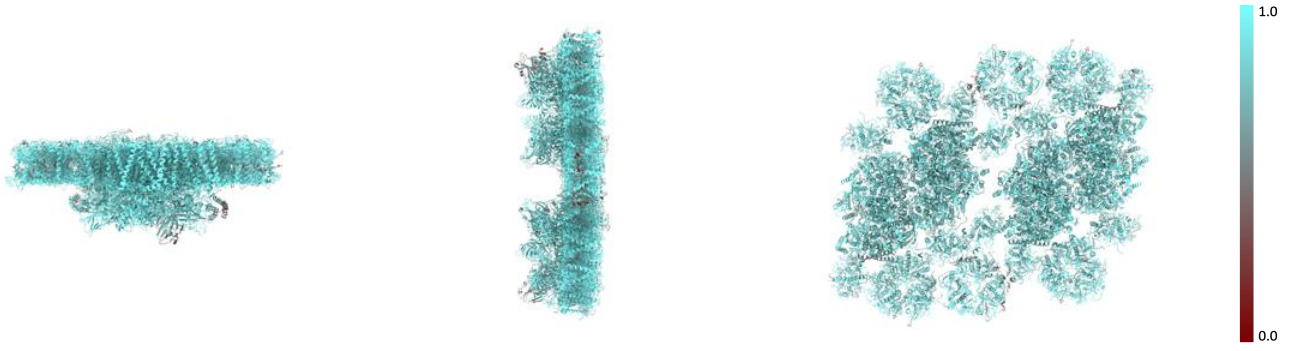
8.2 Q-score mapped to coordinate model (i)



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.

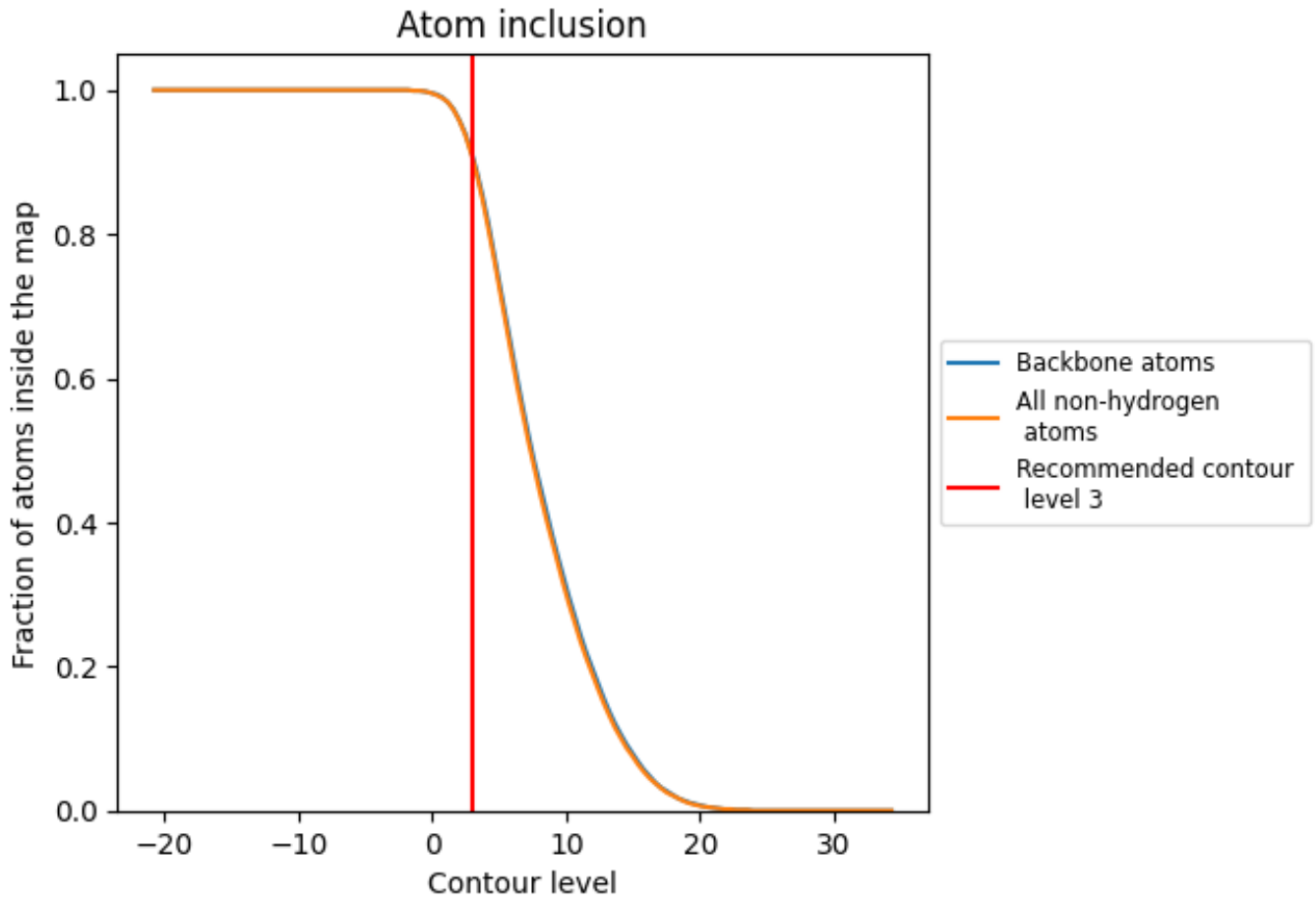
8.3 Atom inclusion mapped to coordinate model (i)



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 (3).

8.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.4520
0	0.7820	0.4470
00	0.8280	0.4610
1	0.9110	0.2140
11	0.9050	0.2020
2	0.8440	0.1600
22	0.8610	0.1580
3	0.8500	0.2130
33	0.8750	0.2150
4	0.8810	0.3570
44	0.8990	0.3600
5	0.7560	0.4260
55	0.7820	0.4450
A	0.9570	0.5300
AA	0.9670	0.5400
Aa	0.9620	0.5300
B	0.9400	0.5240
BB	0.9600	0.5340
Bb	0.9510	0.5250
C	0.9370	0.5200
CC	0.9590	0.5350
Cc	0.9490	0.5110
D	0.9610	0.5370
DD	0.9730	0.5490
Dd	0.9620	0.5260
E	0.9460	0.5120
EE	0.9570	0.5310
Ee	0.9620	0.4650
F	0.9400	0.5180
FF	0.9630	0.5240
Ff	0.9590	0.4630
G	0.8850	0.3760
GG	0.8850	0.3780
Gg	0.8880	0.4220
H	0.9450	0.5020



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HH	0.9680	0.5110
Hh	0.9590	0.5020
I	0.9610	0.5120
II	0.9360	0.5160
Ii	0.9810	0.5360
J	0.9140	0.5180
JJ	0.9390	0.5160
Jj	0.9170	0.4780
K	0.9280	0.5180
KK	0.9460	0.5210
Kk	0.9330	0.4940
L	0.9450	0.5110
LL	0.9660	0.5290
Ll	0.9600	0.5350
M	0.9070	0.4980
MM	0.9530	0.5190
Mm	0.9300	0.5070
N	0.9150	0.4240
NN	0.9210	0.4310
Nn	0.9130	0.4370
O	0.9310	0.4960
OO	0.9490	0.5030
Oo	0.9220	0.4880
P	0.8840	0.4920
PP	0.9000	0.4970
Pp	0.6740	0.4290
Q	0.7830	0.4040
QQ	0.8270	0.4370
Qq	0.6200	0.3860
R	0.8940	0.4400
RR	0.8960	0.4460
Rr	0.8500	0.4130
S	0.7940	0.3810
SS	0.8480	0.3780
Ss	0.8570	0.3590
T	0.8830	0.5030
TT	0.9150	0.5170
Tt	0.9550	0.5320
U	0.8820	0.4630
UU	0.9210	0.4980
Uu	0.9390	0.4600
W	0.9390	0.4990

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Chain	Atom inclusion	Q-score
WW	0.9440	0.5110
Ww	0.9320	0.4960
X	0.8750	0.4520
XX	0.8870	0.4570
Xx	0.9750	0.4450
Y	0.9120	0.4590
YY	0.9200	0.4640
Yy	0.9240	0.4790
Z	0.8960	0.4590
ZZ	0.9490	0.4830
Zz	0.9030	0.4090
a	0.9510	0.5180
b	0.9400	0.5140
c	0.9320	0.4970
d	0.9470	0.5150
e	0.9380	0.4520
f	0.9430	0.4510
g	0.8810	0.4140
h	0.9510	0.4950
i	0.9510	0.4960
j	0.8720	0.4540
k	0.9070	0.4750
l	0.9480	0.5210
m	0.9000	0.4900
n	0.9050	0.4240
o	0.8960	0.4860
p	0.6280	0.4170
q	0.5550	0.3560
r	0.8720	0.4080
s	0.8580	0.3630
t	0.9260	0.5160
u	0.9130	0.4260
w	0.9130	0.4860
x	0.9370	0.4280
y	0.9190	0.4750
z	0.8800	0.3990