Full wwPDB EM Validation Report

May 7, 2024 – 03:27 PM JST

PDB ID	:	8JJR
EMDB ID	:	EMD-36366
Title	:	Cryo-EM structure of Symbiodinium photosystem I
Authors	:	Zhao, L.S.; Wang, N.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2023-05-31
Resolution	:	2.80 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:

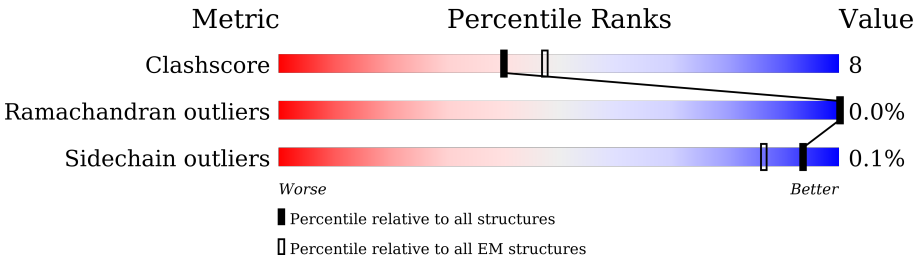
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	256	65% 11% 24%
2	B	269	58% 11% 31%
3	C	193	89% 11%
4	D	177	88% 12%
5	E	253	61% 11% 27%
6	F	286	70% 8% 21%
7	G	228	65% 11% 24%
8	H	271	61% 10% 29%

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Mol	Chain	Length	Quality of chain
9	I	246	78% 12% 10%
10	J	203	71% 14% 15%
11	K	226	12% 51% 17% 32%
12	T	206	10% 54% 14% 32%
13	U	137	20% 65% 11% 24%
14	a	687	97%
15	b	669	98%
16	c	161	53% 47%
17	d	295	73% 27%
18	e	121	60% 40%
19	f	279	61% 39%
20	i	179	67% 33%
21	j	141	70% 30%
22	l	361	70% 30%
23	m	142	56% 44%
24	r	152	86% 14%
25	x	121	65% 35%
26	y	223	8% 58% 42%

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
27	CLA	A	601	X	-	-	-
27	CLA	A	602	X	-	-	-
27	CLA	A	603	X	-	-	-
27	CLA	A	604	X	-	-	-
27	CLA	A	605	X	-	-	-
27	CLA	A	606	X	-	-	-
27	CLA	A	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	609	X	-	-	-
27	CLA	A	610	X	-	-	-
27	CLA	A	611	X	-	-	-
27	CLA	A	612	X	-	-	-
27	CLA	B	601	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	C	201	X	-	-	-
27	CLA	C	202	X	-	-	-
27	CLA	C	203	X	-	-	-
27	CLA	C	204	X	-	-	-
27	CLA	C	205	X	-	-	-
27	CLA	C	206	X	-	-	-
27	CLA	C	207	X	-	-	-
27	CLA	C	208	X	-	-	-
27	CLA	C	209	X	-	-	-
27	CLA	C	211	X	-	-	-
27	CLA	C	212	X	-	-	-
27	CLA	D	601	X	-	-	-
27	CLA	D	602	X	-	-	-
27	CLA	D	603	X	-	-	-
27	CLA	D	604	X	-	-	-
27	CLA	D	605	X	-	-	-
27	CLA	D	606	X	-	-	-
27	CLA	D	607	X	-	-	-
27	CLA	D	608	X	-	-	-
27	CLA	D	609	X	-	-	-
27	CLA	D	610	X	-	-	-
27	CLA	D	611	X	-	-	-
27	CLA	D	612	X	-	-	-
27	CLA	E	602	X	-	-	-
27	CLA	E	603	X	-	-	-
27	CLA	E	604	X	-	-	-
27	CLA	E	605	X	-	-	-
27	CLA	E	606	X	-	-	-
27	CLA	E	607	X	-	-	-
27	CLA	E	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	E	609	X	-	-	-
27	CLA	E	611	X	-	-	-
27	CLA	E	612	X	-	-	-
27	CLA	F	601	X	-	-	-
27	CLA	F	602	X	-	-	-
27	CLA	F	603	X	-	-	-
27	CLA	F	604	X	-	-	-
27	CLA	F	605	X	-	-	-
27	CLA	F	606	X	-	-	-
27	CLA	F	607	X	-	-	-
27	CLA	F	608	X	-	-	-
27	CLA	F	610	X	-	-	-
27	CLA	F	617	X	-	-	-
27	CLA	F	619	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	605	X	-	-	-
27	CLA	G	606	X	-	-	-
27	CLA	G	607	X	-	-	-
27	CLA	G	608	X	-	-	-
27	CLA	G	609	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	H	303	X	-	-	-
27	CLA	H	304	X	-	-	-
27	CLA	H	305	X	-	-	-
27	CLA	H	306	X	-	-	-
27	CLA	H	307	X	-	-	-
27	CLA	H	308	X	-	-	-
27	CLA	H	309	X	-	-	-
27	CLA	H	310	X	-	-	-
27	CLA	H	312	X	-	-	-
27	CLA	H	313	X	-	-	-
27	CLA	H	319	X	-	-	-
27	CLA	I	601	X	-	-	-
27	CLA	I	602	X	-	-	-
27	CLA	I	603	X	-	-	-
27	CLA	I	605	X	-	-	-
27	CLA	I	606	X	-	-	-
27	CLA	I	607	X	-	-	-
27	CLA	I	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	I	609	X	-	-	-
27	CLA	I	610	X	-	-	-
27	CLA	I	611	X	-	-	-
27	CLA	I	616	X	-	-	-
27	CLA	J	601	X	-	-	-
27	CLA	J	603	X	-	-	-
27	CLA	J	605	X	-	-	-
27	CLA	J	607	X	-	-	-
27	CLA	J	609	X	-	-	-
27	CLA	K	601	X	-	-	-
27	CLA	K	602	X	-	-	-
27	CLA	K	603	X	-	-	-
27	CLA	K	604	X	-	-	-
27	CLA	K	605	X	-	-	-
27	CLA	K	606	X	-	-	-
27	CLA	K	608	X	-	-	-
27	CLA	T	601	X	-	-	-
27	CLA	T	602	X	-	-	-
27	CLA	T	603	X	-	-	-
27	CLA	T	604	X	-	-	-
27	CLA	T	605	X	-	-	-
27	CLA	T	606	X	-	-	-
27	CLA	T	607	X	-	-	-
27	CLA	T	609	X	-	-	-
27	CLA	U	601	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	605	X	-	-	-
27	CLA	U	606	X	-	-	-
27	CLA	a	801	X	-	-	-
27	CLA	a	802	X	-	-	-
27	CLA	a	803	X	-	-	-
27	CLA	a	804	X	-	-	-
27	CLA	a	805	X	-	-	-
27	CLA	a	806	X	-	-	-
27	CLA	a	807	X	-	-	-
27	CLA	a	808	X	-	-	-
27	CLA	a	809	X	-	-	-
27	CLA	a	810	X	-	-	-
27	CLA	a	811	X	-	-	-
27	CLA	a	812	X	-	-	-
27	CLA	a	813	X	-	-	-
27	CLA	a	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	a	815	X	-	-	-
27	CLA	a	816	X	-	-	-
27	CLA	a	817	X	-	-	-
27	CLA	a	818	X	-	-	-
27	CLA	a	819	X	-	-	-
27	CLA	a	820	X	-	-	-
27	CLA	a	821	X	-	-	-
27	CLA	a	822	X	-	-	-
27	CLA	a	823	X	-	-	-
27	CLA	a	824	X	-	-	-
27	CLA	a	825	X	-	-	-
27	CLA	a	826	X	-	-	-
27	CLA	a	827	X	-	-	-
27	CLA	a	828	X	-	-	-
27	CLA	a	829	X	-	-	-
27	CLA	a	830	X	-	-	-
27	CLA	a	831	X	-	-	-
27	CLA	a	837	X	-	-	-
27	CLA	a	839	X	-	-	-
27	CLA	b	701	X	-	-	-
27	CLA	b	702	X	-	-	-
27	CLA	b	703	X	-	-	-
27	CLA	b	704	X	-	-	-
27	CLA	b	705	X	-	-	-
27	CLA	b	706	X	-	-	-
27	CLA	b	707	X	-	-	-
27	CLA	b	708	X	-	-	-
27	CLA	b	709	X	-	-	-
27	CLA	b	710	X	-	-	-
27	CLA	b	711	X	-	-	-
27	CLA	b	712	X	-	-	-
27	CLA	b	713	X	-	-	-
27	CLA	b	714	X	-	-	-
27	CLA	b	715	X	-	-	-
27	CLA	b	716	X	-	-	-
27	CLA	b	717	X	-	-	-
27	CLA	b	718	X	-	-	-
27	CLA	b	719	X	-	-	-
27	CLA	b	720	X	-	-	-
27	CLA	b	721	X	-	-	-
27	CLA	b	722	X	-	-	-
27	CLA	b	723	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	724	X	-	-	-
27	CLA	b	725	X	-	-	-
27	CLA	b	726	X	-	-	-
27	CLA	b	727	X	-	-	-
27	CLA	b	728	X	-	-	-
27	CLA	f	302	X	-	-	-
27	CLA	f	303	X	-	-	-
27	CLA	j	202	X	-	-	-
27	CLA	l	402	X	-	-	-
27	CLA	l	403	X	-	-	-
27	CLA	l	404	X	-	-	-
27	CLA	l	405	X	-	-	-
27	CLA	l	406	X	-	-	-
27	CLA	l	407	X	-	-	-
27	CLA	l	408	X	-	-	-
27	CLA	l	409	X	-	-	-
27	CLA	l	410	X	-	-	-
27	CLA	l	411	X	-	-	-
27	CLA	l	412	X	-	-	-
27	CLA	r	203	X	-	-	-
27	CLA	r	204	X	-	-	-
30	DD6	D	613	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total	C	N	O	S	0	0
			1461	941	239	274	7		

- Molecule 2 is a protein called PCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	185	Total	C	N	O	S	0	0
			1412	900	237	264	11		

- Molecule 3 is a protein called PCP-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	192	Total	C	N	O	S	0	0
			1518	990	244	273	11		

- Molecule 4 is a protein called PCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1375	893	226	245	11		

- Molecule 5 is a protein called PCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	184	Total	C	N	O	S	0	0
			1444	940	241	256	7		

- Molecule 6 is a protein called PCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1731	1118	282	314	17		

- Molecule 7 is a protein called PCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	173	Total	C	N	O	S	0	0
			1329	861	220	238	10		

- Molecule 8 is a protein called PCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1458	948	241	261	8		

- Molecule 9 is a protein called PCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	221	Total	C	N	O	S	0	0
			1736	1138	272	315	11		

- Molecule 10 is a protein called PCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	173	Total	C	N	O	S	0	0
			1322	849	220	244	9		

- Molecule 11 is a protein called PCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	154	Total	C	N	O	S	0	0
			1134	718	194	211	11		

- Molecule 12 is a protein called PCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	140	Total	C	N	O	S	0	0
			1065	681	180	196	8		

- Molecule 13 is a protein called PCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	104	Total	C	N	O	S	0	0
			828	535	144	142	7		

- Molecule 14 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	665	Total	C	N	O	S	0	0
			5250	3443	877	904	26		

- Molecule 15 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	659	Total	C	N	O	S	0	0
			5220	3437	845	918	20		

- Molecule 16 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	86	Total	C	N	O	S	0	0
			651	402	109	131	9		

- Molecule 17 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	216	Total	C	N	O	S	0	0
			1765	1123	308	321	13		

- Molecule 18 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	e	73	Total	C	N	O	0	0
			590	386	101	103		

- Molecule 19 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1349	859	238	246	6		

- Molecule 20 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	120	Total	C	N	O	S	0	0
			971	627	165	177	2		

- Molecule 21 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	99	Total	C	N	O	S	0	0
			791	507	130	153	1		

- Molecule 22 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	253	Total	C	N	O	S	0	0
			1974	1290	319	356	9		

- Molecule 23 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	79	Total	C	N	O	S	0	0
			598	391	102	104	1		

- Molecule 24 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	131	Total	C	N	O	S	0	0
			1082	714	168	194	6		

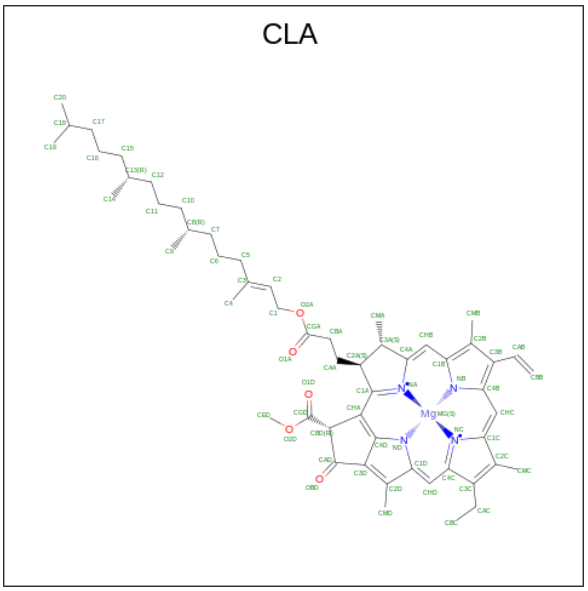
- Molecule 25 is a protein called PsaT.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	79	Total	C	N	O	S	0	0
			642	411	107	123	1		

- Molecule 26 is a protein called PsaU.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	130	Total	C	N	O	S	0	0
			1085	690	184	208	3		

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
27	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms	AltConf
27	a	1	Total C Mg N O 60 50 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 55 45 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 48 38 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 55 45 1 4 5	0
27	a	1	Total C Mg N O 65 55 1 4 5	0
27	a	1	Total C Mg N O 61 51 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0
27	b	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	f	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	f	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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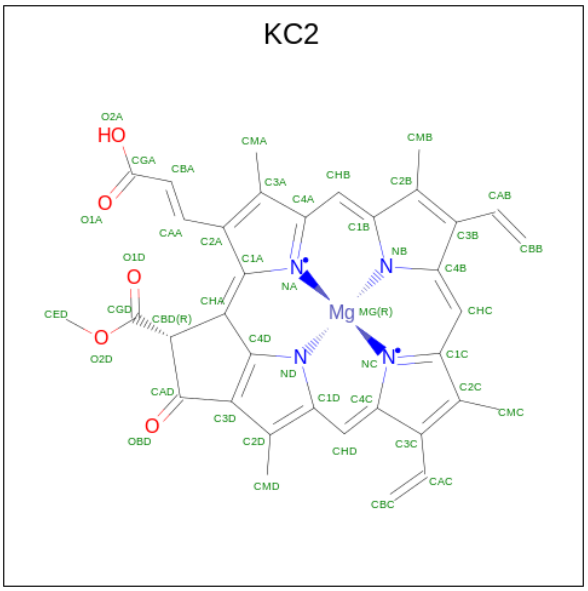
Mol	Chain	Residues	Atoms					AltConf
27	j	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 28 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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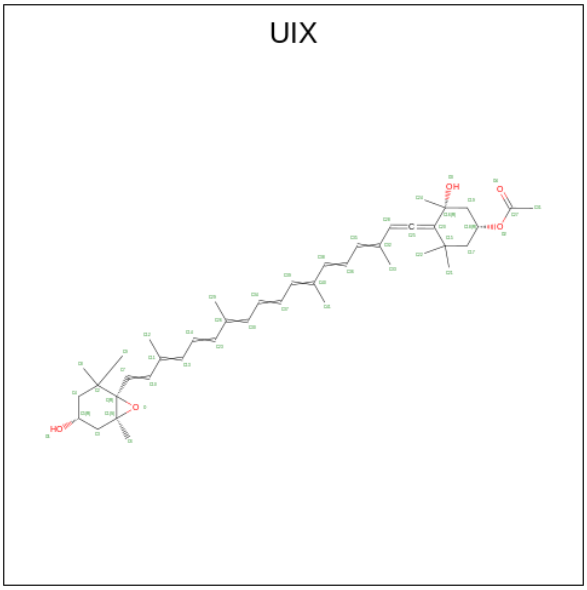
Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (three-letter code: UIX) (formula: $C_{42}H_{58}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			47	42	5	
29	A	1	Total	C	O	0
			47	42	5	
29	B	1	Total	C	O	0
			47	42	5	

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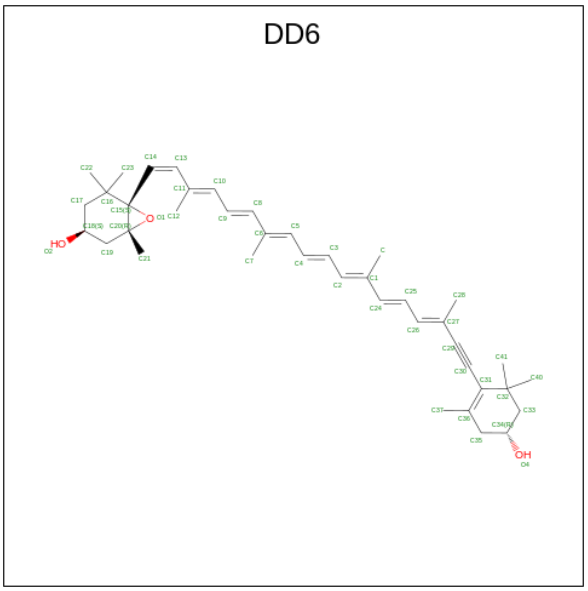
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C O 47 42 5	0
29	C	1	Total C O 47 42 5	0
29	C	1	Total C O 47 42 5	0
29	D	1	Total C O 47 42 5	0
29	E	1	Total C O 47 42 5	0
29	F	1	Total C O 47 42 5	0
29	G	1	Total C O 47 42 5	0
29	H	1	Total C O 47 42 5	0
29	H	1	Total C O 47 42 5	0
29	I	1	Total C O 47 42 5	0
29	J	1	Total C O 47 42 5	0
29	T	1	Total C O 47 42 5	0
29	j	1	Total C O 47 42 5	0

- Molecule 30 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	C	1	Total	C	O	0
			43	40	3	
30	C	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	E	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
30	E	1	Total	C	O	0
			43	40	3	
30	E	1	Total	C	O	0
			43	40	3	
30	E	1	Total	C	O	0
			43	40	3	
30	F	1	Total	C	O	0
			43	40	3	
30	F	1	Total	C	O	0
			43	40	3	
30	G	1	Total	C	O	0
			43	40	3	
30	G	1	Total	C	O	0
			43	40	3	
30	G	1	Total	C	O	0
			43	40	3	
30	G	1	Total	C	O	0
			43	40	3	
30	H	1	Total	C	O	0
			43	40	3	
30	H	1	Total	C	O	0
			43	40	3	
30	H	1	Total	C	O	0
			43	40	3	
30	H	1	Total	C	O	0
			43	40	3	
30	I	1	Total	C	O	0
			43	40	3	
30	I	1	Total	C	O	0
			43	40	3	
30	J	1	Total	C	O	0
			43	40	3	
30	K	1	Total	C	O	0
			43	40	3	
30	K	1	Total	C	O	0
			43	40	3	
30	K	1	Total	C	O	0
			43	40	3	
30	T	1	Total	C	O	0
			43	40	3	
30	T	1	Total	C	O	0
			43	40	3	

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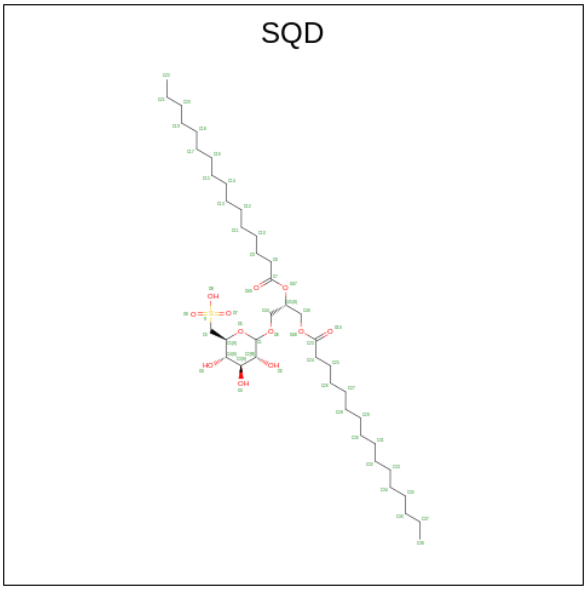
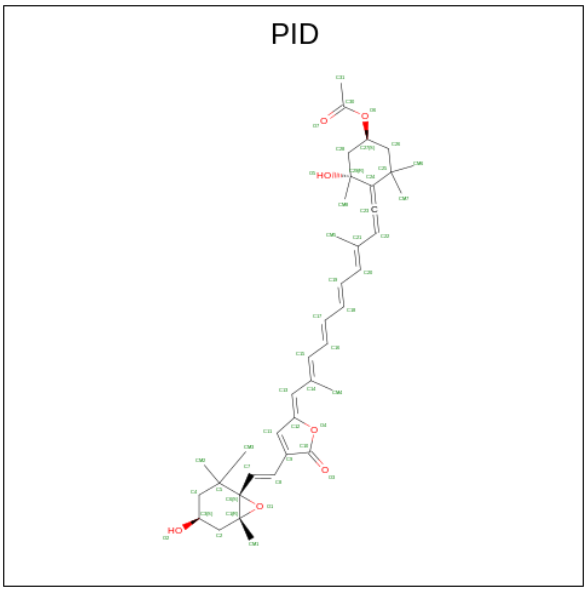
Mol	Chain	Residues	Atoms	AltConf
30	U	1	Total C O 43 40 3	0
30	b	1	Total C O 43 40 3	0
30	i	1	Total C O 43 40 3	0
30	r	1	Total C O 43 40 3	0
30	r	1	Total C O 43 40 3	0
30	r	1	Total C O 43 40 3	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



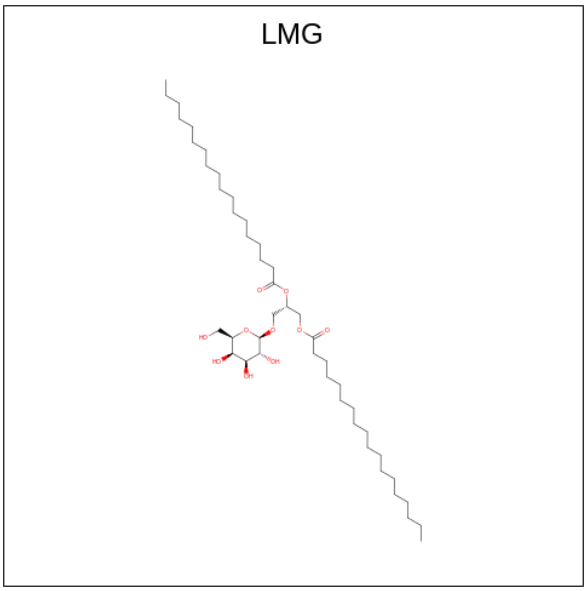
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O S 28 15 12 1	0
31	H	1	Total C O S 46 33 12 1	0
31	y	1	Total C O S 46 33 12 1	0

- Molecule 32 is PERIDININ (three-letter code: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



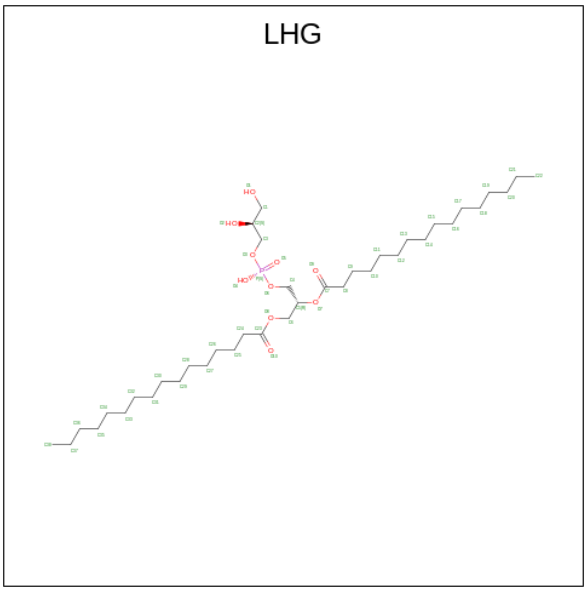
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	I	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	K	1	Total	C	O	0
			46	39	7	
32	U	1	Total	C	O	0
			46	39	7	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



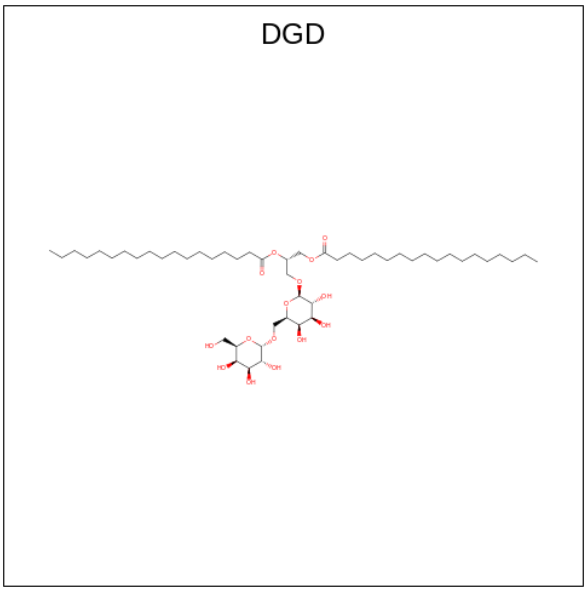
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			34	24	10	
33	D	1	Total	C	O	0
			35	25	10	
33	D	1	Total	C	O	0
			46	36	10	
33	F	1	Total	C	O	0
			46	36	10	
33	K	1	Total	C	O	0
			42	32	10	
33	b	1	Total	C	O	0
			55	45	10	
33	l	1	Total	C	O	0
			50	40	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



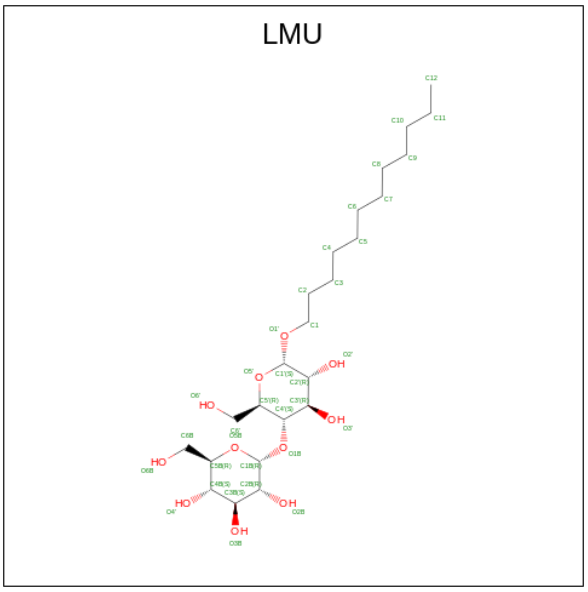
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			46	35	10	1	
34	F	1	Total	C	O	P	0
			37	26	10	1	
34	G	1	Total	C	O	P	0
			34	23	10	1	
34	a	1	Total	C	O	P	0
			48	37	10	1	
34	j	1	Total	C	O	P	0
			37	26	10	1	
34	l	1	Total	C	O	P	0
			46	35	10	1	
34	r	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



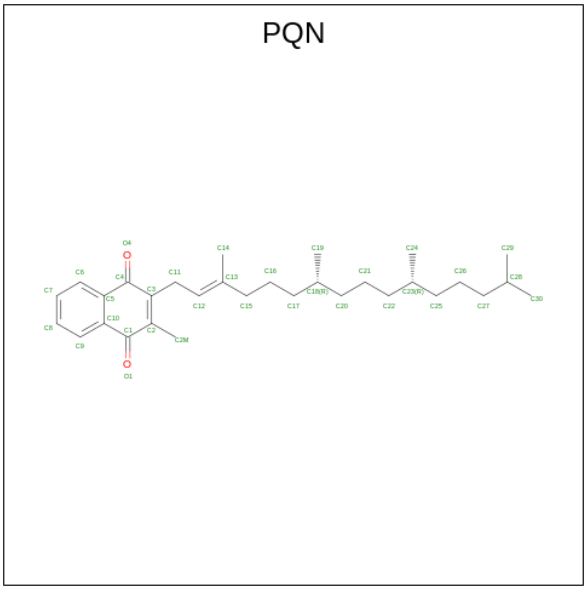
Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total 47	C 32	O 15	0
35	f	1	Total 52	C 37	O 15	0
35	j	1	Total 60	C 45	O 15	0
35	l	1	Total 55	C 40	O 15	0

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



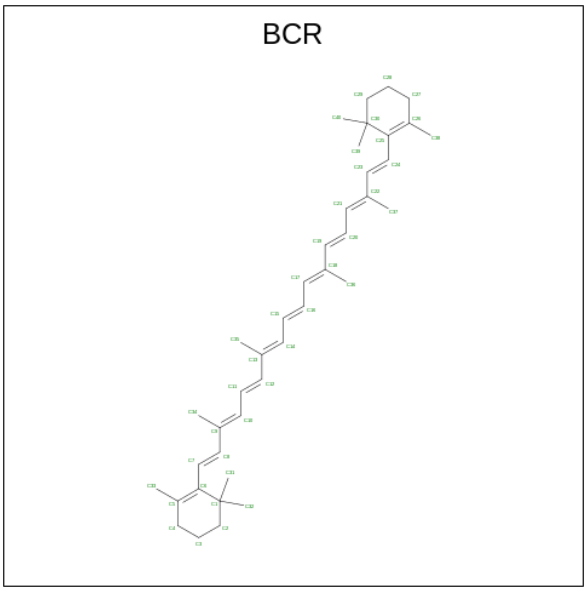
Mol	Chain	Residues	Atoms			AltConf
36	T	1	Total	C	O	0
			35	24	11	

- Molecule 37 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	a	1	Total	C	O	0
			33	31	2	
37	b	1	Total	C	O	0
			33	31	2	

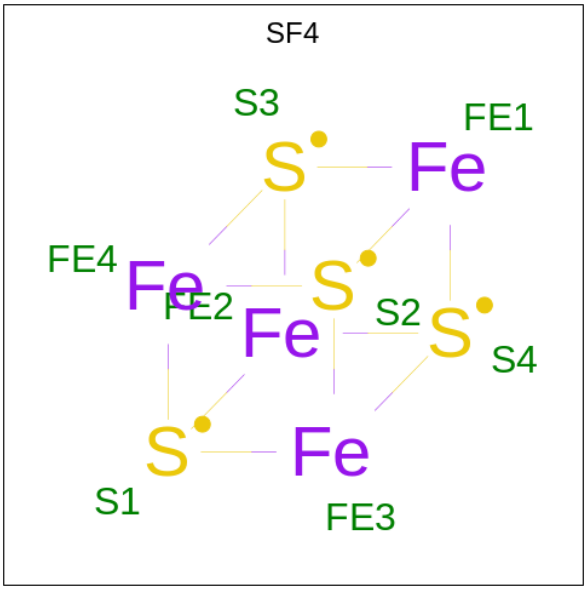
- Molecule 38 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	i	1	Total C 40 40	0
38	j	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	m	1	Total C 40 40	0

- Molecule 39 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled

as "Ligand of Interest" by depositor).



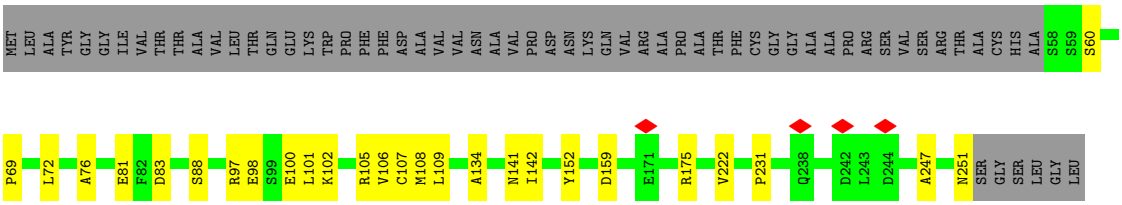
Mol	Chain	Residues	Atoms	AltConf
39	a	1	Total Fe S 8 4 4	0
39	c	1	Total Fe S 8 4 4	0
39	c	1	Total Fe S 8 4 4	0

3 Residue-property plots (i)

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

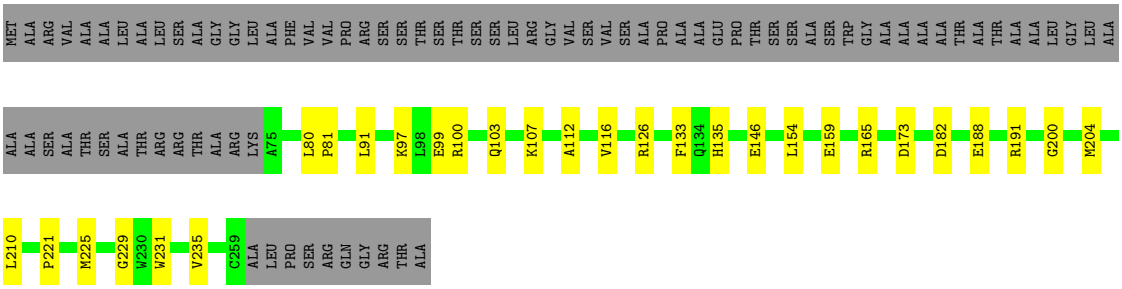
• Molecule 1: PCPI-7

Chain A:



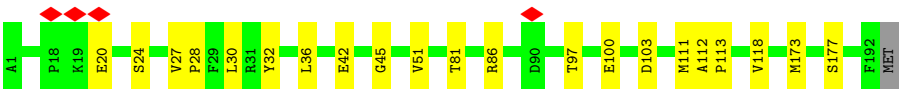
• Molecule 2: PCPI-1

Chain B:



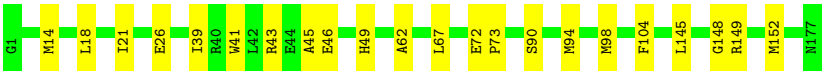
• Molecule 3: PCP-11

Chain C:



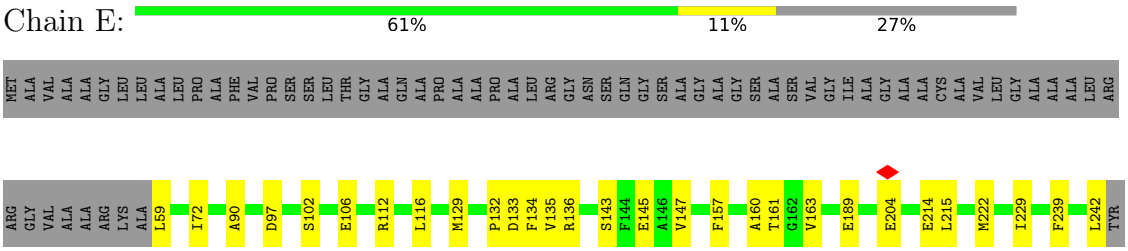
• Molecule 4: PCPI-6

Chain D:



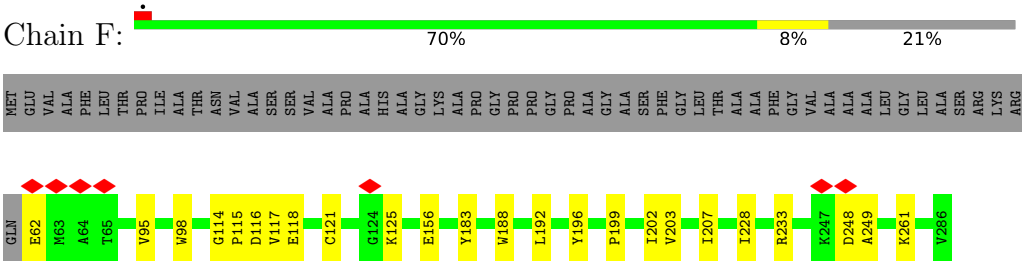
• Molecule 5: PCPI-5

Chain E:



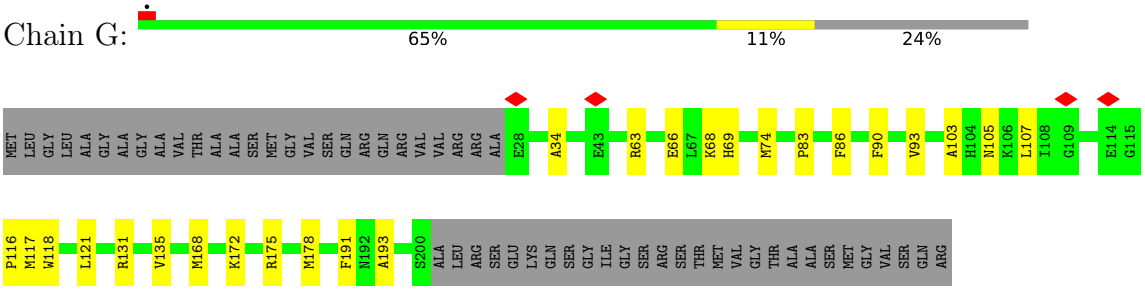
• Molecule 6: PCPI-8

Chain F:



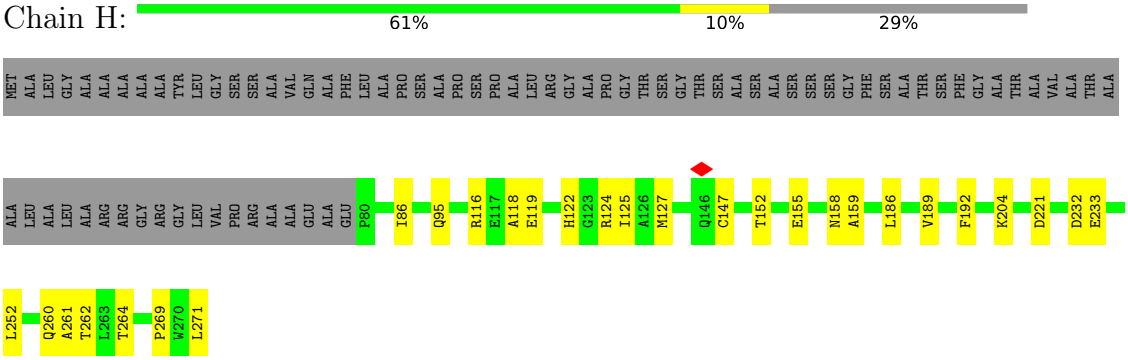
• Molecule 7: PCPI-4

Chain G:



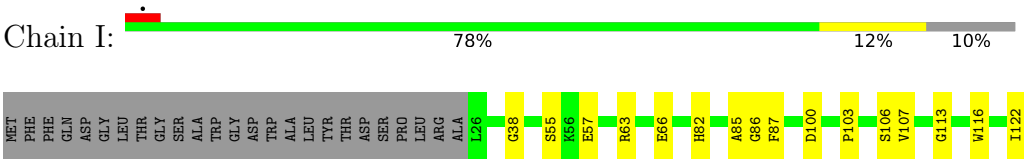
• Molecule 8: PCPI-10

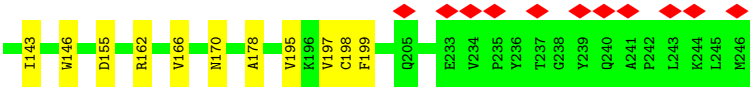
Chain H:



• Molecule 9: PCPI-3

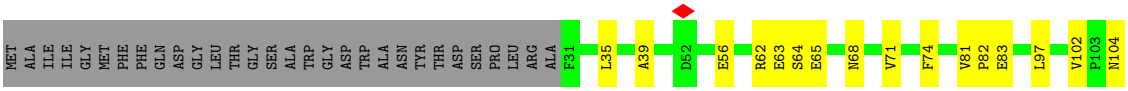
Chain I:

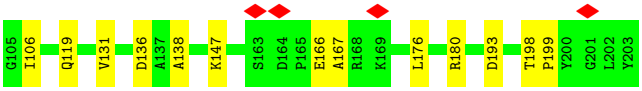




• Molecule 10: PCPI-9

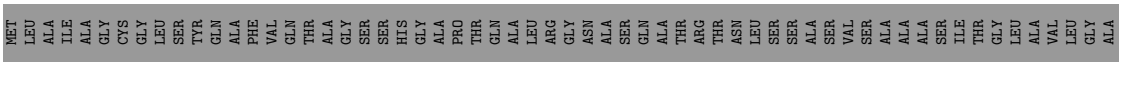
Chain J:

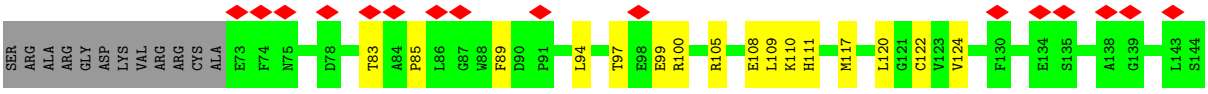




• Molecule 11: PCPI-13

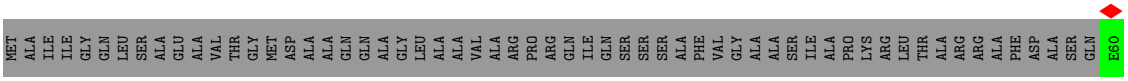
Chain K:

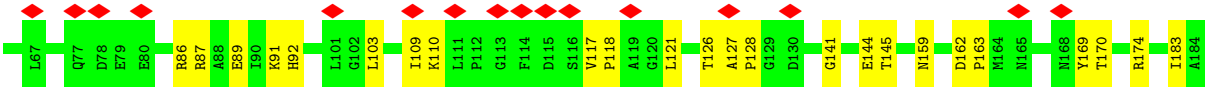


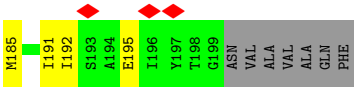


• Molecule 12: PCPI-12

Chain T:

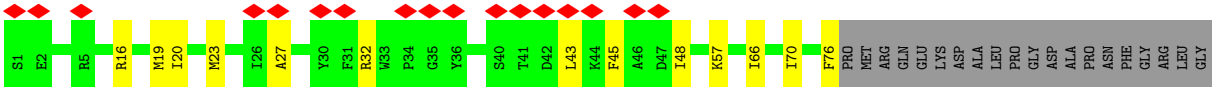


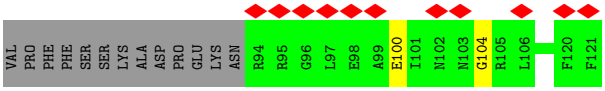




• Molecule 13: PCPI-2

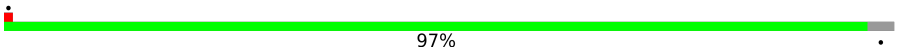
Chain U:

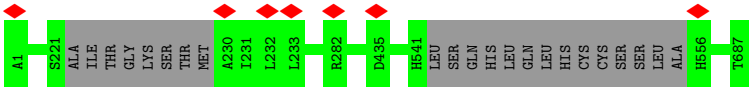




• Molecule 14: PsaA

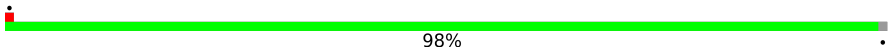
Chain a:

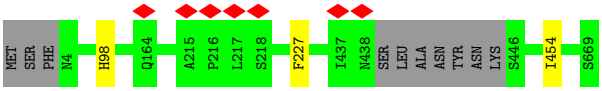




• Molecule 15: PsaB

Chain b:



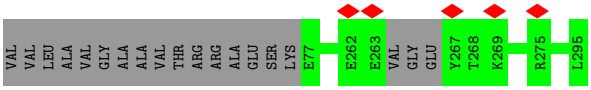


• Molecule 16: PsaC

Chain c:

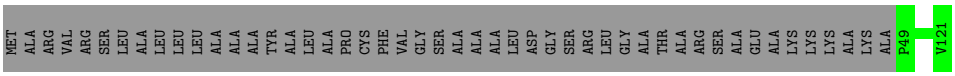
• Molecule 17: PsaD

Chain d:



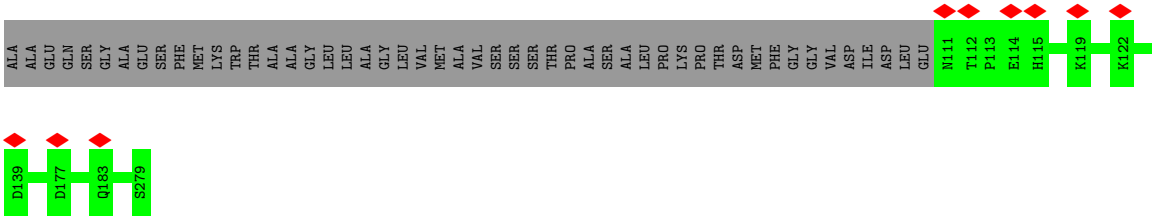
• Molecule 18: PsaE

Chain e:



• Molecule 19: PsaF

Chain f:

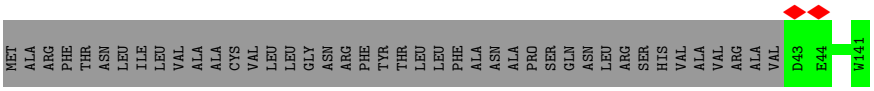


• Molecule 20: PsaI

Chain i:

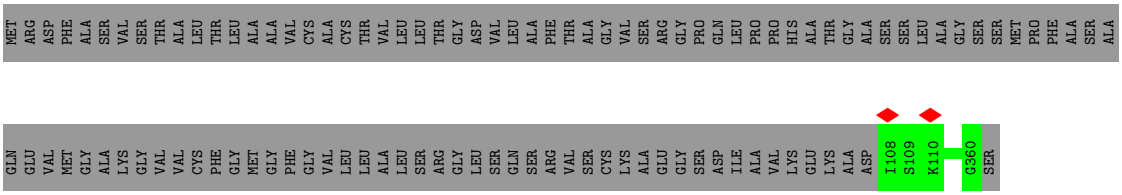
• Molecule 21: PsaJ

Chain j:



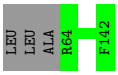
• Molecule 22: PsaL

Chain l:



• Molecule 23: PsaM

Chain m:

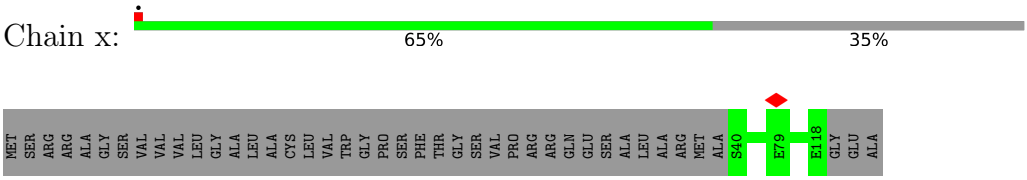


• Molecule 24: PsaR

Chain r:

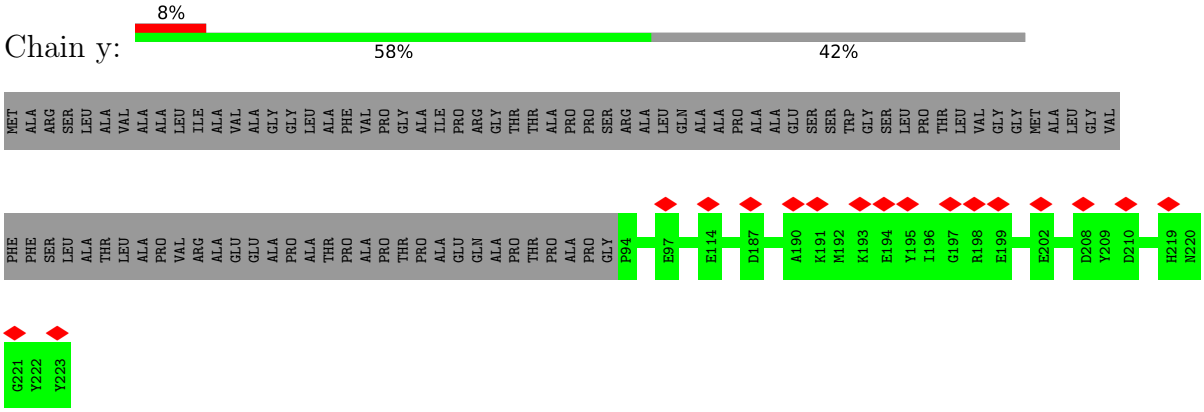
• Molecule 25: PsaT

Chain x:



• Molecule 26: PsaU

Chain y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161863	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.960	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, SQD, LMU, PID, KC2, DD6, BCR, SF4, PQN, DGD, LHG, LMG, UIX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/1501	0.45	0/2037
2	B	0.32	0/1443	0.50	0/1954
3	C	0.26	0/1562	0.43	0/2114
4	D	0.28	0/1413	0.46	0/1912
5	E	0.28	0/1484	0.51	0/2006
6	F	0.27	0/1785	0.44	0/2426
7	G	0.31	0/1365	0.48	0/1841
8	H	0.26	0/1499	0.44	0/2030
9	I	0.34	0/1794	0.48	0/2454
10	J	0.30	0/1355	0.50	0/1835
11	K	0.37	0/1162	0.50	0/1565
12	T	0.32	0/1090	0.52	0/1477
13	U	0.28	0/847	0.50	0/1140
14	a	0.28	0/5412	0.44	0/7363
15	b	0.40	0/5390	0.49	0/7368
16	c	0.36	0/661	0.55	0/901
17	d	0.27	0/1803	0.50	0/2419
18	e	0.27	0/611	0.44	0/836
19	f	0.41	0/1384	0.48	0/1873
20	i	0.27	0/1001	0.47	0/1357
21	j	0.27	0/808	0.47	0/1104
22	l	0.28	0/2031	0.46	0/2755
23	m	0.35	0/608	0.52	0/820
24	r	0.31	0/1118	0.45	0/1513
25	x	0.28	0/667	0.43	0/908
26	y	0.28	0/1119	0.50	0/1515
All	All	0.31	0/40913	0.47	0/55523

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1461	0	1420	19	0
2	B	1412	0	1384	18	0
3	C	1518	0	1491	18	0
4	D	1375	0	1359	15	0
5	E	1444	0	1418	18	0
6	F	1731	0	1691	19	0
7	G	1329	0	1301	27	0
8	H	1458	0	1426	18	0
9	I	1736	0	1687	23	0
10	J	1322	0	1296	19	0
11	K	1134	0	1085	51	0
12	T	1065	0	1042	20	0
13	U	828	0	828	16	0
14	a	5250	0	5201	0	0
15	b	5220	0	5122	0	0
16	c	651	0	634	0	0
17	d	1765	0	1785	0	0
18	e	590	0	582	0	0
19	f	1349	0	1334	0	0
20	i	971	0	951	0	0
21	j	791	0	783	0	0
22	l	1974	0	1950	0	0
23	m	598	0	641	0	0
24	r	1082	0	1041	0	0
25	x	642	0	594	0	0
26	y	1085	0	1025	0	0
27	A	543	0	441	9	0
27	B	454	0	437	5	0
27	C	565	0	489	11	0
27	D	624	0	532	8	0
27	E	537	0	481	4	0
27	F	575	0	500	14	0
27	G	529	0	463	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	H	602	0	559	10	0
27	I	623	0	596	17	0
27	J	248	0	211	7	0
27	K	360	0	309	19	0
27	T	354	0	258	12	0
27	U	198	0	164	12	0
27	a	1927	0	1885	0	0
27	b	1717	0	1790	0	0
27	f	96	0	72	0	0
27	j	56	0	51	0	0
27	l	627	0	600	0	0
27	r	108	0	95	0	0
28	A	45	0	0	0	0
28	B	90	0	0	0	0
28	C	45	0	0	0	0
28	E	90	0	0	0	0
28	F	45	0	0	0	0
28	G	45	0	0	0	0
28	H	90	0	0	0	0
28	I	45	0	0	0	0
28	J	225	0	0	5	0
28	K	45	0	0	6	0
28	T	45	0	0	0	0
28	U	90	0	0	0	0
29	A	94	0	0	0	0
29	B	94	0	0	0	0
29	C	94	0	0	0	0
29	D	47	0	0	0	0
29	E	47	0	0	0	0
29	F	47	0	0	0	0
29	G	47	0	0	0	0
29	H	94	0	0	1	0
29	I	47	0	0	1	0
29	J	47	0	0	0	0
29	T	47	0	0	0	0
29	j	47	0	0	0	0
30	A	129	0	0	2	0
30	B	129	0	0	2	0
30	C	86	0	0	2	0
30	D	215	0	0	3	0
30	E	172	0	0	2	0
30	F	86	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	G	172	0	0	4	0
30	H	172	0	0	3	0
30	I	86	0	0	2	0
30	J	43	0	0	1	0
30	K	129	0	0	3	0
30	T	86	0	0	1	0
30	U	43	0	0	1	0
30	b	43	0	0	0	0
30	i	43	0	0	0	0
30	r	129	0	0	0	0
31	A	28	0	20	0	0
31	H	46	0	56	0	0
31	y	46	0	56	0	0
32	B	46	0	50	1	0
32	F	92	0	100	8	0
32	I	46	0	50	5	0
32	J	184	0	200	21	0
32	K	46	0	50	12	0
32	U	46	0	50	0	0
33	C	34	0	38	1	0
33	D	81	0	105	2	0
33	F	46	0	65	0	0
33	K	42	0	57	1	0
33	b	55	0	86	0	0
33	l	50	0	73	0	0
34	D	46	0	65	0	0
34	F	37	0	44	0	0
34	G	34	0	38	0	0
34	a	48	0	69	0	0
34	j	37	0	44	0	0
34	l	46	0	65	0	0
34	r	46	0	65	0	0
35	K	47	0	52	4	0
35	f	52	0	62	0	0
35	j	60	0	81	0	0
35	l	55	0	71	0	0
36	T	35	0	46	1	0
37	a	33	0	46	0	0
37	b	33	0	46	0	0
38	a	120	0	168	0	0
38	b	80	0	112	0	0
38	f	80	0	112	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i	40	0	56	0	0
38	j	40	0	56	0	0
38	l	120	0	168	0	0
38	m	40	0	56	0	0
39	a	8	0	0	0	0
39	c	16	0	0	0	0
All	All	55980	0	51582	380	0

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

All (380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:PHE:CE1	7:G:93:VAL:HG13	1.79	1.17
11:K:120:LEU:HD12	27:K:603:CLA:HAC1	1.37	1.02
11:K:120:LEU:CD1	27:K:603:CLA:HAC1	1.95	0.96
7:G:90:PHE:HE1	7:G:93:VAL:HG13	1.32	0.90
11:K:120:LEU:HD13	11:K:120:LEU:O	1.71	0.90
1:A:76:ALA:O	1:A:97:ARG:NH2	2.07	0.87
6:F:188:TRP:O	30:F:612:DD6:O4	1.92	0.87
7:G:90:PHE:CE1	7:G:93:VAL:CG1	2.57	0.86
7:G:172:LYS:NZ	27:G:608:CLA:O1D	2.08	0.86
11:K:202:HIS:HE1	28:K:607:KC2:C4D	1.87	0.86
7:G:63:ARG:NH1	7:G:66:GLU:OE1	2.09	0.85
2:B:165:ARG:NH1	2:B:173:ASP:OD2	2.11	0.84
8:H:86:ILE:O	8:H:116:ARG:NH2	2.13	0.82
8:H:158:ASN:OD1	30:H:318:DD6:O2	1.96	0.82
10:J:65:GLU:OE2	10:J:180:ARG:NH1	2.13	0.81
11:K:120:LEU:HD13	11:K:120:LEU:C	2.01	0.81
11:K:198:LYS:O	11:K:202:HIS:CD2	2.34	0.81
5:E:143:SER:OG	5:E:145:GLU:OE1	1.99	0.81
3:C:24:SER:OG	3:C:45:GLY:O	1.97	0.81
35:K:614:DGD:O6E	35:K:614:DGD:O3D	1.98	0.80
11:K:197:ASP:OD1	11:K:201:ASN:ND2	2.15	0.80
32:I:614:PID:HM22	32:I:614:PID:H21	1.63	0.80
5:E:59:LEU:N	5:E:204:GLU:OE2	2.15	0.79
35:K:614:DGD:O5E	35:K:614:DGD:O4E	1.96	0.78
8:H:116:ARG:NH1	8:H:119:GLU:OE2	2.16	0.78
7:G:107:LEU:HD12	7:G:116:PRO:HG2	1.65	0.76
30:C:216:DD6:O2	33:C:217:LMG:O10	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:83:THR:HG22	11:K:85:PRO:HD2	1.69	0.75
32:K:611:PID:H21	32:K:611:PID:HM22	1.68	0.75
32:J:614:PID:HM73	32:J:614:PID:HM51	1.69	0.74
6:F:248:ASP:OD1	6:F:249:ALA:N	2.19	0.74
8:H:152:THR:OG1	8:H:155:GLU:OE1	2.06	0.74
9:I:63:ARG:NH1	9:I:66:GLU:OE1	2.21	0.73
12:T:91:LYS:NZ	12:T:144:GLU:OE2	2.16	0.73
8:H:260:GLN:O	8:H:264:THR:HG22	1.89	0.73
8:H:95:GLN:N	8:H:95:GLN:OE1	2.22	0.73
7:G:34:ALA:O	7:G:63:ARG:NH2	2.22	0.72
11:K:120:LEU:CD1	27:K:603:CLA:CAC	2.67	0.72
32:J:613:PID:HM22	32:J:613:PID:H21	1.70	0.71
7:G:107:LEU:HD12	7:G:116:PRO:CG	2.20	0.71
11:K:97:THR:OG1	11:K:99:GLU:OE1	2.09	0.71
1:A:98:GLU:OE1	1:A:175:ARG:NH2	2.22	0.71
9:I:103:PRO:O	9:I:107:VAL:HG23	1.90	0.71
13:U:45:PHE:HA	27:U:603:CLA:HED1	1.73	0.71
12:T:141:GLY:O	12:T:145:THR:HG23	1.91	0.70
27:I:601:CLA:HMB2	27:I:602:CLA:HED1	1.72	0.70
11:K:120:LEU:HD12	27:K:603:CLA:CAC	2.20	0.69
1:A:141:ASN:OD1	1:A:142:ILE:N	2.25	0.69
6:F:261:LYS:NZ	27:F:608:CLA:O1D	2.22	0.69
11:K:110:LYS:NZ	11:K:163:GLU:OE1	2.23	0.69
11:K:105:ARG:NH1	11:K:108:GLU:OE1	2.26	0.68
27:T:603:CLA:HMC1	27:T:603:CLA:HBC3	1.75	0.67
6:F:62:GLU:OE1	6:F:62:GLU:N	2.27	0.67
12:T:183:ILE:HD12	27:T:607:CLA:HMD2	1.75	0.67
2:B:135:HIS:O	30:B:612:DD6:O4	2.12	0.66
7:G:68:LYS:NZ	27:G:606:CLA:O1D	2.25	0.66
9:I:155:ASP:OD1	9:I:155:ASP:O	2.13	0.65
9:I:85:ALA:HB2	9:I:195:VAL:HG21	1.78	0.65
4:D:90:SER:OG	27:D:605:CLA:OBD	2.14	0.65
1:A:83:ASP:OD2	1:A:88:SER:OG	2.11	0.65
9:I:146:TRP:NE1	27:I:606:CLA:O1A	2.29	0.64
13:U:27:ALA:HB1	27:U:603:CLA:HMD3	1.79	0.64
27:B:601:CLA:HMC2	30:B:612:DD6:C9	2.27	0.64
1:A:247:ALA:O	1:A:251:ASN:ND2	2.30	0.64
32:K:611:PID:HM72	32:K:611:PID:H281	1.80	0.64
5:E:97:ASP:OD2	5:E:102:SER:OG	2.08	0.64
32:J:611:PID:HM22	32:J:611:PID:H21	1.81	0.63
12:T:121:LEU:HD21	12:T:192:ILE:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:I:603:CLA:C4	27:I:610:CLA:HMC2	2.27	0.63
11:K:202:HIS:CE1	28:K:607:KC2:C4D	2.78	0.63
7:G:131:ARG:O	7:G:135:VAL:HG22	1.99	0.62
7:G:74:MET:SD	27:G:607:CLA:HMC3	2.39	0.62
11:K:202:HIS:CD2	27:K:605:CLA:HBB1	2.35	0.62
3:C:32:TYR:OH	3:C:42:GLU:O	2.18	0.62
9:I:85:ALA:HB2	9:I:195:VAL:CG2	2.30	0.61
32:I:614:PID:H282	32:I:614:PID:HM63	1.82	0.61
10:J:136:ASP:OD2	10:J:138:ALA:HB3	2.00	0.61
10:J:63:GLU:HG2	27:J:605:CLA:HED2	1.82	0.61
7:G:103:ALA:O	7:G:107:LEU:HD23	2.01	0.61
9:I:143:ILE:HB	27:I:606:CLA:HMD1	1.82	0.61
13:U:23:MET:HB3	27:U:603:CLA:HBC2	1.82	0.61
3:C:103:ASP:OD2	30:C:216:DD6:O4	2.19	0.61
27:H:303:CLA:HMC2	30:H:315:DD6:C9	2.31	0.61
3:C:27:VAL:HG23	3:C:27:VAL:O	2.01	0.60
11:K:198:LYS:O	11:K:202:HIS:HD2	1.82	0.60
7:G:69:HIS:ND1	27:G:606:CLA:HMD1	2.16	0.60
27:G:608:CLA:HMB2	35:K:614:DGD:O2D	2.01	0.60
11:K:120:LEU:CD1	11:K:120:LEU:C	2.70	0.59
32:J:615:PID:C8	32:J:615:PID:HM11	2.32	0.59
9:I:197:VAL:CG1	9:I:199:PHE:CE2	2.85	0.59
32:J:613:PID:HM82	32:J:613:PID:H262	1.83	0.59
12:T:127:ALA:HB3	12:T:128:PRO:HD3	1.85	0.59
3:C:97:THR:OG1	3:C:100:GLU:OE1	2.21	0.59
27:F:604:CLA:HMC1	27:F:604:CLA:HBC2	1.85	0.58
11:K:122:CYS:HB3	11:K:224:ALA:HB2	1.85	0.58
11:K:180:ASP:OD1	30:K:609:DD6:O2	2.21	0.58
1:A:101:LEU:O	1:A:105:ARG:HG3	2.04	0.58
3:C:20:GLU:N	3:C:20:GLU:OE1	2.36	0.58
11:K:152:MET:CE	27:K:603:CLA:HMA1	2.34	0.58
9:I:82:HIS:CE1	27:I:603:CLA:HMD3	2.39	0.58
27:H:306:CLA:HMC1	27:H:306:CLA:HBC3	1.86	0.58
7:G:90:PHE:HE1	7:G:93:VAL:CG1	2.08	0.57
12:T:86:ARG:NH2	12:T:89:GLU:OE2	2.35	0.57
1:A:60:SER:OG	1:A:81:GLU:O	2.22	0.57
9:I:197:VAL:HG21	27:I:610:CLA:O1A	2.04	0.57
27:G:609:CLA:HMC2	30:G:612:DD6:C9	2.34	0.57
1:A:159:ASP:OD1	1:A:159:ASP:O	2.23	0.57
27:I:605:CLA:HMB3	13:U:76:PHE:CZ	2.40	0.57
11:K:202:HIS:CE1	28:K:607:KC2:CHA	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:208:MET:SD	32:K:611:PID:H11	2.45	0.57
7:G:90:PHE:CZ	7:G:93:VAL:CG1	2.88	0.57
5:E:157:PHE:HA	5:E:161:THR:HG21	1.87	0.56
11:K:202:HIS:CE1	28:K:607:KC2:C1A	2.89	0.56
8:H:262:THR:HG21	27:H:313:CLA:O1D	2.05	0.56
10:J:147:LYS:NZ	28:J:608:KC2:O1A	2.38	0.56
27:I:603:CLA:H43	27:I:610:CLA:HMC2	1.87	0.56
2:B:188:GLU:OE2	2:B:191:ARG:NH1	2.39	0.56
3:C:27:VAL:HG21	3:C:30:LEU:HD12	1.86	0.56
11:K:208:MET:SD	32:K:611:PID:C11	2.93	0.56
2:B:107:LYS:NZ	2:B:159:GLU:OE2	2.23	0.55
3:C:112:ALA:HB3	3:C:113:PRO:HD3	1.88	0.55
9:I:126:GLU:O	9:I:130:THR:HG22	2.06	0.55
2:B:99:GLU:OE2	2:B:100:ARG:N	2.40	0.55
5:E:90:ALA:HB1	27:E:609:CLA:HMB3	1.88	0.55
8:H:125:ILE:HD12	27:H:308:CLA:HMD3	1.88	0.55
11:K:117:MET:O	27:K:603:CLA:HMC3	2.07	0.54
3:C:86:ARG:HA	27:C:205:CLA:HMD1	1.89	0.54
11:K:219:VAL:HG12	11:K:220:THR:HG23	1.89	0.54
3:C:173:MET:SD	27:C:203:CLA:HMC3	2.48	0.54
13:U:16:ARG:NH1	13:U:100:GLU:OE2	2.40	0.54
32:I:614:PID:HM22	32:I:614:PID:C2	2.36	0.54
11:K:225:ALA:O	11:K:226:GLN:HG3	2.08	0.54
6:F:202:ILE:HG22	27:F:605:CLA:HED2	1.90	0.53
11:K:210:ILE:HG21	30:K:610:DD6:C24	2.37	0.53
27:T:603:CLA:HMB3	30:T:611:DD6:C14	2.38	0.53
5:E:239:PHE:O	5:E:242:LEU:N	2.41	0.53
8:H:269:PRO:O	29:H:314:UIX:O1	2.27	0.53
27:F:601:CLA:HMC2	30:F:612:DD6:C9	2.38	0.53
9:I:197:VAL:HG13	9:I:199:PHE:CE2	2.44	0.53
27:D:609:CLA:HMB3	33:D:618:LMG:O4	2.09	0.53
6:F:116:ASP:O	6:F:118:GLU:N	2.40	0.53
11:K:120:LEU:HD11	27:K:603:CLA:HAC1	1.87	0.53
32:J:613:PID:H312	32:J:614:PID:HM82	1.91	0.53
27:F:606:CLA:HMB2	27:F:619:CLA:H43	1.91	0.52
13:U:27:ALA:CB	27:U:603:CLA:HMD3	2.38	0.52
6:F:207:ILE:HG21	27:F:604:CLA:HBC3	1.90	0.52
11:K:202:HIS:HE1	28:K:607:KC2:CHA	2.21	0.52
13:U:70:ILE:HG21	27:U:605:CLA:HMC3	1.90	0.52
12:T:185:MET:SD	27:T:601:CLA:HMC3	2.49	0.52
32:F:614:PID:CM1	32:F:614:PID:C8	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:614:PID:C8	32:F:614:PID:HM21	2.39	0.51
8:H:124:ARG:HA	8:H:127:MET:HE3	1.92	0.51
11:K:89:PHE:N	27:K:601:CLA:OBD	2.43	0.51
27:T:603:CLA:HBB1	27:T:603:CLA:HMB1	1.92	0.51
8:H:192:PHE:CE2	27:H:306:CLA:HMC3	2.46	0.51
27:H:304:CLA:HBB1	27:H:304:CLA:HMB1	1.93	0.51
2:B:91:LEU:O	2:B:97:LYS:NZ	2.39	0.51
2:B:146:GLU:N	2:B:146:GLU:OE1	2.40	0.51
11:K:152:MET:HE2	27:K:603:CLA:HMA1	1.92	0.51
7:G:90:PHE:CZ	7:G:93:VAL:HG11	2.45	0.51
4:D:26:GLU:OE2	30:D:615:DD6:O2	2.29	0.50
9:I:122:ILE:HG21	27:I:605:CLA:HMC3	1.93	0.50
10:J:198:THR:HG22	10:J:199:PRO:HD2	1.92	0.50
9:I:55:SER:OG	9:I:57:GLU:OE1	2.28	0.50
10:J:35:LEU:O	10:J:62:ARG:NH2	2.42	0.50
27:T:601:CLA:HMB1	27:T:601:CLA:HBB1	1.93	0.50
27:I:606:CLA:HMB1	27:I:606:CLA:HBB1	1.93	0.50
8:H:118:ALA:O	8:H:122:HIS:ND1	2.41	0.50
28:J:608:KC2:CHC	32:J:611:PID:HM43	2.42	0.50
27:J:609:CLA:CMB	32:J:611:PID:HM13	2.41	0.50
12:T:169:TYR:CD1	27:T:606:CLA:HED3	2.47	0.50
7:G:191:PHE:O	7:G:193:ALA:N	2.44	0.49
3:C:177:SER:OG	27:C:211:CLA:HMC3	2.12	0.49
6:F:196:TYR:CG	27:F:604:CLA:HMD3	2.47	0.49
27:F:604:CLA:HMB1	27:F:604:CLA:HBB1	1.94	0.49
11:K:100:ARG:NH1	12:T:162:ASP:O	2.45	0.49
27:F:602:CLA:HMA3	32:F:614:PID:C18	2.42	0.49
11:K:100:ARG:NH2	12:T:163:PRO:O	2.41	0.49
32:K:611:PID:HM72	32:K:611:PID:C28	2.43	0.49
13:U:70:ILE:HG21	27:U:605:CLA:CMC	2.43	0.49
11:K:202:HIS:HE1	28:K:607:KC2:ND	2.10	0.49
32:J:615:PID:HM22	32:J:615:PID:H21	1.95	0.49
12:T:117:VAL:HG12	12:T:126:THR:HB	1.95	0.49
27:U:601:CLA:HMC2	30:U:607:DD6:C24	2.43	0.49
27:B:606:CLA:HMB1	27:B:606:CLA:HBB1	1.95	0.49
4:D:43:ARG:NH1	4:D:145:LEU:HD11	2.28	0.49
5:E:133:ASP:OD1	5:E:134:PHE:N	2.45	0.49
5:E:222:MET:HG2	30:E:614:DD6:C5	2.43	0.49
4:D:41:TRP:NE1	27:D:603:CLA:O1A	2.43	0.48
4:D:62:ALA:HB1	4:D:67:LEU:HD23	1.95	0.48
6:F:156:GLU:OE2	6:F:233:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:K:611:PID:CM1	32:K:611:PID:C8	2.91	0.48
7:G:117:MET:HB3	27:G:605:CLA:HMD3	1.95	0.48
13:U:43:LEU:CD2	13:U:48:ILE:HD11	2.44	0.48
27:U:603:CLA:HBC3	27:U:603:CLA:HHD	1.95	0.48
2:B:231:TRP:HB3	2:B:235:VAL:HG23	1.95	0.48
32:J:615:PID:HM11	32:J:615:PID:H8	1.96	0.48
27:A:604:CLA:HMB1	27:A:604:CLA:HBB1	1.95	0.48
2:B:103:GLN:HG2	27:B:605:CLA:HED2	1.96	0.48
5:E:129:MET:CE	5:E:229:ILE:HD12	2.43	0.48
6:F:192:LEU:HD23	32:F:615:PID:HM23	1.96	0.48
27:I:601:CLA:HMC2	30:I:613:DD6:C25	2.44	0.48
27:K:602:CLA:O1A	27:K:602:CLA:C2	2.62	0.48
12:T:92:HIS:HB3	12:T:185:MET:HE2	1.95	0.48
3:C:81:THR:CG2	27:C:205:CLA:HED1	2.43	0.48
33:D:619:LMG:O2	30:D:621:DD6:O4	2.31	0.48
13:U:48:ILE:HB	27:U:603:CLA:CED	2.43	0.48
27:F:605:CLA:HMC1	27:F:605:CLA:HBC3	1.94	0.48
8:H:147:CYS:HA	8:H:159:ALA:HB1	1.95	0.48
11:K:109:LEU:HD13	11:K:176:GLY:HA3	1.96	0.48
27:T:602:CLA:HMD1	27:T:605:CLA:HBA2	1.96	0.48
3:C:51:VAL:HG13	27:H:319:CLA:CMB	2.44	0.47
32:K:611:PID:HM13	32:K:611:PID:H8	1.96	0.47
1:A:97:ARG:NH1	1:A:100:GLU:OE1	2.41	0.47
5:E:189:GLU:N	5:E:189:GLU:OE1	2.46	0.47
27:G:607:CLA:HBB1	27:G:607:CLA:HMB1	1.96	0.47
28:J:604:KC2:CBC	32:J:613:PID:C17	2.93	0.47
27:J:605:CLA:HBC3	32:J:613:PID:HM21	1.97	0.47
8:H:204:LYS:NZ	8:H:221:ASP:O	2.45	0.47
9:I:38:GLY:HA2	27:I:601:CLA:HMD1	1.97	0.47
32:F:614:PID:H21	32:F:614:PID:HM22	1.97	0.47
11:K:204:ARG:HB2	32:K:611:PID:HM23	1.96	0.47
1:A:222:VAL:HG13	1:A:231:PRO:HG3	1.97	0.47
3:C:51:VAL:HG13	27:H:319:CLA:HMB1	1.96	0.47
8:H:252:LEU:HD13	30:H:316:DD6:C26	2.44	0.47
10:J:166:GLU:OE1	10:J:167:ALA:N	2.48	0.47
5:E:163:VAL:HG13	27:E:605:CLA:HMD1	1.95	0.46
30:D:615:DD6:O4	5:E:160:ALA:O	2.34	0.46
6:F:228:ILE:O	6:F:228:ILE:HG22	2.15	0.46
2:B:210:LEU:HD23	2:B:221:PRO:HG2	1.97	0.46
3:C:118:VAL:HG11	27:C:207:CLA:HMC3	1.97	0.46
11:K:111:HIS:CD2	27:K:604:CLA:HMD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:176:LEU:O	10:J:180:ARG:HG3	2.16	0.46
32:J:611:PID:HM72	32:J:611:PID:HM51	1.97	0.46
32:J:614:PID:HM51	32:J:614:PID:CM7	2.44	0.46
9:I:162:ARG:O	9:I:166:VAL:HG23	2.16	0.46
1:A:69:PRO:CG	1:A:72:LEU:HD21	2.46	0.46
1:A:109:LEU:O	27:A:604:CLA:HMC3	2.16	0.46
4:D:14:MET:HG3	4:D:18:LEU:HD11	1.97	0.46
27:F:619:CLA:H62	27:F:619:CLA:H41	1.82	0.46
27:H:304:CLA:HAA1	27:H:304:CLA:CGD	2.46	0.46
11:K:145:ASN:OD1	11:K:148:ALA:N	2.45	0.46
11:K:120:LEU:HD12	27:K:603:CLA:HMC1	1.98	0.46
1:A:152:TYR:HB2	27:A:612:CLA:HMB3	1.98	0.45
5:E:72:ILE:HG23	5:E:106:GLU:HB2	1.98	0.45
6:F:228:ILE:N	6:F:228:ILE:HD13	2.30	0.45
2:B:200:GLY:O	2:B:204:MET:HG3	2.17	0.45
3:C:111:MET:HB3	27:C:206:CLA:HMD3	1.97	0.45
27:C:204:CLA:HED3	27:C:204:CLA:H141	1.99	0.45
8:H:261:ALA:HB2	8:H:271:LEU:C	2.36	0.45
9:I:130:THR:HG23	9:I:131:TYR:CD2	2.52	0.45
12:T:159:ASN:OD1	27:T:606:CLA:HED2	2.16	0.45
7:G:107:LEU:HD12	7:G:116:PRO:HG3	1.97	0.45
1:A:108:MET:SD	27:A:606:CLA:HMC3	2.56	0.45
4:D:72:GLU:N	4:D:73:PRO:CD	2.79	0.45
27:H:304:CLA:HMB1	27:H:304:CLA:CBB	2.47	0.45
10:J:64:SER:O	10:J:68:ASN:ND2	2.45	0.45
13:U:20:ILE:HG22	27:U:603:CLA:CAB	2.47	0.45
27:D:608:CLA:HBB1	27:D:608:CLA:HMB1	1.97	0.45
4:D:46:GLU:OE2	4:D:149:ARG:NE	2.44	0.45
27:J:601:CLA:HMC2	30:J:612:DD6:C9	2.47	0.44
4:D:94:MET:O	4:D:98:MET:HG2	2.17	0.44
32:K:611:PID:HM51	32:K:611:PID:HM83	1.97	0.44
2:B:225:MET:O	2:B:229:GLY:N	2.50	0.44
6:F:121:CYS:HB3	6:F:125:LYS:O	2.18	0.44
6:F:183:TYR:CE2	6:F:203:VAL:HG23	2.52	0.44
7:G:105:ASN:OD1	30:G:616:DD6:O2	2.36	0.44
10:J:74:PHE:CD2	32:J:613:PID:HM11	2.51	0.44
12:T:118:PRO:CD	12:T:126:THR:HG21	2.47	0.44
27:D:612:CLA:H61	27:D:612:CLA:H41	1.84	0.44
11:K:204:ARG:CB	32:K:611:PID:HM23	2.47	0.44
2:B:182:ASP:OD1	2:B:182:ASP:C	2.56	0.44
7:G:168:MET:HE3	7:G:172:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:71:VAL:HG22	32:J:613:PID:HM13	2.00	0.44
10:J:131:VAL:HG22	10:J:131:VAL:O	2.18	0.44
35:K:614:DGD:O5D	35:K:614:DGD:O4D	2.19	0.44
12:T:87:ARG:HG2	27:T:605:CLA:HED2	2.00	0.44
13:U:19:MET:SD	13:U:104:GLY:HA2	2.58	0.44
27:A:605:CLA:H61	27:A:605:CLA:H41	1.89	0.44
2:B:154:LEU:HD21	27:B:610:CLA:HMB3	2.00	0.44
5:E:136:ARG:NH1	5:E:147:VAL:O	2.51	0.44
8:H:186:LEU:HA	8:H:189:VAL:HG22	2.00	0.44
6:F:95:VAL:HG21	32:F:615:PID:O7	2.18	0.43
6:F:196:TYR:HB3	27:F:604:CLA:HMD3	2.00	0.43
11:K:152:MET:HE1	27:K:603:CLA:HMA1	1.99	0.43
32:B:613:PID:H16	32:B:613:PID:HM41	1.78	0.43
10:J:81:VAL:HB	10:J:82:PRO:HD3	2.00	0.43
11:K:94:LEU:O	11:K:100:ARG:NE	2.43	0.43
12:T:191:ILE:O	12:T:195:GLU:HG2	2.18	0.43
1:A:107:CYS:SG	30:A:614:DD6:C2	3.07	0.43
7:G:69:HIS:HB3	7:G:178:MET:SD	2.57	0.43
9:I:113:GLY:HA2	9:I:116:TRP:CD1	2.54	0.43
5:E:112:ARG:NH1	5:E:215:LEU:HD11	2.33	0.43
6:F:98:TRP:CZ3	6:F:228:ILE:HD11	2.54	0.43
11:K:213:GLN:O	11:K:217:GLU:HG3	2.18	0.43
27:E:608:CLA:HMC2	30:E:613:DD6:C25	2.48	0.43
4:D:21:ILE:HD12	4:D:39:ILE:HG12	2.00	0.43
5:E:112:ARG:HD3	5:E:112:ARG:O	2.19	0.43
27:K:601:CLA:HMC2	30:K:610:DD6:C9	2.49	0.43
4:D:18:LEU:HB2	27:D:602:CLA:HED1	2.00	0.43
9:I:100:ASP:O	9:I:106:SER:OG	2.30	0.43
11:K:120:LEU:HD11	11:K:124:VAL:HG21	2.01	0.43
9:I:86:GLY:O	9:I:87:PHE:C	2.55	0.43
10:J:97:LEU:HD11	10:J:102:VAL:CG1	2.49	0.43
2:B:182:ASP:OD1	2:B:182:ASP:O	2.36	0.43
32:J:611:PID:O7	32:J:611:PID:C26	2.67	0.43
11:K:94:LEU:HD13	27:K:601:CLA:H2	2.01	0.43
12:T:109:ILE:HG22	12:T:110:LYS:N	2.34	0.43
13:U:70:ILE:CG2	27:U:605:CLA:HMC3	2.49	0.43
30:A:615:DD6:C41	27:D:605:CLA:HED2	2.49	0.42
2:B:112:ALA:O	2:B:116:VAL:HG23	2.19	0.42
7:G:175:ARG:HB2	30:G:614:DD6:C41	2.49	0.42
8:H:232:ASP:OD1	8:H:233:GLU:N	2.52	0.42
6:F:114:GLY:N	6:F:115:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:LEU:HD12	27:G:606:CLA:HMC2	2.01	0.42
27:K:601:CLA:HAC2	32:K:611:PID:HM22	2.01	0.42
2:B:80:LEU:N	2:B:81:PRO:HD2	2.34	0.42
12:T:117:VAL:HG12	12:T:126:THR:CB	2.50	0.42
32:F:614:PID:H262	32:F:614:PID:H313	2.01	0.42
7:G:118:TRP:CD1	27:G:605:CLA:HMD1	2.55	0.42
9:I:82:HIS:ND1	27:I:603:CLA:HMD3	2.34	0.42
10:J:56:GLU:OE2	10:J:56:GLU:C	2.58	0.42
9:I:178:ALA:CB	29:I:612:UIX:C13	2.98	0.42
11:K:202:HIS:CD2	27:K:605:CLA:CBB	3.02	0.42
27:F:604:CLA:HMB1	27:F:604:CLA:CBB	2.50	0.42
10:J:119:GLN:OE1	28:J:604:KC2:ND	2.52	0.42
7:G:83:PRO:HA	7:G:86:PHE:O	2.20	0.42
27:I:609:CLA:HMD1	32:I:614:PID:CM7	2.50	0.42
32:J:613:PID:HM22	32:J:613:PID:C2	2.44	0.42
1:A:102:LYS:O	1:A:106:VAL:HG13	2.19	0.42
10:J:83:GLU:OE2	10:J:104:ASN:ND2	2.50	0.42
13:U:43:LEU:HD11	13:U:57:LYS:HD2	2.01	0.42
1:A:108:MET:HG3	27:A:606:CLA:HMC3	2.02	0.42
32:I:614:PID:H16	32:I:614:PID:HM41	1.96	0.42
11:K:120:LEU:HD11	27:K:603:CLA:CAC	2.47	0.42
27:C:205:CLA:H61	27:C:205:CLA:H41	1.94	0.42
10:J:106:ILE:N	10:J:193:ASP:OD2	2.47	0.41
4:D:148:GLY:O	4:D:152:MET:HG3	2.19	0.41
11:K:217:GLU:HG2	11:K:222:MET:O	2.20	0.41
1:A:97:ARG:HD2	1:A:101:LEU:CD2	2.49	0.41
2:B:126:ARG:NH1	2:B:133:PHE:O	2.50	0.41
32:F:614:PID:H313	32:F:614:PID:C26	2.51	0.41
13:U:32:ARG:HH21	27:U:603:CLA:HED2	1.85	0.41
3:C:36:LEU:HB2	27:C:203:CLA:HED1	2.02	0.41
27:G:611:CLA:HMB1	27:G:611:CLA:HBB1	2.03	0.41
11:K:200:ILE:O	11:K:204:ARG:HG3	2.21	0.41
11:K:110:LYS:NZ	11:K:169:ASP:OD1	2.35	0.41
1:A:134:ALA:HB1	27:A:604:CLA:HED3	2.03	0.41
27:G:602:CLA:HMC2	30:G:613:DD6:C9	2.50	0.41
4:D:45:ALA:O	4:D:49:HIS:ND1	2.50	0.41
4:D:67:LEU:O	4:D:67:LEU:HG	2.20	0.41
27:D:610:CLA:HMB1	27:D:610:CLA:HBB1	2.03	0.41
5:E:132:PRO:HA	5:E:135:VAL:O	2.20	0.41
7:G:175:ARG:HA	7:G:178:MET:HE3	2.03	0.41
12:T:103:LEU:HD13	12:T:191:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:601:CLA:HMB1	27:T:601:CLA:CBB	2.50	0.41
27:T:603:CLA:HMB1	27:T:603:CLA:CBB	2.51	0.41
28:J:604:KC2:CBC	32:J:613:PID:H17	2.51	0.41
32:J:613:PID:H11	32:J:614:PID:HM22	2.01	0.41
33:K:613:LMG:O5	33:K:613:LMG:O4	2.32	0.41
3:C:28:PRO:HG3	27:C:202:CLA:HMB3	2.03	0.40
6:F:199:PRO:HA	6:F:203:VAL:HG13	2.02	0.40
27:G:607:CLA:HMB1	27:G:607:CLA:CBB	2.50	0.40
9:I:170:ASN:ND2	27:I:607:CLA:O1D	2.53	0.40
10:J:39:ALA:HB3	27:J:607:CLA:HMB3	2.03	0.40
12:T:170:THR:O	12:T:174:ARG:HG3	2.22	0.40
27:B:606:CLA:HMB1	27:B:606:CLA:CBB	2.52	0.40
27:I:601:CLA:HMC2	30:I:613:DD6:C24	2.51	0.40
36:T:613:LMU:O3'	36:T:613:LMU:C1B	2.69	0.40
27:F:602:CLA:HMB1	27:F:602:CLA:HBB1	2.02	0.40
27:J:609:CLA:HBB1	27:J:609:CLA:HMB1	2.03	0.40
27:J:609:CLA:HMB3	32:J:611:PID:HM13	2.04	0.40
32:K:611:PID:HM51	32:K:611:PID:CM8	2.51	0.40
5:E:116:LEU:HD22	5:E:214:GLU:OE2	2.20	0.40
27:E:611:CLA:H43	27:G:605:CLA:H43	2.04	0.40
27:A:601:CLA:CBC	4:D:104:PHE:CZ	3.05	0.40
27:A:604:CLA:HMB1	27:A:604:CLA:CBB	2.52	0.40
27:C:205:CLA:HMB1	27:C:205:CLA:HBB1	2.04	0.40
27:I:603:CLA:O2A	27:I:603:CLA:C1A	2.69	0.40
13:U:66:ILE:O	13:U:70:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/256 (75%)	186 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	183/269 (68%)	177 (97%)	6 (3%)	0	100	100
3	C	190/193 (98%)	186 (98%)	4 (2%)	0	100	100
4	D	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
5	E	182/253 (72%)	175 (96%)	7 (4%)	0	100	100
6	F	223/286 (78%)	212 (95%)	10 (4%)	1 (0%)	34	66
7	G	171/228 (75%)	162 (95%)	9 (5%)	0	100	100
8	H	190/271 (70%)	186 (98%)	4 (2%)	0	100	100
9	I	219/246 (89%)	207 (94%)	12 (6%)	0	100	100
10	J	171/203 (84%)	168 (98%)	3 (2%)	0	100	100
11	K	152/226 (67%)	147 (97%)	5 (3%)	0	100	100
12	T	138/206 (67%)	128 (93%)	10 (7%)	0	100	100
13	U	100/137 (73%)	96 (96%)	4 (4%)	0	100	100
14	a	659/687 (96%)	642 (97%)	17 (3%)	0	100	100
15	b	655/669 (98%)	634 (97%)	20 (3%)	1 (0%)	47	78
16	c	84/161 (52%)	78 (93%)	6 (7%)	0	100	100
17	d	212/295 (72%)	206 (97%)	6 (3%)	0	100	100
18	e	71/121 (59%)	68 (96%)	3 (4%)	0	100	100
19	f	167/279 (60%)	162 (97%)	5 (3%)	0	100	100
20	i	118/179 (66%)	116 (98%)	2 (2%)	0	100	100
21	j	97/141 (69%)	96 (99%)	1 (1%)	0	100	100
22	l	251/361 (70%)	246 (98%)	5 (2%)	0	100	100
23	m	77/142 (54%)	75 (97%)	2 (3%)	0	100	100
24	r	129/152 (85%)	126 (98%)	3 (2%)	0	100	100
25	x	77/121 (64%)	73 (95%)	4 (5%)	0	100	100
26	y	128/223 (57%)	127 (99%)	1 (1%)	0	100	100
All	All	5011/6482 (77%)	4849 (97%)	160 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	117	VAL
15	b	454	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	149/195 (76%)	149 (100%)	0	100 100
2	B	149/202 (74%)	149 (100%)	0	100 100
3	C	155/156 (99%)	155 (100%)	0	100 100
4	D	140/140 (100%)	140 (100%)	0	100 100
5	E	145/181 (80%)	145 (100%)	0	100 100
6	F	183/220 (83%)	183 (100%)	0	100 100
7	G	134/172 (78%)	134 (100%)	0	100 100
8	H	143/188 (76%)	143 (100%)	0	100 100
9	I	186/205 (91%)	185 (100%)	1 (0%)	88 96
10	J	134/156 (86%)	134 (100%)	0	100 100
11	K	107/155 (69%)	107 (100%)	0	100 100
12	T	108/152 (71%)	108 (100%)	0	100 100
13	U	83/110 (76%)	83 (100%)	0	100 100
14	a	565/584 (97%)	565 (100%)	0	100 100
15	b	559/568 (98%)	557 (100%)	2 (0%)	91 97
16	c	75/119 (63%)	75 (100%)	0	100 100
17	d	193/242 (80%)	193 (100%)	0	100 100
18	e	64/93 (69%)	64 (100%)	0	100 100
19	f	140/212 (66%)	140 (100%)	0	100 100
20	i	102/143 (71%)	102 (100%)	0	100 100
21	j	90/124 (73%)	90 (100%)	0	100 100
22	l	201/280 (72%)	201 (100%)	0	100 100
23	m	63/108 (58%)	63 (100%)	0	100 100
24	r	115/124 (93%)	114 (99%)	1 (1%)	78 94
25	x	67/97 (69%)	67 (100%)	0	100 100
26	y	115/175 (66%)	115 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4165/5101 (82%)	4161 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	198	CYS
15	b	98	HIS
15	b	227	PHE
24	r	141	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
8	H	158	ASN
8	H	181	HIS
11	K	202	HIS
11	K	213	GLN
14	a	532	GLN
15	b	245	HIS
15	b	495	HIS
17	d	220	HIS
20	i	93	GLN
24	r	51	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

323 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	DD6	D	615	-	39,45,45	0.16	0	52,67,67	0.63	1 (1%)
34	LHG	F	618	-	36,36,48	0.58	0	39,42,54	0.56	0
28	KC2	U	602	-	48,53,53	1.52	8 (16%)	54,89,89	1.07	5 (9%)
27	CLA	l	411	22	48,56,73	2.55	8 (16%)	55,92,113	1.66	7 (12%)
30	DD6	G	614	-	39,45,45	0.16	0	52,67,67	0.75	3 (5%)
27	CLA	A	604	-	45,53,73	2.67	8 (17%)	52,89,113	1.66	7 (13%)
27	CLA	K	603	-	45,53,73	2.73	8 (17%)	52,89,113	1.71	7 (13%)
27	CLA	E	606	-	60,68,73	2.33	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	b	728	-	65,73,73	2.19	8 (12%)	76,113,113	1.36	8 (10%)
30	DD6	E	617	-	39,45,45	0.15	0	52,67,67	0.82	2 (3%)
27	CLA	A	610	-	55,63,73	2.39	8 (14%)	64,101,113	1.51	7 (10%)
27	CLA	a	807	-	65,73,73	2.21	8 (12%)	76,113,113	1.43	9 (11%)
34	LHG	G	617	-	33,33,48	0.60	0	36,39,54	0.55	0
27	CLA	a	837	-	65,73,73	2.06	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	E	602	5	55,63,73	2.41	8 (14%)	64,101,113	1.53	7 (10%)
30	DD6	A	617	-	39,45,45	0.18	0	52,67,67	0.66	2 (3%)
27	CLA	a	810	-	50,58,73	2.54	8 (16%)	58,95,113	1.60	9 (15%)
27	CLA	C	208	-	47,55,73	2.61	8 (17%)	54,91,113	1.63	7 (12%)
27	CLA	C	202	3	45,53,73	2.69	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	I	610	-	55,63,73	2.41	8 (14%)	64,101,113	1.63	6 (9%)
27	CLA	B	607	-	60,68,73	2.30	8 (13%)	70,107,113	1.42	8 (11%)
27	CLA	A	605	1	55,63,73	2.42	8 (14%)	64,101,113	1.51	7 (10%)
28	KC2	H	302	30	48,53,53	1.50	8 (16%)	54,89,89	1.11	5 (9%)
27	CLA	H	308	8	55,63,73	2.36	8 (14%)	64,101,113	1.47	7 (10%)
27	CLA	F	619	-	55,63,73	2.38	8 (14%)	64,101,113	1.50	7 (10%)
27	CLA	D	604	-	55,63,73	2.39	8 (14%)	64,101,113	1.53	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	PID	B	613	-	41,49,49	1.56	7 (17%)	49,76,76	3.46	21 (42%)
27	CLA	b	721	-	50,58,73	2.55	8 (16%)	58,95,113	1.60	7 (12%)
27	CLA	C	212	-	47,55,73	2.65	8 (17%)	54,91,113	1.64	7 (12%)
27	CLA	F	610	6	47,55,73	2.67	8 (17%)	54,91,113	1.66	7 (12%)
32	PID	J	615	-	41,49,49	1.51	5 (12%)	49,76,76	3.56	18 (36%)
27	CLA	D	602	-	55,63,73	2.39	8 (14%)	64,101,113	1.57	6 (9%)
30	DD6	I	615	-	39,45,45	0.18	0	52,67,67	0.59	2 (3%)
27	CLA	F	608	6	45,53,73	2.72	8 (17%)	52,89,113	1.67	7 (13%)
27	CLA	B	604	2	47,55,73	2.67	8 (17%)	54,91,113	1.69	7 (12%)
27	CLA	H	312	-	42,50,73	2.72	8 (19%)	48,85,113	1.74	8 (16%)
30	DD6	G	616	-	39,45,45	0.15	0	52,67,67	0.47	0
27	CLA	K	601	11	57,65,73	2.38	8 (14%)	66,103,113	1.52	7 (10%)
27	CLA	b	723	-	65,73,73	2.21	8 (12%)	76,113,113	1.42	7 (9%)
27	CLA	K	606	-	41,49,73	2.91	9 (21%)	47,84,113	1.90	8 (17%)
27	CLA	H	307	-	45,53,73	2.66	8 (17%)	52,89,113	1.64	7 (13%)
28	KC2	B	608	2	48,53,53	1.47	8 (16%)	54,89,89	1.09	5 (9%)
27	CLA	b	717	-	65,73,73	2.15	8 (12%)	76,113,113	1.38	7 (9%)
30	DD6	E	613	-	39,45,45	0.18	0	52,67,67	0.87	4 (7%)
27	CLA	a	805	-	65,73,73	2.22	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	f	302	-	48,56,73	2.60	8 (16%)	55,92,113	1.60	8 (14%)
27	CLA	A	602	1	60,68,73	2.33	8 (13%)	70,107,113	1.48	7 (10%)
30	DD6	B	612	-	39,45,45	0.17	0	52,67,67	0.64	2 (3%)
27	CLA	I	605	9	55,63,73	2.37	8 (14%)	64,101,113	1.46	7 (10%)
27	CLA	H	303	8	60,68,73	2.26	8 (13%)	70,107,113	1.46	8 (11%)
30	DD6	B	616	-	39,45,45	0.14	0	52,67,67	0.58	0
28	KC2	G	601	-	48,53,53	1.50	8 (16%)	54,89,89	1.13	6 (11%)
30	DD6	b	730	-	39,45,45	0.18	0	52,67,67	0.61	1 (1%)
28	KC2	C	210	-	48,53,53	1.53	8 (16%)	54,89,89	1.07	5 (9%)
27	CLA	l	408	-	47,55,73	2.61	8 (17%)	54,91,113	1.70	7 (12%)
38	BCR	l	415	-	41,41,41	0.33	0	56,56,56	0.57	0
34	LHG	D	620	-	45,45,48	0.53	0	48,51,54	0.51	0
38	BCR	a	833	-	41,41,41	0.30	0	56,56,56	0.61	0
27	CLA	a	816	-	60,68,73	2.33	8 (13%)	70,107,113	1.46	7 (10%)
32	PID	U	608	-	41,49,49	1.55	6 (14%)	49,76,76	3.57	17 (34%)
30	DD6	G	612	-	39,45,45	0.17	0	52,67,67	0.94	3 (5%)
27	CLA	b	719	-	65,73,73	2.20	8 (12%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	f	303	19	48,56,73	2.62	8 (16%)	55,92,113	1.59	8 (14%)
27	CLA	a	802	-	55,63,73	2.37	8 (14%)	64,101,113	1.47	8 (12%)
27	CLA	b	701	-	65,73,73	2.20	8 (12%)	76,113,113	1.37	7 (9%)
39	SF4	c	202	-	0,12,12	-	-	-		
27	CLA	B	609	2	65,73,73	2.20	8 (12%)	76,113,113	1.38	8 (10%)
27	CLA	J	603	-	60,68,73	2.32	8 (13%)	70,107,113	1.46	7 (10%)
36	LMU	T	613	-	36,36,36	0.41	0	47,47,47	0.95	2 (4%)
28	KC2	U	604	13	48,53,53	1.54	8 (16%)	54,89,89	1.08	5 (9%)
38	BCR	a	836	-	41,41,41	0.85	2 (4%)	56,56,56	2.18	19 (33%)
27	CLA	a	809	-	47,55,73	2.64	8 (17%)	54,91,113	1.74	5 (9%)
30	DD6	C	214	-	39,45,45	0.19	0	52,67,67	0.69	2 (3%)
27	CLA	a	826	-	55,63,73	2.32	8 (14%)	64,101,113	1.47	7 (10%)
28	KC2	E	601	27	48,53,53	1.52	8 (16%)	54,89,89	1.10	5 (9%)
27	CLA	a	820	-	65,73,73	2.20	8 (12%)	76,113,113	1.36	7 (9%)
29	UIX	A	616	-	41,49,49	1.27	4 (9%)	52,74,74	1.91	16 (30%)
27	CLA	b	710	-	55,63,73	2.42	8 (14%)	64,101,113	1.55	8 (12%)
27	CLA	D	612	-	55,63,73	2.42	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	a	808	14	55,63,73	2.45	8 (14%)	64,101,113	1.54	9 (14%)
27	CLA	U	603	-	50,58,73	2.56	8 (16%)	58,95,113	1.69	7 (12%)
27	CLA	E	605	5	45,53,73	2.69	8 (17%)	52,89,113	1.73	8 (15%)
28	KC2	J	604	10	48,53,53	1.51	8 (16%)	54,89,89	1.08	5 (9%)
27	CLA	r	204	-	60,68,73	2.30	8 (13%)	70,107,113	1.41	7 (10%)
27	CLA	b	718	-	65,73,73	2.15	8 (12%)	76,113,113	1.52	8 (10%)
30	DD6	G	613	-	39,45,45	0.15	0	52,67,67	0.78	2 (3%)
27	CLA	T	604	12	41,49,73	2.86	9 (21%)	47,84,113	1.77	7 (14%)
27	CLA	b	703	-	65,73,73	2.16	8 (12%)	76,113,113	1.44	11 (14%)
28	KC2	H	311	-	48,53,53	1.51	8 (16%)	54,89,89	1.09	5 (9%)
30	DD6	I	613	-	39,45,45	0.19	0	52,67,67	0.89	4 (7%)
32	PID	K	611	-	41,49,49	1.62	5 (12%)	49,76,76	3.72	19 (38%)
37	PQN	a	832	-	34,34,34	0.35	0	42,45,45	0.68	0
30	DD6	K	610	-	39,45,45	0.17	0	52,67,67	0.81	2 (3%)
27	CLA	b	711	-	60,68,73	2.31	8 (13%)	70,107,113	1.47	7 (10%)
32	PID	F	614	-	41,49,49	1.55	5 (12%)	49,76,76	3.83	17 (34%)
29	UIX	B	615	-	41,49,49	1.25	4 (9%)	52,74,74	1.89	15 (28%)
27	CLA	b	714	-	48,56,73	2.60	8 (16%)	55,92,113	1.74	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	DD6	F	612	-	39,45,45	0.16	0	52,67,67	0.50	0
27	CLA	a	827	-	65,73,73	2.23	8 (12%)	76,113,113	1.51	8 (10%)
27	CLA	D	605	4	47,55,73	2.59	8 (17%)	54,91,113	1.57	8 (14%)
28	KC2	T	608	-	48,53,53	1.57	7 (14%)	54,89,89	1.09	4 (7%)
30	DD6	i	202	-	39,45,45	0.18	0	52,67,67	0.87	2 (3%)
27	CLA	T	605	12	45,53,73	2.62	8 (17%)	52,89,113	1.59	6 (11%)
38	BCR	b	732	-	41,41,41	0.30	0	56,56,56	0.75	0
29	UIX	H	314	-	41,49,49	1.23	3 (7%)	52,74,74	1.94	18 (34%)
38	BCR	f	301	-	41,41,41	0.30	0	56,56,56	0.73	0
27	CLA	F	602	-	56,64,73	2.39	8 (14%)	65,102,113	1.50	8 (12%)
27	CLA	C	205	-	55,63,73	2.43	8 (14%)	64,101,113	1.70	7 (10%)
27	CLA	H	310	-	45,53,73	2.73	8 (17%)	52,89,113	1.75	8 (15%)
35	DGD	f	305	-	53,53,67	0.97	3 (5%)	67,67,81	1.51	11 (16%)
30	DD6	F	611	-	39,45,45	0.16	0	52,67,67	0.93	4 (7%)
27	CLA	T	602	-	45,53,73	2.70	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	D	608	4	55,63,73	2.39	8 (14%)	64,101,113	1.55	8 (12%)
27	CLA	l	407	-	48,56,73	2.62	8 (16%)	55,92,113	1.61	7 (12%)
34	LHG	l	401	-	45,45,48	0.52	0	48,51,54	0.47	0
30	DD6	r	201	-	39,45,45	0.16	0	52,67,67	0.87	2 (3%)
27	CLA	C	206	-	47,55,73	2.58	8 (17%)	54,91,113	1.61	7 (12%)
28	KC2	B	602	-	48,53,53	1.46	7 (14%)	54,89,89	1.04	5 (9%)
27	CLA	a	825	-	65,73,73	2.22	8 (12%)	76,113,113	1.37	7 (9%)
29	UIX	A	613	-	41,49,49	1.23	3 (7%)	52,74,74	1.86	13 (25%)
27	CLA	a	817	-	55,63,73	2.43	8 (14%)	64,101,113	1.52	8 (12%)
27	CLA	B	606	-	65,73,73	2.22	8 (12%)	76,113,113	1.45	8 (10%)
38	BCR	f	304	-	41,41,41	0.30	0	56,56,56	0.52	0
38	BCR	j	203	-	41,41,41	0.32	0	56,56,56	0.57	0
27	CLA	G	608	-	60,68,73	2.35	8 (13%)	70,107,113	1.51	7 (10%)
27	CLA	H	304	-	60,68,73	2.30	8 (13%)	70,107,113	1.51	11 (15%)
29	UIX	B	611	-	41,49,49	1.31	4 (9%)	52,74,74	2.00	21 (40%)
30	DD6	D	613	-	39,45,45	0.43	0	52,67,67	0.81	3 (5%)
30	DD6	A	615	-	39,45,45	0.16	0	52,67,67	0.86	3 (5%)
27	CLA	D	609	-	45,53,73	2.70	8 (17%)	52,89,113	1.67	7 (13%)
29	UIX	j	204	-	41,49,49	1.25	3 (7%)	52,74,74	2.02	18 (34%)
28	KC2	A	608	-	48,53,53	1.48	7 (14%)	54,89,89	1.15	6 (11%)
27	CLA	a	823	-	65,73,73	2.22	8 (12%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PQN	b	729	-	34,34,34	0.36	0	42,45,45	0.61	1 (2%)
27	CLA	A	607	-	45,53,73	2.70	8 (17%)	52,89,113	1.66	7 (13%)
27	CLA	a	831	-	55,63,73	2.39	8 (14%)	64,101,113	1.52	8 (12%)
27	CLA	l	410	-	48,56,73	2.62	8 (16%)	55,92,113	1.68	7 (12%)
27	CLA	T	609	-	41,49,73	2.91	9 (21%)	47,84,113	1.83	7 (14%)
27	CLA	b	702	-	65,73,73	2.09	8 (12%)	76,113,113	1.28	9 (11%)
27	CLA	D	607	4	60,68,73	2.30	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	J	607	-	42,50,73	2.81	8 (19%)	48,85,113	1.73	7 (14%)
33	LMG	D	618	-	35,35,55	0.55	0	43,43,63	0.78	1 (2%)
27	CLA	B	601	-	60,68,73	2.26	8 (13%)	70,107,113	1.49	8 (11%)
31	SQD	y	301	-	45,46,54	1.29	4 (8%)	54,57,65	1.08	5 (9%)
29	UIX	H	317	-	41,49,49	1.21	3 (7%)	52,74,74	1.91	16 (30%)
35	DGD	j	201	-	61,61,67	0.92	4 (6%)	75,75,81	1.44	13 (17%)
27	CLA	T	603	-	45,53,73	2.66	8 (17%)	52,89,113	1.62	7 (13%)
27	CLA	G	611	-	45,53,73	2.69	8 (17%)	52,89,113	1.65	7 (13%)
38	BCR	l	413	-	41,41,41	0.32	0	56,56,56	0.54	0
39	SF4	a	838	14	0,12,12	-	-	-		
27	CLA	I	602	-	55,63,73	2.37	8 (14%)	64,101,113	1.45	7 (10%)
29	UIX	T	612	-	41,49,49	1.24	4 (9%)	52,74,74	2.02	18 (34%)
30	DD6	B	614	-	39,45,45	0.42	0	52,67,67	0.85	1 (1%)
27	CLA	l	403	-	65,73,73	2.18	8 (12%)	76,113,113	1.35	7 (9%)
35	DGD	K	614	-	48,48,67	1.00	3 (6%)	62,62,81	1.43	10 (16%)
33	LMG	C	217	-	34,34,55	0.58	0	42,42,63	0.71	1 (2%)
28	KC2	E	610	5	48,53,53	1.51	8 (16%)	54,89,89	1.08	5 (9%)
30	DD6	K	609	-	39,45,45	0.16	0	52,67,67	0.59	1 (1%)
27	CLA	C	203	3	65,73,73	2.19	8 (12%)	76,113,113	1.44	8 (10%)
27	CLA	A	612	1	47,55,73	2.64	8 (17%)	54,91,113	1.86	10 (18%)
27	CLA	I	606	9	55,63,73	2.41	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	l	405	22	61,69,73	2.28	8 (13%)	71,108,113	1.44	7 (9%)
27	CLA	G	605	-	60,68,73	2.32	8 (13%)	70,107,113	1.56	8 (11%)
35	DGD	l	416	-	56,56,67	0.92	2 (3%)	70,70,81	1.40	7 (10%)
30	DD6	U	607	-	39,45,45	0.14	0	52,67,67	0.59	1 (1%)
30	DD6	E	615	-	39,45,45	0.17	0	52,67,67	0.71	3 (5%)
27	CLA	U	601	-	43,51,73	2.80	8 (18%)	49,86,113	1.87	6 (12%)
27	CLA	U	605	13	60,68,73	2.34	8 (13%)	70,107,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	DD6	H	316	-	39,45,45	0.20	0	52,67,67	0.77	3 (5%)
28	KC2	J	606	-	48,53,53	1.49	7 (14%)	54,89,89	1.07	4 (7%)
33	LMG	F	616	-	46,46,55	0.52	0	54,54,63	0.69	0
27	CLA	T	601	12	47,55,73	2.67	8 (17%)	54,91,113	1.70	8 (14%)
28	KC2	F	609	6	48,53,53	1.54	8 (16%)	54,89,89	1.07	5 (9%)
30	DD6	C	216	-	39,45,45	0.16	0	52,67,67	0.77	2 (3%)
27	CLA	J	601	-	45,53,73	2.68	8 (17%)	52,89,113	1.75	6 (11%)
27	CLA	T	606	12	45,53,73	2.72	8 (17%)	52,89,113	1.66	5 (9%)
27	CLA	F	606	6	65,73,73	2.19	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	l	406	-	65,73,73	2.20	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	a	839	-	61,69,73	2.25	8 (13%)	71,108,113	1.40	7 (9%)
27	CLA	F	607	6	45,53,73	2.66	8 (17%)	52,89,113	1.72	7 (13%)
27	CLA	l	402	-	60,68,73	2.33	8 (13%)	70,107,113	1.49	7 (10%)
27	CLA	C	201	-	42,50,73	2.79	8 (19%)	48,85,113	1.77	9 (18%)
27	CLA	H	319	-	65,73,73	2.20	8 (12%)	76,113,113	1.39	7 (9%)
38	BCR	b	731	-	41,41,41	0.31	0	56,56,56	0.73	1 (1%)
27	CLA	A	603	-	55,63,73	2.38	8 (14%)	64,101,113	1.51	8 (12%)
27	CLA	b	720	-	48,56,73	2.59	8 (16%)	55,92,113	1.62	7 (12%)
30	DD6	K	612	-	39,45,45	0.15	0	52,67,67	0.68	3 (5%)
27	CLA	T	607	-	45,53,73	2.71	8 (17%)	52,89,113	1.67	7 (13%)
27	CLA	E	608	5	60,68,73	2.31	8 (13%)	70,107,113	1.47	5 (7%)
27	CLA	b	726	-	60,68,73	2.30	8 (13%)	70,107,113	1.43	7 (10%)
38	BCR	i	201	-	41,41,41	0.31	0	56,56,56	0.94	1 (1%)
27	CLA	I	608	9	60,68,73	2.30	8 (13%)	70,107,113	1.39	8 (11%)
27	CLA	E	607	5	65,73,73	2.17	8 (12%)	76,113,113	1.33	8 (10%)
27	CLA	F	617	-	60,68,73	2.30	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	a	821	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	I	603	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	9 (11%)
27	CLA	a	822	-	60,68,73	2.31	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	F	604	-	45,53,73	2.59	8 (17%)	52,89,113	1.64	8 (15%)
27	CLA	G	607	7	45,53,73	2.67	8 (17%)	52,89,113	1.76	7 (13%)
30	DD6	D	617	-	39,45,45	0.19	0	52,67,67	0.64	3 (5%)
31	SQD	A	618	-	27,28,54	1.50	4 (14%)	36,39,65	1.32	4 (11%)
27	CLA	b	707	-	65,73,73	2.15	8 (12%)	76,113,113	1.43	7 (9%)
34	LHG	a	835	-	47,47,48	0.52	0	50,53,54	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	l	404	-	55,63,73	2.32	8 (14%)	64,101,113	1.55	8 (12%)
27	CLA	K	605	11	60,68,73	2.29	8 (13%)	70,107,113	1.42	6 (8%)
28	KC2	J	610	-	48,53,53	1.49	8 (16%)	54,89,89	1.10	5 (9%)
28	KC2	J	602	10	48,53,53	1.50	8 (16%)	54,89,89	1.06	4 (7%)
27	CLA	B	603	-	65,73,73	2.25	8 (12%)	76,113,113	1.50	7 (9%)
38	BCR	a	834	-	41,41,41	0.28	0	56,56,56	0.53	0
27	CLA	b	725	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	8 (10%)
29	UIX	C	215	-	41,49,49	1.22	3 (7%)	52,74,74	2.12	21 (40%)
27	CLA	C	209	-	45,53,73	2.71	8 (17%)	52,89,113	1.69	8 (15%)
27	CLA	G	603	-	50,58,73	2.50	8 (16%)	58,95,113	1.58	8 (13%)
29	UIX	C	213	-	41,49,49	1.26	3 (7%)	52,74,74	1.89	16 (30%)
34	LHG	j	205	-	36,36,48	0.57	0	39,42,54	0.53	0
27	CLA	a	818	-	55,63,73	2.36	8 (14%)	64,101,113	1.49	6 (9%)
30	DD6	D	621	-	39,45,45	0.18	0	52,67,67	0.75	2 (3%)
27	CLA	B	610	-	47,55,73	2.61	8 (17%)	54,91,113	1.66	7 (12%)
30	DD6	r	206	-	39,45,45	0.18	0	52,67,67	0.83	3 (5%)
30	DD6	r	205	-	39,45,45	0.18	0	52,67,67	0.86	2 (3%)
27	CLA	a	815	-	60,68,73	2.27	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	a	829	27	65,73,73	2.23	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	J	609	-	41,49,73	2.89	9 (21%)	47,84,113	1.87	7 (14%)
30	DD6	T	610	-	39,45,45	0.15	0	52,67,67	0.64	1 (1%)
27	CLA	K	608	-	45,53,73	2.73	8 (17%)	52,89,113	1.67	8 (15%)
32	PID	F	615	-	41,49,49	1.53	5 (12%)	49,76,76	3.48	16 (32%)
27	CLA	l	409	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	b	727	-	65,73,73	2.20	8 (12%)	76,113,113	1.44	8 (10%)
38	BCR	m	201	-	41,41,41	0.30	0	56,56,56	0.69	0
34	LHG	r	202	-	45,45,48	0.53	0	48,51,54	0.51	0
27	CLA	G	606	7	65,73,73	2.22	8 (12%)	76,113,113	1.45	9 (11%)
27	CLA	G	604	-	47,55,73	2.66	8 (17%)	54,91,113	1.70	5 (9%)
27	CLA	F	605	6	45,53,73	2.67	8 (17%)	52,89,113	1.71	8 (15%)
30	DD6	T	611	-	39,45,45	0.17	0	52,67,67	0.77	4 (7%)
30	DD6	H	318	28	39,45,45	0.15	0	52,67,67	0.74	3 (5%)
27	CLA	a	813	-	48,56,73	2.63	8 (16%)	55,92,113	1.62	7 (12%)
33	LMG	b	733	-	55,55,55	0.48	0	63,63,63	0.57	0
27	CLA	a	814	-	55,63,73	2.42	8 (14%)	64,101,113	1.49	7 (10%)
27	CLA	b	724	-	65,73,73	2.21	8 (12%)	76,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	KC2	J	608	-	48,53,53	1.53	7 (14%)	54,89,89	1.09	5 (9%)
27	CLA	C	211	-	47,55,73	2.62	8 (17%)	54,91,113	1.59	7 (12%)
33	LMG	l	417	-	50,50,55	0.49	0	58,58,63	0.61	0
27	CLA	a	828	-	48,56,73	2.65	8 (16%)	55,92,113	1.73	6 (10%)
30	DD6	H	301	-	39,45,45	0.19	0	52,67,67	0.75	2 (3%)
27	CLA	a	824	-	65,73,73	2.19	8 (12%)	76,113,113	1.41	8 (10%)
27	CLA	b	722	-	48,56,73	2.57	8 (16%)	55,92,113	1.66	7 (12%)
27	CLA	D	603	-	55,63,73	2.40	8 (14%)	64,101,113	1.55	7 (10%)
27	CLA	E	609	28	45,53,73	2.69	8 (17%)	52,89,113	1.63	7 (13%)
38	BCR	l	414	-	41,41,41	0.33	0	56,56,56	0.81	0
30	DD6	J	612	-	39,45,45	0.19	0	52,67,67	0.67	2 (3%)
27	CLA	a	801	-	65,73,73	2.10	7 (10%)	76,113,113	1.30	9 (11%)
27	CLA	G	609	7	55,63,73	2.42	8 (14%)	64,101,113	1.51	9 (14%)
27	CLA	a	804	-	65,73,73	2.19	8 (12%)	76,113,113	1.49	10 (13%)
39	SF4	c	201	16	0,12,12	-	-	-		
27	CLA	l	412	22	65,73,73	2.19	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	G	602	7	55,63,73	2.41	8 (14%)	64,101,113	1.51	7 (10%)
27	CLA	A	601	1	42,50,73	2.74	8 (19%)	48,85,113	1.73	8 (16%)
27	CLA	I	616	-	65,73,73	2.25	8 (12%)	76,113,113	1.33	7 (9%)
27	CLA	G	610	7	47,55,73	2.64	8 (17%)	54,91,113	1.61	7 (12%)
27	CLA	E	604	-	55,63,73	2.40	8 (14%)	64,101,113	1.53	8 (12%)
27	CLA	D	611	-	60,68,73	2.30	8 (13%)	70,107,113	1.42	8 (11%)
27	CLA	A	606	1	47,55,73	2.59	8 (17%)	54,91,113	1.65	7 (12%)
27	CLA	j	202	27	56,64,73	2.42	7 (12%)	65,102,113	1.44	7 (10%)
27	CLA	D	601	4	45,53,73	2.66	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	b	704	-	65,73,73	2.19	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	D	606	-	45,53,73	2.63	8 (17%)	52,89,113	1.66	7 (13%)
30	DD6	H	315	-	39,45,45	0.17	0	52,67,67	0.65	1 (1%)
27	CLA	A	609	-	47,55,73	2.60	8 (17%)	54,91,113	1.62	7 (12%)
30	DD6	A	614	-	39,45,45	0.16	0	52,67,67	0.71	2 (3%)
27	CLA	C	204	-	65,73,73	2.21	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	I	601	9	65,73,73	2.20	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	b	709	15	65,73,73	2.12	8 (12%)	76,113,113	1.34	7 (9%)
27	CLA	r	203	-	48,56,73	2.61	8 (16%)	55,92,113	1.65	5 (9%)
30	DD6	D	614	-	39,45,45	0.15	0	52,67,67	0.66	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	F	603	-	52,60,73	2.44	8 (15%)	60,97,113	1.55	7 (11%)
27	CLA	a	812	-	50,58,73	2.59	8 (16%)	58,95,113	1.71	10 (17%)
27	CLA	a	819	-	60,68,73	2.29	8 (13%)	70,107,113	1.43	7 (10%)
27	CLA	I	609	9	45,53,73	2.66	8 (17%)	52,89,113	1.72	8 (15%)
29	UIX	F	613	-	41,49,49	1.21	3 (7%)	52,74,74	2.03	14 (26%)
29	UIX	D	616	-	41,49,49	1.22	3 (7%)	52,74,74	2.11	16 (30%)
32	PID	I	614	-	41,49,49	1.58	5 (12%)	49,76,76	3.86	22 (44%)
27	CLA	I	607	-	61,69,73	2.28	8 (13%)	71,108,113	1.43	7 (9%)
27	CLA	K	604	-	57,65,73	2.36	8 (14%)	66,103,113	1.46	6 (9%)
27	CLA	I	611	-	42,50,73	2.85	8 (19%)	48,85,113	1.84	9 (18%)
32	PID	J	611	-	41,49,49	1.53	6 (14%)	49,76,76	4.07	21 (42%)
27	CLA	C	207	3	60,68,73	2.31	8 (13%)	70,107,113	1.46	8 (11%)
27	CLA	H	309	-	65,73,73	2.23	8 (12%)	76,113,113	1.41	7 (9%)
27	CLA	b	708	-	65,73,73	2.12	8 (12%)	76,113,113	1.30	6 (7%)
27	CLA	b	713	-	65,73,73	2.20	8 (12%)	76,113,113	1.48	8 (10%)
27	CLA	b	705	-	65,73,73	2.21	8 (12%)	76,113,113	1.49	5 (6%)
27	CLA	E	612	-	45,53,73	2.70	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	H	305	-	60,68,73	2.31	8 (13%)	70,107,113	1.54	10 (14%)
27	CLA	A	611	27	45,53,73	2.71	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	B	605	2	45,53,73	2.64	8 (17%)	52,89,113	1.67	8 (15%)
28	KC2	I	604	9	48,53,53	1.51	8 (16%)	54,89,89	1.09	5 (9%)
29	UIX	J	616	-	41,49,49	1.22	3 (7%)	52,74,74	1.87	14 (26%)
27	CLA	b	715	-	65,73,73	2.21	8 (12%)	76,113,113	1.51	9 (11%)
27	CLA	E	603	-	47,55,73	2.61	8 (17%)	54,91,113	1.64	7 (12%)
31	SQD	H	320	-	45,46,54	1.27	4 (8%)	54,57,65	1.09	6 (11%)
27	CLA	F	601	6	60,68,73	2.32	8 (13%)	70,107,113	1.46	7 (10%)
29	UIX	E	616	-	41,49,49	1.24	4 (9%)	52,74,74	1.97	15 (28%)
27	CLA	K	602	-	55,63,73	2.43	8 (14%)	64,101,113	1.51	8 (12%)
28	KC2	K	607	-	48,53,53	1.53	7 (14%)	54,89,89	1.09	5 (9%)
27	CLA	D	610	4	47,55,73	2.64	8 (17%)	54,91,113	1.60	8 (14%)
27	CLA	a	830	-	65,73,73	2.19	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	b	716	-	65,73,73	2.21	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	E	611	5	60,68,73	2.32	8 (13%)	70,107,113	1.49	8 (11%)
27	CLA	U	606	-	45,53,73	2.75	8 (17%)	52,89,113	1.67	7 (13%)
29	UIX	I	612	-	41,49,49	1.29	3 (7%)	52,74,74	2.14	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	H	313	-	60,68,73	2.33	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	a	806	-	55,63,73	2.41	8 (14%)	64,101,113	1.51	6 (9%)
33	LMG	K	613	-	42,42,55	0.53	0	50,50,63	0.66	0
32	PID	J	614	-	41,49,49	1.54	5 (12%)	49,76,76	3.27	15 (30%)
27	CLA	H	306	-	45,53,73	2.65	8 (17%)	52,89,113	1.64	8 (15%)
29	UIX	G	615	-	41,49,49	1.24	3 (7%)	52,74,74	1.97	17 (32%)
27	CLA	b	712	-	48,56,73	2.58	8 (16%)	55,92,113	1.66	8 (14%)
33	LMG	D	619	-	46,46,55	0.52	0	54,54,63	0.71	1 (1%)
27	CLA	J	605	10	60,68,73	2.29	8 (13%)	70,107,113	1.39	7 (10%)
30	DD6	E	614	-	39,45,45	0.17	0	52,67,67	0.52	0
27	CLA	b	706	-	65,73,73	2.19	8 (12%)	76,113,113	1.37	8 (10%)
32	PID	J	613	-	41,49,49	1.61	6 (14%)	49,76,76	4.24	20 (40%)
27	CLA	a	803	27	50,58,73	2.52	8 (16%)	58,95,113	1.67	6 (10%)
27	CLA	a	811	-	48,56,73	2.63	8 (16%)	55,92,113	1.63	8 (14%)

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
30	DD6	D	615	-	-	2/26/80/80	0/3/3/3
34	LHG	F	618	-	-	21/41/41/53	-
28	KC2	U	602	-	-	5/15/71/71	-
27	CLA	l	411	22	1/1/11/20	1/17/95/115	-
30	DD6	G	614	-	-	2/26/80/80	0/3/3/3
27	CLA	A	604	-	1/1/11/20	4/13/91/115	-
27	CLA	K	603	-	1/1/11/20	3/13/91/115	-
27	CLA	E	606	-	1/1/14/20	8/31/109/115	-
27	CLA	b	728	-	1/1/15/20	8/37/115/115	-
30	DD6	E	617	-	-	2/26/80/80	0/3/3/3
27	CLA	A	610	-	1/1/13/20	4/25/103/115	-
27	CLA	a	807	-	1/1/15/20	10/37/115/115	-
34	LHG	G	617	-	-	23/38/38/53	-
27	CLA	a	837	-	1/1/15/20	3/37/115/115	-
27	CLA	E	602	5	1/1/13/20	0/25/103/115	-
30	DD6	A	617	-	-	4/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	810	-	1/1/12/20	1/19/97/115	-
27	CLA	C	208	-	1/1/11/20	2/16/94/115	-
27	CLA	C	202	3	1/1/11/20	1/13/91/115	-
27	CLA	I	610	-	1/1/13/20	4/25/103/115	-
27	CLA	B	607	-	1/1/14/20	7/31/109/115	-
27	CLA	A	605	1	1/1/13/20	4/25/103/115	-
28	KC2	H	302	30	-	8/15/71/71	-
27	CLA	H	308	8	1/1/13/20	2/25/103/115	-
27	CLA	F	619	-	1/1/13/20	5/25/103/115	-
27	CLA	D	604	-	1/1/13/20	8/25/103/115	-
32	PID	B	613	-	-	3/24/93/93	0/4/4/4
27	CLA	b	721	-	1/1/12/20	2/19/97/115	-
27	CLA	C	212	-	1/1/11/20	0/16/94/115	-
27	CLA	F	610	6	1/1/11/20	6/16/94/115	-
32	PID	J	615	-	-	6/24/93/93	0/4/4/4
27	CLA	D	602	-	1/1/13/20	7/25/103/115	-
30	DD6	I	615	-	-	0/26/80/80	0/3/3/3
27	CLA	F	608	6	1/1/11/20	1/13/91/115	-
27	CLA	B	604	2	1/1/11/20	0/16/94/115	-
27	CLA	H	312	-	1/1/10/20	5/10/88/115	-
30	DD6	G	616	-	-	1/26/80/80	0/3/3/3
27	CLA	K	601	11	1/1/13/20	1/28/106/115	-
27	CLA	b	723	-	1/1/15/20	5/37/115/115	-
27	CLA	K	606	-	1/1/10/20	0/8/86/115	-
27	CLA	H	307	-	1/1/11/20	4/13/91/115	-
28	KC2	B	608	2	-	4/15/71/71	-
27	CLA	b	717	-	1/1/15/20	7/37/115/115	-
30	DD6	E	613	-	-	1/26/80/80	0/3/3/3
27	CLA	a	805	-	1/1/15/20	9/37/115/115	-
27	CLA	f	302	-	1/1/11/20	1/17/95/115	-
27	CLA	A	602	1	1/1/14/20	2/31/109/115	-
30	DD6	B	612	-	-	1/26/80/80	0/3/3/3
27	CLA	I	605	9	1/1/13/20	3/25/103/115	-
27	CLA	H	303	8	1/1/14/20	4/31/109/115	-
30	DD6	B	616	-	-	2/26/80/80	0/3/3/3
28	KC2	G	601	-	-	8/15/71/71	-
30	DD6	b	730	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	KC2	C	210	-	-	6/15/71/71	-
27	CLA	l	408	-	1/1/11/20	3/16/94/115	-
38	BCR	l	415	-	-	12/29/63/63	0/2/2/2
34	LHG	D	620	-	-	22/50/50/53	-
38	BCR	a	833	-	-	8/29/63/63	0/2/2/2
27	CLA	a	816	-	1/1/14/20	7/31/109/115	-
32	PID	U	608	-	-	4/24/93/93	1/4/4/4
30	DD6	G	612	-	-	0/26/80/80	0/3/3/3
27	CLA	b	719	-	1/1/15/20	7/37/115/115	-
27	CLA	f	303	19	1/1/11/20	0/17/95/115	-
27	CLA	a	802	-	1/1/13/20	4/25/103/115	-
27	CLA	b	701	-	1/1/15/20	9/37/115/115	-
39	SF4	c	202	-	-	-	0/6/5/5
27	CLA	B	609	2	1/1/15/20	6/37/115/115	-
27	CLA	J	603	-	1/1/14/20	4/31/109/115	-
36	LMU	T	613	-	-	5/21/61/61	0/2/2/2
28	KC2	U	604	13	-	8/15/71/71	-
38	BCR	a	836	-	-	13/29/63/63	0/2/2/2
27	CLA	a	809	-	1/1/11/20	3/16/94/115	-
30	DD6	C	214	-	-	1/26/80/80	0/3/3/3
27	CLA	a	826	-	1/1/13/20	4/25/103/115	-
28	KC2	E	601	27	-	10/15/71/71	-
27	CLA	a	820	-	1/1/15/20	8/37/115/115	-
29	UIX	A	616	-	-	6/31/87/87	0/3/3/3
27	CLA	b	710	-	1/1/13/20	3/25/103/115	-
27	CLA	D	612	-	1/1/13/20	5/25/103/115	-
27	CLA	a	808	14	1/1/13/20	5/25/103/115	-
27	CLA	U	603	-	1/1/12/20	6/19/97/115	-
27	CLA	E	605	5	1/1/11/20	4/13/91/115	-
28	KC2	J	604	10	-	5/15/71/71	-
27	CLA	r	204	-	1/1/14/20	12/31/109/115	-
27	CLA	b	718	-	1/1/15/20	7/37/115/115	-
30	DD6	G	613	-	-	2/26/80/80	0/3/3/3
27	CLA	T	604	12	1/1/10/20	0/8/86/115	-
27	CLA	b	703	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	KC2	H	311	-	-	10/15/71/71	-
30	DD6	I	613	-	-	1/26/80/80	0/3/3/3
32	PID	K	611	-	-	6/24/93/93	1/4/4/4
37	PQN	a	832	-	-	6/23/43/43	0/2/2/2
30	DD6	K	610	-	-	3/26/80/80	0/3/3/3
27	CLA	b	711	-	1/1/14/20	6/31/109/115	-
32	PID	F	614	-	-	5/24/93/93	0/4/4/4
29	UIX	B	615	-	-	3/31/87/87	1/3/3/3
27	CLA	b	714	-	1/1/11/20	5/17/95/115	-
30	DD6	F	612	-	-	0/26/80/80	0/3/3/3
27	CLA	a	827	-	1/1/15/20	12/37/115/115	-
27	CLA	D	605	4	1/1/11/20	0/16/94/115	-
28	KC2	T	608	-	-	5/15/71/71	-
30	DD6	i	202	-	-	3/26/80/80	0/3/3/3
27	CLA	T	605	12	1/1/11/20	0/13/91/115	-
38	BCR	b	732	-	-	1/29/63/63	0/2/2/2
29	UIX	H	314	-	-	2/31/87/87	0/3/3/3
38	BCR	f	301	-	-	9/29/63/63	0/2/2/2
27	CLA	F	602	-	1/1/13/20	5/27/105/115	-
27	CLA	C	205	-	1/1/13/20	7/25/103/115	-
27	CLA	H	310	-	1/1/11/20	5/13/91/115	-
35	DGD	f	305	-	-	17/41/81/95	0/2/2/2
30	DD6	F	611	-	-	2/26/80/80	0/3/3/3
27	CLA	T	602	-	1/1/11/20	5/13/91/115	-
27	CLA	D	608	4	1/1/13/20	2/25/103/115	-
27	CLA	l	407	-	1/1/11/20	4/17/95/115	-
34	LHG	l	401	-	-	23/50/50/53	-
30	DD6	r	201	-	-	2/26/80/80	0/3/3/3
27	CLA	C	206	-	1/1/11/20	2/16/94/115	-
28	KC2	B	602	-	-	2/15/71/71	-
27	CLA	a	825	-	1/1/15/20	9/37/115/115	-
29	UIX	A	613	-	-	2/31/87/87	0/3/3/3
27	CLA	a	817	-	1/1/13/20	3/25/103/115	-
27	CLA	B	606	-	1/1/15/20	8/37/115/115	-
38	BCR	f	304	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	BCR	j	203	-	-	10/29/63/63	0/2/2/2
27	CLA	G	608	-	1/1/14/20	5/31/109/115	-
27	CLA	H	304	-	1/1/14/20	9/31/109/115	-
29	UIX	B	611	-	-	2/31/87/87	0/3/3/3
30	DD6	D	613	-	1/1/12/24	2/26/80/80	0/3/3/3
30	DD6	A	615	-	-	3/26/80/80	0/3/3/3
27	CLA	D	609	-	1/1/11/20	2/13/91/115	-
29	UIX	j	204	-	-	6/31/87/87	0/3/3/3
28	KC2	A	608	-	-	6/15/71/71	-
27	CLA	a	823	-	1/1/15/20	13/37/115/115	-
37	PQN	b	729	-	-	10/23/43/43	0/2/2/2
27	CLA	A	607	-	1/1/11/20	0/13/91/115	-
27	CLA	a	831	-	1/1/13/20	2/25/103/115	-
27	CLA	l	410	-	1/1/11/20	3/17/95/115	-
27	CLA	T	609	-	1/1/10/20	0/8/86/115	-
27	CLA	b	702	-	1/1/15/20	13/37/115/115	-
27	CLA	D	607	4	1/1/14/20	3/31/109/115	-
27	CLA	J	607	-	1/1/10/20	2/10/88/115	-
33	LMG	D	618	-	-	17/30/50/70	0/1/1/1
27	CLA	B	601	-	1/1/14/20	4/31/109/115	-
31	SQD	y	301	-	-	6/41/61/69	0/1/1/1
29	UIX	H	317	-	-	4/31/87/87	0/3/3/3
35	DGD	j	201	-	-	17/49/89/95	0/2/2/2
27	CLA	T	603	-	1/1/11/20	4/13/91/115	-
27	CLA	G	611	-	1/1/11/20	1/13/91/115	-
38	BCR	l	413	-	-	3/29/63/63	0/2/2/2
39	SF4	a	838	14	-	-	0/6/5/5
27	CLA	I	602	-	1/1/13/20	7/25/103/115	-
29	UIX	T	612	-	-	5/31/87/87	0/3/3/3
30	DD6	B	614	-	-	5/26/80/80	0/3/3/3
27	CLA	l	403	-	1/1/15/20	7/37/115/115	-
35	DGD	K	614	-	-	19/36/76/95	0/2/2/2
33	LMG	C	217	-	-	14/29/49/70	0/1/1/1
28	KC2	E	610	5	-	7/15/71/71	-
30	DD6	K	609	-	-	4/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	C	203	3	1/1/15/20	4/37/115/115	-
27	CLA	A	612	1	1/1/11/20	3/16/94/115	-
27	CLA	I	606	9	1/1/13/20	3/25/103/115	-
27	CLA	l	405	22	1/1/14/20	5/33/111/115	-
27	CLA	G	605	-	1/1/14/20	2/31/109/115	-
35	DGD	l	416	-	-	17/44/84/95	0/2/2/2
30	DD6	U	607	-	-	0/26/80/80	0/3/3/3
30	DD6	E	615	-	-	1/26/80/80	0/3/3/3
27	CLA	U	601	-	1/1/10/20	3/11/89/115	-
27	CLA	U	605	13	1/1/14/20	6/31/109/115	-
30	DD6	H	316	-	-	1/26/80/80	0/3/3/3
28	KC2	J	606	-	-	5/15/71/71	-
33	LMG	F	616	-	-	14/41/61/70	0/1/1/1
27	CLA	T	601	12	1/1/11/20	3/16/94/115	-
28	KC2	F	609	6	-	7/15/71/71	-
30	DD6	C	216	-	-	1/26/80/80	0/3/3/3
27	CLA	J	601	-	1/1/11/20	4/13/91/115	-
27	CLA	T	606	12	1/1/11/20	1/13/91/115	-
27	CLA	F	606	6	1/1/15/20	12/37/115/115	-
27	CLA	l	406	-	1/1/15/20	3/37/115/115	-
27	CLA	a	839	-	1/1/14/20	7/33/111/115	-
27	CLA	F	607	6	1/1/11/20	5/13/91/115	-
27	CLA	l	402	-	1/1/14/20	3/31/109/115	-
27	CLA	C	201	-	1/1/10/20	2/10/88/115	-
27	CLA	H	319	-	1/1/15/20	8/37/115/115	-
38	BCR	b	731	-	-	8/29/63/63	0/2/2/2
27	CLA	A	603	-	1/1/13/20	1/25/103/115	-
27	CLA	b	720	-	1/1/11/20	1/17/95/115	-
30	DD6	K	612	-	-	5/26/80/80	0/3/3/3
27	CLA	T	607	-	1/1/11/20	3/13/91/115	-
27	CLA	E	608	5	1/1/14/20	5/31/109/115	-
27	CLA	b	726	-	1/1/14/20	4/31/109/115	-
38	BCR	i	201	-	-	6/29/63/63	0/2/2/2
27	CLA	I	608	9	1/1/14/20	4/31/109/115	-
27	CLA	E	607	5	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	F	617	-	1/1/14/20	8/31/109/115	-
27	CLA	a	821	-	1/1/15/20	8/37/115/115	-
27	CLA	I	603	-	1/1/15/20	8/37/115/115	-
27	CLA	a	822	-	1/1/14/20	7/31/109/115	-
27	CLA	F	604	-	1/1/11/20	4/13/91/115	-
27	CLA	G	607	7	1/1/11/20	7/13/91/115	-
30	DD6	D	617	-	-	0/26/80/80	0/3/3/3
31	SQD	A	618	-	-	8/22/42/69	0/1/1/1
27	CLA	b	707	-	1/1/15/20	3/37/115/115	-
34	LHG	a	835	-	-	21/52/52/53	-
27	CLA	l	404	-	1/1/13/20	1/25/103/115	-
27	CLA	K	605	11	1/1/14/20	8/31/109/115	-
28	KC2	J	610	-	-	6/15/71/71	-
28	KC2	J	602	10	-	6/15/71/71	-
27	CLA	B	603	-	1/1/15/20	9/37/115/115	-
38	BCR	a	834	-	-	5/29/63/63	0/2/2/2
27	CLA	b	725	-	1/1/15/20	4/37/115/115	-
29	UIX	C	215	-	-	3/31/87/87	0/3/3/3
27	CLA	C	209	-	1/1/11/20	1/13/91/115	-
27	CLA	G	603	-	1/1/12/20	4/19/97/115	-
29	UIX	C	213	-	-	2/31/87/87	0/3/3/3
34	LHG	j	205	-	-	16/41/41/53	-
27	CLA	a	818	-	1/1/13/20	5/25/103/115	-
30	DD6	D	621	-	-	5/26/80/80	0/3/3/3
27	CLA	B	610	-	1/1/11/20	5/16/94/115	-
30	DD6	r	206	-	-	3/26/80/80	0/3/3/3
30	DD6	r	205	-	-	3/26/80/80	0/3/3/3
27	CLA	a	815	-	1/1/14/20	5/31/109/115	-
27	CLA	a	829	27	1/1/15/20	16/37/115/115	-
27	CLA	J	609	-	1/1/10/20	5/8/86/115	-
30	DD6	T	610	-	-	4/26/80/80	0/3/3/3
27	CLA	K	608	-	1/1/11/20	2/13/91/115	-
32	PID	F	615	-	-	4/24/93/93	0/4/4/4
27	CLA	l	409	-	1/1/15/20	12/37/115/115	-
27	CLA	b	727	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	BCR	m	201	-	-	10/29/63/63	0/2/2/2
34	LHG	r	202	-	-	20/50/50/53	-
27	CLA	G	606	7	1/1/15/20	8/37/115/115	-
27	CLA	G	604	-	1/1/11/20	1/16/94/115	-
27	CLA	F	605	6	1/1/11/20	7/13/91/115	-
30	DD6	T	611	-	-	2/26/80/80	0/3/3/3
30	DD6	H	318	28	-	0/26/80/80	0/3/3/3
27	CLA	a	813	-	1/1/11/20	4/17/95/115	-
33	LMG	b	733	-	-	26/50/70/70	0/1/1/1
27	CLA	a	814	-	1/1/13/20	2/25/103/115	-
27	CLA	b	724	-	1/1/15/20	6/37/115/115	-
28	KC2	J	608	-	-	4/15/71/71	-
27	CLA	C	211	-	1/1/11/20	2/16/94/115	-
33	LMG	l	417	-	-	21/45/65/70	0/1/1/1
27	CLA	a	828	-	1/1/11/20	6/17/95/115	-
30	DD6	H	301	-	-	3/26/80/80	0/3/3/3
27	CLA	a	824	-	1/1/15/20	10/37/115/115	-
27	CLA	b	722	-	1/1/11/20	5/17/95/115	-
27	CLA	D	603	-	1/1/13/20	3/25/103/115	-
27	CLA	E	609	28	1/1/11/20	2/13/91/115	-
38	BCR	l	414	-	-	5/29/63/63	0/2/2/2
30	DD6	J	612	-	-	1/26/80/80	0/3/3/3
27	CLA	a	801	-	1/1/15/20	6/37/115/115	-
27	CLA	G	609	7	1/1/13/20	6/25/103/115	-
27	CLA	a	804	-	1/1/15/20	12/37/115/115	-
39	SF4	c	201	16	-	-	0/6/5/5
27	CLA	l	412	22	1/1/15/20	10/37/115/115	-
27	CLA	G	602	7	1/1/13/20	2/25/103/115	-
27	CLA	A	601	1	1/1/10/20	2/10/88/115	-
27	CLA	I	616	-	1/1/15/20	1/37/115/115	-
27	CLA	G	610	7	1/1/11/20	4/16/94/115	-
27	CLA	E	604	-	1/1/13/20	4/25/103/115	-
27	CLA	D	611	-	1/1/14/20	6/31/109/115	-
27	CLA	A	606	1	1/1/11/20	3/16/94/115	-
27	CLA	j	202	27	1/1/13/20	5/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	D	601	4	1/1/11/20	3/13/91/115	-
27	CLA	b	704	-	1/1/15/20	9/37/115/115	-
27	CLA	D	606	-	1/1/11/20	2/13/91/115	-
30	DD6	H	315	-	-	0/26/80/80	0/3/3/3
27	CLA	A	609	-	1/1/11/20	2/16/94/115	-
30	DD6	A	614	-	-	1/26/80/80	0/3/3/3
27	CLA	C	204	-	1/1/15/20	7/37/115/115	-
27	CLA	I	601	9	1/1/15/20	7/37/115/115	-
27	CLA	b	709	15	1/1/15/20	7/37/115/115	-
27	CLA	r	203	-	1/1/11/20	4/17/95/115	-
30	DD6	D	614	-	-	0/26/80/80	0/3/3/3
27	CLA	F	603	-	1/1/12/20	6/22/100/115	-
27	CLA	a	812	-	1/1/12/20	2/19/97/115	-
27	CLA	a	819	-	1/1/14/20	5/31/109/115	-
27	CLA	I	609	9	1/1/11/20	3/13/91/115	-
29	UIX	F	613	-	-	4/31/87/87	0/3/3/3
29	UIX	D	616	-	-	5/31/87/87	0/3/3/3
32	PID	I	614	-	-	5/24/93/93	0/4/4/4
27	CLA	I	607	-	1/1/14/20	3/33/111/115	-
27	CLA	K	604	-	1/1/13/20	6/28/106/115	-
27	CLA	I	611	-	1/1/10/20	4/10/88/115	-
32	PID	J	611	-	-	4/24/93/93	0/4/4/4
27	CLA	C	207	3	1/1/14/20	4/31/109/115	-
27	CLA	H	309	-	1/1/15/20	6/37/115/115	-
27	CLA	b	708	-	1/1/15/20	8/37/115/115	-
27	CLA	b	713	-	1/1/15/20	7/37/115/115	-
27	CLA	b	705	-	1/1/15/20	9/37/115/115	-
27	CLA	E	612	-	1/1/11/20	0/13/91/115	-
27	CLA	H	305	-	1/1/14/20	14/31/109/115	-
27	CLA	A	611	27	1/1/11/20	3/13/91/115	-
27	CLA	B	605	2	1/1/11/20	5/13/91/115	-
28	KC2	I	604	9	-	2/15/71/71	-
29	UIX	J	616	-	-	3/31/87/87	0/3/3/3
27	CLA	b	715	-	1/1/15/20	6/37/115/115	-
27	CLA	E	603	-	1/1/11/20	1/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	H	320	-	-	15/41/61/69	0/1/1/1
27	CLA	F	601	6	1/1/14/20	5/31/109/115	-
29	UIX	E	616	-	-	3/31/87/87	0/3/3/3
27	CLA	K	602	-	1/1/13/20	8/25/103/115	-
28	KC2	K	607	-	-	3/15/71/71	-
27	CLA	D	610	4	1/1/11/20	4/16/94/115	-
27	CLA	a	830	-	1/1/15/20	11/37/115/115	-
27	CLA	b	716	-	1/1/15/20	5/37/115/115	-
27	CLA	E	611	5	1/1/14/20	6/31/109/115	-
27	CLA	U	606	-	1/1/11/20	7/13/91/115	-
29	UIX	I	612	-	-	2/31/87/87	1/3/3/3
27	CLA	H	313	-	1/1/14/20	2/31/109/115	-
27	CLA	a	806	-	1/1/13/20	4/25/103/115	-
33	LMG	K	613	-	-	11/37/57/70	0/1/1/1
32	PID	J	614	-	-	0/24/93/93	0/4/4/4
27	CLA	H	306	-	1/1/11/20	3/13/91/115	-
29	UIX	G	615	-	-	4/31/87/87	0/3/3/3
27	CLA	b	712	-	1/1/11/20	3/17/95/115	-
33	LMG	D	619	-	-	21/41/61/70	0/1/1/1
27	CLA	J	605	10	1/1/14/20	4/31/109/115	-
30	DD6	E	614	-	-	0/26/80/80	0/3/3/3
27	CLA	b	706	-	1/1/15/20	11/37/115/115	-
32	PID	J	613	-	-	3/24/93/93	0/4/4/4
27	CLA	a	803	27	1/1/12/20	2/19/97/115	-
27	CLA	a	811	-	1/1/11/20	2/17/95/115	-

All (1858) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	603	CLA	C1B-NB	10.82	1.44	1.35
27	I	611	CLA	C1B-NB	10.78	1.44	1.35
27	U	606	CLA	C1B-NB	10.77	1.44	1.35
27	B	604	CLA	C1B-NB	10.77	1.44	1.35
27	K	606	CLA	C1B-NB	10.75	1.44	1.35
27	T	609	CLA	C1B-NB	10.75	1.44	1.35
27	a	828	CLA	C1B-NB	10.73	1.44	1.35
27	a	812	CLA	C1B-NB	10.72	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	608	CLA	C1B-NB	10.71	1.44	1.35
27	U	603	CLA	C1B-NB	10.70	1.44	1.35
27	U	601	CLA	C1B-NB	10.68	1.44	1.35
27	C	209	CLA	C1B-NB	10.68	1.44	1.35
27	T	606	CLA	C1B-NB	10.67	1.44	1.35
27	F	608	CLA	C1B-NB	10.66	1.44	1.35
27	T	607	CLA	C1B-NB	10.66	1.44	1.35
27	J	607	CLA	C1B-NB	10.66	1.44	1.35
27	T	601	CLA	C1B-NB	10.66	1.44	1.35
27	C	201	CLA	C1B-NB	10.65	1.44	1.35
27	G	604	CLA	C1B-NB	10.64	1.44	1.35
27	J	609	CLA	C1B-NB	10.64	1.44	1.35
27	F	610	CLA	C1B-NB	10.64	1.44	1.35
27	H	310	CLA	C1B-NB	10.63	1.44	1.35
27	a	813	CLA	C1B-NB	10.62	1.44	1.35
27	r	203	CLA	C1B-NB	10.61	1.44	1.35
27	l	407	CLA	C1B-NB	10.60	1.44	1.35
27	A	607	CLA	C1B-NB	10.59	1.44	1.35
27	E	612	CLA	C1B-NB	10.59	1.44	1.35
27	C	212	CLA	C1B-NB	10.58	1.44	1.35
27	A	611	CLA	C1B-NB	10.57	1.44	1.35
27	T	604	CLA	C1B-NB	10.57	1.44	1.35
27	l	402	CLA	C1B-NB	10.57	1.44	1.35
27	E	606	CLA	C1B-NB	10.57	1.44	1.35
27	F	605	CLA	C1B-NB	10.56	1.44	1.35
27	T	602	CLA	C1B-NB	10.55	1.44	1.35
27	C	202	CLA	C1B-NB	10.54	1.44	1.35
27	D	610	CLA	C1B-NB	10.54	1.44	1.35
27	G	608	CLA	C1B-NB	10.54	1.44	1.35
27	E	605	CLA	C1B-NB	10.54	1.44	1.35
27	a	803	CLA	C1B-NB	10.53	1.44	1.35
27	G	610	CLA	C1B-NB	10.52	1.44	1.35
27	U	605	CLA	C1B-NB	10.52	1.44	1.35
27	l	410	CLA	C1B-NB	10.52	1.44	1.35
27	a	811	CLA	C1B-NB	10.51	1.44	1.35
27	K	601	CLA	C1B-NB	10.50	1.44	1.35
27	H	313	CLA	C1B-NB	10.50	1.44	1.35
27	b	711	CLA	C1B-NB	10.49	1.44	1.35
27	A	602	CLA	C1B-NB	10.49	1.44	1.35
27	b	714	CLA	C1B-NB	10.49	1.44	1.35
27	a	806	CLA	C1B-NB	10.49	1.44	1.35
27	E	609	CLA	C1B-NB	10.48	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	808	CLA	C1B-NB	10.48	1.44	1.35
27	G	611	CLA	C1B-NB	10.47	1.44	1.35
27	B	603	CLA	C1B-NB	10.46	1.44	1.35
27	H	309	CLA	C1B-NB	10.46	1.44	1.35
27	j	202	CLA	C1B-NB	10.46	1.44	1.35
27	a	814	CLA	C1B-NB	10.45	1.44	1.35
27	G	602	CLA	C1B-NB	10.45	1.44	1.35
27	C	207	CLA	C1B-NB	10.45	1.44	1.35
27	D	609	CLA	C1B-NB	10.45	1.44	1.35
27	b	721	CLA	C1B-NB	10.45	1.44	1.35
27	b	720	CLA	C1B-NB	10.44	1.44	1.35
27	l	405	CLA	C1B-NB	10.44	1.44	1.35
27	f	303	CLA	C1B-NB	10.43	1.44	1.35
27	H	306	CLA	C1B-NB	10.42	1.44	1.35
27	a	816	CLA	C1B-NB	10.42	1.44	1.35
27	K	604	CLA	C1B-NB	10.41	1.44	1.35
27	a	809	CLA	C1B-NB	10.41	1.44	1.35
27	b	723	CLA	C1B-NB	10.41	1.44	1.35
27	F	601	CLA	C1B-NB	10.40	1.44	1.35
27	E	611	CLA	C1B-NB	10.40	1.44	1.35
27	D	607	CLA	C1B-NB	10.38	1.44	1.35
27	b	710	CLA	C1B-NB	10.38	1.44	1.35
27	E	602	CLA	C1B-NB	10.38	1.44	1.35
27	G	605	CLA	C1B-NB	10.38	1.44	1.35
27	a	825	CLA	C1B-NB	10.38	1.44	1.35
27	a	817	CLA	C1B-NB	10.37	1.44	1.35
27	G	609	CLA	C1B-NB	10.37	1.44	1.35
27	I	606	CLA	C1B-NB	10.37	1.44	1.35
27	r	204	CLA	C1B-NB	10.37	1.44	1.35
27	I	610	CLA	C1B-NB	10.36	1.44	1.35
27	D	612	CLA	C1B-NB	10.36	1.44	1.35
27	B	610	CLA	C1B-NB	10.36	1.44	1.35
27	b	722	CLA	C1B-NB	10.36	1.44	1.35
27	A	605	CLA	C1B-NB	10.36	1.44	1.35
27	b	715	CLA	C1B-NB	10.35	1.44	1.35
27	D	601	CLA	C1B-NB	10.35	1.44	1.35
27	D	604	CLA	C1B-NB	10.34	1.44	1.35
27	J	601	CLA	C1B-NB	10.34	1.44	1.35
27	K	605	CLA	C1B-NB	10.34	1.44	1.35
27	G	607	CLA	C1B-NB	10.34	1.44	1.35
27	a	827	CLA	C1B-NB	10.34	1.44	1.35
27	b	701	CLA	C1B-NB	10.34	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	616	CLA	C1B-NB	10.34	1.44	1.35
27	E	603	CLA	C1B-NB	10.34	1.44	1.35
27	f	302	CLA	C1B-NB	10.34	1.44	1.35
27	K	602	CLA	C1B-NB	10.33	1.44	1.35
27	G	606	CLA	C1B-NB	10.33	1.44	1.35
27	B	607	CLA	C1B-NB	10.33	1.44	1.35
27	A	612	CLA	C1B-NB	10.33	1.44	1.35
27	F	607	CLA	C1B-NB	10.33	1.44	1.35
27	B	606	CLA	C1B-NB	10.33	1.44	1.35
27	J	603	CLA	C1B-NB	10.32	1.44	1.35
27	a	829	CLA	C1B-NB	10.32	1.44	1.35
27	T	603	CLA	C1B-NB	10.32	1.44	1.35
27	C	208	CLA	C1B-NB	10.31	1.44	1.35
27	b	713	CLA	C1B-NB	10.31	1.44	1.35
27	C	211	CLA	C1B-NB	10.31	1.44	1.35
27	A	609	CLA	C1B-NB	10.31	1.44	1.35
27	b	726	CLA	C1B-NB	10.30	1.44	1.35
27	A	604	CLA	C1B-NB	10.30	1.44	1.35
27	I	609	CLA	C1B-NB	10.29	1.44	1.35
27	H	307	CLA	C1B-NB	10.29	1.44	1.35
27	b	705	CLA	C1B-NB	10.28	1.44	1.35
27	C	205	CLA	C1B-NB	10.28	1.44	1.35
27	A	601	CLA	C1B-NB	10.28	1.44	1.35
27	b	724	CLA	C1B-NB	10.27	1.44	1.35
27	J	605	CLA	C1B-NB	10.27	1.44	1.35
27	a	819	CLA	C1B-NB	10.27	1.44	1.35
27	A	610	CLA	C1B-NB	10.26	1.44	1.35
27	b	727	CLA	C1B-NB	10.26	1.44	1.35
27	a	822	CLA	C1B-NB	10.26	1.44	1.35
27	E	604	CLA	C1B-NB	10.26	1.44	1.35
27	A	606	CLA	C1B-NB	10.26	1.44	1.35
27	a	805	CLA	C1B-NB	10.25	1.44	1.35
27	I	603	CLA	C1B-NB	10.25	1.44	1.35
27	C	206	CLA	C1B-NB	10.25	1.44	1.35
27	D	603	CLA	C1B-NB	10.24	1.44	1.35
27	B	605	CLA	C1B-NB	10.24	1.44	1.35
27	D	608	CLA	C1B-NB	10.24	1.44	1.35
27	l	411	CLA	C1B-NB	10.24	1.44	1.35
27	D	605	CLA	C1B-NB	10.24	1.44	1.35
27	b	728	CLA	C1B-NB	10.23	1.44	1.35
27	a	823	CLA	C1B-NB	10.22	1.44	1.35
27	F	602	CLA	C1B-NB	10.22	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	830	CLA	C1B-NB	10.22	1.44	1.35
27	I	607	CLA	C1B-NB	10.22	1.44	1.35
27	C	204	CLA	C1B-NB	10.21	1.44	1.35
27	F	606	CLA	C1B-NB	10.21	1.44	1.35
27	l	408	CLA	C1B-NB	10.21	1.44	1.35
27	I	605	CLA	C1B-NB	10.20	1.44	1.35
27	E	608	CLA	C1B-NB	10.19	1.44	1.35
27	H	312	CLA	C1B-NB	10.19	1.44	1.35
27	a	824	CLA	C1B-NB	10.19	1.44	1.35
27	a	807	CLA	C1B-NB	10.18	1.44	1.35
27	H	319	CLA	C1B-NB	10.18	1.44	1.35
27	b	716	CLA	C1B-NB	10.18	1.44	1.35
27	D	606	CLA	C1B-NB	10.17	1.44	1.35
27	I	601	CLA	C1B-NB	10.17	1.44	1.35
27	D	602	CLA	C1B-NB	10.17	1.44	1.35
27	a	810	CLA	C1B-NB	10.17	1.44	1.35
27	F	619	CLA	C1B-NB	10.17	1.44	1.35
27	l	412	CLA	C1B-NB	10.17	1.44	1.35
27	A	603	CLA	C1B-NB	10.16	1.44	1.35
27	a	839	CLA	C1B-NB	10.16	1.44	1.35
27	G	603	CLA	C1B-NB	10.15	1.44	1.35
27	b	725	CLA	C1B-NB	10.15	1.44	1.35
27	b	719	CLA	C1B-NB	10.15	1.44	1.35
27	B	601	CLA	C1B-NB	10.14	1.44	1.35
27	b	712	CLA	C1B-NB	10.14	1.44	1.35
27	F	617	CLA	C1B-NB	10.14	1.44	1.35
27	I	602	CLA	C1B-NB	10.14	1.44	1.35
27	T	605	CLA	C1B-NB	10.13	1.44	1.35
27	l	406	CLA	C1B-NB	10.13	1.44	1.35
27	B	609	CLA	C1B-NB	10.13	1.44	1.35
27	H	305	CLA	C1B-NB	10.13	1.44	1.35
27	a	804	CLA	C1B-NB	10.12	1.44	1.35
27	l	409	CLA	C1B-NB	10.12	1.44	1.35
27	a	818	CLA	C1B-NB	10.12	1.44	1.35
27	D	611	CLA	C1B-NB	10.10	1.44	1.35
27	H	308	CLA	C1B-NB	10.10	1.44	1.35
27	F	603	CLA	C1B-NB	10.09	1.44	1.35
27	b	706	CLA	C1B-NB	10.09	1.44	1.35
27	b	704	CLA	C1B-NB	10.09	1.44	1.35
27	l	403	CLA	C1B-NB	10.08	1.44	1.35
27	E	607	CLA	C1B-NB	10.08	1.44	1.35
27	a	831	CLA	C1B-NB	10.06	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	604	CLA	C1B-NB	10.05	1.44	1.35
27	C	203	CLA	C1B-NB	10.04	1.44	1.35
27	I	608	CLA	C1B-NB	10.04	1.44	1.35
27	a	821	CLA	C1B-NB	10.02	1.44	1.35
27	H	303	CLA	C1B-NB	10.01	1.44	1.35
27	a	802	CLA	C1B-NB	9.99	1.44	1.35
27	H	304	CLA	C1B-NB	9.93	1.44	1.35
27	a	815	CLA	C1B-NB	9.92	1.44	1.35
27	b	717	CLA	C1B-NB	9.91	1.44	1.35
27	a	820	CLA	C1B-NB	9.88	1.44	1.35
27	b	703	CLA	C1B-NB	9.86	1.44	1.35
27	b	707	CLA	C1B-NB	9.76	1.43	1.35
27	b	709	CLA	C1B-NB	9.72	1.43	1.35
27	l	404	CLA	C1B-NB	9.67	1.43	1.35
27	a	801	CLA	C1B-NB	9.66	1.43	1.35
27	b	708	CLA	C1B-NB	9.66	1.43	1.35
27	b	718	CLA	C1B-NB	9.50	1.43	1.35
27	a	826	CLA	C1B-NB	9.48	1.43	1.35
27	a	837	CLA	C1B-NB	9.36	1.43	1.35
27	b	702	CLA	C1B-NB	9.17	1.43	1.35
27	U	606	CLA	C4B-NB	8.98	1.43	1.35
27	f	302	CLA	C4B-NB	8.90	1.43	1.35
27	I	616	CLA	C4B-NB	8.84	1.43	1.35
27	F	608	CLA	C4B-NB	8.76	1.43	1.35
27	A	611	CLA	C4B-NB	8.75	1.43	1.35
27	a	811	CLA	C4B-NB	8.74	1.43	1.35
27	K	603	CLA	C4B-NB	8.72	1.43	1.35
27	U	605	CLA	C4B-NB	8.72	1.43	1.35
27	G	610	CLA	C4B-NB	8.72	1.43	1.35
27	F	610	CLA	C4B-NB	8.71	1.43	1.35
27	T	606	CLA	C4B-NB	8.70	1.43	1.35
27	T	607	CLA	C4B-NB	8.69	1.43	1.35
27	T	609	CLA	C4B-NB	8.69	1.43	1.35
27	D	609	CLA	C4B-NB	8.67	1.42	1.35
27	D	610	CLA	C4B-NB	8.67	1.42	1.35
27	J	607	CLA	C4B-NB	8.66	1.42	1.35
27	a	813	CLA	C4B-NB	8.66	1.42	1.35
27	j	202	CLA	C4B-NB	8.65	1.42	1.35
27	C	202	CLA	C4B-NB	8.63	1.42	1.35
27	C	212	CLA	C4B-NB	8.63	1.42	1.35
27	A	604	CLA	C4B-NB	8.63	1.42	1.35
27	a	810	CLA	C4B-NB	8.63	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	814	CLA	C4B-NB	8.62	1.42	1.35
27	E	609	CLA	C4B-NB	8.62	1.42	1.35
27	G	604	CLA	C4B-NB	8.62	1.42	1.35
27	I	611	CLA	C4B-NB	8.62	1.42	1.35
27	A	607	CLA	C4B-NB	8.62	1.42	1.35
27	A	605	CLA	C4B-NB	8.61	1.42	1.35
27	T	604	CLA	C4B-NB	8.61	1.42	1.35
27	l	402	CLA	C4B-NB	8.60	1.42	1.35
27	f	303	CLA	C4B-NB	8.59	1.42	1.35
27	F	601	CLA	C4B-NB	8.58	1.42	1.35
27	a	808	CLA	C4B-NB	8.58	1.42	1.35
27	T	602	CLA	C4B-NB	8.57	1.42	1.35
27	K	606	CLA	C4B-NB	8.57	1.42	1.35
27	l	406	CLA	C4B-NB	8.57	1.42	1.35
27	B	610	CLA	C4B-NB	8.57	1.42	1.35
27	E	612	CLA	C4B-NB	8.56	1.42	1.35
27	a	829	CLA	C4B-NB	8.55	1.42	1.35
27	E	602	CLA	C4B-NB	8.55	1.42	1.35
27	b	724	CLA	C4B-NB	8.54	1.42	1.35
27	G	611	CLA	C4B-NB	8.53	1.42	1.35
27	C	209	CLA	C4B-NB	8.53	1.42	1.35
27	a	817	CLA	C4B-NB	8.53	1.42	1.35
27	G	608	CLA	C4B-NB	8.53	1.42	1.35
27	a	805	CLA	C4B-NB	8.52	1.42	1.35
27	K	602	CLA	C4B-NB	8.52	1.42	1.35
27	E	606	CLA	C4B-NB	8.52	1.42	1.35
27	J	609	CLA	C4B-NB	8.51	1.42	1.35
27	l	410	CLA	C4B-NB	8.50	1.42	1.35
27	I	608	CLA	C4B-NB	8.50	1.42	1.35
27	H	305	CLA	C4B-NB	8.49	1.42	1.35
27	K	605	CLA	C4B-NB	8.49	1.42	1.35
27	l	407	CLA	C4B-NB	8.49	1.42	1.35
27	F	617	CLA	C4B-NB	8.49	1.42	1.35
27	U	601	CLA	C4B-NB	8.49	1.42	1.35
27	D	611	CLA	C4B-NB	8.47	1.42	1.35
27	D	612	CLA	C4B-NB	8.47	1.42	1.35
27	K	608	CLA	C4B-NB	8.47	1.42	1.35
27	H	310	CLA	C4B-NB	8.47	1.42	1.35
27	G	609	CLA	C4B-NB	8.47	1.42	1.35
27	A	602	CLA	C4B-NB	8.47	1.42	1.35
27	C	211	CLA	C4B-NB	8.47	1.42	1.35
27	H	309	CLA	C4B-NB	8.47	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	605	CLA	C4B-NB	8.46	1.42	1.35
27	T	601	CLA	C4B-NB	8.46	1.42	1.35
27	B	603	CLA	C4B-NB	8.45	1.42	1.35
27	E	608	CLA	C4B-NB	8.45	1.42	1.35
27	B	607	CLA	C4B-NB	8.44	1.42	1.35
27	J	603	CLA	C4B-NB	8.44	1.42	1.35
27	b	716	CLA	C4B-NB	8.44	1.42	1.35
27	F	607	CLA	C4B-NB	8.44	1.42	1.35
27	B	609	CLA	C4B-NB	8.43	1.42	1.35
27	a	825	CLA	C4B-NB	8.43	1.42	1.35
27	a	822	CLA	C4B-NB	8.42	1.42	1.35
27	H	313	CLA	C4B-NB	8.42	1.42	1.35
27	C	208	CLA	C4B-NB	8.42	1.42	1.35
27	K	604	CLA	C4B-NB	8.42	1.42	1.35
27	I	607	CLA	C4B-NB	8.42	1.42	1.35
27	b	728	CLA	C4B-NB	8.42	1.42	1.35
27	E	603	CLA	C4B-NB	8.42	1.42	1.35
27	a	827	CLA	C4B-NB	8.41	1.42	1.35
27	B	604	CLA	C4B-NB	8.41	1.42	1.35
27	H	319	CLA	C4B-NB	8.41	1.42	1.35
27	G	607	CLA	C4B-NB	8.41	1.42	1.35
27	D	605	CLA	C4B-NB	8.40	1.42	1.35
27	E	611	CLA	C4B-NB	8.40	1.42	1.35
27	G	606	CLA	C4B-NB	8.40	1.42	1.35
27	C	206	CLA	C4B-NB	8.39	1.42	1.35
27	b	704	CLA	C4B-NB	8.39	1.42	1.35
27	a	815	CLA	C4B-NB	8.39	1.42	1.35
27	a	809	CLA	C4B-NB	8.39	1.42	1.35
27	C	207	CLA	C4B-NB	8.39	1.42	1.35
27	b	721	CLA	C4B-NB	8.38	1.42	1.35
27	T	605	CLA	C4B-NB	8.38	1.42	1.35
27	F	619	CLA	C4B-NB	8.38	1.42	1.35
27	A	601	CLA	C4B-NB	8.38	1.42	1.35
27	a	828	CLA	C4B-NB	8.38	1.42	1.35
27	a	806	CLA	C4B-NB	8.38	1.42	1.35
27	C	201	CLA	C4B-NB	8.37	1.42	1.35
27	b	701	CLA	C4B-NB	8.37	1.42	1.35
27	A	610	CLA	C4B-NB	8.36	1.42	1.35
27	a	807	CLA	C4B-NB	8.36	1.42	1.35
27	a	816	CLA	C4B-NB	8.36	1.42	1.35
27	K	601	CLA	C4B-NB	8.36	1.42	1.35
27	I	605	CLA	C4B-NB	8.35	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	726	CLA	C4B-NB	8.34	1.42	1.35
27	b	720	CLA	C4B-NB	8.34	1.42	1.35
27	I	601	CLA	C4B-NB	8.34	1.42	1.35
27	D	601	CLA	C4B-NB	8.33	1.42	1.35
27	E	604	CLA	C4B-NB	8.32	1.42	1.35
27	r	204	CLA	C4B-NB	8.32	1.42	1.35
27	F	605	CLA	C4B-NB	8.32	1.42	1.35
27	a	812	CLA	C4B-NB	8.32	1.42	1.35
27	G	603	CLA	C4B-NB	8.32	1.42	1.35
27	I	606	CLA	C4B-NB	8.32	1.42	1.35
27	a	819	CLA	C4B-NB	8.31	1.42	1.35
27	A	609	CLA	C4B-NB	8.31	1.42	1.35
27	b	713	CLA	C4B-NB	8.31	1.42	1.35
27	H	304	CLA	C4B-NB	8.31	1.42	1.35
27	C	205	CLA	C4B-NB	8.31	1.42	1.35
27	r	203	CLA	C4B-NB	8.31	1.42	1.35
27	A	606	CLA	C4B-NB	8.30	1.42	1.35
27	H	303	CLA	C4B-NB	8.30	1.42	1.35
27	b	712	CLA	C4B-NB	8.29	1.42	1.35
27	C	204	CLA	C4B-NB	8.29	1.42	1.35
27	E	605	CLA	C4B-NB	8.29	1.42	1.35
27	T	603	CLA	C4B-NB	8.29	1.42	1.35
27	a	804	CLA	C4B-NB	8.29	1.42	1.35
27	G	602	CLA	C4B-NB	8.29	1.42	1.35
27	I	609	CLA	C4B-NB	8.28	1.42	1.35
27	a	820	CLA	C4B-NB	8.28	1.42	1.35
27	b	711	CLA	C4B-NB	8.28	1.42	1.35
27	D	607	CLA	C4B-NB	8.27	1.42	1.35
27	I	602	CLA	C4B-NB	8.27	1.42	1.35
27	D	608	CLA	C4B-NB	8.27	1.42	1.35
27	F	604	CLA	C4B-NB	8.27	1.42	1.35
27	a	831	CLA	C4B-NB	8.27	1.42	1.35
27	b	710	CLA	C4B-NB	8.27	1.42	1.35
27	D	604	CLA	C4B-NB	8.26	1.42	1.35
27	a	839	CLA	C4B-NB	8.26	1.42	1.35
27	A	612	CLA	C4B-NB	8.26	1.42	1.35
27	B	606	CLA	C4B-NB	8.25	1.42	1.35
27	C	203	CLA	C4B-NB	8.25	1.42	1.35
27	F	606	CLA	C4B-NB	8.24	1.42	1.35
27	l	408	CLA	C4B-NB	8.24	1.42	1.35
27	a	803	CLA	C4B-NB	8.24	1.42	1.35
27	F	602	CLA	C4B-NB	8.24	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	306	CLA	C4B-NB	8.24	1.42	1.35
27	l	411	CLA	C4B-NB	8.24	1.42	1.35
27	b	723	CLA	C4B-NB	8.23	1.42	1.35
27	J	605	CLA	C4B-NB	8.23	1.42	1.35
27	a	823	CLA	C4B-NB	8.22	1.42	1.35
27	D	606	CLA	C4B-NB	8.22	1.42	1.35
27	H	312	CLA	C4B-NB	8.22	1.42	1.35
27	E	607	CLA	C4B-NB	8.21	1.42	1.35
27	I	603	CLA	C4B-NB	8.21	1.42	1.35
27	b	706	CLA	C4B-NB	8.21	1.42	1.35
27	J	601	CLA	C4B-NB	8.21	1.42	1.35
27	G	605	CLA	C4B-NB	8.21	1.42	1.35
27	b	705	CLA	C4B-NB	8.21	1.42	1.35
27	D	603	CLA	C4B-NB	8.20	1.42	1.35
27	A	603	CLA	C4B-NB	8.20	1.42	1.35
27	a	830	CLA	C4B-NB	8.20	1.42	1.35
27	a	802	CLA	C4B-NB	8.20	1.42	1.35
27	l	405	CLA	C4B-NB	8.20	1.42	1.35
27	b	722	CLA	C4B-NB	8.19	1.42	1.35
27	l	409	CLA	C4B-NB	8.19	1.42	1.35
27	H	307	CLA	C4B-NB	8.18	1.42	1.35
27	b	715	CLA	C4B-NB	8.16	1.42	1.35
27	b	702	CLA	C4B-NB	8.15	1.42	1.35
27	H	308	CLA	C4B-NB	8.14	1.42	1.35
27	b	727	CLA	C4B-NB	8.13	1.42	1.35
27	b	714	CLA	C4B-NB	8.13	1.42	1.35
27	b	717	CLA	C4B-NB	8.09	1.42	1.35
27	F	603	CLA	C4B-NB	8.08	1.42	1.35
27	D	602	CLA	C4B-NB	8.08	1.42	1.35
27	b	707	CLA	C4B-NB	8.05	1.42	1.35
27	b	719	CLA	C4B-NB	8.04	1.42	1.35
27	B	601	CLA	C4B-NB	8.03	1.42	1.35
27	I	610	CLA	C4B-NB	8.01	1.42	1.35
27	U	603	CLA	C4B-NB	8.01	1.42	1.35
27	a	824	CLA	C4B-NB	8.00	1.42	1.35
27	l	412	CLA	C4B-NB	7.99	1.42	1.35
27	a	821	CLA	C4B-NB	7.97	1.42	1.35
27	b	718	CLA	C4B-NB	7.96	1.42	1.35
27	a	801	CLA	C4B-NB	7.94	1.42	1.35
27	l	403	CLA	C4B-NB	7.93	1.42	1.35
27	b	709	CLA	C4B-NB	7.89	1.42	1.35
27	b	725	CLA	C4B-NB	7.89	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	708	CLA	C4B-NB	7.84	1.42	1.35
27	a	818	CLA	C4B-NB	7.83	1.42	1.35
27	b	703	CLA	C4B-NB	7.81	1.42	1.35
27	a	826	CLA	C4B-NB	7.73	1.42	1.35
27	l	404	CLA	C4B-NB	7.62	1.42	1.35
27	a	817	CLA	C1D-ND	7.59	1.47	1.37
27	a	831	CLA	C1D-ND	7.58	1.47	1.37
27	a	808	CLA	C1D-ND	7.58	1.47	1.37
27	I	616	CLA	C1D-ND	7.57	1.47	1.37
27	U	606	CLA	C1D-ND	7.53	1.47	1.37
27	F	610	CLA	C1D-ND	7.53	1.47	1.37
27	C	211	CLA	C1D-ND	7.53	1.47	1.37
27	T	604	CLA	C1D-ND	7.52	1.47	1.37
27	K	608	CLA	C1D-ND	7.52	1.47	1.37
27	U	603	CLA	C1D-ND	7.51	1.47	1.37
27	D	610	CLA	C1D-ND	7.51	1.47	1.37
27	G	609	CLA	C1D-ND	7.51	1.47	1.37
27	F	608	CLA	C1D-ND	7.49	1.47	1.37
27	a	810	CLA	C1D-ND	7.48	1.47	1.37
27	T	607	CLA	C1D-ND	7.47	1.47	1.37
27	K	602	CLA	C1D-ND	7.45	1.46	1.37
27	A	611	CLA	C1D-ND	7.45	1.46	1.37
27	J	607	CLA	C1D-ND	7.42	1.46	1.37
27	f	302	CLA	C1D-ND	7.42	1.46	1.37
27	T	603	CLA	C1D-ND	7.42	1.46	1.37
27	D	601	CLA	C1D-ND	7.41	1.46	1.37
27	I	608	CLA	C1D-ND	7.40	1.46	1.37
27	K	603	CLA	C1D-ND	7.40	1.46	1.37
27	G	610	CLA	C1D-ND	7.39	1.46	1.37
27	a	813	CLA	C1D-ND	7.39	1.46	1.37
27	D	611	CLA	C1D-ND	7.38	1.46	1.37
27	b	719	CLA	C1D-ND	7.37	1.46	1.37
27	G	607	CLA	C1D-ND	7.36	1.46	1.37
27	T	601	CLA	C1D-ND	7.35	1.46	1.37
27	E	612	CLA	C1D-ND	7.35	1.46	1.37
27	A	607	CLA	C1D-ND	7.34	1.46	1.37
27	E	604	CLA	C1D-ND	7.33	1.46	1.37
27	C	209	CLA	C1D-ND	7.33	1.46	1.37
27	b	726	CLA	C1D-ND	7.32	1.46	1.37
27	G	602	CLA	C1D-ND	7.32	1.46	1.37
27	C	202	CLA	C1D-ND	7.32	1.46	1.37
27	C	206	CLA	C1D-ND	7.32	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	806	CLA	C1D-ND	7.31	1.46	1.37
27	a	816	CLA	C1D-ND	7.30	1.46	1.37
27	B	604	CLA	C1D-ND	7.30	1.46	1.37
27	E	609	CLA	C1D-ND	7.30	1.46	1.37
27	B	607	CLA	C1D-ND	7.29	1.46	1.37
27	J	601	CLA	C1D-ND	7.29	1.46	1.37
27	T	609	CLA	C1D-ND	7.29	1.46	1.37
27	H	307	CLA	C1D-ND	7.29	1.46	1.37
27	A	609	CLA	C1D-ND	7.29	1.46	1.37
27	b	711	CLA	C1D-ND	7.27	1.46	1.37
27	I	611	CLA	C1D-ND	7.27	1.46	1.37
27	a	822	CLA	C1D-ND	7.27	1.46	1.37
27	T	602	CLA	C1D-ND	7.27	1.46	1.37
27	l	403	CLA	C1D-ND	7.27	1.46	1.37
27	B	610	CLA	C1D-ND	7.27	1.46	1.37
27	C	204	CLA	C1D-ND	7.26	1.46	1.37
27	A	604	CLA	C1D-ND	7.25	1.46	1.37
27	D	609	CLA	C1D-ND	7.25	1.46	1.37
27	K	601	CLA	C1D-ND	7.25	1.46	1.37
27	r	204	CLA	C1D-ND	7.24	1.46	1.37
27	E	606	CLA	C1D-ND	7.23	1.46	1.37
27	H	304	CLA	C1D-ND	7.23	1.46	1.37
27	F	617	CLA	C1D-ND	7.23	1.46	1.37
27	F	602	CLA	C1D-ND	7.23	1.46	1.37
27	G	604	CLA	C1D-ND	7.23	1.46	1.37
27	J	609	CLA	C1D-ND	7.22	1.46	1.37
27	a	828	CLA	C1D-ND	7.22	1.46	1.37
27	U	601	CLA	C1D-ND	7.21	1.46	1.37
27	C	212	CLA	C1D-ND	7.21	1.46	1.37
27	l	412	CLA	C1D-ND	7.21	1.46	1.37
27	H	312	CLA	C1D-ND	7.20	1.46	1.37
27	b	712	CLA	C1D-ND	7.20	1.46	1.37
27	U	605	CLA	C1D-ND	7.20	1.46	1.37
27	T	606	CLA	C1D-ND	7.20	1.46	1.37
27	D	612	CLA	C1D-ND	7.19	1.46	1.37
27	l	408	CLA	C1D-ND	7.19	1.46	1.37
27	F	601	CLA	C1D-ND	7.19	1.46	1.37
27	H	309	CLA	C1D-ND	7.19	1.46	1.37
27	F	605	CLA	C1D-ND	7.18	1.46	1.37
27	D	606	CLA	C1D-ND	7.18	1.46	1.37
27	E	602	CLA	C1D-ND	7.18	1.46	1.37
27	A	602	CLA	C1D-ND	7.17	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	201	CLA	C1D-ND	7.17	1.46	1.37
27	a	811	CLA	C1D-ND	7.17	1.46	1.37
27	J	603	CLA	C1D-ND	7.16	1.46	1.37
27	H	310	CLA	C1D-ND	7.16	1.46	1.37
27	K	606	CLA	C1D-ND	7.16	1.46	1.37
27	C	208	CLA	C1D-ND	7.15	1.46	1.37
27	a	837	CLA	C4B-NB	7.15	1.41	1.35
27	b	710	CLA	C1D-ND	7.14	1.46	1.37
27	a	814	CLA	C1D-ND	7.14	1.46	1.37
27	E	608	CLA	C1D-ND	7.14	1.46	1.37
27	A	601	CLA	C1D-ND	7.14	1.46	1.37
27	a	815	CLA	C1D-ND	7.14	1.46	1.37
27	H	303	CLA	C1D-ND	7.13	1.46	1.37
27	b	720	CLA	C1D-ND	7.13	1.46	1.37
27	r	203	CLA	C1D-ND	7.13	1.46	1.37
27	a	819	CLA	C1D-ND	7.13	1.46	1.37
27	G	611	CLA	C1D-ND	7.13	1.46	1.37
27	G	603	CLA	C1D-ND	7.13	1.46	1.37
27	b	725	CLA	C1D-ND	7.12	1.46	1.37
27	a	804	CLA	C1D-ND	7.12	1.46	1.37
27	F	619	CLA	C1D-ND	7.12	1.46	1.37
27	F	607	CLA	C1D-ND	7.11	1.46	1.37
27	a	820	CLA	C1D-ND	7.11	1.46	1.37
27	b	722	CLA	C1D-ND	7.11	1.46	1.37
27	E	611	CLA	C1D-ND	7.10	1.46	1.37
27	b	701	CLA	C1D-ND	7.10	1.46	1.37
27	F	603	CLA	C1D-ND	7.10	1.46	1.37
27	H	313	CLA	C1D-ND	7.10	1.46	1.37
27	I	607	CLA	C1D-ND	7.10	1.46	1.37
27	H	319	CLA	C1D-ND	7.10	1.46	1.37
27	a	825	CLA	C1D-ND	7.09	1.46	1.37
27	A	603	CLA	C1D-ND	7.09	1.46	1.37
27	I	610	CLA	C1D-ND	7.09	1.46	1.37
27	I	606	CLA	C1D-ND	7.08	1.46	1.37
27	J	605	CLA	C1D-ND	7.08	1.46	1.37
27	B	609	CLA	C1D-ND	7.08	1.46	1.37
27	l	402	CLA	C1D-ND	7.08	1.46	1.37
27	b	721	CLA	C1D-ND	7.08	1.46	1.37
27	A	606	CLA	C1D-ND	7.08	1.46	1.37
27	G	608	CLA	C1D-ND	7.08	1.46	1.37
27	H	305	CLA	C1D-ND	7.06	1.46	1.37
27	b	728	CLA	C1D-ND	7.06	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	829	CLA	C1D-ND	7.06	1.46	1.37
27	A	610	CLA	C1D-ND	7.06	1.46	1.37
27	b	714	CLA	C1D-ND	7.05	1.46	1.37
27	A	605	CLA	C1D-ND	7.05	1.46	1.37
27	b	723	CLA	C1D-ND	7.05	1.46	1.37
27	l	406	CLA	C1D-ND	7.05	1.46	1.37
27	I	601	CLA	C1D-ND	7.04	1.46	1.37
27	I	603	CLA	C1D-ND	7.04	1.46	1.37
27	a	807	CLA	C1D-ND	7.04	1.46	1.37
27	I	609	CLA	C1D-ND	7.04	1.46	1.37
27	H	308	CLA	C1D-ND	7.04	1.46	1.37
27	D	605	CLA	C1D-ND	7.03	1.46	1.37
27	a	803	CLA	C1D-ND	7.02	1.46	1.37
27	I	605	CLA	C1D-ND	7.02	1.46	1.37
27	K	604	CLA	C1D-ND	7.02	1.46	1.37
27	b	706	CLA	C1D-ND	7.02	1.46	1.37
27	b	704	CLA	C1D-ND	7.01	1.46	1.37
27	j	202	CLA	C1D-ND	7.01	1.46	1.37
27	D	603	CLA	C1D-ND	7.01	1.46	1.37
27	a	805	CLA	C1D-ND	7.01	1.46	1.37
27	l	407	CLA	C1D-ND	7.01	1.46	1.37
27	F	606	CLA	C1D-ND	7.01	1.46	1.37
27	D	607	CLA	C1D-ND	7.00	1.46	1.37
27	T	605	CLA	C1D-ND	7.00	1.46	1.37
27	f	303	CLA	C1D-ND	7.00	1.46	1.37
27	H	306	CLA	C1D-ND	6.99	1.46	1.37
27	a	830	CLA	C1D-ND	6.99	1.46	1.37
27	l	409	CLA	C1D-ND	6.99	1.46	1.37
27	E	603	CLA	C1D-ND	6.98	1.46	1.37
27	b	724	CLA	C1D-ND	6.98	1.46	1.37
27	D	608	CLA	C1D-ND	6.98	1.46	1.37
27	a	824	CLA	C1D-ND	6.98	1.46	1.37
27	K	605	CLA	C1D-ND	6.98	1.46	1.37
27	B	601	CLA	C1D-ND	6.97	1.46	1.37
27	b	713	CLA	C1D-ND	6.97	1.46	1.37
27	B	603	CLA	C1D-ND	6.96	1.46	1.37
27	l	410	CLA	C1D-ND	6.96	1.46	1.37
27	B	606	CLA	C1D-ND	6.95	1.46	1.37
27	b	727	CLA	C1D-ND	6.95	1.46	1.37
27	b	716	CLA	C1D-ND	6.95	1.46	1.37
27	l	405	CLA	C1D-ND	6.94	1.46	1.37
27	a	812	CLA	C1D-ND	6.94	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	823	CLA	C1D-ND	6.94	1.46	1.37
27	D	602	CLA	C1D-ND	6.93	1.46	1.37
27	I	602	CLA	C1D-ND	6.93	1.46	1.37
27	E	605	CLA	C1D-ND	6.92	1.46	1.37
27	a	827	CLA	C1D-ND	6.92	1.46	1.37
27	C	207	CLA	C1D-ND	6.91	1.46	1.37
27	l	411	CLA	C1D-ND	6.90	1.46	1.37
27	a	839	CLA	C1D-ND	6.90	1.46	1.37
27	A	612	CLA	C1D-ND	6.89	1.46	1.37
27	a	818	CLA	C1D-ND	6.89	1.46	1.37
27	G	605	CLA	C1D-ND	6.87	1.46	1.37
27	B	605	CLA	C1D-ND	6.87	1.46	1.37
27	C	203	CLA	C1D-ND	6.85	1.46	1.37
27	b	705	CLA	C1D-ND	6.85	1.46	1.37
27	b	707	CLA	C1D-ND	6.83	1.46	1.37
27	a	821	CLA	C1D-ND	6.83	1.46	1.37
27	b	709	CLA	C1D-ND	6.82	1.46	1.37
27	b	717	CLA	C1D-ND	6.81	1.46	1.37
27	a	826	CLA	C1D-ND	6.78	1.46	1.37
27	b	708	CLA	C1D-ND	6.76	1.46	1.37
27	b	715	CLA	C1D-ND	6.76	1.46	1.37
27	F	604	CLA	C1D-ND	6.74	1.46	1.37
27	b	718	CLA	C1D-ND	6.74	1.46	1.37
27	G	606	CLA	C1D-ND	6.73	1.46	1.37
27	E	607	CLA	C1D-ND	6.73	1.46	1.37
27	a	809	CLA	C1D-ND	6.67	1.46	1.37
27	l	404	CLA	C1D-ND	6.66	1.46	1.37
27	b	703	CLA	C1D-ND	6.64	1.46	1.37
27	C	205	CLA	C1D-ND	6.62	1.45	1.37
27	D	604	CLA	C1D-ND	6.58	1.45	1.37
27	a	802	CLA	C1D-ND	6.49	1.45	1.37
27	b	702	CLA	C1D-ND	6.44	1.45	1.37
27	a	837	CLA	MG-ND	-6.31	1.93	2.05
27	a	837	CLA	C1D-ND	6.26	1.45	1.37
27	a	801	CLA	MG-ND	-6.22	1.93	2.05
28	T	608	KC2	C4B-NB	6.10	1.45	1.37
27	D	605	CLA	MG-ND	-5.96	1.94	2.05
27	b	702	CLA	MG-ND	-5.94	1.94	2.05
27	a	801	CLA	C1D-ND	5.91	1.45	1.37
27	a	826	CLA	MG-ND	-5.90	1.94	2.05
27	l	404	CLA	MG-ND	-5.88	1.94	2.05
27	C	205	CLA	MG-NA	-5.87	1.92	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	703	CLA	MG-ND	-5.86	1.94	2.05
28	E	601	KC2	C4B-NB	5.84	1.45	1.37
27	E	607	CLA	MG-ND	-5.83	1.94	2.05
27	E	605	CLA	MG-ND	-5.82	1.94	2.05
28	U	604	KC2	C4B-NB	5.82	1.44	1.37
27	A	612	CLA	MG-NA	-5.82	1.92	2.06
27	a	812	CLA	MG-ND	-5.81	1.94	2.05
27	b	718	CLA	MG-ND	-5.81	1.94	2.05
28	C	210	KC2	C4B-NB	5.80	1.44	1.37
28	F	609	KC2	C4B-NB	5.80	1.44	1.37
27	a	809	CLA	MG-NA	-5.78	1.92	2.06
28	J	602	KC2	C4B-NB	5.78	1.44	1.37
27	a	828	CLA	MG-NA	-5.76	1.92	2.06
28	H	311	KC2	C4B-NB	5.76	1.44	1.37
27	a	802	CLA	MG-ND	-5.76	1.94	2.05
27	C	205	CLA	MG-ND	-5.75	1.94	2.05
28	J	604	KC2	C4B-NB	5.74	1.44	1.37
27	G	605	CLA	MG-ND	-5.74	1.94	2.05
27	f	303	CLA	MG-ND	-5.73	1.94	2.05
28	H	302	KC2	C4B-NB	5.72	1.44	1.37
27	A	612	CLA	MG-ND	-5.72	1.94	2.05
28	J	608	KC2	C4B-NB	5.70	1.44	1.37
27	a	818	CLA	MG-ND	-5.70	1.94	2.05
27	F	602	CLA	MG-ND	-5.70	1.94	2.05
28	E	610	KC2	C4B-NB	5.69	1.44	1.37
27	b	706	CLA	MG-ND	-5.68	1.94	2.05
28	K	607	KC2	C4B-NB	5.68	1.44	1.37
27	a	812	CLA	MG-NA	-5.68	1.92	2.06
27	C	207	CLA	MG-ND	-5.67	1.94	2.05
27	T	605	CLA	MG-ND	-5.67	1.94	2.05
27	H	308	CLA	MG-ND	-5.66	1.94	2.05
27	b	715	CLA	MG-NA	-5.66	1.92	2.06
27	H	307	CLA	MG-ND	-5.65	1.94	2.05
27	K	604	CLA	MG-ND	-5.63	1.94	2.05
27	b	727	CLA	MG-ND	-5.63	1.94	2.05
28	A	608	KC2	C4B-NB	5.63	1.44	1.37
27	b	708	CLA	MG-ND	-5.62	1.94	2.05
28	G	601	KC2	C4B-NB	5.62	1.44	1.37
27	U	603	CLA	MG-ND	-5.62	1.94	2.05
27	a	811	CLA	MG-ND	-5.62	1.94	2.05
27	l	411	CLA	MG-ND	-5.62	1.94	2.05
27	a	809	CLA	MG-ND	-5.60	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	725	CLA	MG-ND	-5.60	1.94	2.05
27	a	805	CLA	MG-ND	-5.60	1.94	2.05
27	B	609	CLA	MG-ND	-5.60	1.94	2.05
27	b	717	CLA	MG-ND	-5.60	1.94	2.05
27	G	611	CLA	MG-ND	-5.59	1.94	2.05
27	H	306	CLA	MG-ND	-5.59	1.94	2.05
27	H	310	CLA	MG-ND	-5.59	1.94	2.05
27	K	608	CLA	MG-ND	-5.59	1.94	2.05
27	b	720	CLA	MG-ND	-5.59	1.94	2.05
27	a	827	CLA	MG-ND	-5.59	1.94	2.05
27	H	304	CLA	MG-ND	-5.59	1.94	2.05
27	K	606	CLA	MG-NA	-5.59	1.93	2.06
27	C	204	CLA	MG-ND	-5.58	1.94	2.05
27	b	709	CLA	MG-ND	-5.58	1.94	2.05
27	l	409	CLA	MG-ND	-5.58	1.94	2.05
27	U	601	CLA	MG-NA	-5.58	1.93	2.06
27	D	607	CLA	MG-ND	-5.58	1.94	2.05
27	F	604	CLA	MG-ND	-5.57	1.94	2.05
28	J	610	KC2	C4B-NB	5.57	1.44	1.37
27	l	407	CLA	MG-ND	-5.57	1.94	2.05
27	K	606	CLA	MG-ND	-5.57	1.94	2.05
28	U	602	KC2	C4B-NB	5.57	1.44	1.37
27	J	605	CLA	MG-ND	-5.56	1.94	2.05
27	D	606	CLA	MG-ND	-5.56	1.94	2.05
27	a	804	CLA	MG-ND	-5.56	1.94	2.05
27	a	823	CLA	MG-ND	-5.55	1.94	2.05
27	C	201	CLA	MG-ND	-5.55	1.94	2.05
27	U	605	CLA	MG-ND	-5.55	1.94	2.05
27	F	606	CLA	MG-ND	-5.54	1.94	2.05
27	K	605	CLA	MG-ND	-5.54	1.94	2.05
27	H	312	CLA	MG-ND	-5.54	1.94	2.05
27	G	606	CLA	MG-ND	-5.54	1.94	2.05
27	I	605	CLA	MG-ND	-5.54	1.94	2.05
27	G	605	CLA	MG-NA	-5.54	1.93	2.06
27	I	611	CLA	MG-NA	-5.54	1.93	2.06
28	B	608	KC2	C4B-NB	5.54	1.44	1.37
27	F	617	CLA	MG-ND	-5.53	1.94	2.05
27	b	714	CLA	MG-ND	-5.53	1.94	2.05
27	I	608	CLA	MG-ND	-5.53	1.94	2.05
27	B	603	CLA	MG-NA	-5.53	1.93	2.06
28	I	604	KC2	C4B-NB	5.53	1.44	1.37
27	F	605	CLA	MG-ND	-5.53	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	l	410	CLA	MG-ND	-5.53	1.94	2.05
27	a	829	CLA	MG-ND	-5.53	1.94	2.05
27	I	602	CLA	MG-ND	-5.52	1.94	2.05
27	a	820	CLA	MG-NA	-5.52	1.93	2.06
27	A	605	CLA	MG-ND	-5.52	1.94	2.05
27	E	611	CLA	MG-ND	-5.51	1.94	2.05
28	B	602	KC2	C4B-NB	5.51	1.44	1.37
27	G	608	CLA	MG-NA	-5.51	1.93	2.06
27	D	604	CLA	MG-ND	-5.51	1.94	2.05
27	a	819	CLA	MG-ND	-5.51	1.94	2.05
27	l	403	CLA	MG-ND	-5.51	1.94	2.05
27	b	713	CLA	MG-ND	-5.50	1.94	2.05
27	A	610	CLA	MG-ND	-5.50	1.94	2.05
27	a	815	CLA	MG-ND	-5.50	1.94	2.05
27	l	408	CLA	MG-ND	-5.50	1.94	2.05
27	j	202	CLA	MG-ND	-5.50	1.94	2.05
27	l	410	CLA	MG-NA	-5.50	1.93	2.06
27	H	305	CLA	MG-ND	-5.50	1.94	2.05
27	a	839	CLA	MG-ND	-5.50	1.94	2.05
27	B	605	CLA	MG-ND	-5.49	1.94	2.05
27	B	606	CLA	MG-NA	-5.49	1.93	2.06
27	b	721	CLA	MG-ND	-5.49	1.94	2.05
27	B	610	CLA	MG-ND	-5.49	1.94	2.05
27	a	821	CLA	MG-ND	-5.49	1.94	2.05
27	l	405	CLA	MG-ND	-5.49	1.94	2.05
27	b	701	CLA	MG-ND	-5.49	1.94	2.05
27	B	603	CLA	MG-ND	-5.49	1.94	2.05
27	H	310	CLA	MG-NA	-5.49	1.93	2.06
27	I	609	CLA	MG-ND	-5.48	1.94	2.05
27	a	817	CLA	MG-ND	-5.48	1.94	2.05
28	J	606	KC2	C4B-NB	5.48	1.44	1.37
27	A	603	CLA	MG-ND	-5.48	1.94	2.05
27	l	412	CLA	MG-ND	-5.47	1.94	2.05
27	a	816	CLA	MG-ND	-5.47	1.94	2.05
27	G	603	CLA	MG-ND	-5.47	1.94	2.05
27	b	718	CLA	MG-NA	-5.47	1.93	2.06
27	b	726	CLA	MG-ND	-5.47	1.94	2.05
27	I	610	CLA	MG-ND	-5.47	1.95	2.05
27	b	722	CLA	MG-ND	-5.46	1.95	2.05
27	a	823	CLA	MG-NA	-5.46	1.93	2.06
27	E	608	CLA	MG-ND	-5.46	1.95	2.05
27	b	723	CLA	MG-ND	-5.46	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	603	CLA	MG-ND	-5.46	1.95	2.05
27	b	710	CLA	MG-ND	-5.46	1.95	2.05
27	J	609	CLA	MG-ND	-5.45	1.95	2.05
27	D	602	CLA	MG-ND	-5.45	1.95	2.05
27	a	822	CLA	MG-ND	-5.45	1.95	2.05
27	b	707	CLA	MG-ND	-5.45	1.95	2.05
27	b	711	CLA	MG-ND	-5.44	1.95	2.05
27	H	303	CLA	MG-ND	-5.44	1.95	2.05
27	I	607	CLA	MG-ND	-5.44	1.95	2.05
27	D	601	CLA	MG-ND	-5.44	1.95	2.05
27	B	607	CLA	MG-ND	-5.44	1.95	2.05
27	G	608	CLA	MG-ND	-5.44	1.95	2.05
27	r	204	CLA	MG-ND	-5.44	1.95	2.05
27	T	607	CLA	MG-ND	-5.44	1.95	2.05
27	b	710	CLA	MG-NA	-5.43	1.93	2.06
27	a	825	CLA	MG-ND	-5.43	1.95	2.05
27	J	603	CLA	MG-ND	-5.43	1.95	2.05
27	a	807	CLA	MG-ND	-5.43	1.95	2.05
27	r	203	CLA	MG-ND	-5.43	1.95	2.05
27	A	602	CLA	MG-ND	-5.42	1.95	2.05
27	T	609	CLA	MG-ND	-5.42	1.95	2.05
27	T	601	CLA	MG-ND	-5.42	1.95	2.05
27	J	607	CLA	MG-ND	-5.42	1.95	2.05
27	b	714	CLA	MG-NA	-5.42	1.93	2.06
27	a	814	CLA	MG-ND	-5.42	1.95	2.05
27	b	719	CLA	MG-NA	-5.42	1.93	2.06
27	T	602	CLA	MG-ND	-5.42	1.95	2.05
27	H	319	CLA	MG-ND	-5.42	1.95	2.05
27	b	724	CLA	MG-ND	-5.42	1.95	2.05
27	b	705	CLA	MG-NA	-5.41	1.93	2.06
27	a	808	CLA	MG-ND	-5.41	1.95	2.05
27	D	603	CLA	MG-ND	-5.41	1.95	2.05
27	a	831	CLA	MG-ND	-5.41	1.95	2.05
27	a	813	CLA	MG-ND	-5.41	1.95	2.05
27	a	830	CLA	MG-ND	-5.41	1.95	2.05
27	G	606	CLA	MG-NA	-5.41	1.93	2.06
27	A	606	CLA	MG-ND	-5.41	1.95	2.05
27	K	602	CLA	MG-ND	-5.41	1.95	2.05
27	U	601	CLA	MG-ND	-5.41	1.95	2.05
27	D	610	CLA	MG-ND	-5.41	1.95	2.05
27	B	604	CLA	MG-ND	-5.41	1.95	2.05
27	J	601	CLA	MG-ND	-5.40	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	820	CLA	MG-ND	-5.40	1.95	2.05
27	a	828	CLA	MG-ND	-5.40	1.95	2.05
27	J	609	CLA	MG-NA	-5.40	1.93	2.06
27	a	803	CLA	MG-ND	-5.40	1.95	2.05
27	b	712	CLA	MG-ND	-5.40	1.95	2.05
27	G	609	CLA	MG-ND	-5.40	1.95	2.05
27	T	606	CLA	MG-ND	-5.40	1.95	2.05
27	C	203	CLA	MG-ND	-5.40	1.95	2.05
27	a	824	CLA	MG-NA	-5.40	1.93	2.06
27	C	206	CLA	MG-ND	-5.40	1.95	2.05
27	D	603	CLA	MG-NA	-5.40	1.93	2.06
27	C	212	CLA	MG-ND	-5.39	1.95	2.05
27	E	609	CLA	MG-ND	-5.39	1.95	2.05
27	A	601	CLA	MG-ND	-5.39	1.95	2.05
27	a	827	CLA	MG-NA	-5.39	1.93	2.06
27	b	712	CLA	MG-NA	-5.39	1.93	2.06
27	T	609	CLA	MG-NA	-5.39	1.93	2.06
27	A	609	CLA	MG-ND	-5.39	1.95	2.05
27	I	601	CLA	MG-ND	-5.39	1.95	2.05
27	I	610	CLA	MG-NA	-5.39	1.93	2.06
27	H	309	CLA	MG-ND	-5.38	1.95	2.05
27	a	802	CLA	MG-NA	-5.38	1.93	2.06
27	D	612	CLA	MG-ND	-5.38	1.95	2.05
27	I	611	CLA	MG-ND	-5.38	1.95	2.05
27	I	603	CLA	MG-ND	-5.38	1.95	2.05
27	b	721	CLA	MG-NA	-5.37	1.93	2.06
27	C	202	CLA	MG-ND	-5.37	1.95	2.05
27	T	603	CLA	MG-ND	-5.37	1.95	2.05
27	E	605	CLA	MG-NA	-5.37	1.93	2.06
27	H	313	CLA	MG-ND	-5.37	1.95	2.05
27	H	313	CLA	MG-NA	-5.36	1.93	2.06
27	B	601	CLA	MG-ND	-5.36	1.95	2.05
27	D	611	CLA	MG-ND	-5.36	1.95	2.05
27	I	616	CLA	MG-ND	-5.36	1.95	2.05
27	B	606	CLA	MG-ND	-5.36	1.95	2.05
27	b	728	CLA	MG-ND	-5.36	1.95	2.05
27	b	705	CLA	MG-ND	-5.36	1.95	2.05
27	E	611	CLA	MG-NA	-5.36	1.93	2.06
27	E	606	CLA	MG-ND	-5.36	1.95	2.05
27	G	602	CLA	MG-ND	-5.36	1.95	2.05
27	l	408	CLA	MG-NA	-5.36	1.93	2.06
27	D	608	CLA	MG-ND	-5.35	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	l	402	CLA	MG-ND	-5.35	1.95	2.05
27	b	716	CLA	MG-NA	-5.35	1.93	2.06
27	b	716	CLA	MG-ND	-5.35	1.95	2.05
27	B	604	CLA	MG-NA	-5.35	1.93	2.06
27	A	604	CLA	MG-ND	-5.35	1.95	2.05
27	C	209	CLA	MG-ND	-5.35	1.95	2.05
27	a	824	CLA	MG-ND	-5.34	1.95	2.05
27	A	607	CLA	MG-ND	-5.34	1.95	2.05
27	D	602	CLA	MG-NA	-5.34	1.93	2.06
27	b	719	CLA	MG-ND	-5.34	1.95	2.05
27	l	406	CLA	MG-ND	-5.34	1.95	2.05
27	T	601	CLA	MG-NA	-5.34	1.93	2.06
27	F	619	CLA	MG-ND	-5.33	1.95	2.05
27	G	610	CLA	MG-ND	-5.33	1.95	2.05
27	J	601	CLA	MG-NA	-5.33	1.93	2.06
27	K	601	CLA	MG-ND	-5.33	1.95	2.05
27	b	715	CLA	MG-ND	-5.33	1.95	2.05
27	b	704	CLA	MG-ND	-5.33	1.95	2.05
27	a	806	CLA	MG-ND	-5.33	1.95	2.05
27	f	302	CLA	MG-ND	-5.33	1.95	2.05
27	F	603	CLA	MG-NA	-5.33	1.93	2.06
27	b	727	CLA	MG-NA	-5.33	1.93	2.06
27	E	602	CLA	MG-ND	-5.33	1.95	2.05
27	C	208	CLA	MG-ND	-5.32	1.95	2.05
27	C	211	CLA	MG-ND	-5.32	1.95	2.05
27	T	604	CLA	MG-ND	-5.32	1.95	2.05
27	F	601	CLA	MG-ND	-5.32	1.95	2.05
27	r	203	CLA	MG-NA	-5.32	1.93	2.06
27	E	612	CLA	MG-ND	-5.32	1.95	2.05
27	l	405	CLA	MG-NA	-5.32	1.93	2.06
27	G	604	CLA	MG-NA	-5.31	1.93	2.06
27	D	609	CLA	MG-ND	-5.31	1.95	2.05
27	a	807	CLA	MG-NA	-5.30	1.93	2.06
27	H	305	CLA	MG-NA	-5.30	1.93	2.06
27	f	303	CLA	MG-NA	-5.29	1.93	2.06
27	a	810	CLA	MG-ND	-5.29	1.95	2.05
27	C	203	CLA	MG-NA	-5.29	1.93	2.06
27	G	604	CLA	MG-ND	-5.28	1.95	2.05
27	I	609	CLA	MG-NA	-5.28	1.93	2.06
27	E	604	CLA	MG-ND	-5.28	1.95	2.05
27	l	407	CLA	MG-NA	-5.28	1.93	2.06
27	l	404	CLA	MG-NA	-5.28	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	602	CLA	MG-NA	-5.27	1.93	2.06
27	I	606	CLA	MG-ND	-5.27	1.95	2.05
27	a	816	CLA	MG-NA	-5.27	1.93	2.06
27	F	603	CLA	MG-ND	-5.26	1.95	2.05
27	F	607	CLA	MG-ND	-5.26	1.95	2.05
27	a	818	CLA	MG-NA	-5.26	1.93	2.06
27	K	603	CLA	MG-ND	-5.25	1.95	2.05
27	F	608	CLA	MG-ND	-5.25	1.95	2.05
27	C	208	CLA	MG-NA	-5.25	1.93	2.06
27	b	707	CLA	MG-NA	-5.24	1.93	2.06
27	b	703	CLA	MG-NA	-5.24	1.93	2.06
27	F	610	CLA	MG-ND	-5.24	1.95	2.05
27	A	611	CLA	MG-ND	-5.22	1.95	2.05
27	E	603	CLA	MG-NA	-5.21	1.93	2.06
27	U	606	CLA	MG-ND	-5.21	1.95	2.05
27	a	829	CLA	MG-NA	-5.20	1.93	2.06
27	J	603	CLA	MG-NA	-5.19	1.93	2.06
27	D	608	CLA	MG-NA	-5.19	1.93	2.06
27	j	202	CLA	MG-NA	-5.19	1.93	2.06
27	F	607	CLA	MG-NA	-5.19	1.93	2.06
27	l	403	CLA	MG-NA	-5.18	1.94	2.06
27	D	604	CLA	MG-NA	-5.18	1.94	2.06
27	b	713	CLA	MG-NA	-5.17	1.94	2.06
27	b	722	CLA	MG-NA	-5.15	1.94	2.06
27	a	811	CLA	MG-NA	-5.15	1.94	2.06
27	K	608	CLA	MG-NA	-5.15	1.94	2.06
27	G	607	CLA	MG-ND	-5.14	1.95	2.05
27	b	724	CLA	MG-NA	-5.14	1.94	2.06
27	T	606	CLA	MG-NA	-5.13	1.94	2.06
27	F	610	CLA	MG-NA	-5.13	1.94	2.06
27	I	606	CLA	MG-NA	-5.13	1.94	2.06
27	D	612	CLA	MG-NA	-5.13	1.94	2.06
27	C	209	CLA	MG-NA	-5.13	1.94	2.06
27	a	839	CLA	MG-NA	-5.12	1.94	2.06
27	C	212	CLA	MG-NA	-5.11	1.94	2.06
27	B	601	CLA	MG-NA	-5.11	1.94	2.06
27	a	821	CLA	MG-NA	-5.10	1.94	2.06
27	D	609	CLA	MG-NA	-5.10	1.94	2.06
27	T	602	CLA	MG-NA	-5.09	1.94	2.06
27	a	813	CLA	MG-NA	-5.09	1.94	2.06
27	b	723	CLA	MG-NA	-5.09	1.94	2.06
27	G	611	CLA	MG-NA	-5.08	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	l	412	CLA	MG-NA	-5.08	1.94	2.06
27	U	603	CLA	MG-NA	-5.08	1.94	2.06
27	a	805	CLA	MG-NA	-5.08	1.94	2.06
27	l	411	CLA	MG-NA	-5.07	1.94	2.06
27	C	207	CLA	MG-NA	-5.07	1.94	2.06
27	a	808	CLA	MG-NA	-5.07	1.94	2.06
27	A	611	CLA	MG-NA	-5.07	1.94	2.06
27	a	830	CLA	MG-NA	-5.06	1.94	2.06
27	H	309	CLA	MG-NA	-5.06	1.94	2.06
27	I	607	CLA	MG-NA	-5.06	1.94	2.06
27	I	603	CLA	MG-NA	-5.06	1.94	2.06
27	a	803	CLA	MG-NA	-5.05	1.94	2.06
27	F	606	CLA	MG-NA	-5.05	1.94	2.06
27	E	608	CLA	MG-NA	-5.05	1.94	2.06
27	b	704	CLA	MG-NA	-5.05	1.94	2.06
27	l	406	CLA	MG-NA	-5.05	1.94	2.06
27	l	402	CLA	MG-NA	-5.05	1.94	2.06
27	a	825	CLA	MG-NA	-5.05	1.94	2.06
27	H	307	CLA	MG-NA	-5.04	1.94	2.06
27	a	810	CLA	MG-NA	-5.04	1.94	2.06
27	J	605	CLA	MG-NA	-5.04	1.94	2.06
27	D	607	CLA	MG-NA	-5.04	1.94	2.06
27	A	610	CLA	MG-NA	-5.04	1.94	2.06
27	C	201	CLA	MG-NA	-5.04	1.94	2.06
27	J	607	CLA	MG-NA	-5.03	1.94	2.06
27	K	601	CLA	MG-NA	-5.03	1.94	2.06
27	G	603	CLA	MG-NA	-5.02	1.94	2.06
27	A	601	CLA	MG-NA	-5.01	1.94	2.06
27	A	602	CLA	MG-NA	-5.01	1.94	2.06
27	H	319	CLA	MG-NA	-5.01	1.94	2.06
27	b	720	CLA	MG-NA	-5.01	1.94	2.06
27	b	706	CLA	MG-NA	-5.01	1.94	2.06
27	b	708	CLA	MG-NA	-5.00	1.94	2.06
27	a	815	CLA	MG-NA	-5.00	1.94	2.06
27	E	609	CLA	MG-NA	-5.00	1.94	2.06
27	A	605	CLA	MG-NA	-5.00	1.94	2.06
27	T	603	CLA	MG-NA	-5.00	1.94	2.06
27	a	822	CLA	MG-NA	-4.99	1.94	2.06
27	E	612	CLA	MG-NA	-4.99	1.94	2.06
27	E	606	CLA	MG-NA	-4.99	1.94	2.06
27	E	602	CLA	MG-NA	-4.98	1.94	2.06
27	K	604	CLA	MG-NA	-4.98	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	609	CLA	MG-NA	-4.98	1.94	2.06
27	U	606	CLA	MG-NA	-4.98	1.94	2.06
27	E	604	CLA	MG-NA	-4.98	1.94	2.06
27	b	711	CLA	MG-NA	-4.97	1.94	2.06
27	F	617	CLA	MG-NA	-4.97	1.94	2.06
27	G	607	CLA	MG-NA	-4.97	1.94	2.06
27	A	606	CLA	MG-NA	-4.96	1.94	2.06
27	C	204	CLA	MG-NA	-4.96	1.94	2.06
27	B	605	CLA	MG-NA	-4.96	1.94	2.06
27	F	608	CLA	MG-NA	-4.96	1.94	2.06
27	a	819	CLA	MG-NA	-4.96	1.94	2.06
27	r	204	CLA	MG-NA	-4.96	1.94	2.06
27	C	211	CLA	MG-NA	-4.96	1.94	2.06
27	F	601	CLA	MG-NA	-4.95	1.94	2.06
27	C	202	CLA	MG-NA	-4.95	1.94	2.06
27	U	605	CLA	MG-NA	-4.95	1.94	2.06
27	I	602	CLA	MG-NA	-4.95	1.94	2.06
27	b	709	CLA	MG-NA	-4.95	1.94	2.06
27	H	304	CLA	MG-NA	-4.95	1.94	2.06
27	I	601	CLA	MG-NA	-4.94	1.94	2.06
27	K	602	CLA	MG-NA	-4.94	1.94	2.06
27	H	306	CLA	MG-NA	-4.94	1.94	2.06
27	b	717	CLA	MG-NA	-4.94	1.94	2.06
27	A	604	CLA	MG-NA	-4.94	1.94	2.06
27	H	312	CLA	MG-NA	-4.93	1.94	2.06
27	F	605	CLA	MG-NA	-4.93	1.94	2.06
27	D	611	CLA	MG-NA	-4.93	1.94	2.06
27	F	619	CLA	MG-NA	-4.93	1.94	2.06
27	b	728	CLA	MG-NA	-4.92	1.94	2.06
27	l	409	CLA	MG-NA	-4.91	1.94	2.06
27	B	609	CLA	MG-NA	-4.90	1.94	2.06
27	A	607	CLA	MG-NA	-4.90	1.94	2.06
27	H	308	CLA	MG-NA	-4.89	1.94	2.06
27	A	603	CLA	MG-NA	-4.89	1.94	2.06
27	K	603	CLA	MG-NA	-4.88	1.94	2.06
27	b	702	CLA	MG-NA	-4.88	1.94	2.06
27	a	814	CLA	MG-NA	-4.88	1.94	2.06
27	I	616	CLA	MG-NA	-4.88	1.94	2.06
27	b	701	CLA	MG-NA	-4.88	1.94	2.06
27	G	602	CLA	MG-NA	-4.87	1.94	2.06
27	E	607	CLA	MG-NA	-4.87	1.94	2.06
27	T	607	CLA	MG-NA	-4.87	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	806	CLA	MG-NA	-4.87	1.94	2.06
27	K	605	CLA	MG-NA	-4.86	1.94	2.06
27	I	605	CLA	MG-NA	-4.85	1.94	2.06
27	D	601	CLA	MG-NA	-4.85	1.94	2.06
27	a	837	CLA	MG-NA	-4.84	1.94	2.06
27	D	606	CLA	MG-NA	-4.84	1.94	2.06
27	G	610	CLA	MG-NA	-4.83	1.94	2.06
27	F	604	CLA	MG-NA	-4.83	1.94	2.06
27	B	607	CLA	MG-NA	-4.82	1.94	2.06
27	a	826	CLA	MG-NA	-4.82	1.94	2.06
27	b	725	CLA	MG-NA	-4.82	1.94	2.06
32	J	615	PID	O6-C30	4.81	1.46	1.35
29	F	613	UIX	O2-C27	4.80	1.46	1.35
27	a	801	CLA	MG-NA	-4.80	1.94	2.06
32	U	608	PID	O6-C30	4.80	1.46	1.35
27	B	610	CLA	MG-NA	-4.80	1.94	2.06
27	b	726	CLA	MG-NA	-4.80	1.94	2.06
27	a	804	CLA	MG-NA	-4.79	1.94	2.06
27	C	206	CLA	MG-NA	-4.78	1.94	2.06
29	D	616	UIX	O2-C27	4.77	1.46	1.35
32	B	613	PID	O6-C30	4.77	1.46	1.35
27	a	831	CLA	MG-NA	-4.77	1.94	2.06
29	A	613	UIX	O2-C27	4.76	1.46	1.35
29	G	615	UIX	O2-C27	4.76	1.46	1.35
29	B	611	UIX	O2-C27	4.76	1.45	1.35
27	T	604	CLA	MG-NA	-4.76	1.95	2.06
29	B	615	UIX	O2-C27	4.75	1.45	1.35
29	J	616	UIX	O2-C27	4.75	1.45	1.35
32	I	614	PID	O6-C30	4.75	1.45	1.35
29	E	616	UIX	O2-C27	4.75	1.45	1.35
27	D	605	CLA	MG-NA	-4.74	1.95	2.06
29	j	204	UIX	O2-C27	4.74	1.45	1.35
27	f	302	CLA	MG-NA	-4.74	1.95	2.06
32	F	615	PID	O6-C30	4.74	1.45	1.35
29	A	616	UIX	O2-C27	4.73	1.45	1.35
27	I	608	CLA	MG-NA	-4.73	1.95	2.06
27	T	605	CLA	MG-NA	-4.73	1.95	2.06
27	H	303	CLA	MG-NA	-4.73	1.95	2.06
29	C	215	UIX	O2-C27	4.72	1.45	1.35
29	T	612	UIX	O2-C27	4.72	1.45	1.35
32	J	614	PID	O6-C30	4.72	1.45	1.35
27	a	817	CLA	MG-NA	-4.70	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	314	UIX	O2-C27	4.69	1.45	1.35
29	C	213	UIX	O2-C27	4.68	1.45	1.35
29	H	317	UIX	O2-C27	4.68	1.45	1.35
27	D	610	CLA	MG-NA	-4.67	1.95	2.06
32	F	614	PID	O6-C30	4.66	1.45	1.35
32	J	614	PID	C13-C12	4.65	1.49	1.36
32	K	611	PID	O6-C30	4.65	1.45	1.35
32	J	613	PID	O6-C30	4.64	1.45	1.35
32	F	615	PID	C13-C12	4.64	1.49	1.36
31	y	301	SQD	O8-S	4.62	1.64	1.47
31	H	320	SQD	O8-S	4.59	1.63	1.47
32	I	614	PID	C13-C12	4.59	1.49	1.36
31	A	618	SQD	O8-S	4.58	1.63	1.47
32	K	611	PID	C13-C12	4.57	1.49	1.36
32	B	613	PID	C13-C12	4.56	1.49	1.36
32	J	611	PID	O6-C30	4.55	1.45	1.35
27	G	609	CLA	MG-NA	-4.55	1.95	2.06
29	I	612	UIX	O2-C27	4.54	1.45	1.35
32	J	615	PID	C13-C12	4.50	1.48	1.36
32	U	608	PID	C13-C12	4.49	1.48	1.36
32	F	614	PID	C13-C12	4.49	1.48	1.36
32	J	613	PID	C13-C12	4.36	1.48	1.36
32	J	611	PID	C13-C12	4.31	1.48	1.36
31	y	301	SQD	O47-C7	4.29	1.46	1.34
31	y	301	SQD	O48-C23	4.28	1.45	1.33
31	H	320	SQD	O48-C23	4.23	1.45	1.33
29	j	204	UIX	C25-C28	-4.11	1.25	1.32
29	B	611	UIX	C25-C28	-4.10	1.25	1.32
31	A	618	SQD	O47-C7	4.07	1.45	1.34
28	U	602	KC2	C1B-NB	4.06	1.42	1.37
28	T	608	KC2	C3D-C4D	4.06	1.44	1.40
32	K	611	PID	C23-C22	-4.04	1.25	1.32
29	I	612	UIX	C25-C28	-4.03	1.25	1.32
28	J	604	KC2	C1B-NB	4.02	1.42	1.37
32	J	613	PID	C23-C22	-3.98	1.25	1.32
27	a	828	CLA	MG-NC	-3.97	1.96	2.06
28	K	607	KC2	C3D-C4D	3.96	1.44	1.40
28	K	607	KC2	C1B-NB	3.95	1.42	1.37
27	a	812	CLA	MG-NC	-3.94	1.96	2.06
31	H	320	SQD	O47-C7	3.93	1.45	1.34
28	F	609	KC2	C1B-NB	3.93	1.42	1.37
28	I	604	KC2	C4C-NC	3.92	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	205	CLA	MG-NC	-3.91	1.97	2.06
27	U	601	CLA	MG-NC	-3.90	1.97	2.06
28	C	210	KC2	C1B-NB	3.89	1.42	1.37
27	A	612	CLA	MG-NC	-3.89	1.97	2.06
27	I	611	CLA	MG-NC	-3.89	1.97	2.06
28	J	608	KC2	C1B-NB	3.88	1.42	1.37
27	b	703	CLA	MG-NC	-3.87	1.97	2.06
28	U	604	KC2	C1B-NB	3.87	1.42	1.37
28	E	610	KC2	C1B-NB	3.86	1.42	1.37
27	G	605	CLA	MG-NC	-3.85	1.97	2.06
28	J	606	KC2	C4C-NC	3.84	1.43	1.37
27	B	606	CLA	MG-NC	-3.83	1.97	2.06
28	J	608	KC2	C3D-C4D	3.83	1.43	1.40
27	H	313	CLA	MG-NC	-3.82	1.97	2.06
28	H	302	KC2	C1B-NB	3.81	1.42	1.37
27	a	809	CLA	MG-NC	-3.81	1.97	2.06
28	U	604	KC2	C3D-C4D	3.80	1.43	1.40
27	a	820	CLA	MG-NC	-3.80	1.97	2.06
27	b	721	CLA	MG-NC	-3.79	1.97	2.06
27	B	604	CLA	MG-NC	-3.79	1.97	2.06
27	a	823	CLA	MG-NC	-3.79	1.97	2.06
27	H	310	CLA	MG-NC	-3.77	1.97	2.06
28	C	210	KC2	C3D-C4D	3.77	1.43	1.40
28	G	601	KC2	C1B-NB	3.77	1.42	1.37
27	b	712	CLA	MG-NC	-3.77	1.97	2.06
27	I	610	CLA	MG-NC	-3.76	1.97	2.06
28	F	609	KC2	C3D-C4D	3.76	1.43	1.40
28	T	608	KC2	C4C-NC	3.76	1.43	1.37
27	b	705	CLA	MG-NC	-3.76	1.97	2.06
28	H	311	KC2	C1B-NB	3.76	1.42	1.37
27	K	606	CLA	MG-NC	-3.76	1.97	2.06
27	l	410	CLA	MG-NC	-3.75	1.97	2.06
27	l	408	CLA	MG-NC	-3.75	1.97	2.06
27	B	603	CLA	MG-NC	-3.75	1.97	2.06
27	T	601	CLA	MG-NC	-3.74	1.97	2.06
28	K	607	KC2	C4C-NC	3.74	1.43	1.37
28	F	609	KC2	C4C-NC	3.74	1.43	1.37
27	G	608	CLA	MG-NC	-3.74	1.97	2.06
27	a	824	CLA	MG-NC	-3.74	1.97	2.06
28	C	210	KC2	C4C-NC	3.73	1.43	1.37
29	C	215	UIX	C25-C28	-3.73	1.25	1.32
29	H	314	UIX	C25-C28	-3.73	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	714	CLA	MG-NC	-3.73	1.97	2.06
27	D	602	CLA	MG-NC	-3.73	1.97	2.06
27	b	715	CLA	MG-NC	-3.73	1.97	2.06
29	A	616	UIX	C25-C28	-3.72	1.25	1.32
27	j	202	CLA	MG-NC	-3.72	1.97	2.06
28	J	602	KC2	C1B-NB	3.71	1.42	1.37
27	a	802	CLA	MG-NC	-3.71	1.97	2.06
29	G	615	UIX	C25-C28	-3.71	1.25	1.32
27	T	609	CLA	MG-NC	-3.71	1.97	2.06
27	l	404	CLA	MG-NC	-3.69	1.97	2.06
27	I	609	CLA	MG-NC	-3.69	1.97	2.06
27	b	718	CLA	MG-NC	-3.69	1.97	2.06
32	F	614	PID	C23-C22	-3.69	1.25	1.32
27	b	719	CLA	MG-NC	-3.69	1.97	2.06
27	f	303	CLA	MG-NC	-3.69	1.97	2.06
28	J	608	KC2	C4C-NC	3.69	1.43	1.37
27	D	603	CLA	MG-NC	-3.69	1.97	2.06
28	H	311	KC2	C4C-NC	3.68	1.43	1.37
28	E	601	KC2	C4C-NC	3.68	1.43	1.37
28	J	610	KC2	C3D-C4D	3.68	1.43	1.40
29	T	612	UIX	C25-C28	-3.68	1.25	1.32
27	E	611	CLA	MG-NC	-3.68	1.97	2.06
27	b	716	CLA	MG-NC	-3.68	1.97	2.06
27	a	807	CLA	MG-NC	-3.68	1.97	2.06
28	E	601	KC2	C1B-NB	3.68	1.42	1.37
32	I	614	PID	C23-C22	-3.68	1.25	1.32
29	B	615	UIX	C25-C28	-3.67	1.25	1.32
28	U	602	KC2	C3D-C4D	3.67	1.43	1.40
27	a	808	CLA	MG-NC	-3.67	1.97	2.06
27	T	602	CLA	MG-NC	-3.67	1.97	2.06
28	I	604	KC2	C1B-NB	3.67	1.42	1.37
28	T	608	KC2	C1B-NB	3.66	1.42	1.37
28	J	610	KC2	C1B-NB	3.66	1.42	1.37
27	b	707	CLA	MG-NC	-3.66	1.97	2.06
27	G	604	CLA	MG-NC	-3.66	1.97	2.06
28	E	610	KC2	C4C-NC	3.66	1.43	1.37
27	E	603	CLA	MG-NC	-3.65	1.97	2.06
27	C	209	CLA	MG-NC	-3.65	1.97	2.06
27	C	203	CLA	MG-NC	-3.65	1.97	2.06
27	l	407	CLA	MG-NC	-3.65	1.97	2.06
27	I	606	CLA	MG-NC	-3.64	1.97	2.06
28	B	602	KC2	C1B-NB	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J	601	CLA	MG-NC	-3.64	1.97	2.06
27	r	203	CLA	MG-NC	-3.64	1.97	2.06
27	H	305	CLA	MG-NC	-3.64	1.97	2.06
27	a	801	CLA	MG-NC	-3.64	1.97	2.06
27	E	605	CLA	MG-NC	-3.63	1.97	2.06
28	G	601	KC2	C3D-C4D	3.63	1.43	1.40
29	A	613	UIX	C25-C28	-3.63	1.25	1.32
27	F	603	CLA	MG-NC	-3.63	1.97	2.06
27	b	710	CLA	MG-NC	-3.63	1.97	2.06
28	U	604	KC2	C4C-NC	3.63	1.43	1.37
27	G	606	CLA	MG-NC	-3.63	1.97	2.06
27	l	405	CLA	MG-NC	-3.62	1.97	2.06
28	E	601	KC2	C3D-C4D	3.62	1.43	1.40
27	U	603	CLA	MG-NC	-3.62	1.97	2.06
27	I	607	CLA	MG-NC	-3.62	1.97	2.06
27	K	608	CLA	MG-NC	-3.62	1.97	2.06
28	J	610	KC2	C4C-NC	3.61	1.43	1.37
28	J	606	KC2	C1B-NB	3.61	1.42	1.37
27	l	412	CLA	MG-NC	-3.61	1.97	2.06
27	a	829	CLA	MG-NC	-3.61	1.97	2.06
27	J	609	CLA	MG-NC	-3.60	1.97	2.06
28	H	311	KC2	C3D-C4D	3.60	1.43	1.40
28	U	602	KC2	C4C-NC	3.60	1.43	1.37
27	a	816	CLA	MG-NC	-3.60	1.97	2.06
27	F	610	CLA	MG-NC	-3.60	1.97	2.06
28	A	608	KC2	C3D-C4D	3.59	1.43	1.40
27	D	612	CLA	MG-NC	-3.59	1.97	2.06
29	H	317	UIX	C25-C28	-3.59	1.26	1.32
28	J	604	KC2	C4C-NC	3.59	1.43	1.37
28	J	602	KC2	C4C-NC	3.59	1.43	1.37
27	D	608	CLA	MG-NC	-3.59	1.97	2.06
27	a	827	CLA	MG-NC	-3.58	1.97	2.06
27	F	602	CLA	MG-NC	-3.58	1.97	2.06
29	E	616	UIX	C25-C28	-3.58	1.26	1.32
27	F	607	CLA	MG-NC	-3.57	1.97	2.06
27	J	603	CLA	MG-NC	-3.57	1.97	2.06
28	H	302	KC2	C4C-NC	3.56	1.43	1.37
27	C	204	CLA	MG-NC	-3.56	1.97	2.06
27	G	607	CLA	MG-NC	-3.56	1.97	2.06
28	G	601	KC2	C4C-NC	3.56	1.43	1.37
29	D	616	UIX	C25-C28	-3.56	1.26	1.32
27	G	611	CLA	MG-NC	-3.56	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	208	CLA	MG-NC	-3.55	1.97	2.06
28	B	608	KC2	C3D-C4D	3.55	1.43	1.40
32	U	608	PID	C23-C22	-3.55	1.26	1.32
27	K	602	CLA	MG-NC	-3.55	1.97	2.06
27	C	212	CLA	MG-NC	-3.55	1.97	2.06
29	J	616	UIX	C25-C28	-3.55	1.26	1.32
27	D	609	CLA	MG-NC	-3.55	1.97	2.06
27	a	818	CLA	MG-NC	-3.54	1.97	2.06
27	a	811	CLA	MG-NC	-3.54	1.97	2.06
27	b	711	CLA	MG-NC	-3.54	1.97	2.06
27	l	403	CLA	MG-NC	-3.54	1.97	2.06
32	U	608	PID	O3-C10	3.54	1.28	1.21
32	J	613	PID	O3-C10	3.54	1.28	1.21
28	B	608	KC2	C4C-NC	3.53	1.43	1.37
27	a	839	CLA	MG-NC	-3.53	1.97	2.06
28	B	608	KC2	C1B-NB	3.53	1.42	1.37
27	b	727	CLA	MG-NC	-3.53	1.97	2.06
32	J	615	PID	O3-C10	3.53	1.28	1.21
27	H	307	CLA	MG-NC	-3.53	1.97	2.06
28	A	608	KC2	C4C-NC	3.53	1.43	1.37
27	A	602	CLA	MG-NC	-3.52	1.97	2.06
27	a	810	CLA	MG-NC	-3.52	1.97	2.06
27	J	607	CLA	MG-NC	-3.52	1.97	2.06
27	l	402	CLA	MG-NC	-3.52	1.97	2.06
27	D	604	CLA	MG-NC	-3.52	1.97	2.06
27	B	605	CLA	MG-NC	-3.52	1.97	2.06
27	b	706	CLA	MG-NC	-3.52	1.97	2.06
27	a	825	CLA	MG-NC	-3.51	1.97	2.06
27	J	605	CLA	MG-NC	-3.51	1.97	2.06
28	J	606	KC2	C3D-C4D	3.51	1.43	1.40
28	H	302	KC2	C3D-C4D	3.51	1.43	1.40
27	E	606	CLA	MG-NC	-3.51	1.97	2.06
27	A	603	CLA	MG-NC	-3.50	1.97	2.06
27	l	411	CLA	MG-NC	-3.50	1.97	2.06
27	E	604	CLA	MG-NC	-3.50	1.98	2.06
27	J	609	CLA	C3A-C2A	-3.50	1.51	1.54
29	C	213	UIX	C25-C28	-3.50	1.26	1.32
32	B	613	PID	C23-C22	-3.50	1.26	1.32
27	E	609	CLA	MG-NC	-3.49	1.98	2.06
27	b	704	CLA	MG-NC	-3.49	1.98	2.06
27	b	722	CLA	MG-NC	-3.49	1.98	2.06
32	F	615	PID	O3-C10	3.49	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	304	CLA	MG-NC	-3.49	1.98	2.06
27	H	309	CLA	MG-NC	-3.49	1.98	2.06
27	b	713	CLA	MG-NC	-3.49	1.98	2.06
27	C	211	CLA	MG-NC	-3.49	1.98	2.06
27	E	608	CLA	MG-NC	-3.48	1.98	2.06
27	a	803	CLA	MG-NC	-3.48	1.98	2.06
27	C	201	CLA	MG-NC	-3.48	1.98	2.06
27	b	720	CLA	MG-NC	-3.48	1.98	2.06
28	B	602	KC2	C4C-NC	3.48	1.43	1.37
27	A	605	CLA	MG-NC	-3.47	1.98	2.06
29	F	613	UIX	C25-C28	-3.47	1.26	1.32
27	C	207	CLA	MG-NC	-3.47	1.98	2.06
27	E	612	CLA	MG-NC	-3.47	1.98	2.06
27	G	603	CLA	MG-NC	-3.47	1.98	2.06
32	F	615	PID	C23-C22	-3.47	1.26	1.32
32	J	614	PID	O3-C10	3.46	1.28	1.21
32	F	614	PID	O3-C10	3.46	1.28	1.21
27	A	607	CLA	MG-NC	-3.46	1.98	2.06
28	B	602	KC2	C3D-C4D	3.46	1.43	1.40
27	a	805	CLA	MG-NC	-3.46	1.98	2.06
27	T	606	CLA	MG-NC	-3.46	1.98	2.06
27	B	601	CLA	MG-NC	-3.46	1.98	2.06
27	b	724	CLA	MG-NC	-3.46	1.98	2.06
27	r	204	CLA	MG-NC	-3.46	1.98	2.06
27	U	606	CLA	MG-NC	-3.45	1.98	2.06
27	A	611	CLA	MG-NC	-3.45	1.98	2.06
27	U	605	CLA	MG-NC	-3.45	1.98	2.06
27	a	830	CLA	MG-NC	-3.45	1.98	2.06
27	l	406	CLA	MG-NC	-3.45	1.98	2.06
27	A	601	CLA	MG-NC	-3.45	1.98	2.06
27	D	611	CLA	MG-NC	-3.45	1.98	2.06
27	A	606	CLA	MG-NC	-3.45	1.98	2.06
27	A	609	CLA	MG-NC	-3.45	1.98	2.06
28	J	602	KC2	C3D-C4D	3.44	1.43	1.40
28	A	608	KC2	C1B-NB	3.44	1.42	1.37
27	I	601	CLA	MG-NC	-3.44	1.98	2.06
28	E	610	KC2	C3D-C4D	3.44	1.43	1.40
27	a	822	CLA	MG-NC	-3.43	1.98	2.06
27	E	607	CLA	MG-NC	-3.43	1.98	2.06
27	D	607	CLA	MG-NC	-3.43	1.98	2.06
27	b	723	CLA	MG-NC	-3.43	1.98	2.06
32	B	613	PID	O3-C10	3.43	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	I	614	PID	O3-C10	3.42	1.28	1.21
27	a	813	CLA	MG-NC	-3.42	1.98	2.06
27	K	601	CLA	MG-NC	-3.42	1.98	2.06
27	H	312	CLA	MG-NC	-3.42	1.98	2.06
27	a	821	CLA	MG-NC	-3.42	1.98	2.06
27	A	604	CLA	MG-NC	-3.42	1.98	2.06
27	I	616	CLA	MG-NC	-3.42	1.98	2.06
27	K	603	CLA	MG-NC	-3.42	1.98	2.06
27	C	202	CLA	MG-NC	-3.41	1.98	2.06
27	F	601	CLA	MG-NC	-3.41	1.98	2.06
27	H	319	CLA	MG-NC	-3.41	1.98	2.06
28	I	604	KC2	C3D-C4D	3.41	1.43	1.40
27	K	606	CLA	C3A-C2A	-3.41	1.51	1.54
27	T	607	CLA	MG-NC	-3.40	1.98	2.06
27	A	610	CLA	MG-NC	-3.39	1.98	2.06
27	F	617	CLA	MG-NC	-3.39	1.98	2.06
32	J	614	PID	C23-C22	-3.39	1.26	1.32
27	G	610	CLA	MG-NC	-3.39	1.98	2.06
27	F	608	CLA	MG-NC	-3.39	1.98	2.06
27	E	602	CLA	MG-NC	-3.39	1.98	2.06
27	B	609	CLA	MG-NC	-3.38	1.98	2.06
27	a	826	CLA	MG-NC	-3.38	1.98	2.06
27	a	817	CLA	MG-NC	-3.38	1.98	2.06
27	b	728	CLA	MG-NC	-3.38	1.98	2.06
27	a	804	CLA	MG-NC	-3.38	1.98	2.06
27	I	602	CLA	MG-NC	-3.38	1.98	2.06
27	I	603	CLA	MG-NC	-3.37	1.98	2.06
27	F	606	CLA	MG-NC	-3.37	1.98	2.06
27	I	608	CLA	MG-NC	-3.36	1.98	2.06
27	a	831	CLA	MG-NC	-3.36	1.98	2.06
32	J	611	PID	C23-C22	-3.34	1.26	1.32
27	K	604	CLA	MG-NC	-3.34	1.98	2.06
28	J	604	KC2	C3D-C4D	3.33	1.43	1.40
27	F	619	CLA	MG-NC	-3.32	1.98	2.06
27	F	605	CLA	MG-NC	-3.32	1.98	2.06
27	a	815	CLA	MG-NC	-3.32	1.98	2.06
27	T	604	CLA	MG-NC	-3.31	1.98	2.06
27	T	603	CLA	MG-NC	-3.31	1.98	2.06
27	B	607	CLA	MG-NC	-3.31	1.98	2.06
32	J	611	PID	O3-C10	3.31	1.28	1.21
27	a	837	CLA	MG-NC	-3.30	1.98	2.06
27	b	726	CLA	MG-NC	-3.30	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	819	CLA	MG-NC	-3.30	1.98	2.06
27	b	701	CLA	MG-NC	-3.30	1.98	2.06
27	D	606	CLA	MG-NC	-3.29	1.98	2.06
27	b	702	CLA	MG-NC	-3.29	1.98	2.06
27	B	610	CLA	MG-NC	-3.29	1.98	2.06
27	b	708	CLA	MG-NC	-3.29	1.98	2.06
27	G	609	CLA	MG-NC	-3.28	1.98	2.06
27	b	717	CLA	MG-NC	-3.28	1.98	2.06
27	H	308	CLA	MG-NC	-3.28	1.98	2.06
27	D	601	CLA	MG-NC	-3.27	1.98	2.06
27	K	605	CLA	MG-NC	-3.27	1.98	2.06
27	H	306	CLA	MG-NC	-3.27	1.98	2.06
27	f	302	CLA	MG-NC	-3.27	1.98	2.06
27	G	602	CLA	MG-NC	-3.26	1.98	2.06
27	D	605	CLA	MG-NC	-3.24	1.98	2.06
27	a	814	CLA	MG-NC	-3.24	1.98	2.06
32	J	615	PID	C23-C22	-3.24	1.26	1.32
27	l	409	CLA	MG-NC	-3.23	1.98	2.06
27	b	709	CLA	MG-NC	-3.23	1.98	2.06
27	F	604	CLA	MG-NC	-3.20	1.98	2.06
27	H	303	CLA	MG-NC	-3.19	1.98	2.06
27	I	605	CLA	MG-NC	-3.19	1.98	2.06
27	C	206	CLA	MG-NC	-3.18	1.98	2.06
28	J	608	KC2	C1D-ND	3.18	1.38	1.35
27	b	725	CLA	MG-NC	-3.18	1.98	2.06
28	T	608	KC2	C1D-ND	3.18	1.38	1.35
27	a	806	CLA	MG-NC	-3.18	1.98	2.06
27	D	610	CLA	MG-NC	-3.15	1.98	2.06
28	H	302	KC2	C1D-ND	3.15	1.38	1.35
27	T	605	CLA	MG-NC	-3.14	1.98	2.06
28	H	311	KC2	C1D-ND	3.11	1.38	1.35
27	T	609	CLA	C3A-C2A	-3.09	1.51	1.54
32	K	611	PID	O3-C10	3.09	1.28	1.21
28	G	601	KC2	C1D-ND	3.07	1.37	1.35
28	J	610	KC2	C1D-ND	3.06	1.37	1.35
28	C	210	KC2	C1D-ND	3.05	1.37	1.35
28	J	604	KC2	C1D-ND	3.05	1.37	1.35
28	I	604	KC2	C1D-ND	3.04	1.37	1.35
28	U	604	KC2	C1D-ND	3.04	1.37	1.35
28	K	607	KC2	C1D-ND	3.03	1.37	1.35
28	E	610	KC2	C1D-ND	3.02	1.37	1.35
28	U	602	KC2	C1D-ND	3.02	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	608	KC2	C1D-ND	3.01	1.37	1.35
28	F	609	KC2	C1D-ND	2.99	1.37	1.35
28	E	601	KC2	C1D-ND	2.96	1.37	1.35
31	H	320	SQD	C6-S	-2.96	1.66	1.77
28	J	602	KC2	C1D-ND	2.96	1.37	1.35
28	J	606	KC2	C1D-ND	2.94	1.37	1.35
28	B	608	KC2	C1D-ND	2.93	1.37	1.35
28	B	602	KC2	C1D-ND	2.93	1.37	1.35
27	T	604	CLA	C3A-C2A	-2.86	1.51	1.54
32	J	613	PID	C11-C12	-2.85	1.38	1.44
31	y	301	SQD	C6-S	-2.80	1.67	1.77
28	J	602	KC2	C3D-C2D	2.80	1.44	1.39
28	F	609	KC2	C3D-C2D	2.80	1.44	1.39
28	J	606	KC2	C3D-C2D	2.79	1.44	1.39
28	C	210	KC2	C3D-C2D	2.79	1.44	1.39
28	T	608	KC2	C3D-C2D	2.78	1.44	1.39
28	H	311	KC2	C3D-C2D	2.78	1.44	1.39
28	U	604	KC2	C3D-C2D	2.77	1.44	1.39
28	B	602	KC2	C3D-C2D	2.77	1.44	1.39
28	U	602	KC2	C3D-C2D	2.77	1.44	1.39
28	E	610	KC2	C3D-C2D	2.77	1.44	1.39
28	J	608	KC2	C3D-C2D	2.76	1.44	1.39
31	A	618	SQD	C6-S	-2.76	1.67	1.77
28	J	610	KC2	C3D-C2D	2.76	1.44	1.39
32	K	611	PID	C25-C24	-2.75	1.49	1.54
28	J	604	KC2	C3D-C2D	2.75	1.44	1.39
28	E	601	KC2	C3D-C2D	2.74	1.44	1.39
28	K	607	KC2	C3D-C2D	2.74	1.44	1.39
28	G	601	KC2	C3D-C2D	2.73	1.44	1.39
28	B	608	KC2	C3D-C2D	2.73	1.44	1.39
28	H	302	KC2	C3D-C2D	2.72	1.44	1.39
28	A	608	KC2	C3D-C2D	2.72	1.44	1.39
28	I	604	KC2	C3D-C2D	2.71	1.44	1.39
28	J	606	KC2	C4D-CHA	-2.68	1.41	1.45
32	J	611	PID	C11-C12	-2.56	1.39	1.44
28	I	604	KC2	C4D-CHA	-2.55	1.41	1.45
31	A	618	SQD	O48-C23	2.55	1.46	1.33
32	J	613	PID	C25-C24	-2.54	1.50	1.54
28	K	607	KC2	C4D-CHA	-2.54	1.41	1.45
29	I	612	UIX	C15-C20	-2.50	1.50	1.54
29	C	213	UIX	C15-C20	-2.50	1.50	1.54
29	B	611	UIX	C15-C20	-2.49	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	837	CLA	C3D-C4D	-2.48	1.38	1.44
27	b	702	CLA	C1D-C2D	-2.42	1.40	1.45
28	U	604	KC2	C4D-CHA	-2.39	1.42	1.45
27	D	604	CLA	C1D-C2D	-2.38	1.40	1.45
28	E	601	KC2	C4D-ND	2.38	1.37	1.35
27	H	304	CLA	C1D-C2D	-2.37	1.40	1.45
28	T	608	KC2	C4D-ND	2.37	1.37	1.35
27	K	605	CLA	C1D-C2D	-2.37	1.40	1.45
27	a	830	CLA	C1D-C2D	-2.37	1.40	1.45
29	A	616	UIX	O-C1	-2.36	1.42	1.46
35	l	416	DGD	O1G-C1G	-2.36	1.39	1.45
27	I	608	CLA	C1D-C2D	-2.35	1.40	1.45
27	G	606	CLA	C1D-C2D	-2.35	1.40	1.45
35	j	201	DGD	O2G-C2G	-2.35	1.40	1.46
27	T	605	CLA	C1D-C2D	-2.34	1.40	1.45
27	I	602	CLA	C1D-C2D	-2.34	1.40	1.45
27	b	708	CLA	C1D-C2D	-2.33	1.40	1.45
27	a	827	CLA	C1D-C2D	-2.32	1.40	1.45
35	l	416	DGD	O2G-C2G	-2.32	1.40	1.46
27	A	606	CLA	C1D-C2D	-2.32	1.40	1.45
27	a	839	CLA	C1D-C2D	-2.32	1.40	1.45
28	J	604	KC2	C4D-CHA	-2.32	1.42	1.45
27	D	606	CLA	C1D-C2D	-2.32	1.40	1.45
27	a	817	CLA	C1D-C2D	-2.31	1.40	1.45
27	K	604	CLA	C1D-C2D	-2.31	1.40	1.45
27	D	610	CLA	C1D-C2D	-2.31	1.40	1.45
28	B	602	KC2	C4D-CHA	-2.31	1.42	1.45
27	D	605	CLA	C1D-C2D	-2.30	1.40	1.45
27	C	204	CLA	C1D-C2D	-2.30	1.40	1.45
27	l	406	CLA	C1D-C2D	-2.30	1.40	1.45
27	a	801	CLA	C1D-C2D	-2.29	1.40	1.45
28	J	610	KC2	C4D-ND	2.29	1.37	1.35
27	F	602	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	822	CLA	C1D-C2D	-2.29	1.40	1.45
28	A	608	KC2	C4D-ND	2.29	1.37	1.35
27	a	804	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	831	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	805	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	818	CLA	C1D-C2D	-2.29	1.40	1.45
27	E	603	CLA	C1D-C2D	-2.28	1.40	1.45
27	B	609	CLA	C1D-C2D	-2.28	1.40	1.45
27	B	607	CLA	C1D-C2D	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	604	CLA	C1D-C2D	-2.28	1.40	1.45
27	l	411	CLA	C1D-C2D	-2.28	1.40	1.45
29	E	616	UIX	C15-C20	-2.28	1.50	1.54
27	G	609	CLA	C1D-C2D	-2.28	1.40	1.45
27	E	607	CLA	C1D-C2D	-2.28	1.40	1.45
27	H	305	CLA	C1D-C2D	-2.28	1.40	1.45
27	f	302	CLA	C1D-C2D	-2.28	1.40	1.45
27	b	717	CLA	C1D-C2D	-2.28	1.40	1.45
27	C	205	CLA	C1D-C2D	-2.28	1.40	1.45
27	a	824	CLA	C3D-C4D	-2.28	1.39	1.44
27	D	611	CLA	C1D-C2D	-2.28	1.40	1.45
27	A	603	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	809	CLA	C1D-C2D	-2.27	1.40	1.45
32	F	614	PID	C11-C12	-2.27	1.39	1.44
27	F	617	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	826	CLA	C3D-C4D	-2.27	1.39	1.44
27	I	616	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	802	CLA	C1D-C2D	-2.27	1.40	1.45
27	b	705	CLA	C1D-C2D	-2.27	1.40	1.45
27	C	203	CLA	C3D-C4D	-2.27	1.39	1.44
27	a	826	CLA	C1D-C2D	-2.27	1.40	1.45
27	I	601	CLA	C1D-C2D	-2.27	1.40	1.45
27	j	202	CLA	C1D-C2D	-2.27	1.40	1.45
27	b	723	CLA	C1D-C2D	-2.27	1.40	1.45
28	J	602	KC2	C4D-CHA	-2.27	1.42	1.45
27	D	603	CLA	C1D-C2D	-2.27	1.40	1.45
27	b	725	CLA	C1D-C2D	-2.27	1.40	1.45
27	F	619	CLA	C1D-C2D	-2.27	1.40	1.45
27	G	603	CLA	C1D-C2D	-2.27	1.40	1.45
29	C	215	UIX	O-C1	-2.27	1.43	1.46
27	b	727	CLA	C1D-C2D	-2.27	1.40	1.45
27	l	409	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	821	CLA	C3D-C4D	-2.27	1.39	1.44
27	C	204	CLA	C3D-C4D	-2.26	1.39	1.44
27	a	823	CLA	C1D-C2D	-2.26	1.40	1.45
27	b	706	CLA	C1D-C2D	-2.26	1.40	1.45
27	l	403	CLA	C1D-C2D	-2.26	1.40	1.45
35	K	614	DGD	C4D-C5D	2.26	1.57	1.53
27	A	609	CLA	C1D-C2D	-2.26	1.40	1.45
27	b	703	CLA	C1D-C2D	-2.26	1.40	1.45
27	b	726	CLA	C1D-C2D	-2.26	1.40	1.45
27	l	408	CLA	C1D-C2D	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	602	CLA	C1D-C2D	-2.26	1.40	1.45
27	G	602	CLA	C1D-C2D	-2.26	1.40	1.45
27	H	307	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	724	CLA	C1D-C2D	-2.25	1.40	1.45
27	C	212	CLA	C1D-C2D	-2.25	1.40	1.45
27	l	411	CLA	C3D-C4D	-2.25	1.39	1.44
32	U	608	PID	C25-C24	-2.25	1.50	1.54
27	r	204	CLA	C1D-C2D	-2.25	1.40	1.45
27	D	605	CLA	C3D-C4D	-2.25	1.39	1.44
27	E	609	CLA	C1D-C2D	-2.25	1.40	1.45
27	H	319	CLA	C1D-C2D	-2.25	1.40	1.45
27	a	803	CLA	C3D-C4D	-2.25	1.39	1.44
27	C	203	CLA	C1D-C2D	-2.25	1.40	1.45
27	K	602	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	701	CLA	C1D-C2D	-2.25	1.40	1.45
27	I	606	CLA	C1D-C2D	-2.25	1.40	1.45
27	I	607	CLA	C1D-C2D	-2.25	1.40	1.45
27	a	810	CLA	C1D-C2D	-2.25	1.40	1.45
38	a	836	BCR	C1-C6	-2.25	1.50	1.53
27	B	605	CLA	C1D-C2D	-2.25	1.40	1.45
27	l	403	CLA	C3D-C4D	-2.25	1.39	1.44
27	b	710	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	718	CLA	C1D-C2D	-2.25	1.40	1.45
27	C	208	CLA	C1D-C2D	-2.25	1.40	1.45
27	B	601	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	728	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	706	CLA	C3D-C4D	-2.24	1.39	1.44
27	D	612	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	825	CLA	C1D-C2D	-2.24	1.40	1.45
27	E	603	CLA	C3D-C4D	-2.24	1.39	1.44
27	A	602	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	830	CLA	C3D-C4D	-2.24	1.39	1.44
27	D	601	CLA	C1D-C2D	-2.24	1.40	1.45
27	I	610	CLA	C3D-C4D	-2.24	1.39	1.44
27	b	715	CLA	C3D-C4D	-2.24	1.39	1.44
27	a	814	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	829	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	718	CLA	C3D-C4D	-2.24	1.39	1.44
27	l	404	CLA	C3D-C4D	-2.24	1.39	1.44
27	b	725	CLA	C3D-C4D	-2.24	1.39	1.44
27	b	709	CLA	C1D-C2D	-2.24	1.40	1.45
35	j	201	DGD	O5D-C6D	-2.24	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	815	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	820	CLA	C1D-C2D	-2.24	1.40	1.45
27	C	211	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	813	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	720	CLA	C1D-C2D	-2.24	1.40	1.45
27	B	604	CLA	C3D-C4D	-2.24	1.39	1.44
27	T	602	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	704	CLA	C1D-C2D	-2.23	1.40	1.45
35	f	305	DGD	O2G-C2G	-2.23	1.41	1.46
27	A	610	CLA	C1D-C2D	-2.23	1.40	1.45
27	l	402	CLA	C1D-C2D	-2.23	1.40	1.45
27	a	825	CLA	C3D-C4D	-2.23	1.39	1.44
27	a	820	CLA	C3D-C4D	-2.23	1.39	1.44
27	F	607	CLA	C1D-C2D	-2.23	1.40	1.45
27	A	602	CLA	C3D-C4D	-2.23	1.39	1.44
27	A	604	CLA	C1D-C2D	-2.23	1.40	1.45
27	I	610	CLA	C1D-C2D	-2.23	1.40	1.45
27	F	601	CLA	C1D-C2D	-2.23	1.40	1.45
27	b	722	CLA	C1D-C2D	-2.23	1.40	1.45
27	G	606	CLA	C3D-C4D	-2.23	1.39	1.44
27	D	603	CLA	C3D-C4D	-2.23	1.39	1.44
27	F	601	CLA	C3D-C4D	-2.23	1.39	1.44
27	F	606	CLA	C3D-C4D	-2.23	1.39	1.44
27	H	303	CLA	C1D-C2D	-2.23	1.40	1.45
27	J	601	CLA	C1D-C2D	-2.23	1.40	1.45
27	l	402	CLA	C3D-C4D	-2.23	1.39	1.44
27	b	723	CLA	C3D-C4D	-2.23	1.39	1.44
27	l	407	CLA	C1D-C2D	-2.23	1.40	1.45
27	D	604	CLA	C3D-C4D	-2.23	1.39	1.44
27	B	603	CLA	C1D-C2D	-2.23	1.40	1.45
27	b	707	CLA	C3D-C4D	-2.23	1.39	1.44
27	a	839	CLA	C3D-C4D	-2.23	1.39	1.44
27	H	319	CLA	C3D-C4D	-2.23	1.39	1.44
27	J	605	CLA	C1D-C2D	-2.23	1.40	1.45
27	U	605	CLA	C1D-C2D	-2.23	1.40	1.45
27	I	603	CLA	C1D-C2D	-2.22	1.40	1.45
27	a	824	CLA	C1D-C2D	-2.22	1.40	1.45
27	b	711	CLA	C1D-C2D	-2.22	1.40	1.45
27	D	602	CLA	C3D-C4D	-2.22	1.39	1.44
27	H	308	CLA	C1D-C2D	-2.22	1.40	1.45
35	K	614	DGD	O1G-C1G	-2.22	1.40	1.45
27	b	719	CLA	C1D-C2D	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	307	CLA	C3D-C4D	-2.22	1.39	1.44
27	A	601	CLA	C1D-C2D	-2.22	1.40	1.45
27	F	606	CLA	C1D-C2D	-2.22	1.40	1.45
27	H	312	CLA	C1D-C2D	-2.22	1.40	1.45
27	J	607	CLA	C1D-C2D	-2.22	1.40	1.45
27	l	406	CLA	C3D-C4D	-2.22	1.39	1.44
27	E	611	CLA	C1D-C2D	-2.22	1.40	1.45
27	a	819	CLA	C1D-C2D	-2.22	1.40	1.45
27	l	404	CLA	C1D-C2D	-2.22	1.40	1.45
27	I	603	CLA	C3D-C4D	-2.22	1.39	1.44
27	G	605	CLA	C1D-C2D	-2.22	1.40	1.45
28	H	311	KC2	C4D-ND	2.22	1.37	1.35
27	I	606	CLA	C3D-C4D	-2.22	1.39	1.44
27	l	409	CLA	C3D-C4D	-2.22	1.39	1.44
27	C	201	CLA	C1D-C2D	-2.22	1.40	1.45
27	G	608	CLA	C1D-C2D	-2.22	1.40	1.45
27	b	705	CLA	C3D-C4D	-2.22	1.39	1.44
27	D	607	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	816	CLA	C1D-C2D	-2.21	1.41	1.45
27	G	611	CLA	C1D-C2D	-2.21	1.41	1.45
27	K	608	CLA	C1D-C2D	-2.21	1.41	1.45
27	b	712	CLA	C1D-C2D	-2.21	1.41	1.45
27	l	412	CLA	C1D-C2D	-2.21	1.41	1.45
27	D	608	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	719	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	807	CLA	C1D-C2D	-2.21	1.41	1.45
27	l	405	CLA	C1D-C2D	-2.21	1.41	1.45
27	a	809	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	812	CLA	C1D-C2D	-2.21	1.41	1.45
27	H	310	CLA	C3D-C4D	-2.21	1.39	1.44
27	G	610	CLA	C1D-C2D	-2.21	1.41	1.45
27	A	612	CLA	C3D-C4D	-2.21	1.39	1.44
27	F	603	CLA	C1D-C2D	-2.21	1.41	1.45
27	b	716	CLA	C3D-C4D	-2.21	1.39	1.44
27	C	205	CLA	C3D-C4D	-2.21	1.39	1.44
27	I	602	CLA	C3D-C4D	-2.21	1.39	1.44
27	E	602	CLA	C1D-C2D	-2.21	1.41	1.45
27	b	712	CLA	C3D-C4D	-2.21	1.39	1.44
27	C	201	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	714	CLA	C1D-C2D	-2.21	1.41	1.45
32	J	611	PID	O1-C1	-2.21	1.43	1.46
27	I	605	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	303	CLA	C1D-C2D	-2.21	1.41	1.45
28	G	601	KC2	C4D-ND	2.21	1.37	1.35
27	H	312	CLA	C3D-C4D	-2.21	1.39	1.44
27	E	604	CLA	C1D-C2D	-2.21	1.41	1.45
27	E	608	CLA	C1D-C2D	-2.21	1.41	1.45
27	E	612	CLA	C1D-C2D	-2.21	1.41	1.45
27	G	604	CLA	C1D-C2D	-2.20	1.41	1.45
27	r	203	CLA	C1D-C2D	-2.20	1.41	1.45
27	H	303	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	714	CLA	C3D-C4D	-2.20	1.39	1.44
27	H	313	CLA	C3D-C4D	-2.20	1.39	1.44
27	C	202	CLA	C1D-C2D	-2.20	1.41	1.45
27	G	607	CLA	C1D-C2D	-2.20	1.41	1.45
27	a	811	CLA	C1D-C2D	-2.20	1.41	1.45
27	G	603	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	728	CLA	C3D-C4D	-2.20	1.39	1.44
29	D	616	UIX	O-C1	-2.20	1.43	1.46
27	l	410	CLA	C1D-C2D	-2.20	1.41	1.45
27	r	203	CLA	C3D-C4D	-2.20	1.39	1.44
27	A	607	CLA	C1D-C2D	-2.20	1.41	1.45
27	H	306	CLA	C1D-C2D	-2.20	1.41	1.45
27	U	603	CLA	C1D-C2D	-2.20	1.41	1.45
27	b	711	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	713	CLA	C3D-C4D	-2.20	1.39	1.44
32	B	613	PID	C25-C24	-2.20	1.50	1.54
27	E	605	CLA	C1D-C2D	-2.20	1.41	1.45
27	a	805	CLA	C3D-C4D	-2.20	1.39	1.44
27	F	619	CLA	C3D-C4D	-2.20	1.39	1.44
27	B	604	CLA	C1D-C2D	-2.20	1.41	1.45
29	B	615	UIX	O-C1	-2.20	1.43	1.46
27	a	816	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	721	CLA	C3D-C4D	-2.20	1.39	1.44
27	C	208	CLA	C3D-C4D	-2.20	1.39	1.44
28	E	610	KC2	C4D-ND	2.20	1.37	1.35
27	T	603	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	606	CLA	C3D-C4D	-2.20	1.39	1.44
27	a	823	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	720	CLA	C3D-C4D	-2.20	1.39	1.44
27	C	207	CLA	C1D-C2D	-2.19	1.41	1.45
27	C	209	CLA	C1D-C2D	-2.19	1.41	1.45
27	D	609	CLA	C1D-C2D	-2.19	1.41	1.45
27	l	408	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	821	CLA	C1D-C2D	-2.19	1.41	1.45
28	F	609	KC2	C4D-ND	2.19	1.37	1.35
27	a	804	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	716	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	612	CLA	C1D-C2D	-2.19	1.41	1.45
27	a	810	CLA	C3D-C4D	-2.19	1.39	1.44
27	G	611	CLA	C3D-C4D	-2.19	1.39	1.44
27	J	603	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	724	CLA	C3D-C4D	-2.19	1.39	1.44
27	F	610	CLA	C1D-C2D	-2.19	1.41	1.45
27	H	313	CLA	C1D-C2D	-2.19	1.41	1.45
27	b	709	CLA	C3D-C4D	-2.19	1.39	1.44
27	T	604	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	605	CLA	C1D-C2D	-2.19	1.41	1.45
27	D	611	CLA	C3D-C4D	-2.19	1.39	1.44
27	l	405	CLA	C3D-C4D	-2.19	1.39	1.44
27	a	829	CLA	C3D-C4D	-2.19	1.39	1.44
27	E	611	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	708	CLA	C3D-C4D	-2.19	1.39	1.44
27	A	603	CLA	C3D-C4D	-2.19	1.39	1.44
27	a	828	CLA	C3D-C4D	-2.19	1.39	1.44
27	J	603	CLA	C1D-C2D	-2.19	1.41	1.45
27	G	605	CLA	C3D-C4D	-2.19	1.39	1.44
27	J	605	CLA	C3D-C4D	-2.19	1.39	1.44
27	K	601	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	606	CLA	C3D-C4D	-2.18	1.39	1.44
27	b	717	CLA	C3D-C4D	-2.18	1.39	1.44
27	K	603	CLA	C3D-C4D	-2.18	1.39	1.44
27	b	704	CLA	C3D-C4D	-2.18	1.39	1.44
27	H	310	CLA	C1D-C2D	-2.18	1.41	1.45
28	J	608	KC2	C4D-ND	2.18	1.37	1.35
27	I	601	CLA	C3D-C4D	-2.18	1.39	1.44
27	D	612	CLA	C3D-C4D	-2.18	1.39	1.44
27	B	609	CLA	C3D-C4D	-2.18	1.39	1.44
27	E	602	CLA	C3D-C4D	-2.18	1.39	1.44
27	F	605	CLA	C1D-C2D	-2.18	1.41	1.45
27	a	808	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	601	CLA	C3D-C4D	-2.18	1.39	1.44
27	b	727	CLA	C3D-C4D	-2.18	1.39	1.44
28	B	608	KC2	C4D-ND	2.18	1.37	1.35
27	l	410	CLA	C3D-C4D	-2.18	1.39	1.44
27	b	701	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	U	602	KC2	C4D-CHA	-2.18	1.42	1.45
27	H	309	CLA	C3D-C4D	-2.18	1.39	1.44
27	H	309	CLA	C1D-C2D	-2.18	1.41	1.45
27	F	603	CLA	C3D-C4D	-2.18	1.39	1.44
27	A	609	CLA	C3D-C4D	-2.18	1.39	1.44
27	T	601	CLA	C3D-C4D	-2.18	1.39	1.44
28	F	609	KC2	C4D-CHA	-2.18	1.42	1.45
27	b	721	CLA	C1D-C2D	-2.17	1.41	1.45
27	b	722	CLA	C3D-C4D	-2.17	1.39	1.44
27	a	806	CLA	C3D-C4D	-2.17	1.39	1.44
27	a	815	CLA	C3D-C4D	-2.17	1.39	1.44
27	b	710	CLA	C3D-C4D	-2.17	1.39	1.44
27	B	610	CLA	C1D-C2D	-2.17	1.41	1.45
27	D	608	CLA	C1D-C2D	-2.17	1.41	1.45
27	a	818	CLA	C3D-C4D	-2.17	1.39	1.44
27	C	206	CLA	C1D-C2D	-2.17	1.41	1.45
27	F	608	CLA	C1D-C2D	-2.17	1.41	1.45
27	B	610	CLA	C3D-C4D	-2.17	1.39	1.44
27	a	837	CLA	C1D-C2D	-2.17	1.41	1.45
28	C	210	KC2	C4D-CHA	-2.17	1.42	1.45
27	f	302	CLA	C3D-C4D	-2.17	1.39	1.44
27	E	606	CLA	C3D-C4D	-2.17	1.39	1.44
27	G	607	CLA	C3D-C4D	-2.17	1.39	1.44
27	T	601	CLA	C1D-C2D	-2.17	1.41	1.45
29	E	616	UIX	O-C1	-2.17	1.43	1.46
27	E	608	CLA	C3D-C4D	-2.17	1.39	1.44
27	T	606	CLA	C1D-C2D	-2.17	1.41	1.45
27	a	806	CLA	C1D-C2D	-2.17	1.41	1.45
27	A	605	CLA	C3D-C4D	-2.17	1.39	1.44
27	F	617	CLA	C3D-C4D	-2.17	1.39	1.44
27	I	609	CLA	C3D-C4D	-2.17	1.39	1.44
27	D	607	CLA	C1D-C2D	-2.17	1.41	1.45
32	U	608	PID	C11-C12	-2.17	1.40	1.44
27	l	412	CLA	C3D-C4D	-2.17	1.39	1.44
27	E	605	CLA	C3D-C4D	-2.17	1.39	1.44
27	F	602	CLA	C3D-C4D	-2.17	1.39	1.44
27	K	606	CLA	C3D-C4D	-2.16	1.39	1.44
27	E	606	CLA	C1D-C2D	-2.16	1.41	1.45
27	b	707	CLA	C1D-C2D	-2.16	1.41	1.45
27	C	212	CLA	C3D-C4D	-2.16	1.39	1.44
27	A	601	CLA	C3D-C4D	-2.16	1.39	1.44
27	I	607	CLA	C3D-C4D	-2.16	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	607	CLA	C1D-C2D	-2.16	1.41	1.45
27	A	607	CLA	C3D-C4D	-2.16	1.39	1.44
32	J	615	PID	C11-C12	-2.16	1.40	1.44
27	T	602	CLA	C3D-C4D	-2.16	1.39	1.44
27	l	407	CLA	C3D-C4D	-2.16	1.39	1.44
27	K	604	CLA	C3D-C4D	-2.16	1.39	1.44
27	A	604	CLA	C3D-C4D	-2.16	1.39	1.44
27	C	207	CLA	C3D-C4D	-2.16	1.39	1.44
27	K	601	CLA	C3D-C4D	-2.16	1.39	1.44
27	a	803	CLA	C1D-C2D	-2.16	1.41	1.45
27	a	802	CLA	C3D-C4D	-2.16	1.39	1.44
27	B	606	CLA	C1D-C2D	-2.16	1.41	1.45
27	H	308	CLA	C3D-C4D	-2.16	1.39	1.44
27	U	601	CLA	C1D-C2D	-2.16	1.41	1.45
27	C	206	CLA	C3D-C4D	-2.16	1.39	1.44
27	b	713	CLA	C1D-C2D	-2.16	1.41	1.45
27	U	606	CLA	C1D-C2D	-2.15	1.41	1.45
27	U	603	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	808	CLA	C3D-C4D	-2.15	1.39	1.44
27	K	602	CLA	C3D-C4D	-2.15	1.39	1.44
28	U	602	KC2	C4D-ND	2.15	1.37	1.35
27	a	827	CLA	C3D-C4D	-2.15	1.39	1.44
27	b	726	CLA	C3D-C4D	-2.15	1.39	1.44
28	I	604	KC2	C4D-ND	2.15	1.37	1.35
28	B	608	KC2	C4D-CHA	-2.15	1.42	1.45
32	I	614	PID	C25-C24	-2.15	1.50	1.54
27	F	604	CLA	C3D-C4D	-2.15	1.39	1.44
27	T	607	CLA	C3D-C4D	-2.15	1.39	1.44
27	C	202	CLA	C3D-C4D	-2.15	1.39	1.44
27	I	611	CLA	C1D-C2D	-2.15	1.41	1.45
27	C	209	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	812	CLA	C3D-C4D	-2.15	1.39	1.44
27	G	602	CLA	C3D-C4D	-2.15	1.39	1.44
27	D	609	CLA	C3D-C4D	-2.15	1.39	1.44
29	H	314	UIX	O-C1	-2.14	1.43	1.46
27	B	607	CLA	C3D-C4D	-2.14	1.39	1.44
27	I	605	CLA	C3D-C4D	-2.14	1.39	1.44
27	I	609	CLA	C1D-C2D	-2.14	1.41	1.45
27	B	605	CLA	C3D-C4D	-2.14	1.39	1.44
27	E	604	CLA	C3D-C4D	-2.14	1.39	1.44
27	a	811	CLA	C3D-C4D	-2.14	1.39	1.44
27	F	607	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	814	CLA	C3D-C4D	-2.14	1.39	1.44
27	r	204	CLA	C3D-C4D	-2.14	1.39	1.44
27	G	604	CLA	C3D-C4D	-2.14	1.39	1.44
27	G	608	CLA	C3D-C4D	-2.14	1.39	1.44
27	J	609	CLA	C3D-C4D	-2.14	1.39	1.44
27	E	607	CLA	C3D-C4D	-2.14	1.39	1.44
27	B	603	CLA	C3D-C4D	-2.14	1.39	1.44
27	D	601	CLA	C3D-C4D	-2.14	1.39	1.44
27	H	306	CLA	C3D-C4D	-2.14	1.39	1.44
27	a	822	CLA	C3D-C4D	-2.14	1.39	1.44
27	a	831	CLA	C3D-C4D	-2.14	1.39	1.44
27	K	603	CLA	C1D-C2D	-2.14	1.41	1.45
27	a	807	CLA	C3D-C4D	-2.14	1.39	1.44
27	F	605	CLA	C3D-C4D	-2.14	1.39	1.44
27	b	703	CLA	C3D-C4D	-2.14	1.39	1.44
27	T	609	CLA	C1D-C2D	-2.14	1.41	1.45
27	E	612	CLA	C3D-C4D	-2.13	1.39	1.44
27	D	610	CLA	C3D-C4D	-2.13	1.39	1.44
27	b	702	CLA	C3D-C4D	-2.13	1.39	1.44
28	H	302	KC2	C4D-ND	2.13	1.37	1.35
27	A	611	CLA	C1D-C2D	-2.13	1.41	1.45
27	U	605	CLA	C3D-C4D	-2.13	1.39	1.44
27	D	606	CLA	C3D-C4D	-2.13	1.39	1.44
27	I	611	CLA	C3D-C4D	-2.13	1.39	1.44
27	J	601	CLA	C3D-C4D	-2.13	1.39	1.44
27	a	819	CLA	C3D-C4D	-2.13	1.39	1.44
27	J	609	CLA	C1D-C2D	-2.13	1.41	1.45
27	K	606	CLA	C1D-C2D	-2.13	1.41	1.45
27	E	609	CLA	C3D-C4D	-2.13	1.39	1.44
27	J	607	CLA	C3D-C4D	-2.13	1.39	1.44
27	A	610	CLA	C3D-C4D	-2.12	1.39	1.44
27	U	601	CLA	C3D-C4D	-2.12	1.39	1.44
29	j	204	UIX	C15-C20	-2.12	1.51	1.54
27	H	305	CLA	C3D-C4D	-2.12	1.39	1.44
27	C	211	CLA	C3D-C4D	-2.12	1.39	1.44
27	H	304	CLA	C3D-C4D	-2.12	1.39	1.44
27	K	605	CLA	C3D-C4D	-2.12	1.39	1.44
29	B	611	UIX	O-C1	-2.12	1.43	1.46
27	b	715	CLA	C1D-C2D	-2.11	1.41	1.45
27	G	609	CLA	C3D-C4D	-2.11	1.39	1.44
28	J	602	KC2	C4D-ND	2.11	1.37	1.35
35	f	305	DGD	O1G-C1G	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	604	KC2	C4D-ND	2.11	1.37	1.35
27	G	610	CLA	C3D-C4D	-2.11	1.39	1.44
27	T	604	CLA	C3D-C4D	-2.10	1.39	1.44
27	T	605	CLA	C3D-C4D	-2.10	1.39	1.44
27	a	817	CLA	C3D-C4D	-2.10	1.39	1.44
27	F	610	CLA	C3D-C4D	-2.10	1.39	1.44
27	K	608	CLA	C3D-C4D	-2.10	1.39	1.44
35	K	614	DGD	C4D-C3D	2.10	1.57	1.52
38	a	836	BCR	C30-C25	-2.10	1.50	1.53
27	F	608	CLA	C3D-C4D	-2.09	1.39	1.44
27	T	606	CLA	C3D-C4D	-2.09	1.39	1.44
27	a	813	CLA	C3D-C4D	-2.09	1.39	1.44
29	B	615	UIX	C15-C20	-2.09	1.51	1.54
28	C	210	KC2	C4D-ND	2.09	1.37	1.35
27	U	606	CLA	C3D-C4D	-2.08	1.39	1.44
29	J	616	UIX	O-C1	-2.08	1.43	1.46
27	I	616	CLA	C3D-C4D	-2.08	1.39	1.44
27	I	608	CLA	C3D-C4D	-2.08	1.39	1.44
29	A	613	UIX	O-C1	-2.08	1.43	1.46
28	H	302	KC2	C4D-CHA	-2.07	1.42	1.45
27	A	611	CLA	C3D-C4D	-2.07	1.39	1.44
27	T	609	CLA	C3D-C4D	-2.06	1.39	1.44
27	T	603	CLA	C3D-C4D	-2.06	1.39	1.44
29	F	613	UIX	O-C1	-2.06	1.43	1.46
28	E	601	KC2	C4D-CHA	-2.06	1.42	1.45
28	J	610	KC2	C4D-CHA	-2.06	1.42	1.45
27	a	828	CLA	C1D-C2D	-2.06	1.41	1.45
32	F	615	PID	C11-C12	-2.06	1.40	1.44
27	f	303	CLA	C3D-C4D	-2.04	1.39	1.44
29	G	615	UIX	O-C1	-2.03	1.43	1.46
29	A	616	UIX	C15-C20	-2.03	1.51	1.54
28	E	610	KC2	C4D-CHA	-2.03	1.42	1.45
28	H	311	KC2	C4D-CHA	-2.03	1.42	1.45
35	j	201	DGD	O1G-C1G	-2.03	1.40	1.45
29	H	317	UIX	C15-C20	-2.02	1.51	1.54
35	f	305	DGD	C4E-C5E	2.02	1.57	1.53
32	J	614	PID	O1-C1	-2.02	1.43	1.46
28	U	604	KC2	C4D-ND	2.02	1.37	1.35
32	B	613	PID	C11-C12	-2.02	1.40	1.44
35	j	201	DGD	O6D-C5D	-2.02	1.39	1.44
28	G	601	KC2	C4D-CHA	-2.01	1.42	1.45
32	B	613	PID	O1-C1	-2.01	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	612	UIX	O-C1	-2.01	1.43	1.46
29	T	612	UIX	C15-C20	-2.00	1.51	1.54

All (2164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	613	PID	O4-C12-C11	16.67	117.47	107.36
32	J	615	PID	O4-C12-C11	16.54	117.39	107.36
32	J	611	PID	O4-C12-C11	16.54	117.39	107.36
32	U	608	PID	O4-C12-C11	16.19	117.17	107.36
32	F	614	PID	O4-C12-C11	16.13	117.14	107.36
32	F	615	PID	O4-C12-C11	16.02	117.07	107.36
32	I	614	PID	O4-C12-C11	15.86	116.97	107.36
32	B	613	PID	O4-C12-C11	15.71	116.88	107.36
32	K	611	PID	O4-C12-C11	15.64	116.84	107.36
32	J	614	PID	O4-C12-C11	15.46	116.73	107.36
32	J	613	PID	C12-O4-C10	-12.96	100.91	107.65
32	J	611	PID	C12-O4-C10	-12.62	101.09	107.65
32	J	615	PID	C12-O4-C10	-11.79	101.52	107.65
32	F	615	PID	C12-O4-C10	-11.70	101.56	107.65
32	F	614	PID	C12-O4-C10	-11.60	101.62	107.65
32	J	613	PID	O1-C1-C2	11.59	122.09	113.38
32	U	608	PID	C12-O4-C10	-11.44	101.70	107.65
32	I	614	PID	O1-C1-C2	11.15	121.76	113.38
32	K	611	PID	C12-O4-C10	-11.12	101.86	107.65
32	B	613	PID	C12-O4-C10	-10.94	101.96	107.65
32	I	614	PID	C12-O4-C10	-10.67	102.10	107.65
32	J	614	PID	C12-O4-C10	-10.52	102.18	107.65
32	K	611	PID	O1-C1-C2	9.66	120.64	113.38
32	J	611	PID	O1-C1-C2	8.06	119.44	113.38
32	F	614	PID	O1-C1-C2	7.68	119.15	113.38
27	A	612	CLA	C4A-NA-C1A	-7.61	103.28	106.71
27	C	205	CLA	C4A-NA-C1A	-7.60	103.29	106.71
32	F	614	PID	O1-C1-CM1	7.54	124.10	115.06
27	b	718	CLA	C4A-NA-C1A	-7.19	103.47	106.71
27	a	827	CLA	C4A-NA-C1A	-7.10	103.51	106.71
27	U	601	CLA	C4A-NA-C1A	-7.04	103.54	106.71
32	J	611	PID	CM1-C1-C6	-7.01	110.52	122.26
27	K	606	CLA	C4A-NA-C1A	-6.92	103.59	106.71
27	b	705	CLA	C4A-NA-C1A	-6.90	103.60	106.71
27	G	605	CLA	C4A-NA-C1A	-6.90	103.61	106.71
27	b	714	CLA	C4A-NA-C1A	-6.88	103.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	809	CLA	C4A-NA-C1A	-6.84	103.63	106.71
27	a	812	CLA	C4A-NA-C1A	-6.77	103.66	106.71
27	B	603	CLA	C4A-NA-C1A	-6.76	103.67	106.71
27	J	609	CLA	C4A-NA-C1A	-6.68	103.70	106.71
27	H	310	CLA	C4A-NA-C1A	-6.68	103.70	106.71
27	I	610	CLA	C4A-NA-C1A	-6.66	103.71	106.71
27	a	823	CLA	C4A-NA-C1A	-6.61	103.73	106.71
27	b	727	CLA	C4A-NA-C1A	-6.46	103.80	106.71
27	E	605	CLA	C4A-NA-C1A	-6.45	103.80	106.71
27	H	305	CLA	C4A-NA-C1A	-6.44	103.81	106.71
27	G	607	CLA	C1D-ND-C4D	-6.43	101.77	106.33
32	U	608	PID	CM1-C1-C2	6.41	121.49	114.28
27	G	608	CLA	C4A-NA-C1A	-6.37	103.84	106.71
27	a	828	CLA	C4A-NA-C1A	-6.36	103.85	106.71
29	E	616	UIX	C6-C1-C3	6.34	121.41	114.28
27	E	611	CLA	C4A-NA-C1A	-6.33	103.86	106.71
27	K	603	CLA	C1D-ND-C4D	-6.31	101.85	106.33
27	l	404	CLA	C4A-NA-C1A	-6.30	103.87	106.71
27	b	715	CLA	C4A-NA-C1A	-6.29	103.88	106.71
27	b	713	CLA	C4A-NA-C1A	-6.28	103.88	106.71
27	B	604	CLA	C1D-ND-C4D	-6.27	101.88	106.33
27	I	611	CLA	C4A-NA-C1A	-6.26	103.89	106.71
27	T	607	CLA	C1D-ND-C4D	-6.25	101.90	106.33
27	b	711	CLA	C1D-ND-C4D	-6.24	101.90	106.33
27	a	828	CLA	C1D-ND-C4D	-6.23	101.91	106.33
27	T	609	CLA	C4A-NA-C1A	-6.23	103.91	106.71
27	l	408	CLA	C4A-NA-C1A	-6.22	103.91	106.71
27	U	603	CLA	C1D-ND-C4D	-6.22	101.92	106.33
27	G	604	CLA	C1D-ND-C4D	-6.22	101.92	106.33
32	J	613	PID	CM1-C1-C6	-6.22	111.84	122.26
27	F	610	CLA	C1D-ND-C4D	-6.21	101.93	106.33
27	E	606	CLA	C1D-ND-C4D	-6.20	101.93	106.33
27	C	204	CLA	C1D-ND-C4D	-6.20	101.93	106.33
27	T	604	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	I	609	CLA	C4A-NA-C1A	-6.19	103.92	106.71
27	a	803	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	F	608	CLA	C1D-ND-C4D	-6.18	101.94	106.33
27	b	723	CLA	C1D-ND-C4D	-6.18	101.94	106.33
27	H	309	CLA	C1D-ND-C4D	-6.18	101.94	106.33
27	C	209	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	l	402	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	J	601	CLA	C4A-NA-C1A	-6.17	103.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	U	606	CLA	C1D-ND-C4D	-6.16	101.96	106.33
27	I	603	CLA	C1D-ND-C4D	-6.16	101.96	106.33
27	J	603	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	l	410	CLA	C4A-NA-C1A	-6.14	103.95	106.71
27	H	313	CLA	C1D-ND-C4D	-6.14	101.98	106.33
27	F	607	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	b	710	CLA	C4A-NA-C1A	-6.13	103.95	106.71
27	C	202	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	K	602	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	D	612	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	A	604	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	b	719	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	C	212	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	b	712	CLA	C1D-ND-C4D	-6.12	101.98	106.33
27	A	602	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	I	607	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	A	601	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	D	608	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	T	602	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	a	810	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	G	604	CLA	C4A-NA-C1A	-6.11	103.96	106.71
27	a	808	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	D	603	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	a	813	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	H	312	CLA	C1D-ND-C4D	-6.11	102.00	106.33
27	C	207	CLA	C4A-NA-C1A	-6.11	103.96	106.71
27	I	606	CLA	C1D-ND-C4D	-6.11	102.00	106.33
27	b	715	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	D	602	CLA	C4A-NA-C1A	-6.10	103.96	106.71
27	A	609	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	A	607	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	I	611	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	G	602	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	U	601	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	B	610	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	B	606	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	b	713	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	K	601	CLA	C1D-ND-C4D	-6.08	102.01	106.33
27	F	603	CLA	C1D-ND-C4D	-6.08	102.02	106.33
27	D	609	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	a	806	CLA	C1D-ND-C4D	-6.07	102.02	106.33
32	J	613	PID	C11-C12-C13	-6.07	114.91	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	611	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	E	602	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	F	605	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	G	610	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	a	817	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	T	603	CLA	C1D-ND-C4D	-6.07	102.03	106.33
27	C	208	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	E	604	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	C	203	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	D	611	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	F	601	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	E	612	CLA	C1D-ND-C4D	-6.05	102.03	106.33
27	I	610	CLA	C1D-ND-C4D	-6.05	102.04	106.33
27	r	203	CLA	C1D-ND-C4D	-6.05	102.04	106.33
27	b	716	CLA	C1D-ND-C4D	-6.05	102.04	106.33
27	T	601	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	b	726	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	A	606	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	B	601	CLA	C1D-ND-C4D	-6.04	102.05	106.33
27	C	211	CLA	C1D-ND-C4D	-6.04	102.05	106.33
27	J	607	CLA	C1D-ND-C4D	-6.04	102.05	106.33
27	E	603	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	I	601	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	K	608	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	a	816	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	b	707	CLA	C1D-ND-C4D	-6.02	102.06	106.33
27	F	619	CLA	C1D-ND-C4D	-6.02	102.06	106.33
27	a	804	CLA	C4A-NA-C1A	-6.02	104.00	106.71
27	a	822	CLA	C1D-ND-C4D	-6.02	102.06	106.33
27	H	303	CLA	C1D-ND-C4D	-6.01	102.06	106.33
27	a	825	CLA	C1D-ND-C4D	-6.01	102.06	106.33
27	D	604	CLA	C1D-ND-C4D	-6.00	102.07	106.33
27	K	606	CLA	C1D-ND-C4D	-6.00	102.07	106.33
27	l	412	CLA	C1D-ND-C4D	-5.99	102.08	106.33
27	G	609	CLA	C1D-ND-C4D	-5.98	102.08	106.33
27	G	611	CLA	C1D-ND-C4D	-5.98	102.08	106.33
27	a	831	CLA	C1D-ND-C4D	-5.98	102.08	106.33
27	B	606	CLA	C4A-NA-C1A	-5.98	104.02	106.71
27	C	201	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	T	601	CLA	C4A-NA-C1A	-5.98	104.02	106.71
27	b	707	CLA	C4A-NA-C1A	-5.98	104.02	106.71
27	A	603	CLA	C1D-ND-C4D	-5.97	102.09	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	722	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	l	403	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	H	307	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	C	206	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	G	608	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	D	601	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	H	319	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	a	824	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	E	611	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	b	721	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	l	408	CLA	C1D-ND-C4D	-5.95	102.11	106.33
27	T	609	CLA	C1D-ND-C4D	-5.95	102.11	106.33
27	b	725	CLA	C1D-ND-C4D	-5.95	102.11	106.33
27	D	606	CLA	C1D-ND-C4D	-5.95	102.11	106.33
27	l	411	CLA	C1D-ND-C4D	-5.95	102.11	106.33
27	E	609	CLA	C1D-ND-C4D	-5.94	102.11	106.33
27	G	606	CLA	C1D-ND-C4D	-5.94	102.11	106.33
27	D	610	CLA	C1D-ND-C4D	-5.94	102.11	106.33
27	J	601	CLA	C1D-ND-C4D	-5.94	102.11	106.33
27	a	814	CLA	C1D-ND-C4D	-5.94	102.11	106.33
32	I	614	PID	CM1-C1-C6	-5.94	112.31	122.26
27	E	608	CLA	C1D-ND-C4D	-5.94	102.12	106.33
27	J	609	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	l	410	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	b	720	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	a	830	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	l	409	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	G	603	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	a	805	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	K	604	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	r	203	CLA	C4A-NA-C1A	-5.92	104.05	106.71
27	f	302	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	A	610	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	a	815	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	b	728	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	a	821	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	r	204	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	a	839	CLA	C1D-ND-C4D	-5.90	102.14	106.33
27	a	807	CLA	C1D-ND-C4D	-5.90	102.14	106.33
27	I	609	CLA	C1D-ND-C4D	-5.89	102.15	106.33
27	A	605	CLA	C1D-ND-C4D	-5.89	102.15	106.33
27	B	607	CLA	C1D-ND-C4D	-5.88	102.16	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	705	CLA	C1D-ND-C4D	-5.88	102.16	106.33
27	C	201	CLA	C4A-NA-C1A	-5.88	104.06	106.71
27	B	605	CLA	C1D-ND-C4D	-5.88	102.16	106.33
27	I	608	CLA	C1D-ND-C4D	-5.88	102.16	106.33
27	b	701	CLA	C1D-ND-C4D	-5.88	102.16	106.33
27	a	829	CLA	C1D-ND-C4D	-5.87	102.16	106.33
27	D	602	CLA	C1D-ND-C4D	-5.87	102.16	106.33
27	B	603	CLA	C1D-ND-C4D	-5.87	102.16	106.33
27	b	704	CLA	C1D-ND-C4D	-5.87	102.17	106.33
27	b	724	CLA	C1D-ND-C4D	-5.87	102.17	106.33
27	l	406	CLA	C1D-ND-C4D	-5.87	102.17	106.33
27	b	710	CLA	C1D-ND-C4D	-5.86	102.17	106.33
27	H	306	CLA	C1D-ND-C4D	-5.86	102.17	106.33
27	T	606	CLA	C1D-ND-C4D	-5.86	102.17	106.33
27	F	606	CLA	C1D-ND-C4D	-5.86	102.17	106.33
27	K	605	CLA	C1D-ND-C4D	-5.86	102.17	106.33
27	H	310	CLA	C1D-ND-C4D	-5.86	102.17	106.33
27	F	617	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	B	609	CLA	C1D-ND-C4D	-5.85	102.18	106.33
32	J	611	PID	O3-C10-C9	-5.85	124.08	130.74
27	b	714	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	l	405	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	E	608	CLA	C4A-NA-C1A	-5.85	104.08	106.71
27	F	604	CLA	C1D-ND-C4D	-5.84	102.18	106.33
27	a	804	CLA	C1D-ND-C4D	-5.84	102.19	106.33
27	I	605	CLA	C1D-ND-C4D	-5.83	102.19	106.33
27	a	811	CLA	C4A-NA-C1A	-5.83	104.08	106.71
27	a	837	CLA	C1D-ND-C4D	-5.83	102.19	106.33
27	J	605	CLA	C1D-ND-C4D	-5.82	102.20	106.33
27	b	727	CLA	C1D-ND-C4D	-5.82	102.20	106.33
27	A	612	CLA	C1D-ND-C4D	-5.82	102.20	106.33
27	a	819	CLA	C1D-ND-C4D	-5.81	102.20	106.33
27	a	827	CLA	C1D-ND-C4D	-5.81	102.21	106.33
27	C	205	CLA	C1D-ND-C4D	-5.81	102.21	106.33
27	D	607	CLA	C1D-ND-C4D	-5.81	102.21	106.33
27	B	604	CLA	C4A-NA-C1A	-5.81	104.10	106.71
27	b	722	CLA	C4A-NA-C1A	-5.81	104.10	106.71
27	I	616	CLA	C1D-ND-C4D	-5.80	102.21	106.33
27	H	308	CLA	C1D-ND-C4D	-5.80	102.21	106.33
27	l	407	CLA	C1D-ND-C4D	-5.80	102.22	106.33
27	b	706	CLA	C1D-ND-C4D	-5.80	102.22	106.33
27	a	837	CLA	C4A-NA-C1A	-5.79	104.10	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	610	CLA	C4A-NA-C1A	-5.78	104.11	106.71
27	I	602	CLA	C1D-ND-C4D	-5.78	102.23	106.33
27	a	811	CLA	C1D-ND-C4D	-5.77	102.23	106.33
27	a	823	CLA	C1D-ND-C4D	-5.76	102.24	106.33
27	a	820	CLA	C1D-ND-C4D	-5.76	102.24	106.33
27	b	720	CLA	C4A-NA-C1A	-5.75	104.12	106.71
27	F	602	CLA	C1D-ND-C4D	-5.74	102.26	106.33
27	H	305	CLA	C1D-ND-C4D	-5.74	102.26	106.33
27	G	605	CLA	C1D-ND-C4D	-5.73	102.26	106.33
27	E	605	CLA	C1D-ND-C4D	-5.72	102.27	106.33
27	D	603	CLA	C4A-NA-C1A	-5.71	104.14	106.71
29	C	215	UIX	O-C1-C3	-5.71	109.09	113.38
27	D	607	CLA	C4A-NA-C1A	-5.71	104.14	106.71
27	A	602	CLA	C4A-NA-C1A	-5.70	104.14	106.71
27	F	605	CLA	C4A-NA-C1A	-5.69	104.15	106.71
27	b	717	CLA	C1D-ND-C4D	-5.69	102.30	106.33
27	b	709	CLA	C1D-ND-C4D	-5.68	102.30	106.33
32	J	611	PID	O1-C1-CM1	5.67	121.85	115.06
27	U	605	CLA	C1D-ND-C4D	-5.67	102.31	106.33
27	a	809	CLA	C1D-ND-C4D	-5.67	102.31	106.33
27	F	617	CLA	C4A-NA-C1A	-5.66	104.16	106.71
27	C	203	CLA	C4A-NA-C1A	-5.66	104.16	106.71
27	l	411	CLA	C4A-NA-C1A	-5.66	104.16	106.71
32	F	615	PID	O3-C10-C9	-5.65	124.30	130.74
27	D	605	CLA	C1D-ND-C4D	-5.65	102.32	106.33
27	a	812	CLA	C1D-ND-C4D	-5.65	102.32	106.33
27	T	605	CLA	C1D-ND-C4D	-5.65	102.32	106.33
27	a	803	CLA	C4A-NA-C1A	-5.65	104.17	106.71
27	a	818	CLA	C1D-ND-C4D	-5.63	102.33	106.33
27	K	601	CLA	C4A-NA-C1A	-5.62	104.18	106.71
27	C	207	CLA	C1D-ND-C4D	-5.62	102.35	106.33
27	I	606	CLA	C4A-NA-C1A	-5.61	104.19	106.71
27	b	718	CLA	C1D-ND-C4D	-5.60	102.36	106.33
27	j	202	CLA	C1D-ND-C4D	-5.60	102.36	106.33
27	l	402	CLA	C4A-NA-C1A	-5.59	104.19	106.71
32	K	611	PID	O1-C1-CM1	5.59	121.75	115.06
27	H	304	CLA	C1D-ND-C4D	-5.57	102.38	106.33
32	J	613	PID	O3-C10-C9	-5.57	124.40	130.74
27	b	721	CLA	C4A-NA-C1A	-5.57	104.20	106.71
27	F	606	CLA	C4A-NA-C1A	-5.57	104.20	106.71
27	A	605	CLA	C4A-NA-C1A	-5.56	104.21	106.71
27	F	602	CLA	C4A-NA-C1A	-5.56	104.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	404	CLA	C1D-ND-C4D	-5.56	102.39	106.33
29	I	612	UIX	C6-C1-C3	5.56	120.53	114.28
27	H	319	CLA	C4A-NA-C1A	-5.55	104.21	106.71
27	a	826	CLA	C1D-ND-C4D	-5.55	102.39	106.33
29	G	615	UIX	C6-C1-C3	5.54	120.52	114.28
27	a	806	CLA	C4A-NA-C1A	-5.54	104.21	106.71
27	l	407	CLA	C4A-NA-C1A	-5.54	104.22	106.71
27	l	405	CLA	C4A-NA-C1A	-5.54	104.22	106.71
32	J	611	PID	C11-C12-C13	-5.52	116.14	128.34
27	a	829	CLA	C4A-NA-C1A	-5.51	104.23	106.71
27	a	805	CLA	C4A-NA-C1A	-5.50	104.23	106.71
27	A	603	CLA	C4A-NA-C1A	-5.49	104.24	106.71
27	b	724	CLA	C4A-NA-C1A	-5.47	104.25	106.71
27	H	306	CLA	C4A-NA-C1A	-5.47	104.25	106.71
27	A	611	CLA	C4A-NA-C1A	-5.46	104.25	106.71
27	C	202	CLA	C4A-NA-C1A	-5.46	104.25	106.71
32	I	614	PID	O1-C1-CM1	5.45	121.58	115.06
27	f	303	CLA	C4A-NA-C1A	-5.45	104.26	106.71
27	l	409	CLA	C4A-NA-C1A	-5.44	104.26	106.71
27	b	708	CLA	C1D-ND-C4D	-5.44	102.47	106.33
27	J	603	CLA	C4A-NA-C1A	-5.44	104.26	106.71
27	D	608	CLA	C4A-NA-C1A	-5.44	104.26	106.71
27	a	801	CLA	CHD-C1D-ND	-5.42	119.47	124.45
27	a	825	CLA	C4A-NA-C1A	-5.41	104.27	106.71
27	f	303	CLA	C1D-ND-C4D	-5.41	102.49	106.33
27	F	607	CLA	C4A-NA-C1A	-5.40	104.28	106.71
27	E	603	CLA	C4A-NA-C1A	-5.39	104.28	106.71
27	K	603	CLA	C4A-NA-C1A	-5.39	104.28	106.71
27	B	601	CLA	C4A-NA-C1A	-5.39	104.28	106.71
27	a	815	CLA	C4A-NA-C1A	-5.38	104.29	106.71
27	F	601	CLA	C4A-NA-C1A	-5.37	104.29	106.71
27	U	603	CLA	C4A-NA-C1A	-5.37	104.29	106.71
27	b	723	CLA	C4A-NA-C1A	-5.36	104.30	106.71
27	a	816	CLA	C4A-NA-C1A	-5.36	104.30	106.71
27	D	609	CLA	C4A-NA-C1A	-5.35	104.30	106.71
27	E	602	CLA	C4A-NA-C1A	-5.35	104.30	106.71
32	K	611	PID	CM1-C1-C6	-5.34	113.31	122.26
27	a	802	CLA	C1D-ND-C4D	-5.33	102.55	106.33
27	a	814	CLA	C4A-NA-C1A	-5.32	104.31	106.71
27	E	607	CLA	C1D-ND-C4D	-5.32	102.55	106.33
27	F	610	CLA	C4A-NA-C1A	-5.32	104.31	106.71
27	a	802	CLA	C4A-NA-C1A	-5.32	104.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	606	CLA	C4A-NA-C1A	-5.32	104.32	106.71
27	C	204	CLA	C4A-NA-C1A	-5.30	104.32	106.71
27	l	412	CLA	C4A-NA-C1A	-5.30	104.32	106.71
27	b	703	CLA	C1D-ND-C4D	-5.30	102.57	106.33
27	J	607	CLA	C4A-NA-C1A	-5.30	104.32	106.71
27	E	606	CLA	C4A-NA-C1A	-5.30	104.33	106.71
27	H	312	CLA	C4A-NA-C1A	-5.29	104.33	106.71
27	F	604	CLA	C4A-NA-C1A	-5.29	104.33	106.71
27	G	609	CLA	C4A-NA-C1A	-5.28	104.33	106.71
27	C	208	CLA	C4A-NA-C1A	-5.28	104.33	106.71
27	b	701	CLA	C4A-NA-C1A	-5.28	104.33	106.71
27	a	819	CLA	C4A-NA-C1A	-5.27	104.34	106.71
32	J	615	PID	O3-C10-C9	-5.27	124.75	130.74
27	C	209	CLA	C4A-NA-C1A	-5.25	104.35	106.71
27	a	817	CLA	C4A-NA-C1A	-5.25	104.35	106.71
27	C	212	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	H	309	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	A	607	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	U	603	CLA	CHD-C1D-ND	-5.24	119.64	124.45
27	D	612	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	b	711	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	a	821	CLA	C4A-NA-C1A	-5.23	104.35	106.71
27	K	608	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	A	610	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	a	826	CLA	C4A-NA-C1A	-5.21	104.36	106.71
27	D	604	CLA	C4A-NA-C1A	-5.21	104.36	106.71
27	a	831	CLA	C4A-NA-C1A	-5.21	104.36	106.71
27	a	808	CLA	C4A-NA-C1A	-5.21	104.36	106.71
27	K	604	CLA	C4A-NA-C1A	-5.20	104.37	106.71
32	U	608	PID	O3-C10-C9	-5.20	124.82	130.74
27	H	308	CLA	C4A-NA-C1A	-5.17	104.38	106.71
27	D	606	CLA	C4A-NA-C1A	-5.17	104.38	106.71
27	G	607	CLA	CHD-C1D-ND	-5.16	119.71	124.45
27	D	610	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	G	603	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	I	603	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	G	602	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	a	822	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	A	606	CLA	C4A-NA-C1A	-5.15	104.39	106.71
29	F	613	UIX	O2-C27-C31	5.15	120.56	111.09
27	T	601	CLA	CHD-C1D-ND	-5.13	119.74	124.45
27	b	703	CLA	CHD-C1D-ND	-5.13	119.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	605	CLA	CHD-C1D-ND	-5.12	119.75	124.45
27	a	818	CLA	C4A-NA-C1A	-5.12	104.41	106.71
27	A	609	CLA	C4A-NA-C1A	-5.11	104.41	106.71
27	F	608	CLA	C4A-NA-C1A	-5.11	104.41	106.71
27	F	603	CLA	C4A-NA-C1A	-5.11	104.41	106.71
27	a	837	CLA	CHD-C1D-ND	-5.11	119.76	124.45
27	b	716	CLA	C4A-NA-C1A	-5.10	104.41	106.71
27	b	707	CLA	CHD-C1D-ND	-5.10	119.77	124.45
27	G	607	CLA	C4A-NA-C1A	-5.09	104.42	106.71
27	j	202	CLA	CHD-C1D-ND	-5.08	119.79	124.45
27	b	726	CLA	C4A-NA-C1A	-5.08	104.42	106.71
27	B	603	CLA	CHD-C1D-ND	-5.08	119.79	124.45
32	F	614	PID	CM1-C1-C6	-5.07	113.76	122.26
27	D	601	CLA	C4A-NA-C1A	-5.07	104.43	106.71
27	b	713	CLA	CHD-C1D-ND	-5.07	119.80	124.45
27	a	830	CLA	C4A-NA-C1A	-5.07	104.43	106.71
27	a	824	CLA	CHD-C1D-ND	-5.06	119.80	124.45
27	C	206	CLA	C4A-NA-C1A	-5.05	104.44	106.71
27	b	721	CLA	CHD-C1D-ND	-5.05	119.81	124.45
27	T	602	CLA	C4A-NA-C1A	-5.05	104.44	106.71
27	B	604	CLA	CHD-C1D-ND	-5.05	119.81	124.45
27	H	309	CLA	CHD-C1D-ND	-5.05	119.82	124.45
27	B	605	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	a	808	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	B	609	CLA	C4A-NA-C1A	-5.04	104.44	106.71
27	B	606	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	a	818	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	I	601	CLA	C4A-NA-C1A	-5.04	104.44	106.71
27	E	603	CLA	CHD-C1D-ND	-5.04	119.83	124.45
27	l	404	CLA	CHD-C1D-ND	-5.04	119.83	124.45
27	b	714	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	f	303	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	I	610	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	b	705	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	A	612	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	I	611	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	l	412	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	T	607	CLA	C4A-NA-C1A	-5.03	104.45	106.71
27	D	608	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	F	613	UIX	C6-C1-C3	5.02	119.93	114.28
27	D	602	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	a	824	CLA	C4A-NA-C1A	-5.02	104.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	812	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	K	608	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	A	601	CLA	C4A-NA-C1A	-5.02	104.45	106.71
27	H	307	CLA	C4A-NA-C1A	-5.02	104.45	106.71
27	a	826	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	b	715	CLA	CHD-C1D-ND	-5.01	119.85	124.45
29	D	616	UIX	O-C1-C3	-5.01	109.62	113.38
27	b	712	CLA	C4A-NA-C1A	-5.01	104.45	106.71
27	E	607	CLA	CHD-C1D-ND	-5.00	119.86	124.45
27	U	601	CLA	CHD-C1D-ND	-5.00	119.86	124.45
27	K	603	CLA	CHD-C1D-ND	-5.00	119.86	124.45
27	a	809	CLA	CHD-C1D-ND	-5.00	119.86	124.45
32	B	613	PID	O3-C10-C9	-4.99	125.06	130.74
27	I	607	CLA	C4A-NA-C1A	-4.99	104.46	106.71
27	a	829	CLA	CHD-C1D-ND	-4.99	119.87	124.45
27	b	719	CLA	CHD-C1D-ND	-4.98	119.87	124.45
27	l	411	CLA	CHD-C1D-ND	-4.98	119.87	124.45
27	G	604	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	I	607	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	l	406	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	a	804	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	b	711	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	G	611	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	r	203	CLA	CHD-C1D-ND	-4.98	119.88	124.45
32	F	614	PID	O3-C10-C9	-4.98	125.07	130.74
27	C	203	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	I	606	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	l	410	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	H	303	CLA	C4A-NA-C1A	-4.98	104.47	106.71
27	E	608	CLA	CHD-C1D-ND	-4.97	119.88	124.45
27	J	603	CLA	CHD-C1D-ND	-4.97	119.88	124.45
27	J	601	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	E	609	CLA	C4A-NA-C1A	-4.97	104.47	106.71
27	b	706	CLA	C4A-NA-C1A	-4.97	104.47	106.71
27	F	610	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	E	605	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	F	619	CLA	C4A-NA-C1A	-4.97	104.47	106.71
29	j	204	UIX	C6-C1-C3	4.97	119.87	114.28
27	b	712	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	U	606	CLA	C4A-NA-C1A	-4.97	104.47	106.71
27	F	607	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	K	601	CLA	CHD-C1D-ND	-4.96	119.89	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	828	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	b	718	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	a	823	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	C	212	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	a	803	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	E	604	CLA	CHD-C1D-ND	-4.95	119.90	124.45
27	a	816	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	b	716	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	E	602	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	I	609	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	T	607	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	b	722	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	K	606	CLA	CHD-C1D-ND	-4.94	119.92	124.45
27	T	606	CLA	CHD-C1D-ND	-4.94	119.92	124.45
27	A	602	CLA	CHD-C1D-ND	-4.94	119.92	124.45
27	H	304	CLA	C4A-NA-C1A	-4.94	104.49	106.71
29	A	616	UIX	C6-C1-C3	4.94	119.83	114.28
27	A	610	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	D	612	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	a	807	CLA	C4A-NA-C1A	-4.93	104.49	106.71
27	T	609	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	U	605	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	H	313	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	a	839	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	a	820	CLA	C4A-NA-C1A	-4.92	104.49	106.71
27	b	704	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	G	608	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	l	407	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	l	408	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	G	606	CLA	C4A-NA-C1A	-4.92	104.50	106.71
27	b	709	CLA	C4A-NA-C1A	-4.91	104.50	106.71
27	a	802	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	T	604	CLA	C4A-NA-C1A	-4.91	104.50	106.71
27	C	209	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	D	603	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	C	202	CLA	CHD-C1D-ND	-4.91	119.95	124.45
27	l	403	CLA	C4A-NA-C1A	-4.90	104.50	106.71
27	a	810	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	a	811	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	A	605	CLA	CHD-C1D-ND	-4.90	119.95	124.45
32	J	614	PID	O3-C10-C9	-4.90	125.17	130.74
27	U	606	CLA	CHD-C1D-ND	-4.90	119.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	611	CLA	C4A-NA-C1A	-4.89	104.51	106.71
27	D	611	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	J	605	CLA	CHD-C1D-ND	-4.89	119.96	124.45
38	a	836	BCR	C15-C14-C13	-4.89	120.33	127.31
27	C	205	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	H	310	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	a	820	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	b	717	CLA	C4A-NA-C1A	-4.89	104.51	106.71
27	C	208	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	H	303	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	A	611	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	T	605	CLA	C4A-NA-C1A	-4.88	104.51	106.71
27	a	807	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	l	402	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	J	609	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	b	710	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	E	607	CLA	C4A-NA-C1A	-4.88	104.51	106.71
27	F	617	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	I	601	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	b	728	CLA	C4A-NA-C1A	-4.88	104.51	106.71
27	D	609	CLA	CHD-C1D-ND	-4.87	119.98	124.45
27	T	603	CLA	C4A-NA-C1A	-4.87	104.52	106.71
29	D	616	UIX	C14-C13-C11	-4.87	120.36	127.31
27	I	608	CLA	C4A-NA-C1A	-4.86	104.52	106.71
27	E	609	CLA	CHD-C1D-ND	-4.86	119.98	124.45
27	F	619	CLA	CHD-C1D-ND	-4.86	119.98	124.45
27	K	602	CLA	C4A-NA-C1A	-4.86	104.52	106.71
27	b	702	CLA	C1D-ND-C4D	-4.86	102.88	106.33
27	C	204	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	l	405	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	F	601	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	b	727	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	B	609	CLA	CHD-C1D-ND	-4.85	119.99	124.45
27	D	607	CLA	CHD-C1D-ND	-4.85	119.99	124.45
27	H	319	CLA	CHD-C1D-ND	-4.85	119.99	124.45
27	A	606	CLA	CHD-C1D-ND	-4.85	120.00	124.45
27	a	821	CLA	CHD-C1D-ND	-4.85	120.00	124.45
32	U	608	PID	O6-C30-C31	4.85	120.01	111.09
27	b	701	CLA	CHD-C1D-ND	-4.85	120.00	124.45
27	B	601	CLA	CHD-C1D-ND	-4.84	120.00	124.45
27	r	204	CLA	C4A-NA-C1A	-4.84	104.53	106.71
27	J	607	CLA	CHD-C1D-ND	-4.84	120.01	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	724	CLA	CHD-C1D-ND	-4.84	120.01	124.45
27	b	720	CLA	CHD-C1D-ND	-4.84	120.01	124.45
27	b	726	CLA	CHD-C1D-ND	-4.84	120.01	124.45
27	F	602	CLA	CHD-C1D-ND	-4.83	120.01	124.45
27	A	604	CLA	CHD-C1D-ND	-4.83	120.01	124.45
27	A	601	CLA	CHD-C1D-ND	-4.83	120.01	124.45
27	E	612	CLA	CHD-C1D-ND	-4.83	120.02	124.45
32	F	615	PID	O6-C30-C31	4.83	119.97	111.09
27	C	207	CLA	CHD-C1D-ND	-4.83	120.02	124.45
27	G	602	CLA	CHD-C1D-ND	-4.83	120.02	124.45
27	A	603	CLA	CHD-C1D-ND	-4.83	120.02	124.45
27	E	606	CLA	CHD-C1D-ND	-4.82	120.02	124.45
27	F	608	CLA	CHD-C1D-ND	-4.82	120.02	124.45
27	H	305	CLA	CHD-C1D-ND	-4.81	120.03	124.45
27	C	201	CLA	CHD-C1D-ND	-4.81	120.04	124.45
27	G	610	CLA	CHD-C1D-ND	-4.81	120.04	124.45
27	a	806	CLA	CHD-C1D-ND	-4.81	120.04	124.45
27	b	723	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	a	819	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	a	814	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	K	602	CLA	CHD-C1D-ND	-4.80	120.05	124.45
27	a	805	CLA	CHD-C1D-ND	-4.80	120.05	124.45
27	a	825	CLA	CHD-C1D-ND	-4.80	120.05	124.45
27	b	706	CLA	CHD-C1D-ND	-4.79	120.05	124.45
27	E	611	CLA	CHD-C1D-ND	-4.79	120.05	124.45
27	a	815	CLA	CHD-C1D-ND	-4.79	120.05	124.45
27	C	211	CLA	CHD-C1D-ND	-4.78	120.06	124.45
27	a	830	CLA	CHD-C1D-ND	-4.78	120.06	124.45
27	G	610	CLA	C4A-NA-C1A	-4.78	104.56	106.71
27	b	704	CLA	C4A-NA-C1A	-4.78	104.56	106.71
27	a	827	CLA	CHD-C1D-ND	-4.78	120.06	124.45
27	b	728	CLA	CHD-C1D-ND	-4.78	120.06	124.45
27	a	831	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	a	813	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	l	403	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	A	604	CLA	C4A-NA-C1A	-4.77	104.56	106.71
27	G	603	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	T	604	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	a	817	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	A	609	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	F	603	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	b	717	CLA	CHD-C1D-ND	-4.76	120.08	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	822	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	D	605	CLA	C4A-NA-C1A	-4.75	104.57	106.71
29	H	317	UIX	C6-C1-C3	4.75	119.62	114.28
27	f	302	CLA	C4A-NA-C1A	-4.74	104.57	106.71
27	b	702	CLA	CHD-C1D-ND	-4.74	120.09	124.45
27	A	607	CLA	CHD-C1D-ND	-4.74	120.10	124.45
27	r	204	CLA	CHD-C1D-ND	-4.74	120.10	124.45
27	I	605	CLA	CHD-C1D-ND	-4.74	120.10	124.45
32	B	613	PID	O6-C30-C31	4.73	119.80	111.09
27	G	606	CLA	CHD-C1D-ND	-4.73	120.11	124.45
27	H	313	CLA	C4A-NA-C1A	-4.73	104.58	106.71
27	b	725	CLA	C4A-NA-C1A	-4.73	104.58	106.71
27	E	612	CLA	C4A-NA-C1A	-4.72	104.58	106.71
27	H	307	CLA	CHD-C1D-ND	-4.72	120.11	124.45
27	C	206	CLA	CHD-C1D-ND	-4.72	120.12	124.45
27	f	302	CLA	CHD-C1D-ND	-4.71	120.12	124.45
27	a	810	CLA	C4A-NA-C1A	-4.71	104.59	106.71
27	I	603	CLA	CHD-C1D-ND	-4.71	120.12	124.45
27	F	606	CLA	CHD-C1D-ND	-4.71	120.13	124.45
32	J	615	PID	O6-C30-C31	4.70	119.74	111.09
27	G	609	CLA	CHD-C1D-ND	-4.70	120.14	124.45
27	H	308	CLA	CHD-C1D-ND	-4.70	120.14	124.45
27	I	602	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	T	602	CLA	CHD-C1D-ND	-4.69	120.14	124.45
27	B	610	CLA	CHD-C1D-ND	-4.69	120.14	124.45
27	B	605	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	J	605	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	F	604	CLA	CHD-C1D-ND	-4.68	120.15	124.45
27	H	306	CLA	CHD-C1D-ND	-4.68	120.16	124.45
27	D	605	CLA	CHD-C1D-ND	-4.68	120.16	124.45
27	I	605	CLA	C4A-NA-C1A	-4.68	104.60	106.71
27	F	605	CLA	CHD-C1D-ND	-4.67	120.16	124.45
27	I	616	CLA	CHD-C1D-ND	-4.67	120.17	124.45
27	T	603	CLA	CHD-C1D-ND	-4.66	120.17	124.45
38	a	836	BCR	C11-C10-C9	-4.66	120.66	127.31
27	U	605	CLA	C4A-NA-C1A	-4.66	104.61	106.71
27	B	607	CLA	CHD-C1D-ND	-4.66	120.17	124.45
27	D	606	CLA	CHD-C1D-ND	-4.66	120.17	124.45
27	E	604	CLA	C4A-NA-C1A	-4.66	104.61	106.71
32	J	613	PID	C6-C7-C8	-4.65	116.15	125.99
32	J	613	PID	C8-C9-C11	-4.64	118.44	127.37
32	I	614	PID	O3-C10-C9	-4.64	125.45	130.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	836	BCR	C20-C21-C22	-4.64	120.68	127.31
27	I	602	CLA	CHD-C1D-ND	-4.64	120.19	124.45
27	D	601	CLA	CHD-C1D-ND	-4.63	120.20	124.45
27	b	709	CLA	CHD-C1D-ND	-4.63	120.20	124.45
27	a	813	CLA	C4A-NA-C1A	-4.63	104.62	106.71
32	J	615	PID	CM1-C1-C2	4.63	119.49	114.28
29	A	613	UIX	C6-C1-C3	4.62	119.48	114.28
27	D	610	CLA	CHD-C1D-ND	-4.62	120.21	124.45
27	b	725	CLA	CHD-C1D-ND	-4.61	120.22	124.45
27	C	211	CLA	C4A-NA-C1A	-4.61	104.64	106.71
27	H	304	CLA	CHD-C1D-ND	-4.60	120.23	124.45
27	B	607	CLA	C4A-NA-C1A	-4.60	104.64	106.71
27	I	608	CLA	CHD-C1D-ND	-4.58	120.25	124.45
27	K	605	CLA	CHD-C1D-ND	-4.58	120.25	124.45
29	B	615	UIX	C6-C1-C3	4.56	119.41	114.28
27	H	312	CLA	CHD-C1D-ND	-4.55	120.27	124.45
27	l	409	CLA	CHD-C1D-ND	-4.55	120.27	124.45
29	H	314	UIX	O2-C27-C31	4.55	119.46	111.09
32	I	614	PID	O6-C30-C31	4.54	119.44	111.09
29	C	213	UIX	C6-C1-C3	4.53	119.37	114.28
32	F	614	PID	O6-C30-C31	4.52	119.41	111.09
29	G	615	UIX	O2-C27-C31	4.52	119.40	111.09
29	B	615	UIX	O2-C27-C31	4.51	119.39	111.09
27	K	604	CLA	CHD-C1D-ND	-4.50	120.31	124.45
29	A	616	UIX	O2-C27-C31	4.50	119.36	111.09
27	b	703	CLA	C4A-NA-C1A	-4.50	104.69	106.71
27	b	708	CLA	CHD-C1D-ND	-4.50	120.32	124.45
27	l	406	CLA	C4A-NA-C1A	-4.48	104.69	106.71
27	D	611	CLA	C4A-NA-C1A	-4.48	104.69	106.71
29	A	613	UIX	O2-C27-C31	4.48	119.33	111.09
27	b	708	CLA	C4A-NA-C1A	-4.48	104.69	106.71
29	I	612	UIX	O2-C27-C31	4.47	119.32	111.09
27	j	202	CLA	C4A-NA-C1A	-4.47	104.69	106.71
32	J	613	PID	O6-C30-C31	4.46	119.29	111.09
38	a	836	BCR	C24-C23-C22	-4.45	119.51	126.23
29	j	204	UIX	O2-C27-C31	4.45	119.27	111.09
29	C	213	UIX	O2-C27-C31	4.43	119.25	111.09
29	E	616	UIX	O2-C27-C31	4.43	119.25	111.09
29	H	314	UIX	C6-C1-C3	4.43	119.27	114.28
27	D	604	CLA	CHD-C1D-ND	-4.43	120.38	124.45
29	C	215	UIX	O2-C27-C31	4.43	119.23	111.09
27	b	719	CLA	C4A-NA-C1A	-4.42	104.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	616	UIX	O2-C27-C31	4.41	119.21	111.09
32	J	611	PID	O6-C30-C31	4.41	119.20	111.09
27	T	605	CLA	CHD-C1D-ND	-4.38	120.43	124.45
29	T	612	UIX	O2-C27-C31	4.37	119.12	111.09
32	K	611	PID	O6-C30-C31	4.36	119.11	111.09
35	f	305	DGD	O3G-C3G-C2G	-4.36	100.39	110.90
29	J	616	UIX	O2-C27-C31	4.34	119.08	111.09
27	a	801	CLA	C1D-ND-C4D	-4.34	103.25	106.33
32	J	613	PID	O1-C1-CM1	4.34	120.25	115.06
29	H	317	UIX	O2-C27-C31	4.33	119.06	111.09
27	a	839	CLA	C4A-NA-C1A	-4.27	104.79	106.71
38	a	836	BCR	C16-C17-C18	-4.27	121.22	127.31
30	i	202	DD6	O1-C20-C19	-4.26	110.18	113.38
38	a	836	BCR	C33-C5-C6	-4.26	119.74	124.53
29	F	613	UIX	O-C1-C3	-4.26	110.18	113.38
29	J	616	UIX	O-C1-C3	-4.25	110.19	113.38
32	J	611	PID	C8-C9-C11	-4.25	119.20	127.37
27	I	616	CLA	C4A-NA-C1A	-4.24	104.80	106.71
29	B	611	UIX	O2-C27-C31	4.23	118.87	111.09
32	F	614	PID	C11-C12-C13	-4.23	118.99	128.34
29	D	616	UIX	C6-C1-C3	4.22	119.03	114.28
35	K	614	DGD	O3G-C3G-C2G	-4.21	100.74	110.90
35	j	201	DGD	O3G-C3G-C2G	-4.17	100.84	110.90
29	G	615	UIX	C14-C13-C11	-4.15	121.39	127.31
32	F	615	PID	CM1-C1-C2	4.14	118.94	114.28
32	J	614	PID	O6-C30-C31	4.14	118.70	111.09
27	b	702	CLA	C4A-NA-C1A	-4.13	104.85	106.71
32	J	611	PID	C6-C7-C8	-4.13	117.26	125.99
32	J	615	PID	C11-C12-C13	-4.12	119.22	128.34
27	G	606	CLA	CAA-C2A-C1A	-4.11	98.52	111.97
30	E	617	DD6	C14-C13-C11	4.10	131.89	125.53
29	T	612	UIX	O-C1-C3	-4.10	110.31	113.38
29	H	314	UIX	O-C1-C6	-4.08	110.17	115.06
35	l	416	DGD	O3G-C3G-C2G	-4.08	101.06	110.90
27	K	605	CLA	C4A-NA-C1A	-4.07	104.87	106.71
29	J	616	UIX	C6-C1-C3	4.06	118.85	114.28
29	I	612	UIX	O-C1-C3	-4.04	110.35	113.38
32	K	611	PID	O4-C10-C9	4.02	111.40	108.04
29	C	215	UIX	C12-C11-C10	4.02	124.41	118.08
32	U	608	PID	C19-C20-C21	-4.01	121.58	127.31
29	D	616	UIX	C34-C30-C26	-3.99	121.61	127.31
29	E	616	UIX	C34-C30-C26	-3.97	121.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	614	PID	CM1-C1-C2	3.97	118.75	114.28
27	a	801	CLA	C4A-NA-C1A	-3.97	104.92	106.71
30	B	614	DD6	O1-C20-C19	-3.95	110.41	113.38
32	I	614	PID	C19-C20-C21	-3.95	121.68	127.31
32	K	611	PID	C8-C9-C11	-3.95	119.79	127.37
32	F	615	PID	C11-C12-C13	-3.93	119.64	128.34
29	T	612	UIX	C6-C1-C3	3.93	118.70	114.28
30	r	201	DD6	C14-C13-C11	3.93	131.62	125.53
29	D	616	UIX	O-C1-C6	-3.92	110.36	115.06
32	U	608	PID	C11-C12-C13	-3.92	119.67	128.34
32	J	611	PID	C19-C20-C21	-3.91	121.72	127.31
32	B	613	PID	C11-C12-C13	-3.91	119.69	128.34
30	K	610	DD6	C14-C13-C11	3.88	131.55	125.53
29	H	317	UIX	C34-C30-C26	-3.87	121.78	127.31
29	B	611	UIX	C12-C11-C10	3.85	124.14	118.08
32	J	613	PID	C19-C20-C21	-3.82	121.86	127.31
32	F	614	PID	O4-C10-C9	3.81	111.23	108.04
27	b	703	CLA	O2A-C1-C2	3.80	118.62	108.64
29	T	612	UIX	C34-C30-C26	-3.79	121.89	127.31
32	F	615	PID	O4-C10-C9	3.78	111.20	108.04
32	K	611	PID	C19-C20-C21	-3.78	121.91	127.31
30	D	621	DD6	C14-C13-C11	3.77	131.37	125.53
30	A	615	DD6	C14-C13-C11	3.76	131.36	125.53
29	B	611	UIX	C29-C26-C23	3.74	123.97	118.08
29	B	611	UIX	C6-C1-C3	3.73	118.48	114.28
31	A	618	SQD	O47-C7-C8	3.73	119.54	111.50
31	y	301	SQD	O47-C7-C8	3.71	119.49	111.50
32	J	613	PID	O4-C10-C9	3.69	111.13	108.04
32	J	615	PID	C19-C20-C21	-3.69	122.04	127.31
29	C	215	UIX	C6-C1-C3	3.69	118.43	114.28
32	J	611	PID	O4-C10-C9	3.69	111.12	108.04
29	I	612	UIX	O-C1-C6	-3.68	110.64	115.06
32	B	613	PID	C19-C20-C21	-3.68	122.06	127.31
32	F	614	PID	C19-C20-C21	-3.65	122.10	127.31
29	T	612	UIX	C29-C26-C23	3.64	123.81	118.08
29	j	204	UIX	C34-C30-C26	-3.64	122.11	127.31
29	A	616	UIX	C12-C11-C10	3.62	123.77	118.08
29	j	204	UIX	C14-C13-C11	-3.61	122.15	127.31
32	J	615	PID	C8-C9-C11	-3.61	120.43	127.37
29	D	616	UIX	C10-C11-C13	3.61	124.48	118.94
32	B	613	PID	O4-C10-C9	3.61	111.05	108.04
32	J	614	PID	C11-C12-C13	-3.58	120.41	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	611	UIX	O-C1-C6	-3.57	110.78	115.06
32	F	614	PID	C29-C24-C25	3.57	123.24	119.70
32	J	614	PID	C16-C15-C14	-3.57	122.22	127.31
30	G	613	DD6	C14-C13-C11	3.57	131.06	125.53
29	B	615	UIX	C12-C11-C10	3.55	123.66	118.08
32	J	611	PID	C17-C16-C15	-3.54	116.23	123.47
29	C	215	UIX	C29-C26-C23	3.53	123.64	118.08
29	A	613	UIX	O-C1-C6	-3.53	110.82	115.06
38	a	836	BCR	C38-C26-C25	-3.53	120.56	124.53
29	E	616	UIX	C14-C13-C11	-3.53	122.28	127.31
29	D	616	UIX	C-C7-C10	-3.52	118.54	125.99
29	j	204	UIX	O-C1-C3	-3.52	110.73	113.38
29	T	612	UIX	C12-C11-C10	3.52	123.62	118.08
29	E	616	UIX	C12-C11-C10	3.52	123.62	118.08
30	r	205	DD6	C32-C31-C36	-3.51	117.67	122.63
32	K	611	PID	O3-C10-C9	-3.50	126.75	130.74
29	G	615	UIX	C34-C30-C26	-3.50	122.31	127.31
30	G	612	DD6	C14-C13-C11	3.50	130.96	125.53
29	A	613	UIX	C29-C26-C23	3.50	123.58	118.08
32	I	614	PID	O4-C10-C9	3.49	110.96	108.04
32	J	615	PID	O4-C10-C9	3.49	110.95	108.04
30	G	612	DD6	C32-C31-C36	-3.49	117.71	122.63
29	H	317	UIX	C12-C11-C10	3.48	123.56	118.08
29	j	204	UIX	C41-C40-C38	3.48	123.56	118.08
30	r	206	DD6	C14-C13-C11	3.47	130.91	125.53
29	I	612	UIX	C34-C37-C39	-3.46	116.38	123.47
29	I	612	UIX	C41-C40-C38	3.46	123.53	118.08
29	A	616	UIX	C34-C30-C26	-3.46	122.37	127.31
32	U	608	PID	C8-C9-C11	-3.46	120.72	127.37
29	H	317	UIX	O-C1-C6	-3.45	110.92	115.06
29	I	612	UIX	C14-C13-C11	-3.45	122.39	127.31
29	G	615	UIX	C36-C35-C32	-3.45	122.39	127.31
35	j	201	DGD	O6D-C1D-O3G	-3.44	101.82	109.97
32	B	613	PID	C16-C15-C14	-3.44	122.40	127.31
30	C	216	DD6	C14-C13-C11	3.44	130.87	125.53
32	B	613	PID	CM1-C1-C2	3.44	118.15	114.28
27	U	603	CLA	C1-C2-C3	-3.44	121.19	126.75
29	F	613	UIX	C34-C30-C26	-3.44	122.41	127.31
32	J	613	PID	C27-O6-C30	-3.44	111.49	117.90
29	B	611	UIX	C-C7-C10	-3.43	118.73	125.99
29	H	314	UIX	C29-C26-C23	3.43	123.48	118.08
32	J	614	PID	O4-C10-C9	3.43	110.91	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	213	UIX	C12-C11-C10	3.43	123.48	118.08
29	B	615	UIX	C29-C26-C23	3.42	123.47	118.08
30	F	611	DD6	O1-C20-C19	-3.42	110.81	113.38
29	J	616	UIX	O-C1-C6	-3.42	110.96	115.06
29	C	213	UIX	C29-C26-C23	3.42	123.47	118.08
29	I	612	UIX	C34-C30-C26	-3.42	122.43	127.31
29	J	616	UIX	C12-C11-C10	3.42	123.46	118.08
38	a	836	BCR	C38-C26-C27	3.41	120.17	113.62
29	C	213	UIX	C34-C30-C26	-3.41	122.45	127.31
29	F	613	UIX	C29-C26-C23	3.40	123.44	118.08
32	K	611	PID	C27-O6-C30	-3.40	111.55	117.90
29	H	314	UIX	C12-C11-C10	3.38	123.40	118.08
32	U	608	PID	O4-C10-C9	3.38	110.86	108.04
30	E	613	DD6	C14-C13-C11	3.36	130.74	125.53
29	j	204	UIX	C29-C26-C23	3.35	123.35	118.08
29	T	612	UIX	C18-O2-C27	-3.35	111.66	117.90
29	J	616	UIX	C14-C13-C11	-3.35	122.54	127.31
29	C	215	UIX	C34-C30-C26	-3.34	122.54	127.31
32	U	608	PID	C6-C7-C8	-3.34	118.94	125.99
30	H	318	DD6	C32-C31-C36	-3.34	117.92	122.63
35	f	305	DGD	O6D-C1D-O3G	-3.34	102.07	109.97
29	I	612	UIX	C38-C40-C39	-3.33	113.83	118.94
29	T	612	UIX	C14-C13-C11	-3.32	122.57	127.31
32	F	615	PID	C19-C20-C21	-3.32	122.58	127.31
30	D	613	DD6	O1-C20-C19	-3.32	110.89	113.38
29	A	616	UIX	C29-C26-C23	3.32	123.30	118.08
29	G	615	UIX	C29-C26-C23	3.31	123.28	118.08
32	F	614	PID	C8-C9-C11	-3.28	121.07	127.37
32	I	614	PID	C6-C7-C8	-3.25	119.12	125.99
32	I	614	PID	C11-C12-C13	-3.24	121.18	128.34
29	H	314	UIX	C34-C30-C26	-3.23	122.69	127.31
30	r	201	DD6	O1-C20-C19	-3.23	110.95	113.38
29	F	613	UIX	C12-C11-C10	3.23	123.16	118.08
29	E	616	UIX	C34-C37-C39	-3.22	116.87	123.47
32	I	614	PID	C27-O6-C30	-3.21	111.91	117.90
29	j	204	UIX	C37-C39-C40	-3.21	122.73	127.31
29	H	317	UIX	C14-C13-C11	-3.20	122.75	127.31
38	i	201	BCR	C24-C23-C22	-3.19	121.42	126.23
29	J	616	UIX	C36-C35-C32	-3.19	122.76	127.31
29	H	314	UIX	C-C7-C10	-3.18	119.27	125.99
27	a	804	CLA	O2A-C1-C2	3.17	116.97	108.64
30	A	614	DD6	O1-C20-C19	-3.16	111.01	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	828	CLA	C3D-C4D-ND	3.16	115.34	110.24
29	D	616	UIX	C29-C26-C23	3.15	123.04	118.08
31	A	618	SQD	O9-S-C6	3.15	110.68	106.94
27	b	715	CLA	C3D-C4D-ND	3.14	115.32	110.24
31	y	301	SQD	O7-S-C6	3.14	110.67	106.94
29	A	613	UIX	O-C1-C3	-3.14	111.03	113.38
29	C	213	UIX	C14-C13-C11	-3.13	122.84	127.31
27	G	607	CLA	C3D-C4D-ND	3.13	115.30	110.24
30	D	615	DD6	C14-C13-C11	3.13	130.38	125.53
32	J	614	PID	C18-C17-C16	-3.12	117.87	124.81
29	A	613	UIX	C-C7-C10	-3.12	119.40	125.99
29	H	317	UIX	C-C7-C10	-3.11	119.43	125.99
32	B	613	PID	O1-C1-CM1	-3.10	111.34	115.06
29	H	317	UIX	C29-C26-C23	3.10	122.96	118.08
27	a	837	CLA	C3D-C4D-ND	3.10	115.25	110.24
27	K	603	CLA	C3D-C4D-ND	3.09	115.24	110.24
27	a	803	CLA	C3D-C4D-ND	3.08	115.22	110.24
27	D	604	CLA	C1-C2-C3	-3.08	120.71	126.04
29	A	613	UIX	C12-C11-C10	3.08	122.93	118.08
29	C	213	UIX	C18-O2-C27	-3.07	112.17	117.90
29	B	611	UIX	C37-C34-C30	-3.07	117.19	123.47
27	b	703	CLA	C1-C2-C3	-3.07	120.74	126.04
27	b	712	CLA	CAA-C2A-C1A	-3.06	101.96	111.97
32	F	615	PID	C8-C9-C11	-3.05	121.50	127.37
27	D	608	CLA	C3D-C4D-ND	3.04	115.16	110.24
27	G	604	CLA	C3D-C4D-ND	3.04	115.16	110.24
27	B	606	CLA	C3D-C4D-ND	3.04	115.15	110.24
29	A	616	UIX	C38-C40-C39	-3.03	114.29	118.94
29	D	616	UIX	C34-C37-C39	-3.02	117.28	123.47
35	K	614	DGD	O6D-C1D-O3G	-3.02	102.82	109.97
29	D	616	UIX	C29-C26-C30	-3.02	118.69	122.92
27	I	606	CLA	C3D-C4D-ND	3.02	115.12	110.24
32	B	613	PID	C27-O6-C30	-3.01	112.28	117.90
27	b	713	CLA	C3D-C4D-ND	3.01	115.11	110.24
27	I	607	CLA	C3D-C4D-ND	3.01	115.11	110.24
30	F	611	DD6	C32-C31-C36	-3.01	118.38	122.63
27	H	309	CLA	C3D-C4D-ND	3.01	115.11	110.24
29	I	612	UIX	C18-O2-C27	-3.01	112.29	117.90
27	a	807	CLA	CAA-C2A-C1A	-3.01	102.12	111.97
27	B	604	CLA	C3D-C4D-ND	3.01	115.10	110.24
27	b	723	CLA	C3D-C4D-ND	3.00	115.10	110.24
32	J	611	PID	C17-C18-C19	-3.00	118.13	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	I	603	CLA	C3D-C4D-ND	3.00	115.09	110.24
27	l	402	CLA	C3D-C4D-ND	3.00	115.09	110.24
27	C	209	CLA	C3D-C4D-ND	3.00	115.08	110.24
27	T	602	CLA	C3D-C4D-ND	2.99	115.08	110.24
27	b	716	CLA	C3D-C4D-ND	2.99	115.07	110.24
27	E	606	CLA	C3D-C4D-ND	2.98	115.06	110.24
27	I	611	CLA	C3D-C4D-ND	2.98	115.06	110.24
27	I	603	CLA	C1-C2-C3	-2.98	120.89	126.04
27	b	707	CLA	C3D-C4D-ND	2.98	115.05	110.24
27	A	602	CLA	C3D-C4D-ND	2.97	115.05	110.24
27	A	601	CLA	C3D-C4D-ND	2.97	115.04	110.24
32	F	615	PID	O1-C1-C2	-2.97	111.15	113.38
27	b	712	CLA	C3D-C4D-ND	2.97	115.04	110.24
27	F	607	CLA	C3D-C4D-ND	2.96	115.03	110.24
27	F	610	CLA	C3D-C4D-ND	2.96	115.03	110.24
27	r	203	CLA	C3D-C4D-ND	2.96	115.03	110.24
27	b	715	CLA	CAA-C2A-C1A	-2.96	102.27	111.97
27	D	604	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	b	711	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	U	601	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	H	313	CLA	C3D-C4D-ND	2.95	115.02	110.24
27	C	204	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	G	608	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	C	203	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	D	603	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	F	605	CLA	C3D-C4D-ND	2.95	115.01	110.24
29	F	613	UIX	C-C7-C10	-2.95	119.76	125.99
27	C	202	CLA	C3D-C4D-ND	2.95	115.00	110.24
28	A	608	KC2	CHB-C4A-NA	2.94	128.84	124.20
27	T	604	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	C	212	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	D	612	CLA	C3D-C4D-ND	2.94	114.99	110.24
38	a	836	BCR	C8-C7-C6	-2.93	118.96	127.20
27	U	603	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	a	824	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
27	J	603	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	a	813	CLA	C3D-C4D-ND	2.93	114.98	110.24
32	J	611	PID	CM1-C1-C2	2.93	117.58	114.28
27	A	611	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	G	602	CLA	C3D-C4D-ND	2.93	114.97	110.24
29	I	612	UIX	C12-C11-C10	2.93	122.69	118.08
27	D	609	CLA	C3D-C4D-ND	2.93	114.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	E	602	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	F	608	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	b	719	CLA	C3D-C4D-ND	2.93	114.97	110.24
29	B	615	UIX	C34-C30-C26	-2.93	123.13	127.31
28	J	606	KC2	CHB-C1B-NB	2.92	127.14	124.45
29	j	204	UIX	C-C7-C10	-2.92	119.81	125.99
27	l	410	CLA	C3D-C4D-ND	2.92	114.97	110.24
29	A	616	UIX	C34-C37-C39	-2.92	117.49	123.47
27	F	603	CLA	C3D-C4D-ND	2.92	114.97	110.24
27	C	208	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	U	606	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	a	821	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	B	610	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	C	201	CLA	C3D-C4D-ND	2.92	114.96	110.24
29	C	215	UIX	C18-O2-C27	-2.92	112.46	117.90
27	I	609	CLA	C3D-C4D-ND	2.92	114.95	110.24
32	B	613	PID	C8-C9-C11	-2.91	121.77	127.37
27	B	601	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	E	604	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	A	606	CLA	C3D-C4D-ND	2.91	114.95	110.24
29	G	615	UIX	C-C7-C10	-2.91	119.84	125.99
27	A	604	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	H	312	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	A	607	CLA	C3D-C4D-ND	2.91	114.94	110.24
32	J	613	PID	C17-C16-C15	-2.91	117.51	123.47
27	K	606	CLA	C3D-C4D-ND	2.91	114.94	110.24
29	C	213	UIX	C-C7-C10	-2.91	119.84	125.99
27	b	722	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	a	825	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	A	609	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	B	607	CLA	C2C-C1C-NC	2.90	112.69	109.97
27	K	601	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	a	806	CLA	C3D-C4D-ND	2.90	114.93	110.24
35	f	305	DGD	O6E-C5E-C4E	2.90	114.97	109.69
27	E	612	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	I	601	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	H	319	CLA	C3D-C4D-ND	2.90	114.93	110.24
29	B	615	UIX	C14-C13-C11	-2.90	123.18	127.31
27	a	816	CLA	C3D-C4D-ND	2.89	114.92	110.24
27	B	605	CLA	C3D-C4D-ND	2.89	114.92	110.24
27	A	612	CLA	C3D-C4D-ND	2.89	114.92	110.24
27	b	721	CLA	C3D-C4D-ND	2.89	114.91	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	601	CLA	C3D-C4D-ND	2.89	114.91	110.24
27	J	609	CLA	C3D-C4D-ND	2.89	114.91	110.24
27	J	607	CLA	C3D-C4D-ND	2.89	114.91	110.24
29	B	611	UIX	C34-C30-C26	-2.89	123.19	127.31
29	A	616	UIX	C6-C1-C	-2.89	117.42	122.26
27	G	606	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	T	609	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	D	607	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	a	814	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	I	610	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	a	807	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	I	614	PID	C8-C9-C11	-2.88	121.84	127.37
27	F	619	CLA	C3D-C4D-ND	2.88	114.89	110.24
28	G	601	KC2	CHB-C4A-NA	2.88	128.73	124.20
27	a	808	CLA	C3D-C4D-ND	2.87	114.89	110.24
29	G	615	UIX	C18-O2-C27	-2.87	112.54	117.90
29	D	616	UIX	C21-C15-C20	-2.87	107.90	110.47
27	F	601	CLA	C3D-C4D-ND	2.87	114.88	110.24
29	A	613	UIX	C34-C30-C26	-2.87	123.22	127.31
27	T	607	CLA	C3D-C4D-ND	2.87	114.88	110.24
27	G	611	CLA	C3D-C4D-ND	2.86	114.87	110.24
27	B	609	CLA	C3D-C4D-ND	2.86	114.86	110.24
27	a	817	CLA	C2C-C1C-NC	2.86	112.65	109.97
27	C	205	CLA	C3D-C4D-ND	2.86	114.86	110.24
27	a	824	CLA	C3D-C4D-ND	2.86	114.86	110.24
27	a	839	CLA	C3D-C4D-ND	2.86	114.86	110.24
27	A	610	CLA	C3D-C4D-ND	2.86	114.86	110.24
27	F	606	CLA	C3D-C4D-ND	2.85	114.86	110.24
27	H	310	CLA	C3D-C4D-ND	2.85	114.86	110.24
27	l	409	CLA	C3D-C4D-ND	2.85	114.86	110.24
27	a	810	CLA	C3D-C4D-ND	2.85	114.85	110.24
27	b	722	CLA	C2C-C1C-NC	2.85	112.64	109.97
29	E	616	UIX	C29-C26-C23	2.85	122.57	118.08
27	l	412	CLA	C3D-C4D-ND	2.85	114.85	110.24
29	J	616	UIX	C-C7-C10	-2.85	119.97	125.99
27	b	726	CLA	C3D-C4D-ND	2.85	114.85	110.24
27	H	306	CLA	C3D-C4D-ND	2.85	114.85	110.24
27	E	603	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	J	615	PID	C17-C16-C15	-2.85	117.64	123.47
35	l	416	DGD	O6D-C1D-O3G	-2.85	103.23	109.97
29	B	615	UIX	O-C1-C6	-2.85	111.64	115.06
27	H	303	CLA	C3D-C4D-ND	2.85	114.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	720	CLA	C3D-C4D-ND	2.85	114.84	110.24
30	I	613	DD6	C14-C13-C11	2.85	129.95	125.53
27	a	822	CLA	C3D-C4D-ND	2.85	114.84	110.24
27	l	405	CLA	C3D-C4D-ND	2.85	114.84	110.24
32	J	614	PID	C18-C19-C20	-2.85	117.64	123.47
27	A	605	CLA	C3D-C4D-ND	2.84	114.84	110.24
27	T	603	CLA	C3D-C4D-ND	2.84	114.84	110.24
27	D	611	CLA	C3D-C4D-ND	2.84	114.84	110.24
27	K	608	CLA	C3D-C4D-ND	2.84	114.84	110.24
27	l	408	CLA	C3D-C4D-ND	2.84	114.83	110.24
27	E	604	CLA	C1-C2-C3	-2.84	121.13	126.04
27	E	611	CLA	C3D-C4D-ND	2.84	114.83	110.24
29	C	215	UIX	C38-C40-C39	-2.84	114.58	118.94
27	b	724	CLA	C3D-C4D-ND	2.84	114.83	110.24
27	B	603	CLA	C3D-C4D-ND	2.84	114.83	110.24
27	a	829	CLA	C3D-C4D-ND	2.84	114.83	110.24
27	G	610	CLA	C3D-C4D-ND	2.84	114.83	110.24
30	U	607	DD6	C14-C13-C11	2.84	129.93	125.53
29	F	613	UIX	C14-C13-C11	-2.83	123.26	127.31
27	D	606	CLA	C2C-C1C-NC	2.83	112.63	109.97
27	A	603	CLA	C3D-C4D-ND	2.83	114.82	110.24
27	G	603	CLA	C3D-C4D-ND	2.83	114.82	110.24
27	b	727	CLA	C3D-C4D-ND	2.83	114.82	110.24
27	I	605	CLA	C3D-C4D-ND	2.83	114.81	110.24
27	a	805	CLA	C3D-C4D-ND	2.83	114.81	110.24
27	C	206	CLA	C3D-C4D-ND	2.83	114.81	110.24
27	H	308	CLA	C3D-C4D-ND	2.83	114.81	110.24
27	K	602	CLA	C3D-C4D-ND	2.83	114.81	110.24
27	l	403	CLA	C3D-C4D-ND	2.83	114.81	110.24
27	l	411	CLA	C3D-C4D-ND	2.83	114.81	110.24
30	A	615	DD6	C32-C31-C36	-2.82	118.65	122.63
27	K	604	CLA	C3D-C4D-ND	2.82	114.81	110.24
27	a	815	CLA	C3D-C4D-ND	2.82	114.81	110.24
27	b	728	CLA	C3D-C4D-ND	2.82	114.81	110.24
29	I	612	UIX	C22-C15-C20	-2.82	107.95	110.47
30	G	614	DD6	C32-C31-C36	-2.82	118.65	122.63
27	a	819	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	I	614	PID	CM6-C25-C24	-2.82	107.95	110.47
27	E	608	CLA	C3D-C4D-ND	2.82	114.80	110.24
30	r	205	DD6	C14-C13-C11	2.82	129.90	125.53
27	b	704	CLA	C3D-C4D-ND	2.82	114.80	110.24
27	E	609	CLA	C3D-C4D-ND	2.82	114.79	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	601	CLA	C3D-C4D-ND	2.82	114.79	110.24
27	D	606	CLA	C3D-C4D-ND	2.82	114.79	110.24
27	b	708	CLA	C2C-C1C-NC	2.81	112.61	109.97
27	b	725	CLA	C3D-C4D-ND	2.81	114.79	110.24
27	a	830	CLA	C3D-C4D-ND	2.81	114.79	110.24
27	b	714	CLA	C3D-C4D-ND	2.81	114.79	110.24
29	B	611	UIX	C21-C15-C20	-2.81	107.96	110.47
29	T	612	UIX	C-C7-C10	-2.81	120.06	125.99
27	T	606	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	C	211	CLA	C3D-C4D-ND	2.80	114.77	110.24
29	A	616	UIX	C14-C13-C11	-2.80	123.31	127.31
27	a	812	CLA	C3D-C4D-ND	2.80	114.77	110.24
27	H	307	CLA	C3D-C4D-ND	2.80	114.77	110.24
27	b	705	CLA	C3D-C4D-ND	2.80	114.77	110.24
27	b	701	CLA	C3D-C4D-ND	2.80	114.77	110.24
27	E	605	CLA	C3D-C4D-ND	2.80	114.77	110.24
30	I	613	DD6	C33-C34-C35	2.80	114.14	110.30
27	J	605	CLA	C3D-C4D-ND	2.80	114.76	110.24
35	f	305	DGD	C3D-C4D-C5D	-2.79	105.25	110.24
27	l	407	CLA	C3D-C4D-ND	2.79	114.76	110.24
27	b	710	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	F	604	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	C	207	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	b	709	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	D	602	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	H	314	UIX	C41-C40-C38	2.79	122.47	118.08
32	F	615	PID	O1-C1-CM1	-2.78	111.72	115.06
27	D	601	CLA	C3D-C4D-ND	2.78	114.74	110.24
27	r	204	CLA	C3D-C4D-ND	2.78	114.74	110.24
29	E	616	UIX	C18-O2-C27	-2.78	112.72	117.90
27	a	823	CLA	C3D-C4D-ND	2.78	114.73	110.24
27	a	809	CLA	C3D-C4D-ND	2.78	114.73	110.24
27	G	605	CLA	C3D-C4D-ND	2.78	114.73	110.24
29	C	213	UIX	O-C1-C6	-2.78	111.73	115.06
32	J	615	PID	C17-C18-C19	-2.78	118.63	124.81
32	U	608	PID	C27-O6-C30	-2.78	112.72	117.90
30	D	613	DD6	C14-C13-C11	2.77	129.83	125.53
27	l	406	CLA	C3D-C4D-ND	2.77	114.72	110.24
27	b	718	CLA	C3D-C4D-ND	2.77	114.72	110.24
29	H	314	UIX	O-C1-C3	-2.77	111.30	113.38
32	J	614	PID	C8-C9-C11	-2.77	122.05	127.37
30	r	206	DD6	O1-C20-C19	-2.77	111.30	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K	605	CLA	C3D-C4D-ND	2.77	114.72	110.24
27	a	831	CLA	C3D-C4D-ND	2.77	114.72	110.24
29	H	317	UIX	C34-C37-C39	-2.77	117.81	123.47
27	b	717	CLA	C3D-C4D-ND	2.76	114.71	110.24
32	J	614	PID	O1-C1-CM1	-2.76	111.75	115.06
27	a	817	CLA	C3D-C4D-ND	2.76	114.70	110.24
29	j	204	UIX	C38-C40-C39	-2.76	114.71	118.94
32	K	611	PID	C11-C12-C13	-2.76	122.24	128.34
27	B	607	CLA	C3D-C4D-ND	2.75	114.69	110.24
27	a	827	CLA	C3D-C4D-ND	2.75	114.69	110.24
27	l	404	CLA	C3D-C4D-ND	2.75	114.69	110.24
27	b	725	CLA	C2C-C1C-NC	2.75	112.55	109.97
29	B	615	UIX	O-C1-C3	-2.75	111.32	113.38
27	b	706	CLA	C3D-C4D-ND	2.75	114.68	110.24
35	j	201	DGD	CDB-CCB-CBB	-2.75	100.49	114.42
29	B	615	UIX	C18-O2-C27	-2.74	112.78	117.90
27	a	811	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	l	412	CLA	C2C-C1C-NC	2.74	112.54	109.97
27	I	608	CLA	C2C-C1C-NC	2.74	112.54	109.97
32	J	615	PID	C27-O6-C30	-2.74	112.79	117.90
27	a	820	CLA	C3D-C4D-ND	2.74	114.66	110.24
28	J	610	KC2	CHB-C4A-NA	2.73	128.51	124.20
27	I	602	CLA	C3D-C4D-ND	2.73	114.66	110.24
29	C	215	UIX	C-C7-C10	-2.73	120.22	125.99
29	B	615	UIX	C37-C34-C30	-2.73	117.88	123.47
29	C	215	UIX	C34-C37-C39	-2.73	117.88	123.47
27	F	602	CLA	C3D-C4D-ND	2.73	114.65	110.24
28	H	302	KC2	CHB-C4A-NA	2.73	128.50	124.20
27	F	617	CLA	C3D-C4D-ND	2.73	114.65	110.24
32	I	614	PID	C26-C25-C24	2.72	111.86	109.21
38	a	836	BCR	C30-C25-C26	-2.72	118.78	122.61
27	D	610	CLA	C3D-C4D-ND	2.72	114.64	110.24
29	A	613	UIX	C18-O2-C27	-2.72	112.82	117.90
35	K	614	DGD	O5D-C6D-C5D	-2.72	104.02	109.05
29	F	613	UIX	O2-C27-O4	-2.72	117.56	122.96
32	U	608	PID	C17-C18-C19	-2.72	118.76	124.81
29	A	616	UIX	C35-C36-C38	-2.72	114.74	123.22
27	I	605	CLA	C2C-C1C-NC	2.72	112.52	109.97
27	U	605	CLA	C3D-C4D-ND	2.72	114.63	110.24
27	a	818	CLA	C3D-C4D-ND	2.72	114.63	110.24
27	a	826	CLA	C3D-C4D-ND	2.71	114.62	110.24
27	H	305	CLA	C3D-C4D-ND	2.71	114.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	f	302	CLA	C3D-C4D-ND	2.71	114.62	110.24
27	C	206	CLA	C2C-C1C-NC	2.71	112.51	109.97
30	C	214	DD6	C14-C13-C11	2.71	129.73	125.53
29	B	611	UIX	C23-C26-C30	-2.71	114.79	118.94
27	E	606	CLA	C2C-C1C-NC	2.70	112.50	109.97
35	K	614	DGD	C6D-O5D-C1E	2.70	119.01	113.74
27	a	802	CLA	C3D-C4D-ND	2.70	114.60	110.24
27	H	307	CLA	C2C-C1C-NC	2.70	112.50	109.97
27	f	302	CLA	C2C-C1C-NC	2.70	112.50	109.97
27	a	831	CLA	C2C-C1C-NC	2.69	112.50	109.97
28	T	608	KC2	CHB-C4A-NA	2.69	128.44	124.20
31	A	618	SQD	O7-S-C6	2.69	110.14	106.94
27	G	609	CLA	C3D-C4D-ND	2.69	114.59	110.24
27	T	605	CLA	C3D-C4D-ND	2.69	114.59	110.24
29	I	612	UIX	C35-C36-C38	-2.69	114.83	123.22
29	H	314	UIX	C18-O2-C27	-2.69	112.89	117.90
29	C	215	UIX	C10-C11-C13	-2.68	114.83	118.94
28	B	608	KC2	CHB-C4A-NA	2.68	128.43	124.20
28	H	311	KC2	CHB-C4A-NA	2.68	128.43	124.20
27	I	602	CLA	C2C-C1C-NC	2.68	112.48	109.97
27	D	605	CLA	C3D-C4D-ND	2.68	114.57	110.24
29	F	613	UIX	C17-C15-C20	2.68	111.81	109.21
28	T	608	KC2	CHB-C1B-NB	2.68	126.91	124.45
29	B	615	UIX	C36-C35-C32	-2.67	123.50	127.31
29	F	613	UIX	O-C1-C6	-2.67	111.86	115.06
28	E	601	KC2	CHB-C4A-NA	2.67	128.41	124.20
30	G	614	DD6	C14-C13-C11	2.67	129.67	125.53
29	A	613	UIX	C14-C13-C11	-2.67	123.50	127.31
27	a	804	CLA	C3D-C4D-ND	2.67	114.55	110.24
29	j	204	UIX	C35-C36-C38	-2.66	114.91	123.22
27	I	608	CLA	C3D-C4D-ND	2.66	114.55	110.24
35	f	305	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
29	j	204	UIX	C34-C37-C39	-2.65	118.04	123.47
27	a	820	CLA	C2C-C1C-NC	2.65	112.46	109.97
29	T	612	UIX	C34-C37-C39	-2.65	118.05	123.47
32	B	613	PID	C29-C24-C25	2.65	122.33	119.70
32	B	613	PID	CM4-C14-C15	-2.65	119.21	122.92
35	l	416	DGD	O5D-C6D-C5D	-2.65	104.15	109.05
29	C	215	UIX	C16-C20-C15	2.65	122.32	119.70
27	I	616	CLA	C2C-C1C-NC	2.64	112.45	109.97
32	B	613	PID	C6-C7-C8	-2.64	120.41	125.99
30	H	316	DD6	C14-C13-C11	2.64	129.62	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	j	204	UIX	C6-C1-C	-2.64	117.84	122.26
29	G	615	UIX	C22-C15-C20	-2.63	108.12	110.47
27	a	801	CLA	CHA-C1A-NA	-2.63	120.37	126.40
27	j	202	CLA	C3D-C4D-ND	2.63	114.49	110.24
29	B	611	UIX	C19-C18-C17	2.63	114.46	109.88
27	U	606	CLA	C2C-C1C-NC	2.63	112.43	109.97
30	F	611	DD6	C14-C13-C11	2.63	129.61	125.53
35	K	614	DGD	C1E-O6E-C5E	2.63	118.84	113.69
28	U	604	KC2	CHB-C1B-NB	2.62	126.86	124.45
27	E	609	CLA	C2C-C1C-NC	2.62	112.43	109.97
27	b	708	CLA	C3D-C4D-ND	2.62	114.48	110.24
27	b	703	CLA	C3D-C4D-ND	2.62	114.48	110.24
27	a	805	CLA	C2C-C1C-NC	2.62	112.42	109.97
28	J	602	KC2	CHB-C1B-NB	2.62	126.86	124.45
27	I	616	CLA	C3D-C4D-ND	2.62	114.47	110.24
29	B	611	UIX	C10-C11-C13	-2.62	114.93	118.94
30	K	610	DD6	C32-C31-C36	-2.61	118.94	122.63
27	b	723	CLA	C1-C2-C3	-2.61	121.52	126.04
28	B	602	KC2	CHB-C1B-NB	2.61	126.85	124.45
28	H	311	KC2	CHB-C1B-NB	2.61	126.85	124.45
27	T	605	CLA	C2C-C1C-NC	2.61	112.41	109.97
32	K	611	PID	C18-C17-C16	-2.61	119.01	124.81
28	E	610	KC2	CHB-C4A-NA	2.60	128.31	124.20
29	C	215	UIX	C35-C36-C38	-2.60	115.09	123.22
27	E	607	CLA	C3D-C4D-ND	2.60	114.45	110.24
27	a	813	CLA	C2C-C1C-NC	2.60	112.41	109.97
28	K	607	KC2	CHB-C1B-NB	2.60	126.84	124.45
27	B	610	CLA	C2C-C1C-NC	2.60	112.41	109.97
32	F	615	PID	C6-C7-C8	-2.60	120.50	125.99
32	F	615	PID	O6-C30-O7	-2.60	117.80	122.96
27	a	810	CLA	C2C-C1C-NC	2.59	112.40	109.97
27	a	822	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	C	215	UIX	C22-C15-C20	-2.59	108.15	110.47
27	A	611	CLA	C2C-C1C-NC	2.59	112.40	109.97
27	a	808	CLA	C2C-C1C-NC	2.59	112.40	109.97
27	a	815	CLA	C2C-C1C-NC	2.59	112.40	109.97
28	C	210	KC2	CHB-C1B-NB	2.59	126.83	124.45
28	C	210	KC2	CHB-C4A-NA	2.58	128.28	124.20
27	K	602	CLA	C2C-C1C-NC	2.58	112.39	109.97
30	H	301	DD6	O1-C20-C19	-2.58	111.44	113.38
27	f	303	CLA	C3D-C4D-ND	2.58	114.41	110.24
29	H	317	UIX	C36-C35-C32	-2.58	123.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	601	CLA	C2C-C1C-NC	2.58	112.39	109.97
27	G	610	CLA	C2C-C1C-NC	2.58	112.39	109.97
27	l	405	CLA	C2C-C1C-NC	2.58	112.39	109.97
32	J	615	PID	C6-C7-C8	-2.58	120.54	125.99
28	J	608	KC2	CHB-C4A-NA	2.58	128.26	124.20
27	H	305	CLA	C1-C2-C3	-2.57	121.59	126.04
27	b	726	CLA	C2C-C1C-NC	2.57	112.38	109.97
27	F	606	CLA	C2C-C1C-NC	2.57	112.38	109.97
27	H	304	CLA	C2C-C1C-NC	2.57	112.38	109.97
27	F	608	CLA	C2C-C1C-NC	2.57	112.38	109.97
31	y	301	SQD	O48-C23-C24	2.57	119.97	111.91
28	I	604	KC2	CHB-C1B-NB	2.57	126.81	124.45
29	j	204	UIX	O-C1-C6	-2.57	111.98	115.06
30	E	613	DD6	C33-C34-C35	2.56	113.81	110.30
30	I	615	DD6	C14-C13-C11	2.56	129.50	125.53
27	l	411	CLA	C2C-C1C-NC	2.56	112.37	109.97
27	b	713	CLA	C1-C2-C3	-2.56	121.62	126.04
35	j	201	DGD	O5D-C6D-C5D	-2.56	104.31	109.05
32	K	611	PID	C16-C15-C14	-2.56	123.66	127.31
28	U	602	KC2	CHB-C4A-NA	2.55	128.23	124.20
29	H	317	UIX	O-C1-C3	-2.55	111.47	113.38
27	C	202	CLA	C2C-C1C-NC	2.55	112.36	109.97
27	T	604	CLA	C2C-C1C-NC	2.55	112.36	109.97
29	G	615	UIX	C10-C11-C13	2.55	122.85	118.94
32	U	608	PID	C17-C16-C15	-2.55	118.26	123.47
28	B	608	KC2	CHB-C1B-NB	2.55	126.79	124.45
29	B	611	UIX	O-C1-C3	-2.54	111.47	113.38
30	i	202	DD6	C21-C20-C19	2.54	117.14	114.28
27	G	609	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	F	613	UIX	C34-C37-C39	-2.54	118.27	123.47
27	b	706	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	E	601	KC2	CHB-C1B-NB	2.54	126.79	124.45
28	F	609	KC2	CHB-C1B-NB	2.54	126.79	124.45
27	C	204	CLA	C2C-C1C-NC	2.54	112.35	109.97
27	D	605	CLA	C2C-C1C-NC	2.54	112.35	109.97
27	B	609	CLA	C2C-C1C-NC	2.54	112.35	109.97
27	T	607	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	J	604	KC2	CHB-C4A-NA	2.54	128.20	124.20
29	B	615	UIX	C-C7-C10	-2.53	120.63	125.99
29	C	215	UIX	C14-C13-C11	-2.53	123.69	127.31
32	F	614	PID	O1-C1-C6	-2.53	56.87	58.96
29	E	616	UIX	C38-C40-C39	-2.53	115.06	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	603	CLA	C2C-C1C-NC	2.53	112.34	109.97
29	H	314	UIX	C38-C40-C39	-2.52	115.07	118.94
38	a	836	BCR	C7-C8-C9	-2.52	122.42	126.23
30	H	301	DD6	C14-C13-C11	2.52	129.44	125.53
28	F	609	KC2	CHB-C4A-NA	2.52	128.18	124.20
32	B	613	PID	C17-C18-C19	-2.52	119.20	124.81
29	H	314	UIX	C35-C36-C38	-2.52	115.36	123.22
27	E	612	CLA	C2C-C1C-NC	2.52	112.33	109.97
27	A	601	CLA	C2C-C1C-NC	2.52	112.33	109.97
27	a	816	CLA	C2C-C1C-NC	2.52	112.33	109.97
27	b	709	CLA	C2C-C1C-NC	2.51	112.33	109.97
30	A	615	DD6	C33-C34-C35	2.51	113.74	110.30
27	A	609	CLA	C2C-C1C-NC	2.51	112.32	109.97
27	b	719	CLA	C2C-C1C-NC	2.51	112.32	109.97
32	U	608	PID	O6-C30-O7	-2.51	117.98	122.96
28	I	604	KC2	CHB-C4A-NA	2.50	128.15	124.20
30	A	614	DD6	C14-C13-C11	2.50	129.41	125.53
27	H	312	CLA	C2C-C1C-NC	2.50	112.32	109.97
27	K	608	CLA	C2C-C1C-NC	2.50	112.31	109.97
29	j	204	UIX	C37-C34-C30	-2.50	118.35	123.47
37	b	729	PQN	C11-C3-C4	-2.50	115.83	118.50
38	a	836	BCR	C28-C27-C26	-2.50	109.62	114.08
30	D	617	DD6	C14-C13-C11	2.49	129.40	125.53
28	H	302	KC2	CHB-C1B-NB	2.49	126.75	124.45
29	I	612	UIX	C37-C39-C40	-2.49	123.75	127.31
30	r	206	DD6	C21-C20-C19	2.49	117.08	114.28
27	D	609	CLA	C2C-C1C-NC	2.49	112.30	109.97
32	B	613	PID	O6-C30-O7	-2.49	118.02	122.96
27	A	607	CLA	C2C-C1C-NC	2.49	112.30	109.97
27	r	204	CLA	C2C-C1C-NC	2.49	112.30	109.97
28	K	607	KC2	CHB-C4A-NA	2.49	128.12	124.20
29	A	613	UIX	C37-C34-C30	-2.48	118.39	123.47
27	D	610	CLA	C2C-C1C-NC	2.48	112.30	109.97
27	a	830	CLA	C1-C2-C3	-2.48	121.75	126.04
27	C	204	CLA	C1-C2-C3	-2.48	121.75	126.04
28	G	601	KC2	CHB-C1B-NB	2.48	126.73	124.45
38	a	836	BCR	C2-C1-C6	-2.48	106.66	110.48
30	K	612	DD6	C14-C13-C11	2.48	129.38	125.53
27	b	702	CLA	C2C-C1C-NC	2.48	112.30	109.97
27	a	839	CLA	C2C-C1C-NC	2.48	112.29	109.97
32	K	611	PID	O1-C1-C6	-2.48	56.91	58.96
27	D	611	CLA	C2C-C1C-NC	2.47	112.29	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	J	616	UIX	C34-C30-C26	-2.47	123.78	127.31
27	D	612	CLA	C2C-C1C-NC	2.47	112.29	109.97
28	J	610	KC2	CHB-C1B-NB	2.47	126.72	124.45
27	J	607	CLA	C2C-C1C-NC	2.47	112.28	109.97
35	l	416	DGD	C3G-C2G-C1G	-2.47	105.95	111.79
27	l	412	CLA	C1-C2-C3	-2.46	121.78	126.04
27	a	807	CLA	C2C-C1C-NC	2.46	112.28	109.97
27	F	602	CLA	C2C-C1C-NC	2.46	112.28	109.97
35	j	201	DGD	O6E-C1E-O5D	-2.46	104.15	109.97
32	B	613	PID	O1-C1-C2	-2.46	111.53	113.38
29	I	612	UIX	O2-C27-O4	-2.46	118.08	122.96
27	a	824	CLA	C2C-C1C-NC	2.46	112.28	109.97
29	B	611	UIX	C22-C15-C20	-2.46	108.27	110.47
29	C	213	UIX	C6-C1-C	-2.46	118.14	122.26
32	J	615	PID	CM7-C25-C24	-2.46	108.27	110.47
29	H	314	UIX	C34-C37-C39	-2.46	118.44	123.47
27	B	605	CLA	C2C-C1C-NC	2.46	112.27	109.97
27	C	201	CLA	C2C-C1C-NC	2.45	112.27	109.97
27	H	319	CLA	C2C-C1C-NC	2.45	112.27	109.97
28	E	610	KC2	CHB-C1B-NB	2.45	126.70	124.45
28	J	602	KC2	CHB-C4A-NA	2.45	128.06	124.20
27	B	603	CLA	C1-C2-C3	-2.44	121.81	126.04
29	F	613	UIX	C6-C1-C	-2.44	118.17	122.26
27	K	604	CLA	C2C-C1C-NC	2.44	112.26	109.97
35	f	305	DGD	O5D-C6D-C5D	-2.44	104.53	109.05
36	T	613	LMU	O1B-C4'-C3'	2.44	113.77	107.28
29	E	616	UIX	C-C7-C10	-2.44	120.84	125.99
27	A	603	CLA	C2C-C1C-NC	2.44	112.26	109.97
27	C	203	CLA	C1-C2-C3	-2.44	121.83	126.04
27	A	610	CLA	C2C-C1C-NC	2.44	112.25	109.97
27	G	611	CLA	C2C-C1C-NC	2.43	112.25	109.97
30	H	316	DD6	C21-C20-C19	2.43	117.02	114.28
27	H	304	CLA	C3D-C4D-ND	2.43	114.17	110.24
27	H	303	CLA	C2C-C1C-NC	2.43	112.25	109.97
32	J	613	PID	C17-C18-C19	-2.43	119.40	124.81
29	B	611	UIX	C13-C14-C23	-2.43	115.63	123.22
28	U	604	KC2	C4C-C3C-C2C	2.43	109.05	107.11
28	A	608	KC2	CHB-C1B-NB	2.43	126.69	124.45
28	E	610	KC2	CHD-C4C-NC	2.43	127.89	124.20
29	I	612	UIX	C-C7-C10	-2.43	120.86	125.99
28	U	602	KC2	CHC-C4B-NB	2.43	126.69	124.45
27	I	611	CLA	CAA-C2A-C1A	-2.42	106.77	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	H	315	DD6	C14-C13-C11	2.42	129.29	125.53
32	J	611	PID	O4-C10-O3	2.42	124.79	120.12
29	C	215	UIX	C17-C15-C20	2.42	111.56	109.21
27	b	701	CLA	C2C-C1C-NC	2.42	112.24	109.97
33	C	217	LMG	C8-O7-C10	2.42	123.75	117.79
38	a	836	BCR	C33-C5-C4	2.42	118.26	113.62
31	H	320	SQD	O47-C7-C8	2.42	116.71	111.50
30	K	612	DD6	O1-C20-C19	-2.42	111.57	113.38
27	l	402	CLA	C2C-C1C-NC	2.42	112.23	109.97
29	J	616	UIX	C37-C34-C30	-2.42	118.53	123.47
32	F	614	PID	C17-C16-C15	-2.41	118.53	123.47
27	H	308	CLA	C2C-C1C-NC	2.41	112.23	109.97
29	I	612	UIX	C19-C18-C17	2.41	114.08	109.88
27	F	604	CLA	C2C-C1C-NC	2.41	112.23	109.97
32	J	615	PID	O6-C30-O7	-2.41	118.17	122.96
27	C	205	CLA	C3A-C2A-C1A	-2.41	97.73	101.34
27	l	403	CLA	C2C-C1C-NC	2.41	112.23	109.97
28	U	604	KC2	CHD-C4C-NC	2.41	127.86	124.20
27	I	607	CLA	C2C-C1C-NC	2.41	112.23	109.97
27	T	602	CLA	C2C-C1C-NC	2.41	112.23	109.97
28	H	302	KC2	CHD-C4C-NC	2.40	127.85	124.20
29	T	612	UIX	O-C1-C6	-2.40	112.17	115.06
27	b	716	CLA	C2C-C1C-NC	2.40	112.22	109.97
27	I	606	CLA	C2C-C1C-NC	2.40	112.22	109.97
27	a	819	CLA	C2C-C1C-NC	2.39	112.22	109.97
32	F	614	PID	O6-C30-O7	-2.39	118.21	122.96
30	I	613	DD6	C32-C31-C36	-2.39	119.26	122.63
27	a	821	CLA	C2C-C1C-NC	2.39	112.21	109.97
32	I	614	PID	C16-C15-C14	-2.39	123.90	127.31
27	b	713	CLA	C2C-C1C-NC	2.39	112.21	109.97
27	E	605	CLA	C2C-C1C-NC	2.39	112.21	109.97
28	J	604	KC2	CHD-C4C-NC	2.39	127.83	124.20
32	B	613	PID	C17-C16-C15	-2.39	118.58	123.47
27	a	801	CLA	CHD-C1D-C2D	2.39	130.49	125.48
28	A	608	KC2	CHD-C4C-NC	2.39	127.82	124.20
28	U	604	KC2	CHC-C4B-NB	2.39	126.65	124.45
27	a	801	CLA	C4D-CHA-C1A	-2.39	118.35	121.25
38	a	836	BCR	C27-C26-C25	-2.38	119.27	122.73
27	C	211	CLA	C2C-C1C-NC	2.38	112.20	109.97
29	C	215	UIX	C13-C14-C23	-2.38	115.78	123.22
27	b	707	CLA	C2C-C1C-NC	2.38	112.20	109.97
29	A	616	UIX	C-C7-C10	-2.37	120.97	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	727	CLA	C2C-C1C-NC	2.37	112.19	109.97
27	K	605	CLA	C2C-C1C-NC	2.37	112.19	109.97
32	U	608	PID	CM1-C1-C6	-2.37	118.29	122.26
28	F	609	KC2	CHD-C4C-NC	2.37	127.80	124.20
29	T	612	UIX	C36-C35-C32	-2.37	123.93	127.31
27	a	814	CLA	C2C-C1C-NC	2.37	112.19	109.97
31	H	320	SQD	O8-S-C6	2.37	109.52	105.74
27	F	610	CLA	C2C-C1C-NC	2.37	112.19	109.97
32	J	613	PID	O6-C30-O7	-2.37	118.26	122.96
27	F	605	CLA	C2C-C1C-NC	2.37	112.19	109.97
32	B	613	PID	CM4-C14-C13	2.37	124.51	119.05
27	a	831	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
29	B	611	UIX	C14-C13-C11	-2.36	123.94	127.31
32	J	611	PID	C1-C2-C3	-2.36	108.07	112.75
27	b	710	CLA	C2C-C1C-NC	2.36	112.19	109.97
28	B	608	KC2	CHD-C4C-NC	2.36	127.79	124.20
30	J	612	DD6	C33-C34-C35	2.36	113.54	110.30
30	H	318	DD6	C14-C13-C11	2.36	129.19	125.53
29	C	213	UIX	C34-C37-C39	-2.36	118.64	123.47
28	H	311	KC2	CHD-C4C-NC	2.36	127.78	124.20
27	B	607	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
27	b	712	CLA	C2C-C1C-NC	2.36	112.18	109.97
27	a	810	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
28	E	610	KC2	CHC-C4B-NB	2.36	126.62	124.45
27	a	817	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
27	H	304	CLA	C4D-CHA-C1A	-2.35	118.38	121.25
27	A	612	CLA	C2A-C3A-C4A	-2.35	98.07	101.87
29	D	616	UIX	C17-C15-C20	2.35	111.50	109.21
28	B	602	KC2	CHB-C4A-NA	2.35	127.91	124.20
29	E	616	UIX	C35-C36-C38	-2.35	115.88	123.22
27	D	606	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
27	J	603	CLA	C2C-C1C-NC	2.35	112.17	109.97
27	b	718	CLA	C2C-C1C-NC	2.35	112.17	109.97
27	G	605	CLA	C2C-C1C-NC	2.35	112.17	109.97
28	J	604	KC2	CHB-C1B-NB	2.35	126.61	124.45
28	A	608	KC2	CHC-C4B-NB	2.35	126.61	124.45
27	a	829	CLA	C2C-C1C-NC	2.35	112.17	109.97
35	f	305	DGD	C1E-O6E-C5E	2.35	118.29	113.69
27	E	606	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
27	H	313	CLA	C2C-C1C-NC	2.34	112.17	109.97
31	H	320	SQD	O47-C45-C44	2.34	116.88	108.40
29	H	314	UIX	C37-C39-C40	-2.34	123.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	210	KC2	CHD-C4C-NC	2.34	127.75	124.20
27	l	412	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
28	H	302	KC2	CHC-C4B-NB	2.34	126.60	124.45
32	J	611	PID	C28-C27-C26	-2.34	105.80	109.88
35	j	201	DGD	C3G-C2G-C1G	-2.34	106.26	111.79
27	C	212	CLA	C2C-C1C-NC	2.34	112.16	109.97
27	j	202	CLA	C2C-C1C-NC	2.34	112.16	109.97
27	B	610	CLA	CHC-C1C-C2C	-2.33	120.26	126.72
28	U	604	KC2	CHB-C4A-NA	2.33	127.88	124.20
29	G	615	UIX	O2-C27-O4	-2.33	118.33	122.96
29	J	616	UIX	C29-C26-C23	2.33	121.75	118.08
28	G	601	KC2	CHD-C4C-NC	2.33	127.74	124.20
30	E	613	DD6	C32-C31-C36	-2.33	119.34	122.63
27	b	728	CLA	C2C-C1C-NC	2.33	112.16	109.97
27	E	604	CLA	C2C-C1C-NC	2.33	112.15	109.97
29	C	213	UIX	O-C1-C3	-2.33	111.63	113.38
29	E	616	UIX	C12-C11-C13	-2.33	119.66	122.92
27	C	206	CLA	CHC-C1C-C2C	-2.33	120.29	126.72
27	F	619	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	T	612	UIX	C38-C40-C39	-2.32	115.38	118.94
28	U	602	KC2	CHB-C1B-NB	2.32	126.59	124.45
28	K	607	KC2	CHD-C4C-NC	2.32	127.73	124.20
27	C	207	CLA	C2C-C1C-NC	2.32	112.15	109.97
28	E	601	KC2	CHD-C4C-NC	2.32	127.72	124.20
27	C	209	CLA	C2C-C1C-NC	2.32	112.14	109.97
27	b	725	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
32	I	614	PID	O6-C30-O7	-2.32	118.36	122.96
35	K	614	DGD	C3G-C2G-C1G	-2.32	106.31	111.79
32	K	611	PID	O6-C30-O7	-2.32	118.36	122.96
27	B	604	CLA	C2C-C1C-NC	2.32	112.14	109.97
30	D	614	DD6	C14-C13-C11	2.32	129.12	125.53
27	b	711	CLA	C2C-C1C-NC	2.32	112.14	109.97
27	F	617	CLA	C2C-C1C-NC	2.31	112.14	109.97
27	b	722	CLA	CHC-C1C-C2C	-2.31	120.32	126.72
29	C	215	UIX	C23-C26-C30	-2.31	115.39	118.94
27	a	820	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
27	f	302	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
27	F	608	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
38	b	731	BCR	C8-C9-C10	-2.31	115.40	118.94
27	b	717	CLA	C2C-C1C-NC	2.31	112.14	109.97
28	E	610	KC2	C4C-C3C-C2C	2.31	108.95	107.11
27	E	602	CLA	C2C-C1C-NC	2.31	112.13	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	409	CLA	C2C-C1C-NC	2.31	112.13	109.97
28	B	602	KC2	CHD-C4C-NC	2.31	127.70	124.20
27	F	603	CLA	C2C-C1C-NC	2.31	112.13	109.97
29	j	204	UIX	C23-C26-C30	-2.31	115.40	118.94
28	J	602	KC2	CHD-C4C-NC	2.30	127.70	124.20
27	a	825	CLA	C2C-C1C-NC	2.30	112.13	109.97
27	A	602	CLA	C2C-C1C-NC	2.30	112.13	109.97
29	T	612	UIX	O2-C27-O4	-2.30	118.39	122.96
27	b	703	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	A	616	UIX	O2-C27-O4	-2.30	118.39	122.96
27	A	604	CLA	C2C-C1C-NC	2.30	112.12	109.97
28	J	608	KC2	CHB-C1B-NB	2.30	126.57	124.45
27	B	606	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
29	G	615	UIX	C34-C37-C39	-2.30	118.77	123.47
27	a	823	CLA	C1-C2-C3	-2.29	122.08	126.04
29	T	612	UIX	C16-C20-C15	2.29	121.97	119.70
27	a	827	CLA	CHA-C1A-NA	-2.29	121.15	126.40
27	G	603	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
27	l	407	CLA	C2C-C1C-NC	2.29	112.12	109.97
27	H	307	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
27	b	708	CLA	CHC-C1C-C2C	-2.29	120.40	126.72
27	D	604	CLA	C2C-C1C-NC	2.29	112.11	109.97
29	C	213	UIX	O2-C27-O4	-2.28	118.42	122.96
29	H	314	UIX	C10-C11-C13	-2.28	115.44	118.94
29	E	616	UIX	O2-C27-O4	-2.28	118.42	122.96
27	r	204	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
27	b	704	CLA	C1-C2-C3	-2.28	122.09	126.04
29	B	615	UIX	C37-C39-C40	-2.28	124.05	127.31
27	E	603	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	D	601	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
27	T	609	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	F	606	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	I	608	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
29	H	314	UIX	O2-C27-O4	-2.28	118.44	122.96
28	I	604	KC2	C4C-C3C-C2C	2.28	108.92	107.11
27	T	605	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	a	837	CLA	CHD-C1D-C2D	2.28	130.26	125.48
27	I	609	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	a	804	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	l	410	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	a	808	CLA	CHC-C1C-C2C	-2.28	120.43	126.72
30	G	614	DD6	C33-C34-C35	2.28	113.42	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	804	CLA	CHA-C1A-NA	-2.28	121.19	126.40
27	C	208	CLA	C2C-C1C-NC	2.27	112.10	109.97
32	J	614	PID	C6-C7-C8	-2.27	121.18	125.99
27	l	406	CLA	C2C-C1C-NC	2.27	112.10	109.97
32	I	614	PID	C18-C17-C16	-2.27	119.76	124.81
27	I	605	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
29	G	615	UIX	C12-C11-C13	-2.27	119.74	122.92
27	A	611	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
28	J	610	KC2	CHD-C4C-NC	2.27	127.65	124.20
27	A	605	CLA	C2C-C1C-NC	2.27	112.10	109.97
27	a	808	CLA	C1-C2-C3	-2.27	122.12	126.04
32	F	615	PID	O4-C10-O3	2.27	124.49	120.12
27	H	308	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
27	I	603	CLA	O2A-C1-C2	2.26	114.59	108.64
27	C	202	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
27	H	312	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
31	A	618	SQD	O8-S-C6	2.26	109.35	105.74
27	a	805	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
29	A	616	UIX	C18-O2-C27	-2.26	113.68	117.90
27	b	703	CLA	CHD-C1D-C2D	2.26	130.23	125.48
27	a	815	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
29	B	615	UIX	O2-C27-O4	-2.26	118.47	122.96
27	E	609	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
27	H	309	CLA	C2C-C1C-NC	2.26	112.09	109.97
27	J	609	CLA	C2C-C1C-NC	2.26	112.09	109.97
27	b	706	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
27	G	605	CLA	CHD-C1D-C2D	2.26	130.22	125.48
27	b	719	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
32	J	613	PID	O1-C1-C6	-2.26	57.09	58.96
28	T	608	KC2	CHD-C4C-NC	2.26	127.62	124.20
32	J	613	PID	O4-C10-O3	2.26	124.47	120.12
27	T	607	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
27	a	824	CLA	CHD-C1D-C2D	2.25	130.21	125.48
27	l	404	CLA	CHD-C1D-C2D	2.25	130.20	125.48
29	H	317	UIX	O2-C27-O4	-2.25	118.49	122.96
28	G	601	KC2	CHC-C4B-NB	2.25	126.52	124.45
27	a	826	CLA	CHA-C1A-NA	-2.25	121.25	126.40
27	H	304	CLA	C1-C2-C3	-2.25	122.15	126.04
31	y	301	SQD	O8-S-C6	2.25	109.32	105.74
27	J	605	CLA	C2C-C1C-NC	2.25	112.08	109.97
29	H	317	UIX	C18-O2-C27	-2.25	113.71	117.90
27	b	707	CLA	CHD-C1D-C2D	2.25	130.19	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	611	PID	O1-C1-C6	-2.25	57.10	58.96
27	I	616	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
27	G	606	CLA	C2C-C1C-NC	2.25	112.08	109.97
28	H	311	KC2	C4C-C3C-C2C	2.25	108.90	107.11
28	J	608	KC2	CHD-C4C-NC	2.25	127.61	124.20
27	B	605	CLA	CAA-C2A-C1A	-2.25	104.62	111.97
27	b	726	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
27	b	724	CLA	C2C-C1C-NC	2.24	112.07	109.97
28	J	606	KC2	C4C-C3C-C2C	2.24	108.90	107.11
28	H	311	KC2	CHC-C4B-NB	2.24	126.52	124.45
28	H	302	KC2	C4C-C3C-C2C	2.24	108.89	107.11
27	b	702	CLA	CHA-C1A-NA	-2.24	121.27	126.40
27	F	607	CLA	C2C-C1C-NC	2.24	112.07	109.97
27	l	404	CLA	C2C-C1C-NC	2.24	112.07	109.97
27	K	604	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
27	B	606	CLA	C2C-C1C-NC	2.24	112.07	109.97
32	U	608	PID	O1-C1-C2	-2.24	111.70	113.38
27	A	601	CLA	CAA-C2A-C1A	-2.24	107.19	112.14
27	a	812	CLA	CHD-C1D-C2D	2.24	130.17	125.48
30	B	612	DD6	C14-C13-C11	2.24	129.00	125.53
28	U	602	KC2	CHD-C4C-NC	2.24	127.59	124.20
29	B	611	UIX	C37-C39-C40	-2.23	124.12	127.31
32	K	611	PID	C17-C18-C19	-2.23	119.84	124.81
28	K	607	KC2	CHC-C4B-NB	2.23	126.51	124.45
30	D	613	DD6	C32-C31-C36	2.23	125.79	122.63
27	T	601	CLA	CHD-C1D-C2D	2.23	130.16	125.48
28	F	609	KC2	CHC-C4B-NB	2.23	126.50	124.45
27	f	303	CLA	CHD-C1D-C2D	2.23	130.16	125.48
27	G	608	CLA	C2C-C1C-NC	2.23	112.06	109.97
29	j	204	UIX	C13-C14-C23	-2.23	116.26	123.22
27	H	304	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
27	U	606	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
35	l	416	DGD	CDB-CCB-CBB	-2.23	103.11	114.42
27	U	603	CLA	CHA-C1A-NA	-2.23	121.30	126.40
30	T	611	DD6	C21-C20-C19	2.23	116.79	114.28
27	b	727	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
27	U	605	CLA	C2C-C1C-NC	2.23	112.06	109.97
29	C	215	UIX	C37-C34-C30	-2.23	118.91	123.47
27	D	607	CLA	C2C-C1C-NC	2.23	112.06	109.97
27	b	721	CLA	CHD-C1D-C2D	2.23	130.15	125.48
32	J	613	PID	C18-C19-C20	-2.23	118.92	123.47
27	a	807	CLA	CHC-C1C-C2C	-2.23	120.57	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	816	CLA	CHC-C1C-C2C	-2.23	120.57	126.72
27	l	405	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
27	a	818	CLA	CHD-C1D-C2D	2.22	130.14	125.48
27	A	607	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
27	a	808	CLA	CHD-C1D-C2D	2.22	130.14	125.48
28	J	604	KC2	CHC-C4B-NB	2.22	126.50	124.45
27	U	603	CLA	CHD-C1D-C2D	2.22	130.14	125.48
27	b	719	CLA	CHD-C1D-C2D	2.22	130.14	125.48
27	G	609	CLA	CHD-C4C-C3C	-2.22	121.58	124.84
32	J	611	PID	O6-C27-C26	2.22	113.12	107.59
27	F	602	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	b	713	CLA	CHD-C1D-C2D	2.22	130.13	125.48
29	A	616	UIX	C3-C5-C4	2.22	115.06	110.77
27	D	605	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	b	714	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	A	601	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	a	813	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
29	T	612	UIX	C37-C34-C30	-2.22	118.93	123.47
28	T	608	KC2	C4C-C3C-C2C	2.22	108.88	107.11
27	A	612	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	I	602	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
27	l	411	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
27	a	828	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	D	608	CLA	C2C-C1C-NC	2.22	112.05	109.97
27	G	607	CLA	CHD-C1D-C2D	2.22	130.13	125.48
29	E	616	UIX	C29-C26-C30	-2.22	119.82	122.92
29	C	213	UIX	C12-C11-C13	-2.21	119.82	122.92
29	H	317	UIX	C6-C1-C	-2.21	118.55	122.26
32	J	613	PID	O4-C12-C13	2.21	127.61	122.89
27	F	604	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
27	I	610	CLA	CHD-C1D-C2D	2.21	130.12	125.48
27	F	605	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
27	a	806	CLA	C2C-C1C-NC	2.21	112.04	109.97
27	G	610	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
27	H	306	CLA	C2C-C1C-NC	2.21	112.04	109.97
29	C	215	UIX	O2-C27-O4	-2.21	118.57	122.96
32	I	614	PID	C17-C18-C19	-2.21	119.89	124.81
27	J	607	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
27	b	718	CLA	CHD-C1D-C2D	2.21	130.12	125.48
31	y	301	SQD	O9-S-C6	2.21	109.56	106.94
30	A	617	DD6	C32-C31-C36	-2.21	119.52	122.63
27	H	313	CLA	CHC-C1C-C2C	-2.21	120.61	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	609	CLA	C1-C2-C3	-2.21	122.22	126.04
27	E	605	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	B	603	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	l	412	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	a	826	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	G	611	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
27	a	822	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
27	E	607	CLA	CHD-C1D-C2D	2.21	130.10	125.48
27	U	605	CLA	CHD-C1D-C2D	2.21	130.10	125.48
29	j	204	UIX	O2-C27-O4	-2.20	118.58	122.96
27	j	202	CLA	CHD-C1D-C2D	2.20	130.10	125.48
27	C	204	CLA	CHC-C1C-C2C	-2.20	120.62	126.72
27	E	605	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
27	I	611	CLA	CHD-C1D-C2D	2.20	130.10	125.48
28	E	601	KC2	C4C-C3C-C2C	2.20	108.86	107.11
27	l	410	CLA	CHD-C1D-C2D	2.20	130.10	125.48
27	B	606	CLA	CHD-C1D-C2D	2.20	130.10	125.48
35	K	614	DGD	C5B-C4B-C3B	-2.20	103.25	114.42
27	H	305	CLA	O2A-C1-C2	2.20	114.41	108.64
27	K	603	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	b	712	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	H	314	UIX	C13-C14-C23	-2.20	116.36	123.22
30	F	611	DD6	C33-C34-C35	2.20	113.31	110.30
32	I	614	PID	O1-C1-C6	-2.20	57.14	58.96
27	b	709	CLA	CHC-C1C-C2C	-2.20	120.65	126.72
27	I	603	CLA	C2C-C1C-NC	2.20	112.03	109.97
28	J	604	KC2	C4C-C3C-C2C	2.20	108.86	107.11
27	B	605	CLA	CHD-C1D-C2D	2.20	130.08	125.48
27	K	602	CLA	CHC-C1C-C2C	-2.20	120.65	126.72
28	J	610	KC2	CHC-C4B-NB	2.19	126.47	124.45
27	F	605	CLA	CAA-C2A-C1A	-2.19	104.78	111.97
27	b	712	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
27	b	715	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
27	b	705	CLA	CHD-C1D-C2D	2.19	130.08	125.48
27	B	604	CLA	CHD-C1D-C2D	2.19	130.08	125.48
27	a	823	CLA	CHD-C1D-C2D	2.19	130.08	125.48
33	D	618	LMG	C8-O7-C10	2.19	123.19	117.79
27	G	602	CLA	C2C-C1C-NC	2.19	112.03	109.97
27	H	310	CLA	C2C-C1C-NC	2.19	112.03	109.97
27	b	715	CLA	CHD-C1D-C2D	2.19	130.08	125.48
27	D	608	CLA	C1-C2-C3	-2.19	122.25	126.04
27	A	609	CLA	CHC-C1C-C2C	-2.19	120.66	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	608	KC2	CHC-C4B-NB	2.19	126.47	124.45
28	I	604	KC2	CHC-C4B-NB	2.19	126.47	124.45
27	C	203	CLA	C2C-C1C-NC	2.19	112.02	109.97
27	l	408	CLA	C2C-C1C-NC	2.19	112.02	109.97
35	K	614	DGD	O2D-C2D-C1D	-2.19	104.73	110.05
27	B	609	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
38	a	836	BCR	C20-C19-C18	-2.19	120.27	126.42
27	I	609	CLA	CHD-C1D-C2D	2.19	130.07	125.48
27	G	604	CLA	CHD-C1D-C2D	2.19	130.07	125.48
27	J	601	CLA	CHD-C1D-C2D	2.19	130.07	125.48
32	J	614	PID	CM4-C14-C15	-2.19	119.86	122.92
27	K	601	CLA	CHD-C1D-C2D	2.19	130.06	125.48
27	a	830	CLA	C2C-C1C-NC	2.19	112.02	109.97
29	I	612	UIX	C6-C1-C	-2.18	118.60	122.26
27	a	809	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	D	602	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	D	608	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	D	612	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	a	816	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	D	609	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
28	J	606	KC2	CHB-C4A-NA	2.18	127.64	124.20
27	A	605	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	D	610	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	F	603	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	a	827	CLA	C2C-C1C-NC	2.18	112.02	109.97
27	E	602	CLA	CHD-C1D-C2D	2.18	130.05	125.48
27	b	722	CLA	CHD-C1D-C2D	2.18	130.05	125.48
27	l	407	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	G	611	CLA	CHD-C1D-C2D	2.18	130.05	125.48
27	B	605	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	K	606	CLA	C2C-C1C-NC	2.18	112.01	109.97
27	a	804	CLA	CHD-C1D-C2D	2.18	130.05	125.48
27	H	309	CLA	CHD-C1D-C2D	2.18	130.05	125.48
29	T	612	UIX	C21-C15-C20	-2.18	108.52	110.47
28	U	602	KC2	C4C-C3C-C2C	2.18	108.84	107.11
27	b	702	CLA	C3D-C4D-ND	2.18	113.76	110.24
29	H	314	UIX	C22-C15-C20	-2.18	108.52	110.47
32	J	611	PID	CM5-C21-C20	-2.18	119.87	122.92
27	J	603	CLA	CHD-C1D-C2D	2.18	130.04	125.48
28	F	609	KC2	C4C-C3C-C2C	2.18	108.84	107.11
27	E	604	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	F	610	CLA	CHD-C1D-C2D	2.18	130.04	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	U	601	CLA	CHD-C1D-C2D	2.18	130.04	125.48
32	F	614	PID	C28-C27-C26	-2.18	106.08	109.88
28	J	608	KC2	CHC-C4B-NB	2.18	126.45	124.45
27	r	203	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	a	818	CLA	C2C-C1C-NC	2.17	112.01	109.97
27	b	715	CLA	C2C-C1C-NC	2.17	112.01	109.97
32	U	608	PID	O4-C10-O3	2.17	124.31	120.12
27	a	829	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	l	406	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	E	612	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
27	T	602	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
29	G	615	UIX	C37-C39-C40	-2.17	124.21	127.31
27	H	310	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	J	609	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
27	a	824	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	I	606	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	E	603	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	G	608	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	C	207	CLA	CHD-C1D-C2D	2.17	130.02	125.48
27	l	408	CLA	CHD-C1D-C2D	2.17	130.02	125.48
27	K	608	CLA	CHD-C1D-C2D	2.17	130.02	125.48
32	I	614	PID	C17-C16-C15	-2.17	119.04	123.47
32	J	615	PID	O4-C10-O3	2.16	124.30	120.12
27	l	403	CLA	CHC-C1C-C2C	-2.16	120.73	126.72
27	A	610	CLA	CHD-C1D-C2D	2.16	130.02	125.48
27	a	810	CLA	CHD-C1D-C2D	2.16	130.02	125.48
30	E	615	DD6	C21-C20-C19	2.16	116.72	114.28
27	E	607	CLA	CHA-C1A-NA	-2.16	121.44	126.40
28	C	210	KC2	C4C-C3C-C2C	2.16	108.83	107.11
27	l	404	CLA	CHA-C1A-NA	-2.16	121.44	126.40
27	T	606	CLA	CHD-C1D-C2D	2.16	130.02	125.48
27	a	803	CLA	CHD-C1D-C2D	2.16	130.02	125.48
27	T	609	CLA	CHD-C1D-C2D	2.16	130.02	125.48
27	a	825	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
27	b	703	CLA	CHA-C1A-NA	-2.16	121.45	126.40
27	A	610	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
27	T	609	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
27	C	203	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	a	810	CLA	C1-C2-C3	-2.16	123.25	126.75
27	l	411	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	G	608	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
27	B	609	CLA	CHD-C1D-C2D	2.16	130.01	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	607	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	T	604	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
29	D	616	UIX	C38-C40-C39	-2.16	115.63	118.94
27	b	704	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	J	609	CLA	CHD-C1D-C2D	2.16	130.01	125.48
32	B	613	PID	CM7-C25-C24	-2.16	108.54	110.47
27	A	606	CLA	C2C-C1C-NC	2.16	111.99	109.97
27	C	212	CLA	CHD-C1D-C2D	2.16	130.01	125.48
28	C	210	KC2	CHC-C4B-NB	2.16	126.44	124.45
27	A	603	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
27	U	606	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	H	305	CLA	C2C-C1C-NC	2.16	111.99	109.97
27	l	409	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
27	A	605	CLA	CHD-C1D-C2D	2.16	130.00	125.48
38	a	836	BCR	C15-C16-C17	-2.16	119.06	123.47
27	D	603	CLA	C2C-C1C-NC	2.16	111.99	109.97
27	b	710	CLA	CHC-C1C-C2C	-2.16	120.76	126.72
27	a	820	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	l	407	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	I	607	CLA	CHC-C1C-C2C	-2.16	120.76	126.72
27	a	801	CLA	C2C-C1C-NC	2.16	111.99	109.97
27	b	710	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	E	608	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	b	711	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	b	711	CLA	CHC-C1C-C2C	-2.15	120.76	126.72
27	F	601	CLA	C2C-C1C-NC	2.15	111.99	109.97
27	a	811	CLA	C2C-C1C-NC	2.15	111.99	109.97
27	C	209	CLA	CHC-C1C-C2C	-2.15	120.76	126.72
27	A	602	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	K	606	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
27	H	319	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
27	C	205	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	b	728	CLA	C1-C2-C3	-2.15	122.32	126.04
27	J	605	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	a	819	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	K	608	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
29	G	615	UIX	C6-C1-C	-2.15	118.66	122.26
27	D	611	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
27	a	811	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	b	716	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
28	E	601	KC2	CHC-C4B-NB	2.15	126.43	124.45
29	C	213	UIX	C19-C18-C17	2.15	113.62	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	306	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
27	C	208	CLA	CHD-C1D-C2D	2.15	129.98	125.48
27	a	821	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
27	a	839	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
27	F	610	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
30	H	316	DD6	O1-C20-C19	-2.15	111.77	113.38
27	G	605	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
27	I	608	CLA	CHA-C1A-NA	-2.15	121.48	126.40
27	b	718	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
27	b	701	CLA	CHD-C1D-C2D	2.15	129.98	125.48
27	D	612	CLA	CHD-C1D-C2D	2.14	129.98	125.48
27	F	607	CLA	CHD-C1D-C2D	2.14	129.98	125.48
27	a	829	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
27	H	313	CLA	CHD-C1D-C2D	2.14	129.98	125.48
27	I	609	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
27	T	603	CLA	C2C-C1C-NC	2.14	111.98	109.97
30	T	611	DD6	C33-C34-C35	2.14	113.24	110.30
27	D	607	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
27	a	821	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	b	714	CLA	C2C-C1C-NC	2.14	111.98	109.97
27	H	303	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	G	609	CLA	CHA-C1A-NA	-2.14	121.49	126.40
27	f	303	CLA	C2C-C1C-NC	2.14	111.98	109.97
27	C	209	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	H	319	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	a	807	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	C	212	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
27	B	604	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
27	A	611	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	b	716	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	a	801	CLA	C3D-C4D-ND	2.14	113.70	110.24
27	E	607	CLA	C2C-C1C-NC	2.14	111.97	109.97
27	b	724	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	l	405	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	C	202	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	a	839	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	b	720	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	l	402	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	a	819	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
27	I	601	CLA	C2C-C1C-NC	2.14	111.97	109.97
27	K	606	CLA	CHD-C1D-C2D	2.14	129.96	125.48
32	F	615	PID	C18-C17-C16	-2.14	120.06	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	j	201	DGD	C4E-C3E-C2E	-2.14	107.09	110.82
27	C	201	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	D	609	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	T	607	CLA	CHD-C1D-C2D	2.14	129.96	125.48
32	F	614	PID	C16-C15-C14	-2.13	124.26	127.31
28	B	602	KC2	CHC-C4B-NB	2.13	126.42	124.45
27	E	612	CLA	CHD-C1D-C2D	2.13	129.96	125.48
27	F	602	CLA	CHD-C1D-C2D	2.13	129.96	125.48
27	a	806	CLA	CHD-C1D-C2D	2.13	129.96	125.48
27	b	727	CLA	CHD-C1D-C2D	2.13	129.96	125.48
27	K	601	CLA	C2C-C1C-NC	2.13	111.97	109.97
27	F	619	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	l	408	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
27	a	802	CLA	C2C-C1C-NC	2.13	111.97	109.97
28	A	608	KC2	CHB-C4A-C3A	-2.13	121.65	124.98
27	l	406	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
27	a	804	CLA	CHB-C4A-NA	2.13	127.46	124.51
27	a	814	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	a	815	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	b	706	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	H	304	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	T	610	DD6	O1-C20-C15	-2.13	57.20	58.96
28	B	602	KC2	C4C-C3C-C2C	2.13	108.81	107.11
27	G	609	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
27	I	601	CLA	CHD-C1D-C2D	2.13	129.94	125.48
29	A	613	UIX	O2-C27-O4	-2.13	118.73	122.96
28	J	606	KC2	CHD-C4C-NC	2.13	127.43	124.20
30	G	613	DD6	C33-C34-C35	-2.13	107.39	110.30
30	b	730	DD6	C32-C31-C36	2.13	125.64	122.63
27	l	402	CLA	CHC-C1C-C2C	-2.13	120.84	126.72
27	J	607	CLA	CHD-C1D-C2D	2.13	129.94	125.48
38	a	836	BCR	C23-C24-C25	-2.13	121.23	127.20
27	H	303	CLA	CMC-C2C-C1C	2.13	128.28	125.04
30	J	612	DD6	C14-C13-C11	2.13	128.83	125.53
27	D	603	CLA	CHD-C1D-C2D	2.13	129.94	125.48
27	I	606	CLA	CHC-C1C-C2C	-2.12	120.84	126.72
27	F	601	CLA	CHD-C1D-C2D	2.12	129.94	125.48
27	G	602	CLA	CHD-C1D-C2D	2.12	129.94	125.48
27	a	807	CLA	CHB-C4A-NA	2.12	127.45	124.51
27	E	611	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	b	702	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
27	b	702	CLA	CHC-C1C-C2C	-2.12	120.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	604	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	I	603	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
33	D	619	LMG	C3-C4-C5	-2.12	106.45	110.24
30	D	617	DD6	C32-C31-C36	2.12	125.63	122.63
27	E	609	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	b	726	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	I	610	CLA	C1-C2-C3	-2.12	122.37	126.04
27	E	611	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
27	b	703	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
27	F	617	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	D	611	CLA	CHD-C1D-C2D	2.12	129.93	125.48
29	D	616	UIX	O2-C27-O4	-2.12	118.75	122.96
27	a	802	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	B	601	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	b	707	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
27	C	204	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	F	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
30	G	612	DD6	C21-C20-C19	2.12	116.66	114.28
28	A	608	KC2	C4C-C3C-C2C	2.12	108.80	107.11
27	I	603	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	I	607	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	C	207	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
27	H	310	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
27	f	303	CLA	CHC-C1C-C2C	-2.11	120.87	126.72
35	j	201	DGD	CFB-CEB-CDB	-2.11	103.69	114.42
28	I	604	KC2	CHC-C1C-NC	2.11	127.54	124.20
27	H	305	CLA	CHD-C1D-C2D	2.11	129.91	125.48
38	a	836	BCR	C30-C25-C24	2.11	121.76	115.78
27	K	602	CLA	O2A-C1-C2	2.11	114.19	108.64
31	H	320	SQD	O9-S-C6	2.11	109.45	106.94
27	a	825	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	a	837	CLA	CHA-C1A-NA	-2.11	121.56	126.40
27	b	728	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
27	C	211	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	H	308	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	D	605	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	U	601	CLA	CHA-C1A-NA	-2.11	121.56	126.40
35	l	416	DGD	CAB-C9B-C8B	-2.11	103.71	114.42
27	l	403	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	E	603	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
35	f	305	DGD	CBB-CAB-C9B	-2.11	103.71	114.42
27	b	717	CLA	CHD-C1D-C2D	2.11	129.91	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	206	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	C	201	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
30	D	621	DD6	O1-C20-C19	-2.11	111.80	113.38
27	G	610	CLA	CHD-C1D-C2D	2.11	129.90	125.48
29	D	616	UIX	C35-C36-C38	-2.11	116.64	123.22
27	A	612	CLA	CHC-C1C-C2C	-2.11	120.90	126.72
27	b	723	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	F	608	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	a	805	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	b	727	CLA	CHA-C1A-NA	-2.11	121.58	126.40
27	C	205	CLA	CHA-C1A-NA	-2.10	121.58	126.40
27	T	604	CLA	CHD-C1D-C2D	2.10	129.89	125.48
35	f	305	DGD	O2D-C2D-C1D	-2.10	104.94	110.05
27	B	606	CLA	CHC-C1C-C2C	-2.10	120.90	126.72
27	J	603	CLA	CHC-C1C-C2C	-2.10	120.90	126.72
28	K	607	KC2	C4C-C3C-C2C	2.10	108.78	107.11
27	D	603	CLA	CHC-C1C-C2C	-2.10	120.90	126.72
29	J	616	UIX	C12-C11-C13	-2.10	119.98	122.92
29	B	611	UIX	C18-O2-C27	-2.10	113.98	117.90
27	D	611	CLA	C1-C2-C3	-2.10	122.41	126.04
29	B	611	UIX	C38-C40-C39	-2.10	115.72	118.94
27	E	605	CLA	CHA-C1A-NA	-2.10	121.59	126.40
27	E	606	CLA	CHD-C1D-C2D	2.10	129.89	125.48
28	G	601	KC2	C4C-C3C-C2C	2.10	108.78	107.11
27	H	304	CLA	CHB-C4A-NA	2.10	127.42	124.51
27	A	603	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	b	728	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	I	611	CLA	C2C-C1C-NC	2.10	111.94	109.97
27	a	817	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	G	615	UIX	C37-C34-C30	-2.10	119.18	123.47
35	f	305	DGD	CAB-C9B-C8B	-2.10	103.78	114.42
27	E	604	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
27	H	305	CLA	CHA-C1A-NA	-2.10	121.60	126.40
27	G	602	CLA	CMC-C2C-C1C	2.10	128.23	125.04
27	I	605	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	C	211	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
27	A	609	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	a	831	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	a	811	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
30	I	615	DD6	O1-C20-C19	-2.10	111.81	113.38
32	K	611	PID	C18-C19-C20	-2.10	119.18	123.47
27	b	713	CLA	CHC-C1C-C2C	-2.09	120.93	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	701	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
27	K	602	CLA	CHD-C1D-C2D	2.09	129.87	125.48
29	E	616	UIX	C6-C1-C	-2.09	118.75	122.26
35	j	201	DGD	CAB-C9B-C8B	-2.09	103.80	114.42
29	J	616	UIX	C37-C39-C40	-2.09	124.32	127.31
27	D	602	CLA	C2C-C1C-NC	2.09	111.93	109.97
27	C	207	CLA	CHA-C1A-NA	-2.09	121.61	126.40
27	H	310	CLA	CHA-C1A-NA	-2.09	121.61	126.40
27	a	811	CLA	CHA-C1A-NA	-2.09	121.61	126.40
27	a	812	CLA	CHA-C1A-NA	-2.09	121.61	126.40
27	a	814	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
27	a	812	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
27	A	612	CLA	CHA-C1A-NA	-2.09	121.61	126.40
27	F	617	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
27	C	209	CLA	CAA-C2A-C1A	-2.09	105.13	111.97
27	a	813	CLA	CHD-C1D-C2D	2.09	129.86	125.48
27	U	605	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
30	I	613	DD6	O1-C20-C15	-2.09	57.23	58.96
27	f	302	CLA	CHD-C1D-C2D	2.09	129.86	125.48
27	a	827	CLA	C1-C2-C3	-2.08	122.44	126.04
27	A	601	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	b	702	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	b	724	CLA	CHC-C1C-C2C	-2.08	120.96	126.72
27	b	704	CLA	C2C-C1C-NC	2.08	111.92	109.97
27	b	720	CLA	C2C-C1C-NC	2.08	111.92	109.97
27	j	202	CLA	CHC-C1C-C2C	-2.08	120.96	126.72
27	B	610	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	F	606	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	A	604	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
27	r	204	CLA	CHD-C1D-C2D	2.08	129.84	125.48
30	T	611	DD6	C32-C31-C36	-2.08	119.70	122.63
30	A	617	DD6	C33-C34-C35	2.08	113.15	110.30
27	B	603	CLA	CHA-C1A-NA	-2.08	121.63	126.40
27	a	822	CLA	CHD-C1D-C2D	2.08	129.84	125.48
27	a	827	CLA	CHD-C1D-C2D	2.08	129.84	125.48
27	a	830	CLA	CHD-C1D-C2D	2.08	129.84	125.48
27	E	611	CLA	C2C-C1C-NC	2.08	111.92	109.97
35	j	201	DGD	C1D-C2D-C3D	-2.08	105.67	110.00
28	J	610	KC2	C4C-C3C-C2C	2.08	108.76	107.11
29	A	616	UIX	C10-C11-C13	-2.08	115.75	118.94
27	b	714	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
35	j	201	DGD	CBB-CAB-C9B	-2.08	103.88	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	803	CLA	C2C-C1C-NC	2.08	111.92	109.97
27	F	607	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
28	J	608	KC2	C4C-C3C-C2C	2.08	108.76	107.11
27	A	607	CLA	CHD-C1D-C2D	2.07	129.83	125.48
32	K	611	PID	C17-C16-C15	-2.07	119.22	123.47
27	F	619	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
27	b	721	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
29	C	213	UIX	C29-C26-C30	-2.07	120.02	122.92
27	F	603	CLA	CHD-C1D-C2D	2.07	129.83	125.48
27	G	607	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
30	E	615	DD6	C32-C31-C36	2.07	125.56	122.63
30	E	615	DD6	O1-C20-C19	-2.07	111.83	113.38
27	G	606	CLA	CBA-CAA-C2A	2.07	119.98	113.86
27	H	304	CLA	C2A-C1A-CHA	2.07	127.48	123.86
27	a	817	CLA	CHD-C1D-C2D	2.07	129.82	125.48
27	a	812	CLA	C2C-C1C-NC	2.07	111.91	109.97
27	a	828	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
27	a	837	CLA	C2C-C1C-NC	2.07	111.91	109.97
27	l	410	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
27	F	605	CLA	CHD-C1D-C2D	2.07	129.82	125.48
29	J	616	UIX	O2-C27-O4	-2.07	118.86	122.96
27	H	307	CLA	CHD-C1D-C2D	2.07	129.81	125.48
28	G	601	KC2	CHB-C4A-C3A	-2.07	121.75	124.98
29	A	616	UIX	C13-C14-C23	-2.07	116.77	123.22
27	I	611	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
27	G	606	CLA	CHD-C1D-C2D	2.07	129.81	125.48
27	A	602	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
27	J	605	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
27	a	823	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
27	a	826	CLA	CHB-C4A-NA	2.06	127.37	124.51
27	b	715	CLA	CHC-C1C-NC	2.06	127.33	124.20
29	B	611	UIX	C35-C36-C38	-2.06	116.78	123.22
27	F	601	CLA	C1-C2-C3	-2.06	122.47	126.04
27	T	601	CLA	C2C-C1C-NC	2.06	111.91	109.97
30	D	614	DD6	O1-C20-C19	-2.06	111.83	113.38
29	H	317	UIX	C12-C11-C13	-2.06	120.03	122.92
30	E	617	DD6	C32-C31-C36	-2.06	119.72	122.63
27	D	601	CLA	CHD-C1D-C2D	2.06	129.81	125.48
28	J	602	KC2	C4C-C3C-C2C	2.06	108.75	107.11
27	a	812	CLA	C3A-C2A-C1A	-2.06	98.25	101.34
27	H	306	CLA	CHD-C1D-C2D	2.06	129.80	125.48
27	C	208	CLA	CHC-C1C-C2C	-2.06	121.02	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	603	CLA	CHD-C1D-C2D	2.06	129.80	125.48
27	T	602	CLA	CHD-C1D-C2D	2.06	129.80	125.48
27	b	703	CLA	C2C-C1C-NC	2.06	111.90	109.97
30	B	612	DD6	C32-C31-C36	2.06	125.54	122.63
27	G	605	CLA	CHA-C1A-NA	-2.06	121.69	126.40
27	b	720	CLA	CHC-C1C-C2C	-2.06	121.04	126.72
29	A	613	UIX	C6-C1-C	-2.06	118.82	122.26
27	b	709	CLA	CHD-C1D-C2D	2.05	129.79	125.48
30	K	609	DD6	O1-C20-C15	-2.05	57.26	58.96
29	C	215	UIX	O-C1-C6	-2.05	112.59	115.06
32	J	614	PID	O6-C30-O7	-2.05	118.89	122.96
27	D	606	CLA	CHD-C1D-C2D	2.05	129.78	125.48
27	E	602	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
27	T	601	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
35	K	614	DGD	C7B-C6B-C5B	-2.05	104.02	114.42
31	H	320	SQD	O48-C23-C24	2.05	118.34	111.91
27	b	718	CLA	CHA-C1A-NA	-2.05	121.71	126.40
27	D	608	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
27	a	831	CLA	CHC-C1C-NC	2.05	127.31	124.20
27	D	604	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
27	G	609	CLA	CHD-C1D-C2D	2.05	129.78	125.48
35	l	416	DGD	O3E-C3E-C2E	-2.05	105.61	110.35
27	b	725	CLA	C1-C2-C3	-2.05	122.50	126.04
27	b	710	CLA	CHA-C1A-NA	-2.05	121.71	126.40
32	J	615	PID	O1-C1-C2	-2.05	111.84	113.38
27	f	303	CLA	CHA-C1A-NA	-2.05	121.71	126.40
29	H	317	UIX	C38-C40-C39	-2.04	115.80	118.94
27	I	616	CLA	CHD-C1D-C2D	2.04	129.77	125.48
35	j	201	DGD	C1E-O6E-C5E	2.04	117.70	113.69
27	A	606	CLA	CHD-C4C-C3C	-2.04	121.84	124.84
30	K	612	DD6	O1-C20-C15	-2.04	57.27	58.96
27	A	606	CLA	CHD-C1D-C2D	2.04	129.76	125.48
27	D	610	CLA	CHD-C1D-C2D	2.04	129.76	125.48
27	I	601	CLA	C1-C2-C3	-2.04	122.51	126.04
27	b	706	CLA	C1-C2-C3	-2.04	122.51	126.04
27	a	810	CLA	CHC-C1C-NC	2.04	127.30	124.20
27	A	612	CLA	C2C-C1C-NC	2.04	111.88	109.97
27	B	601	CLA	C2C-C1C-NC	2.04	111.88	109.97
27	b	721	CLA	C2C-C1C-NC	2.04	111.88	109.97
35	f	305	DGD	C5B-C4B-C3B	-2.04	104.06	114.42
27	D	605	CLA	CHA-C1A-NA	-2.04	121.72	126.40
27	B	601	CLA	CHD-C4C-C3C	-2.04	121.84	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	601	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
27	a	802	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
27	b	723	CLA	C2C-C1C-NC	2.04	111.88	109.97
27	B	607	CLA	CHD-C1D-C2D	2.04	129.75	125.48
27	a	823	CLA	C2C-C1C-NC	2.04	111.88	109.97
28	B	608	KC2	C4C-C3C-C2C	2.04	108.73	107.11
29	B	615	UIX	C23-C26-C30	-2.04	115.82	118.94
27	A	612	CLA	C3A-C2A-C1A	-2.04	98.29	101.34
36	T	613	LMU	O5B-C5B-C4B	2.03	113.39	109.69
27	a	804	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
27	C	201	CLA	CAA-C2A-C1A	-2.03	107.64	112.14
30	T	611	DD6	C14-C13-C11	2.03	128.68	125.53
27	H	312	CLA	CAA-C2A-C1A	-2.03	107.64	112.14
27	T	603	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
27	K	603	CLA	C2C-C1C-NC	2.03	111.88	109.97
27	H	303	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
27	K	608	CLA	CHA-C1A-NA	-2.03	121.75	126.40
27	K	605	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
27	G	607	CLA	CHD-C4C-C3C	-2.03	121.86	124.84
27	F	604	CLA	CHD-C1D-C2D	2.03	129.74	125.48
29	T	612	UIX	C10-C11-C13	-2.03	115.83	118.94
30	E	613	DD6	O1-C20-C15	-2.03	57.28	58.96
30	H	318	DD6	O1-C20-C15	-2.03	57.28	58.96
27	b	725	CLA	CHD-C1D-C2D	2.03	129.74	125.48
29	G	615	UIX	C29-C26-C30	-2.03	120.08	122.92
27	K	601	CLA	CHD-C4C-C3C	-2.03	121.86	124.84
27	G	606	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
27	H	305	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
27	H	306	CLA	CHB-C4A-NA	2.03	127.31	124.51
27	K	606	CLA	CHA-C1A-NA	-2.03	121.76	126.40
27	a	822	CLA	C1-C2-C3	-2.02	122.54	126.04
27	I	608	CLA	CHD-C4C-C3C	-2.02	121.87	124.84
27	b	717	CLA	CHD-C4C-C3C	-2.02	121.87	124.84
27	I	602	CLA	CHD-C1D-C2D	2.02	129.72	125.48
27	J	601	CLA	C2C-C1C-NC	2.02	111.87	109.97
27	l	404	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
35	j	201	DGD	O6D-C5D-C6D	-2.02	102.58	106.67
27	l	409	CLA	CHD-C1D-C2D	2.02	129.72	125.48
27	a	802	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	H	320	SQD	O7-S-C6	2.02	109.34	106.94
27	I	609	CLA	CHA-C1A-NA	-2.02	121.78	126.40
27	T	603	CLA	CHD-C1D-C2D	2.02	129.71	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	I	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
27	C	203	CLA	CHC-C1C-C2C	-2.02	121.15	126.72
27	a	801	CLA	CHC-C1C-C2C	-2.02	121.15	126.72
27	E	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
35	K	614	DGD	C4E-C3E-C2E	-2.02	107.31	110.82
27	D	610	CLA	CHA-C1A-NA	-2.01	121.79	126.40
32	J	615	PID	CM5-C21-C20	-2.01	120.10	122.92
32	I	614	PID	CM7-C25-C24	-2.01	108.67	110.47
27	a	812	CLA	C1-C2-C3	-2.01	123.50	126.75
27	H	309	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
30	C	214	DD6	O1-C20-C15	-2.01	57.29	58.96
27	H	312	CLA	CHD-C1D-C2D	2.01	129.70	125.48
27	T	601	CLA	CHA-C1A-NA	-2.01	121.79	126.40
27	C	201	CLA	CHA-C1A-NA	-2.01	121.80	126.40
27	l	406	CLA	C1-C2-C3	-2.01	122.57	126.04
27	a	808	CLA	CHA-C1A-NA	-2.01	121.80	126.40
30	C	216	DD6	C32-C31-C36	2.01	125.47	122.63
32	F	615	PID	C17-C18-C19	-2.01	120.34	124.81
27	G	603	CLA	C1-C2-C3	-2.01	123.50	126.75
27	E	607	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
27	f	302	CLA	CHA-C1A-NA	-2.01	121.80	126.40
27	K	603	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
29	F	613	UIX	C38-C40-C39	-2.00	115.86	118.94
27	A	603	CLA	CHA-C1A-NA	-2.00	121.81	126.40
27	F	604	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	D	617	DD6	O1-C20-C15	-2.00	57.30	58.96
29	B	611	UIX	O2-C27-O4	-2.00	118.98	122.96
27	B	607	CLA	C1-C2-C3	-2.00	122.58	126.04

All (197) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	601	CLA	ND
27	A	602	CLA	ND
27	A	603	CLA	ND
27	A	604	CLA	ND
27	A	605	CLA	ND
27	A	606	CLA	ND
27	A	607	CLA	ND
27	A	609	CLA	ND
27	A	610	CLA	ND
27	A	611	CLA	ND

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Mol	Chain	Res	Type	Atom
27	A	612	CLA	ND
27	B	601	CLA	ND
27	B	603	CLA	ND
27	B	604	CLA	ND
27	B	605	CLA	ND
27	B	606	CLA	ND
27	B	607	CLA	ND
27	B	609	CLA	ND
27	B	610	CLA	ND
27	C	201	CLA	ND
27	C	202	CLA	ND
27	C	203	CLA	ND
27	C	204	CLA	ND
27	C	205	CLA	ND
27	C	206	CLA	ND
27	C	207	CLA	ND
27	C	208	CLA	ND
27	C	209	CLA	ND
27	C	211	CLA	ND
27	C	212	CLA	ND
27	D	601	CLA	ND
27	D	602	CLA	ND
27	D	603	CLA	ND
27	D	604	CLA	ND
27	D	605	CLA	ND
27	D	606	CLA	ND
27	D	607	CLA	ND
27	D	608	CLA	ND
27	D	609	CLA	ND
27	D	610	CLA	ND
27	D	611	CLA	ND
27	D	612	CLA	ND
27	E	602	CLA	ND
27	E	603	CLA	ND
27	E	604	CLA	ND
27	E	605	CLA	ND
27	E	606	CLA	ND
27	E	607	CLA	ND
27	E	608	CLA	ND
27	E	609	CLA	ND
27	E	611	CLA	ND
27	E	612	CLA	ND

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Mol	Chain	Res	Type	Atom
27	F	601	CLA	ND
27	F	602	CLA	ND
27	F	603	CLA	ND
27	F	604	CLA	ND
27	F	605	CLA	ND
27	F	606	CLA	ND
27	F	607	CLA	ND
27	F	608	CLA	ND
27	F	610	CLA	ND
27	F	617	CLA	ND
27	F	619	CLA	ND
27	G	602	CLA	ND
27	G	603	CLA	ND
27	G	604	CLA	ND
27	G	605	CLA	ND
27	G	606	CLA	ND
27	G	607	CLA	ND
27	G	608	CLA	ND
27	G	609	CLA	ND
27	G	610	CLA	ND
27	G	611	CLA	ND
27	H	303	CLA	ND
27	H	304	CLA	ND
27	H	305	CLA	ND
27	H	306	CLA	ND
27	H	307	CLA	ND
27	H	308	CLA	ND
27	H	309	CLA	ND
27	H	310	CLA	ND
27	H	312	CLA	ND
27	H	313	CLA	ND
27	H	319	CLA	ND
27	I	601	CLA	ND
27	I	602	CLA	ND
27	I	603	CLA	ND
27	I	605	CLA	ND
27	I	606	CLA	ND
27	I	607	CLA	ND
27	I	608	CLA	ND
27	I	609	CLA	ND
27	I	610	CLA	ND
27	I	611	CLA	ND

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Mol	Chain	Res	Type	Atom
27	I	616	CLA	ND
27	J	601	CLA	ND
27	J	603	CLA	ND
27	J	605	CLA	ND
27	J	607	CLA	ND
27	J	609	CLA	ND
27	K	601	CLA	ND
27	K	602	CLA	ND
27	K	603	CLA	ND
27	K	604	CLA	ND
27	K	605	CLA	ND
27	K	606	CLA	ND
27	K	608	CLA	ND
27	T	601	CLA	ND
27	T	602	CLA	ND
27	T	603	CLA	ND
27	T	604	CLA	ND
27	T	605	CLA	ND
27	T	606	CLA	ND
27	T	607	CLA	ND
27	T	609	CLA	ND
27	U	601	CLA	ND
27	U	603	CLA	ND
27	U	605	CLA	ND
27	U	606	CLA	ND
27	a	801	CLA	ND
27	a	802	CLA	ND
27	a	803	CLA	ND
27	a	804	CLA	ND
27	a	805	CLA	ND
27	a	806	CLA	ND
27	a	807	CLA	ND
27	a	808	CLA	ND
27	a	809	CLA	ND
27	a	810	CLA	ND
27	a	811	CLA	ND
27	a	812	CLA	ND
27	a	813	CLA	ND
27	a	814	CLA	ND
27	a	815	CLA	ND
27	a	816	CLA	ND
27	a	817	CLA	ND

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Mol	Chain	Res	Type	Atom
27	a	818	CLA	ND
27	a	819	CLA	ND
27	a	820	CLA	ND
27	a	821	CLA	ND
27	a	822	CLA	ND
27	a	823	CLA	ND
27	a	824	CLA	ND
27	a	825	CLA	ND
27	a	826	CLA	ND
27	a	827	CLA	ND
27	a	828	CLA	ND
27	a	829	CLA	ND
27	a	830	CLA	ND
27	a	831	CLA	ND
27	a	837	CLA	ND
27	a	839	CLA	ND
27	b	701	CLA	ND
27	b	702	CLA	ND
27	b	703	CLA	ND
27	b	704	CLA	ND
27	b	705	CLA	ND
27	b	706	CLA	ND
27	b	707	CLA	ND
27	b	708	CLA	ND
27	b	709	CLA	ND
27	b	710	CLA	ND
27	b	711	CLA	ND
27	b	712	CLA	ND
27	b	713	CLA	ND
27	b	714	CLA	ND
27	b	715	CLA	ND
27	b	716	CLA	ND
27	b	717	CLA	ND
27	b	718	CLA	ND
27	b	719	CLA	ND
27	b	720	CLA	ND
27	b	721	CLA	ND
27	b	722	CLA	ND
27	b	723	CLA	ND
27	b	724	CLA	ND
27	b	725	CLA	ND
27	b	726	CLA	ND

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Mol	Chain	Res	Type	Atom
27	b	727	CLA	ND
27	b	728	CLA	ND
27	f	302	CLA	ND
27	f	303	CLA	ND
27	j	202	CLA	ND
27	l	402	CLA	ND
27	l	403	CLA	ND
27	l	404	CLA	ND
27	l	405	CLA	ND
27	l	406	CLA	ND
27	l	407	CLA	ND
27	l	408	CLA	ND
27	l	409	CLA	ND
27	l	410	CLA	ND
27	l	411	CLA	ND
27	l	412	CLA	ND
27	r	203	CLA	ND
27	r	204	CLA	ND
30	D	613	DD6	C20

All (1715) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	601	CLA	C1A-C2A-CAA-CBA
27	A	602	CLA	CHA-CBD-CGD-O1D
27	A	602	CLA	CHA-CBD-CGD-O2D
27	A	604	CLA	C1A-C2A-CAA-CBA
27	A	606	CLA	C1A-C2A-CAA-CBA
27	A	606	CLA	C3A-C2A-CAA-CBA
27	A	612	CLA	C1A-C2A-CAA-CBA
27	B	601	CLA	C3A-C2A-CAA-CBA
27	B	605	CLA	C1A-C2A-CAA-CBA
27	B	605	CLA	C3A-C2A-CAA-CBA
27	B	606	CLA	CHA-CBD-CGD-O1D
27	B	606	CLA	CHA-CBD-CGD-O2D
27	B	607	CLA	CHA-CBD-CGD-O1D
27	B	607	CLA	CHA-CBD-CGD-O2D
27	C	201	CLA	C3A-C2A-CAA-CBA
27	C	203	CLA	CHA-CBD-CGD-O1D
27	C	203	CLA	CHA-CBD-CGD-O2D
27	C	204	CLA	C2A-CAA-CBA-CGA
27	C	205	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	C	205	CLA	C4-C3-C5-C6
27	C	208	CLA	CHA-CBD-CGD-O1D
27	C	208	CLA	CHA-CBD-CGD-O2D
27	C	211	CLA	CHA-CBD-CGD-O1D
27	C	211	CLA	CHA-CBD-CGD-O2D
27	D	608	CLA	CHA-CBD-CGD-O1D
27	D	608	CLA	CHA-CBD-CGD-O2D
27	D	611	CLA	CHA-CBD-CGD-O1D
27	D	612	CLA	C2-C3-C5-C6
27	D	612	CLA	C4-C3-C5-C6
27	E	608	CLA	CHA-CBD-CGD-O1D
27	E	608	CLA	CHA-CBD-CGD-O2D
27	E	608	CLA	C4-C3-C5-C6
27	E	611	CLA	CHA-CBD-CGD-O1D
27	E	611	CLA	CHA-CBD-CGD-O2D
27	E	611	CLA	C2-C3-C5-C6
27	E	611	CLA	C4-C3-C5-C6
27	F	602	CLA	C1A-C2A-CAA-CBA
27	F	602	CLA	C2-C3-C5-C6
27	F	602	CLA	C4-C3-C5-C6
27	F	603	CLA	CHA-CBD-CGD-O1D
27	F	603	CLA	CHA-CBD-CGD-O2D
27	F	603	CLA	CAD-CBD-CGD-O1D
27	F	605	CLA	C1A-C2A-CAA-CBA
27	F	605	CLA	CHA-CBD-CGD-O1D
27	F	605	CLA	CHA-CBD-CGD-O2D
27	F	607	CLA	C3A-C2A-CAA-CBA
27	F	610	CLA	C1A-C2A-CAA-CBA
27	F	619	CLA	C2-C3-C5-C6
27	F	619	CLA	C4-C3-C5-C6
27	G	607	CLA	C3A-C2A-CAA-CBA
27	G	609	CLA	C4-C3-C5-C6
27	H	303	CLA	CHA-CBD-CGD-O1D
27	H	303	CLA	CHA-CBD-CGD-O2D
27	H	309	CLA	CHA-CBD-CGD-O1D
27	H	309	CLA	CHA-CBD-CGD-O2D
27	H	310	CLA	C3A-C2A-CAA-CBA
27	H	319	CLA	CHA-CBD-CGD-O1D
27	I	602	CLA	CHA-CBD-CGD-O1D
27	I	602	CLA	CHA-CBD-CGD-O2D
27	I	602	CLA	CAD-CBD-CGD-O1D
27	I	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	I	607	CLA	C2A-CAA-CBA-CGA
27	I	607	CLA	C2-C3-C5-C6
27	I	607	CLA	C4-C3-C5-C6
27	I	608	CLA	CHA-CBD-CGD-O1D
27	I	608	CLA	CHA-CBD-CGD-O2D
27	I	611	CLA	C1A-C2A-CAA-CBA
27	J	601	CLA	C1A-C2A-CAA-CBA
27	J	601	CLA	C3A-C2A-CAA-CBA
27	J	601	CLA	CHA-CBD-CGD-O1D
27	J	601	CLA	CHA-CBD-CGD-O2D
27	J	603	CLA	CAD-CBD-CGD-O2D
27	J	609	CLA	CHA-CBD-CGD-O1D
27	J	609	CLA	CHA-CBD-CGD-O2D
27	K	602	CLA	C2-C3-C5-C6
27	K	602	CLA	C4-C3-C5-C6
27	K	605	CLA	C1A-C2A-CAA-CBA
27	K	605	CLA	C3A-C2A-CAA-CBA
27	U	606	CLA	CHA-CBD-CGD-O1D
27	U	606	CLA	CHA-CBD-CGD-O2D
27	U	606	CLA	CAD-CBD-CGD-O1D
27	a	803	CLA	C1A-C2A-CAA-CBA
27	a	803	CLA	C3A-C2A-CAA-CBA
27	a	804	CLA	C2-C3-C5-C6
27	a	804	CLA	C4-C3-C5-C6
27	a	804	CLA	C6-C7-C8-C9
27	a	807	CLA	C1A-C2A-CAA-CBA
27	a	807	CLA	C2-C3-C5-C6
27	a	807	CLA	C4-C3-C5-C6
27	a	809	CLA	C1A-C2A-CAA-CBA
27	a	809	CLA	C2A-CAA-CBA-CGA
27	a	812	CLA	C1A-C2A-CAA-CBA
27	a	813	CLA	C3A-C2A-CAA-CBA
27	a	820	CLA	C1A-C2A-CAA-CBA
27	a	820	CLA	C3A-C2A-CAA-CBA
27	a	822	CLA	C3A-C2A-CAA-CBA
27	a	823	CLA	CHA-CBD-CGD-O1D
27	a	823	CLA	CHA-CBD-CGD-O2D
27	a	824	CLA	C4-C3-C5-C6
27	a	824	CLA	C14-C13-C15-C16
27	a	825	CLA	C1A-C2A-CAA-CBA
27	a	825	CLA	C3A-C2A-CAA-CBA
27	a	826	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	a	826	CLA	C4-C3-C5-C6
27	a	828	CLA	CHA-CBD-CGD-O1D
27	a	828	CLA	CHA-CBD-CGD-O2D
27	a	829	CLA	C1A-C2A-CAA-CBA
27	a	829	CLA	C14-C13-C15-C16
27	a	830	CLA	CHA-CBD-CGD-O1D
27	a	830	CLA	CHA-CBD-CGD-O2D
27	a	831	CLA	CHA-CBD-CGD-O1D
27	a	831	CLA	CHA-CBD-CGD-O2D
27	a	839	CLA	C1A-C2A-CAA-CBA
27	a	839	CLA	C3A-C2A-CAA-CBA
27	b	702	CLA	CHA-CBD-CGD-O1D
27	b	702	CLA	CHA-CBD-CGD-O2D
27	b	703	CLA	C2-C1-O2A-CGA
27	b	705	CLA	C1A-C2A-CAA-CBA
27	b	705	CLA	C3A-C2A-CAA-CBA
27	b	708	CLA	C1A-C2A-CAA-CBA
27	b	708	CLA	CHA-CBD-CGD-O2D
27	b	708	CLA	C4-C3-C5-C6
27	b	713	CLA	C1A-C2A-CAA-CBA
27	b	713	CLA	C3A-C2A-CAA-CBA
27	b	714	CLA	C1A-C2A-CAA-CBA
27	b	717	CLA	C3A-C2A-CAA-CBA
27	b	718	CLA	C1A-C2A-CAA-CBA
27	b	727	CLA	C1A-C2A-CAA-CBA
27	j	202	CLA	CHA-CBD-CGD-O1D
27	j	202	CLA	CHA-CBD-CGD-O2D
27	j	202	CLA	CAD-CBD-CGD-O1D
27	j	202	CLA	CAD-CBD-CGD-O2D
27	l	403	CLA	CHA-CBD-CGD-O1D
27	l	403	CLA	CHA-CBD-CGD-O2D
27	r	203	CLA	C1A-C2A-CAA-CBA
27	r	204	CLA	CHA-CBD-CGD-O1D
27	r	204	CLA	CHA-CBD-CGD-O2D
27	r	204	CLA	CAD-CBD-CGD-O1D
27	r	204	CLA	CAD-CBD-CGD-O2D
28	A	608	KC2	C4B-C3B-CAB-CBB
28	B	608	KC2	C1A-C2A-CAA-CBA
28	B	608	KC2	C3A-C2A-CAA-CBA
28	B	608	KC2	CHA-CBD-CGD-O1D
28	B	608	KC2	CHA-CBD-CGD-O2D
28	C	210	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	C	210	KC2	C4C-C3C-CAC-CBC
28	E	601	KC2	C1A-C2A-CAA-CBA
28	E	601	KC2	CHA-CBD-CGD-O2D
28	G	601	KC2	C1A-C2A-CAA-CBA
28	G	601	KC2	C3A-C2A-CAA-CBA
28	G	601	KC2	C2B-C3B-CAB-CBB
28	G	601	KC2	C4B-C3B-CAB-CBB
28	G	601	KC2	CHA-CBD-CGD-O1D
28	G	601	KC2	CHA-CBD-CGD-O2D
28	H	302	KC2	C1A-C2A-CAA-CBA
28	H	302	KC2	C3A-C2A-CAA-CBA
28	H	302	KC2	C2B-C3B-CAB-CBB
28	H	302	KC2	C4B-C3B-CAB-CBB
28	H	302	KC2	CHA-CBD-CGD-O1D
28	H	302	KC2	CHA-CBD-CGD-O2D
28	H	311	KC2	C1A-C2A-CAA-CBA
28	H	311	KC2	C4C-C3C-CAC-CBC
28	I	604	KC2	C2B-C3B-CAB-CBB
28	I	604	KC2	C4B-C3B-CAB-CBB
28	J	602	KC2	C1A-C2A-CAA-CBA
28	J	602	KC2	C3A-C2A-CAA-CBA
28	J	604	KC2	C1A-C2A-CAA-CBA
28	J	604	KC2	C3A-C2A-CAA-CBA
28	J	604	KC2	C2C-C3C-CAC-CBC
28	J	604	KC2	C4C-C3C-CAC-CBC
28	J	606	KC2	C1A-C2A-CAA-CBA
28	J	608	KC2	C4C-C3C-CAC-CBC
28	U	602	KC2	C2B-C3B-CAB-CBB
28	U	602	KC2	C4B-C3B-CAB-CBB
28	U	604	KC2	C1A-C2A-CAA-CBA
28	U	604	KC2	C3A-C2A-CAA-CBA
28	U	604	KC2	C2C-C3C-CAC-CBC
28	U	604	KC2	C4C-C3C-CAC-CBC
29	A	616	UIX	C2-C-C7-C10
29	B	615	UIX	C1-C-C7-C10
29	B	615	UIX	C31-C27-O2-C18
29	C	213	UIX	C31-C27-O2-C18
29	C	215	UIX	C1-C-C7-C10
29	D	616	UIX	C7-C10-C11-C12
29	D	616	UIX	C7-C10-C11-C13
29	D	616	UIX	C19-C18-O2-C27
29	E	616	UIX	C2-C-C7-C10

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Mol	Chain	Res	Type	Atoms
29	F	613	UIX	C19-C18-O2-C27
29	F	613	UIX	O4-C27-O2-C18
29	F	613	UIX	C31-C27-O2-C18
29	G	615	UIX	C7-C10-C11-C12
29	G	615	UIX	C7-C10-C11-C13
29	G	615	UIX	C31-C27-O2-C18
29	H	314	UIX	C31-C27-O2-C18
29	H	317	UIX	C31-C27-O2-C18
29	I	612	UIX	O4-C27-O2-C18
29	I	612	UIX	C31-C27-O2-C18
29	J	616	UIX	C17-C18-O2-C27
29	T	612	UIX	C1-C-C7-C10
29	j	204	UIX	O-C-C7-C10
29	j	204	UIX	C19-C18-O2-C27
30	A	615	DD6	C10-C11-C13-C14
30	A	615	DD6	C12-C11-C13-C14
30	A	617	DD6	C10-C11-C13-C14
30	A	617	DD6	C13-C14-C15-C16
30	A	617	DD6	C13-C14-C15-C20
30	B	614	DD6	C13-C14-C15-C16
30	B	614	DD6	C13-C14-C15-C20
30	B	616	DD6	C13-C14-C15-C20
30	B	616	DD6	C13-C14-C15-O1
30	C	214	DD6	C27-C29-C30-C31
30	D	613	DD6	C13-C14-C15-O1
30	D	613	DD6	C27-C29-C30-C31
30	D	615	DD6	C10-C11-C13-C14
30	D	615	DD6	C12-C11-C13-C14
30	D	621	DD6	C11-C10-C9-C8
30	D	621	DD6	C10-C11-C13-C14
30	D	621	DD6	C12-C11-C13-C14
30	E	617	DD6	C10-C11-C13-C14
30	E	617	DD6	C12-C11-C13-C14
30	F	611	DD6	C10-C11-C13-C14
30	F	611	DD6	C12-C11-C13-C14
30	G	614	DD6	C10-C11-C13-C14
30	G	614	DD6	C12-C11-C13-C14
30	H	301	DD6	C13-C14-C15-C20
30	H	316	DD6	C13-C14-C15-O1
30	K	609	DD6	C10-C11-C13-C14
30	K	609	DD6	C12-C11-C13-C14
30	K	609	DD6	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	K	609	DD6	C13-C14-C15-C20
30	K	612	DD6	C10-C11-C13-C14
30	K	612	DD6	C12-C11-C13-C14
30	K	612	DD6	C13-C14-C15-C16
30	K	612	DD6	C13-C14-C15-C20
30	K	612	DD6	C13-C14-C15-O1
30	T	610	DD6	C10-C11-C13-C14
30	T	610	DD6	C12-C11-C13-C14
30	T	610	DD6	C13-C14-C15-C16
30	T	610	DD6	C13-C14-C15-C20
30	T	611	DD6	C13-C14-C15-C16
30	i	202	DD6	C13-C14-C15-C16
30	i	202	DD6	C5-C6-C8-C9
30	r	201	DD6	C13-C14-C15-C16
30	r	201	DD6	C13-C14-C15-C20
30	r	205	DD6	C10-C11-C13-C14
30	r	205	DD6	C12-C11-C13-C14
30	r	205	DD6	C13-C14-C15-O1
30	r	206	DD6	C10-C11-C13-C14
30	r	206	DD6	C12-C11-C13-C14
31	A	618	SQD	O5-C5-C6-S
31	A	618	SQD	C5-C6-S-O7
31	A	618	SQD	C5-C6-S-O8
31	A	618	SQD	C5-C6-S-O9
32	B	613	PID	O1-C6-C7-C8
32	B	613	PID	C31-C30-O6-C27
32	F	614	PID	C28-C27-O6-C30
32	F	614	PID	C31-C30-O6-C27
32	F	615	PID	C31-C30-O6-C27
32	F	615	PID	O7-C30-O6-C27
32	I	614	PID	O1-C6-C7-C8
32	I	614	PID	C31-C30-O6-C27
32	J	611	PID	C26-C27-O6-C30
32	J	613	PID	O1-C6-C7-C8
32	J	613	PID	C31-C30-O6-C27
32	J	615	PID	C1-C6-C7-C8
32	J	615	PID	C5-C6-C7-C8
32	J	615	PID	C31-C30-O6-C27
32	J	615	PID	O7-C30-O6-C27
32	K	611	PID	C1-C6-C7-C8
32	K	611	PID	C26-C27-O6-C30
32	K	611	PID	C31-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
32	K	611	PID	O7-C30-O6-C27
32	U	608	PID	C28-C27-O6-C30
32	U	608	PID	C31-C30-O6-C27
32	U	608	PID	O7-C30-O6-C27
33	C	217	LMG	C11-C10-O7-C8
33	D	618	LMG	C2-C1-O1-C7
33	D	618	LMG	O6-C1-O1-C7
33	D	619	LMG	O6-C1-O1-C7
33	D	619	LMG	O9-C10-O7-C8
33	F	616	LMG	C2-C1-O1-C7
33	F	616	LMG	O6-C1-O1-C7
33	F	616	LMG	C11-C10-O7-C8
33	K	613	LMG	O7-C8-C9-O8
33	b	733	LMG	C11-C10-O7-C8
33	l	417	LMG	O1-C7-C8-O7
33	l	417	LMG	O9-C10-O7-C8
34	D	620	LHG	C3-O3-P-O4
34	D	620	LHG	C4-O6-P-O5
34	D	620	LHG	O7-C5-C6-O8
34	F	618	LHG	O1-C1-C2-C3
34	F	618	LHG	C8-C7-O7-C5
34	G	617	LHG	C3-O3-P-O6
34	G	617	LHG	C4-O6-P-O5
34	G	617	LHG	C8-C7-O7-C5
34	a	835	LHG	O2-C2-C3-O3
34	a	835	LHG	C3-O3-P-O4
34	j	205	LHG	C4-O6-P-O5
34	j	205	LHG	C8-C7-O7-C5
34	r	202	LHG	O7-C5-C6-O8
35	K	614	DGD	C2D-C1D-O3G-C3G
35	K	614	DGD	O6D-C1D-O3G-C3G
35	f	305	DGD	O1G-C1G-C2G-O2G
35	j	201	DGD	C2B-C1B-O2G-C2G
35	j	201	DGD	O1B-C1B-O2G-C2G
35	j	201	DGD	C2D-C1D-O3G-C3G
35	j	201	DGD	O6D-C1D-O3G-C3G
35	l	416	DGD	C2B-C1B-O2G-C2G
35	l	416	DGD	O1B-C1B-O2G-C2G
38	a	833	BCR	C19-C20-C21-C22
38	a	833	BCR	C21-C22-C23-C24
38	a	833	BCR	C37-C22-C23-C24
38	a	833	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
38	a	833	BCR	C23-C24-C25-C30
38	a	834	BCR	C1-C6-C7-C8
38	a	834	BCR	C11-C12-C13-C35
38	a	836	BCR	C7-C8-C9-C10
38	a	836	BCR	C7-C8-C9-C34
38	a	836	BCR	C21-C22-C23-C24
38	a	836	BCR	C37-C22-C23-C24
38	a	836	BCR	C23-C24-C25-C26
38	b	731	BCR	C7-C8-C9-C34
38	f	301	BCR	C11-C12-C13-C14
38	f	301	BCR	C11-C12-C13-C35
38	f	301	BCR	C17-C18-C19-C20
38	f	301	BCR	C36-C18-C19-C20
38	i	201	BCR	C17-C18-C19-C20
38	i	201	BCR	C36-C18-C19-C20
38	i	201	BCR	C21-C22-C23-C24
38	i	201	BCR	C37-C22-C23-C24
38	i	201	BCR	C23-C24-C25-C30
38	j	203	BCR	C17-C18-C19-C20
38	j	203	BCR	C36-C18-C19-C20
38	l	413	BCR	C36-C18-C19-C20
38	l	414	BCR	C7-C8-C9-C10
38	l	414	BCR	C7-C8-C9-C34
38	l	415	BCR	C5-C6-C7-C8
38	l	415	BCR	C11-C12-C13-C14
38	l	415	BCR	C11-C12-C13-C35
38	l	415	BCR	C17-C18-C19-C20
38	l	415	BCR	C36-C18-C19-C20
38	l	415	BCR	C23-C24-C25-C26
38	l	415	BCR	C23-C24-C25-C30
38	m	201	BCR	C11-C12-C13-C14
38	m	201	BCR	C11-C12-C13-C35
38	m	201	BCR	C17-C18-C19-C20
38	m	201	BCR	C36-C18-C19-C20
27	a	827	CLA	C4C-C3C-CAC-CBC
29	A	613	UIX	O4-C27-O2-C18
29	A	613	UIX	C31-C27-O2-C18
29	A	616	UIX	C31-C27-O2-C18
29	C	215	UIX	C31-C27-O2-C18
29	D	616	UIX	C31-C27-O2-C18
29	E	616	UIX	C31-C27-O2-C18
29	H	314	UIX	O4-C27-O2-C18

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Mol	Chain	Res	Type	Atoms
29	J	616	UIX	C31-C27-O2-C18
29	T	612	UIX	C31-C27-O2-C18
29	j	204	UIX	C31-C27-O2-C18
32	B	613	PID	O7-C30-O6-C27
32	I	614	PID	O7-C30-O6-C27
27	a	827	CLA	C2C-C3C-CAC-CBC
29	B	615	UIX	O4-C27-O2-C18
29	C	213	UIX	O4-C27-O2-C18
29	C	215	UIX	O4-C27-O2-C18
29	D	616	UIX	O4-C27-O2-C18
29	J	616	UIX	O4-C27-O2-C18
29	T	612	UIX	O4-C27-O2-C18
32	F	614	PID	O7-C30-O6-C27
32	J	611	PID	C31-C30-O6-C27
32	J	613	PID	O7-C30-O6-C27
35	K	614	DGD	O1A-C1A-O1G-C1G
33	C	217	LMG	C29-C28-O8-C9
35	l	416	DGD	C4E-C5E-C6E-O5E
27	a	806	CLA	C4C-C3C-CAC-CBC
29	E	616	UIX	O4-C27-O2-C18
33	C	217	LMG	O10-C28-O8-C9
33	D	619	LMG	O10-C28-O8-C9
33	F	616	LMG	O10-C28-O8-C9
34	G	617	LHG	O10-C23-O8-C6
29	A	616	UIX	O4-C27-O2-C18
29	j	204	UIX	O4-C27-O2-C18
36	T	613	LMU	O5B-C1B-O1B-C4'
33	C	217	LMG	O9-C10-O7-C8
33	F	616	LMG	O9-C10-O7-C8
34	G	617	LHG	O9-C7-O7-C5
34	j	205	LHG	O9-C7-O7-C5
27	a	806	CLA	C2C-C3C-CAC-CBC
29	B	611	UIX	C31-C27-O2-C18
32	J	615	PID	C28-C27-O6-C30
27	A	603	CLA	C3-C5-C6-C7
27	E	606	CLA	C3-C5-C6-C7
27	a	818	CLA	C3-C5-C6-C7
27	a	839	CLA	C3-C5-C6-C7
27	b	706	CLA	C3-C5-C6-C7
27	l	403	CLA	C3-C5-C6-C7
27	r	204	CLA	C3-C5-C6-C7
33	F	616	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	G	617	LHG	C24-C23-O8-C6
29	H	317	UIX	O4-C27-O2-C18
33	D	619	LMG	C11-C10-O7-C8
33	l	417	LMG	C11-C10-O7-C8
29	G	615	UIX	O4-C27-O2-C18
28	J	606	KC2	CAA-CBA-CGA-O1A
28	J	606	KC2	CAA-CBA-CGA-O2A
28	U	602	KC2	CAA-CBA-CGA-O1A
28	U	602	KC2	CAA-CBA-CGA-O2A
27	E	608	CLA	C2-C3-C5-C6
27	a	824	CLA	C2-C3-C5-C6
27	a	807	CLA	C2A-CAA-CBA-CGA
34	D	620	LHG	O10-C23-O8-C6
27	D	602	CLA	C3-C5-C6-C7
27	F	617	CLA	C3-C5-C6-C7
27	a	814	CLA	C3-C5-C6-C7
27	a	825	CLA	C3-C5-C6-C7
27	j	202	CLA	C3-C5-C6-C7
33	D	619	LMG	C29-C28-O8-C9
33	l	417	LMG	C29-C28-O8-C9
35	l	416	DGD	O6E-C5E-C6E-O5E
33	b	733	LMG	O9-C10-O7-C8
34	F	618	LHG	O9-C7-O7-C5
34	r	202	LHG	O10-C23-O8-C6
27	T	603	CLA	C2C-C3C-CAC-CBC
34	G	617	LHG	O2-C2-C3-O3
27	G	608	CLA	C3-C5-C6-C7
37	a	832	PQN	C13-C15-C16-C17
34	D	620	LHG	C24-C23-O8-C6
33	l	417	LMG	O10-C28-O8-C9
33	C	217	LMG	O6-C5-C6-O5
33	D	618	LMG	C11-C10-O7-C8
34	r	202	LHG	C8-C7-O7-C5
33	D	619	LMG	O6-C5-C6-O5
32	I	614	PID	C26-C27-O6-C30
27	B	609	CLA	C3-C5-C6-C7
34	r	202	LHG	C24-C23-O8-C6
35	K	614	DGD	C2A-C1A-O1G-C1G
33	D	618	LMG	O9-C10-O7-C8
28	A	608	KC2	CAA-CBA-CGA-O2A
32	J	611	PID	O7-C30-O6-C27
35	f	305	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
27	D	607	CLA	C4-C3-C5-C6
27	I	603	CLA	C4-C3-C5-C6
27	G	609	CLA	C2-C3-C5-C6
27	I	603	CLA	C2-C3-C5-C6
27	b	708	CLA	C2-C3-C5-C6
27	U	603	CLA	CBD-CGD-O2D-CED
27	F	606	CLA	C2A-CAA-CBA-CGA
36	T	613	LMU	C3'-C4'-O1B-C1B
33	D	618	LMG	O6-C5-C6-O5
35	f	305	DGD	O6E-C1E-O5D-C6D
33	b	733	LMG	C29-C28-O8-C9
27	F	604	CLA	C2C-C3C-CAC-CBC
33	C	217	LMG	C4-C5-C6-O5
33	D	619	LMG	C4-C5-C6-O5
28	A	608	KC2	CAA-CBA-CGA-O1A
28	J	610	KC2	CAA-CBA-CGA-O1A
28	J	610	KC2	CAA-CBA-CGA-O2A
32	I	614	PID	C28-C27-O6-C30
33	l	417	LMG	C4-C5-C6-O5
34	G	617	LHG	C1-C2-C3-O3
34	a	835	LHG	C1-C2-C3-O3
33	b	733	LMG	O10-C28-O8-C9
27	H	305	CLA	C3-C5-C6-C7
27	I	603	CLA	CBA-CGA-O2A-C1
27	a	804	CLA	CBA-CGA-O2A-C1
33	D	618	LMG	C4-C5-C6-O5
28	E	601	KC2	CAA-CBA-CGA-O1A
28	U	604	KC2	CAA-CBA-CGA-O2A
27	a	821	CLA	C10-C11-C12-C13
27	a	824	CLA	C5-C6-C7-C8
27	b	701	CLA	C5-C6-C7-C8
33	D	619	LMG	C2-C1-O1-C7
35	K	614	DGD	C2E-C1E-O5D-C6D
35	K	614	DGD	O1G-C1G-C2G-O2G
27	A	605	CLA	C4-C3-C5-C6
27	D	607	CLA	C2-C3-C5-C6
27	F	606	CLA	C6-C7-C8-C9
27	F	617	CLA	C6-C7-C8-C9
27	H	319	CLA	C14-C13-C15-C16
27	K	605	CLA	C11-C10-C8-C9
27	a	804	CLA	C11-C10-C8-C9
27	a	816	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	a	821	CLA	C11-C10-C8-C9
27	a	825	CLA	C6-C7-C8-C9
27	a	827	CLA	C6-C7-C8-C9
27	a	827	CLA	C11-C12-C13-C14
27	b	708	CLA	C6-C7-C8-C9
27	l	409	CLA	C11-C12-C13-C14
37	a	832	PQN	C21-C22-C23-C24
37	b	729	PQN	C21-C22-C23-C24
27	b	719	CLA	C10-C11-C12-C13
29	j	204	UIX	C7-C10-C11-C12
30	A	617	DD6	C12-C11-C13-C14
30	B	614	DD6	C12-C11-C13-C14
30	D	621	DD6	C7-C6-C8-C9
30	G	613	DD6	C12-C11-C13-C14
30	K	610	DD6	C12-C11-C13-C14
38	a	833	BCR	C36-C18-C19-C20
38	j	203	BCR	C7-C8-C9-C34
38	j	203	BCR	C37-C22-C23-C24
38	l	415	BCR	C37-C22-C23-C24
29	j	204	UIX	C7-C10-C11-C13
30	D	621	DD6	C5-C6-C8-C9
30	G	613	DD6	C10-C11-C13-C14
30	K	610	DD6	C10-C11-C13-C14
38	a	833	BCR	C17-C18-C19-C20
38	j	203	BCR	C7-C8-C9-C10
38	l	415	BCR	C21-C22-C23-C24
38	m	201	BCR	C21-C22-C23-C24
34	r	202	LHG	O9-C7-O7-C5
35	f	305	DGD	C4E-C5E-C6E-O5E
33	K	613	LMG	C10-C11-C12-C13
37	b	729	PQN	C25-C26-C27-C28
34	F	618	LHG	C9-C10-C11-C12
28	C	210	KC2	CAA-CBA-CGA-O1A
28	E	601	KC2	CAA-CBA-CGA-O2A
28	J	602	KC2	CAA-CBA-CGA-O1A
28	J	602	KC2	CAA-CBA-CGA-O2A
28	T	608	KC2	CAA-CBA-CGA-O2A
28	U	604	KC2	CAA-CBA-CGA-O1A
27	b	703	CLA	CBA-CGA-O2A-C1
27	I	603	CLA	C13-C15-C16-C17
27	a	807	CLA	C8-C10-C11-C12
33	b	733	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
34	j	205	LHG	C7-C8-C9-C10
27	G	606	CLA	C15-C16-C17-C18
27	a	820	CLA	C15-C16-C17-C18
27	a	830	CLA	C8-C10-C11-C12
29	B	611	UIX	O4-C27-O2-C18
34	l	401	LHG	O1-C1-C2-O2
27	a	823	CLA	C10-C11-C12-C13
27	b	718	CLA	C10-C11-C12-C13
27	b	725	CLA	C5-C6-C7-C8
32	U	608	PID	C26-C27-O6-C30
28	C	210	KC2	CAA-CBA-CGA-O2A
28	H	311	KC2	CAA-CBA-CGA-O1A
28	T	608	KC2	CAA-CBA-CGA-O1A
27	K	602	CLA	C2-C1-O2A-CGA
27	a	839	CLA	C8-C10-C11-C12
33	b	733	LMG	C10-C11-C12-C13
27	b	702	CLA	CBD-CGD-O2D-CED
27	b	722	CLA	O2A-C1-C2-C3
27	f	302	CLA	O2A-C1-C2-C3
27	I	601	CLA	C10-C11-C12-C13
27	G	606	CLA	C11-C12-C13-C15
38	a	836	BCR	C9-C10-C11-C12
27	F	610	CLA	C2A-CAA-CBA-CGA
27	a	818	CLA	C2A-CAA-CBA-CGA
27	b	716	CLA	C8-C10-C11-C12
27	l	412	CLA	C13-C15-C16-C17
37	b	729	PQN	C15-C16-C17-C18
28	H	311	KC2	CAA-CBA-CGA-O2A
33	l	417	LMG	O6-C5-C6-O5
27	I	603	CLA	O1A-CGA-O2A-C1
27	b	703	CLA	C8-C10-C11-C12
27	a	823	CLA	C3-C5-C6-C7
27	b	704	CLA	C3-C5-C6-C7
27	D	607	CLA	C5-C6-C7-C8
27	H	309	CLA	C10-C11-C12-C13
27	a	818	CLA	C5-C6-C7-C8
27	a	804	CLA	C13-C15-C16-C17
27	l	406	CLA	C10-C11-C12-C13
27	l	409	CLA	C5-C6-C7-C8
37	a	832	PQN	C18-C20-C21-C22
27	H	306	CLA	C2C-C3C-CAC-CBC
34	D	620	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	B	603	CLA	C8-C10-C11-C12
27	K	602	CLA	C5-C6-C7-C8
27	b	706	CLA	C15-C16-C17-C18
37	b	729	PQN	C18-C20-C21-C22
32	J	615	PID	C26-C27-O6-C30
34	D	620	LHG	C3-O3-P-O6
34	D	620	LHG	C4-O6-P-O3
34	F	618	LHG	C4-O6-P-O3
34	a	835	LHG	C3-O3-P-O6
34	r	202	LHG	C3-O3-P-O6
27	G	606	CLA	C5-C6-C7-C8
27	a	829	CLA	C15-C16-C17-C18
27	l	407	CLA	O2A-C1-C2-C3
27	r	203	CLA	O2A-C1-C2-C3
27	T	603	CLA	C4C-C3C-CAC-CBC
27	b	704	CLA	C5-C6-C7-C8
32	F	615	PID	C28-C27-O6-C30
31	H	320	SQD	C24-C23-O48-C46
27	D	611	CLA	C5-C6-C7-C8
35	f	305	DGD	C1B-C2B-C3B-C4B
34	G	617	LHG	C23-C24-C25-C26
33	D	618	LMG	C17-C18-C19-C20
35	l	416	DGD	C4B-C5B-C6B-C7B
27	H	304	CLA	C3-C5-C6-C7
33	K	613	LMG	C17-C18-C19-C20
33	K	613	LMG	C20-C21-C22-C23
33	b	733	LMG	C34-C35-C36-C37
34	G	617	LHG	C10-C11-C12-C13
33	D	619	LMG	C11-C12-C13-C14
33	l	417	LMG	C17-C18-C19-C20
33	l	417	LMG	C21-C22-C23-C24
34	D	620	LHG	C12-C13-C14-C15
33	C	217	LMG	C7-C8-O7-C10
33	D	618	LMG	C9-C8-O7-C10
35	f	305	DGD	C1A-C2A-C3A-C4A
31	H	320	SQD	C24-C25-C26-C27
35	j	201	DGD	C4A-C5A-C6A-C7A
34	G	617	LHG	C2-C3-O3-P
27	a	804	CLA	O1A-CGA-O2A-C1
33	D	619	LMG	C21-C22-C23-C24
35	K	614	DGD	C6B-C7B-C8B-C9B
27	B	607	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	J	605	CLA	C3-C5-C6-C7
27	a	816	CLA	C3-C5-C6-C7
35	f	305	DGD	C2E-C1E-O5D-C6D
33	D	619	LMG	C22-C23-C24-C25
27	b	713	CLA	C5-C6-C7-C8
27	l	409	CLA	C10-C11-C12-C13
27	b	703	CLA	O1A-CGA-O2A-C1
31	H	320	SQD	O10-C23-O48-C46
27	b	707	CLA	C16-C17-C18-C19
37	b	729	PQN	C26-C27-C28-C29
33	b	733	LMG	C31-C32-C33-C34
35	f	305	DGD	C5B-C6B-C7B-C8B
36	T	613	LMU	C5'-C4'-O1B-C1B
35	K	614	DGD	C4E-C5E-C6E-O5E
27	A	605	CLA	C2-C3-C5-C6
27	C	207	CLA	C11-C10-C8-C9
27	G	608	CLA	C11-C10-C8-C9
27	b	702	CLA	C14-C13-C15-C16
27	b	705	CLA	C11-C10-C8-C9
27	b	725	CLA	C11-C12-C13-C14
32	F	615	PID	C26-C27-O6-C30
34	r	202	LHG	C23-C24-C25-C26
27	F	604	CLA	C4C-C3C-CAC-CBC
33	D	619	LMG	C16-C17-C18-C19
34	a	835	LHG	C10-C11-C12-C13
34	j	205	LHG	C25-C26-C27-C28
34	r	202	LHG	C24-C25-C26-C27
34	r	202	LHG	C27-C28-C29-C30
28	G	601	KC2	CAA-CBA-CGA-O1A
28	G	601	KC2	CAA-CBA-CGA-O2A
27	T	603	CLA	C2A-CAA-CBA-CGA
27	a	819	CLA	C2A-CAA-CBA-CGA
27	b	712	CLA	C2A-CAA-CBA-CGA
38	a	836	BCR	C11-C12-C13-C35
38	m	201	BCR	C37-C22-C23-C24
34	r	202	LHG	C28-C29-C30-C31
34	j	205	LHG	O1-C1-C2-C3
34	l	401	LHG	O1-C1-C2-C3
38	a	834	BCR	C11-C12-C13-C14
38	a	836	BCR	C11-C12-C13-C14
38	b	731	BCR	C7-C8-C9-C10
27	G	606	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	I	610	CLA	C3-C5-C6-C7
27	a	827	CLA	C5-C6-C7-C8
33	C	217	LMG	C15-C16-C17-C18
34	a	835	LHG	C24-C25-C26-C27
33	C	217	LMG	C14-C15-C16-C17
35	j	201	DGD	CCB-CDB-CEB-CFB
35	l	416	DGD	CEB-CFB-CGB-CHB
27	D	603	CLA	C6-C7-C8-C9
27	D	603	CLA	C6-C7-C8-C10
37	a	832	PQN	C20-C21-C22-C23
29	F	613	UIX	C17-C18-O2-C27
33	K	613	LMG	C12-C13-C14-C15
31	y	301	SQD	C25-C26-C27-C28
34	a	835	LHG	C11-C10-C9-C8
34	r	202	LHG	C9-C10-C11-C12
35	K	614	DGD	C4B-C5B-C6B-C7B
35	j	201	DGD	C2A-C3A-C4A-C5A
27	A	611	CLA	C3A-C2A-CAA-CBA
27	C	205	CLA	C3A-C2A-CAA-CBA
27	E	605	CLA	C3A-C2A-CAA-CBA
27	F	610	CLA	C3A-C2A-CAA-CBA
27	T	602	CLA	C3A-C2A-CAA-CBA
27	a	805	CLA	C3A-C2A-CAA-CBA
27	a	808	CLA	C3A-C2A-CAA-CBA
27	a	812	CLA	C3A-C2A-CAA-CBA
27	a	821	CLA	C3A-C2A-CAA-CBA
27	b	708	CLA	C3A-C2A-CAA-CBA
27	F	605	CLA	C2C-C3C-CAC-CBC
34	r	202	LHG	C18-C19-C20-C21
33	l	417	LMG	C13-C14-C15-C16
34	a	835	LHG	C4-C5-C6-O8
27	b	724	CLA	O2A-C1-C2-C3
27	D	603	CLA	C3-C5-C6-C7
27	E	611	CLA	C3-C5-C6-C7
31	y	301	SQD	C10-C11-C12-C13
31	y	301	SQD	C11-C12-C13-C14
33	D	619	LMG	C12-C13-C14-C15
34	D	620	LHG	C18-C19-C20-C21
35	K	614	DGD	C7B-C8B-C9B-CAB
27	a	830	CLA	C4-C3-C5-C6
29	A	616	UIX	C17-C18-O2-C27
27	K	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	r	204	CLA	C10-C11-C12-C13
33	D	618	LMG	C13-C14-C15-C16
33	F	616	LMG	C23-C24-C25-C26
34	l	401	LHG	C11-C10-C9-C8
35	f	305	DGD	C8B-C9B-CAB-CBB
27	H	308	CLA	C3-C5-C6-C7
33	D	618	LMG	C14-C15-C16-C17
33	b	733	LMG	C19-C20-C21-C22
27	F	606	CLA	C13-C15-C16-C17
27	U	603	CLA	C2-C1-O2A-CGA
35	l	416	DGD	C9B-CAB-CBB-CCB
27	l	409	CLA	C3-C5-C6-C7
38	a	834	BCR	C5-C6-C7-C8
38	a	836	BCR	C1-C6-C7-C8
38	a	836	BCR	C5-C6-C7-C8
38	a	836	BCR	C23-C24-C25-C30
38	b	731	BCR	C1-C6-C7-C8
38	f	301	BCR	C1-C6-C7-C8
38	f	301	BCR	C5-C6-C7-C8
38	i	201	BCR	C23-C24-C25-C26
38	j	203	BCR	C23-C24-C25-C26
38	l	414	BCR	C5-C6-C7-C8
38	l	415	BCR	C1-C6-C7-C8
38	m	201	BCR	C5-C6-C7-C8
34	l	401	LHG	C28-C29-C30-C31
34	F	618	LHG	C12-C13-C14-C15
27	a	816	CLA	C4-C3-C5-C6
27	F	606	CLA	C11-C10-C8-C7
27	a	816	CLA	C2-C3-C5-C6
27	a	821	CLA	C11-C10-C8-C7
27	a	825	CLA	C6-C7-C8-C10
27	a	829	CLA	C11-C12-C13-C15
27	a	830	CLA	C2-C3-C5-C6
27	a	830	CLA	C11-C10-C8-C7
27	b	706	CLA	C11-C10-C8-C7
27	b	708	CLA	C6-C7-C8-C10
27	l	403	CLA	C6-C7-C8-C10
37	b	729	PQN	C21-C22-C23-C25
33	D	618	LMG	C11-C12-C13-C14
33	b	733	LMG	C35-C36-C37-C38
37	b	729	PQN	C26-C27-C28-C30
35	f	305	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
34	F	618	LHG	C24-C23-O8-C6
34	a	835	LHG	C24-C23-O8-C6
27	b	713	CLA	C2A-CAA-CBA-CGA
27	b	726	CLA	C2A-CAA-CBA-CGA
27	F	601	CLA	C8-C10-C11-C12
27	a	804	CLA	C10-C11-C12-C13
27	b	718	CLA	C13-C15-C16-C17
27	l	412	CLA	C10-C11-C12-C13
27	B	606	CLA	C13-C15-C16-C17
27	b	702	CLA	C5-C6-C7-C8
33	b	733	LMG	C36-C37-C38-C39
28	A	608	KC2	C2B-C3B-CAB-CBB
28	E	601	KC2	C2B-C3B-CAB-CBB
28	E	601	KC2	C2C-C3C-CAC-CBC
28	E	610	KC2	C2C-C3C-CAC-CBC
28	F	609	KC2	C2B-C3B-CAB-CBB
28	H	311	KC2	C2B-C3B-CAB-CBB
28	H	311	KC2	C2C-C3C-CAC-CBC
28	J	608	KC2	C2C-C3C-CAC-CBC
28	J	610	KC2	C2B-C3B-CAB-CBB
28	J	610	KC2	C2C-C3C-CAC-CBC
28	K	607	KC2	C2C-C3C-CAC-CBC
27	H	306	CLA	C4C-C3C-CAC-CBC
31	H	320	SQD	C8-C7-O47-C45
34	D	620	LHG	C8-C7-O7-C5
28	E	601	KC2	C4B-C3B-CAB-CBB
28	E	601	KC2	C4C-C3C-CAC-CBC
28	E	610	KC2	C4C-C3C-CAC-CBC
28	F	609	KC2	C4B-C3B-CAB-CBB
28	H	311	KC2	C4B-C3B-CAB-CBB
28	J	610	KC2	C4B-C3B-CAB-CBB
28	J	610	KC2	C4C-C3C-CAC-CBC
28	K	607	KC2	C4C-C3C-CAC-CBC
27	J	603	CLA	C5-C6-C7-C8
27	b	727	CLA	C8-C10-C11-C12
31	H	320	SQD	O49-C7-O47-C45
34	D	620	LHG	O9-C7-O7-C5
29	A	616	UIX	C19-C18-O2-C27
34	F	618	LHG	C26-C27-C28-C29
27	b	705	CLA	C5-C6-C7-C8
27	b	717	CLA	C10-C11-C12-C13
35	j	201	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
35	l	416	DGD	CBB-CCB-CDB-CEB
36	T	613	LMU	O5B-C5B-C6B-O6B
30	B	614	DD6	C27-C29-C30-C31
30	E	613	DD6	C27-C29-C30-C31
30	E	615	DD6	C27-C29-C30-C31
30	I	613	DD6	C27-C29-C30-C31
30	K	610	DD6	C27-C29-C30-C31
30	r	206	DD6	C27-C29-C30-C31
27	F	606	CLA	C11-C10-C8-C9
27	H	319	CLA	C6-C7-C8-C9
27	a	830	CLA	C11-C10-C8-C9
27	l	412	CLA	C11-C12-C13-C14
27	B	606	CLA	C2A-CAA-CBA-CGA
27	b	724	CLA	C2A-CAA-CBA-CGA
33	F	616	LMG	C30-C31-C32-C33
34	G	617	LHG	C11-C10-C9-C8
34	r	202	LHG	C31-C32-C33-C34
38	l	413	BCR	C17-C18-C19-C20
27	A	605	CLA	C1A-C2A-CAA-CBA
27	A	611	CLA	C1A-C2A-CAA-CBA
27	B	601	CLA	C1A-C2A-CAA-CBA
27	C	205	CLA	C1A-C2A-CAA-CBA
27	D	601	CLA	C1A-C2A-CAA-CBA
27	D	612	CLA	C1A-C2A-CAA-CBA
27	F	607	CLA	C1A-C2A-CAA-CBA
27	F	608	CLA	C1A-C2A-CAA-CBA
27	G	607	CLA	C1A-C2A-CAA-CBA
27	H	310	CLA	C1A-C2A-CAA-CBA
27	K	603	CLA	C1A-C2A-CAA-CBA
27	T	602	CLA	C1A-C2A-CAA-CBA
27	T	607	CLA	C1A-C2A-CAA-CBA
27	a	805	CLA	C1A-C2A-CAA-CBA
27	a	808	CLA	C1A-C2A-CAA-CBA
27	a	813	CLA	C1A-C2A-CAA-CBA
27	a	821	CLA	C1A-C2A-CAA-CBA
27	a	822	CLA	C1A-C2A-CAA-CBA
27	b	717	CLA	C1A-C2A-CAA-CBA
27	b	724	CLA	C1A-C2A-CAA-CBA
27	b	707	CLA	C16-C17-C18-C20
34	a	835	LHG	C16-C17-C18-C19
27	U	605	CLA	C10-C11-C12-C13
32	F	614	PID	C26-C27-O6-C30

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Mol	Chain	Res	Type	Atoms
34	l	401	LHG	C4-O6-P-O3
34	D	620	LHG	C14-C15-C16-C17
27	G	608	CLA	C5-C6-C7-C8
34	l	401	LHG	C18-C19-C20-C21
27	D	604	CLA	C6-C7-C8-C9
27	H	313	CLA	C3-C5-C6-C7
27	E	604	CLA	C4-C3-C5-C6
27	E	604	CLA	C2-C3-C5-C6
27	F	603	CLA	C2-C3-C5-C6
27	I	611	CLA	C3A-C2A-CAA-CBA
27	b	713	CLA	C8-C10-C11-C12
34	a	835	LHG	O10-C23-O8-C6
33	l	417	LMG	C23-C24-C25-C26
27	l	406	CLA	C2A-CAA-CBA-CGA
36	T	613	LMU	O5'-C5'-C6'-O6'
31	H	320	SQD	O6-C44-C45-C46
33	l	417	LMG	O1-C7-C8-C9
34	D	620	LHG	C4-C5-C6-O8
34	l	401	LHG	C4-C5-C6-O8
35	f	305	DGD	O1G-C1G-C2G-C3G
34	D	620	LHG	C19-C20-C21-C22
35	f	305	DGD	C5D-C6D-O5D-C1E
31	H	320	SQD	C27-C28-C29-C30
27	a	805	CLA	C8-C10-C11-C12
34	j	205	LHG	C13-C14-C15-C16
35	K	614	DGD	O6E-C5E-C6E-O5E
34	F	618	LHG	O1-C1-C2-O2
27	a	811	CLA	O2A-C1-C2-C3
33	D	618	LMG	C28-C29-C30-C31
27	E	606	CLA	C8-C10-C11-C12
34	F	618	LHG	O10-C23-O8-C6
33	K	613	LMG	C24-C25-C26-C27
27	F	603	CLA	C4-C3-C5-C6
27	K	604	CLA	C2C-C3C-CAC-CBC
34	F	618	LHG	C24-C25-C26-C27
33	l	417	LMG	C10-C11-C12-C13
27	I	605	CLA	CBA-CGA-O2A-C1
27	K	605	CLA	CBA-CGA-O2A-C1
27	B	607	CLA	C8-C10-C11-C12
27	H	304	CLA	C8-C10-C11-C12
27	a	825	CLA	C15-C16-C17-C18
31	H	320	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	H	320	SQD	C44-C45-O47-C7
33	K	613	LMG	O6-C5-C6-O5
27	H	306	CLA	C2A-CAA-CBA-CGA
27	F	606	CLA	C2-C1-O2A-CGA
27	b	728	CLA	C2-C1-O2A-CGA
35	f	305	DGD	CDB-CEB-CFB-CGB
35	j	201	DGD	CFB-CGB-CHB-CIB
37	b	729	PQN	C13-C15-C16-C17
33	l	417	LMG	C29-C30-C31-C32
35	l	416	DGD	C3B-C4B-C5B-C6B
33	F	616	LMG	C18-C19-C20-C21
34	l	401	LHG	C19-C20-C21-C22
35	K	614	DGD	C3B-C4B-C5B-C6B
27	l	406	CLA	C8-C10-C11-C12
34	r	202	LHG	C11-C10-C9-C8
27	b	706	CLA	C10-C11-C12-C13
31	A	618	SQD	C2-C1-O6-C44
34	a	835	LHG	O7-C5-C6-O8
27	D	604	CLA	C4-C3-C5-C6
33	b	733	LMG	C14-C15-C16-C17
27	F	606	CLA	C2-C3-C5-C6
27	H	319	CLA	C6-C7-C8-C10
27	I	601	CLA	C11-C12-C13-C15
27	U	605	CLA	C11-C10-C8-C7
27	a	823	CLA	C11-C12-C13-C15
27	a	827	CLA	C6-C7-C8-C10
27	l	409	CLA	C11-C12-C13-C15
27	l	412	CLA	C11-C12-C13-C15
37	a	832	PQN	C21-C22-C23-C25
27	I	601	CLA	C11-C12-C13-C14
27	U	605	CLA	C11-C10-C8-C9
27	a	823	CLA	C11-C12-C13-C14
27	a	829	CLA	C11-C12-C13-C14
27	b	709	CLA	C11-C12-C13-C14
27	l	403	CLA	C6-C7-C8-C9
37	b	729	PQN	C24-C23-C25-C26
27	E	607	CLA	CBA-CGA-O2A-C1
27	K	602	CLA	CBA-CGA-O2A-C1
38	m	201	BCR	C7-C8-C9-C34
27	F	605	CLA	C4C-C3C-CAC-CBC
38	f	301	BCR	C7-C8-C9-C10
38	m	201	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
35	K	614	DGD	C2A-C3A-C4A-C5A
27	b	715	CLA	C5-C6-C7-C8
35	l	416	DGD	C4A-C5A-C6A-C7A
27	B	606	CLA	C5-C6-C7-C8
27	b	714	CLA	O2A-C1-C2-C3
27	D	602	CLA	C6-C7-C8-C10
34	G	617	LHG	O6-C4-C5-C6
34	r	202	LHG	O6-C4-C5-C6
34	j	205	LHG	C11-C10-C9-C8
27	a	823	CLA	C8-C10-C11-C12
27	F	606	CLA	C4-C3-C5-C6
27	D	604	CLA	C2-C3-C5-C6
33	D	618	LMG	C12-C13-C14-C15
33	F	616	LMG	C31-C32-C33-C34
27	b	717	CLA	CBA-CGA-O2A-C1
27	A	610	CLA	C3A-C2A-CAA-CBA
27	F	605	CLA	C3A-C2A-CAA-CBA
27	K	608	CLA	C3A-C2A-CAA-CBA
27	a	807	CLA	C3A-C2A-CAA-CBA
27	l	412	CLA	C3A-C2A-CAA-CBA
38	f	301	BCR	C9-C10-C11-C12
27	a	821	CLA	C8-C10-C11-C12
34	l	401	LHG	C12-C13-C14-C15
35	f	305	DGD	C2A-C1A-O1G-C1G
27	H	305	CLA	C5-C6-C7-C8
27	b	715	CLA	C8-C10-C11-C12
31	A	618	SQD	C44-C45-C46-O48
33	D	618	LMG	O1-C7-C8-C9
33	D	619	LMG	O1-C7-C8-C9
33	K	613	LMG	C7-C8-C9-O8
34	G	617	LHG	C4-C5-C6-O8
34	r	202	LHG	C4-C5-C6-O8
35	K	614	DGD	O1G-C1G-C2G-C3G
27	I	610	CLA	O2A-C1-C2-C3
34	G	617	LHG	C14-C15-C16-C17
27	b	725	CLA	C4-C3-C5-C6
27	b	725	CLA	C2-C3-C5-C6
27	J	609	CLA	C2C-C3C-CAC-CBC
32	K	611	PID	C28-C27-O6-C30
34	l	401	LHG	C3-O3-P-O6
27	U	603	CLA	O1D-CGD-O2D-CED
27	I	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
34	G	617	LHG	O1-C1-C2-O2
31	H	320	SQD	C7-C8-C9-C10
27	D	604	CLA	C6-C7-C8-C10
27	a	828	CLA	CAA-CBA-CGA-O2A
33	l	417	LMG	C18-C19-C20-C21
35	l	416	DGD	O1A-C1A-O1G-C1G
27	I	605	CLA	C3-C5-C6-C7
33	D	618	LMG	O1-C7-C8-O7
33	D	619	LMG	O1-C7-C8-O7
33	b	733	LMG	O1-C7-C8-O7
35	j	201	DGD	O1G-C1G-C2G-O2G
33	C	217	LMG	C11-C12-C13-C14
35	l	416	DGD	CFB-CGB-CHB-CIB
31	A	618	SQD	O5-C1-O6-C44
27	a	829	CLA	C4-C3-C5-C6
27	F	619	CLA	C2-C1-O2A-CGA
27	a	815	CLA	C2-C1-O2A-CGA
27	a	830	CLA	C2-C1-O2A-CGA
27	a	839	CLA	C2-C1-O2A-CGA
27	B	603	CLA	C14-C13-C15-C16
27	H	313	CLA	C6-C7-C8-C9
27	I	616	CLA	C11-C12-C13-C14
27	a	819	CLA	C11-C10-C8-C9
27	a	820	CLA	C14-C13-C15-C16
27	a	823	CLA	C6-C7-C8-C9
34	j	205	LHG	C2-C3-O3-P
38	b	731	BCR	C5-C6-C7-C8
38	f	304	BCR	C23-C24-C25-C30
38	j	203	BCR	C1-C6-C7-C8
38	j	203	BCR	C23-C24-C25-C30
38	f	301	BCR	C7-C8-C9-C34
27	H	312	CLA	C1A-C2A-CAA-CBA
38	j	203	BCR	C21-C22-C23-C24
35	K	614	DGD	O6D-C5D-C6D-O5D
27	a	813	CLA	O2A-C1-C2-C3
27	E	606	CLA	C5-C6-C7-C8
33	l	417	LMG	C34-C35-C36-C37
27	D	602	CLA	C6-C7-C8-C9
33	b	733	LMG	C4-C5-C6-O5
34	D	620	LHG	O6-C4-C5-C6
27	B	603	CLA	C12-C13-C15-C16
27	B	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	E	607	CLA	C12-C13-C15-C16
27	H	319	CLA	C12-C13-C15-C16
27	a	804	CLA	C6-C7-C8-C10
27	a	820	CLA	C6-C7-C8-C10
27	a	824	CLA	C11-C12-C13-C15
27	a	829	CLA	C12-C13-C15-C16
27	b	701	CLA	C11-C12-C13-C15
27	b	702	CLA	C12-C13-C15-C16
27	b	723	CLA	C11-C10-C8-C7
27	b	727	CLA	C11-C12-C13-C15
27	b	728	CLA	C12-C13-C15-C16
38	b	731	BCR	C9-C10-C11-C12
38	m	201	BCR	C9-C10-C11-C12
33	b	733	LMG	C23-C24-C25-C26
35	K	614	DGD	C1B-C2B-C3B-C4B
33	K	613	LMG	C15-C16-C17-C18
33	D	619	LMG	C30-C31-C32-C33
27	F	606	CLA	CBA-CGA-O2A-C1
34	a	835	LHG	C31-C32-C33-C34
33	l	417	LMG	C12-C13-C14-C15
27	A	609	CLA	CAD-CBD-CGD-O2D
27	A	611	CLA	CAD-CBD-CGD-O2D
27	A	612	CLA	CAD-CBD-CGD-O2D
27	E	606	CLA	CAD-CBD-CGD-O2D
27	E	607	CLA	CAD-CBD-CGD-O2D
27	F	607	CLA	CAD-CBD-CGD-O2D
27	I	601	CLA	CAD-CBD-CGD-O2D
27	K	602	CLA	CAD-CBD-CGD-O2D
27	a	805	CLA	CAD-CBD-CGD-O2D
27	a	811	CLA	CAD-CBD-CGD-O2D
27	a	816	CLA	CAD-CBD-CGD-O2D
27	a	824	CLA	CAD-CBD-CGD-O2D
27	a	827	CLA	CAD-CBD-CGD-O2D
27	b	706	CLA	CAD-CBD-CGD-O2D
27	b	719	CLA	CAD-CBD-CGD-O2D
27	b	723	CLA	CAD-CBD-CGD-O2D
27	b	726	CLA	CAD-CBD-CGD-O2D
27	b	727	CLA	CAD-CBD-CGD-O2D
27	l	411	CLA	CAD-CBD-CGD-O2D
28	F	609	KC2	C2C-C3C-CAC-CBC
28	H	302	KC2	C2C-C3C-CAC-CBC
28	J	602	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	K	607	KC2	CAD-CBD-CGD-O2D
28	U	604	KC2	C2B-C3B-CAB-CBB
33	l	417	LMG	C9-C8-O7-C10
35	j	201	DGD	C6B-C7B-C8B-C9B
27	H	304	CLA	C5-C6-C7-C8
34	a	835	LHG	C15-C16-C17-C18
27	H	305	CLA	C4-C3-C5-C6
35	K	614	DGD	O6E-C1E-O5D-C6D
33	b	733	LMG	O1-C7-C8-C9
35	l	416	DGD	O1G-C1G-C2G-C3G
27	K	605	CLA	O1A-CGA-O2A-C1
34	G	617	LHG	O6-C4-C5-O7
27	J	605	CLA	C5-C6-C7-C8
29	T	612	UIX	C17-C18-O2-C27
29	T	612	UIX	C19-C18-O2-C27
33	D	619	LMG	C31-C32-C33-C34
27	B	603	CLA	C2A-CAA-CBA-CGA
27	b	716	CLA	C16-C17-C18-C20
27	A	604	CLA	CHA-CBD-CGD-O1D
27	A	604	CLA	CHA-CBD-CGD-O2D
27	B	603	CLA	CHA-CBD-CGD-O1D
27	B	603	CLA	CHA-CBD-CGD-O2D
27	C	205	CLA	CHA-CBD-CGD-O1D
27	C	206	CLA	CHA-CBD-CGD-O1D
27	D	601	CLA	CHA-CBD-CGD-O1D
27	D	601	CLA	CHA-CBD-CGD-O2D
27	D	602	CLA	CHA-CBD-CGD-O1D
27	D	604	CLA	CHA-CBD-CGD-O1D
27	D	604	CLA	CHA-CBD-CGD-O2D
27	D	611	CLA	CHA-CBD-CGD-O2D
27	F	610	CLA	CHA-CBD-CGD-O1D
27	G	603	CLA	CHA-CBD-CGD-O1D
27	G	603	CLA	CHA-CBD-CGD-O2D
27	G	610	CLA	CHA-CBD-CGD-O1D
27	G	610	CLA	CHA-CBD-CGD-O2D
27	H	305	CLA	CHA-CBD-CGD-O1D
27	H	305	CLA	CHA-CBD-CGD-O2D
27	H	307	CLA	CHA-CBD-CGD-O1D
27	H	307	CLA	CHA-CBD-CGD-O2D
27	H	312	CLA	CHA-CBD-CGD-O1D
27	H	312	CLA	CHA-CBD-CGD-O2D
27	J	607	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	T	601	CLA	CHA-CBD-CGD-O1D
27	T	601	CLA	CHA-CBD-CGD-O2D
27	U	601	CLA	CHA-CBD-CGD-O1D
27	a	820	CLA	CHA-CBD-CGD-O1D
27	a	820	CLA	CHA-CBD-CGD-O2D
27	a	822	CLA	CHA-CBD-CGD-O1D
27	a	822	CLA	CHA-CBD-CGD-O2D
27	b	704	CLA	CHA-CBD-CGD-O1D
27	b	704	CLA	CHA-CBD-CGD-O2D
27	b	708	CLA	CHA-CBD-CGD-O1D
27	b	721	CLA	CHA-CBD-CGD-O1D
27	b	721	CLA	CHA-CBD-CGD-O2D
27	l	407	CLA	CHA-CBD-CGD-O1D
27	l	412	CLA	CHA-CBD-CGD-O1D
27	l	412	CLA	CHA-CBD-CGD-O2D
28	A	608	KC2	CHA-CBD-CGD-O1D
28	A	608	KC2	CHA-CBD-CGD-O2D
28	C	210	KC2	CHA-CBD-CGD-O1D
28	C	210	KC2	CHA-CBD-CGD-O2D
28	E	601	KC2	CHA-CBD-CGD-O1D
27	I	605	CLA	O1A-CGA-O2A-C1
35	f	305	DGD	O1A-C1A-O1G-C1G
33	b	733	LMG	C20-C21-C22-C23
31	A	618	SQD	O47-C45-C46-O48
27	b	706	CLA	C5-C6-C7-C8
27	I	608	CLA	C4-C3-C5-C6
27	E	607	CLA	O1A-CGA-O2A-C1
27	K	602	CLA	O1A-CGA-O2A-C1
27	a	829	CLA	C2-C3-C5-C6
30	A	614	DD6	C27-C29-C30-C31
30	B	612	DD6	C27-C29-C30-C31
30	G	616	DD6	C27-C29-C30-C31
30	H	301	DD6	C27-C29-C30-C31
27	r	204	CLA	C5-C6-C7-C8
27	B	606	CLA	C14-C13-C15-C16
27	a	820	CLA	C6-C7-C8-C9
27	a	824	CLA	C11-C12-C13-C14
27	b	702	CLA	C6-C7-C8-C9
27	b	724	CLA	C11-C12-C13-C14
27	b	724	CLA	C14-C13-C15-C16
27	b	727	CLA	C11-C12-C13-C14
27	b	728	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
33	b	733	LMG	C13-C14-C15-C16
28	J	608	KC2	CAA-CBA-CGA-O2A
27	D	611	CLA	C11-C12-C13-C14
27	a	801	CLA	CBD-CGD-O2D-CED
30	B	614	DD6	C10-C11-C13-C14
27	E	605	CLA	C1A-C2A-CAA-CBA
27	U	606	CLA	C1A-C2A-CAA-CBA
27	b	707	CLA	C1A-C2A-CAA-CBA
27	H	319	CLA	C15-C16-C17-C18
27	l	410	CLA	C2-C1-O2A-CGA
34	l	401	LHG	C26-C27-C28-C29
27	K	604	CLA	C4C-C3C-CAC-CBC
27	B	607	CLA	C4-C3-C5-C6
27	a	819	CLA	C4-C3-C5-C6
27	b	726	CLA	C4-C3-C5-C6
34	D	620	LHG	C4-O6-P-O4
34	F	618	LHG	C3-O3-P-O5
34	F	618	LHG	C4-O6-P-O5
34	G	617	LHG	C3-O3-P-O5
34	l	401	LHG	C4-O6-P-O4
34	l	401	LHG	C4-O6-P-O5
34	r	202	LHG	C3-O3-P-O4
27	a	829	CLA	C16-C17-C18-C19
34	j	205	LHG	C27-C28-C29-C30
28	J	608	KC2	CAA-CBA-CGA-O1A
35	j	201	DGD	C3A-C4A-C5A-C6A
27	a	828	CLA	O2A-C1-C2-C3
27	B	603	CLA	CAD-CBD-CGD-O1D
27	B	610	CLA	CAD-CBD-CGD-O1D
27	C	201	CLA	CAD-CBD-CGD-O1D
27	C	205	CLA	CAD-CBD-CGD-O1D
27	D	604	CLA	CAD-CBD-CGD-O1D
27	F	610	CLA	CAD-CBD-CGD-O1D
27	H	305	CLA	CAD-CBD-CGD-O1D
27	H	312	CLA	CAD-CBD-CGD-O1D
27	I	603	CLA	CAD-CBD-CGD-O1D
27	J	609	CLA	CAD-CBD-CGD-O1D
27	K	603	CLA	CAD-CBD-CGD-O1D
27	T	601	CLA	CAD-CBD-CGD-O1D
27	a	823	CLA	CAD-CBD-CGD-O1D
27	b	704	CLA	CAD-CBD-CGD-O1D
27	l	407	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	E	610	KC2	CAD-CBD-CGD-O1D
28	F	609	KC2	CAA-CBA-CGA-O1A
28	F	609	KC2	CAA-CBA-CGA-O2A
33	b	733	LMG	C22-C23-C24-C25
34	a	835	LHG	C27-C28-C29-C30
34	D	620	LHG	C1-C2-C3-O3
27	F	606	CLA	C6-C7-C8-C10
27	a	807	CLA	C6-C7-C8-C10
27	a	815	CLA	C6-C7-C8-C10
27	b	718	CLA	C3A-C2A-CAA-CBA
27	b	719	CLA	C11-C12-C13-C15
27	b	727	CLA	C6-C7-C8-C10
27	l	405	CLA	C6-C7-C8-C10
27	l	409	CLA	C11-C10-C8-C7
34	D	620	LHG	O6-C4-C5-O7
34	r	202	LHG	O6-C4-C5-O7
27	I	602	CLA	C3-C5-C6-C7
33	b	733	LMG	C38-C39-C40-C41
27	b	728	CLA	C13-C15-C16-C17
27	G	608	CLA	C11-C12-C13-C15
27	b	719	CLA	C3-C5-C6-C7
35	j	201	DGD	O1G-C1G-C2G-C3G
31	H	320	SQD	O6-C44-C45-O47
34	G	617	LHG	O7-C5-C6-O8
34	l	401	LHG	O7-C5-C6-O8
31	H	320	SQD	C45-C44-O6-C1
33	b	733	LMG	C8-C7-O1-C1
27	U	601	CLA	C2A-CAA-CBA-CGA
27	b	704	CLA	C15-C16-C17-C18
27	F	617	CLA	C4-C3-C5-C6
27	b	706	CLA	C4-C3-C5-C6
27	b	711	CLA	C4-C3-C5-C6
27	H	304	CLA	CBA-CGA-O2A-C1
27	l	402	CLA	C10-C11-C12-C13
27	C	207	CLA	C6-C7-C8-C9
27	E	607	CLA	C14-C13-C15-C16
27	a	829	CLA	C11-C10-C8-C9
27	a	830	CLA	C14-C13-C15-C16
27	b	701	CLA	C11-C12-C13-C14
27	b	716	CLA	C14-C13-C15-C16
27	b	723	CLA	C11-C10-C8-C9
27	b	727	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	l	409	CLA	C11-C10-C8-C9
27	b	717	CLA	O1A-CGA-O2A-C1
33	D	618	LMG	C16-C17-C18-C19
35	j	201	DGD	O6D-C5D-C6D-O5D
27	b	727	CLA	CAA-CBA-CGA-O2A
33	l	417	LMG	C24-C25-C26-C27
27	G	602	CLA	C6-C7-C8-C9
34	a	835	LHG	C25-C26-C27-C28
27	l	405	CLA	C10-C11-C12-C13
33	b	733	LMG	C17-C18-C19-C20
27	E	607	CLA	C4-C3-C5-C6
27	B	607	CLA	C2-C3-C5-C6
27	a	823	CLA	C5-C6-C7-C8
27	C	203	CLA	C16-C17-C18-C19
34	a	835	LHG	C18-C19-C20-C21
27	F	605	CLA	C2A-CAA-CBA-CGA
27	H	305	CLA	C2-C1-O2A-CGA
27	a	818	CLA	C2-C1-O2A-CGA
27	a	827	CLA	C2-C1-O2A-CGA
27	b	709	CLA	C2-C1-O2A-CGA
27	H	305	CLA	CBA-CGA-O2A-C1
29	H	317	UIX	C17-C18-O2-C27
27	b	709	CLA	C10-C11-C12-C13
27	a	817	CLA	C4-C3-C5-C6
27	I	608	CLA	C2-C3-C5-C6
27	b	726	CLA	C2-C3-C5-C6
33	K	613	LMG	C22-C23-C24-C25
34	a	835	LHG	C13-C14-C15-C16
27	C	203	CLA	C16-C17-C18-C20
27	B	605	CLA	C2A-CAA-CBA-CGA
34	G	617	LHG	C4-O6-P-O3
34	a	835	LHG	C4-O6-P-O3
33	D	619	LMG	C13-C14-C15-C16
27	b	702	CLA	C13-C15-C16-C17
27	U	603	CLA	C2C-C3C-CAC-CBC
27	b	704	CLA	C4-C3-C5-C6
27	a	825	CLA	C11-C12-C13-C15
27	b	705	CLA	C11-C10-C8-C7
27	b	709	CLA	C11-C12-C13-C15
27	F	602	CLA	CAA-CBA-CGA-O2A
27	b	706	CLA	C11-C10-C8-C9
34	r	202	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	E	610	KC2	CAA-CBA-CGA-O1A
31	y	301	SQD	C28-C29-C30-C31
34	l	401	LHG	C10-C11-C12-C13
38	b	731	BCR	C36-C18-C19-C20
27	G	602	CLA	C6-C7-C8-C10
27	a	829	CLA	C16-C17-C18-C20
34	a	835	LHG	O1-C1-C2-C3
34	D	620	LHG	O2-C2-C3-O3
34	l	401	LHG	O2-C2-C3-O3
27	a	813	CLA	CAA-CBA-CGA-O2A
34	l	401	LHG	C1-C2-C3-O3
27	E	607	CLA	C13-C15-C16-C17
27	C	207	CLA	C4-C3-C5-C6
27	F	606	CLA	O1A-CGA-O2A-C1
27	D	611	CLA	C11-C12-C13-C15
27	U	603	CLA	CBA-CGA-O2A-C1
35	j	201	DGD	O1A-C1A-O1G-C1G
29	H	317	UIX	C19-C18-O2-C27
27	b	728	CLA	C15-C16-C17-C18
27	B	601	CLA	C2A-CAA-CBA-CGA
38	a	836	BCR	C13-C14-C15-C16
38	j	203	BCR	C15-C16-C17-C18
34	l	401	LHG	C23-C24-C25-C26
27	F	604	CLA	CAA-CBA-CGA-O2A
34	F	618	LHG	O6-C4-C5-O7
27	J	609	CLA	C4C-C3C-CAC-CBC
28	H	302	KC2	C4C-C3C-CAC-CBC
28	T	608	KC2	C4B-C3B-CAB-CBB
34	F	618	LHG	C28-C29-C30-C31
27	H	304	CLA	CAA-CBA-CGA-O2A
27	D	602	CLA	C2-C1-O2A-CGA
27	F	617	CLA	C2-C1-O2A-CGA
27	K	605	CLA	C2-C1-O2A-CGA
27	U	605	CLA	C2-C1-O2A-CGA
27	b	702	CLA	C2-C1-O2A-CGA
27	r	203	CLA	C2-C1-O2A-CGA
35	l	416	DGD	C1A-C2A-C3A-C4A
27	a	801	CLA	C5-C6-C7-C8
27	G	607	CLA	C2A-CAA-CBA-CGA
27	I	603	CLA	C2A-CAA-CBA-CGA
27	I	606	CLA	C2A-CAA-CBA-CGA
27	a	837	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	b	701	CLA	C2A-CAA-CBA-CGA
27	b	704	CLA	C2A-CAA-CBA-CGA
27	b	705	CLA	C2A-CAA-CBA-CGA
33	C	217	LMG	O7-C8-C9-O8
34	F	618	LHG	O7-C5-C6-O8
35	l	416	DGD	O1G-C1G-C2G-O2G
28	E	610	KC2	CAA-CBA-CGA-O2A
27	A	604	CLA	C3A-C2A-CAA-CBA
27	A	612	CLA	C3A-C2A-CAA-CBA
27	B	603	CLA	C3A-C2A-CAA-CBA
27	F	602	CLA	C3A-C2A-CAA-CBA
27	H	305	CLA	C3A-C2A-CAA-CBA
27	a	827	CLA	C3A-C2A-CAA-CBA
27	a	828	CLA	C3A-C2A-CAA-CBA
27	b	710	CLA	C3A-C2A-CAA-CBA
27	b	714	CLA	C3A-C2A-CAA-CBA
27	b	727	CLA	C3A-C2A-CAA-CBA
27	E	605	CLA	CAA-CBA-CGA-O2A
27	b	719	CLA	C8-C10-C11-C12
38	a	834	BCR	C9-C10-C11-C12
38	a	836	BCR	C19-C20-C21-C22
27	l	409	CLA	C4-C3-C5-C6
27	F	617	CLA	C2-C3-C5-C6
27	b	706	CLA	C2-C3-C5-C6
30	A	615	DD6	C27-C29-C30-C31
30	J	612	DD6	C27-C29-C30-C31
34	D	620	LHG	C11-C12-C13-C14
27	B	601	CLA	C6-C7-C8-C9
27	C	204	CLA	C6-C7-C8-C9
27	a	807	CLA	C6-C7-C8-C9
27	b	715	CLA	C14-C13-C15-C16
27	b	718	CLA	C11-C10-C8-C9
34	j	205	LHG	C28-C29-C30-C31
27	B	605	CLA	CAA-CBA-CGA-O1A
27	H	303	CLA	C5-C6-C7-C8
34	j	205	LHG	C10-C11-C12-C13
34	F	618	LHG	C4-C5-C6-O8
38	f	304	BCR	C35-C13-C14-C15
38	l	415	BCR	C11-C10-C9-C34
27	b	701	CLA	C3-C5-C6-C7
27	B	605	CLA	CAA-CBA-CGA-O2A
27	F	617	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	D	612	CLA	O2A-C1-C2-C3
27	a	822	CLA	O2A-C1-C2-C3
27	b	701	CLA	O2A-C1-C2-C3
27	b	702	CLA	CBA-CGA-O2A-C1
27	E	605	CLA	CAA-CBA-CGA-O1A
33	K	613	LMG	C19-C20-C21-C22
33	b	733	LMG	C9-C8-O7-C10
34	F	618	LHG	C4-C5-O7-C7
27	A	609	CLA	C1A-C2A-CAA-CBA
27	A	610	CLA	C1A-C2A-CAA-CBA
27	I	601	CLA	C1A-C2A-CAA-CBA
27	a	814	CLA	C1A-C2A-CAA-CBA
27	l	412	CLA	C1A-C2A-CAA-CBA
33	D	618	LMG	C15-C16-C17-C18
27	B	609	CLA	C11-C12-C13-C15
27	E	607	CLA	C2-C3-C5-C6
27	K	605	CLA	C11-C10-C8-C7
27	a	816	CLA	C6-C7-C8-C10
27	a	823	CLA	C6-C7-C8-C10
38	l	414	BCR	C15-C16-C17-C18
27	H	307	CLA	CAA-CBA-CGA-O2A
27	l	409	CLA	C4C-C3C-CAC-CBC
27	b	710	CLA	C2A-CAA-CBA-CGA
27	b	728	CLA	C2A-CAA-CBA-CGA
27	b	718	CLA	C8-C10-C11-C12
33	b	733	LMG	C37-C38-C39-C40
27	B	606	CLA	CAA-CBA-CGA-O2A
28	E	601	KC2	C3A-C2A-CAA-CBA
28	H	311	KC2	C3A-C2A-CAA-CBA
28	J	606	KC2	C3A-C2A-CAA-CBA
33	D	619	LMG	C17-C18-C19-C20
27	B	603	CLA	C16-C17-C18-C20
27	F	604	CLA	CAA-CBA-CGA-O1A
33	F	616	LMG	C15-C16-C17-C18
34	l	401	LHG	C30-C31-C32-C33
27	a	837	CLA	C4-C3-C5-C6
27	b	713	CLA	C15-C16-C17-C18
33	D	619	LMG	C28-C29-C30-C31
27	C	207	CLA	C2-C3-C5-C6
27	H	305	CLA	C2-C3-C5-C6
38	f	304	BCR	C12-C13-C14-C15
38	l	415	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	H	307	CLA	CAA-CBA-CGA-O1A
27	U	606	CLA	CAA-CBA-CGA-O2A
27	b	701	CLA	C8-C10-C11-C12
27	E	606	CLA	C4-C3-C5-C6
27	H	304	CLA	C4-C3-C5-C6
27	a	805	CLA	C4-C3-C5-C6
27	I	610	CLA	C2-C1-O2A-CGA
27	a	817	CLA	C2-C3-C5-C6
27	a	819	CLA	C2-C3-C5-C6
27	b	711	CLA	C2-C3-C5-C6
27	b	718	CLA	C15-C16-C17-C18
27	F	606	CLA	C14-C13-C15-C16
27	b	703	CLA	C11-C10-C8-C9
27	r	204	CLA	C6-C7-C8-C9
27	H	305	CLA	O1A-CGA-O2A-C1
27	D	604	CLA	C2A-CAA-CBA-CGA
27	a	825	CLA	C2A-CAA-CBA-CGA
27	H	304	CLA	O1A-CGA-O2A-C1
38	b	731	BCR	C23-C24-C25-C30
38	b	732	BCR	C1-C6-C7-C8
38	l	413	BCR	C23-C24-C25-C30
34	l	401	LHG	C16-C17-C18-C19
27	l	409	CLA	C2C-C3C-CAC-CBC
38	l	414	BCR	C19-C20-C21-C22
27	G	606	CLA	C4-C3-C5-C6
27	H	308	CLA	C4-C3-C5-C6
27	a	815	CLA	C4-C3-C5-C6
27	l	412	CLA	C4-C3-C5-C6
35	f	305	DGD	C2B-C3B-C4B-C5B
27	b	704	CLA	C2-C3-C5-C6
27	a	801	CLA	CAA-CBA-CGA-O2A
27	E	611	CLA	C10-C11-C12-C13
27	T	602	CLA	CAA-CBA-CGA-O2A
27	U	606	CLA	CAA-CBA-CGA-O1A
27	a	827	CLA	C16-C17-C18-C19
27	a	828	CLA	CAA-CBA-CGA-O1A
27	I	609	CLA	CAA-CBA-CGA-O2A
27	l	408	CLA	C2-C1-O2A-CGA
34	F	618	LHG	O6-C4-C5-C6
27	H	309	CLA	C4-C3-C5-C6
27	b	723	CLA	C4-C3-C5-C6
27	b	727	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	a	837	CLA	C2-C3-C5-C6
27	b	702	CLA	C6-C7-C8-C10
27	l	409	CLA	C2-C3-C5-C6
27	E	609	CLA	CAA-CBA-CGA-O1A
27	r	204	CLA	CBA-CGA-O2A-C1
27	B	610	CLA	C2C-C3C-CAC-CBC
27	G	607	CLA	CAA-CBA-CGA-O1A
27	b	711	CLA	CAA-CBA-CGA-O2A
27	E	609	CLA	CAA-CBA-CGA-O2A
27	T	602	CLA	CAA-CBA-CGA-O1A
33	F	616	LMG	C10-C11-C12-C13
27	a	822	CLA	CAA-CBA-CGA-O2A
27	b	705	CLA	CAA-CBA-CGA-O2A
27	B	609	CLA	C4-C3-C5-C6
27	J	605	CLA	C4-C3-C5-C6
27	U	605	CLA	C4-C3-C5-C6
27	b	715	CLA	C4-C3-C5-C6
27	l	402	CLA	C4-C3-C5-C6
37	b	729	PQN	C14-C13-C15-C16
27	a	805	CLA	C2-C3-C5-C6
27	l	412	CLA	C2-C3-C5-C6
34	j	205	LHG	C24-C25-C26-C27
27	a	808	CLA	CAA-CBA-CGA-O2A
35	l	416	DGD	O1G-C1A-C2A-C3A
33	l	417	LMG	C33-C34-C35-C36
27	E	607	CLA	C11-C10-C8-C9
27	b	717	CLA	C14-C13-C15-C16
27	b	719	CLA	C6-C7-C8-C9
27	b	719	CLA	C11-C12-C13-C14
27	l	405	CLA	C6-C7-C8-C9
34	G	617	LHG	C24-C25-C26-C27
27	a	829	CLA	C3A-C2A-CAA-CBA
27	b	722	CLA	C3A-C2A-CAA-CBA
27	l	410	CLA	C3A-C2A-CAA-CBA
27	U	603	CLA	O1A-CGA-O2A-C1
27	a	804	CLA	CAA-CBA-CGA-O2A
35	l	416	DGD	C2A-C3A-C4A-C5A
27	T	607	CLA	CAA-CBA-CGA-O2A
27	A	606	CLA	CAD-CBD-CGD-O2D
27	C	204	CLA	CAD-CBD-CGD-O2D
27	D	612	CLA	CAD-CBD-CGD-O2D
27	E	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	F	603	CLA	CAD-CBD-CGD-O2D
27	G	604	CLA	CAD-CBD-CGD-O2D
27	G	605	CLA	CAD-CBD-CGD-O2D
27	G	611	CLA	CAD-CBD-CGD-O2D
27	H	304	CLA	CAD-CBD-CGD-O2D
27	I	609	CLA	CAD-CBD-CGD-O2D
27	K	604	CLA	CAD-CBD-CGD-O2D
27	T	602	CLA	CAD-CBD-CGD-O2D
27	U	606	CLA	CAD-CBD-CGD-O2D
27	a	806	CLA	CAD-CBD-CGD-O2D
27	a	808	CLA	CAD-CBD-CGD-O2D
27	a	821	CLA	CAD-CBD-CGD-O2D
27	a	826	CLA	CAD-CBD-CGD-O2D
27	a	829	CLA	CAD-CBD-CGD-O2D
27	b	711	CLA	CAD-CBD-CGD-O2D
28	B	602	KC2	C2C-C3C-CAC-CBC
28	J	602	KC2	CAD-CBD-CGD-O2D
28	J	604	KC2	CAD-CBD-CGD-O2D
28	T	608	KC2	CAD-CBD-CGD-O2D
28	U	602	KC2	CAD-CBD-CGD-O2D
27	T	606	CLA	C2A-CAA-CBA-CGA
27	b	727	CLA	C3-C5-C6-C7
27	C	204	CLA	CAA-CBA-CGA-O2A
27	G	603	CLA	CAA-CBA-CGA-O2A
27	l	408	CLA	CAA-CBA-CGA-O2A
27	E	608	CLA	C5-C6-C7-C8
27	U	605	CLA	C2-C3-C5-C6
27	a	805	CLA	CAA-CBA-CGA-O2A
29	A	616	UIX	O-C-C7-C10
30	C	216	DD6	C13-C14-C15-O1
30	H	301	DD6	C13-C14-C15-O1
30	T	611	DD6	C13-C14-C15-O1
30	i	202	DD6	C13-C14-C15-O1
32	F	614	PID	O1-C6-C7-C8
32	K	611	PID	O1-C6-C7-C8
35	K	614	DGD	C1G-C2G-C3G-O3G
27	F	607	CLA	CAA-CBA-CGA-O2A
33	D	619	LMG	C15-C16-C17-C18
27	D	611	CLA	C10-C11-C12-C13
27	B	609	CLA	CAA-CBA-CGA-O2A
27	I	601	CLA	CAA-CBA-CGA-O2A
27	b	722	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	A	605	CLA	O2A-C1-C2-C3
27	F	619	CLA	O2A-C1-C2-C3
27	I	602	CLA	O2A-C1-C2-C3
27	b	713	CLA	O2A-C1-C2-C3
27	b	723	CLA	O2A-C1-C2-C3
27	r	204	CLA	O2A-C1-C2-C3
28	B	602	KC2	C4C-C3C-CAC-CBC
28	F	609	KC2	C4C-C3C-CAC-CBC
28	T	608	KC2	C4C-C3C-CAC-CBC
28	U	604	KC2	C4B-C3B-CAB-CBB
27	F	617	CLA	CBA-CGA-O2A-C1
27	D	602	CLA	C5-C6-C7-C8
34	l	401	LHG	C11-C12-C13-C14
34	l	401	LHG	C7-C8-C9-C10
27	b	712	CLA	CAA-CBA-CGA-O2A
27	I	609	CLA	CAA-CBA-CGA-O1A
34	a	835	LHG	C17-C18-C19-C20
27	A	610	CLA	CHA-CBD-CGD-O1D
27	A	610	CLA	CHA-CBD-CGD-O2D
27	B	610	CLA	CHA-CBD-CGD-O1D
27	B	610	CLA	CHA-CBD-CGD-O2D
27	C	205	CLA	CHA-CBD-CGD-O2D
27	C	206	CLA	CHA-CBD-CGD-O2D
27	D	602	CLA	CHA-CBD-CGD-O2D
27	D	606	CLA	CHA-CBD-CGD-O1D
27	D	606	CLA	CHA-CBD-CGD-O2D
27	D	610	CLA	CHA-CBD-CGD-O1D
27	D	610	CLA	CHA-CBD-CGD-O2D
27	E	604	CLA	CHA-CBD-CGD-O1D
27	E	604	CLA	CHA-CBD-CGD-O2D
27	F	601	CLA	CHA-CBD-CGD-O1D
27	F	601	CLA	CHA-CBD-CGD-O2D
27	F	610	CLA	CHA-CBD-CGD-O2D
27	G	607	CLA	CHA-CBD-CGD-O1D
27	G	607	CLA	CHA-CBD-CGD-O2D
27	G	609	CLA	CHA-CBD-CGD-O1D
27	G	609	CLA	CHA-CBD-CGD-O2D
27	H	310	CLA	CHA-CBD-CGD-O1D
27	H	310	CLA	CHA-CBD-CGD-O2D
27	H	319	CLA	CHA-CBD-CGD-O2D
27	I	611	CLA	CHA-CBD-CGD-O1D
27	I	611	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	J	607	CLA	CHA-CBD-CGD-O2D
27	K	603	CLA	CHA-CBD-CGD-O1D
27	U	601	CLA	CHA-CBD-CGD-O2D
27	a	801	CLA	CHA-CBD-CGD-O1D
27	a	801	CLA	CHA-CBD-CGD-O2D
27	a	802	CLA	CHA-CBD-CGD-O1D
27	a	802	CLA	CHA-CBD-CGD-O2D
27	a	807	CLA	CHA-CBD-CGD-O1D
27	a	807	CLA	CHA-CBD-CGD-O2D
27	a	810	CLA	CHA-CBD-CGD-O1D
27	a	817	CLA	CHA-CBD-CGD-O2D
27	a	829	CLA	CHA-CBD-CGD-O2D
27	b	709	CLA	CHA-CBD-CGD-O1D
27	b	709	CLA	CHA-CBD-CGD-O2D
27	b	720	CLA	CHA-CBD-CGD-O2D
27	l	405	CLA	CHA-CBD-CGD-O1D
27	l	405	CLA	CHA-CBD-CGD-O2D
27	l	407	CLA	CHA-CBD-CGD-O2D
28	E	610	KC2	CHA-CBD-CGD-O1D
28	E	610	KC2	CHA-CBD-CGD-O2D
28	H	311	KC2	CHA-CBD-CGD-O1D
28	H	311	KC2	CHA-CBD-CGD-O2D
28	J	606	KC2	CHA-CBD-CGD-O2D
27	b	714	CLA	CAA-CBA-CGA-O2A
27	H	304	CLA	C2-C3-C5-C6
27	K	604	CLA	C5-C6-C7-C8
27	K	605	CLA	C5-C6-C7-C8
34	r	202	LHG	C32-C33-C34-C35
27	T	607	CLA	CAA-CBA-CGA-O1A
27	D	610	CLA	CAA-CBA-CGA-O2A
27	G	610	CLA	CAA-CBA-CGA-O2A
33	l	417	LMG	C16-C17-C18-C19
35	K	614	DGD	O2G-C2G-C3G-O3G
27	F	607	CLA	CAA-CBA-CGA-O1A
27	l	404	CLA	C5-C6-C7-C8
27	b	703	CLA	CAA-CBA-CGA-O2A
27	b	706	CLA	CAA-CBA-CGA-O2A
34	j	205	LHG	O7-C7-C8-C9
32	J	611	PID	C28-C27-O6-C30
27	B	610	CLA	C4C-C3C-CAC-CBC
27	H	312	CLA	C2C-C3C-CAC-CBC
27	a	830	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	F	618	LHG	C29-C30-C31-C32
27	C	204	CLA	C6-C7-C8-C10
27	a	827	CLA	C11-C10-C8-C7
27	a	827	CLA	C11-C12-C13-C15
27	b	724	CLA	C12-C13-C15-C16
37	a	832	PQN	C16-C17-C18-C20
35	j	201	DGD	CAB-CBB-CCB-CDB
27	E	606	CLA	CAA-CBA-CGA-O2A
27	a	823	CLA	CAA-CBA-CGA-O2A
27	G	607	CLA	CAA-CBA-CGA-O2A
27	G	606	CLA	C11-C12-C13-C14
27	a	815	CLA	C6-C7-C8-C9
33	C	217	LMG	C10-C11-C12-C13
27	a	808	CLA	CAA-CBA-CGA-O1A
34	F	618	LHG	O2-C2-C3-O3
27	a	821	CLA	C13-C15-C16-C17
27	a	805	CLA	CAA-CBA-CGA-O1A
27	b	728	CLA	CAA-CBA-CGA-O2A
33	F	616	LMG	C19-C20-C21-C22
27	a	806	CLA	C6-C7-C8-C10
27	b	715	CLA	C2-C3-C5-C6
27	l	402	CLA	C2-C3-C5-C6
27	I	603	CLA	CAA-CBA-CGA-O2A
27	b	711	CLA	CAA-CBA-CGA-O1A
38	b	731	BCR	C17-C18-C19-C20
35	f	305	DGD	O6D-C5D-C6D-O5D
31	H	320	SQD	C13-C14-C15-C16
27	C	204	CLA	C1A-C2A-CAA-CBA
27	G	606	CLA	C1A-C2A-CAA-CBA
27	K	608	CLA	C1A-C2A-CAA-CBA
27	b	722	CLA	C1A-C2A-CAA-CBA
27	l	410	CLA	C1A-C2A-CAA-CBA
27	b	722	CLA	CAA-CBA-CGA-O1A
27	a	824	CLA	C10-C11-C12-C13
27	a	816	CLA	C5-C6-C7-C8
27	H	305	CLA	C2A-CAA-CBA-CGA
27	a	815	CLA	C2A-CAA-CBA-CGA
27	a	830	CLA	C2A-CAA-CBA-CGA
27	a	829	CLA	C13-C15-C16-C17
33	C	217	LMG	O7-C10-C11-C12
34	G	617	LHG	C5-C4-O6-P
27	B	609	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	I	601	CLA	CAA-CBA-CGA-O1A
27	D	609	CLA	CAA-CBA-CGA-O2A
27	A	601	CLA	C4C-C3C-CAC-CBC
27	G	603	CLA	CAA-CBA-CGA-O1A
27	a	804	CLA	CAA-CBA-CGA-O1A
27	a	822	CLA	CAA-CBA-CGA-O1A
27	b	712	CLA	CAA-CBA-CGA-O1A
27	b	714	CLA	CAA-CBA-CGA-O1A
27	l	408	CLA	CAA-CBA-CGA-O1A
27	C	204	CLA	CAA-CBA-CGA-O1A
27	b	705	CLA	CAA-CBA-CGA-O1A
27	F	601	CLA	CAA-CBA-CGA-O2A
27	I	610	CLA	C6-C7-C8-C10
27	b	715	CLA	C2A-CAA-CBA-CGA
27	E	606	CLA	CAA-CBA-CGA-O1A
27	b	706	CLA	CAA-CBA-CGA-O1A
27	a	829	CLA	C10-C11-C12-C13
31	H	320	SQD	O47-C7-C8-C9
27	J	603	CLA	C10-C11-C12-C13
27	E	606	CLA	C2-C3-C5-C6
27	C	202	CLA	CAD-CBD-CGD-O1D
27	F	619	CLA	CAD-CBD-CGD-O1D
27	G	605	CLA	CAD-CBD-CGD-O1D
27	H	310	CLA	CAD-CBD-CGD-O1D
27	J	603	CLA	CAD-CBD-CGD-O1D
27	T	603	CLA	CAD-CBD-CGD-O1D
27	a	801	CLA	CAD-CBD-CGD-O1D
27	a	802	CLA	CAD-CBD-CGD-O1D
27	a	804	CLA	CAD-CBD-CGD-O1D
27	a	824	CLA	CAD-CBD-CGD-O1D
27	a	826	CLA	CAD-CBD-CGD-O1D
27	b	705	CLA	CAD-CBD-CGD-O1D
27	b	709	CLA	CAD-CBD-CGD-O1D
27	b	711	CLA	CAD-CBD-CGD-O1D
27	b	716	CLA	CAD-CBD-CGD-O1D
28	F	609	KC2	CAD-CBD-CGD-O1D
31	H	320	SQD	O5-C5-C6-S
31	y	301	SQD	O5-C5-C6-S
33	b	733	LMG	C7-C8-O7-C10
34	G	617	LHG	C6-C5-O7-C7
34	l	401	LHG	C6-C5-O7-C7
27	b	702	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	b	728	CLA	CAA-CBA-CGA-O1A
27	B	609	CLA	C11-C12-C13-C14
27	a	825	CLA	C11-C12-C13-C14
31	y	301	SQD	C24-C25-C26-C27
33	F	616	LMG	C24-C25-C26-C27
34	D	620	LHG	C24-C25-C26-C27
27	H	309	CLA	CAA-CBA-CGA-O2A
27	J	605	CLA	CAA-CBA-CGA-O2A
27	K	604	CLA	CAA-CBA-CGA-O2A
33	b	733	LMG	C18-C19-C20-C21
27	I	606	CLA	CAA-CBA-CGA-O2A
27	b	717	CLA	CAA-CBA-CGA-O2A
27	r	204	CLA	C8-C10-C11-C12
27	D	610	CLA	CAA-CBA-CGA-O1A
34	j	205	LHG	O9-C7-C8-C9
27	H	319	CLA	C4-C3-C5-C6
27	a	818	CLA	C4-C3-C5-C6
27	b	710	CLA	C4-C3-C5-C6
27	l	403	CLA	C4-C3-C5-C6
27	F	617	CLA	C6-C7-C8-C10
27	G	606	CLA	C2-C3-C5-C6
27	G	608	CLA	C3A-C2A-CAA-CBA
27	K	601	CLA	C11-C10-C8-C7
27	a	805	CLA	C6-C7-C8-C10
27	a	809	CLA	C3A-C2A-CAA-CBA
27	a	823	CLA	C3A-C2A-CAA-CBA
27	a	824	CLA	C12-C13-C15-C16
27	b	702	CLA	C11-C10-C8-C7
27	b	716	CLA	C12-C13-C15-C16
27	l	403	CLA	C11-C12-C13-C15
27	r	203	CLA	C3A-C2A-CAA-CBA
27	r	204	CLA	C11-C10-C8-C7
27	G	610	CLA	CAA-CBA-CGA-O1A
27	I	606	CLA	CAA-CBA-CGA-O1A
27	K	604	CLA	CAA-CBA-CGA-O1A
27	G	609	CLA	CAA-CBA-CGA-O2A
27	H	305	CLA	CAA-CBA-CGA-O2A
27	b	701	CLA	CAA-CBA-CGA-O2A
34	j	205	LHG	C23-C24-C25-C26
30	b	730	DD6	C5-C6-C8-C9
38	a	833	BCR	C11-C12-C13-C14
27	H	305	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	C	209	CLA	CAA-CBA-CGA-O1A
27	D	609	CLA	CAA-CBA-CGA-O1A
27	a	839	CLA	CAA-CBA-CGA-O2A
27	l	409	CLA	C8-C10-C11-C12
27	F	601	CLA	CAA-CBA-CGA-O1A
27	G	609	CLA	CAA-CBA-CGA-O1A
27	a	839	CLA	CAA-CBA-CGA-O1A
27	b	701	CLA	CAA-CBA-CGA-O1A
33	C	217	LMG	O9-C10-C11-C12
27	H	303	CLA	C10-C11-C12-C13
27	B	607	CLA	C10-C11-C12-C13
27	a	802	CLA	C6-C7-C8-C9
35	j	201	DGD	C2B-C3B-C4B-C5B
27	H	309	CLA	CAA-CBA-CGA-O1A
27	b	703	CLA	CAA-CBA-CGA-O1A
27	a	819	CLA	CAA-CBA-CGA-O2A

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	K	611	PID	C24-C25-C26-C27-C28-C29
29	B	615	UIX	C15-C16-C17-C18-C19-C20
29	I	612	UIX	C15-C16-C17-C18-C19-C20
32	U	608	PID	C24-C25-C26-C27-C28-C29

115 monomers are involved in 212 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	615	DD6	2	0
30	G	614	DD6	1	0
27	A	604	CLA	4	0
27	K	603	CLA	11	0
27	C	202	CLA	1	0
27	I	610	CLA	3	0
27	A	605	CLA	1	0
27	H	308	CLA	1	0
27	F	619	CLA	2	0
32	B	613	PID	1	0
32	J	615	PID	3	0
27	D	602	CLA	1	0
27	F	608	CLA	1	0
30	G	616	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	K	601	CLA	4	0
30	E	613	DD6	1	0
30	B	612	DD6	2	0
27	I	605	CLA	2	0
27	H	303	CLA	1	0
30	G	612	DD6	1	0
36	T	613	LMU	1	0
27	D	612	CLA	1	0
27	U	603	CLA	8	0
27	E	605	CLA	1	0
28	J	604	KC2	3	0
30	G	613	DD6	1	0
30	I	613	DD6	2	0
32	K	611	PID	12	0
30	K	610	DD6	2	0
32	F	614	PID	6	0
30	F	612	DD6	2	0
27	D	605	CLA	2	0
27	T	605	CLA	2	0
29	H	314	UIX	1	0
27	F	602	CLA	2	0
27	C	205	CLA	4	0
27	T	602	CLA	1	0
27	D	608	CLA	1	0
27	C	206	CLA	1	0
27	B	606	CLA	2	0
27	G	608	CLA	2	0
27	H	304	CLA	3	0
30	A	615	DD6	1	0
27	D	609	CLA	1	0
27	J	607	CLA	1	0
33	D	618	LMG	1	0
27	B	601	CLA	1	0
27	T	603	CLA	4	0
27	G	611	CLA	1	0
27	I	602	CLA	1	0
35	K	614	DGD	4	0
33	C	217	LMG	1	0
30	K	609	DD6	1	0
27	C	203	CLA	2	0
27	A	612	CLA	1	0
27	I	606	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	G	605	CLA	3	0
30	U	607	DD6	1	0
27	U	601	CLA	1	0
27	U	605	CLA	3	0
30	H	316	DD6	1	0
27	T	601	CLA	3	0
30	C	216	DD6	2	0
27	J	601	CLA	1	0
27	T	606	CLA	2	0
27	F	606	CLA	1	0
27	H	319	CLA	2	0
27	T	607	CLA	1	0
27	E	608	CLA	1	0
27	I	603	CLA	5	0
27	F	604	CLA	6	0
27	G	607	CLA	3	0
27	K	605	CLA	2	0
30	D	621	DD6	1	0
27	B	610	CLA	1	0
27	J	609	CLA	3	0
32	F	615	PID	2	0
27	G	606	CLA	3	0
27	F	605	CLA	2	0
30	T	611	DD6	1	0
30	H	318	DD6	1	0
28	J	608	KC2	2	0
27	C	211	CLA	1	0
27	D	603	CLA	1	0
27	E	609	CLA	1	0
30	J	612	DD6	1	0
27	G	609	CLA	1	0
27	G	602	CLA	1	0
27	A	601	CLA	1	0
27	A	606	CLA	2	0
30	H	315	DD6	1	0
30	A	614	DD6	1	0
27	C	204	CLA	1	0
27	I	601	CLA	4	0
27	I	609	CLA	1	0
32	I	614	PID	5	0
27	I	607	CLA	1	0
27	K	604	CLA	1	0

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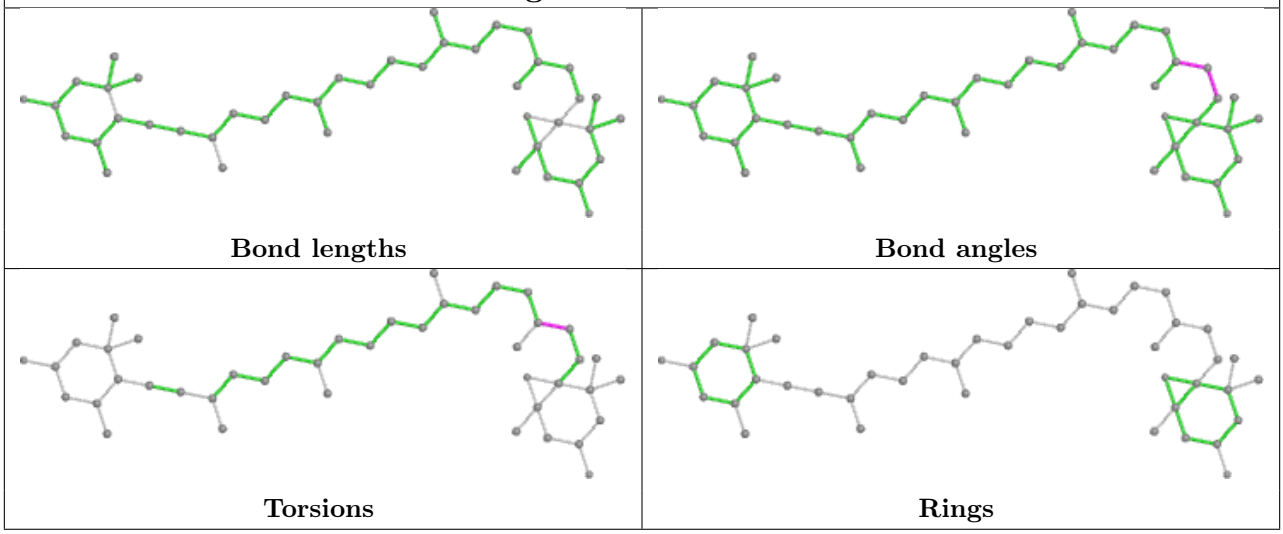
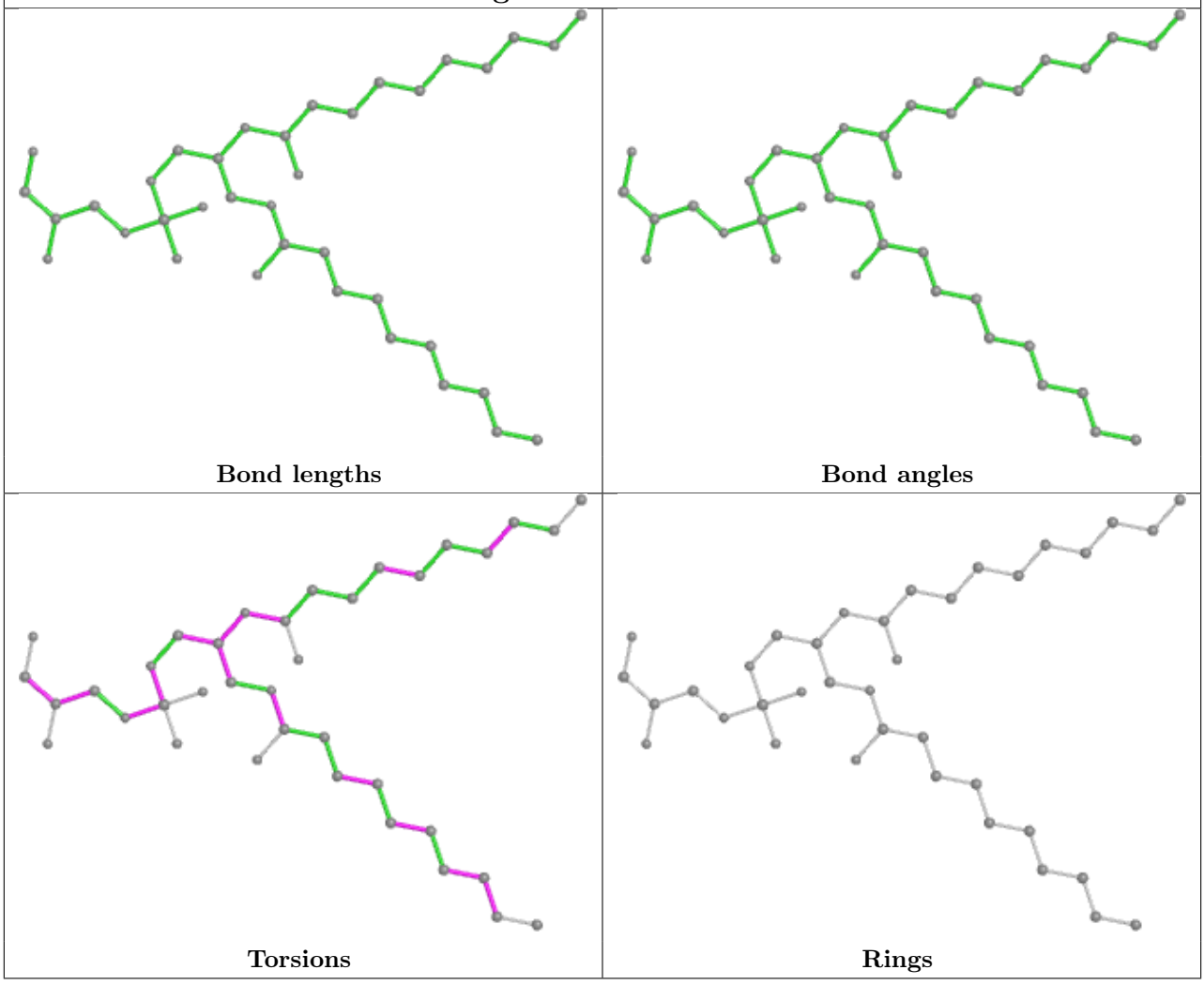
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	J	611	PID	6	0
27	C	207	CLA	1	0
27	B	605	CLA	1	0
27	F	601	CLA	1	0
27	K	602	CLA	1	0
28	K	607	KC2	6	0
27	D	610	CLA	1	0
27	E	611	CLA	1	0
29	I	612	UIX	1	0
27	H	313	CLA	1	0
33	K	613	LMG	1	0
32	J	614	PID	4	0
27	H	306	CLA	2	0
33	D	619	LMG	1	0
27	J	605	CLA	2	0
30	E	614	DD6	1	0
32	J	613	PID	10	0

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

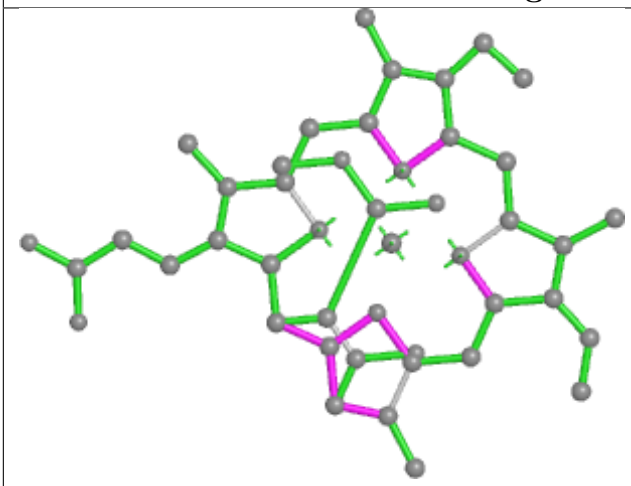
Ligand DD6 D 615



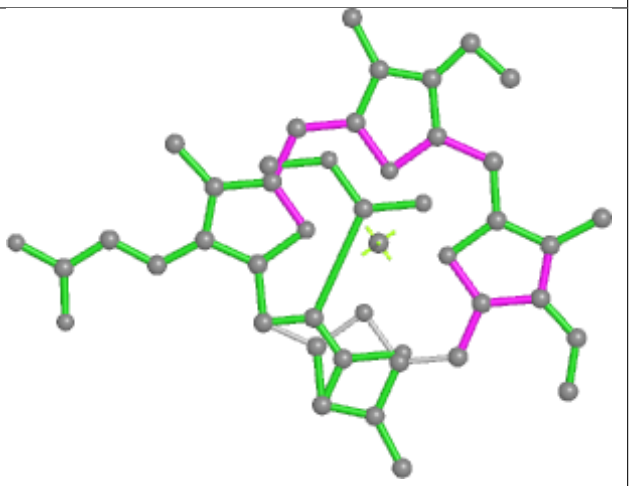
Ligand LHG F 618



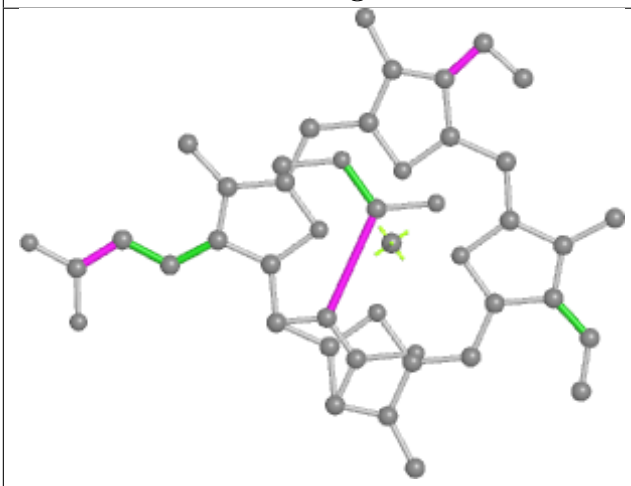
Ligand KC2 U 602



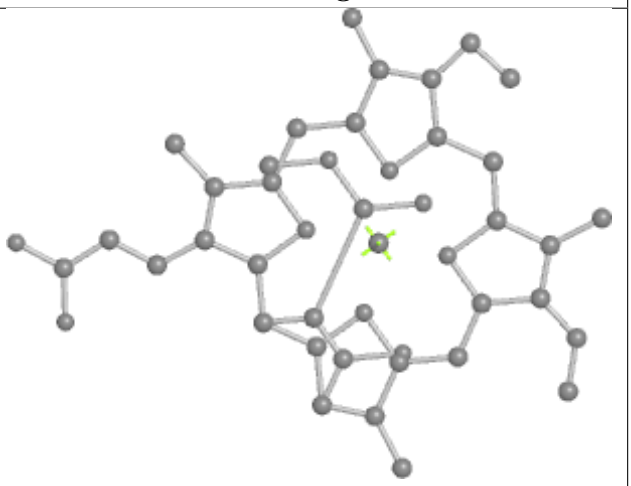
Bond lengths



Bond angles

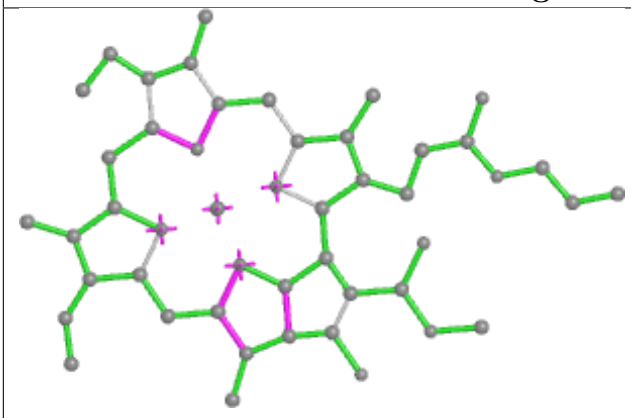


Torsions

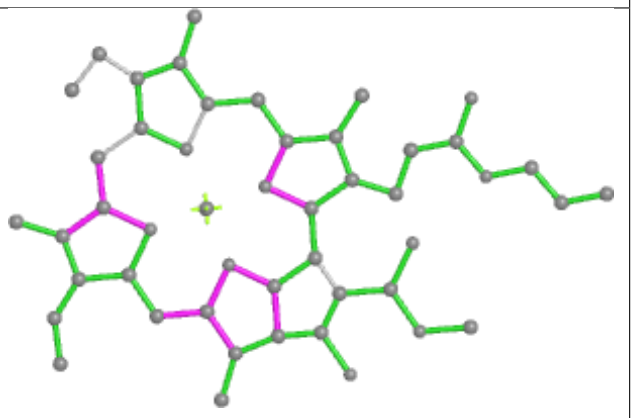


Rings

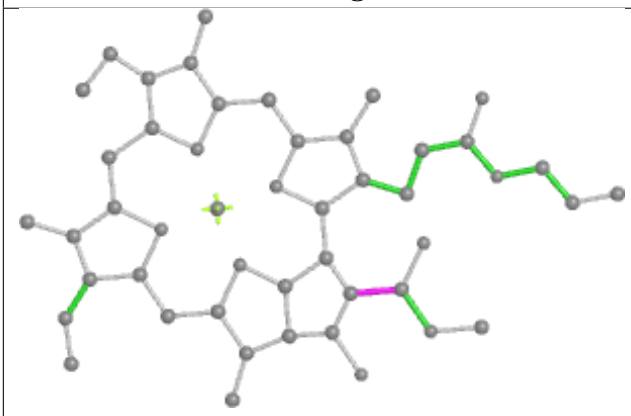
Ligand CLA l 411



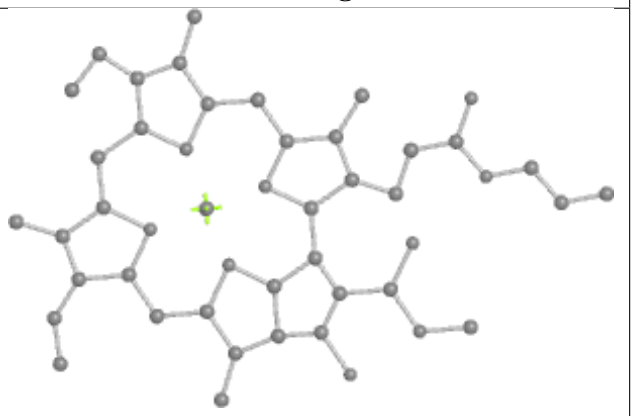
Bond lengths



Bond angles

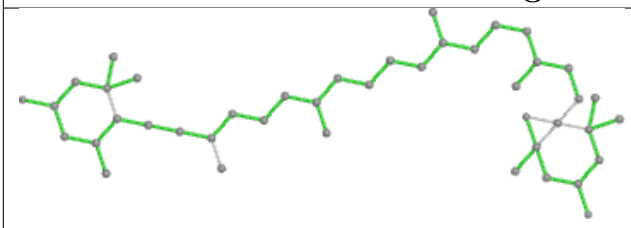


Torsions

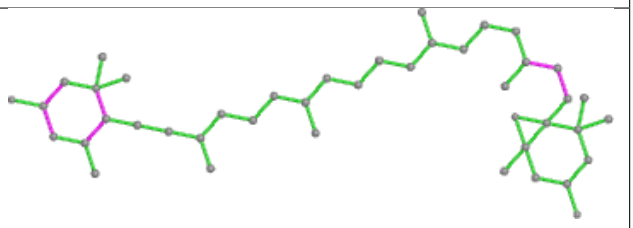


Rings

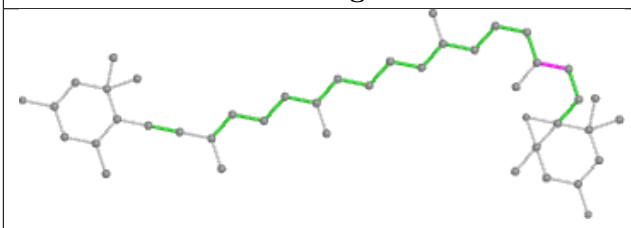
Ligand DD6 G 614



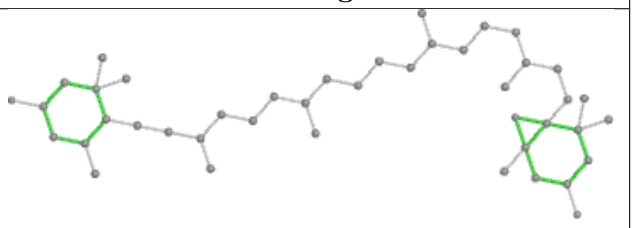
Bond lengths



Bond angles

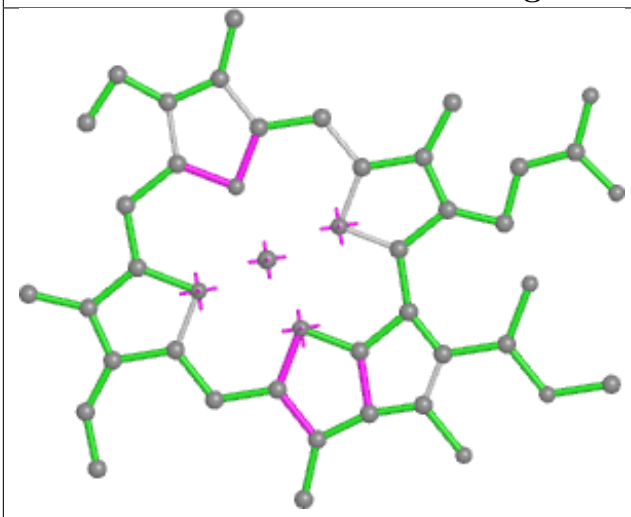


Torsions

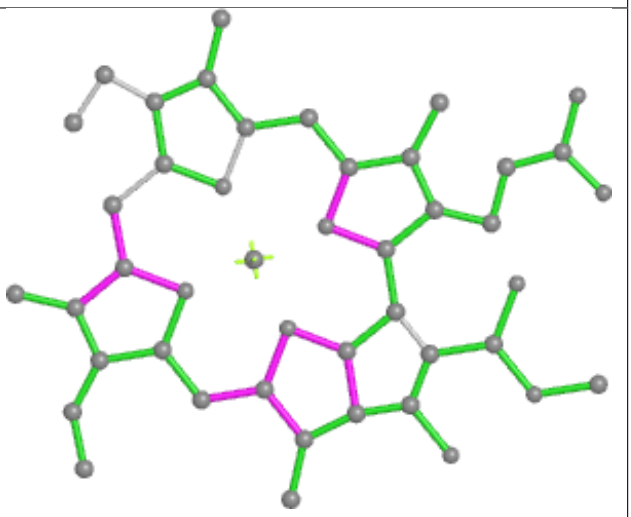


Rings

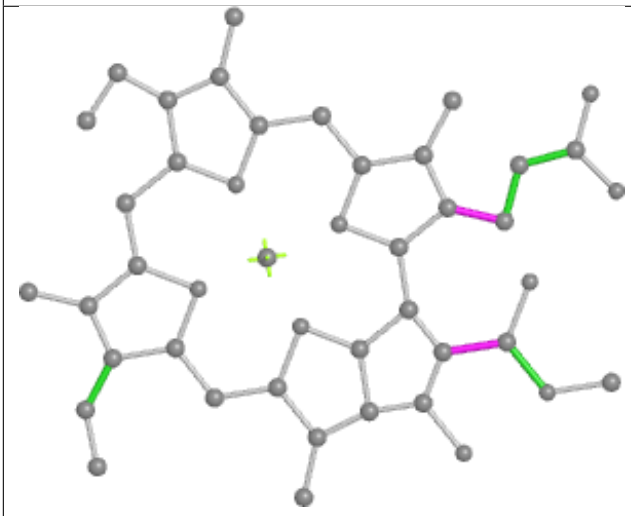
Ligand CLA A 604



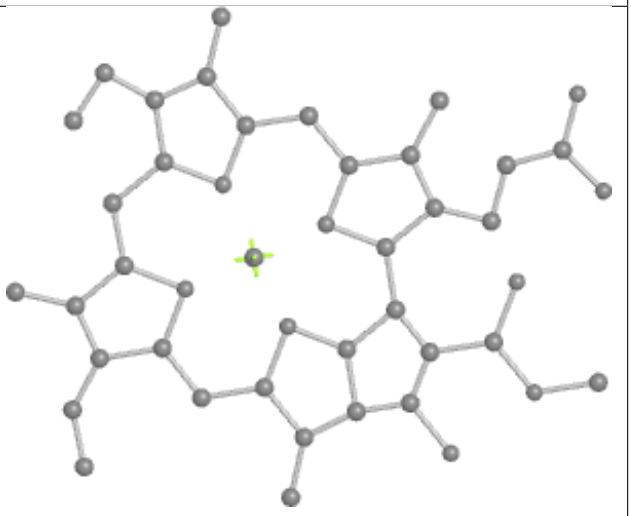
Bond lengths



Bond angles

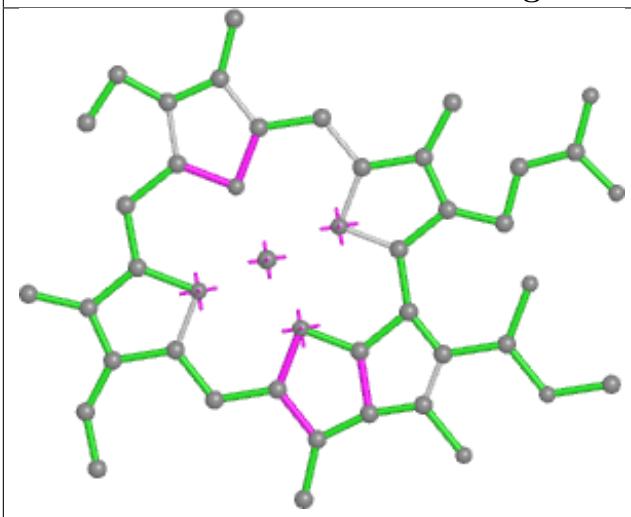


Torsions

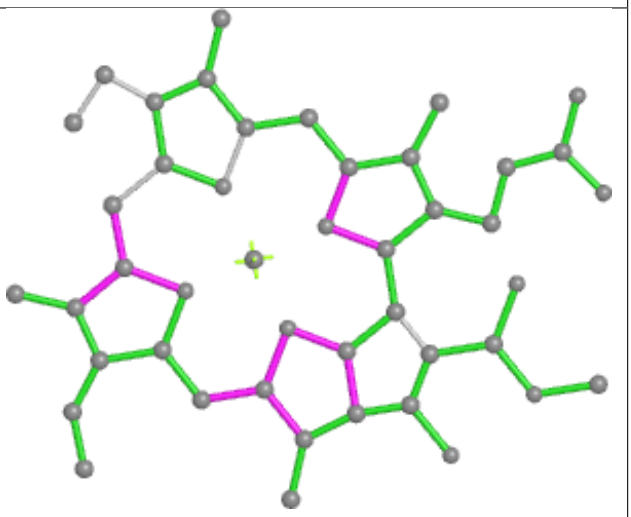


Rings

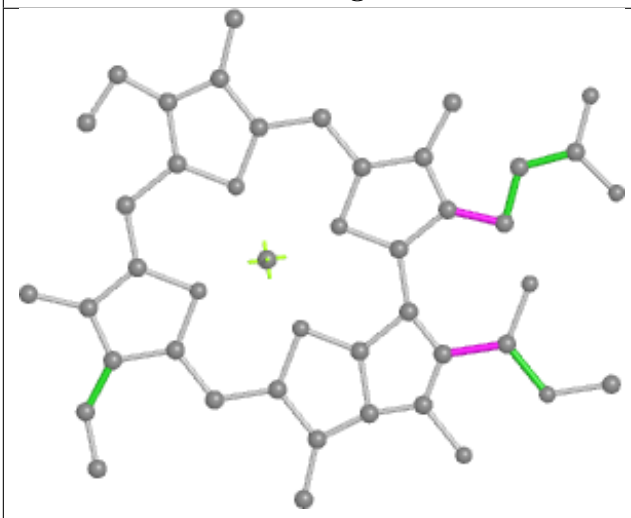
Ligand CLA K 603



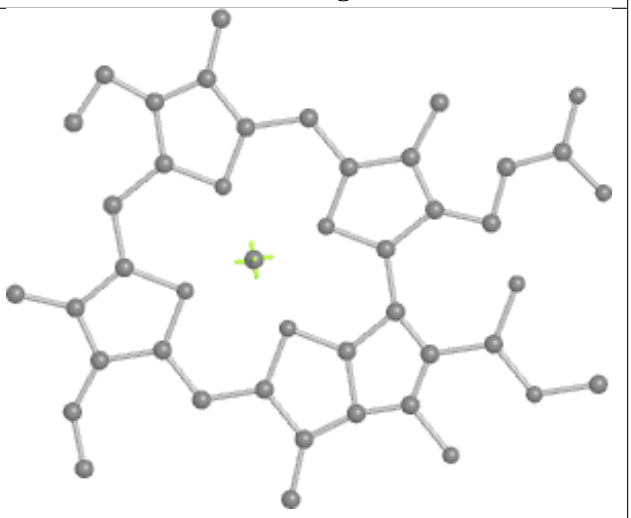
Bond lengths



Bond angles

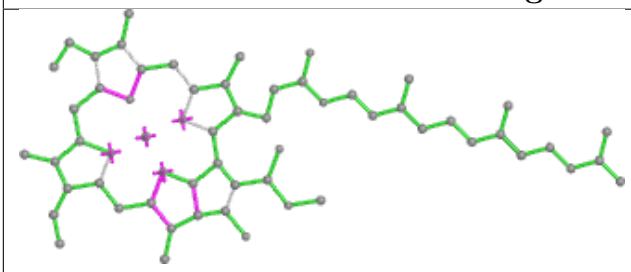


Torsions

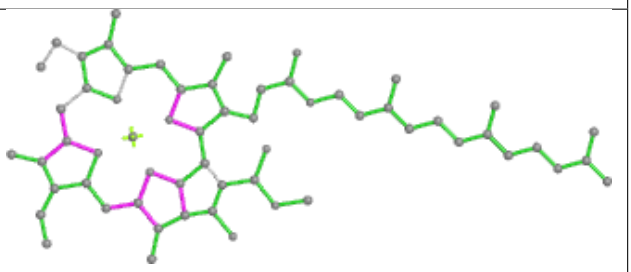


Rings

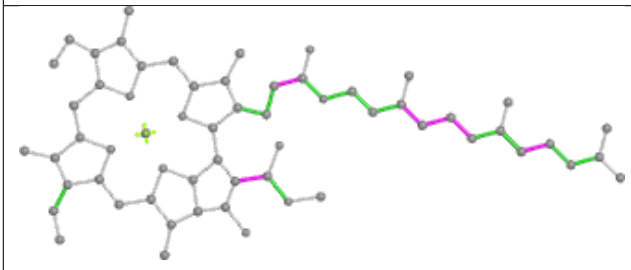
Ligand CLA E 606



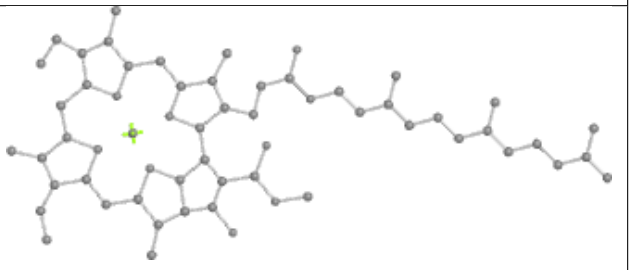
Bond lengths



Bond angles

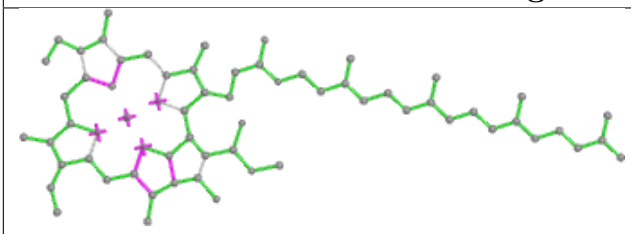


Torsions

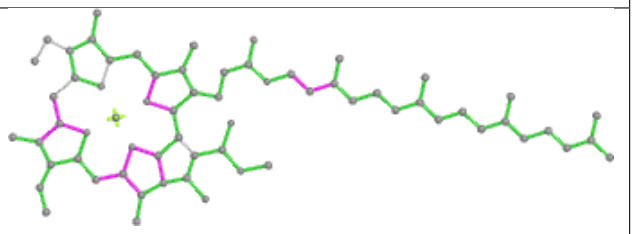


Rings

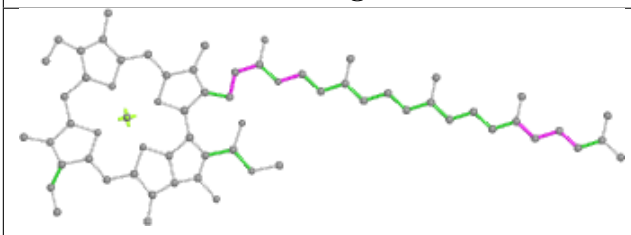
Ligand CLA b 728



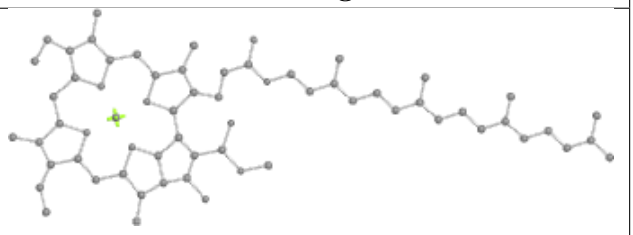
Bond lengths



Bond angles

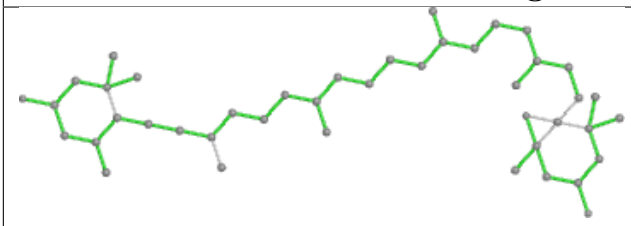


Torsions



Rings

Ligand DD6 E 617



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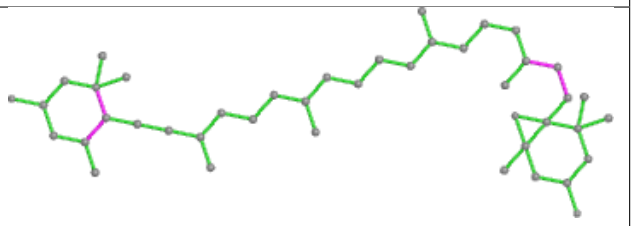
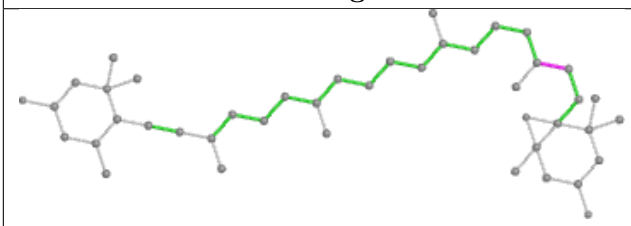


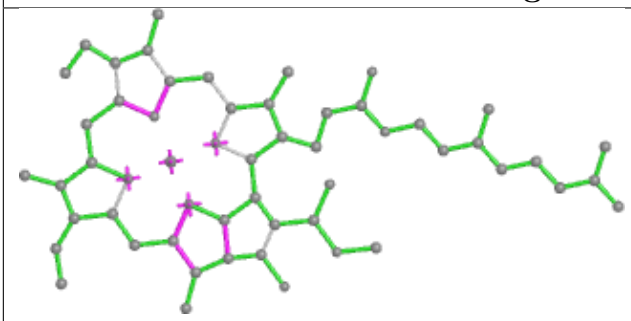
Bond angles



Torsions

Rings

Ligand CLA A 610



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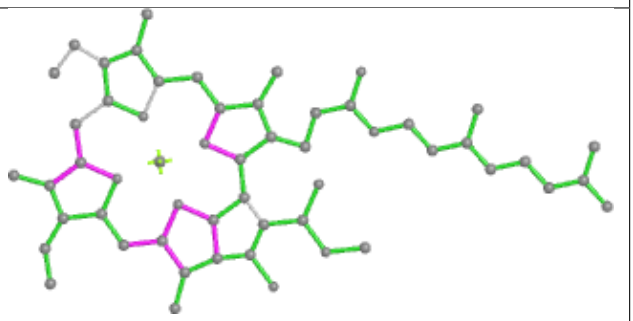
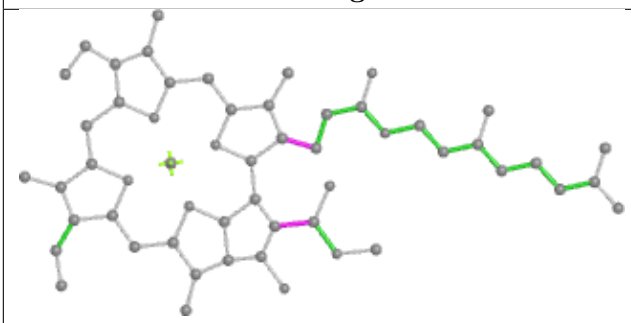
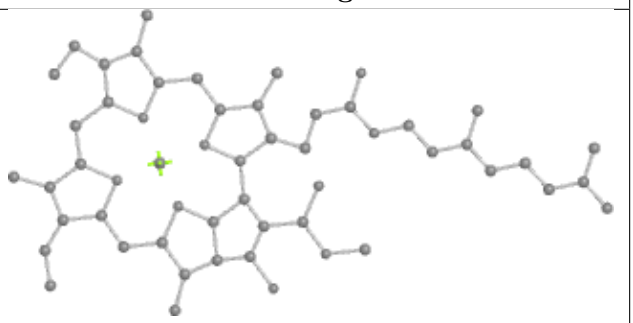


Bond angles

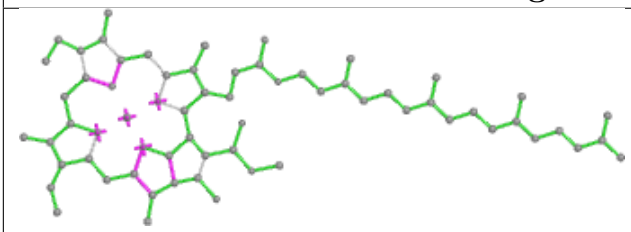


Torsions



Rings

Ligand CLA a 807



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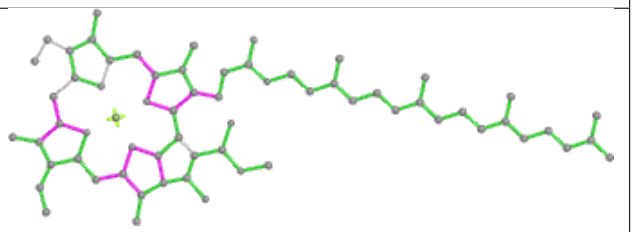
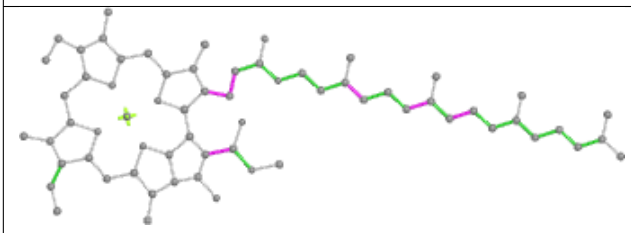


Bond angles



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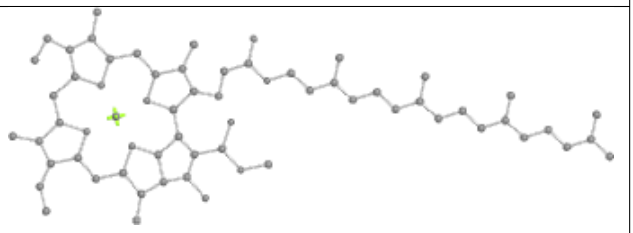
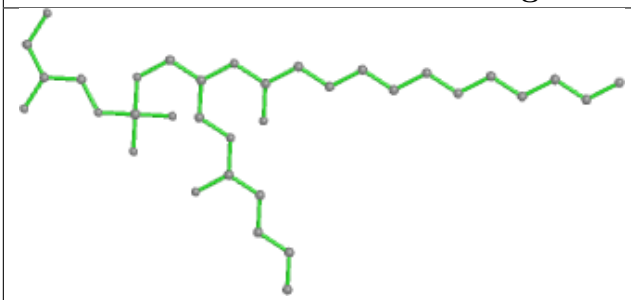


Rings

Ligand LHG G 617



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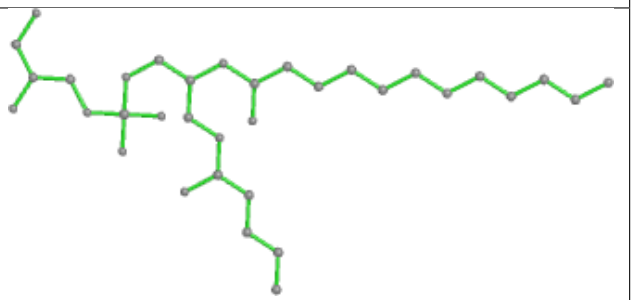
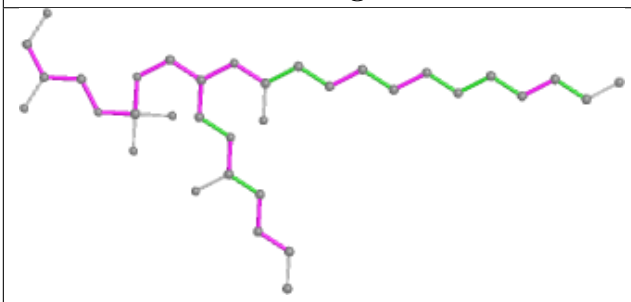
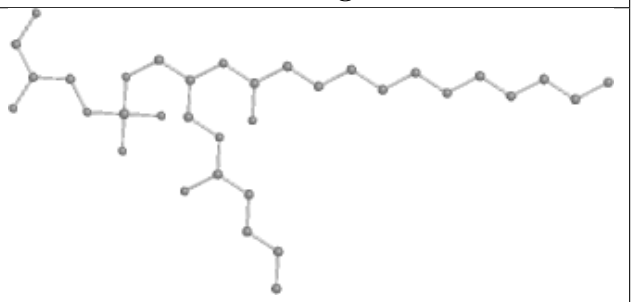


Bond angles

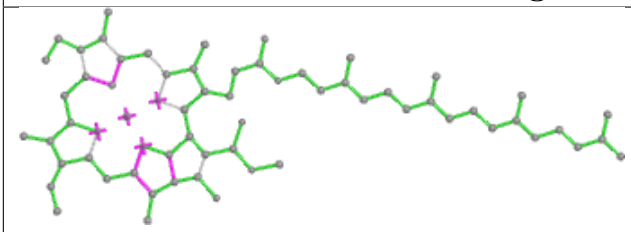


Torsions



Rings

Ligand CLA a 837



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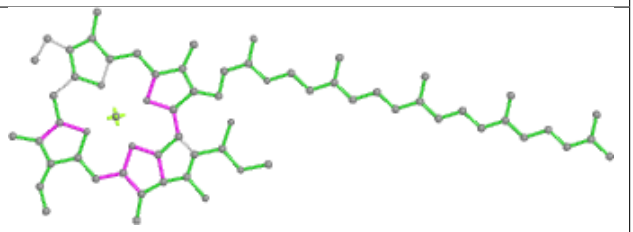
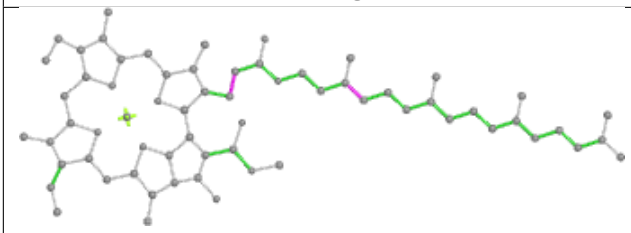


Bond angles



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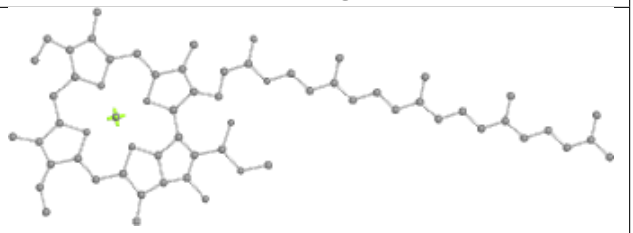
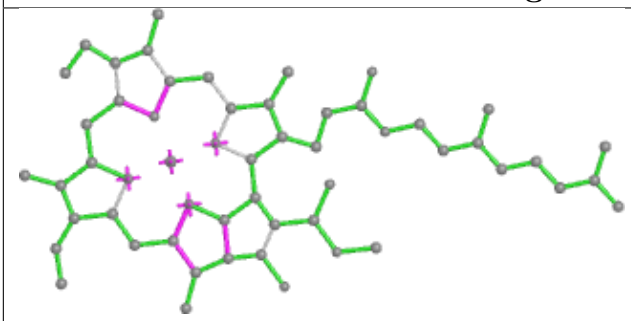


Rings

Ligand CLA E 602



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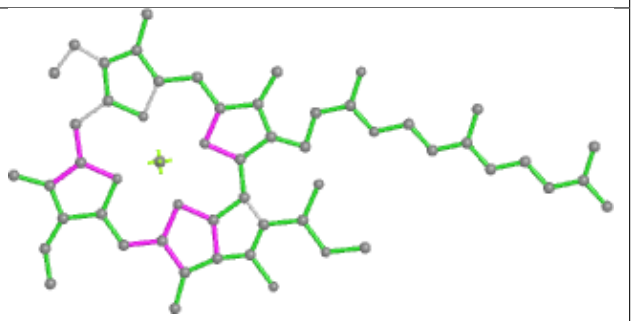
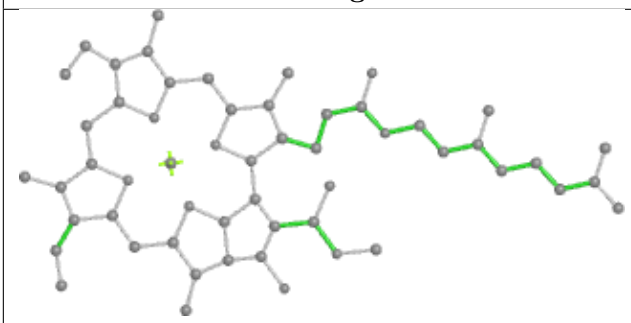
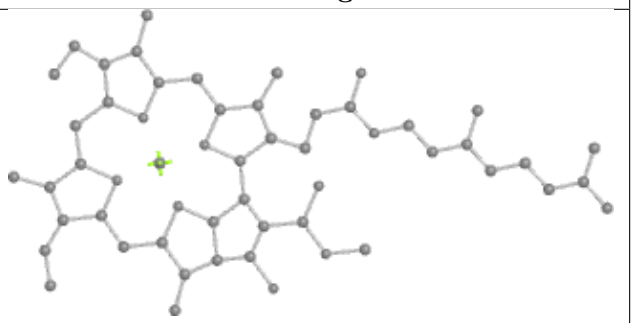


Bond angles

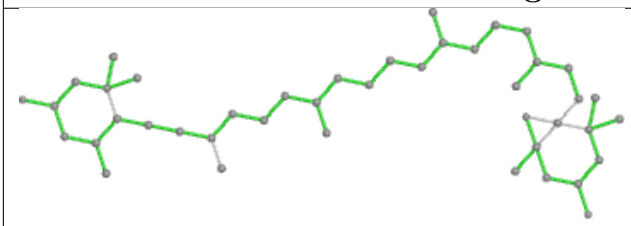


Torsions



Rings

Ligand DD6 A 617



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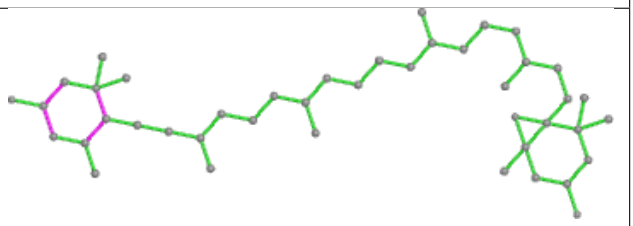
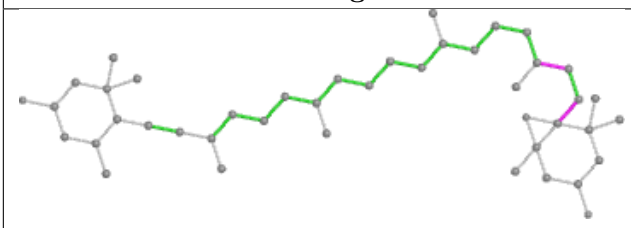
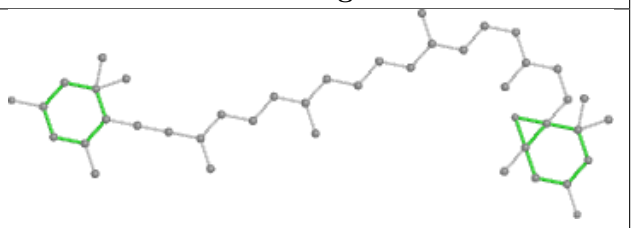


Bond angles

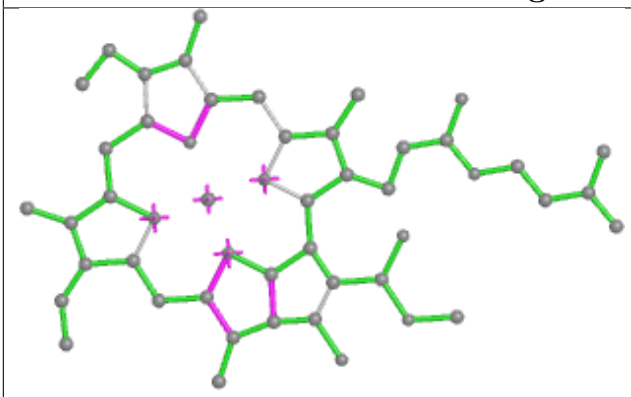


Torsions



Rings

Ligand CLA a 810



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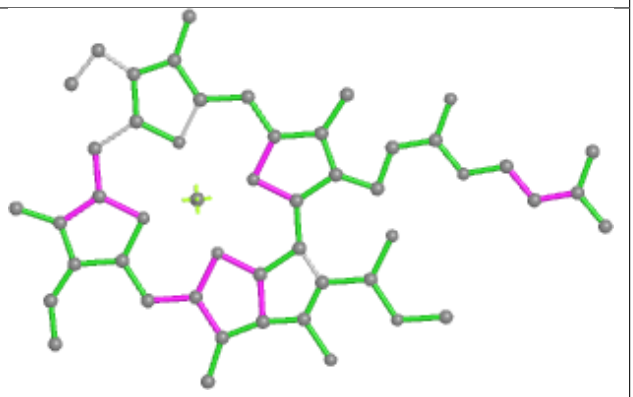
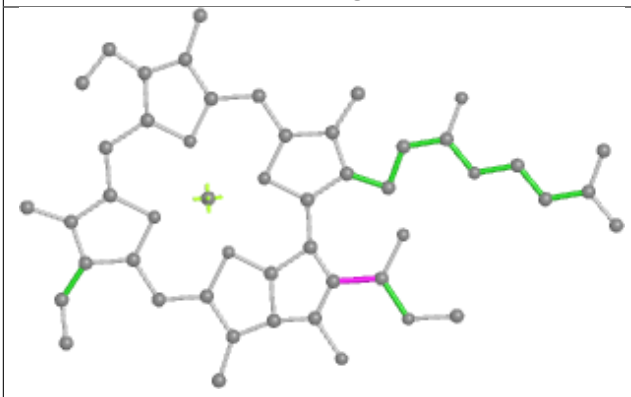
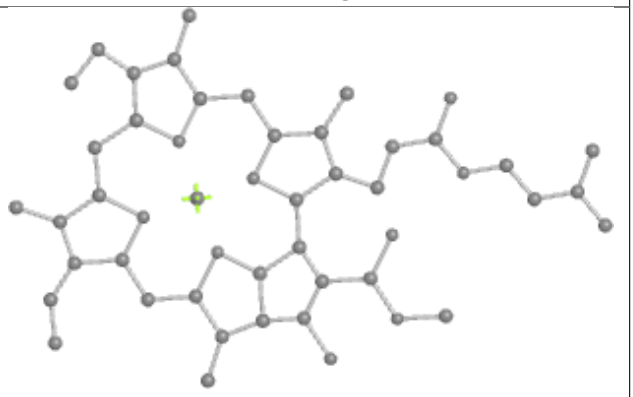


Bond angles

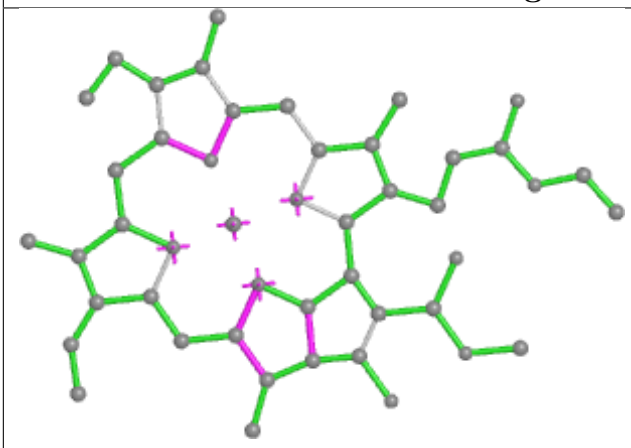


Torsions



Rings

Ligand CLA C 208



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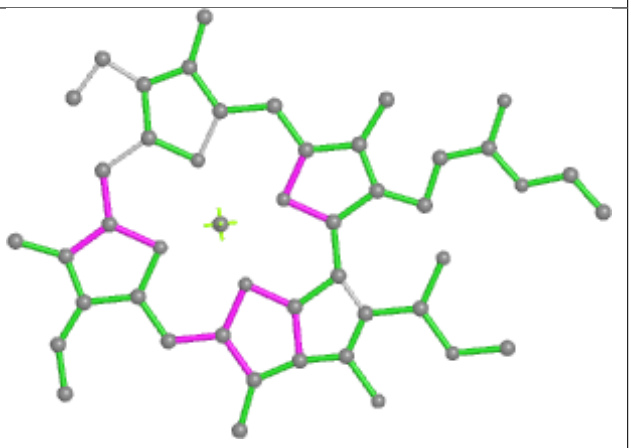
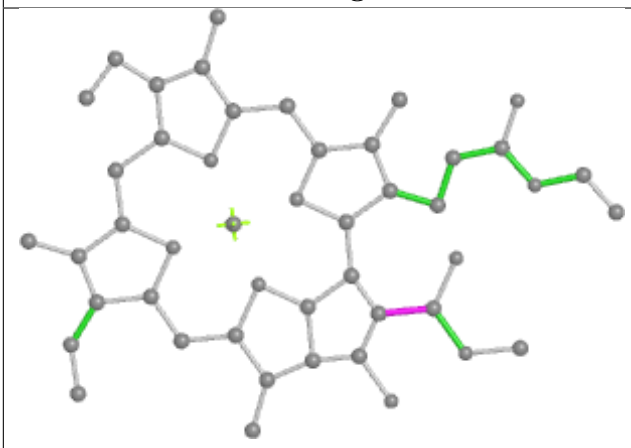


Bond angles



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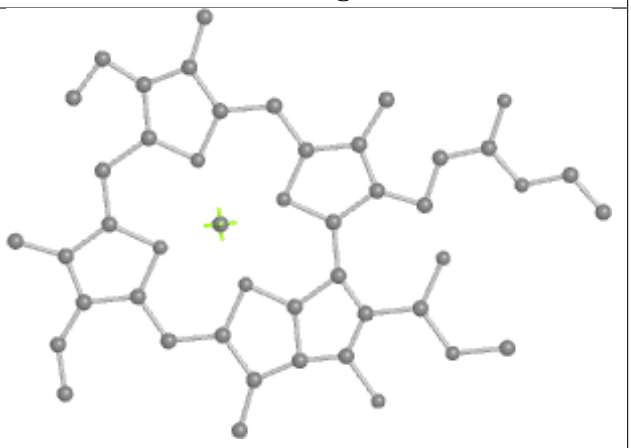
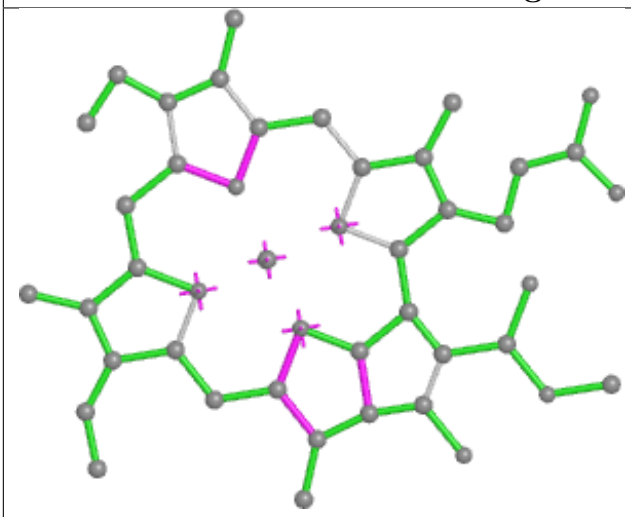
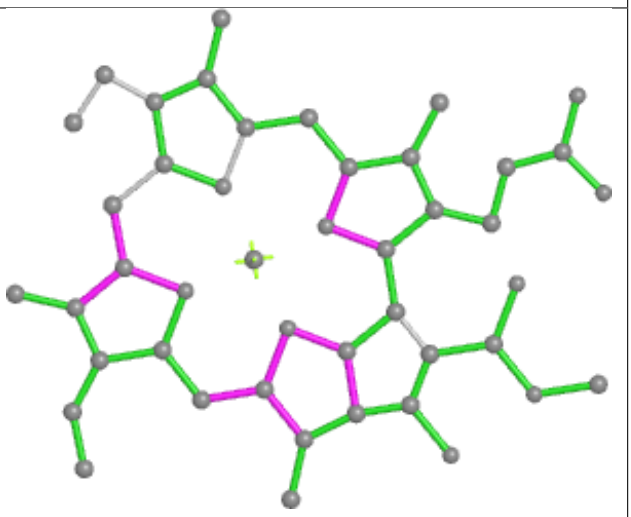


Rings

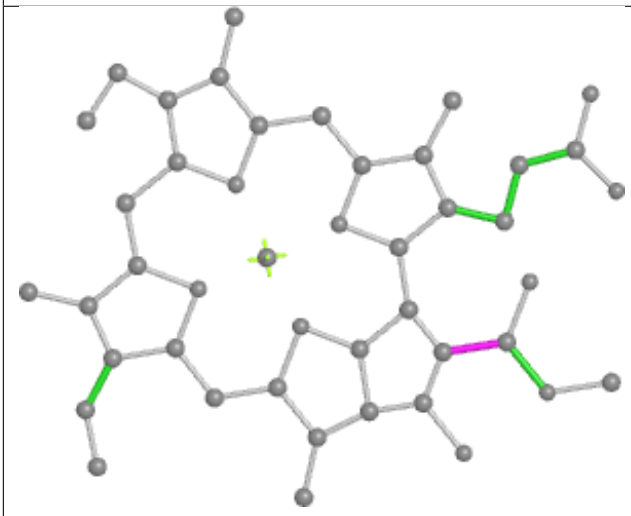
Ligand CLA C 202



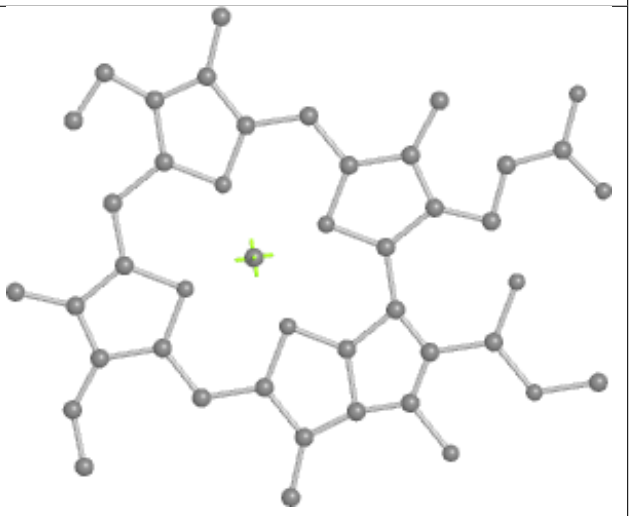
Bond lengths



Bond angles

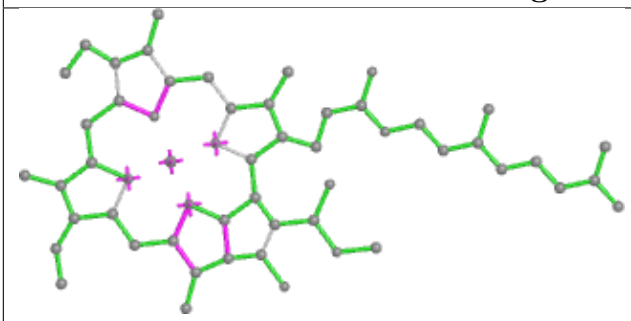


Torsions

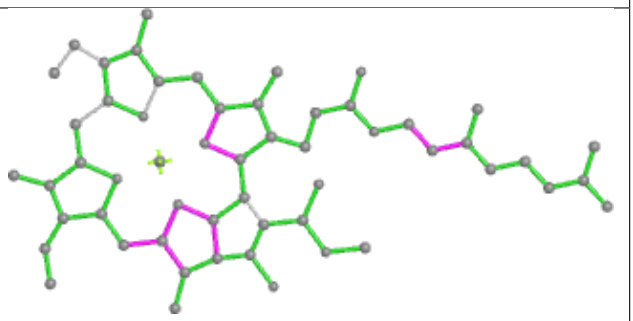


Rings

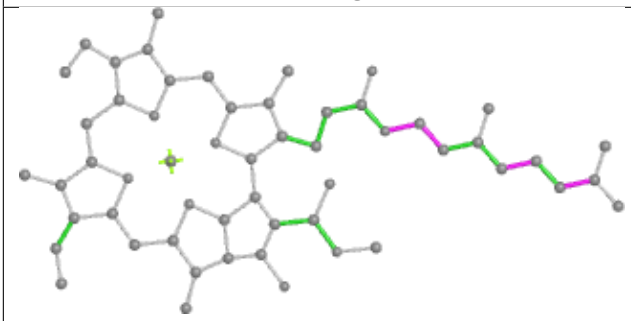
Ligand CLA I 610



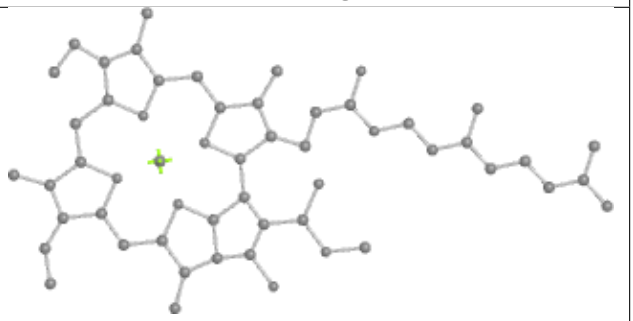
Bond lengths



Bond angles

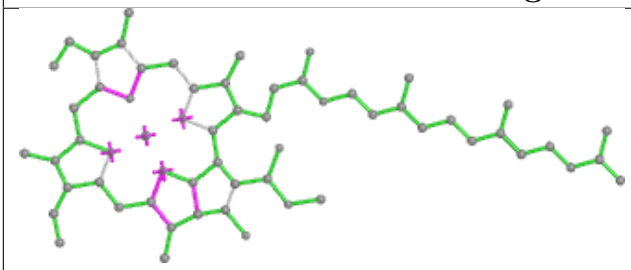


Torsions

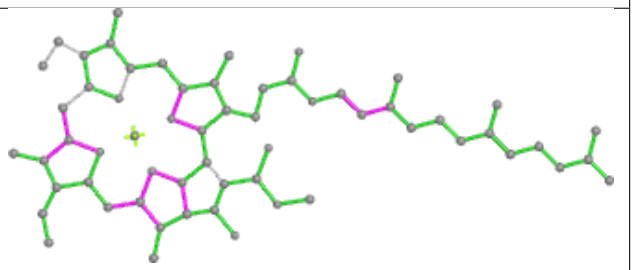


Rings

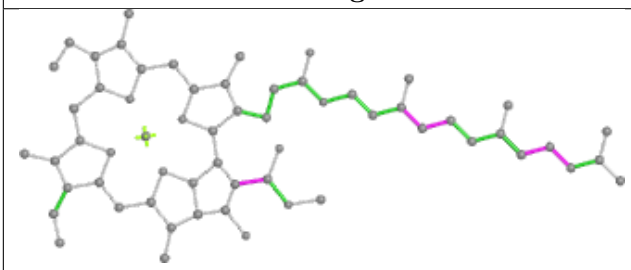
Ligand CLA B 607



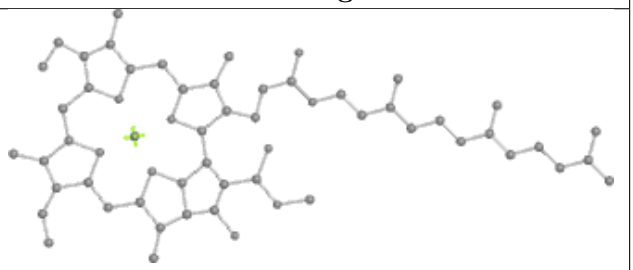
Bond lengths



Bond angles

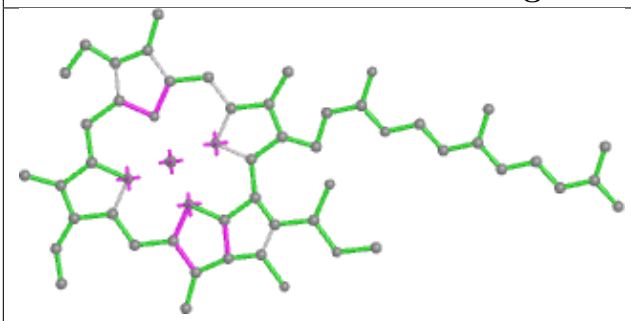


Torsions

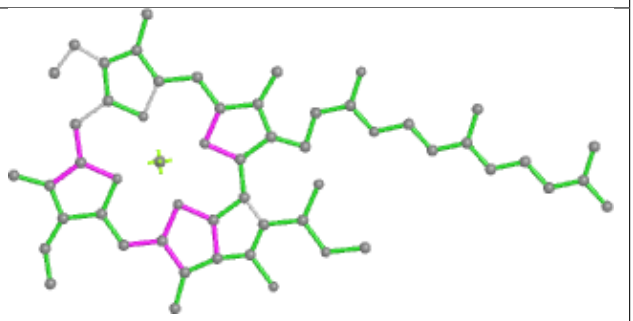


Rings

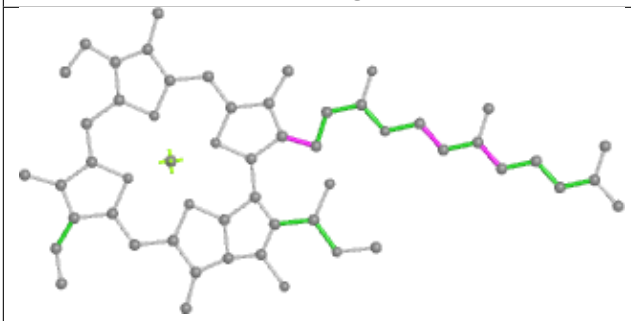
Ligand CLA A 605



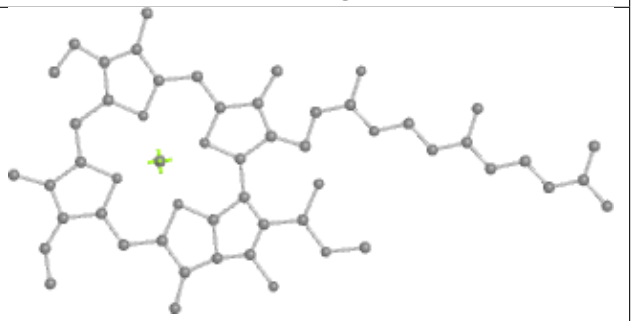
Bond lengths



Bond angles

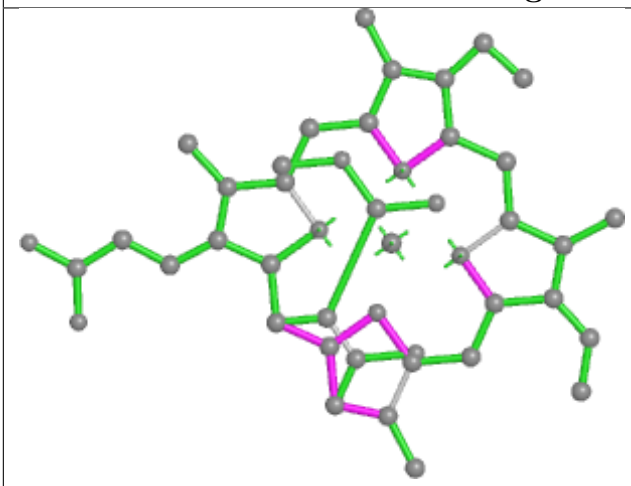


Torsions



Rings

Ligand KC2 H 302



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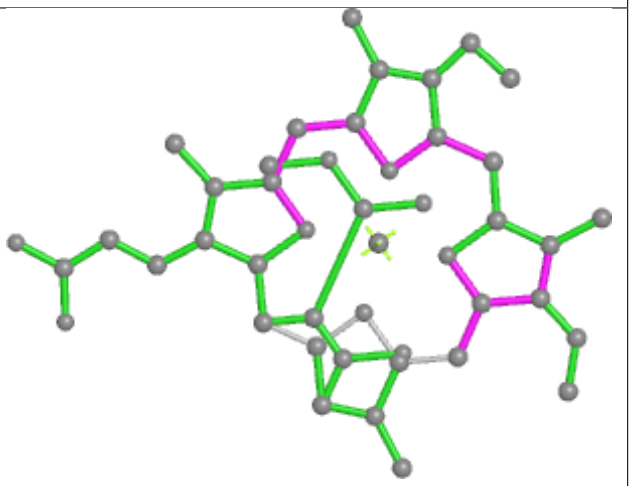
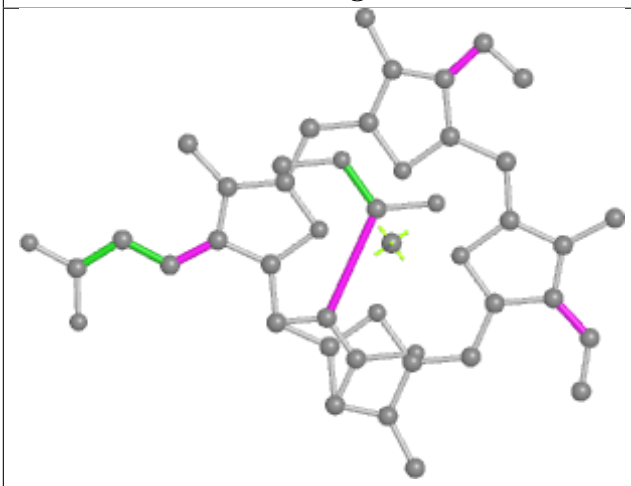


Bond angles



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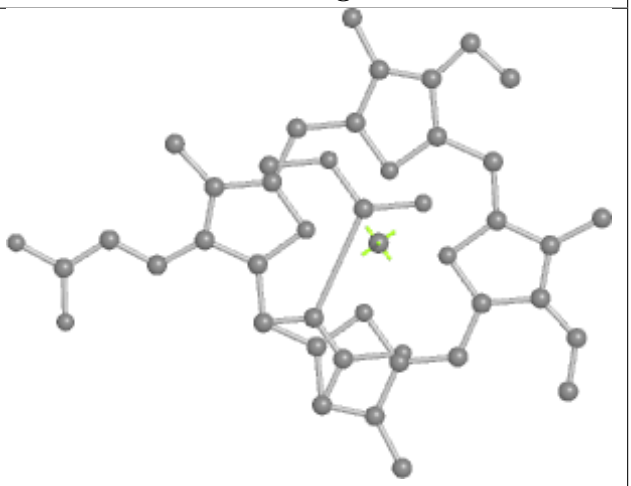
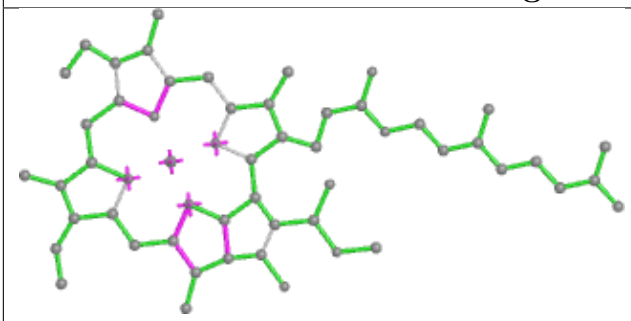


Rings

Ligand CLA H 308



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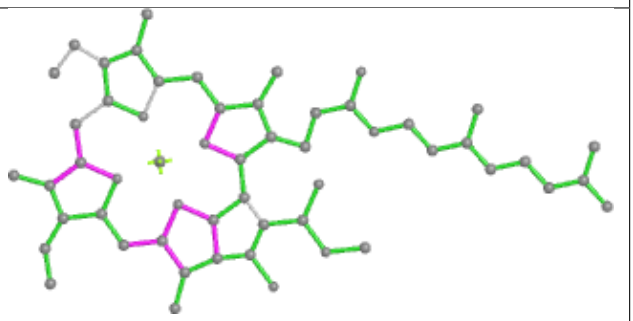

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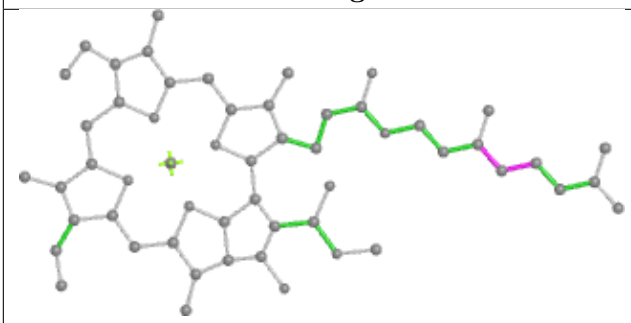
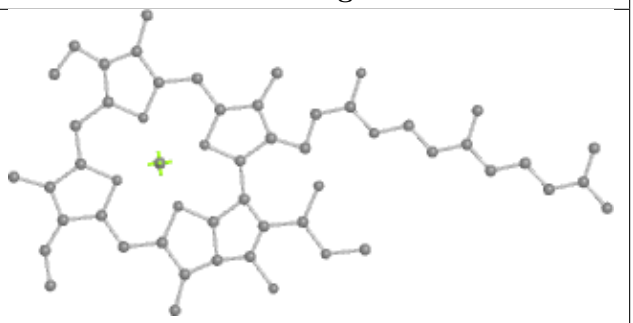
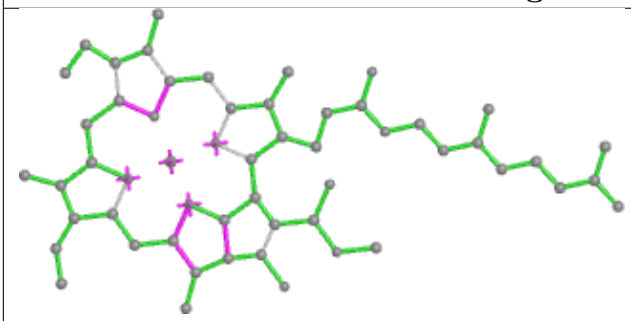


Torsions



Rings

Ligand CLA F 619



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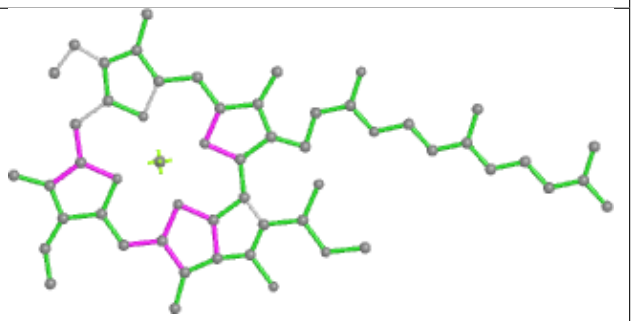
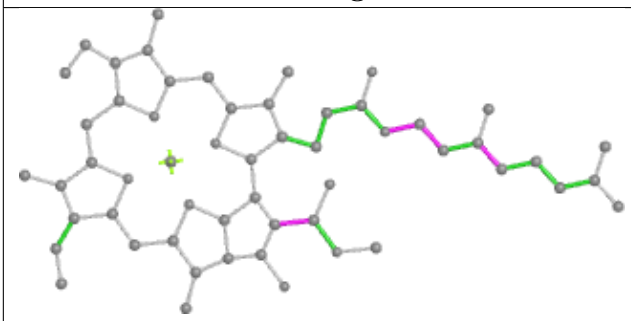
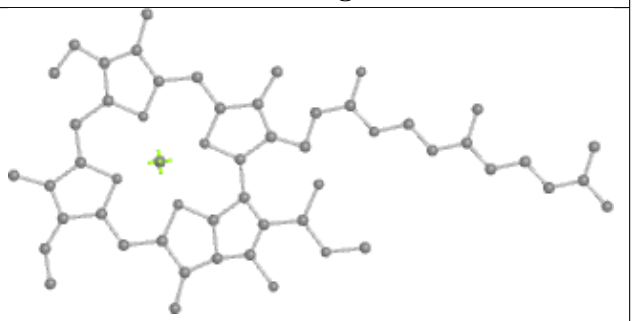


Bond angles

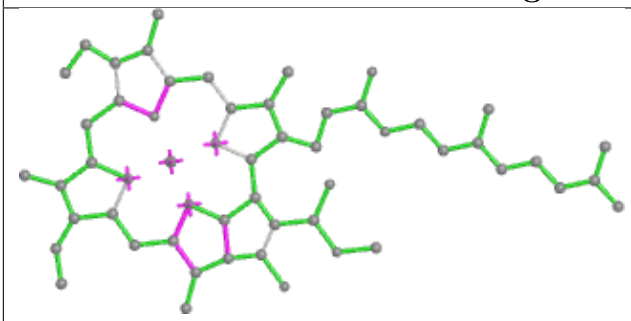


Torsions



Rings

Ligand CLA D 604



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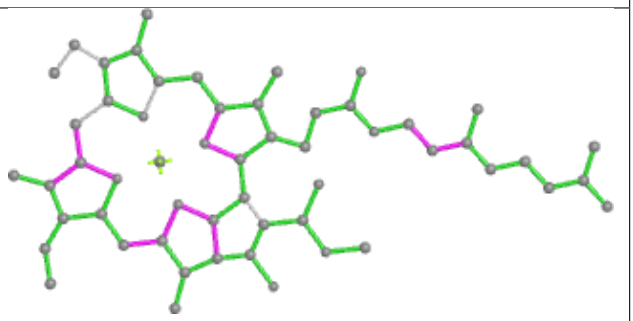
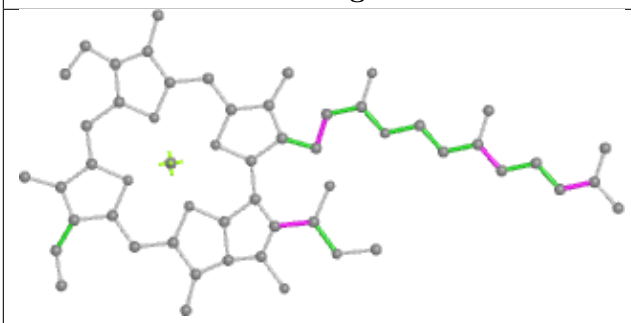


Bond angles



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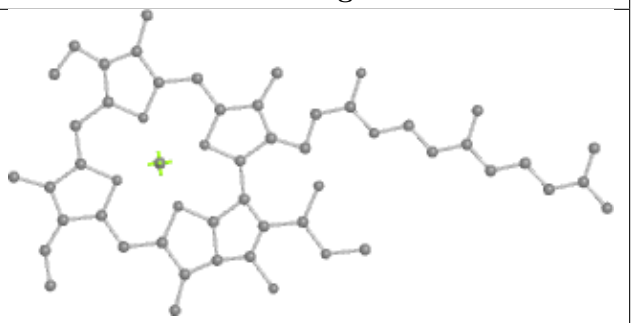
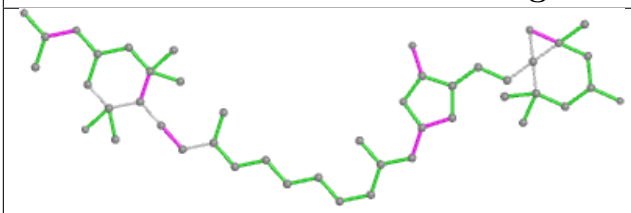


Rings

Ligand PID B 613



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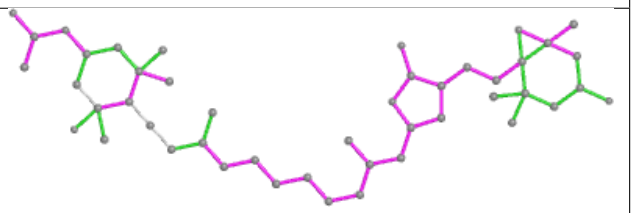
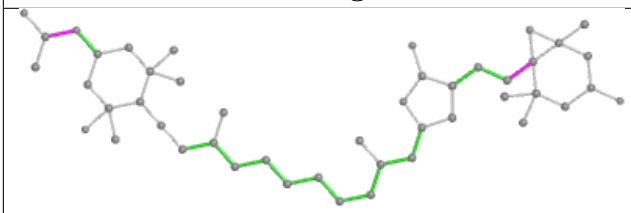


Bond angles



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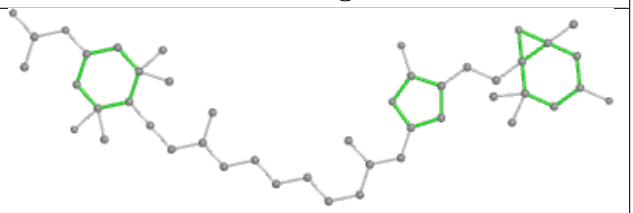
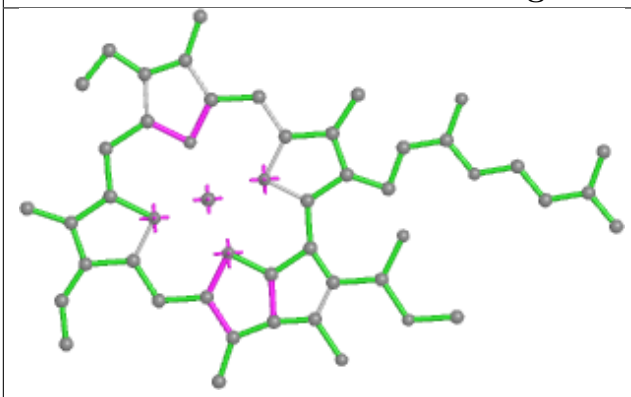
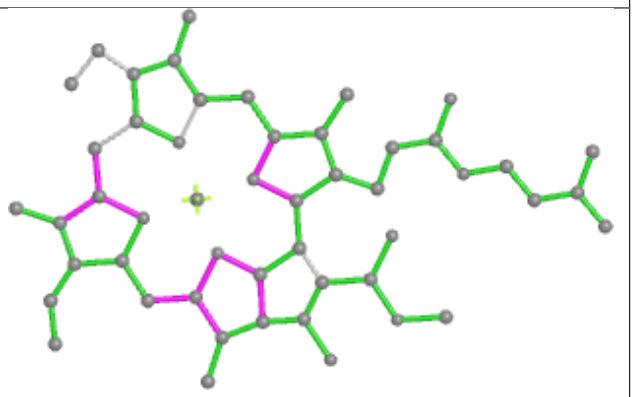


Rings

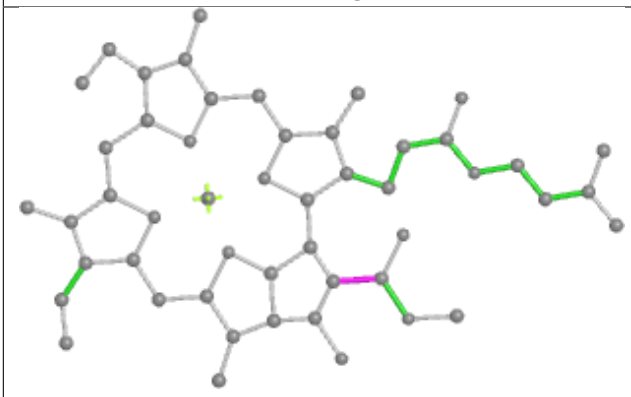
Ligand CLA b 721



Bond lengths



Bond angles



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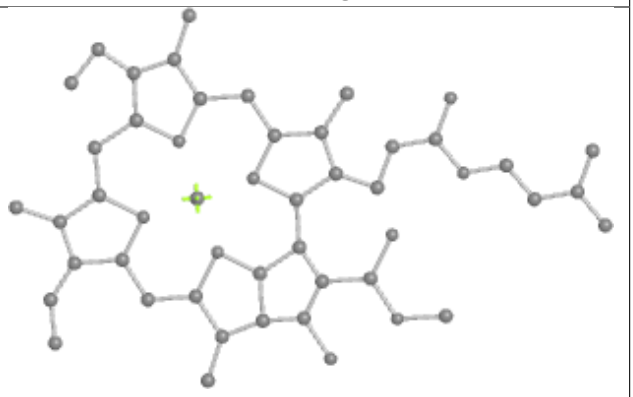
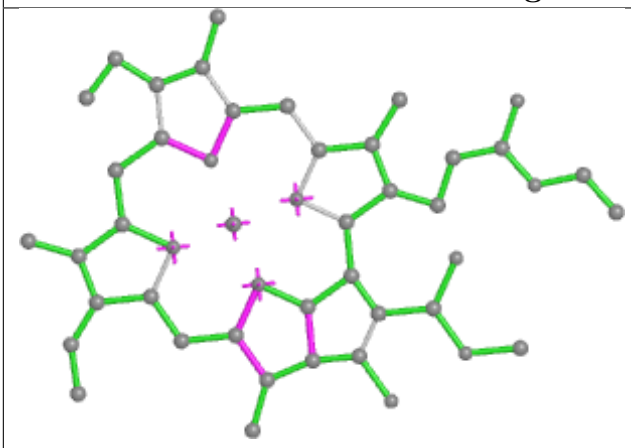
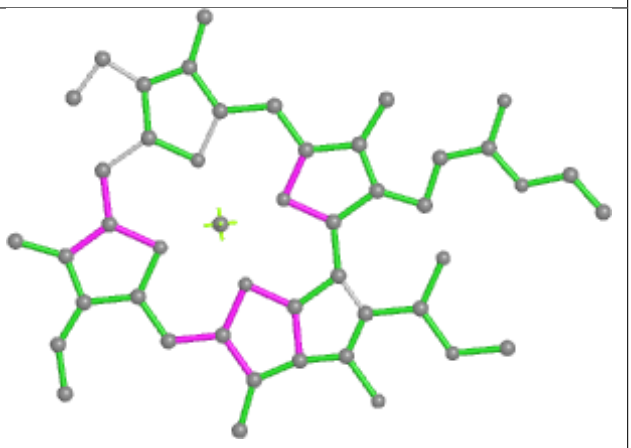


Rings

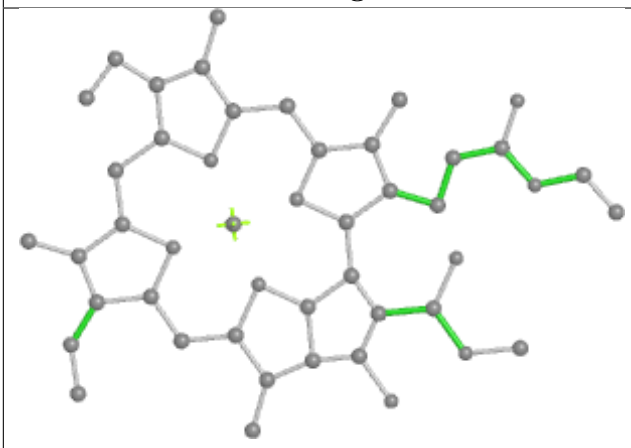
Ligand CLA C 212



Bond lengths



Bond angles



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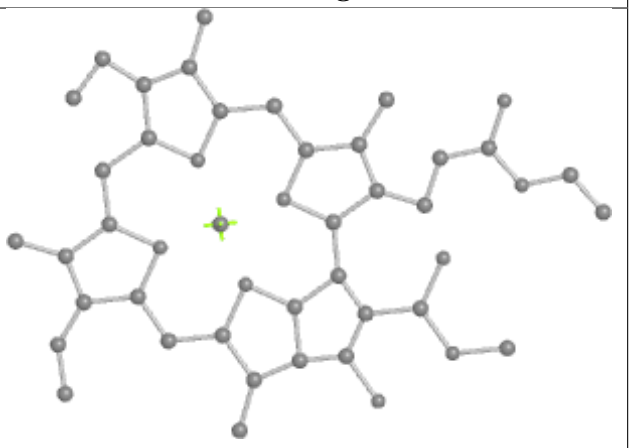
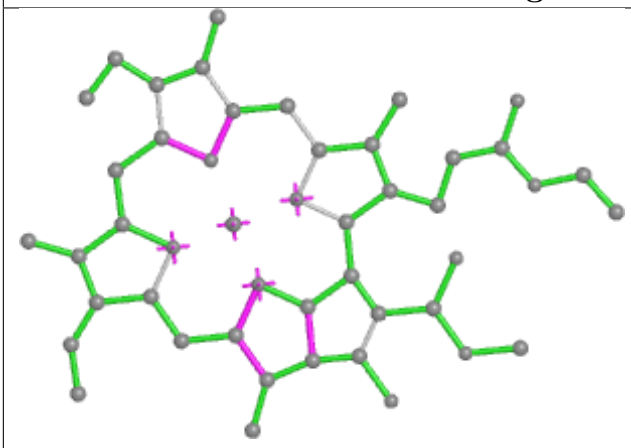


Rings

Ligand CLA F 610



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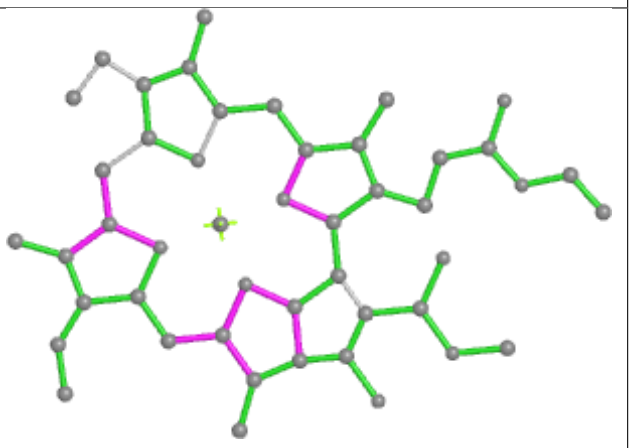
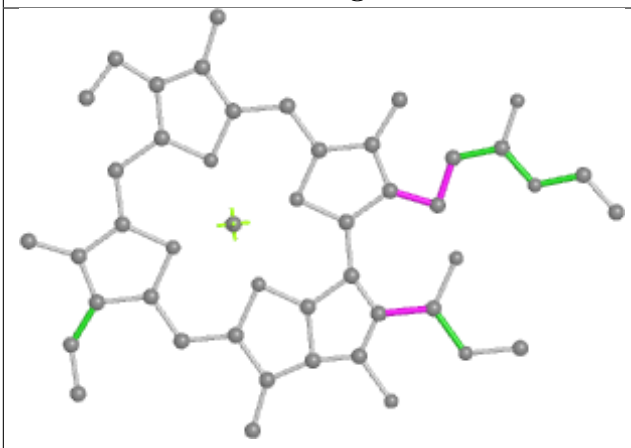
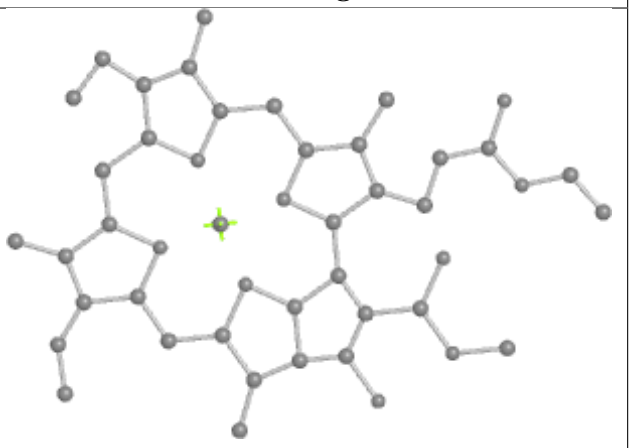


Bond angles

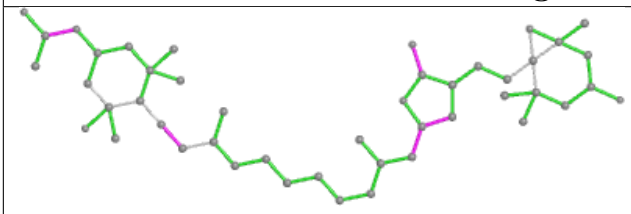


Torsions



Rings

Ligand PID J 615



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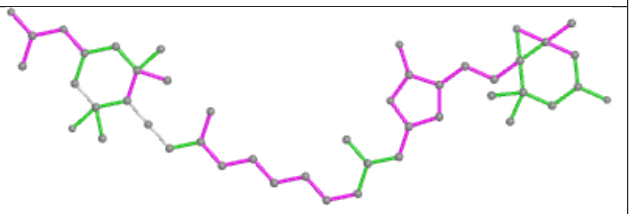
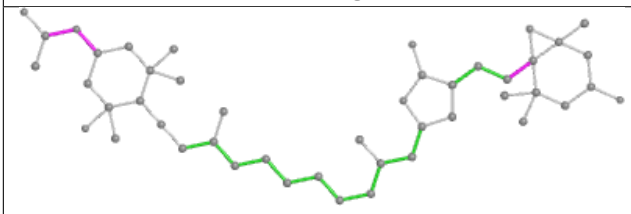


Bond angles



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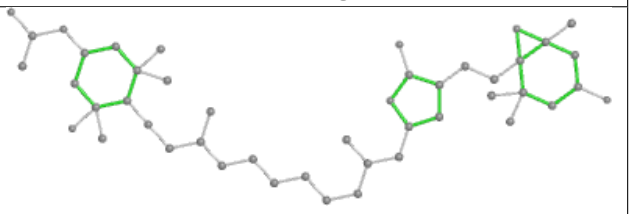
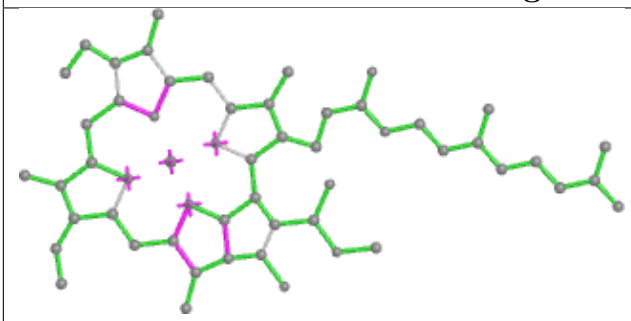


Rings

Ligand CLA D 602



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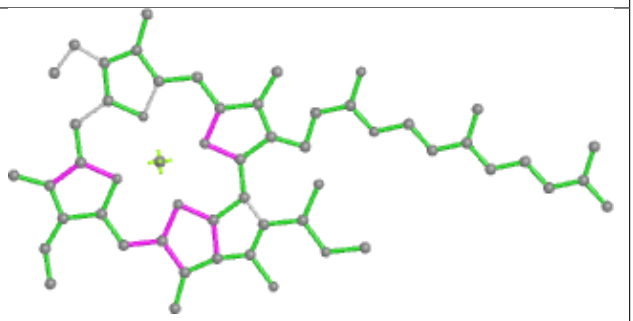
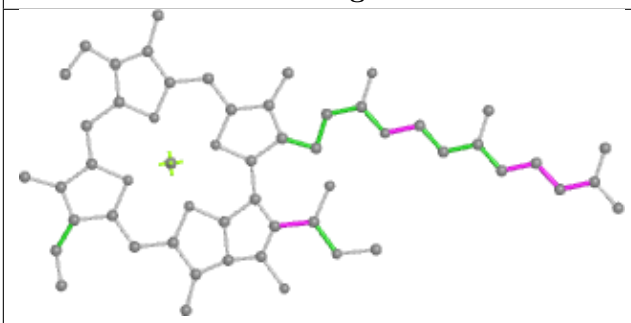
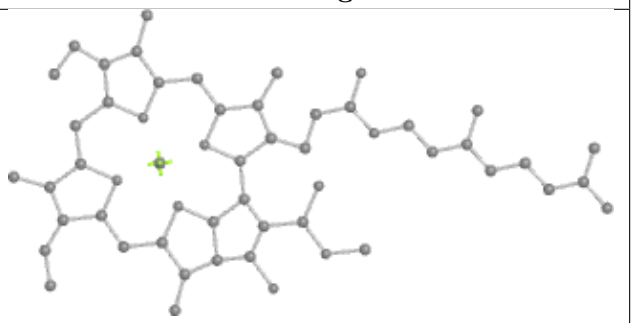


Bond angles

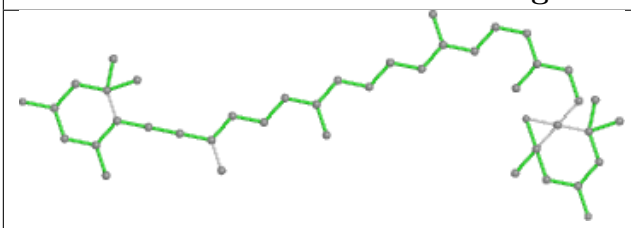


Torsions



Rings

Ligand DD6 I 615



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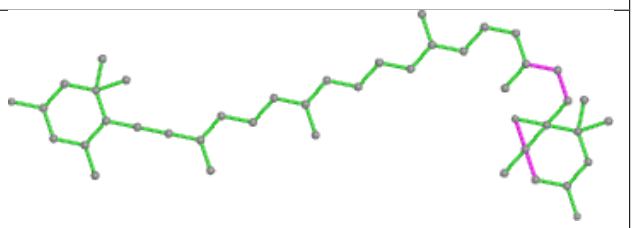
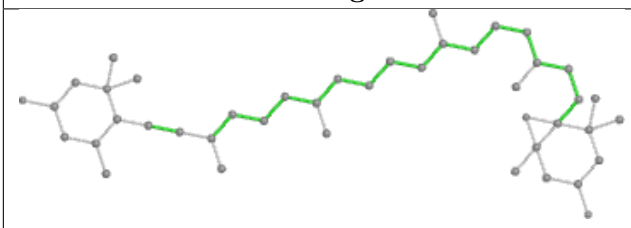


Bond angles



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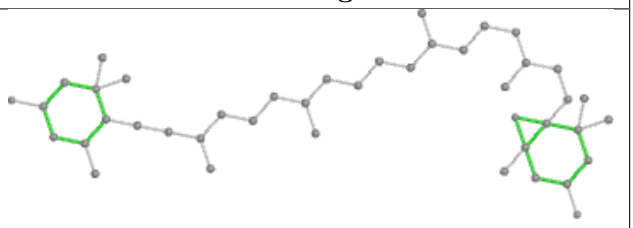
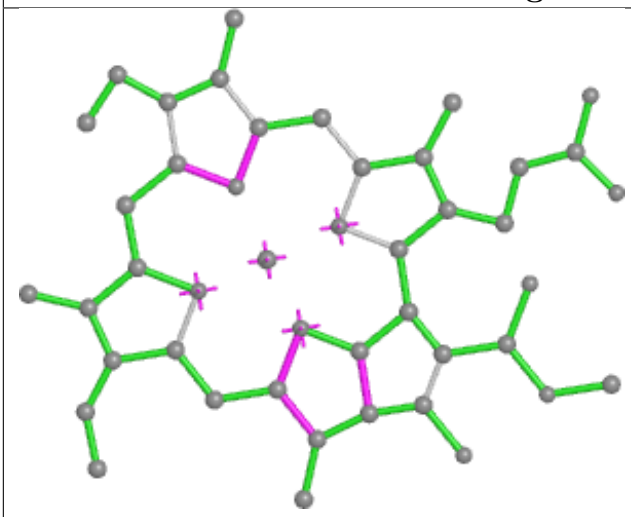


Rings

Ligand CLA F 608



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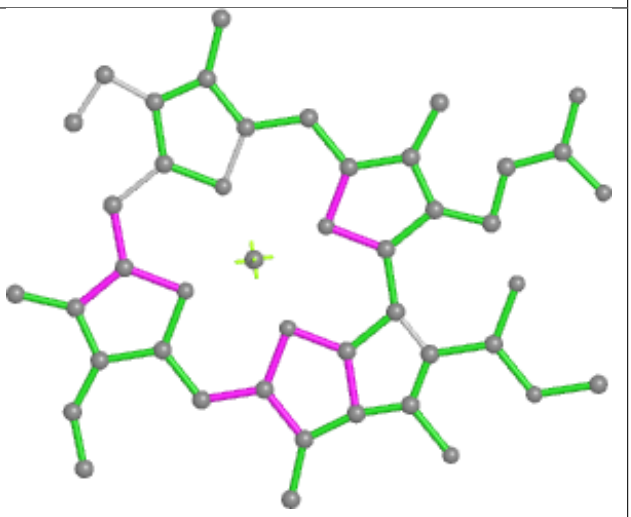
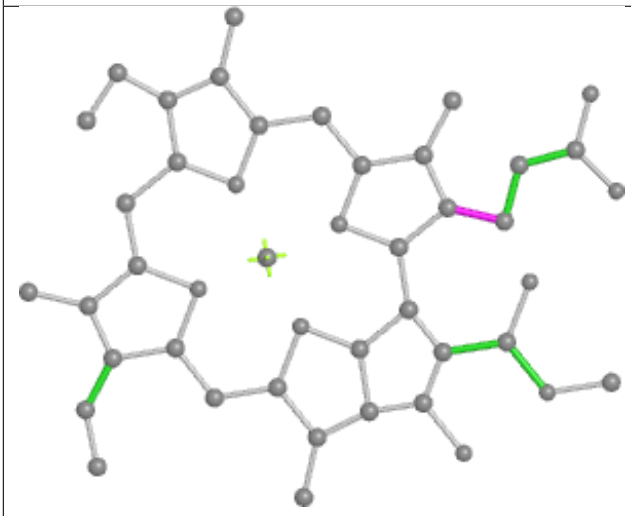
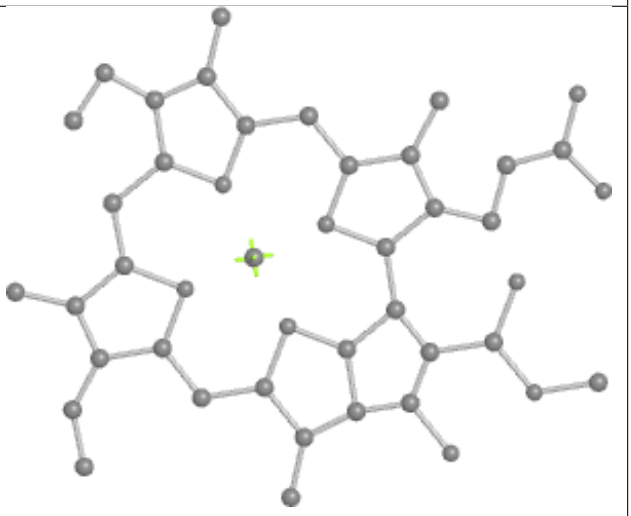


Bond angles

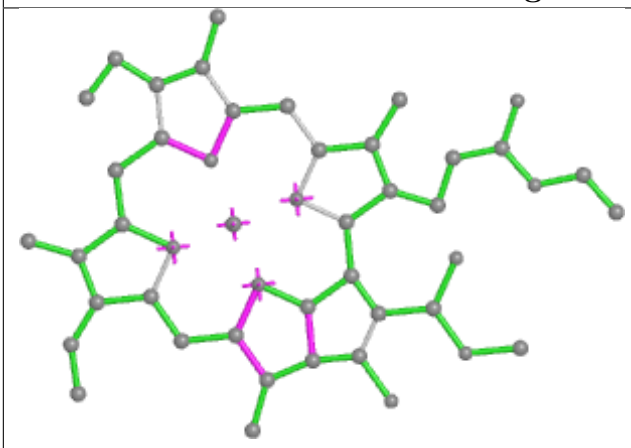


Torsions

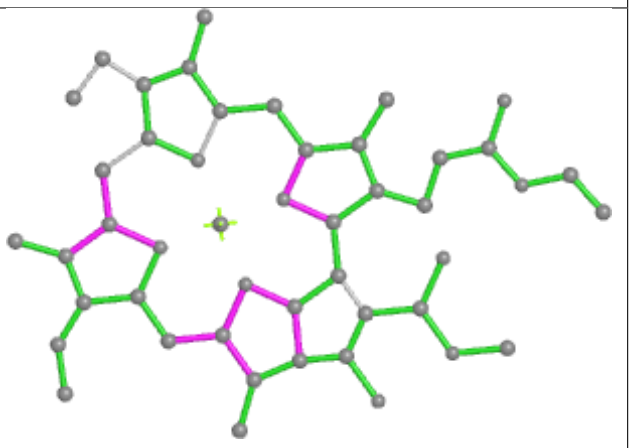


Rings

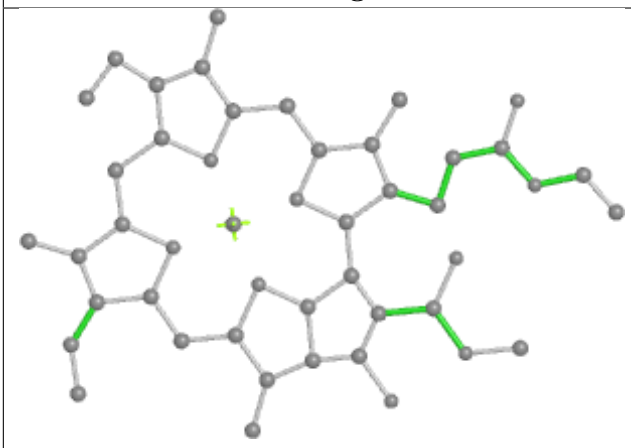
Ligand CLA B 604



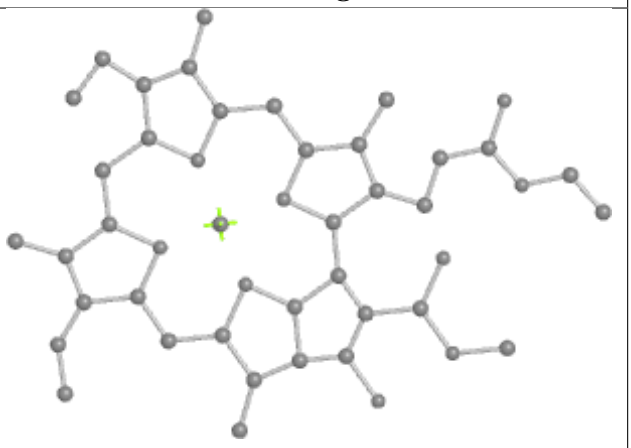
Bond lengths



Bond angles

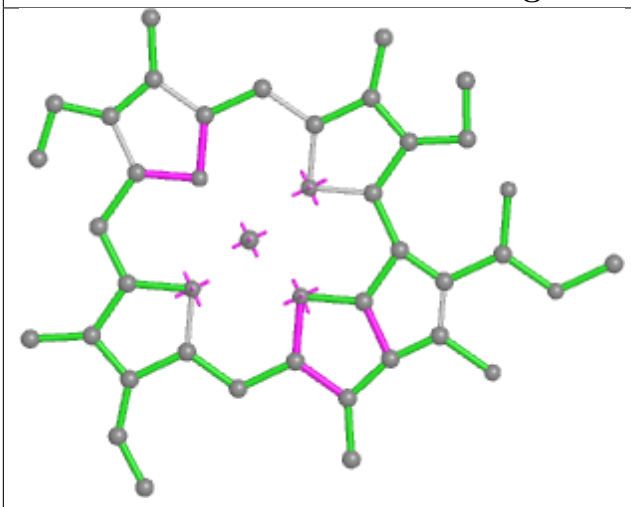


Torsions

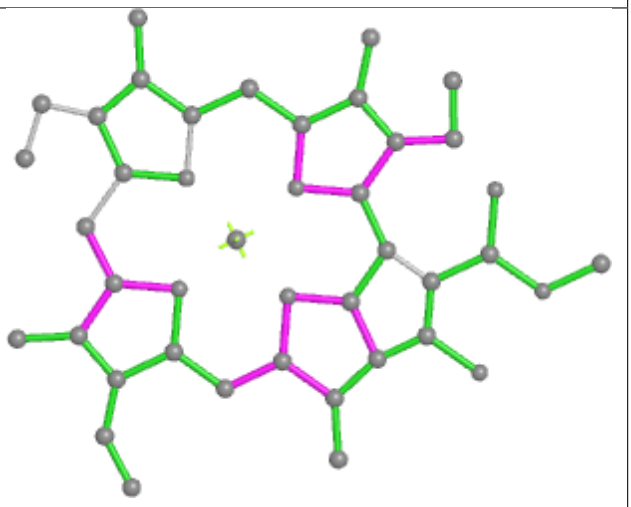


Rings

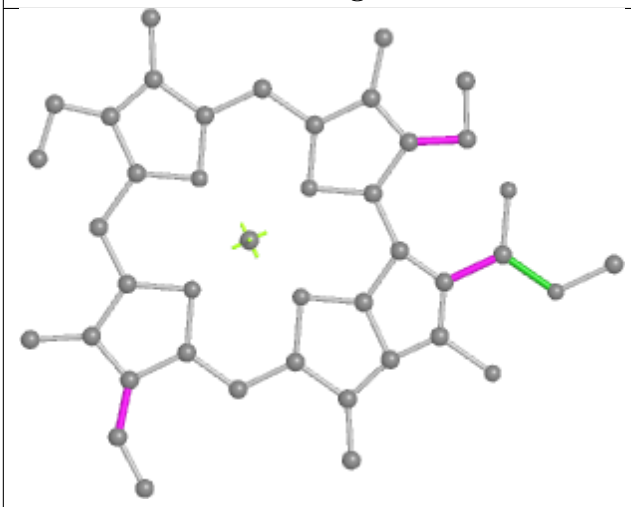
Ligand CLA H 312



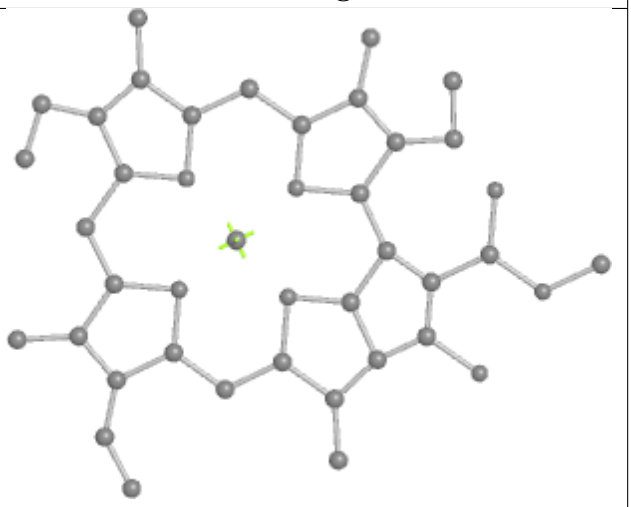
Bond lengths



Bond angles

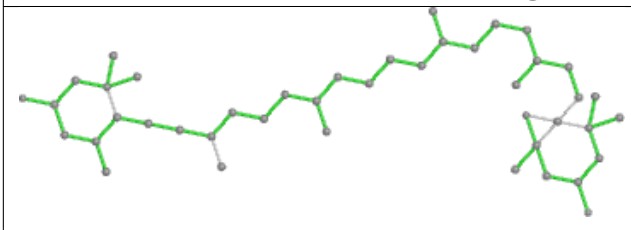


Torsions

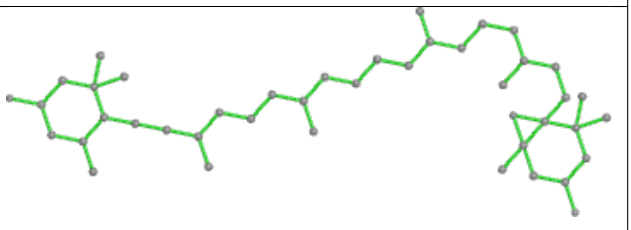


Rings

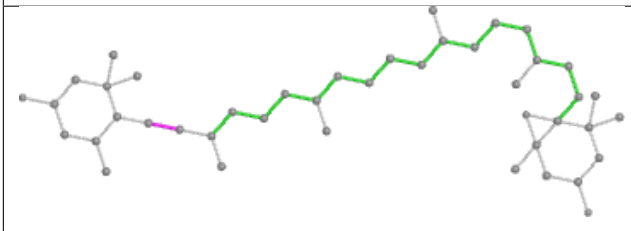
Ligand DD6 G 616



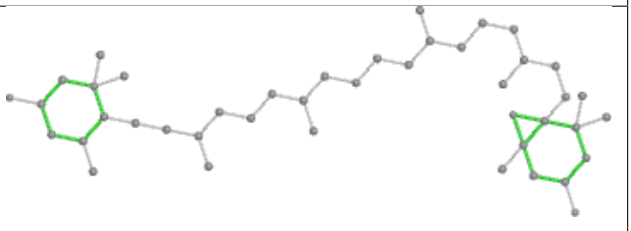
Bond lengths



Bond angles

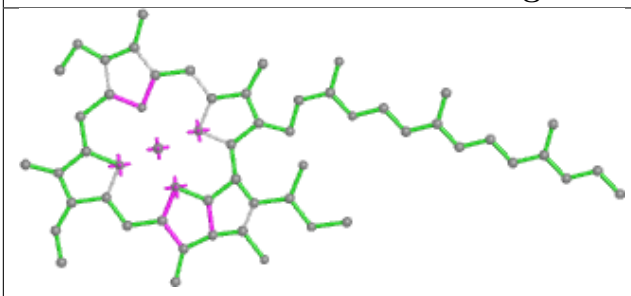


Torsions



Rings

Ligand CLA K 601



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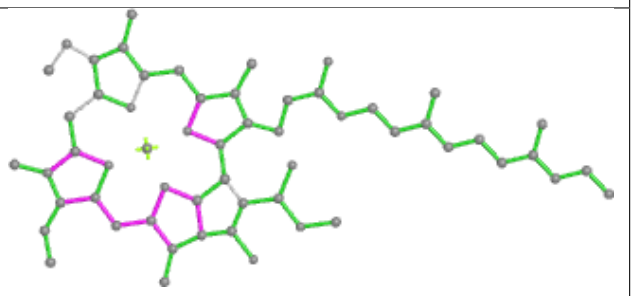
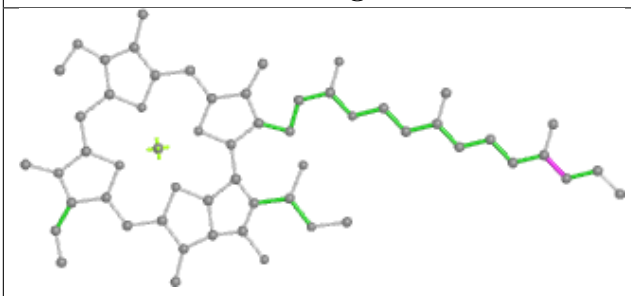
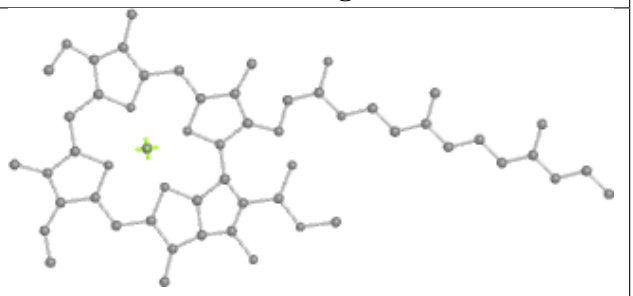


Bond angles

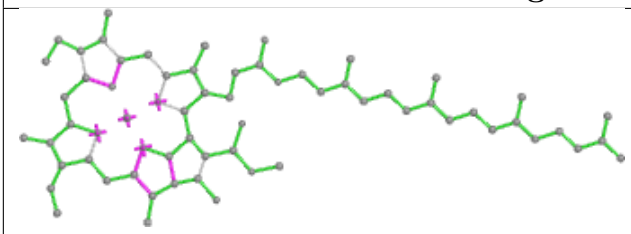


Torsions



Rings

Ligand CLA b 723



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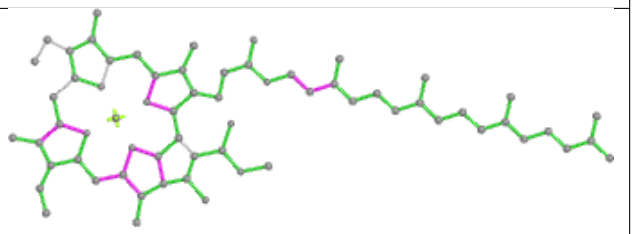
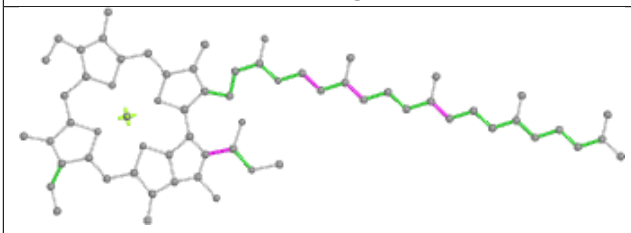
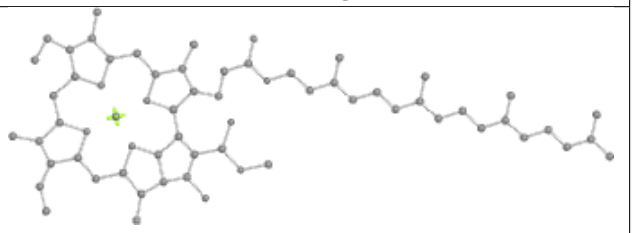


Bond angles

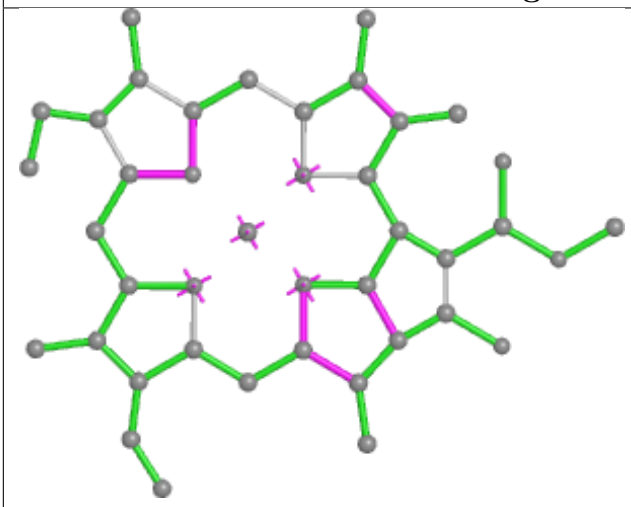


Torsions



Rings

Ligand CLA K 606



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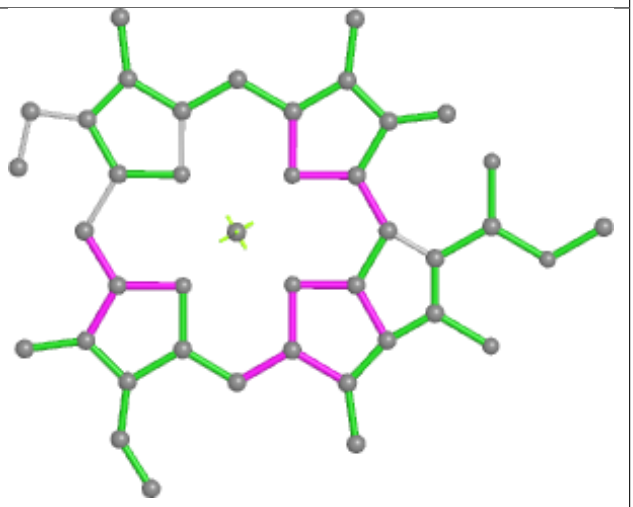
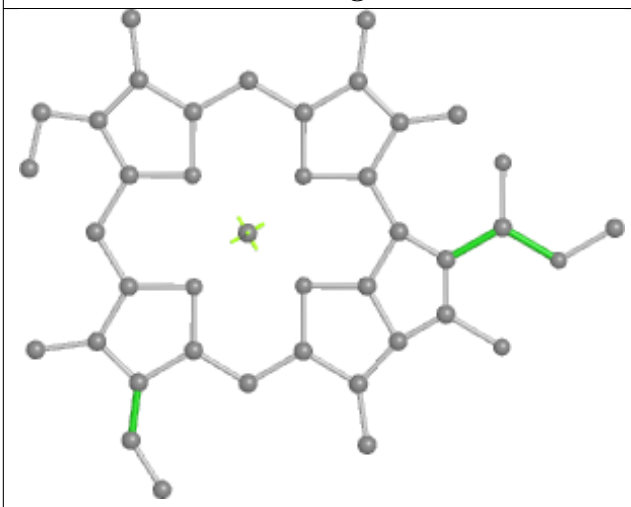
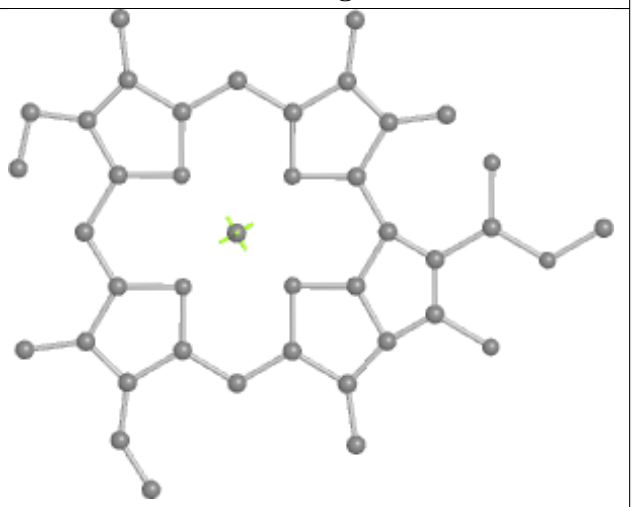


Bond angles

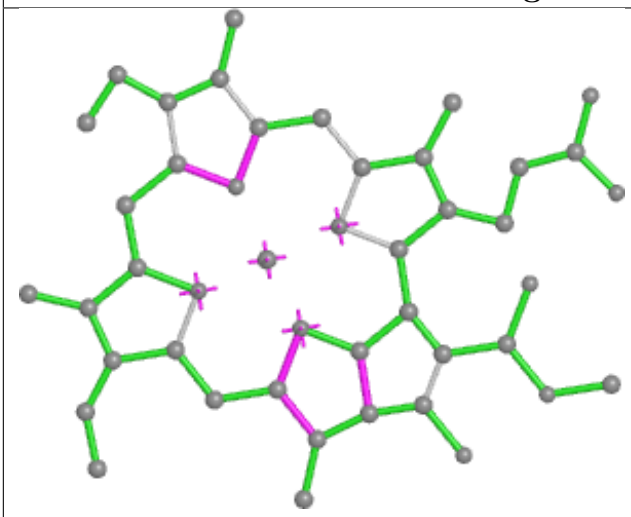


Torsions



Rings

Ligand CLA H 307



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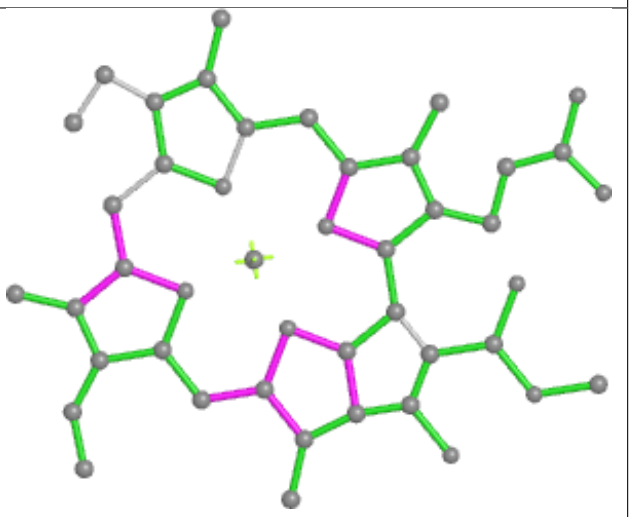
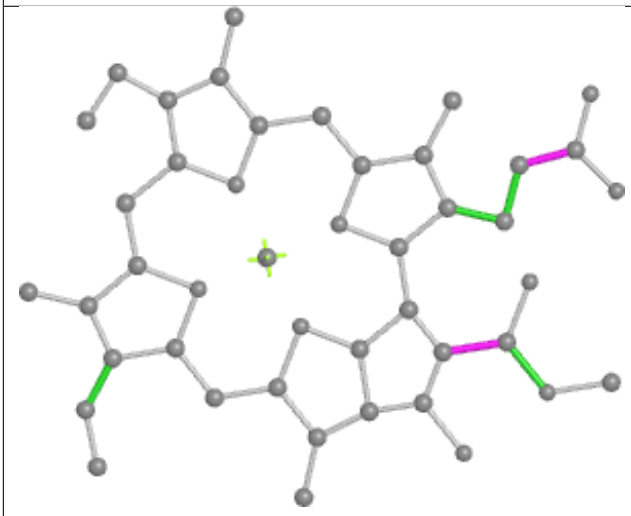


Bond angles



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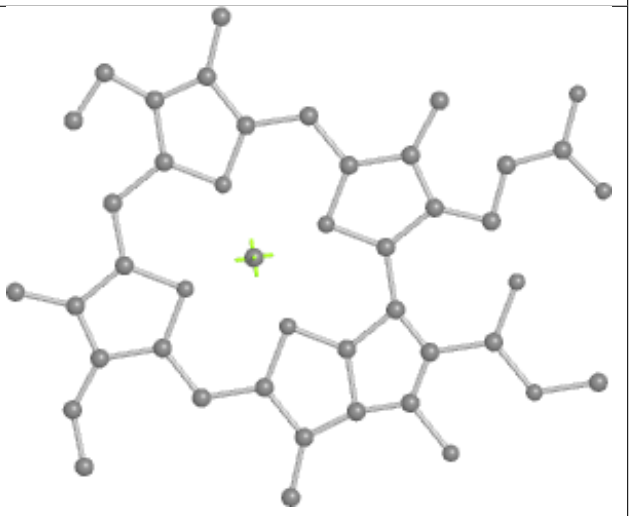
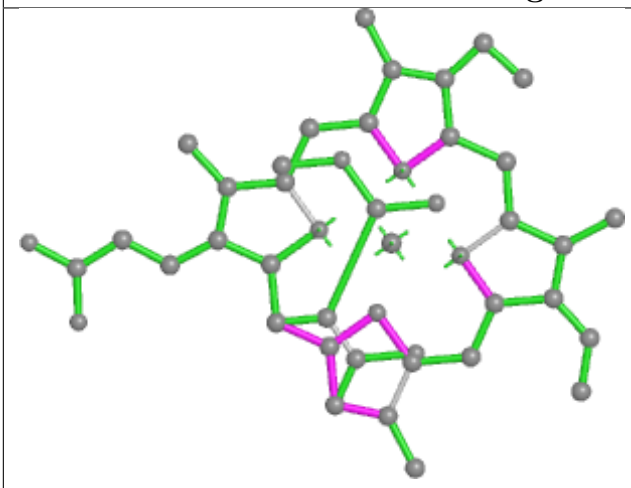
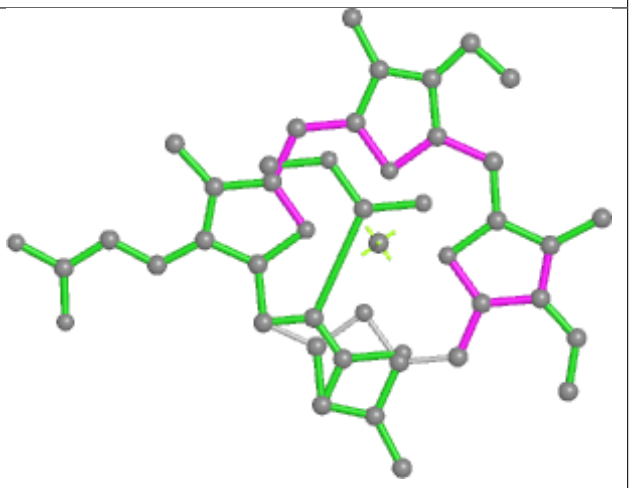


Rings

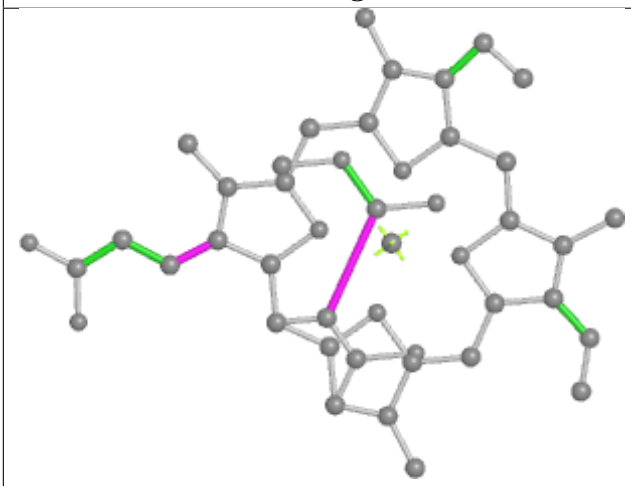
Ligand KC2 B 608



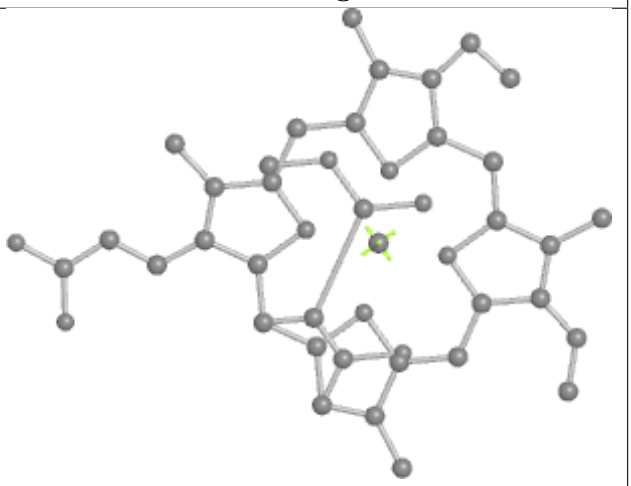
Bond lengths



Bond angles

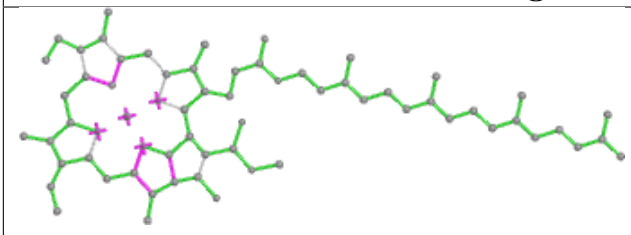


Torsions



Rings

Ligand CLA b 717



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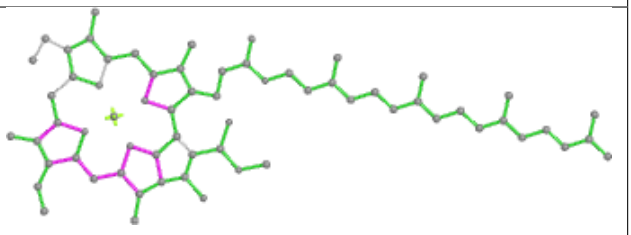
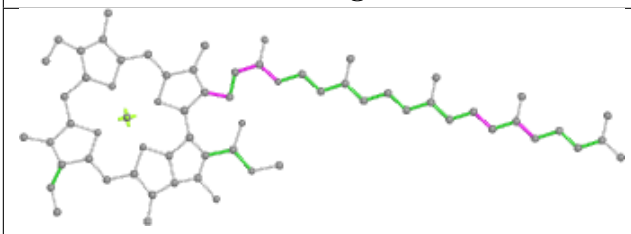


Bond angles



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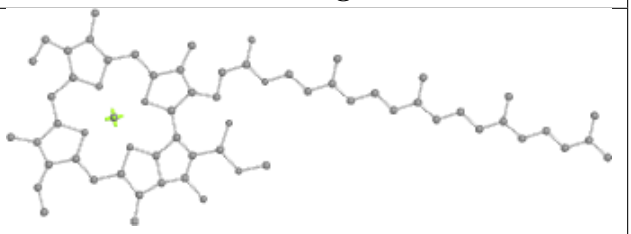
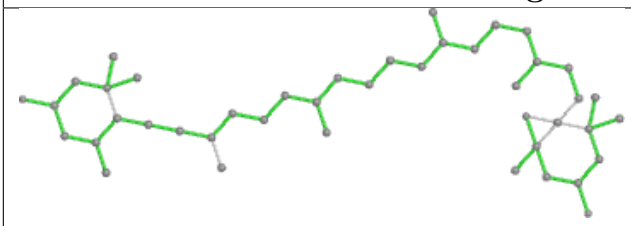


Rings

Ligand DD6 E 613



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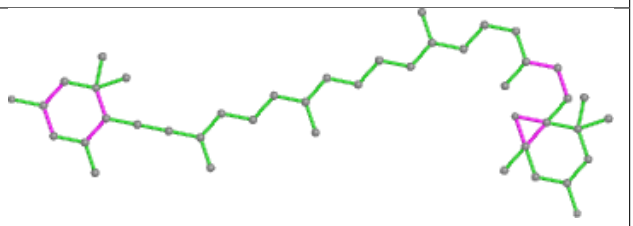
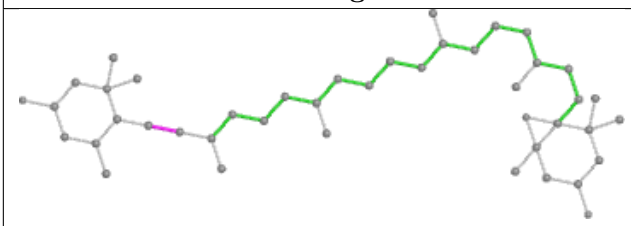


Bond angles



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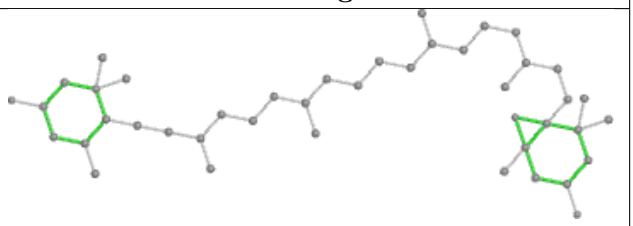
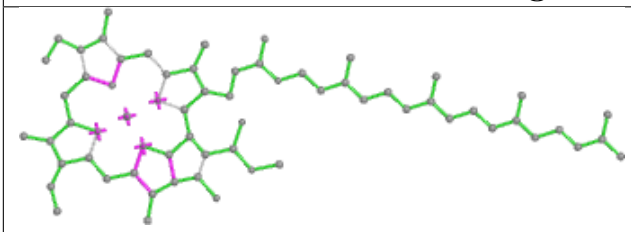
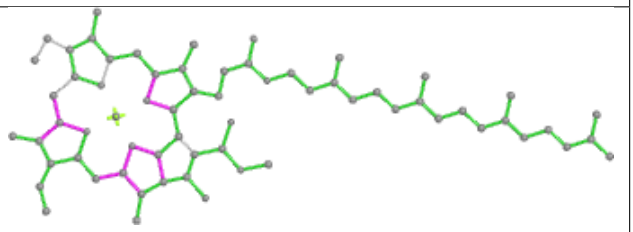


Rings

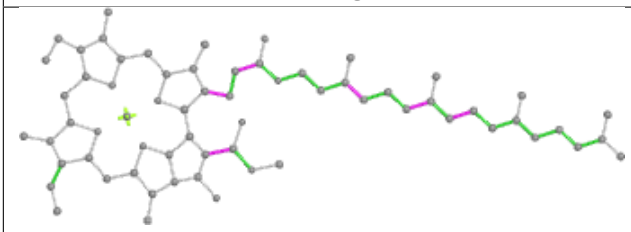
Ligand CLA a 805



Bond lengths



Bond angles



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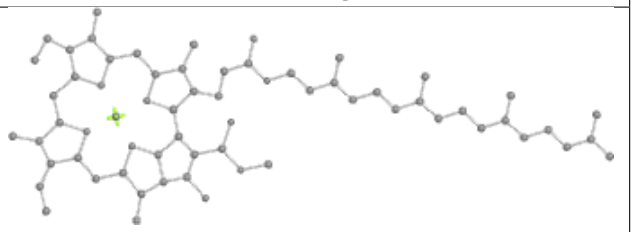
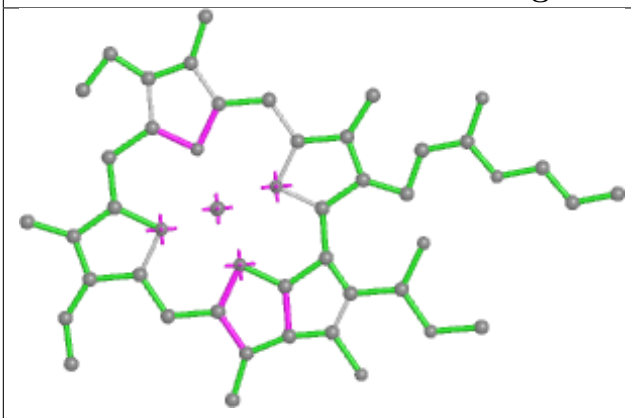


Rings

Ligand CLA f 302



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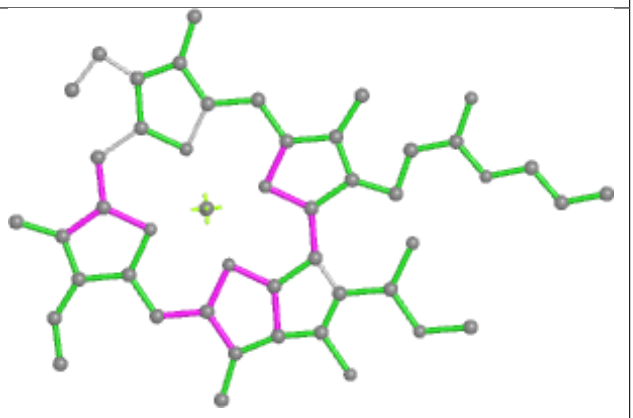
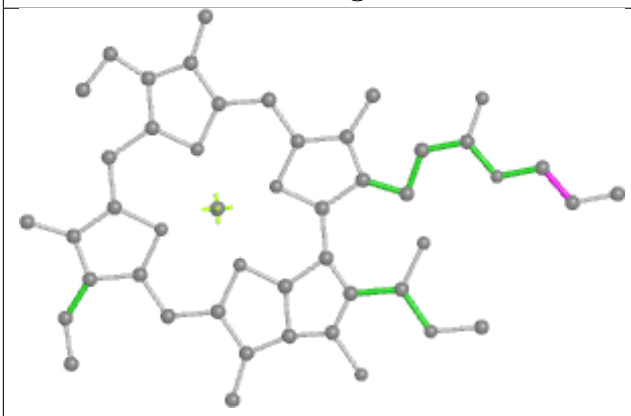


Bond angles



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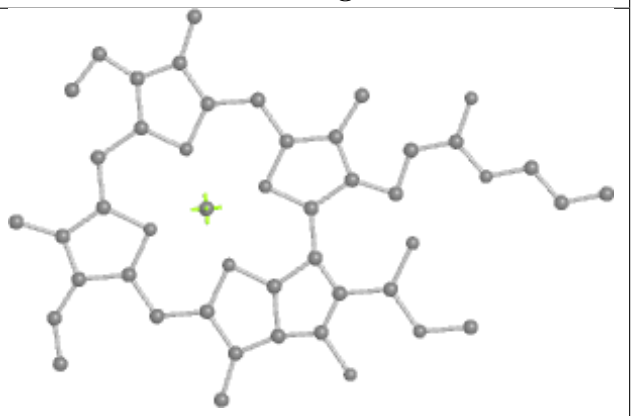
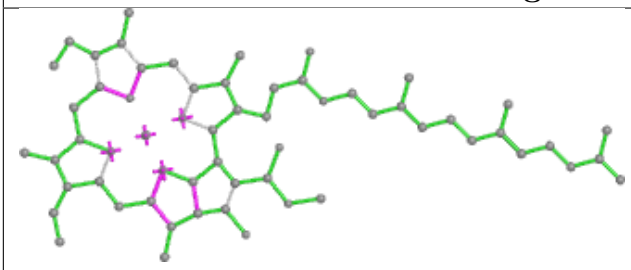


Rings

Ligand CLA A 602



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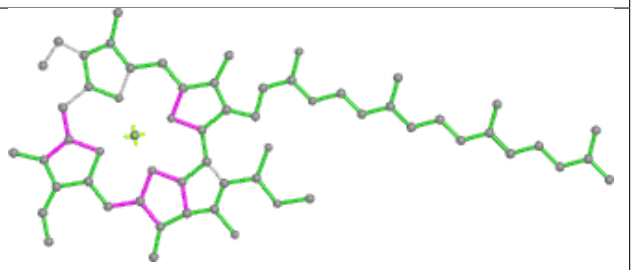
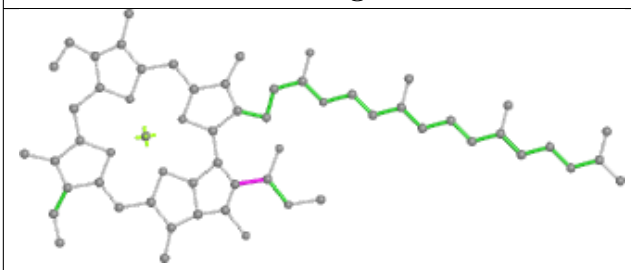


Bond angles



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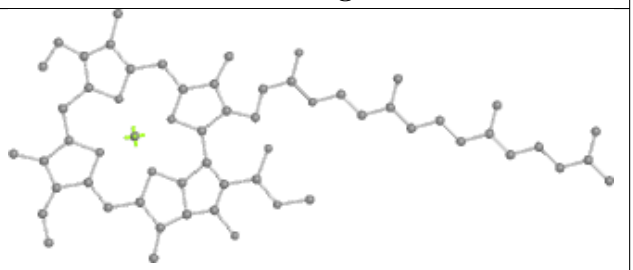
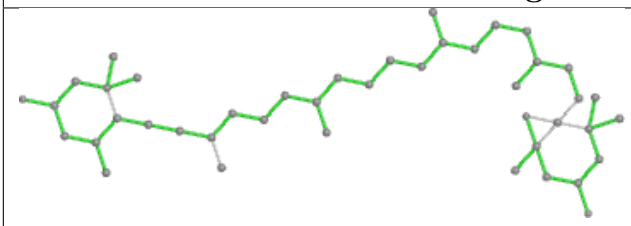


Rings

Ligand DD6 B 612



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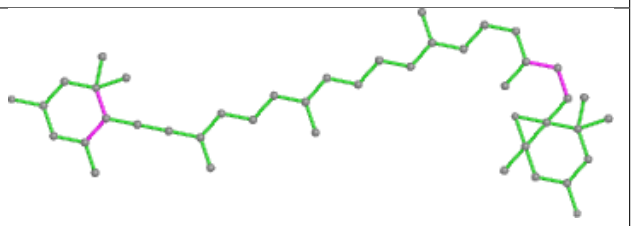
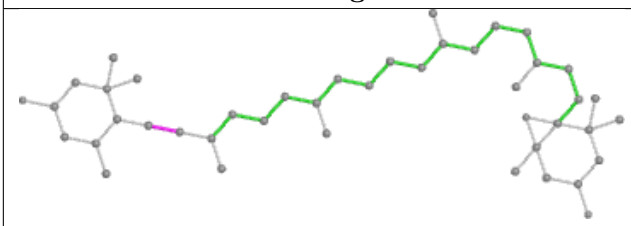


Bond angles



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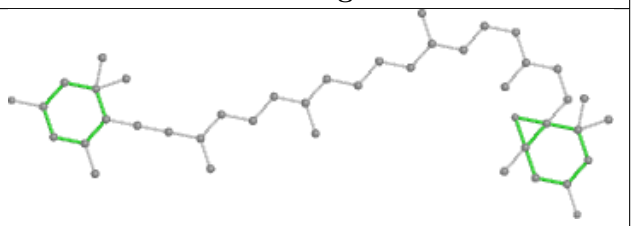
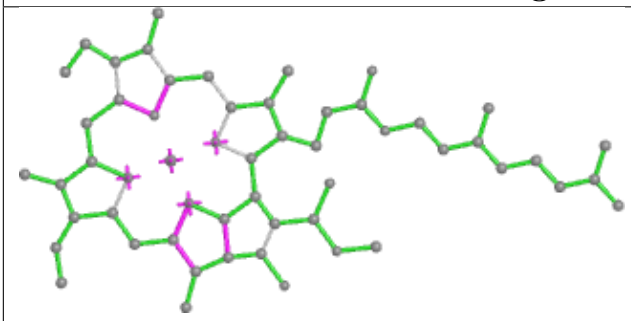


Rings

Ligand CLA I 605



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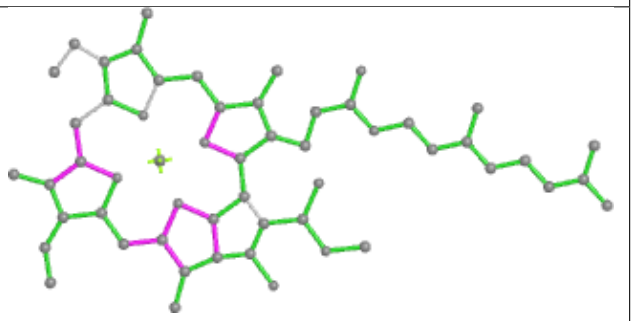
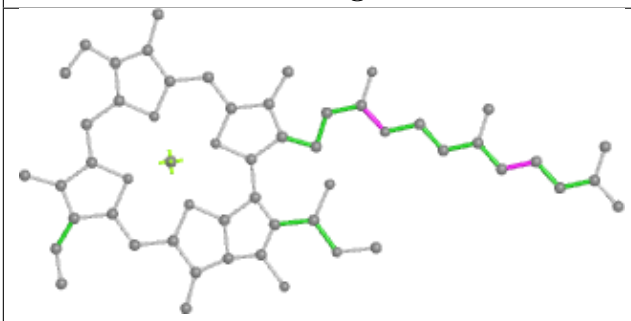
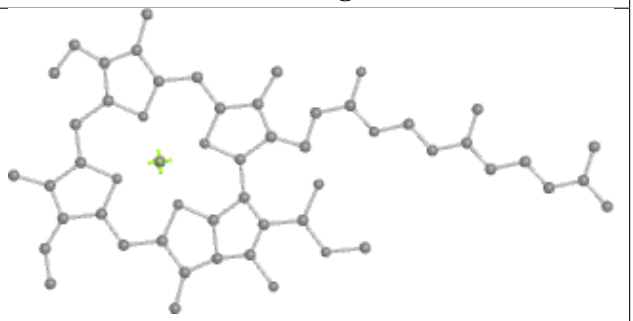


Bond angles

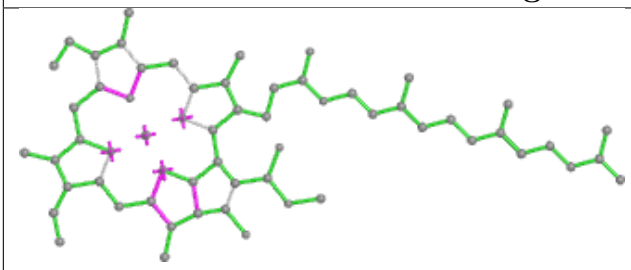


Torsions

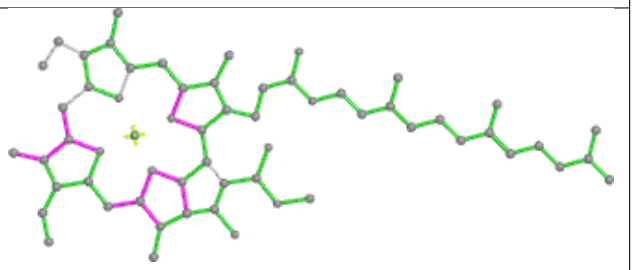


Rings

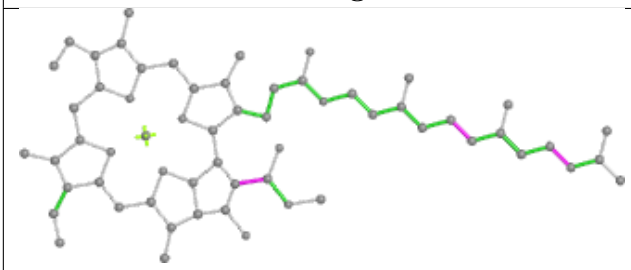
Ligand CLA H 303



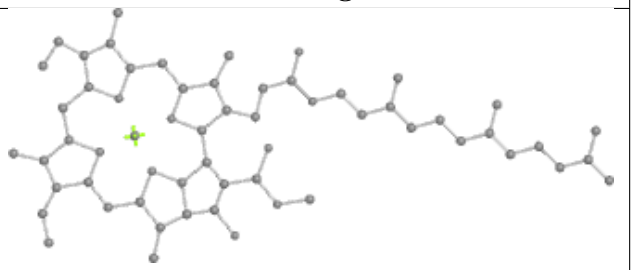
Bond lengths



Bond angles

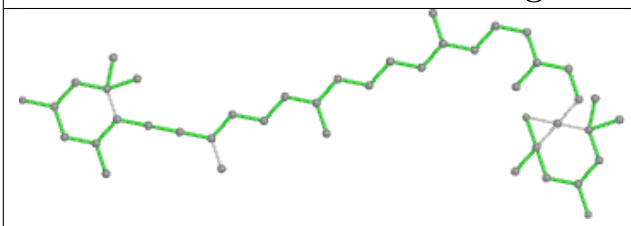


Torsions

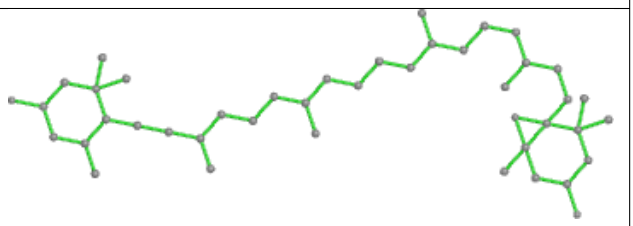


Rings

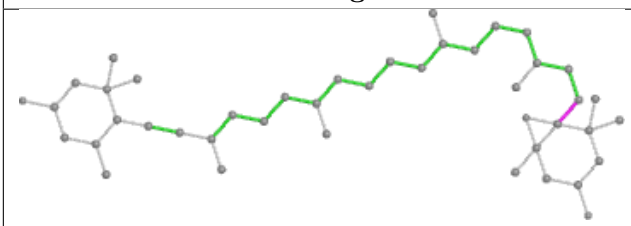
Ligand DD6 B 616



Bond lengths



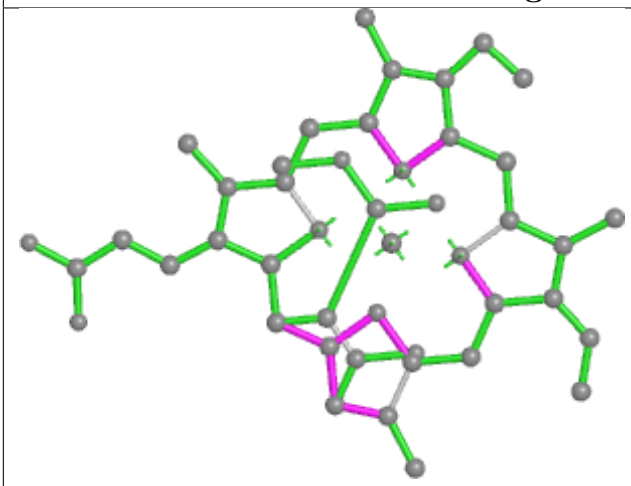
Bond angles



Torsions

Rings

Ligand KC2 G 601



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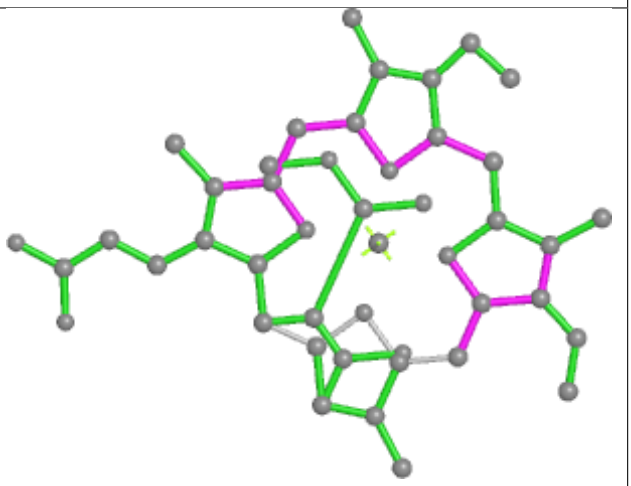
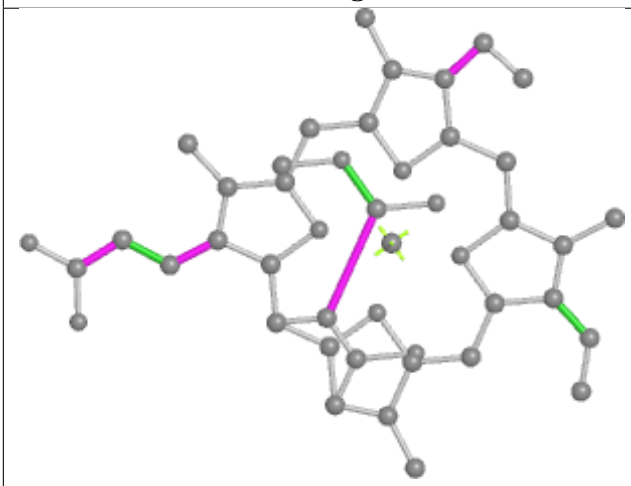
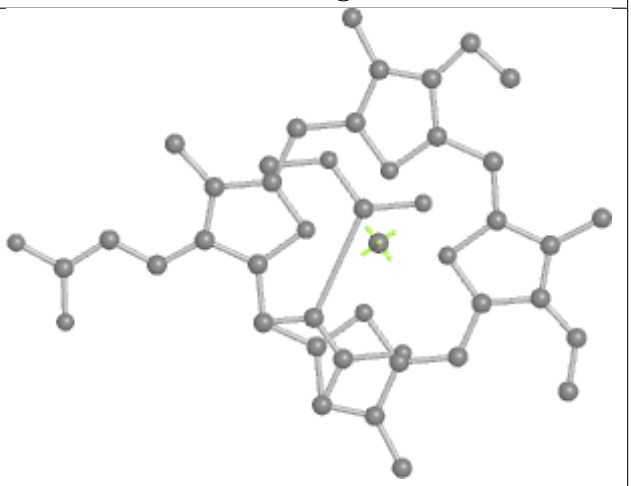


Bond angles

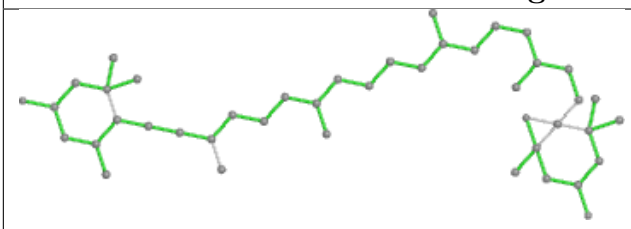


Torsions



Rings

Ligand DD6 b 730



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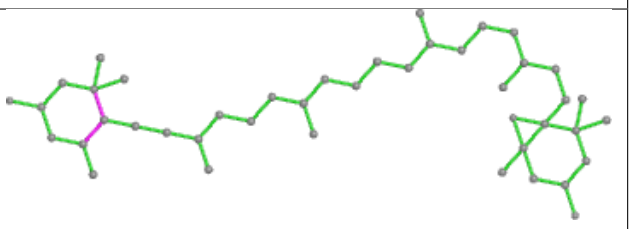
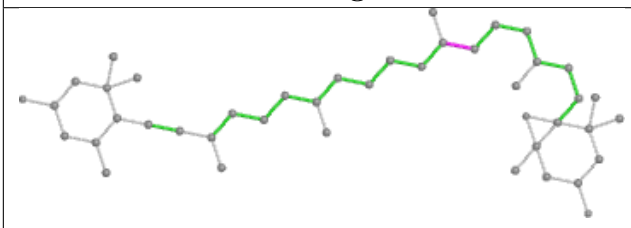
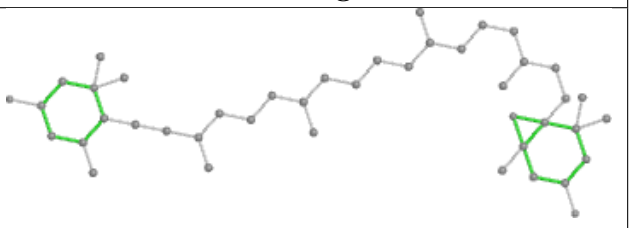


Bond angles

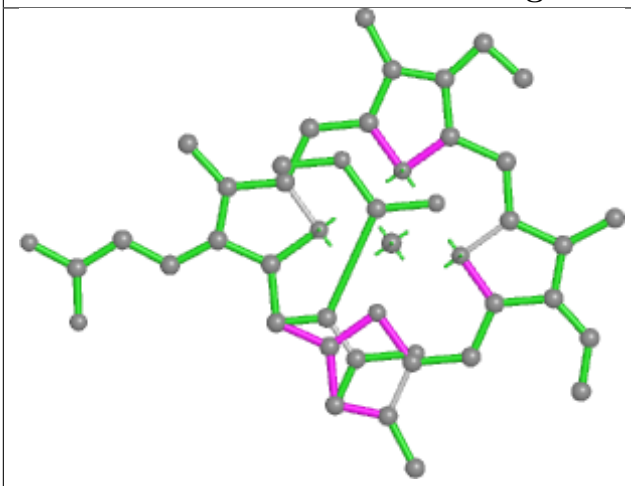


Torsions



Rings

Ligand KC2 C 210



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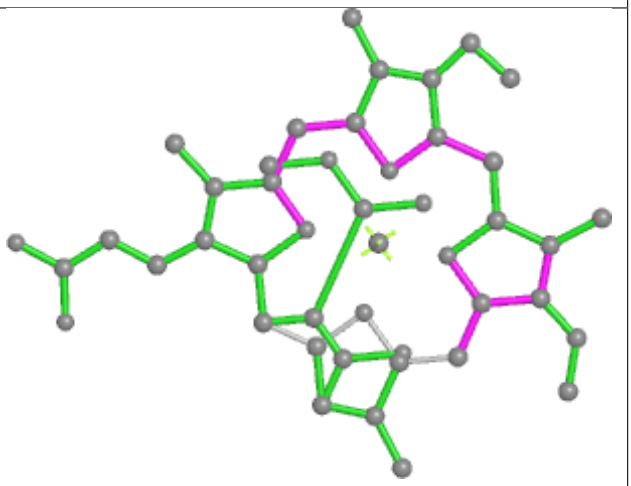
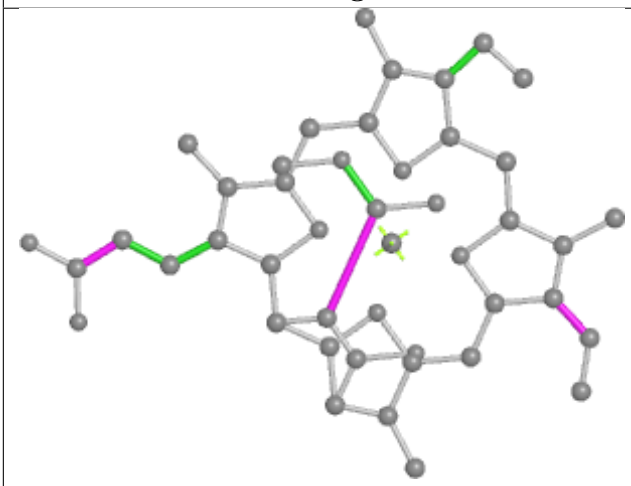
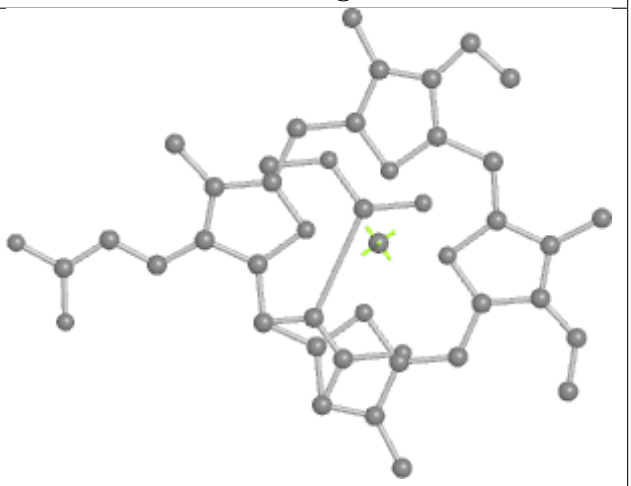


Bond angles

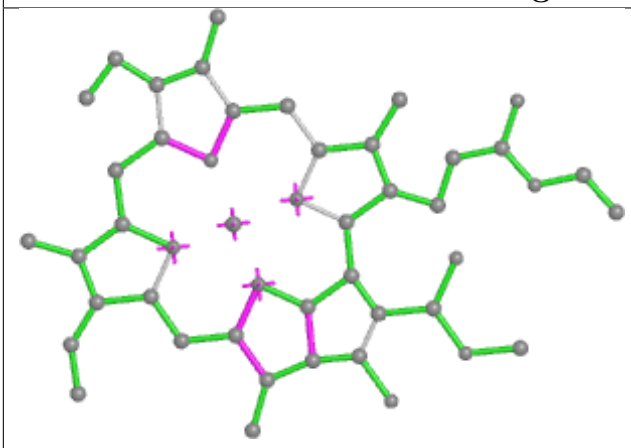


Torsions



Rings

Ligand CLA l 408



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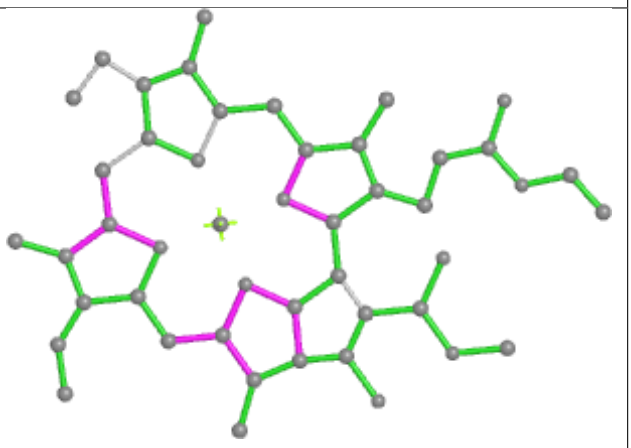
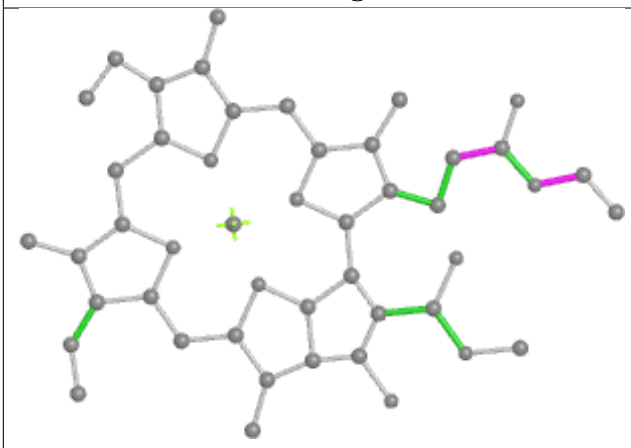
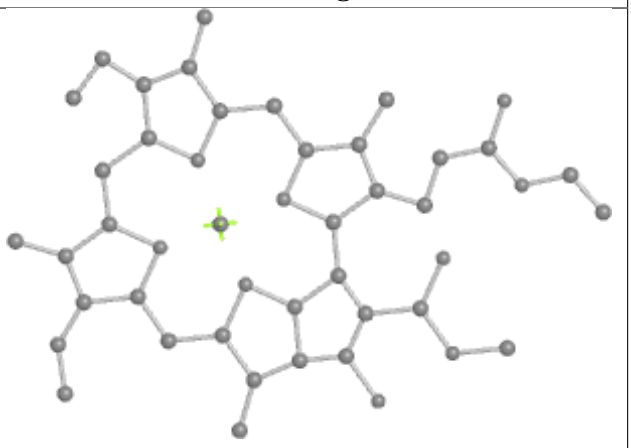


Bond angles

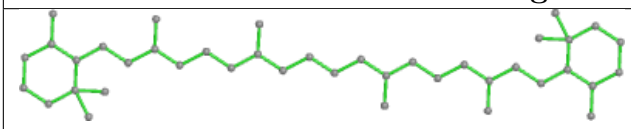


Torsions



Rings

Ligand BCR l 415



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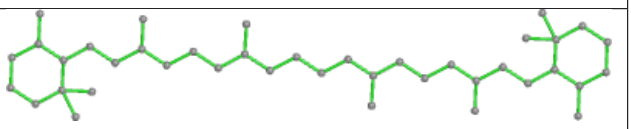
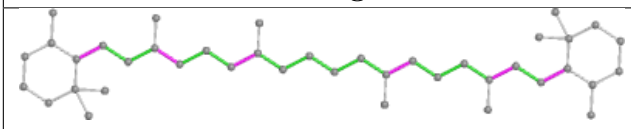


Bond angles



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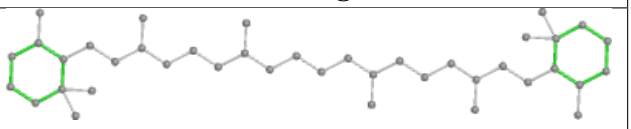
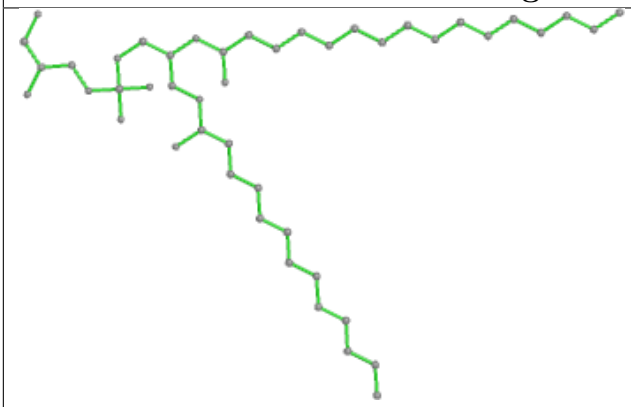


Rings

Ligand LHG D 620



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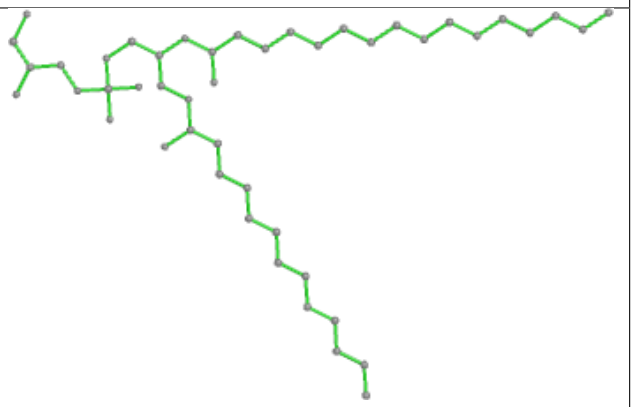
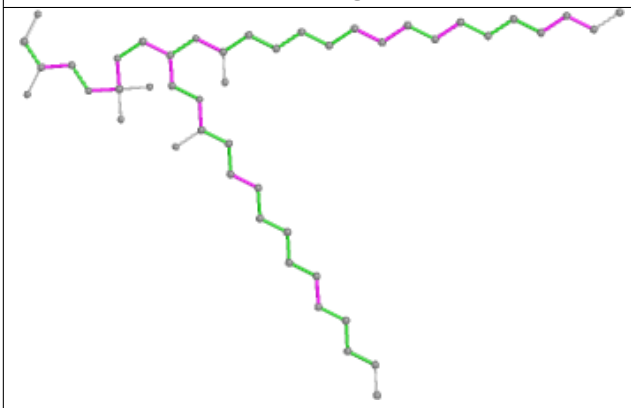


Bond angles



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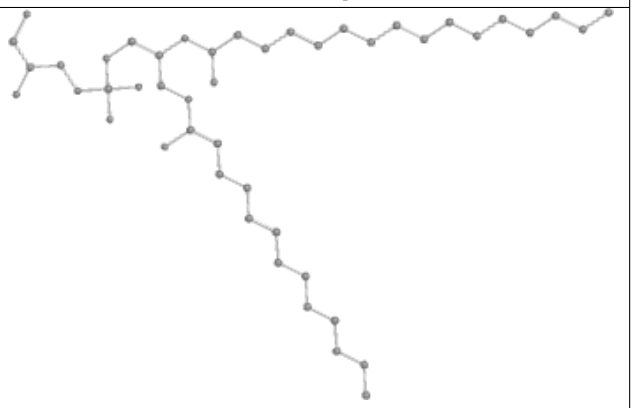
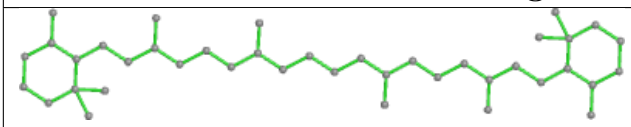


Rings

Ligand BCR a 833



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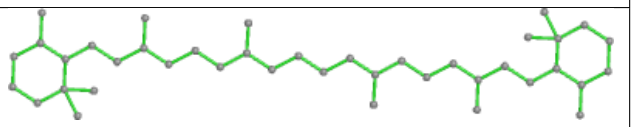
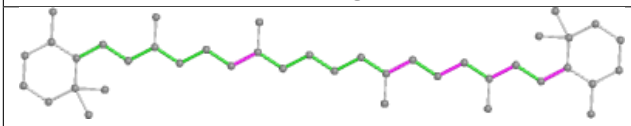


Bond angles



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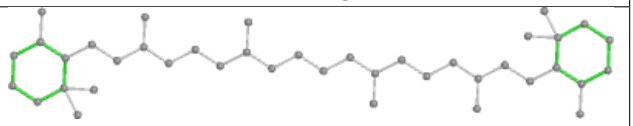
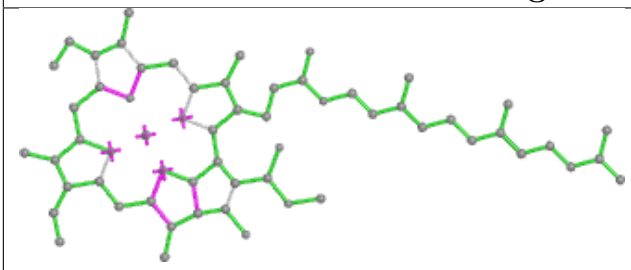


Rings

Ligand CLA a 816



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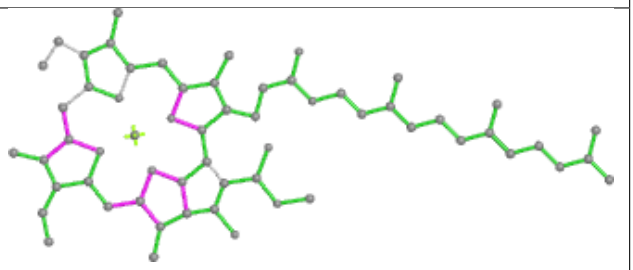
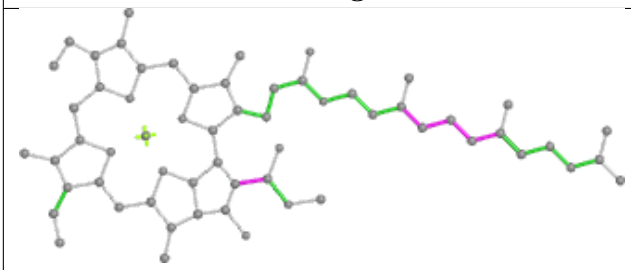
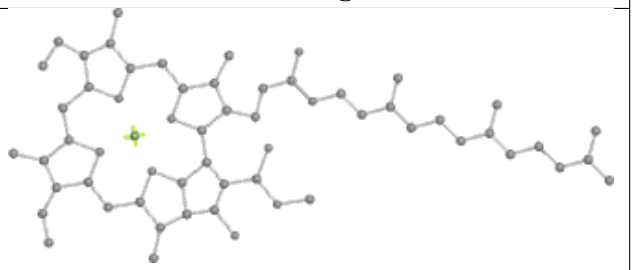


Bond angles

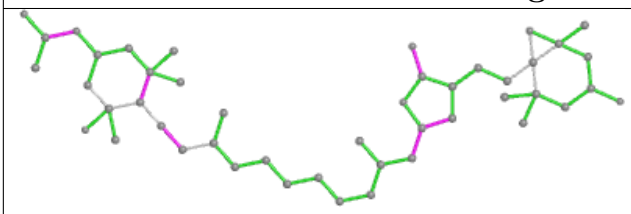


Torsions



Rings

Ligand PID U 608



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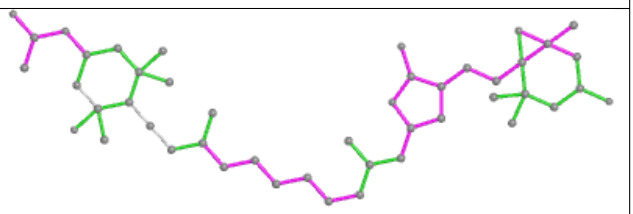
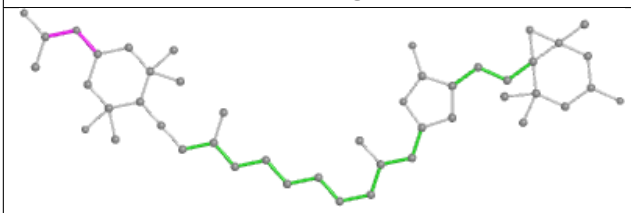


Bond angles



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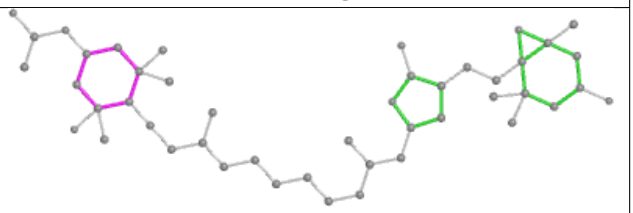
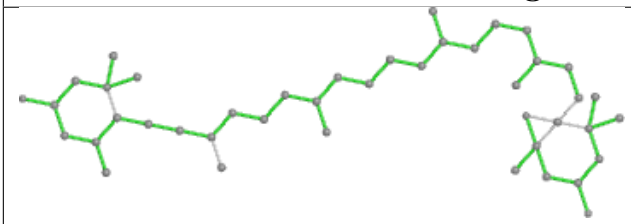


Rings

Ligand DD6 G 612



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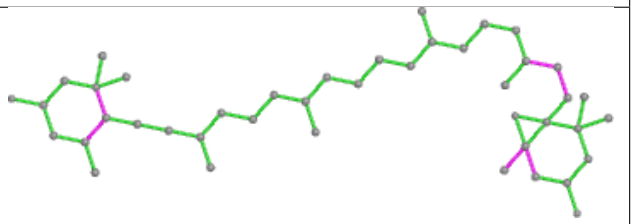
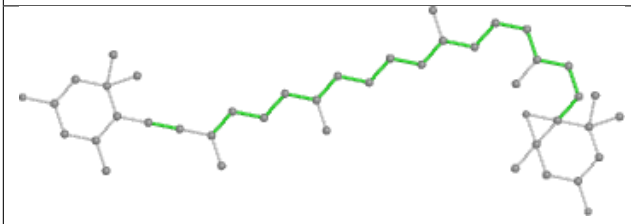


Bond angles



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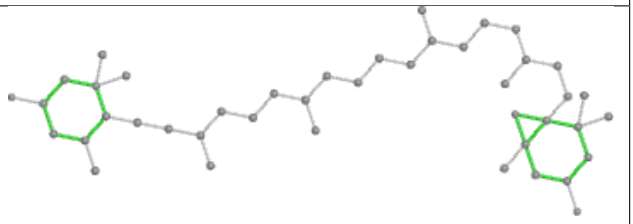
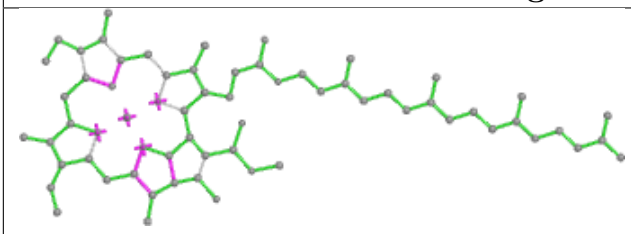


Rings

Ligand CLA b 719



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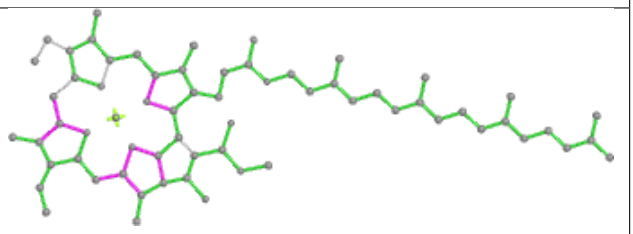
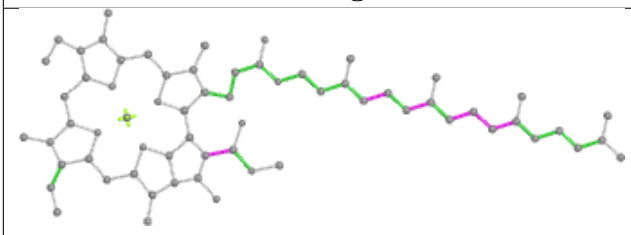


Bond angles



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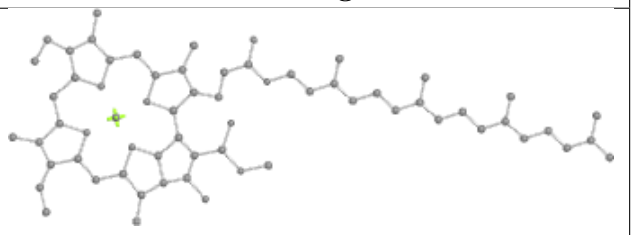
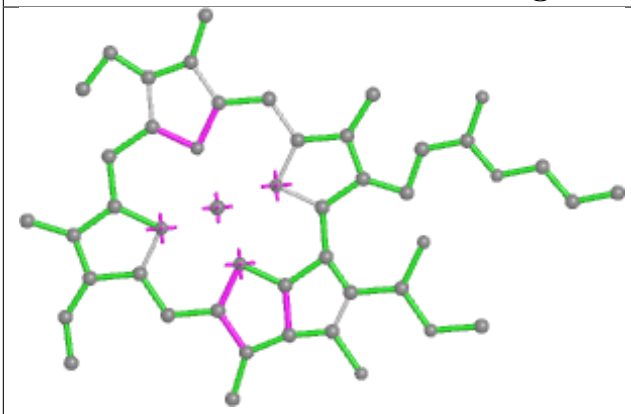
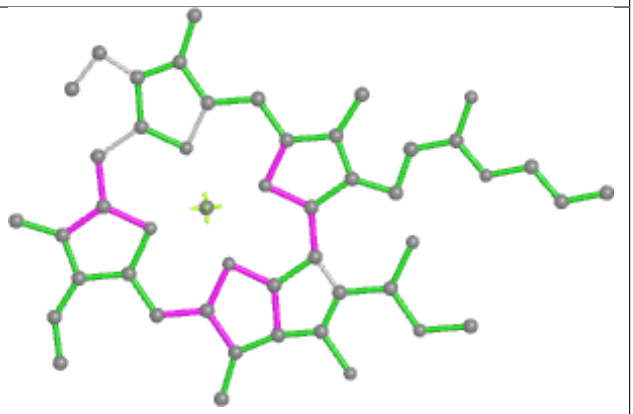


Rings

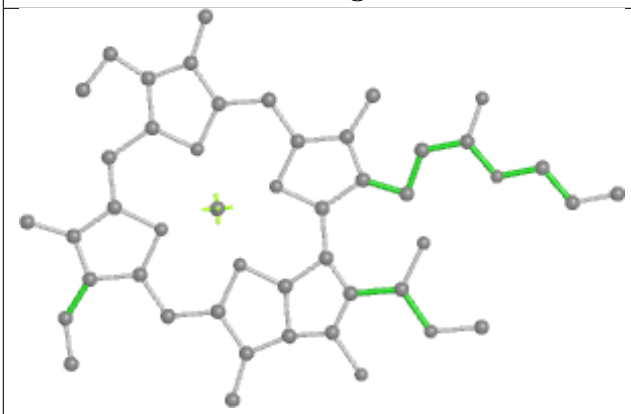
Ligand CLA f 303



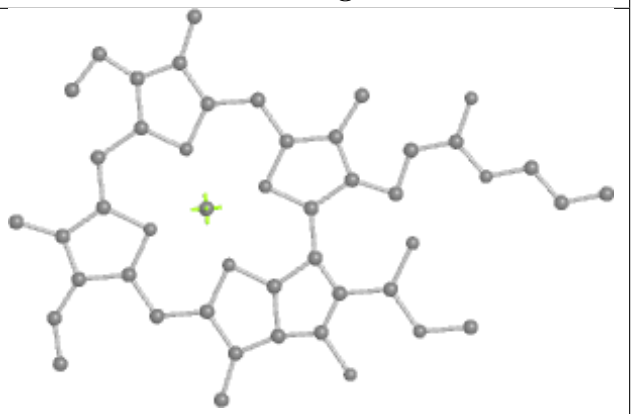
Bond lengths



Bond angles

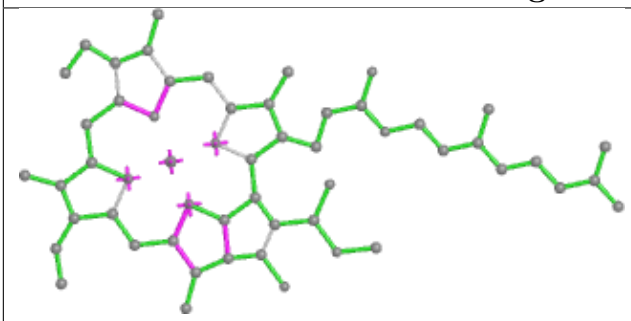


Torsions

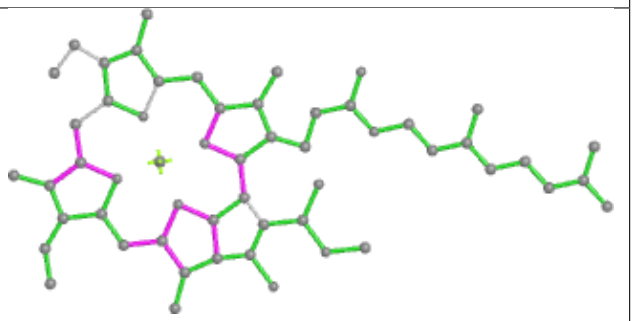


Rings

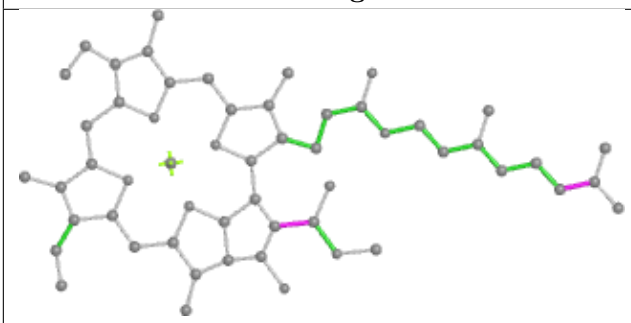
Ligand CLA a 802



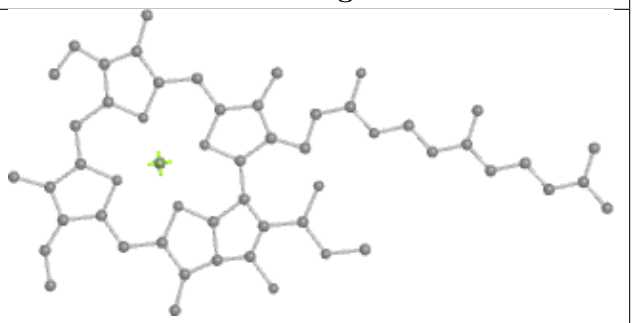
Bond lengths



Bond angles

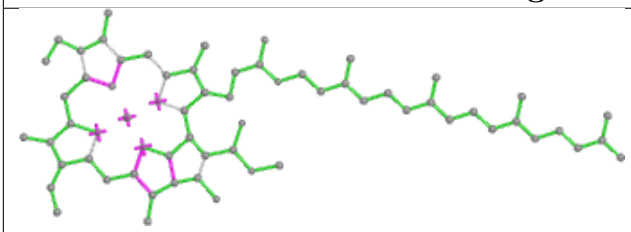


Torsions

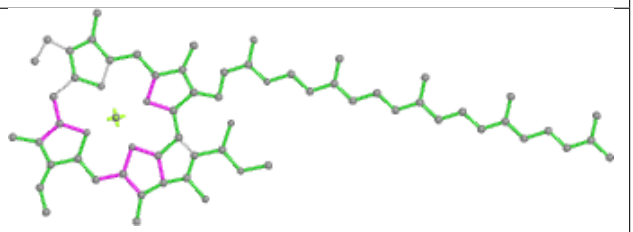


Rings

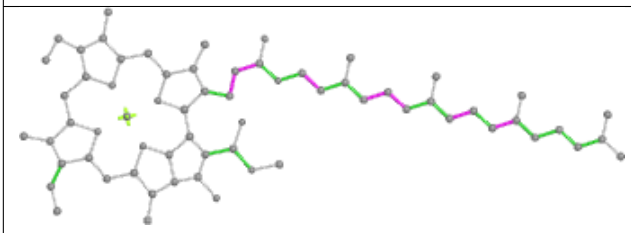
Ligand CLA b 701



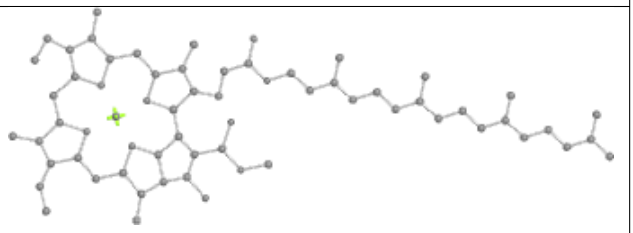
Bond lengths



Bond angles

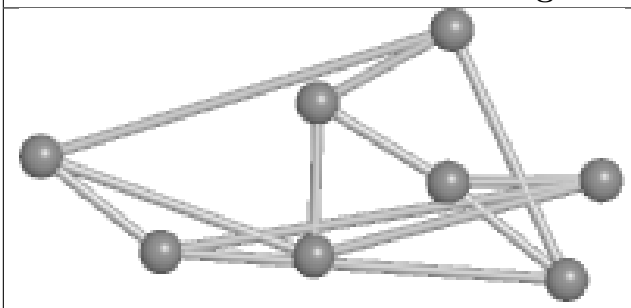


Torsions

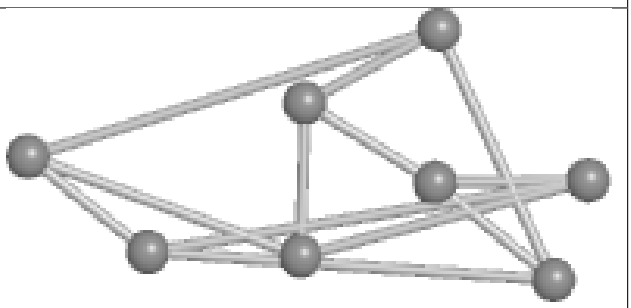


Rings

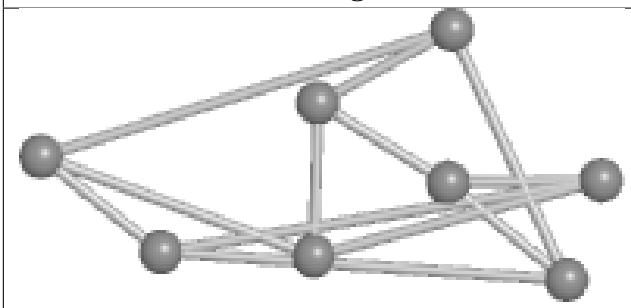
Ligand SF4 c 202



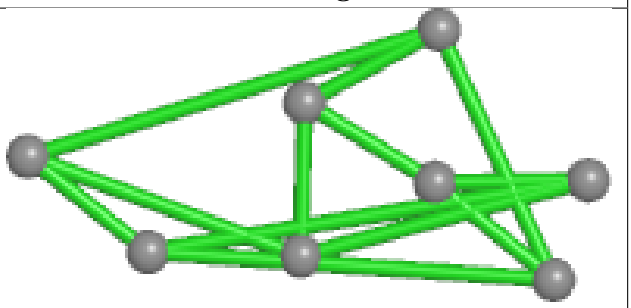
Bond lengths



Bond angles

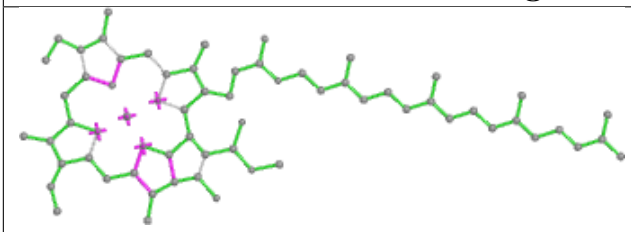


Torsions



Rings

Ligand CLA B 609



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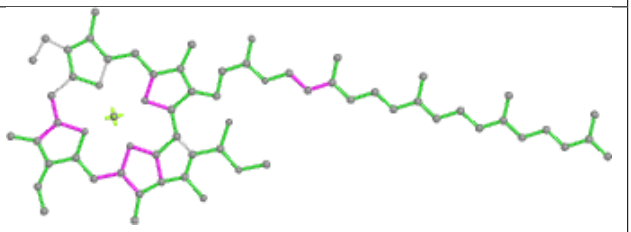

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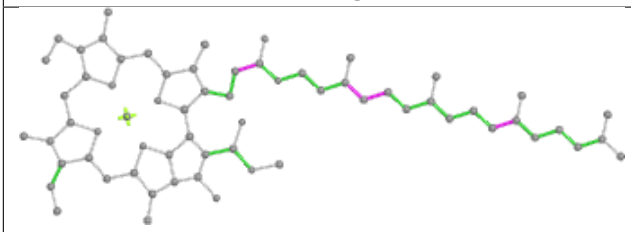

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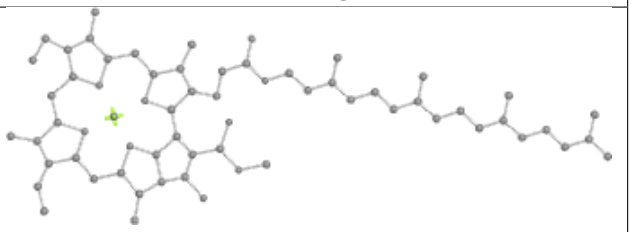
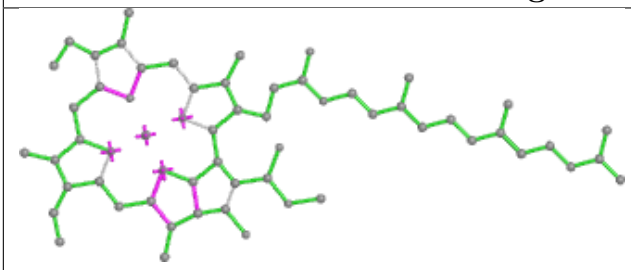


Rings

Ligand CLA J 603



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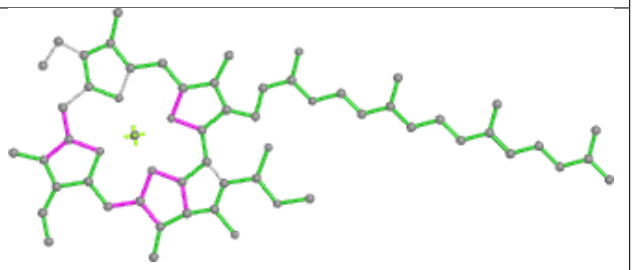
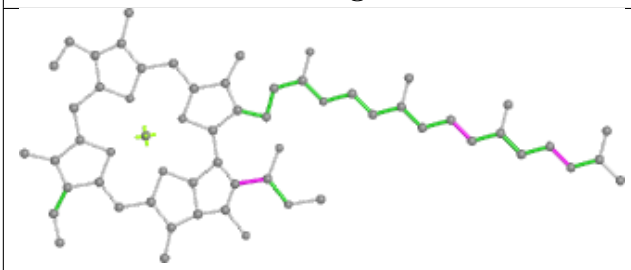


Bond angles



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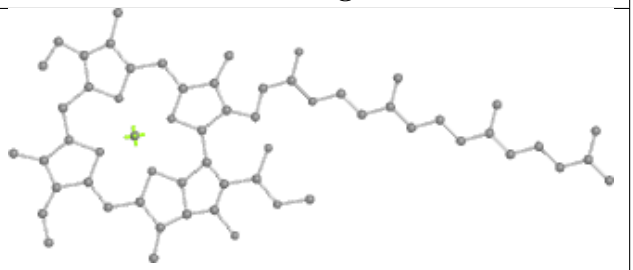
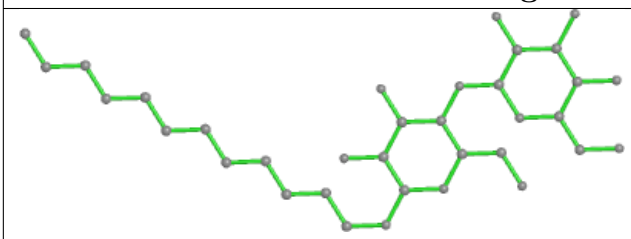


Rings

Ligand LMU T 613



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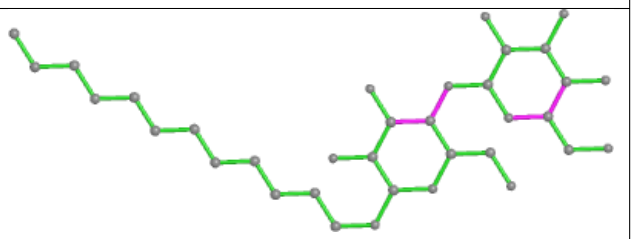

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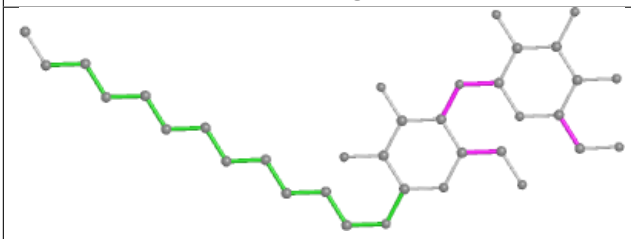

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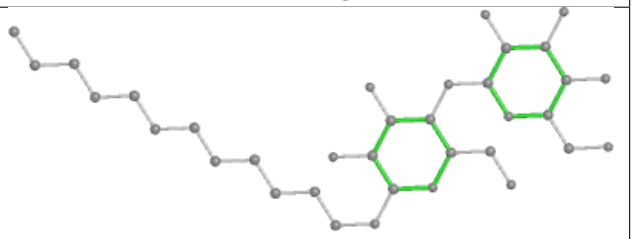
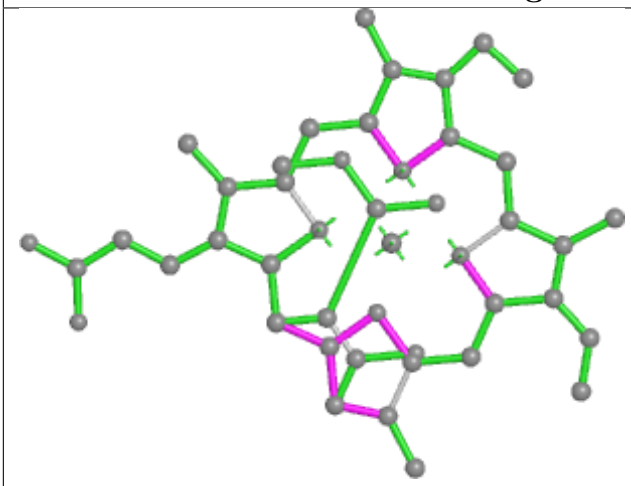


Rings

Ligand KC2 U 604



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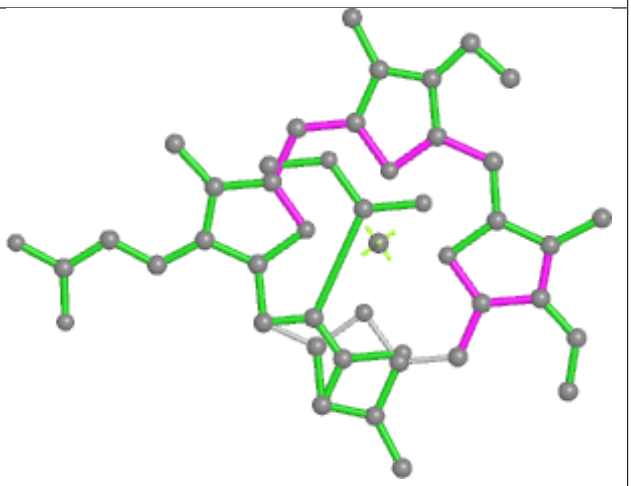

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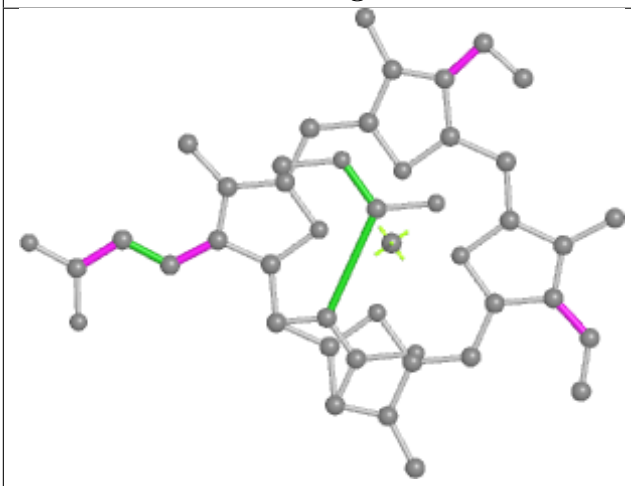

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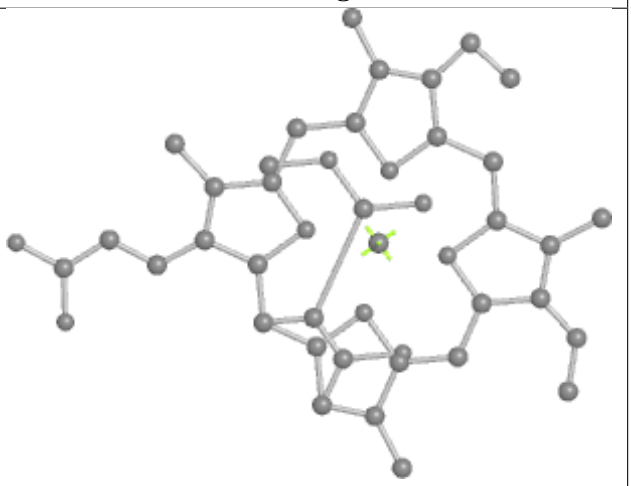
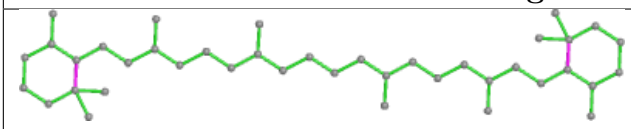


Rings

Ligand BCR a 836



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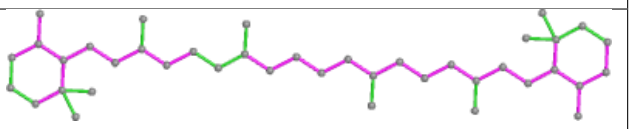

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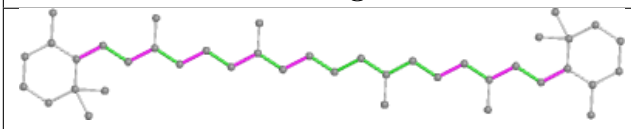
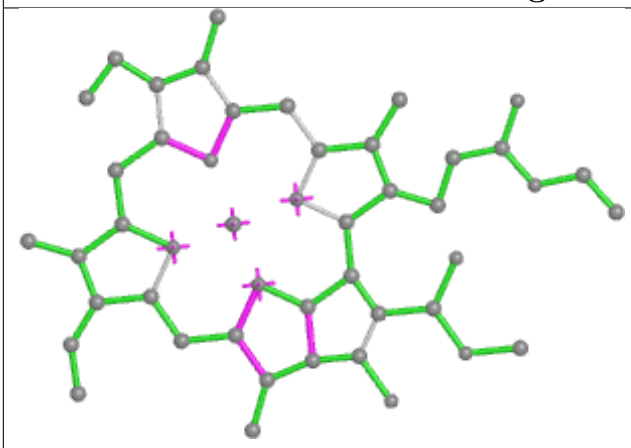


Torsions

Rings

Ligand CLA a 809



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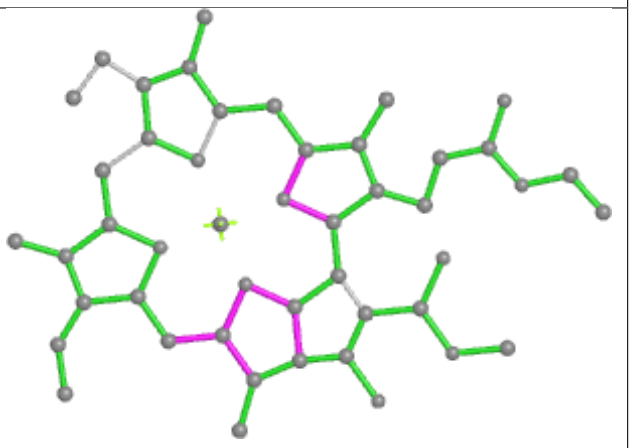
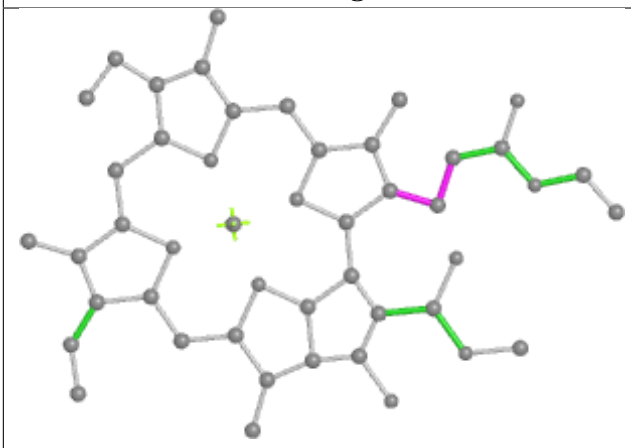


Bond angles



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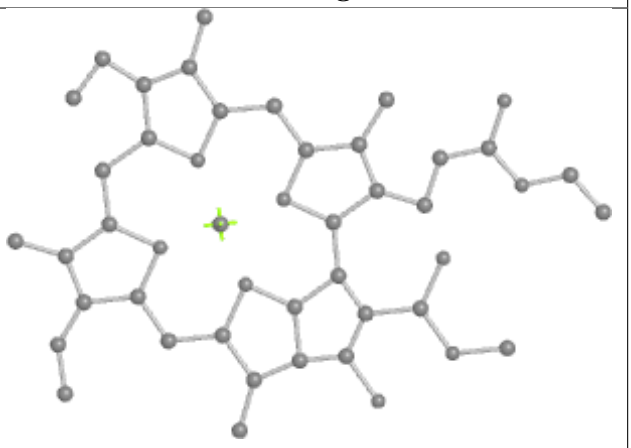
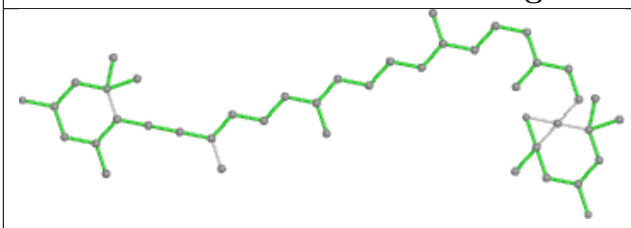


Rings

Ligand DD6 C 214



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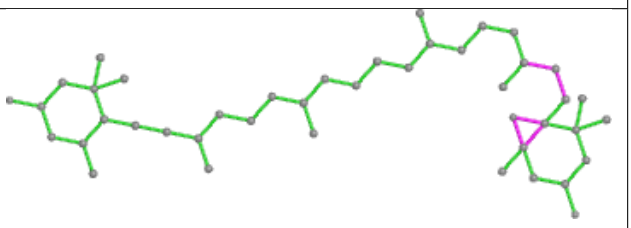

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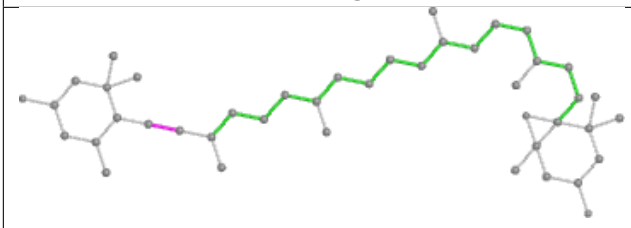
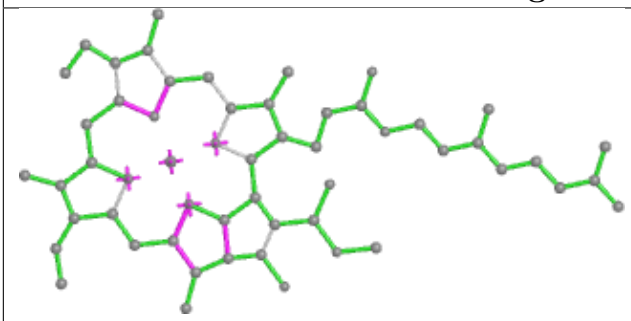


Torsions

Rings

Ligand CLA a 826



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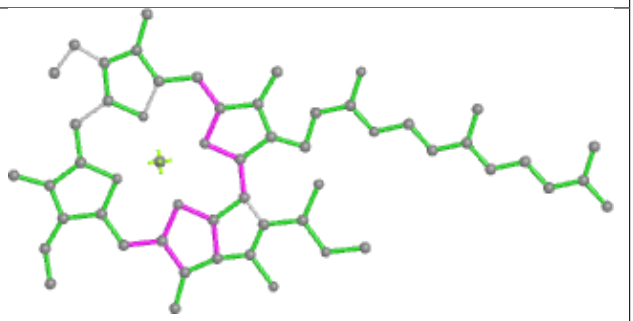
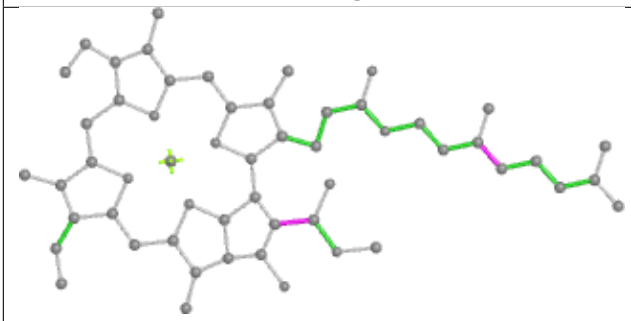


Bond angles



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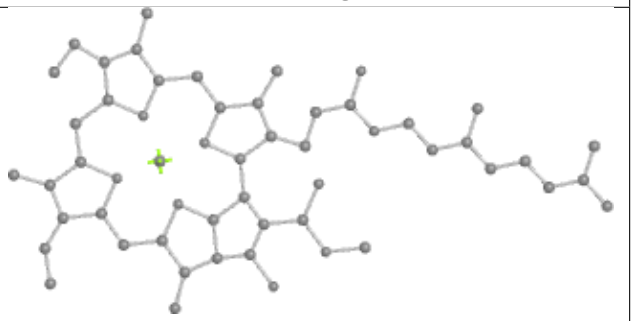
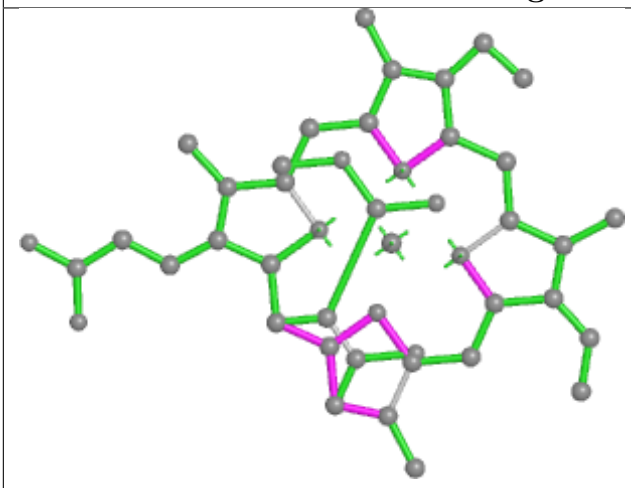


Rings

Ligand KC2 E 601



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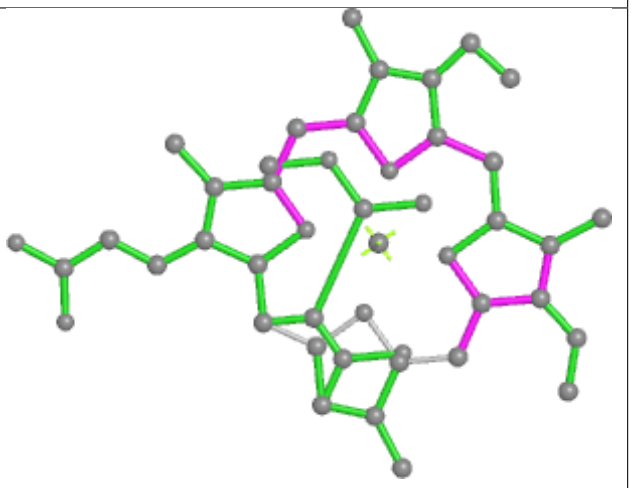

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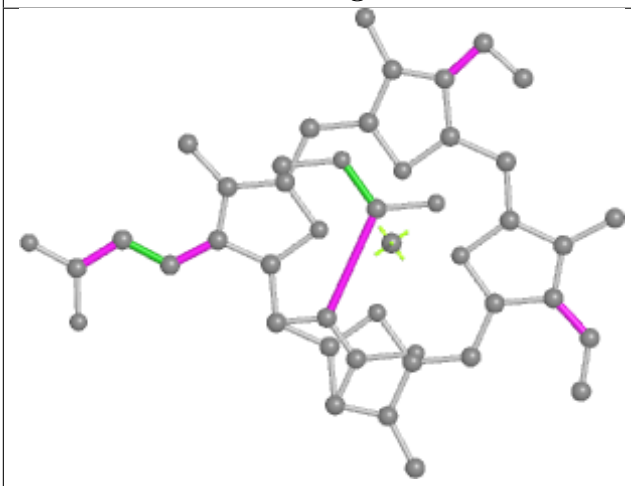

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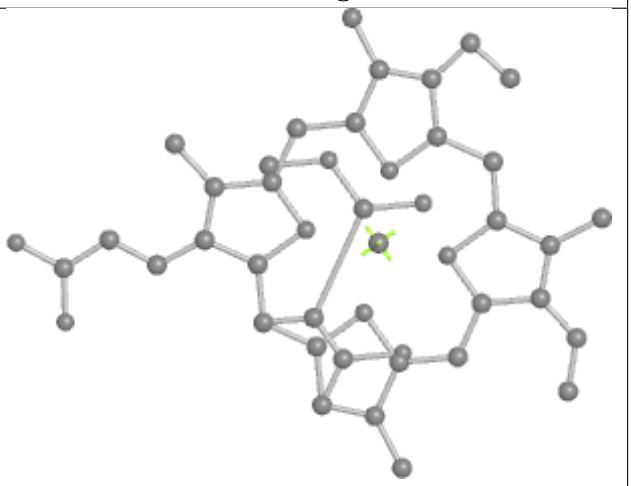
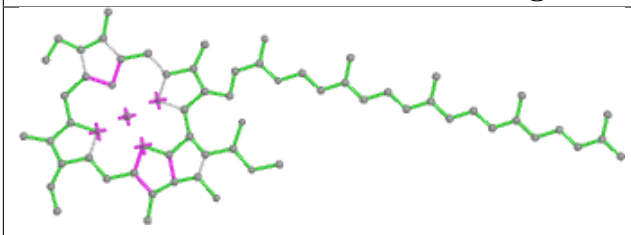


Rings

Ligand CLA a 820



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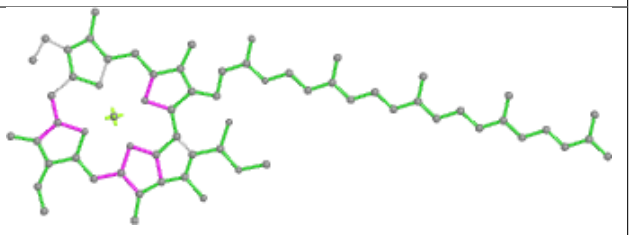

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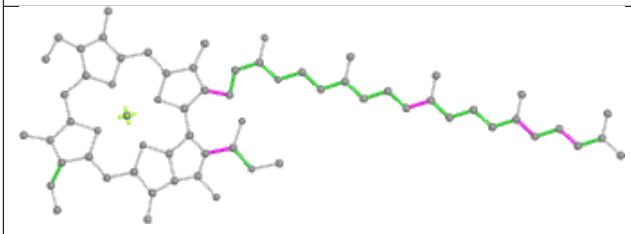

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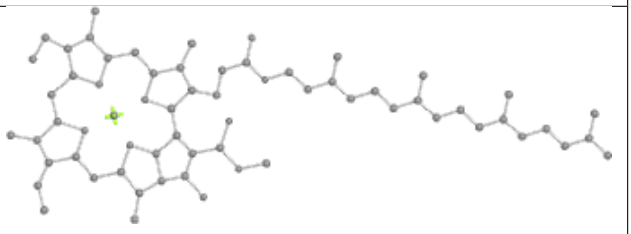
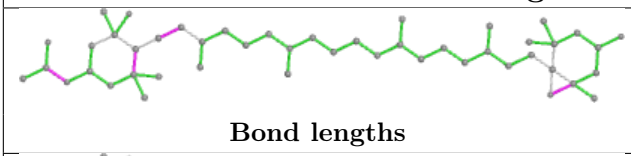


Rings

Ligand UIX A 616



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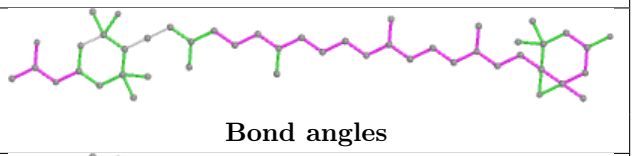

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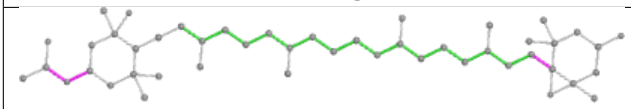
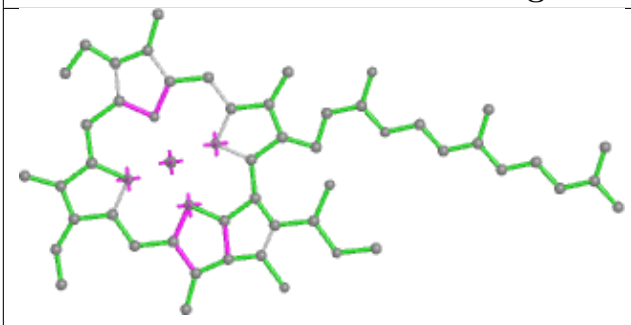


Torsions

Rings

Ligand CLA b 710



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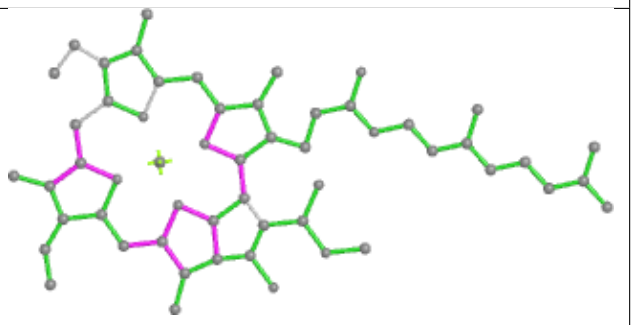
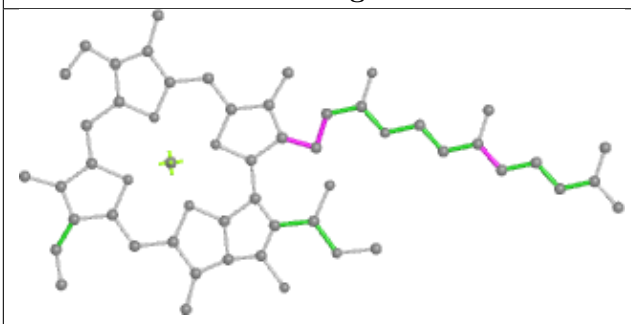
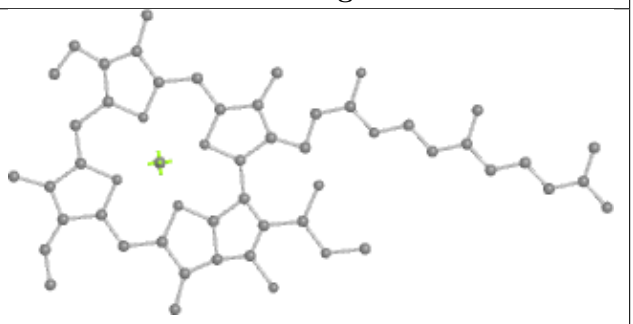


Bond angles

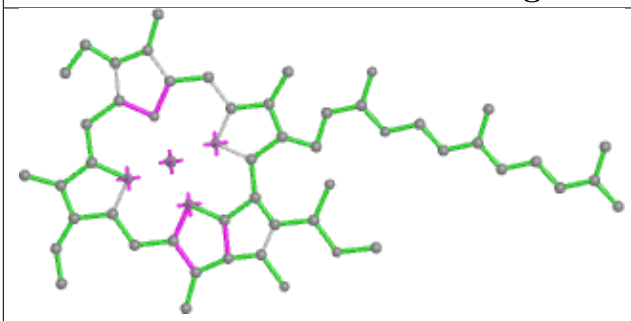


Torsions



Rings

Ligand CLA D 612



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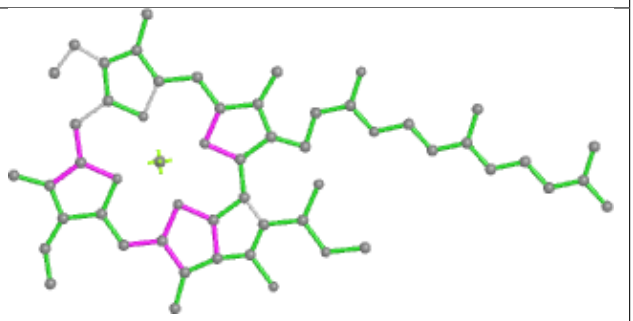
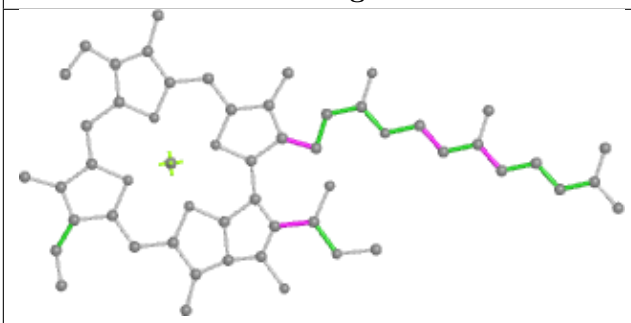


Bond angles



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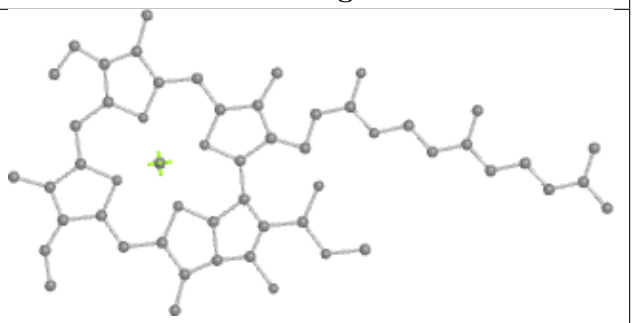
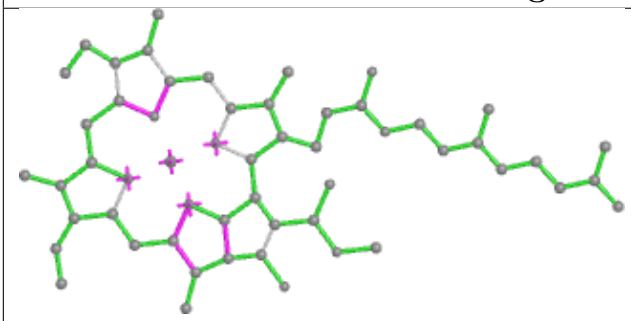


Rings

Ligand CLA a 808



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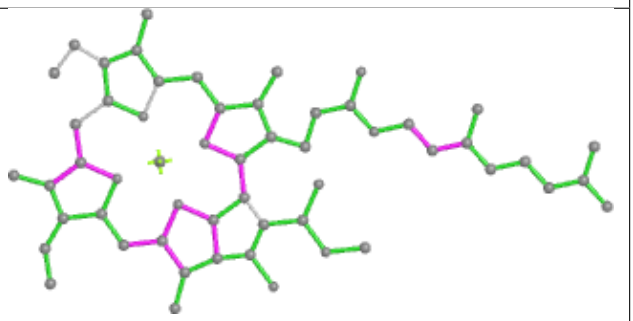
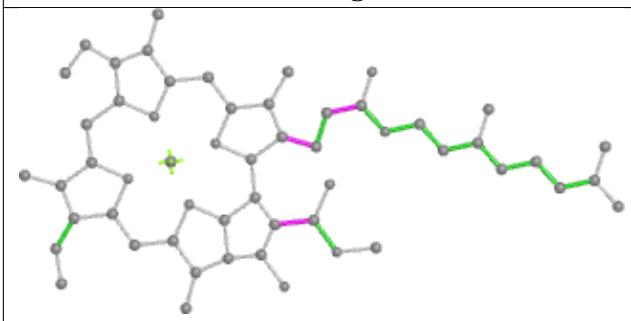


Bond angles



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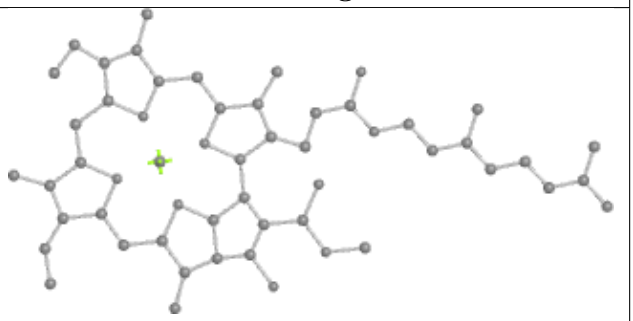
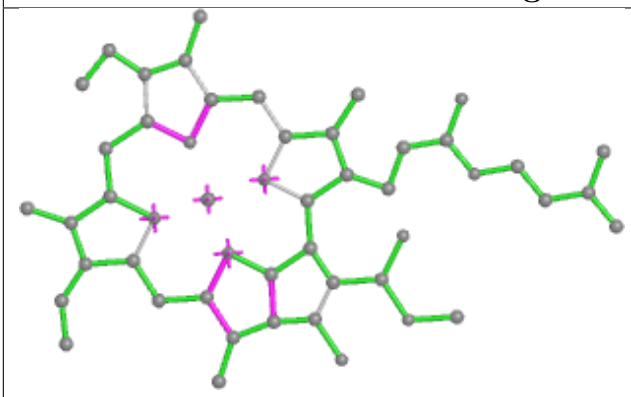


Rings

Ligand CLA U 603



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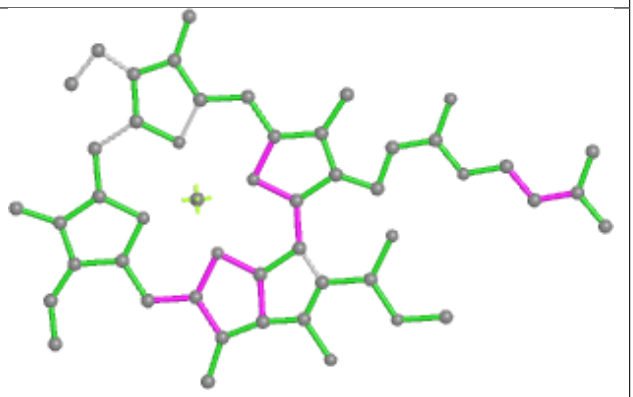
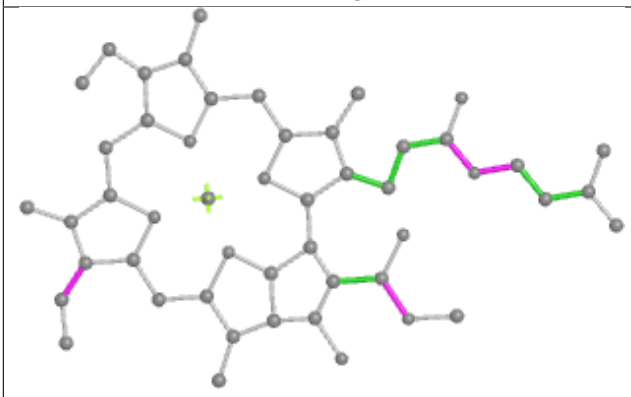
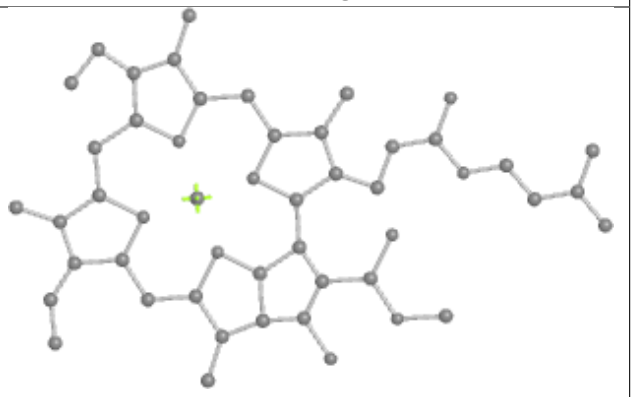


Bond angles

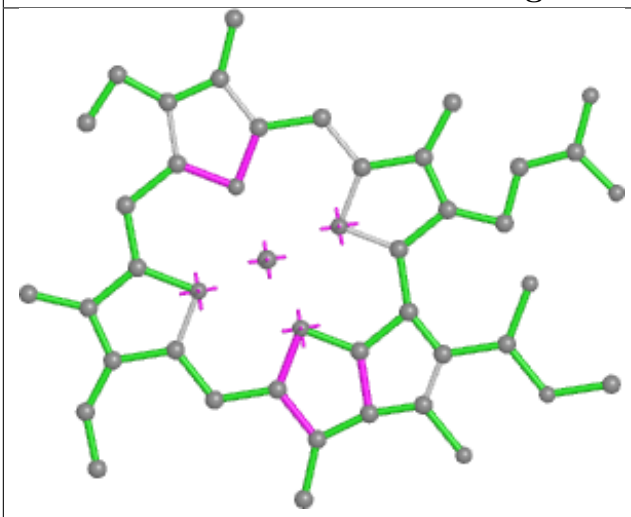


Torsions

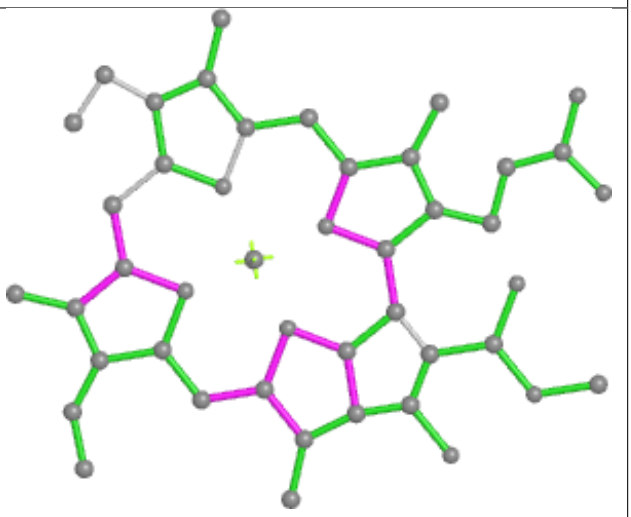


Rings

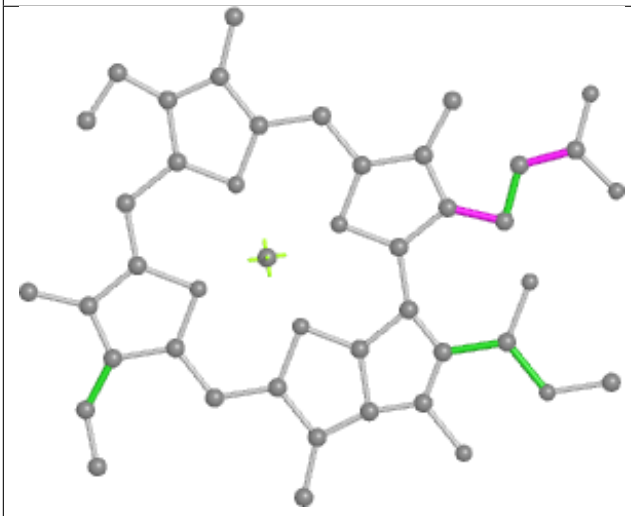
Ligand CLA E 605



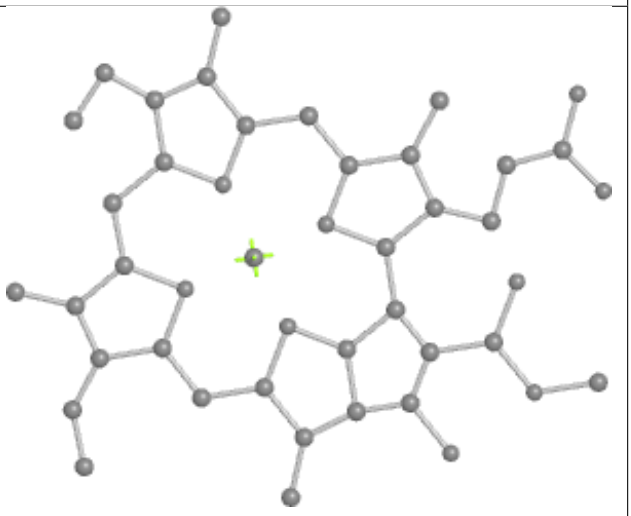
Bond lengths



Bond angles

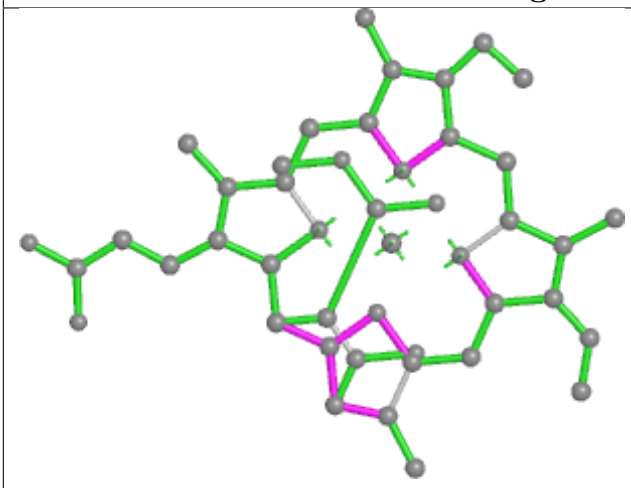


Torsions

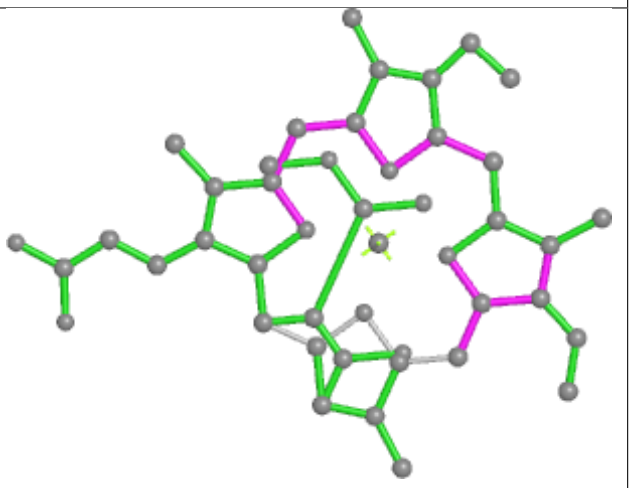


Rings

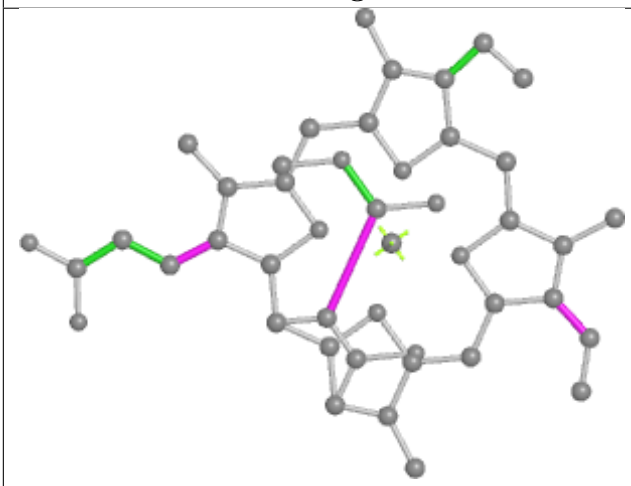
Ligand KC2 J 604



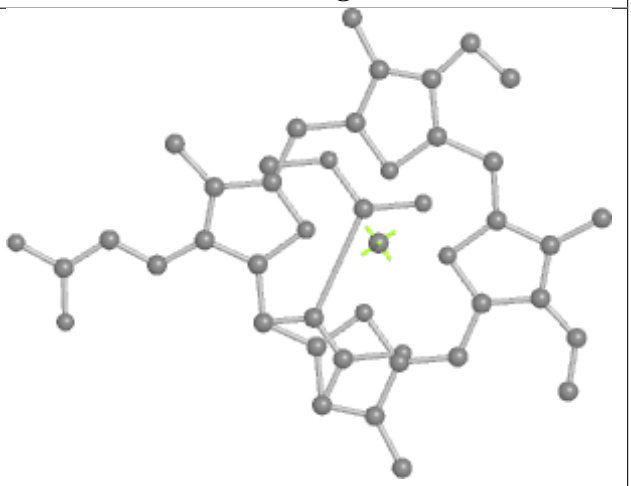
Bond lengths



Bond angles

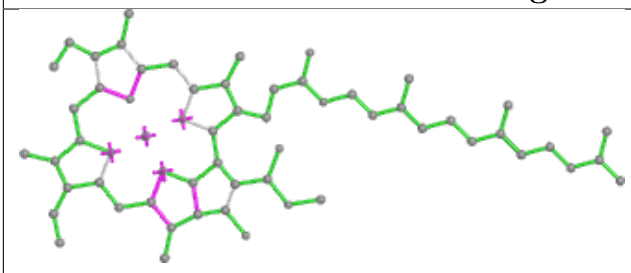


Torsions



Rings

Ligand CLA r 204



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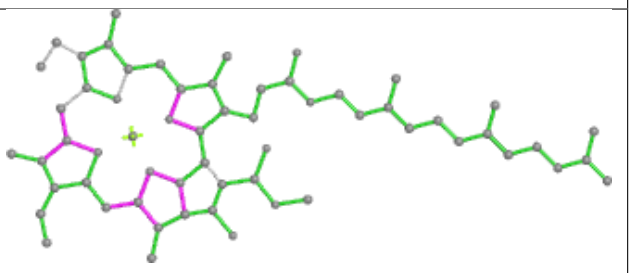
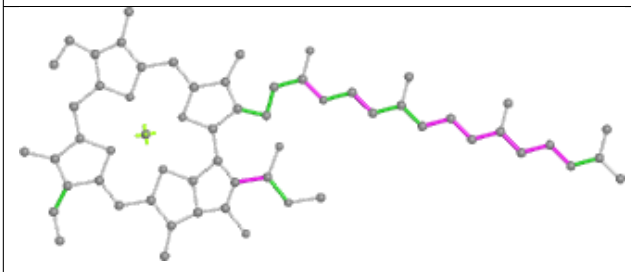
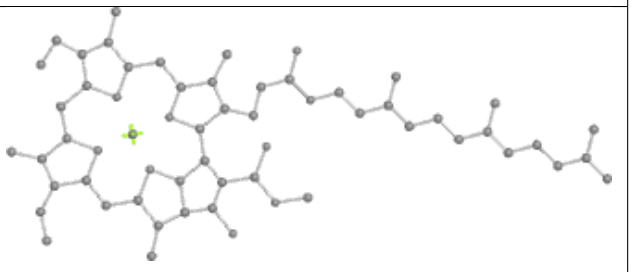


Bond angles

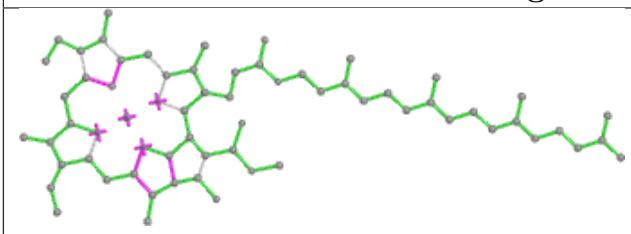


Torsions

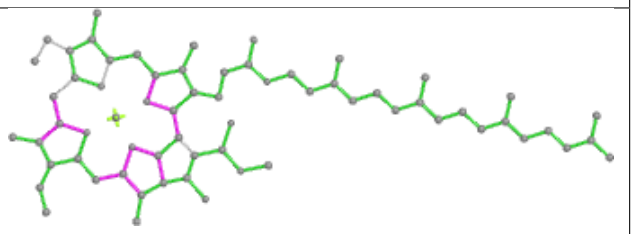


Rings

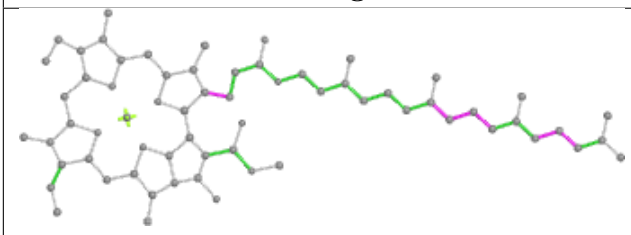
Ligand CLA b 718



Bond lengths



Bond angles



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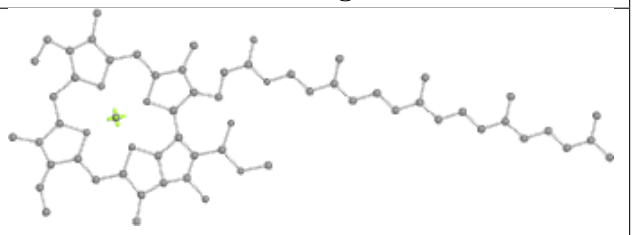
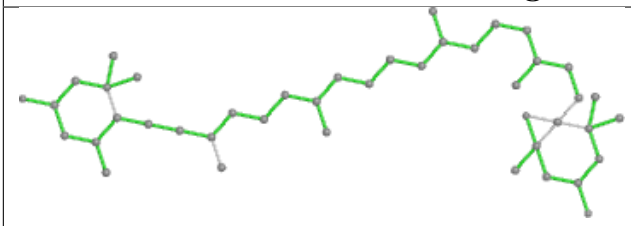


Rings

Ligand DD6 G 613



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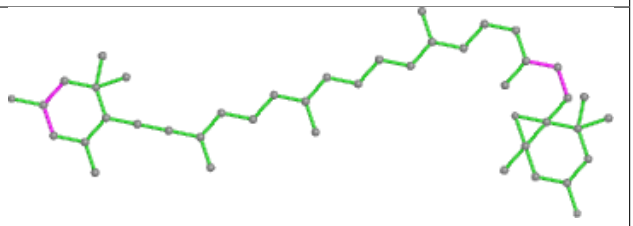

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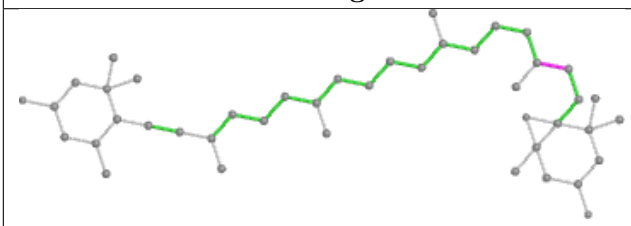
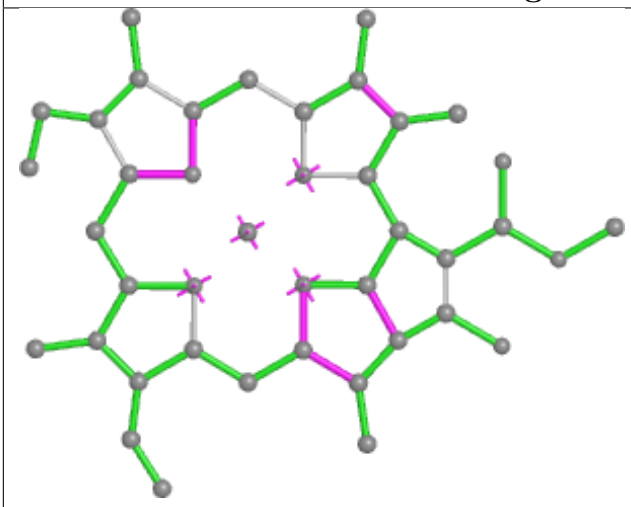


Torsions

Rings

Ligand CLA T 604



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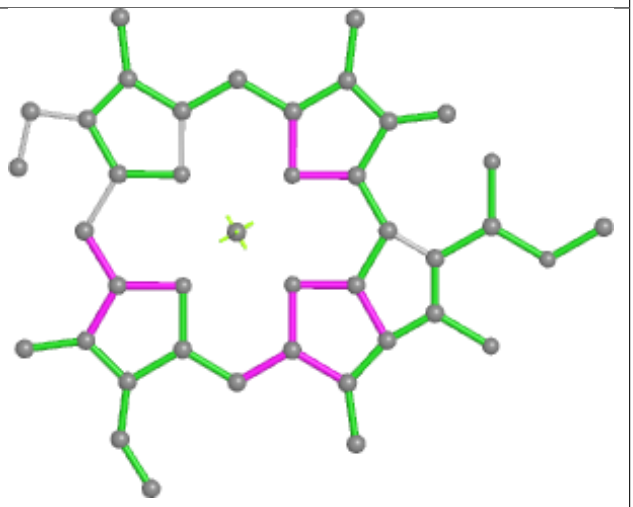
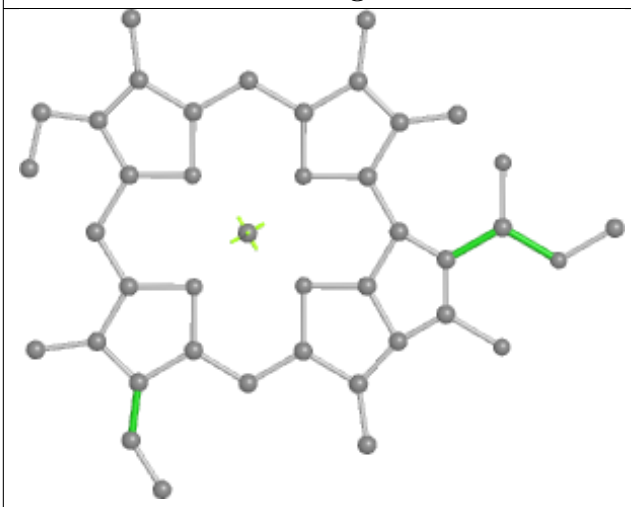
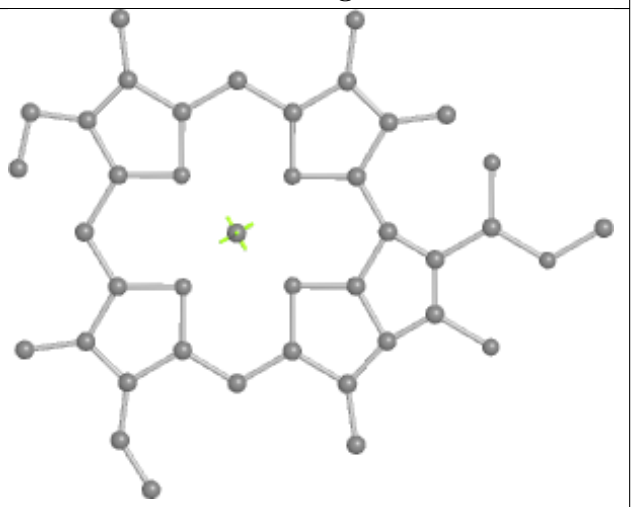


Bond angles

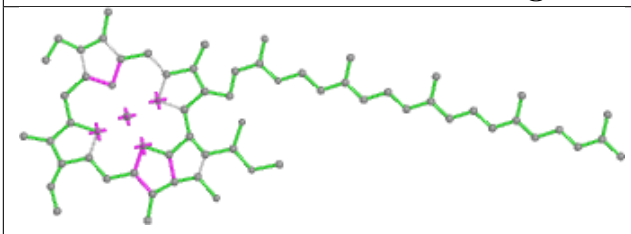


Torsions



Rings

Ligand CLA b 703



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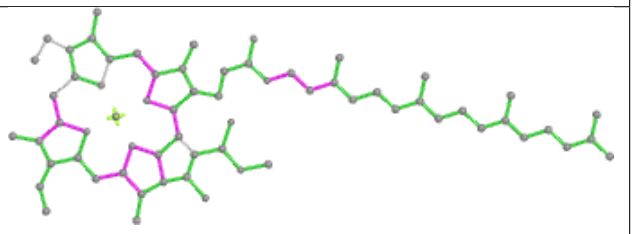
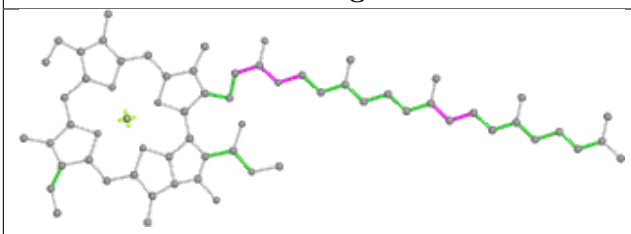


Bond angles



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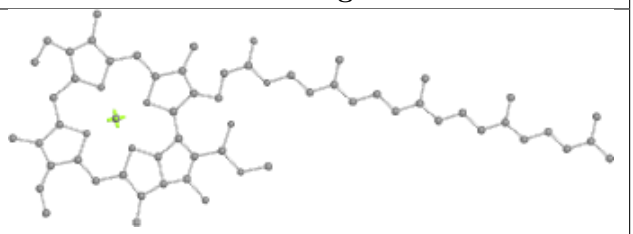
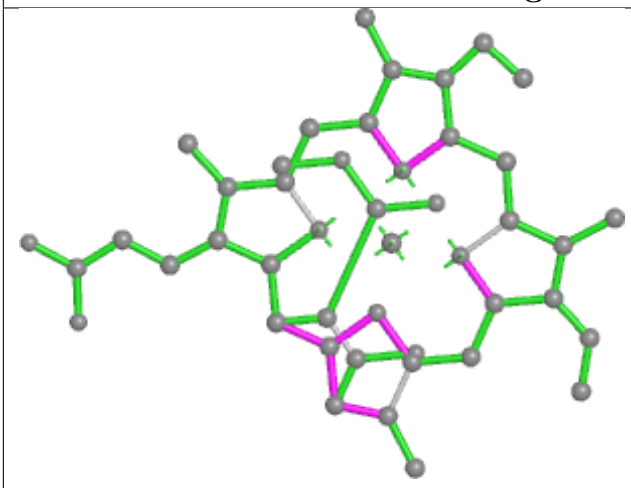


Rings

Ligand KC2 H 311



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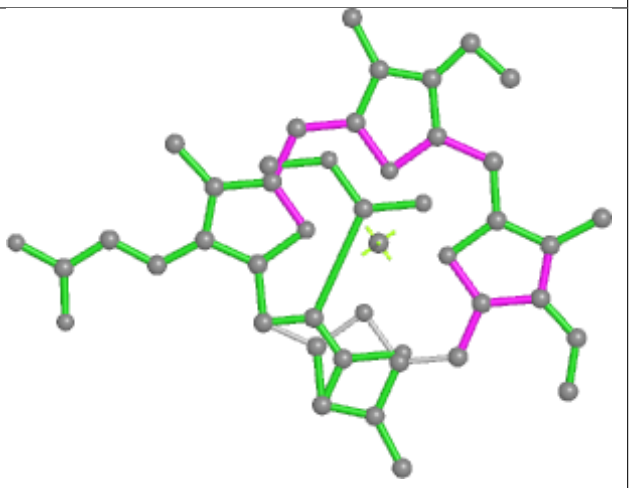
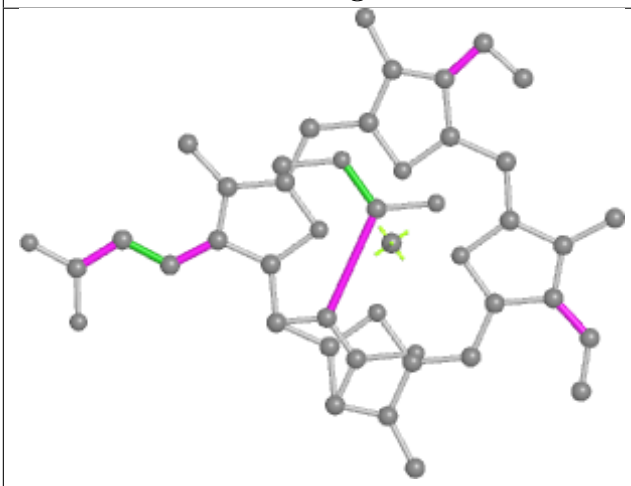
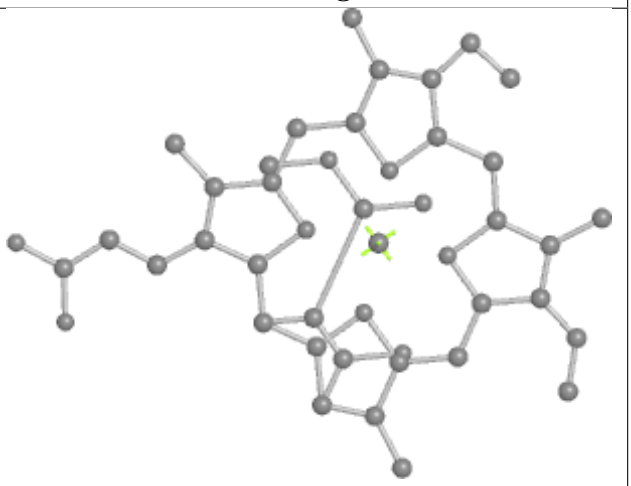


Bond angles

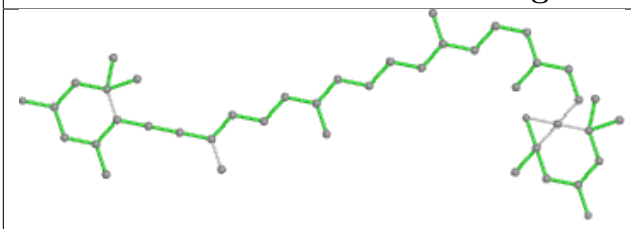


Torsions

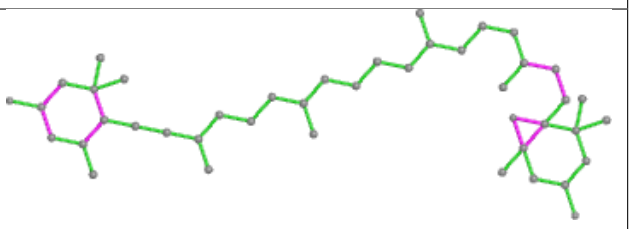


Rings

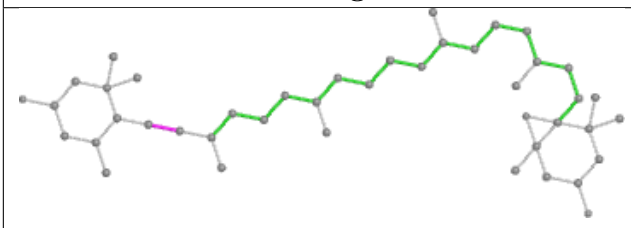
Ligand DD6 I 613



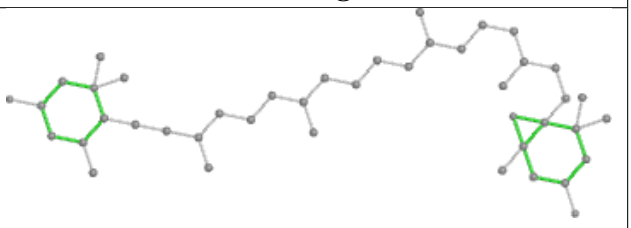
Bond lengths



Bond angles

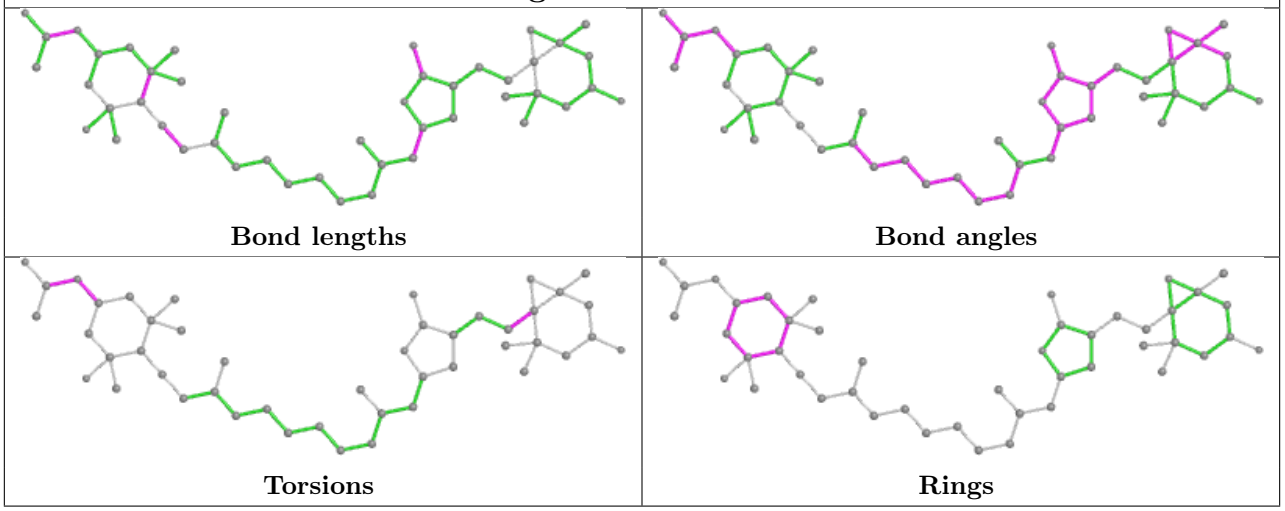


Torsions

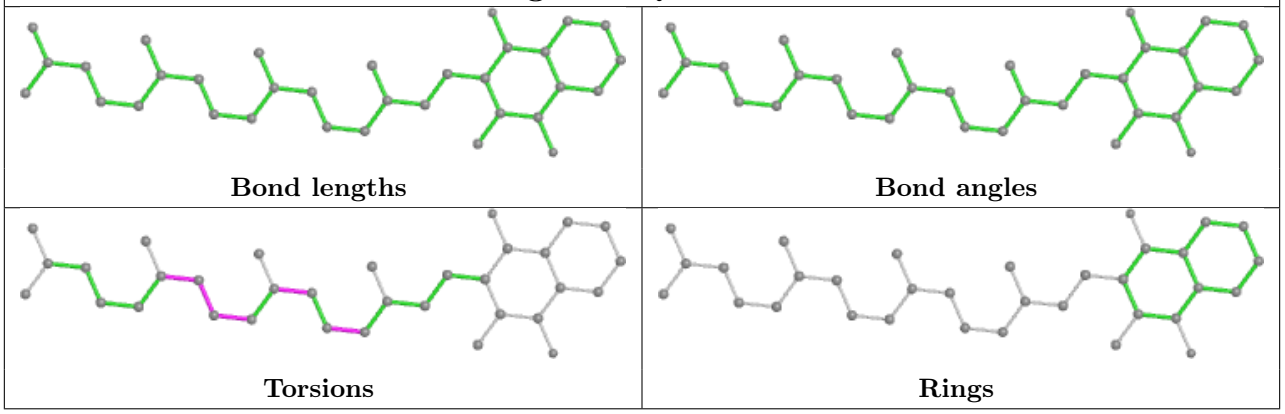


Rings

Ligand PID K 611



Ligand PQN a 832



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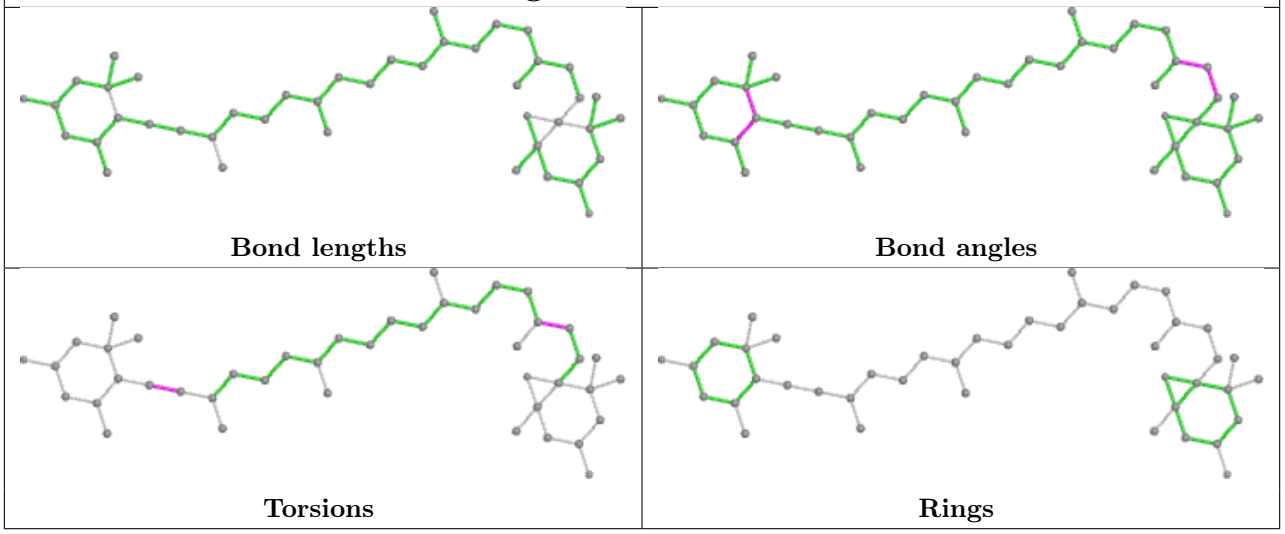
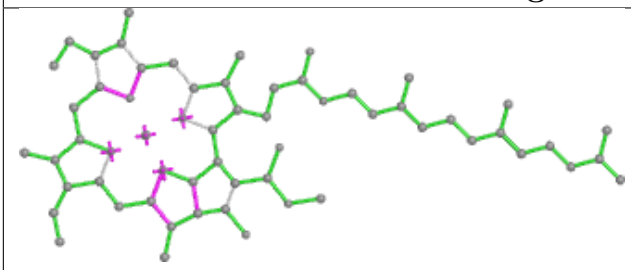
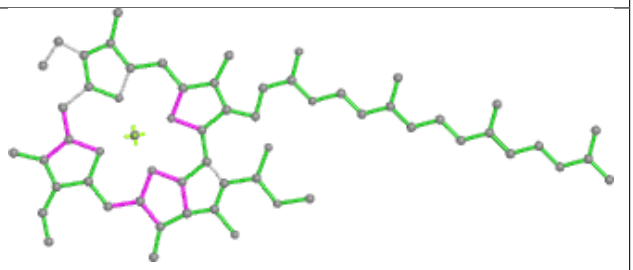


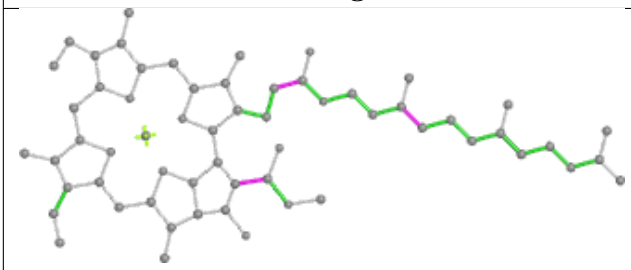
Ligand CLA b 711



Bond lengths



Bond angles



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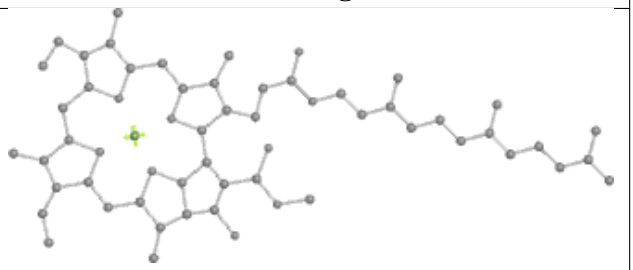
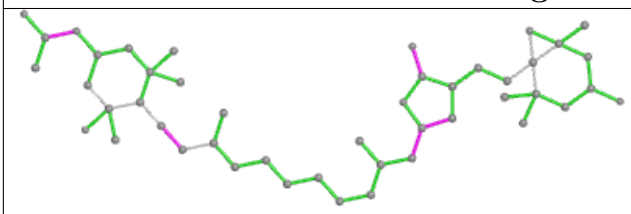


Rings

Ligand PID F 614



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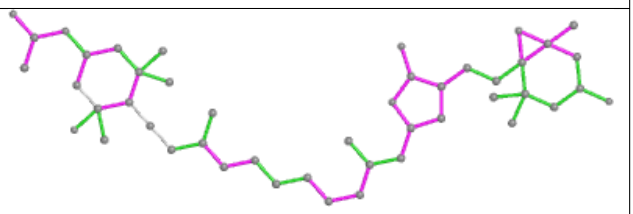
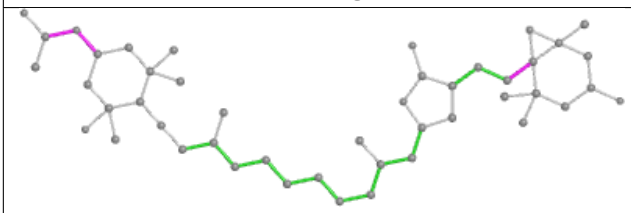


Bond angles



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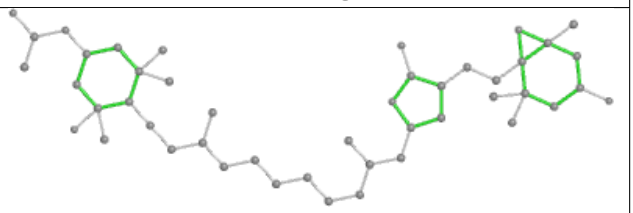
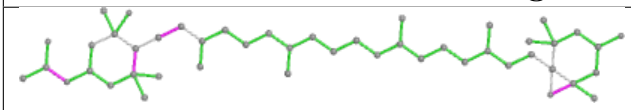
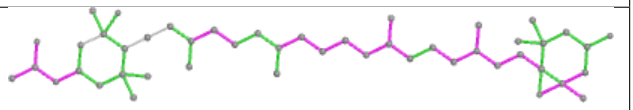


Rings

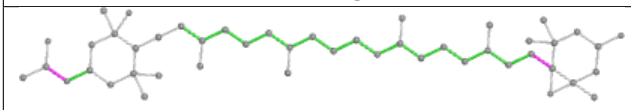
Ligand UIX B 615



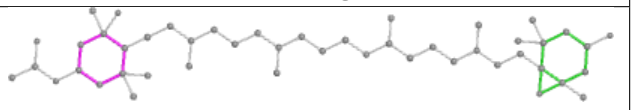
Bond lengths



Bond angles

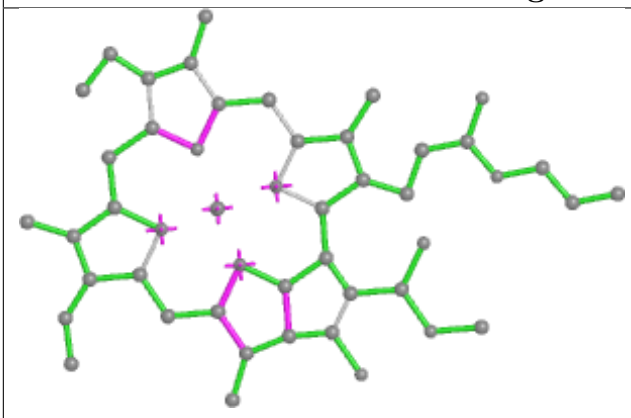


Torsions

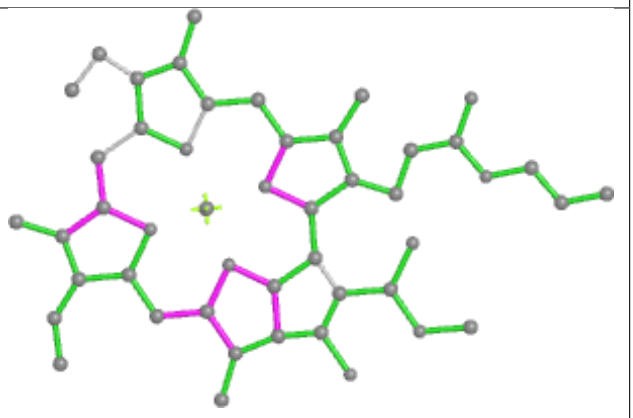


Rings

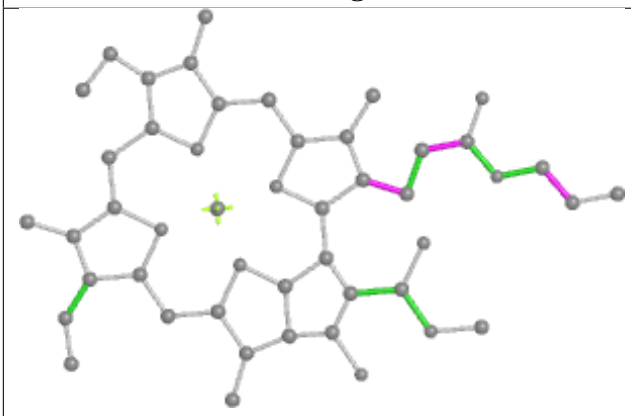
Ligand CLA b 714



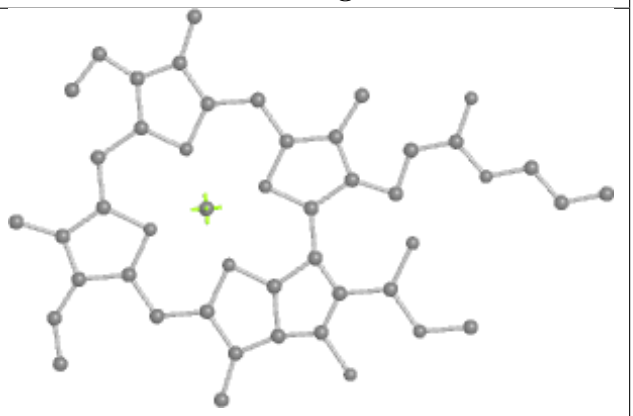
Bond lengths



Bond angles

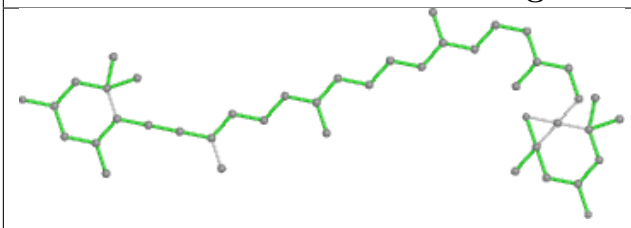


Torsions

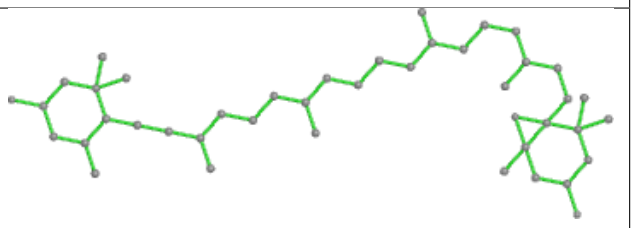


Rings

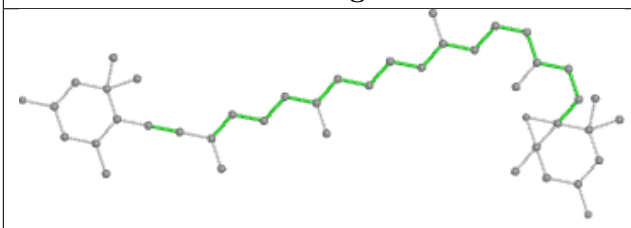
Ligand DD6 F 612



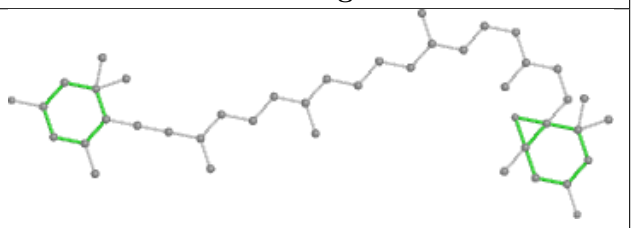
Bond lengths



Bond angles

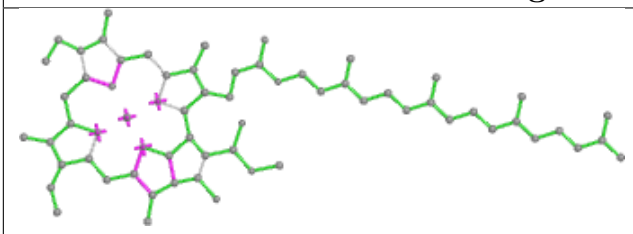


Torsions

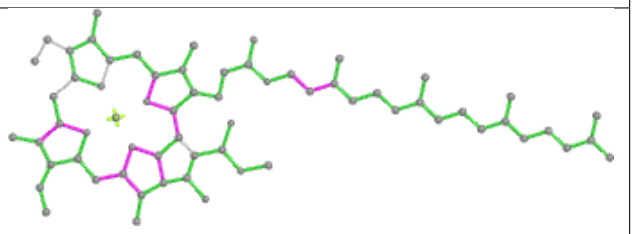


Rings

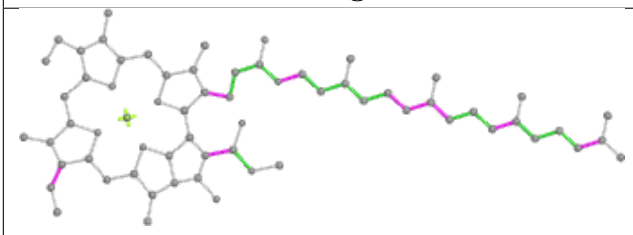
Ligand CLA a 827



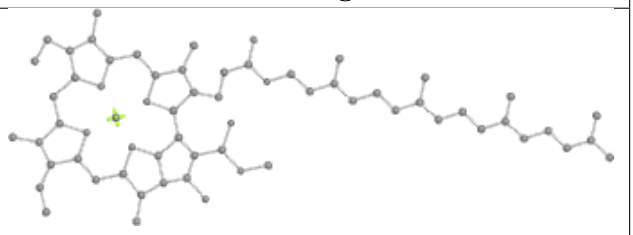
Bond lengths



Bond angles

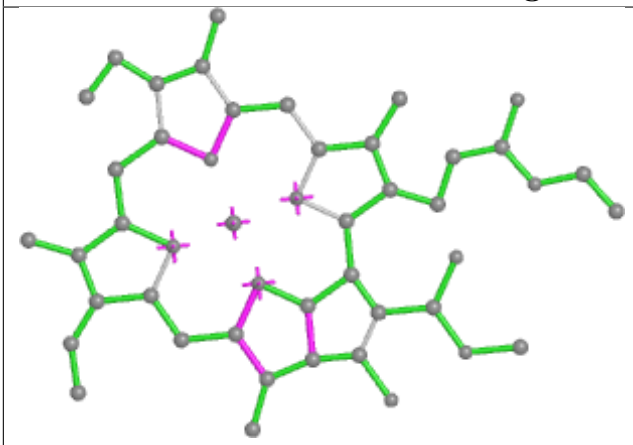


Torsions



Rings

Ligand CLA D 605



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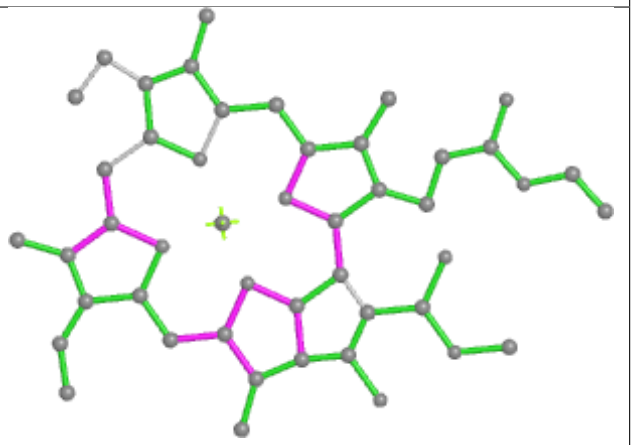

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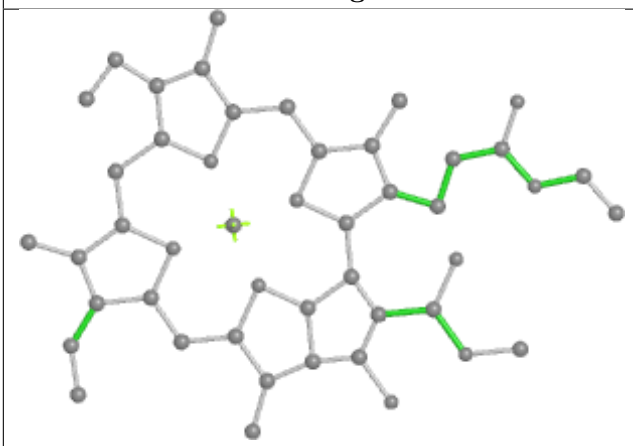

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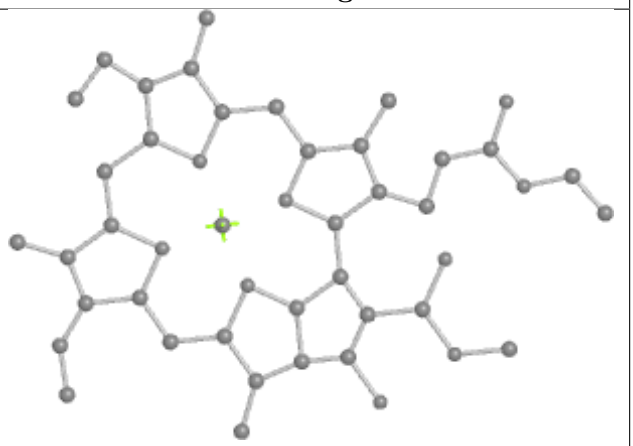
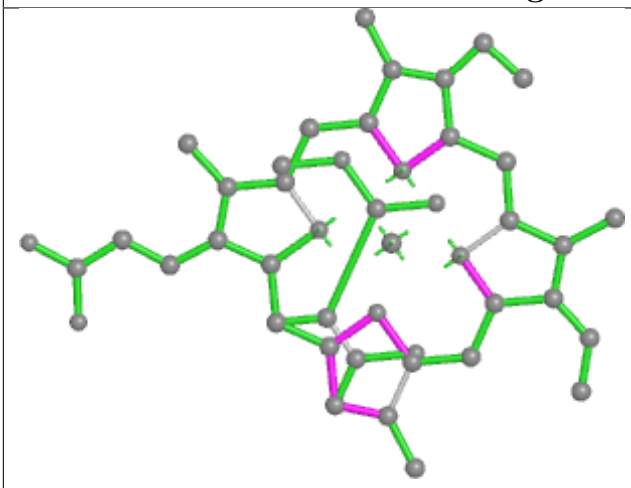


Rings

Ligand KC2 T 608



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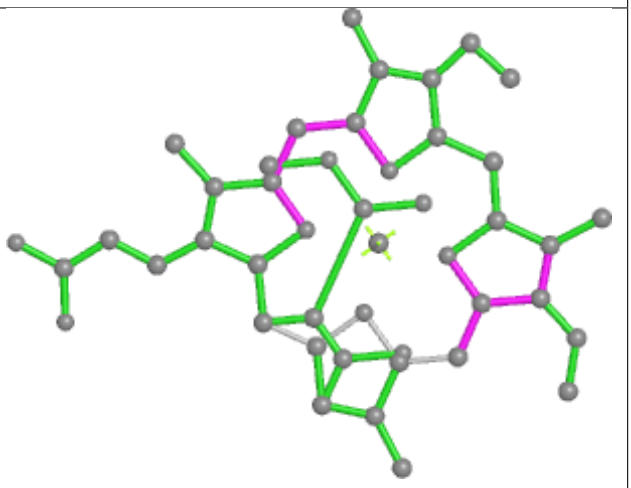
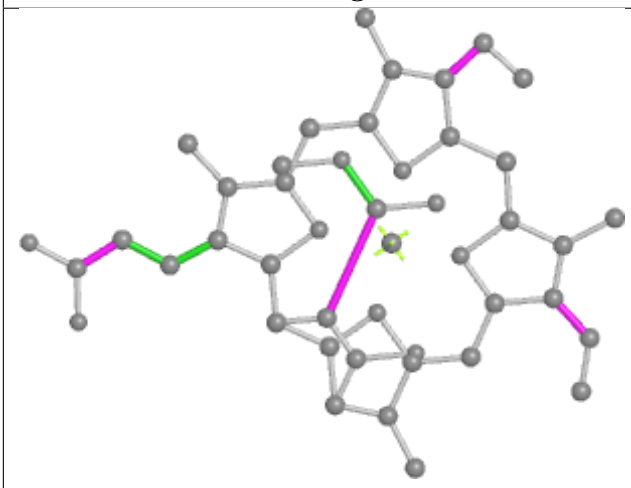


Bond angles



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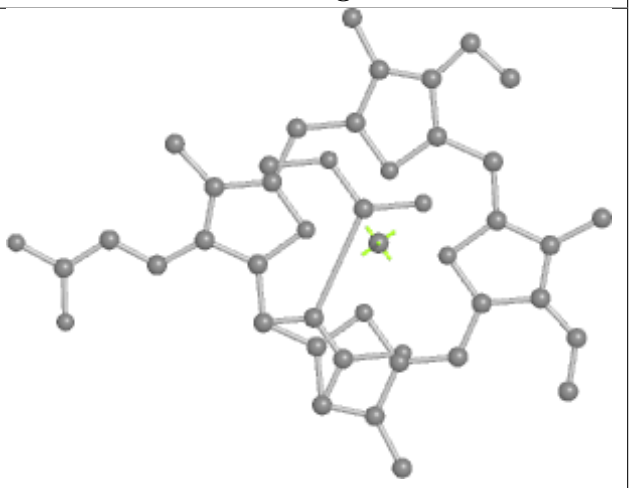
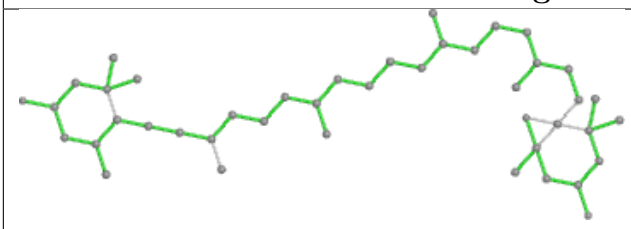


Rings

Ligand DD6 i 202



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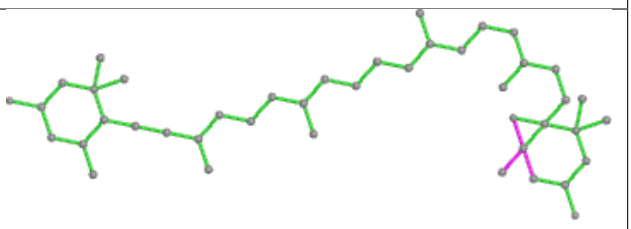

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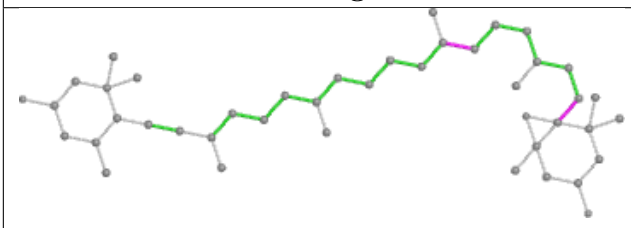

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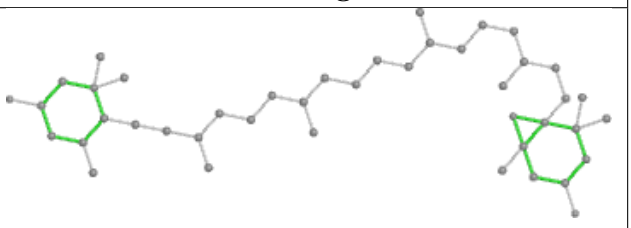
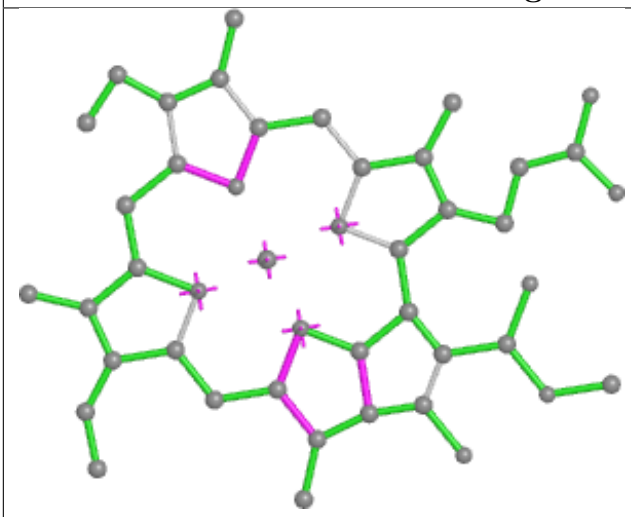


Rings

Ligand CLA T 605



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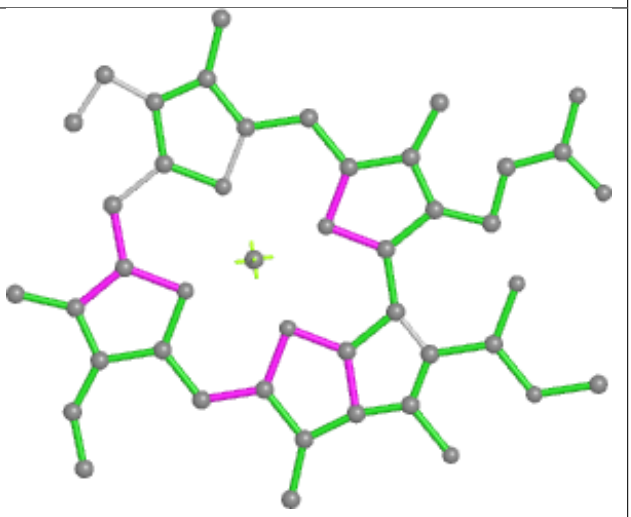

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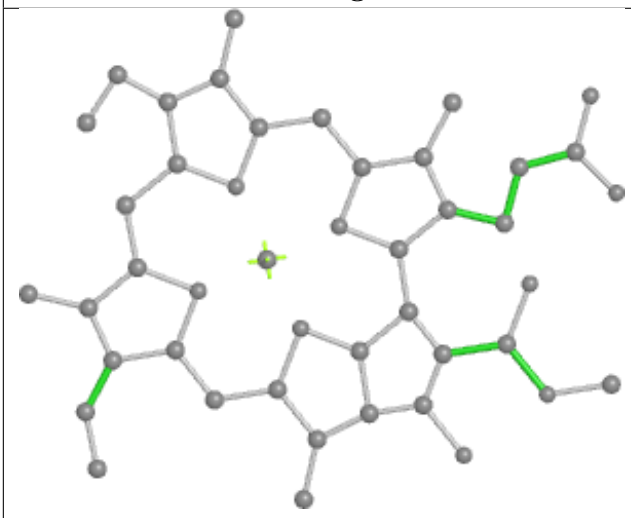

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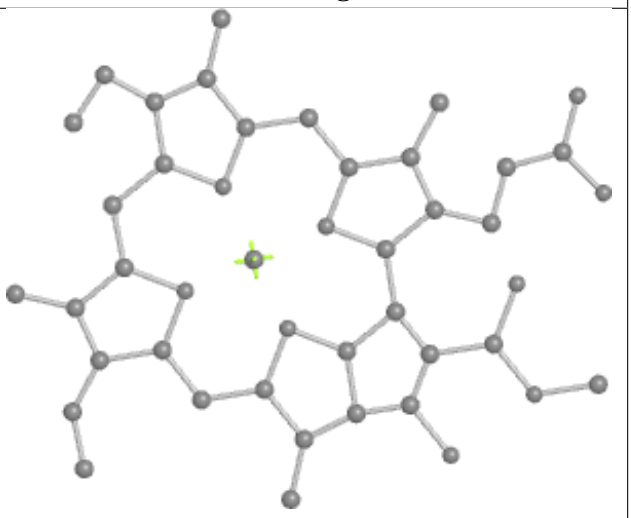
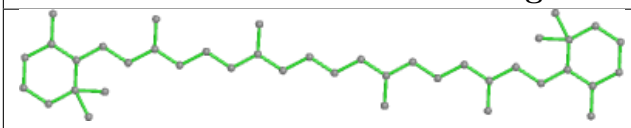


Rings

Ligand BCR b 732



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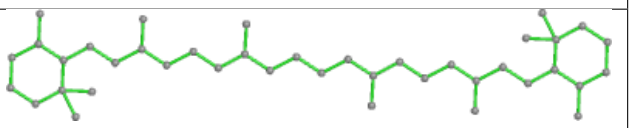
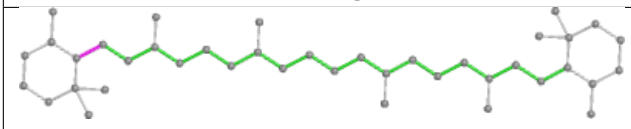


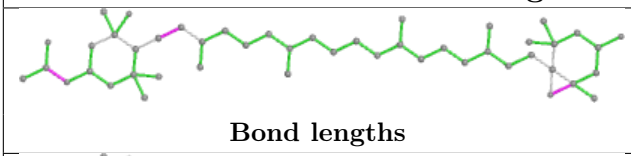
Bond angles



Torsions

Rings

Ligand UIX H 314



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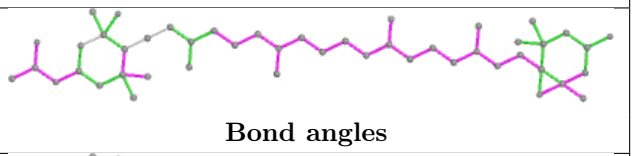
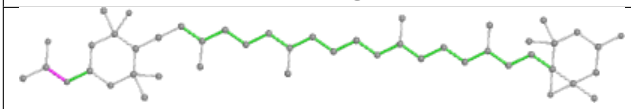


Bond angles



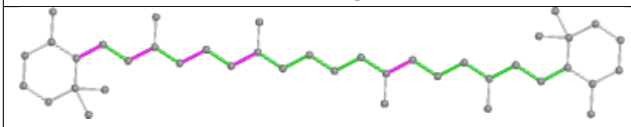
Torsions

Rings

Ligand BCR f 301

Bond lengths

Bond angles



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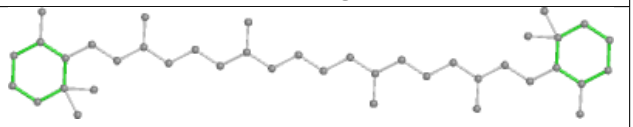
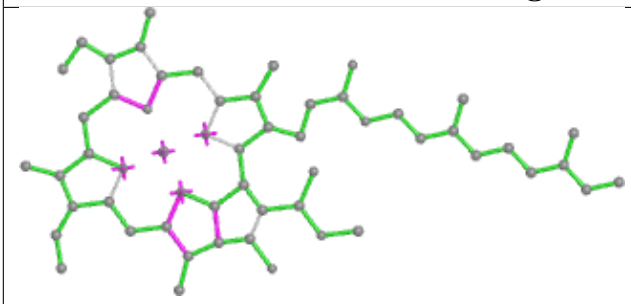


Rings

Ligand CLA F 602



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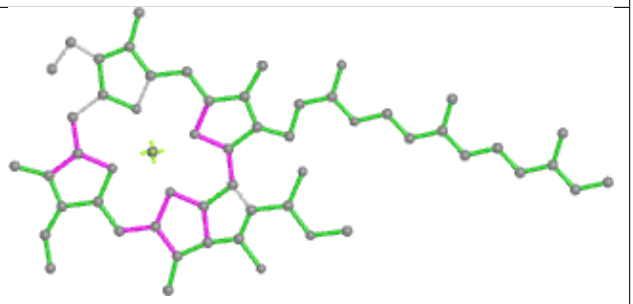
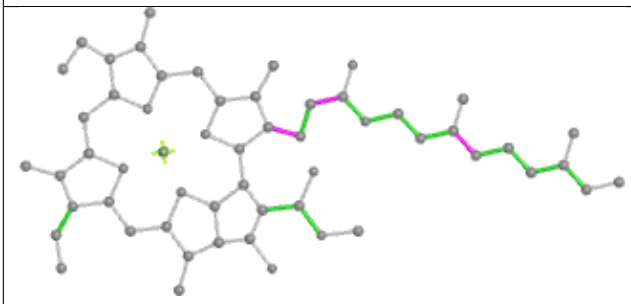


Bond angles



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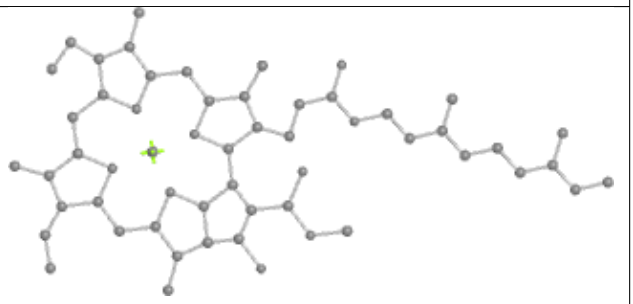
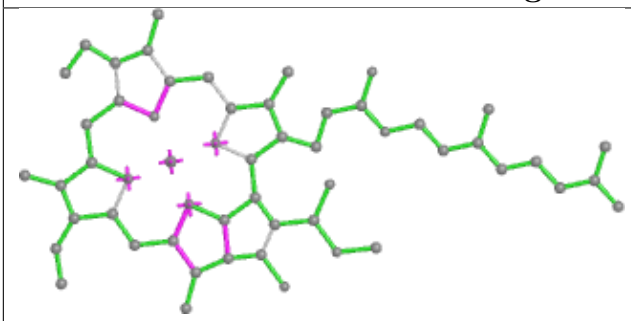


Rings

Ligand CLA C 205



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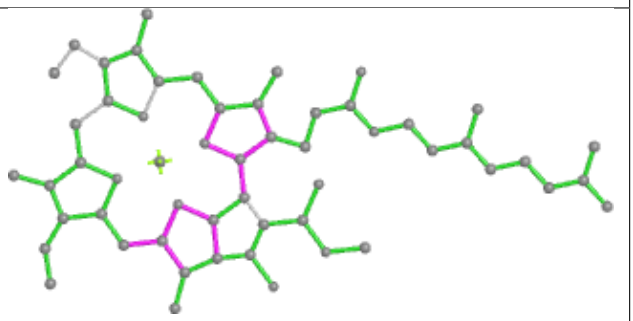
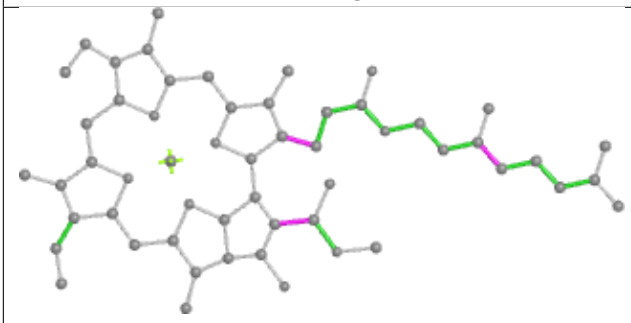
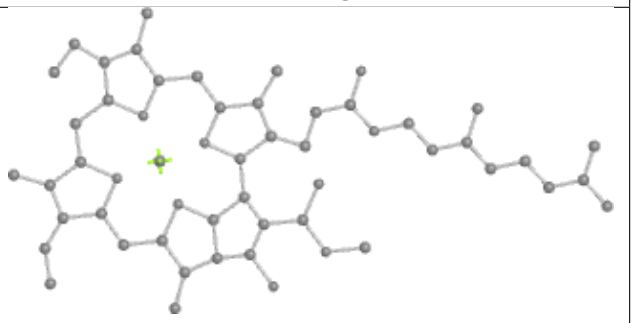


Bond angles

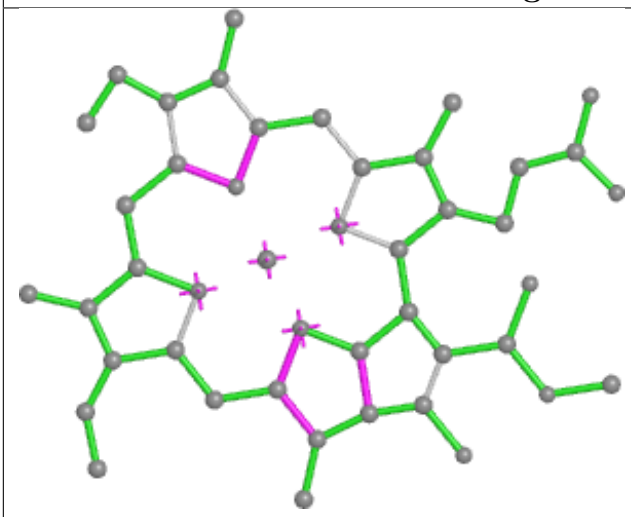


Torsions



Rings

Ligand CLA H 310



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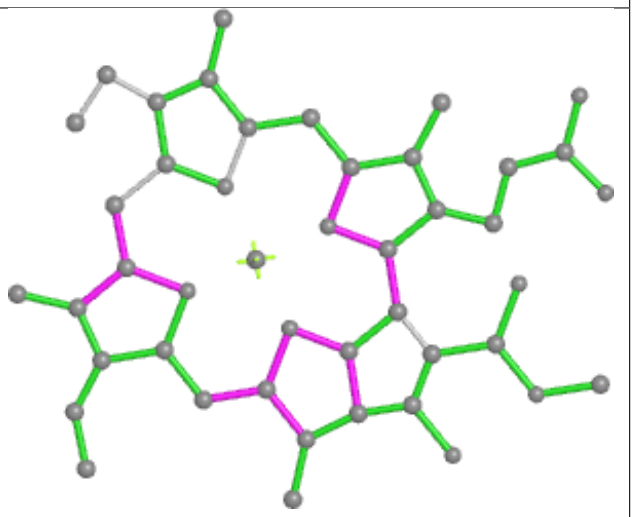
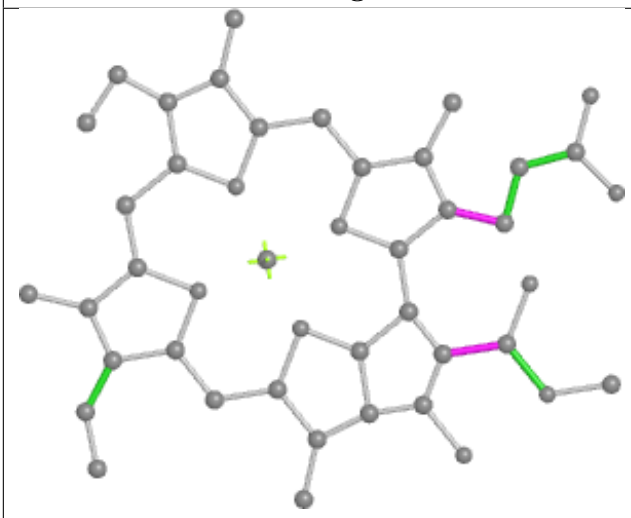


Bond angles



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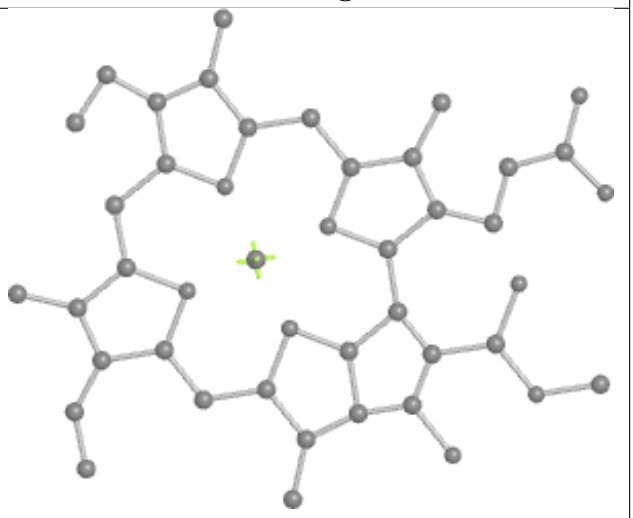
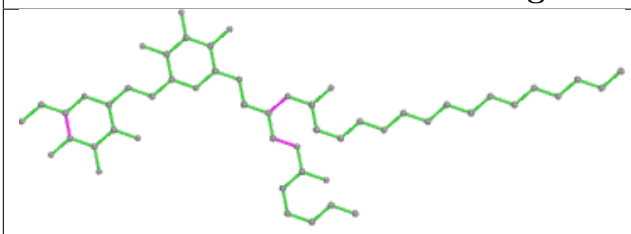


Rings

Ligand DGD f 305



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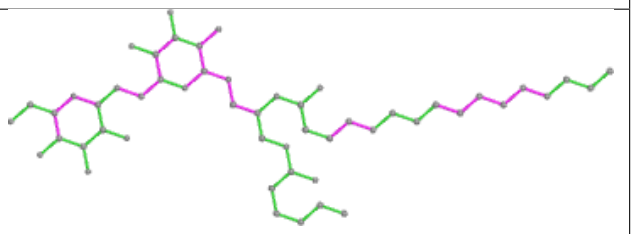
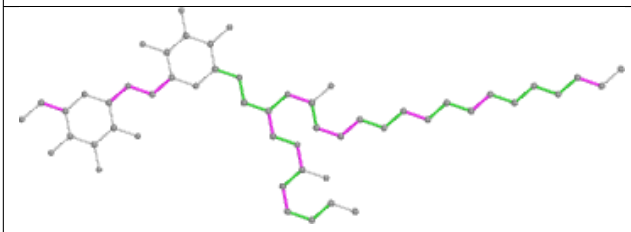


Bond angles



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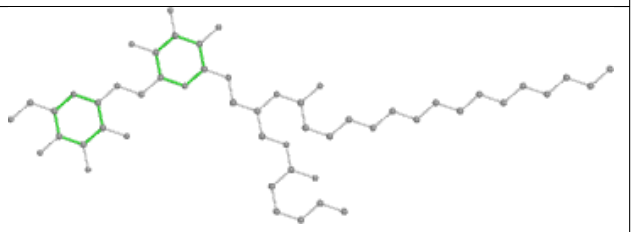
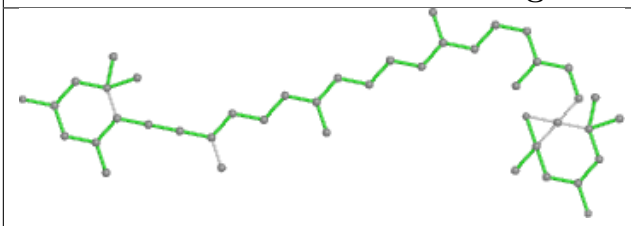


Rings

Ligand DD6 F 611



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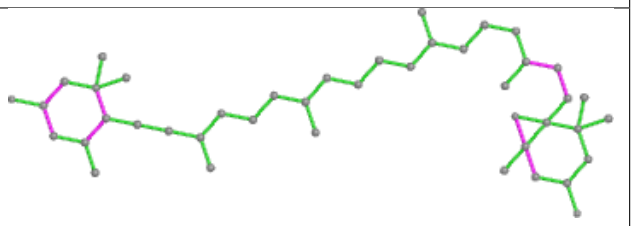
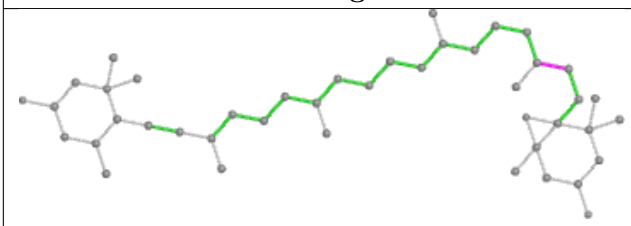


Bond angles



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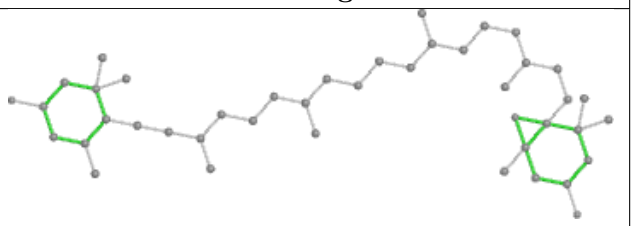
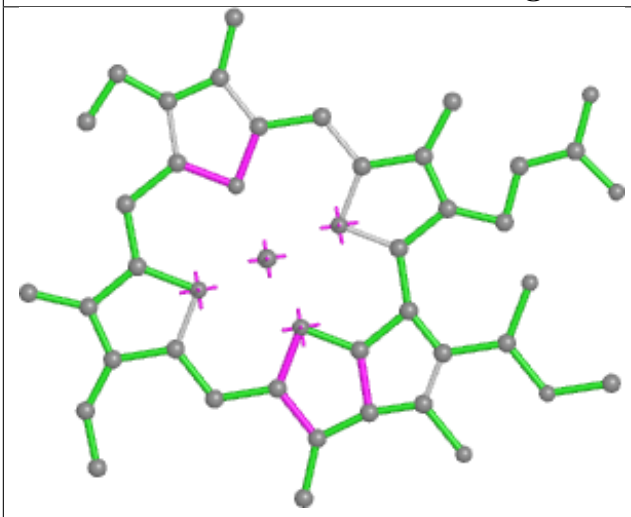


Rings

Ligand CLA T 602



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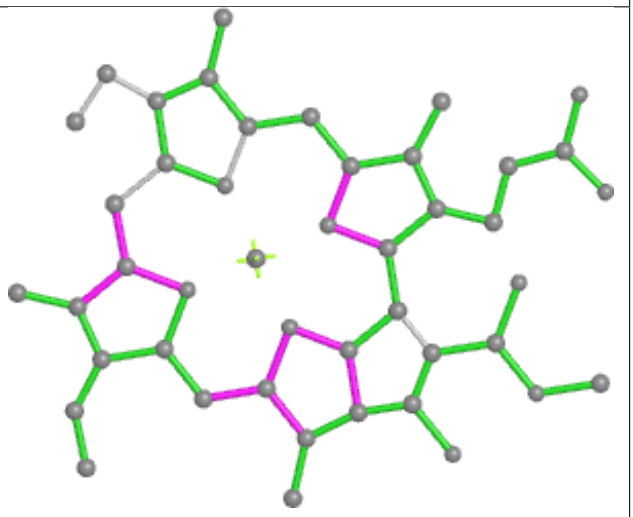
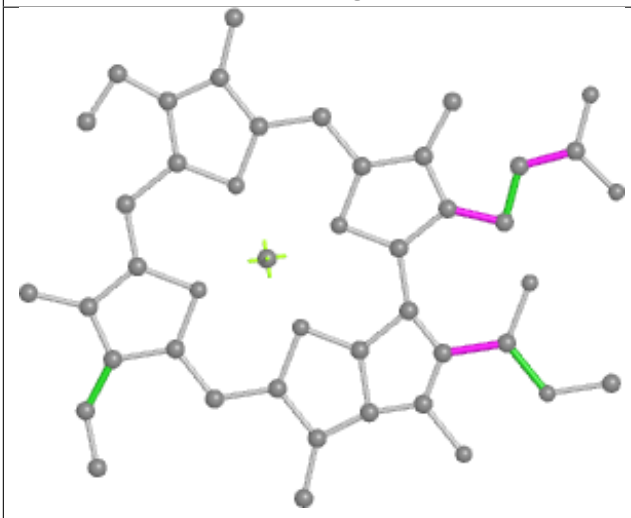


Bond angles



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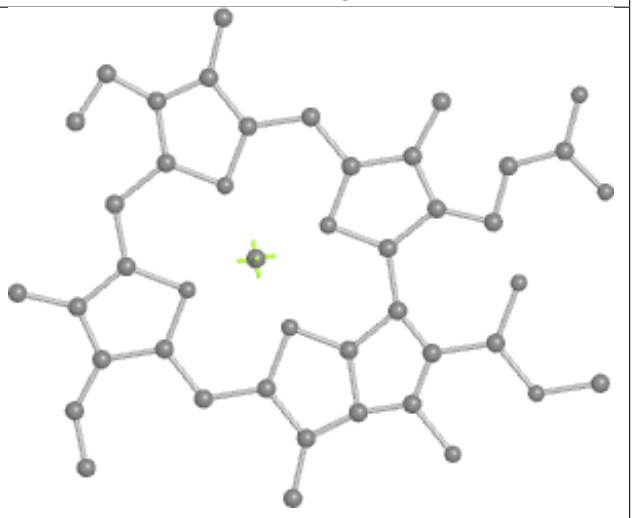
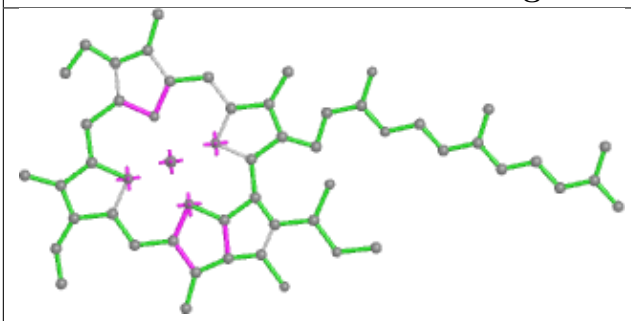


Rings

Ligand CLA D 608



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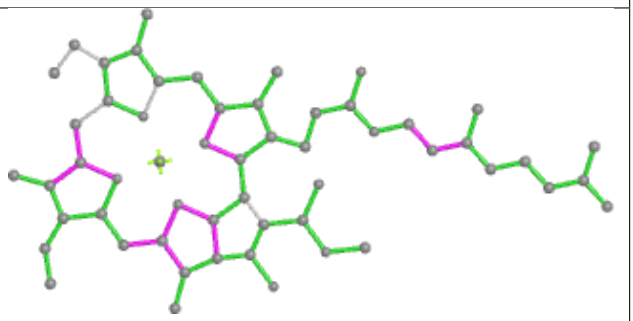
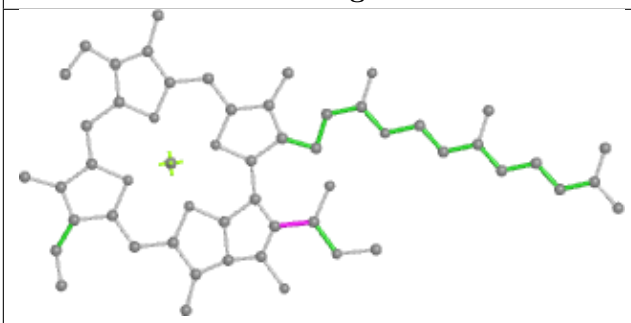


Bond angles



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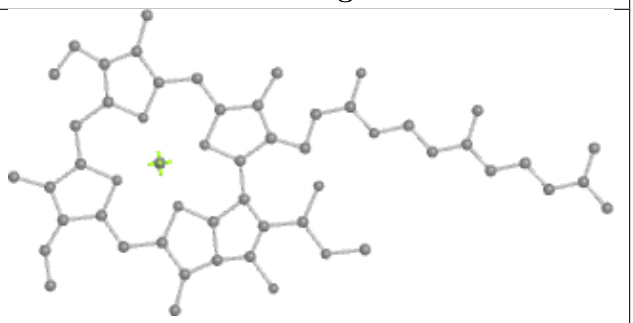
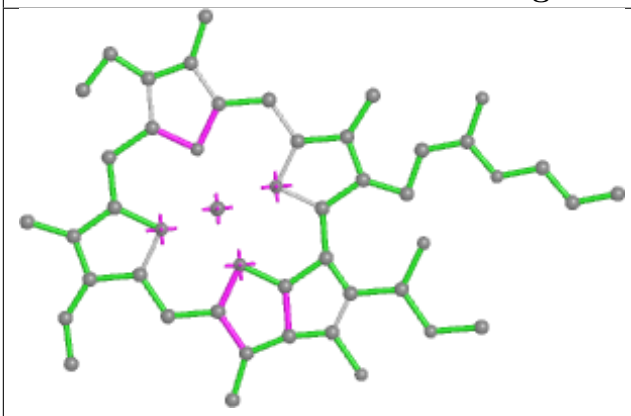
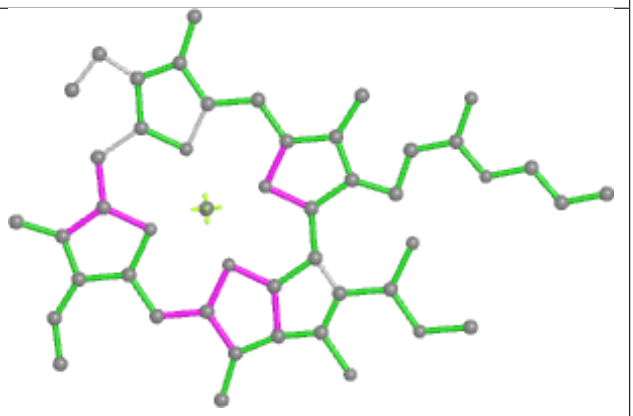


Rings

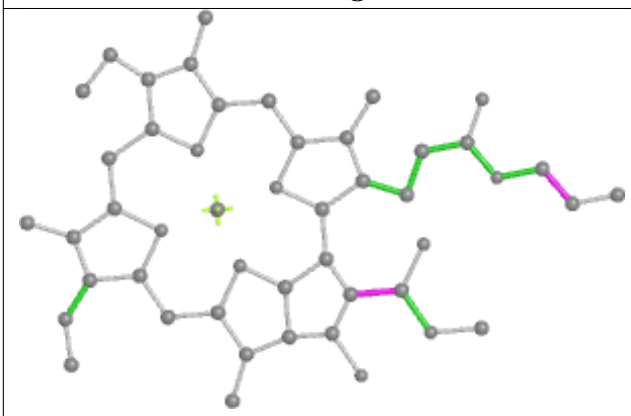
Ligand CLA l 407



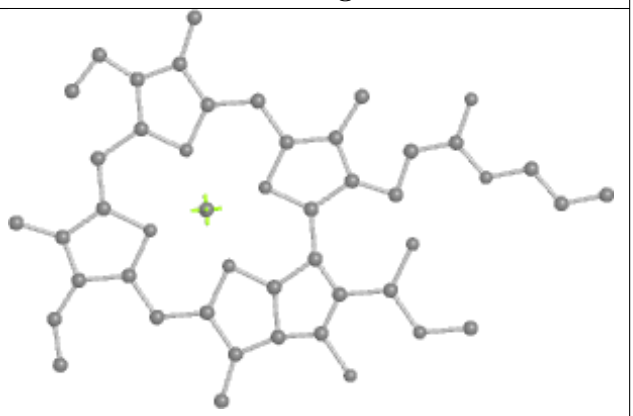
Bond lengths



Bond angles

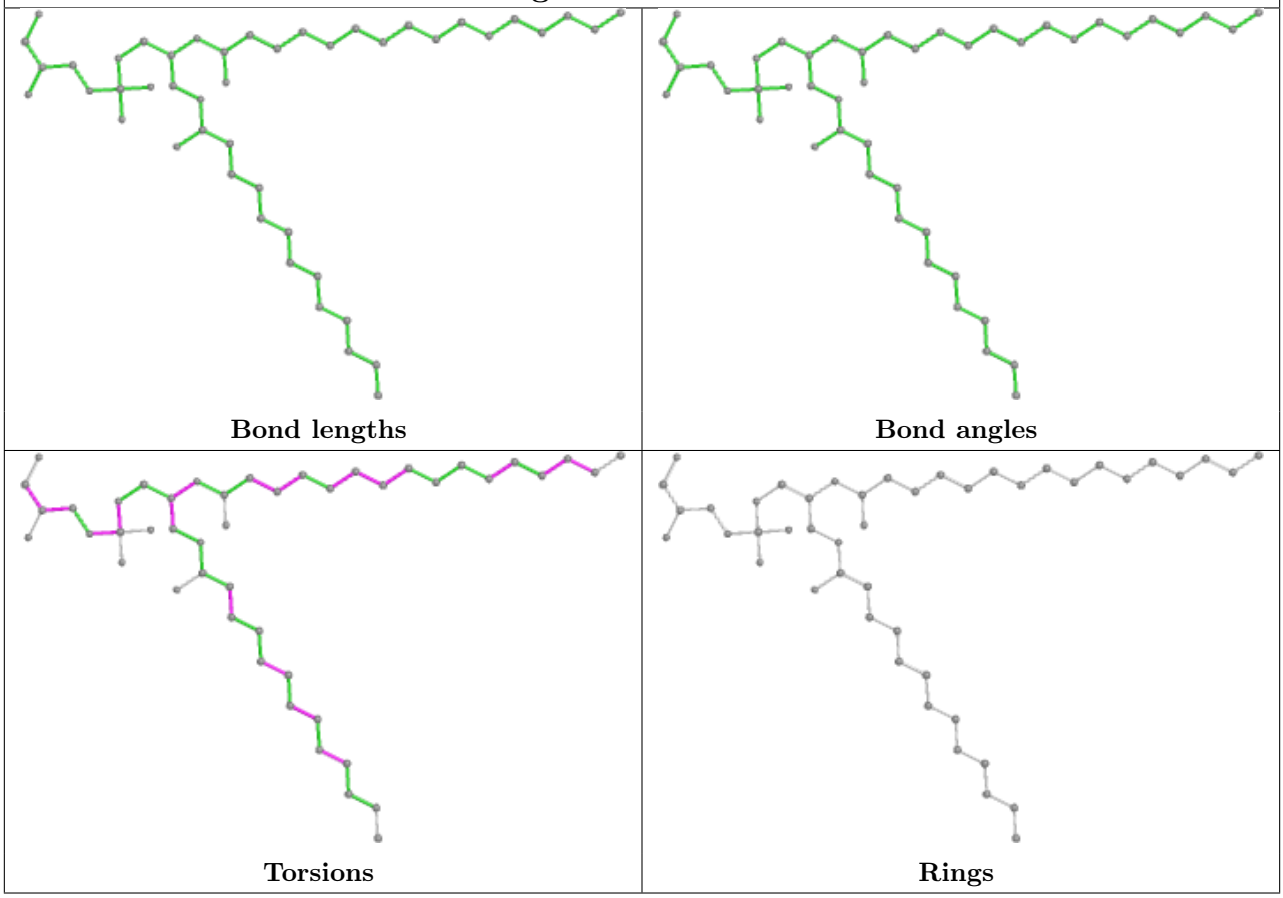


Torsions

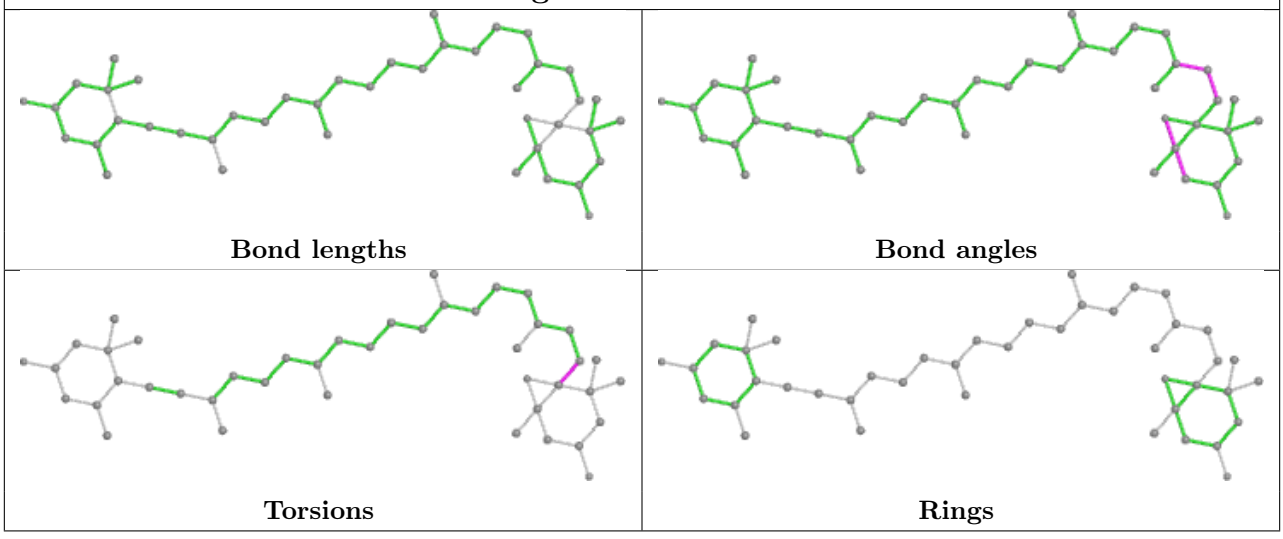


Rings

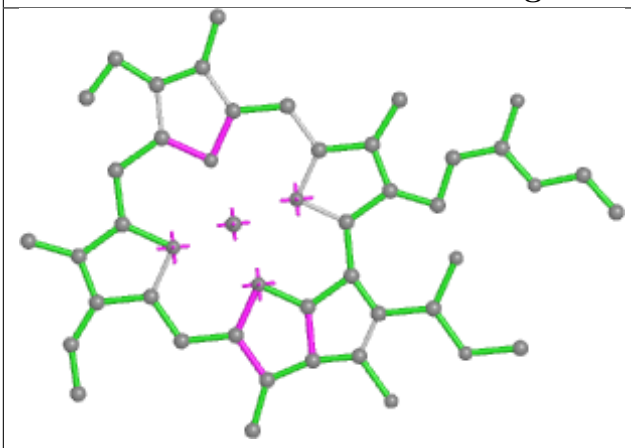
Ligand LHG l 401



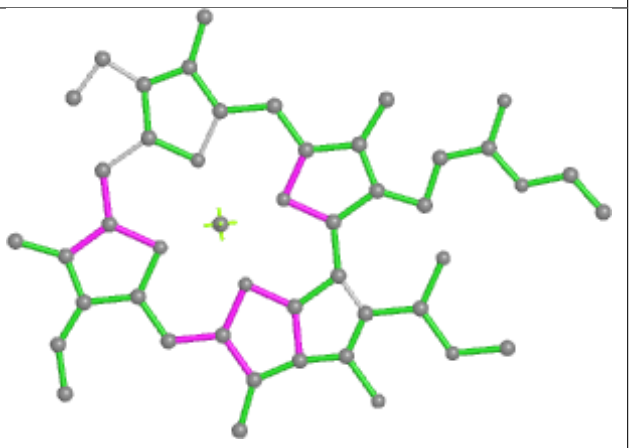
Ligand DD6 r 201



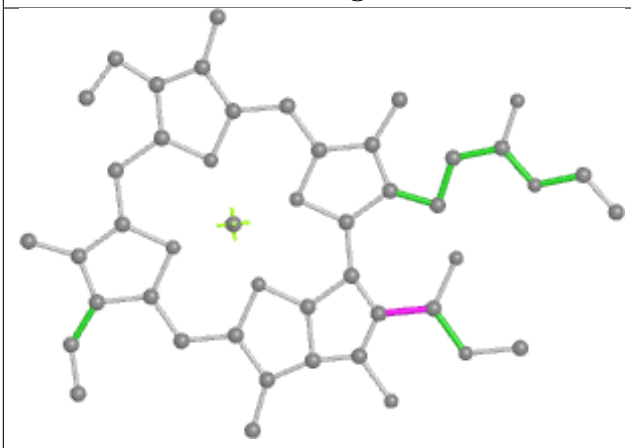
Ligand CLA C 206



Bond lengths



Bond angles



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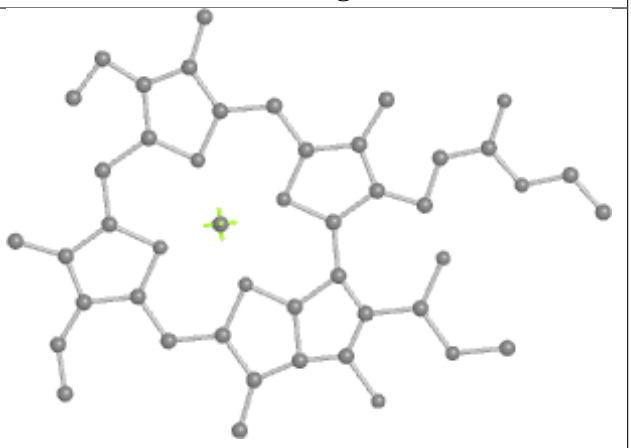
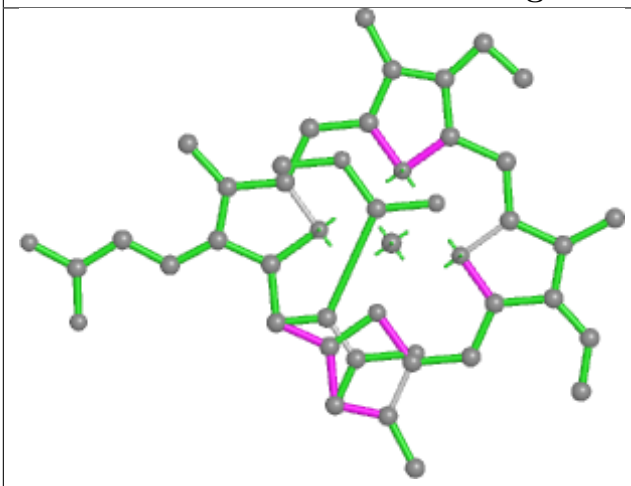


Rings

Ligand KC2 B 602



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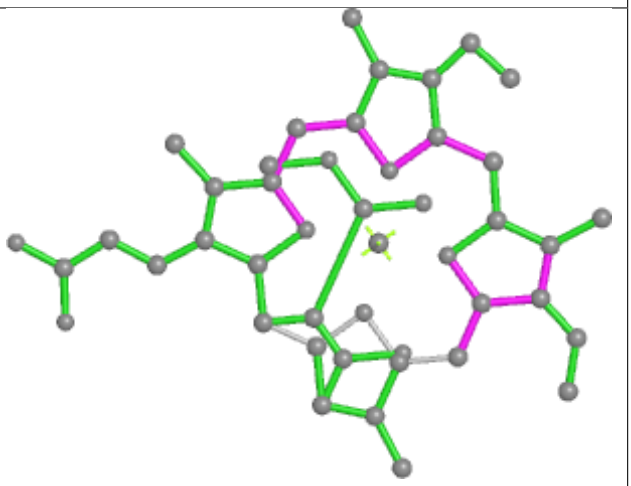
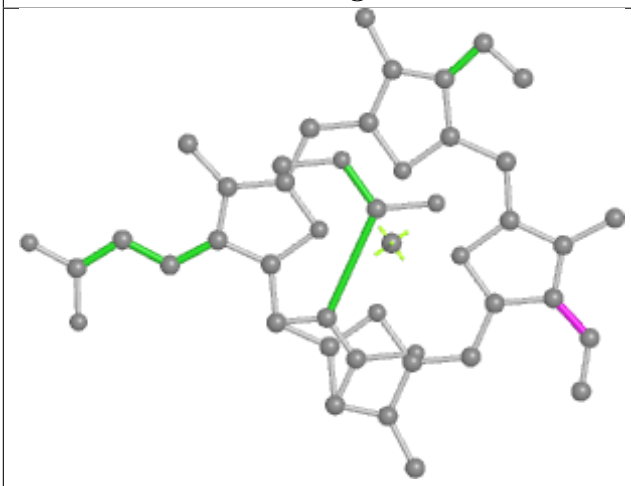


Bond angles



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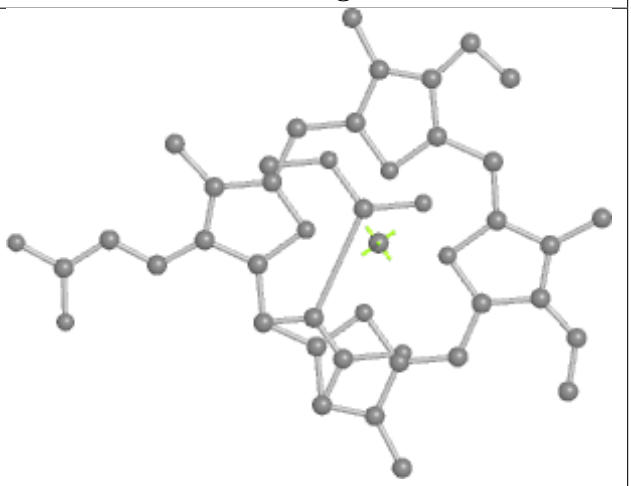
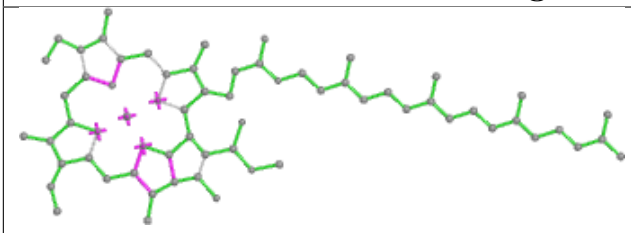


Rings

Ligand CLA a 825



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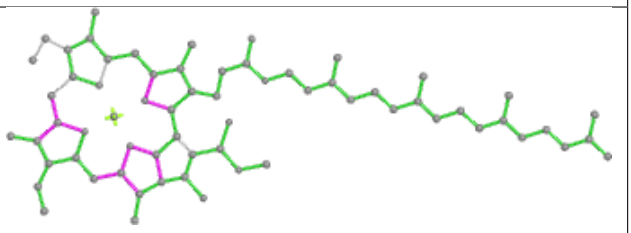
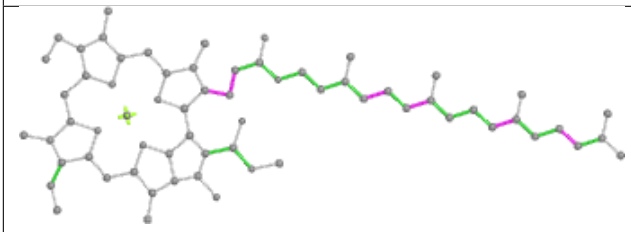


Bond angles



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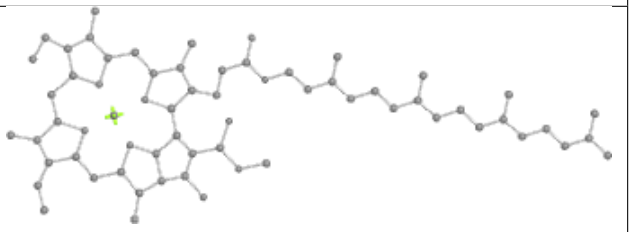
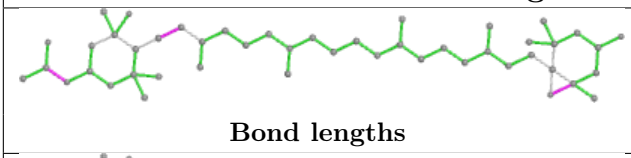


Rings

Ligand UIX A 613



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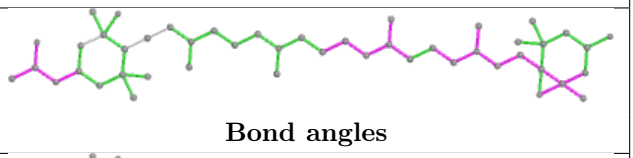
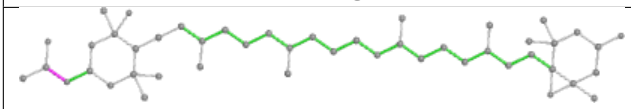


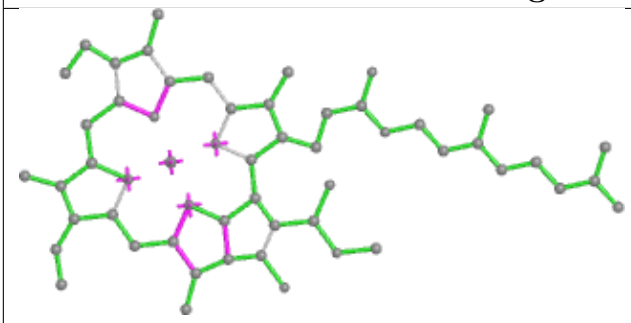
Bond angles



Torsions

Rings

Ligand CLA a 817



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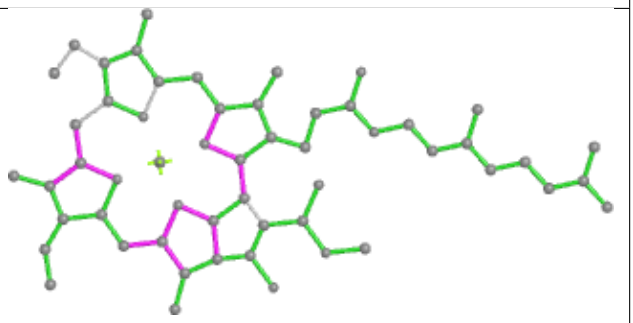
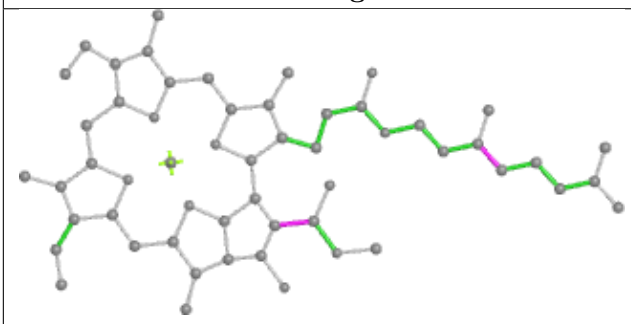


Bond angles



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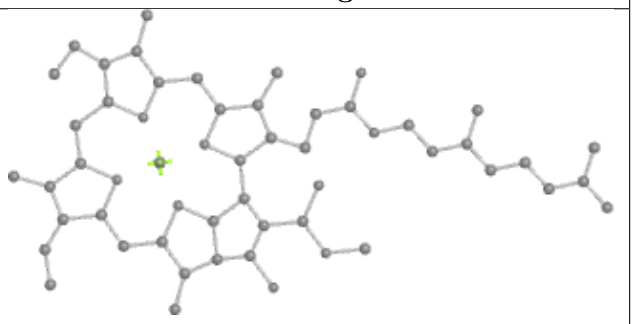
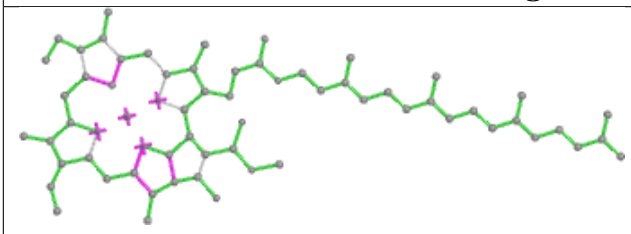


Rings

Ligand CLA B 606



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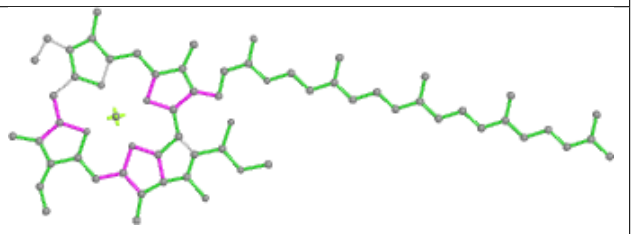
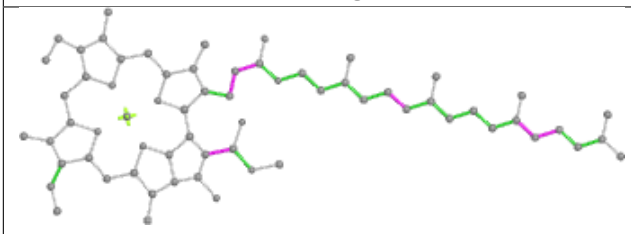


Bond angles



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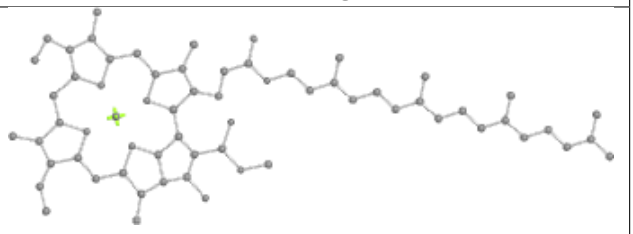
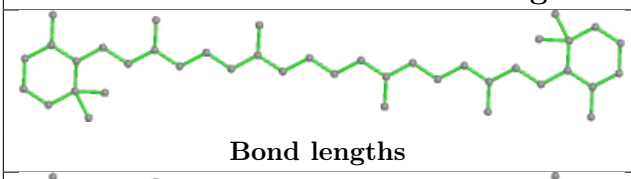


Rings

Ligand BCR f 304



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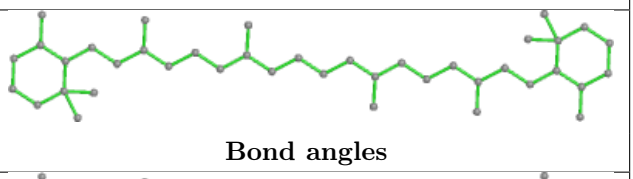
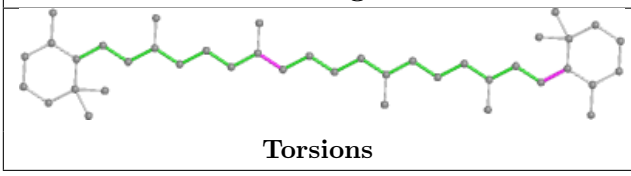


Bond angles



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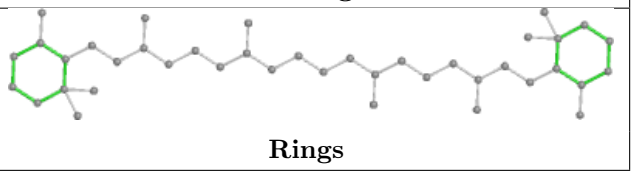
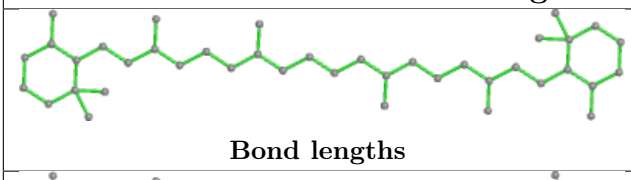


Rings

Ligand BCR j 203



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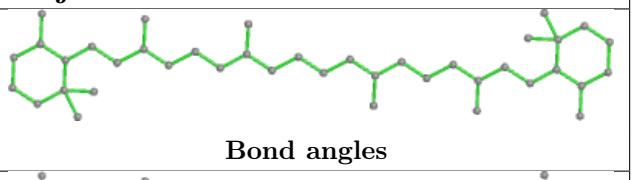
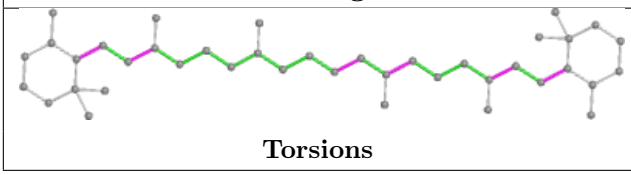
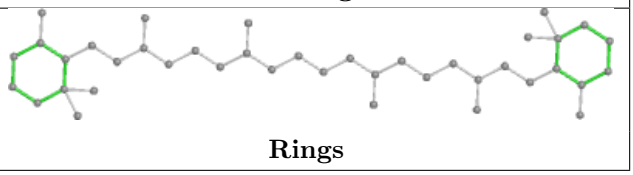


Bond angles

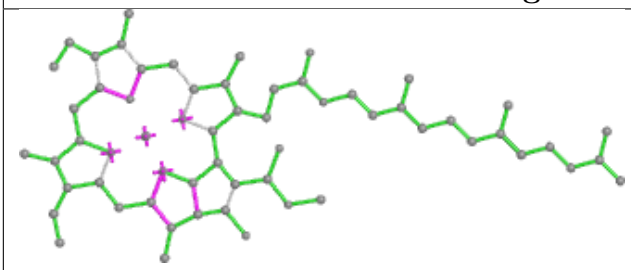


Torsions



Rings

Ligand CLA G 608



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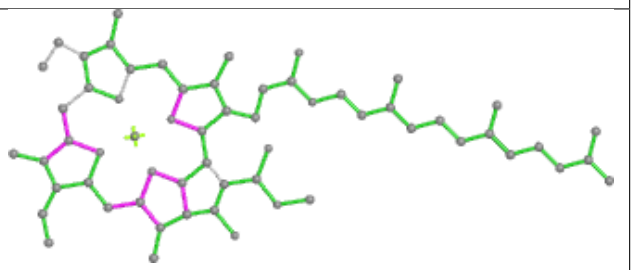
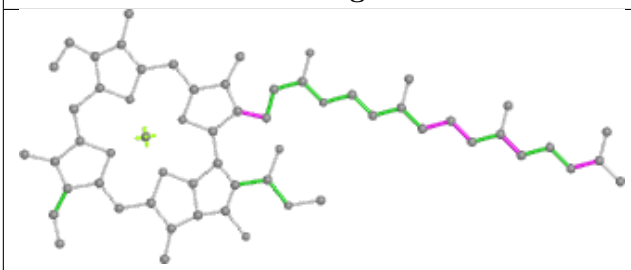


Bond angles



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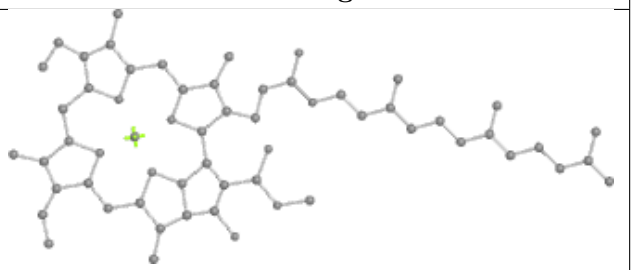
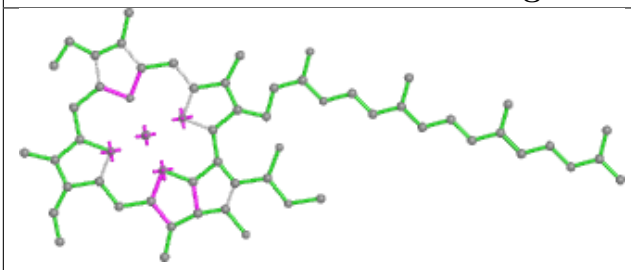


Rings

Ligand CLA H 304



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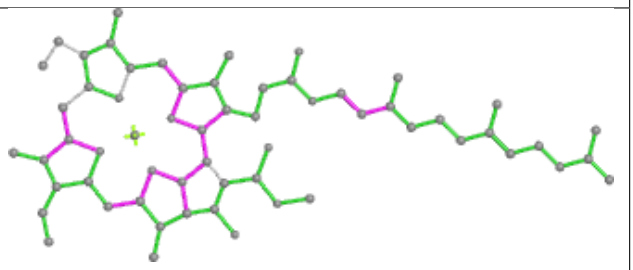
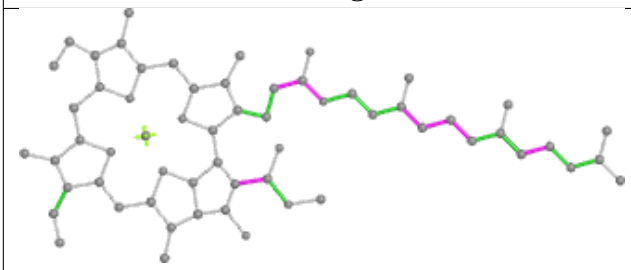


Bond angles



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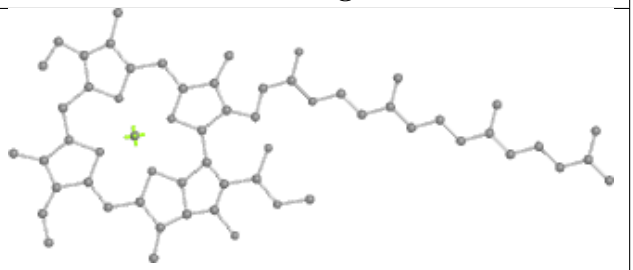
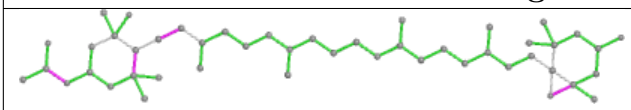


Rings

Ligand UIX B 611



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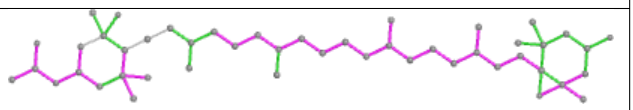
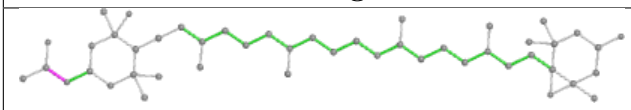


Bond angles



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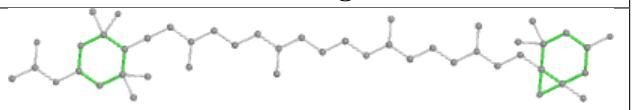
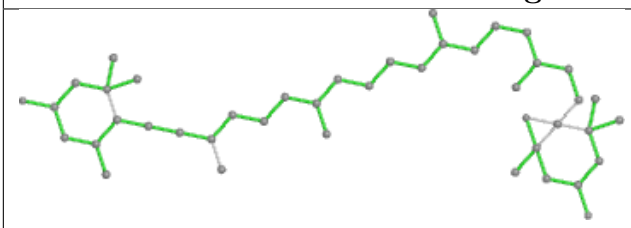


Rings

Ligand DD6 D 613



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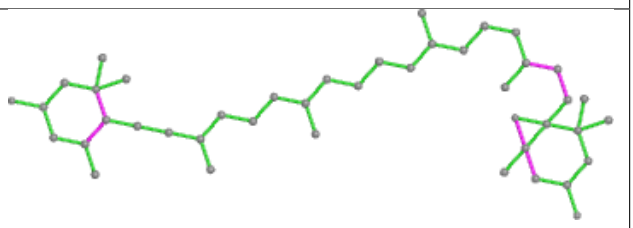
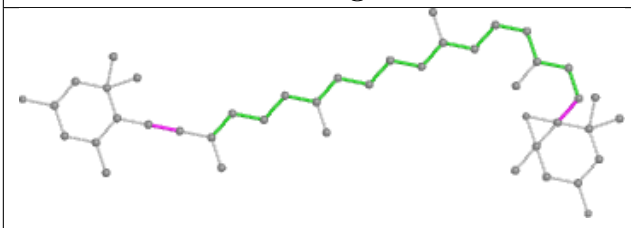


Bond angles



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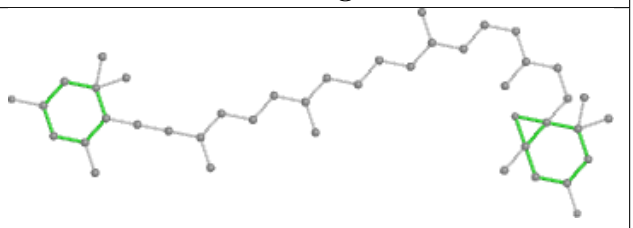
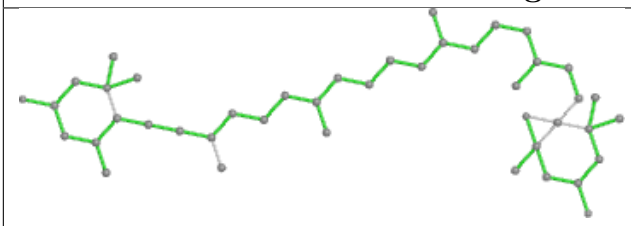
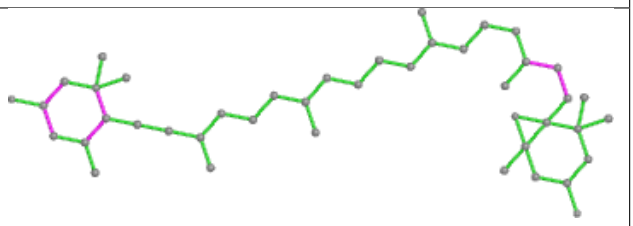


Rings

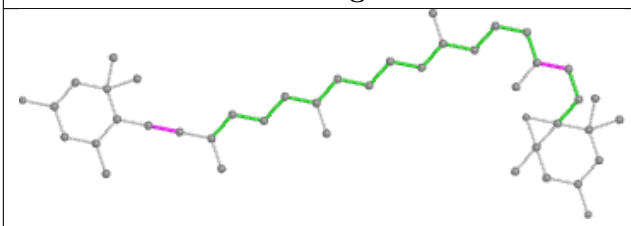
Ligand DD6 A 615



Bond lengths



Bond angles



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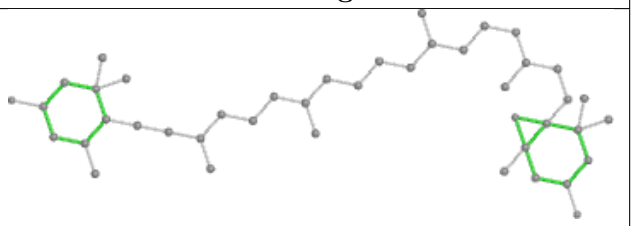
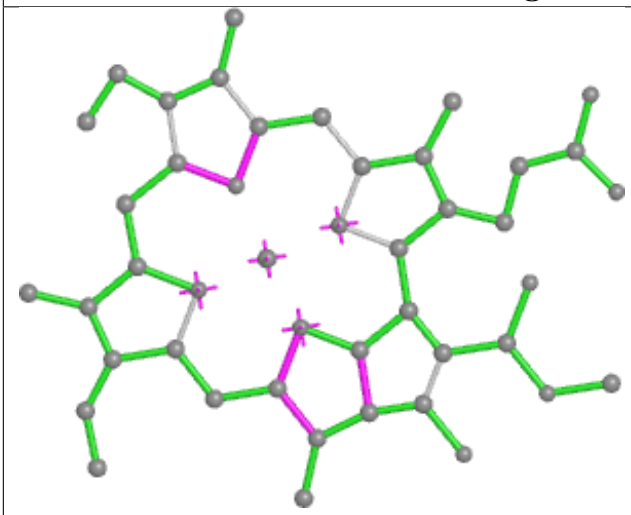
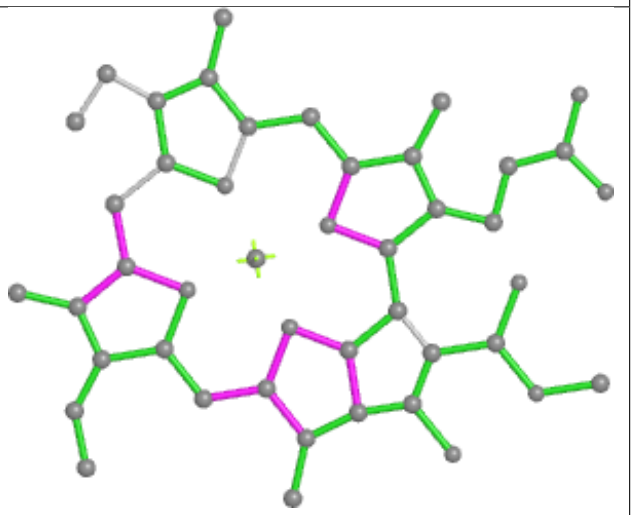


Rings

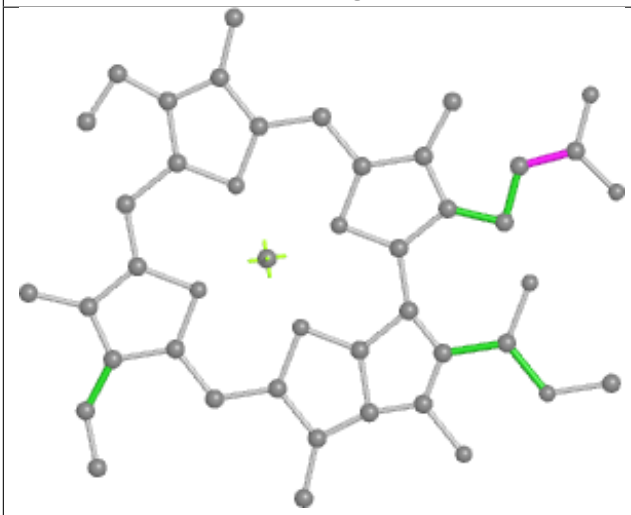
Ligand CLA D 609



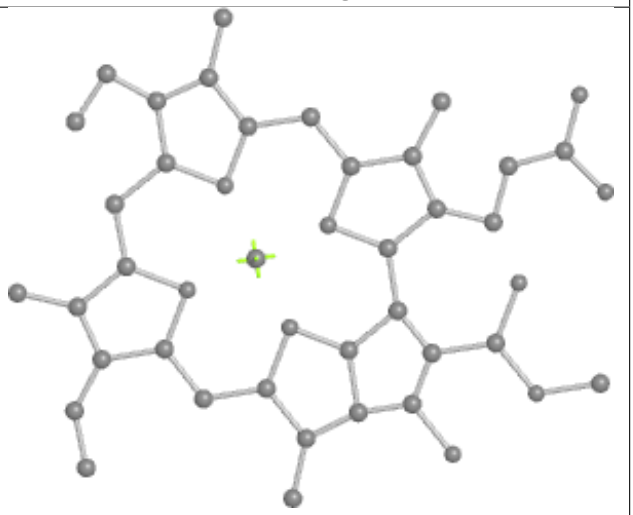
Bond lengths



Bond angles

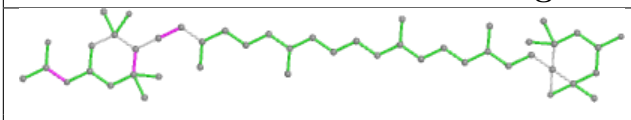


Torsions

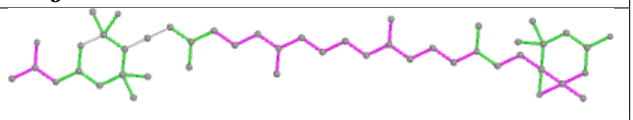


Rings

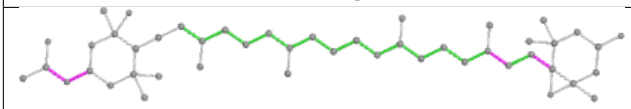
Ligand UIX j 204



Bond lengths



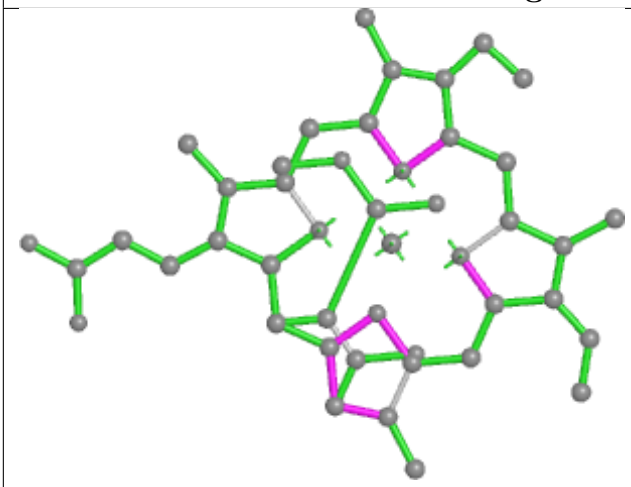
Bond angles



Torsions

Rings

Ligand KC2 A 608



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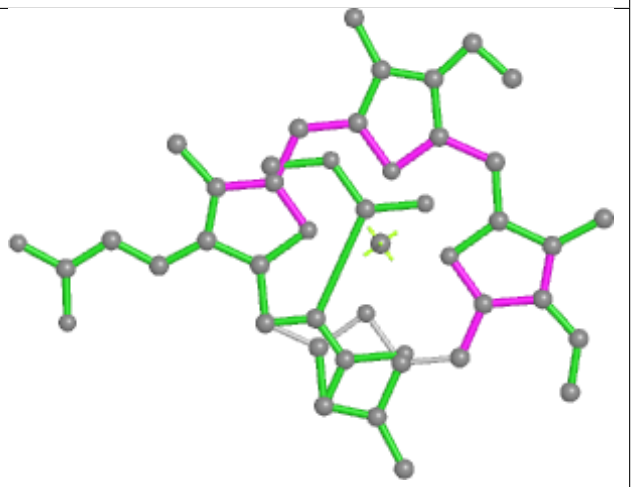
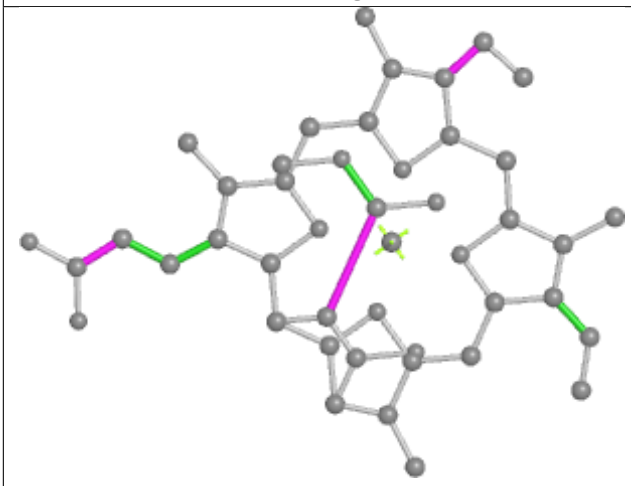
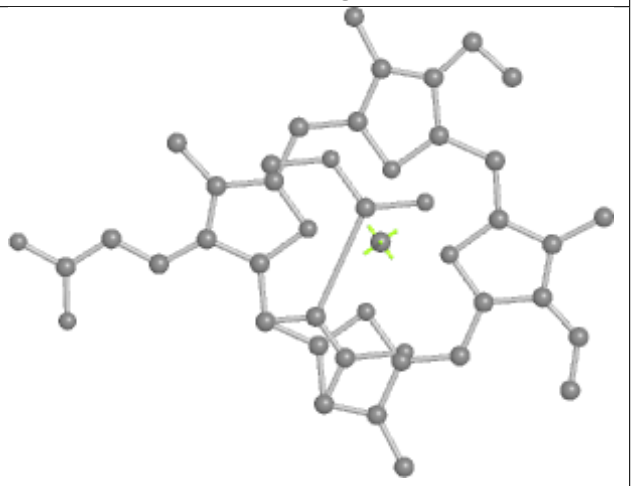


Bond angles

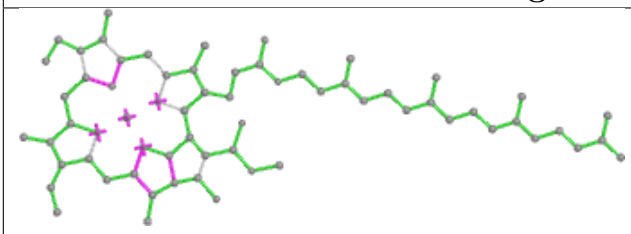


Torsions



Rings

Ligand CLA a 823



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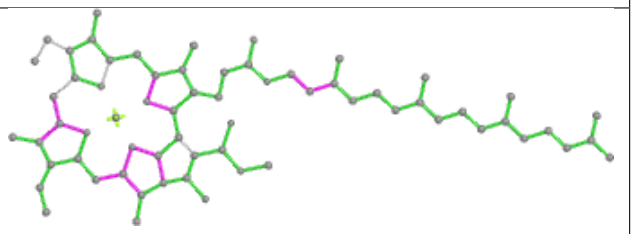
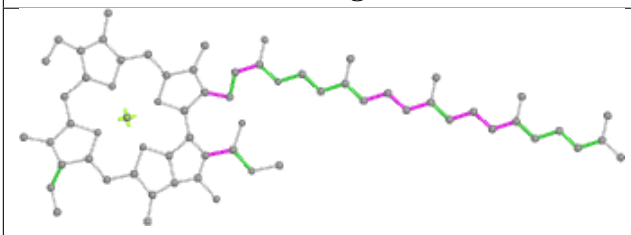
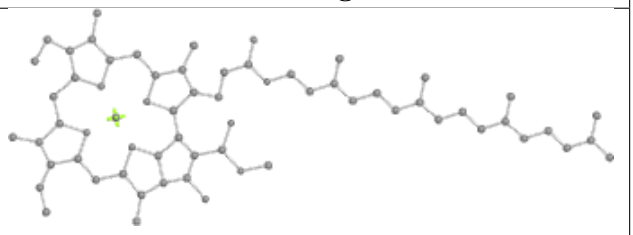


Bond angles

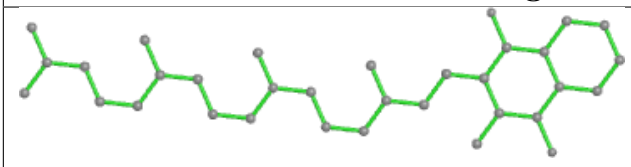


Torsions



Rings

Ligand PQN b 729



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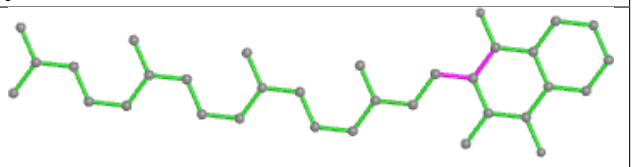
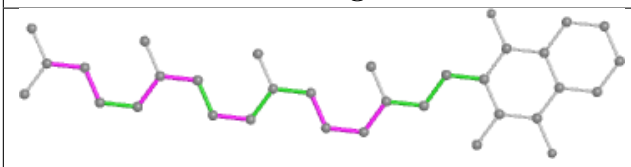


Bond angles



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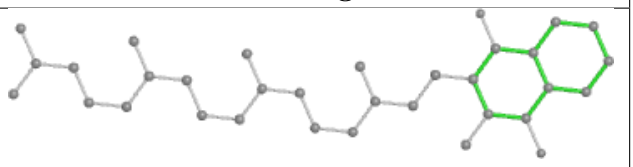
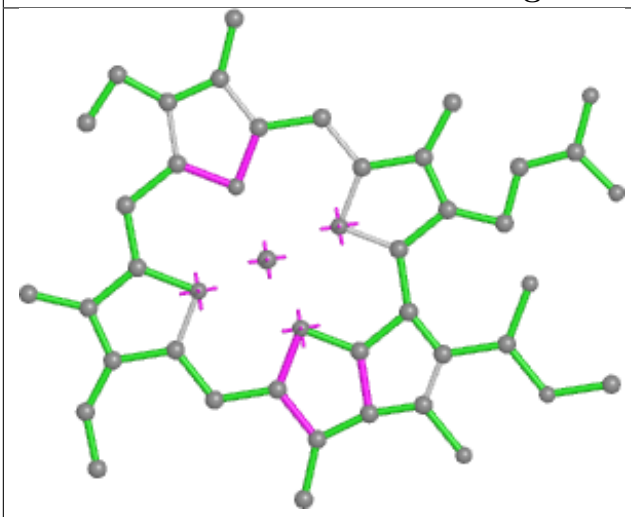


Rings

Ligand CLA A 607



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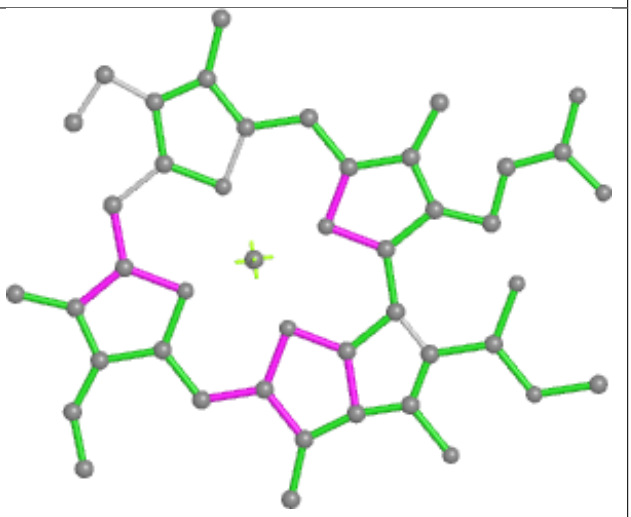
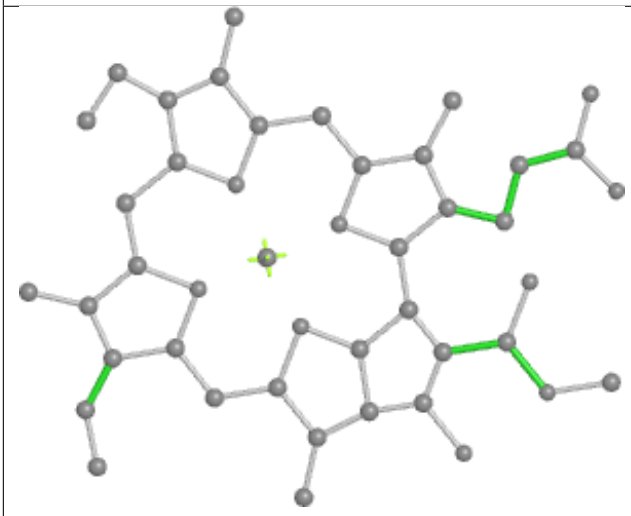


Bond angles



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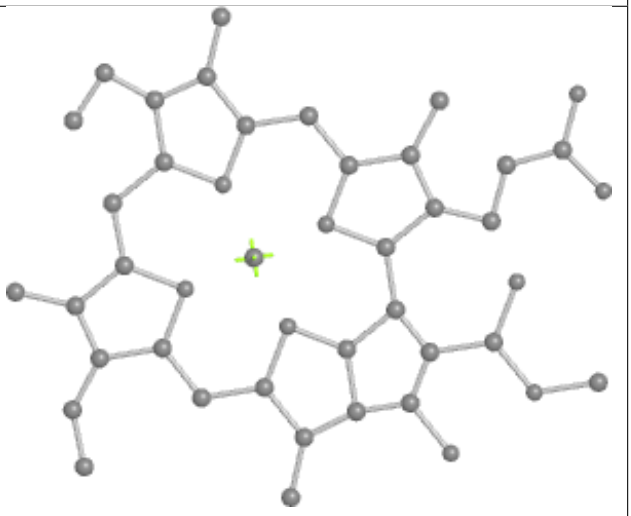
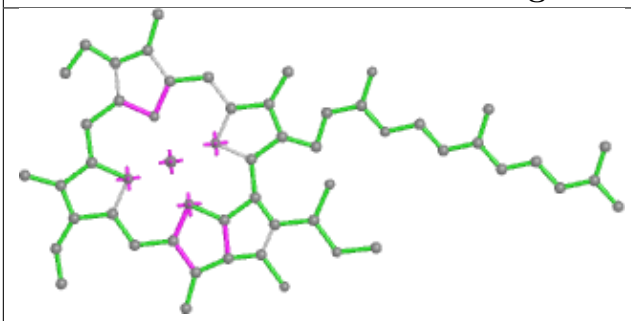


Rings

Ligand CLA a 831



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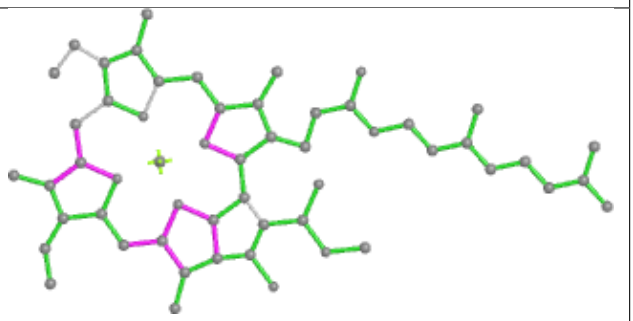
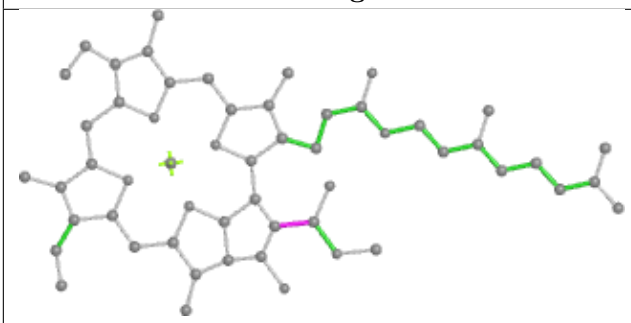
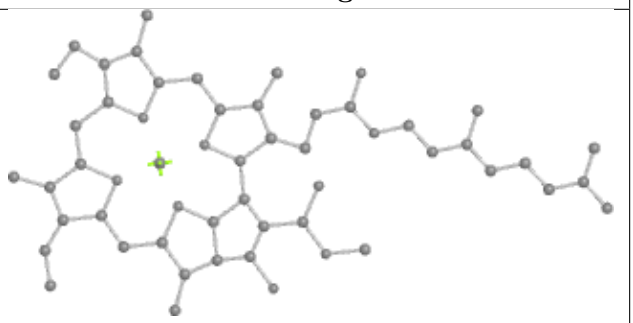


Bond angles

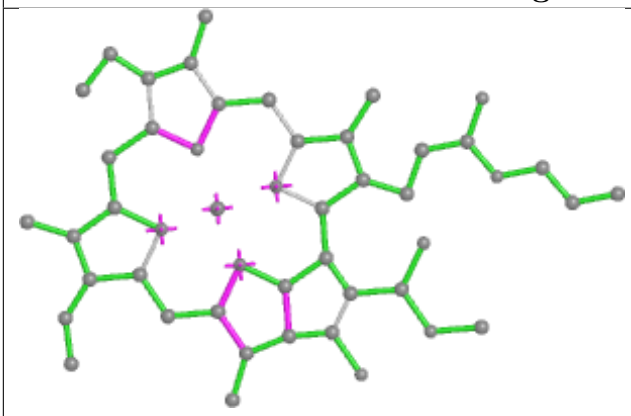


Torsions



Rings

Ligand CLA l 410



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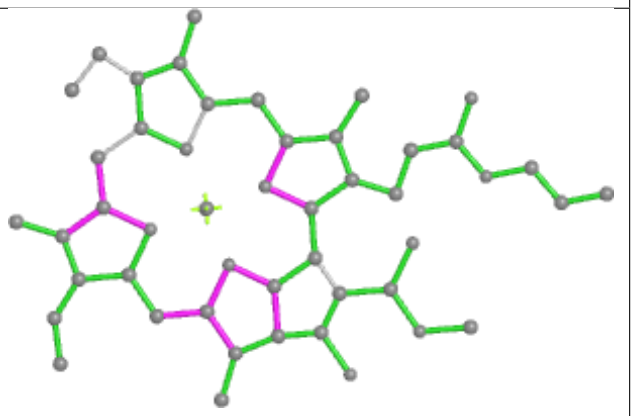
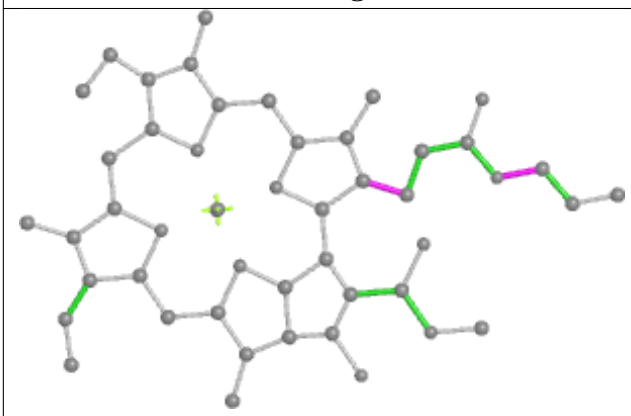


Bond angles



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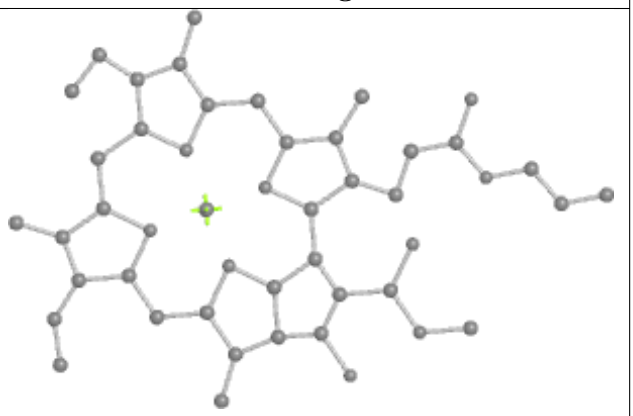
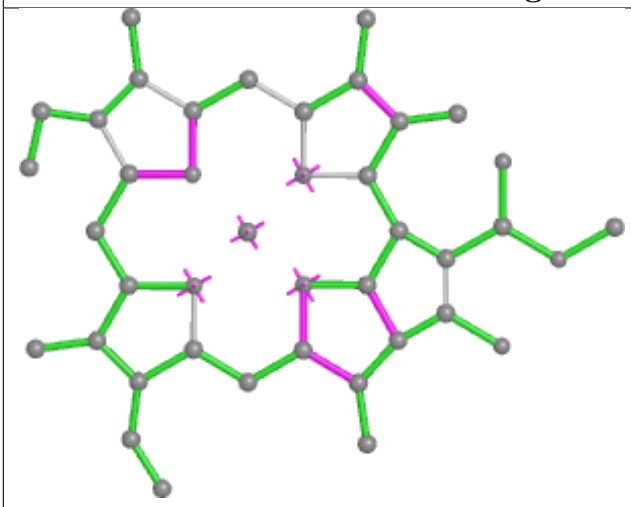
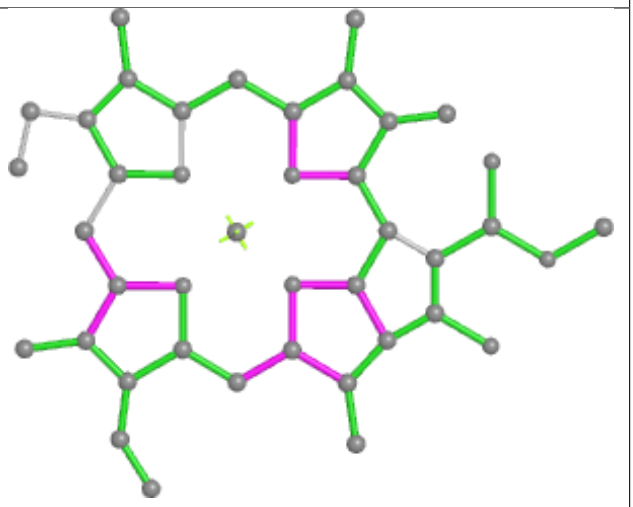


Rings

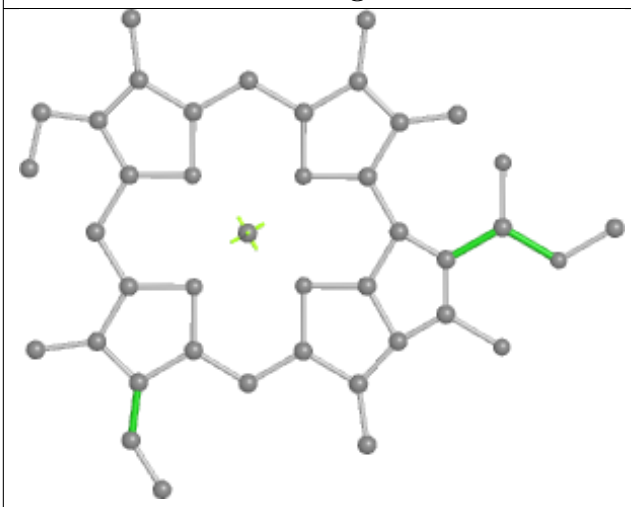
Ligand CLA T 609



Bond lengths



Bond angles



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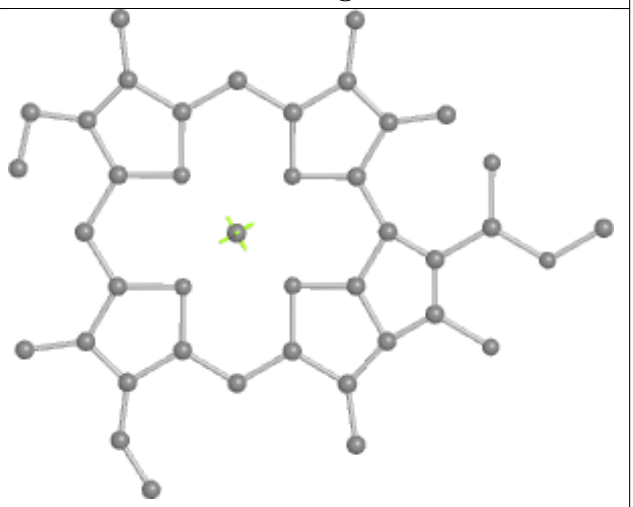
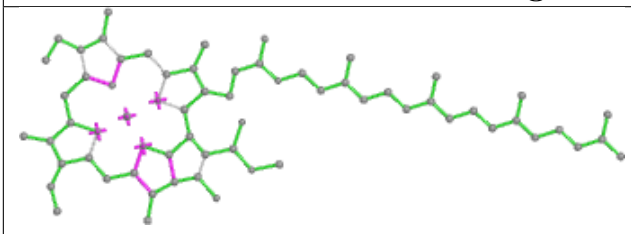
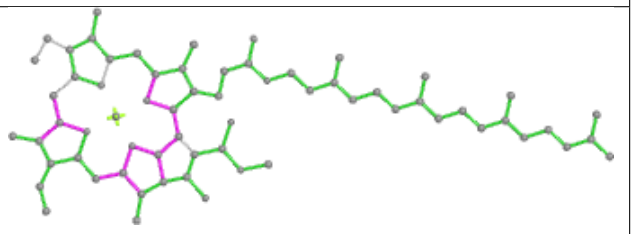


Rings

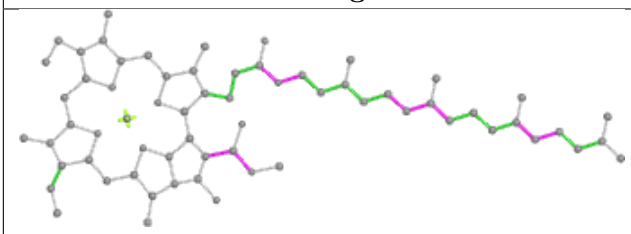
Ligand CLA b 702



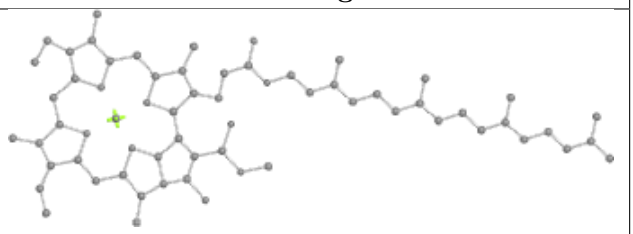
Bond lengths



Bond angles

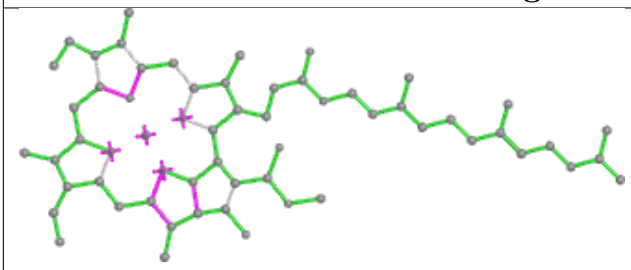


Torsions



Rings

Ligand CLA D 607



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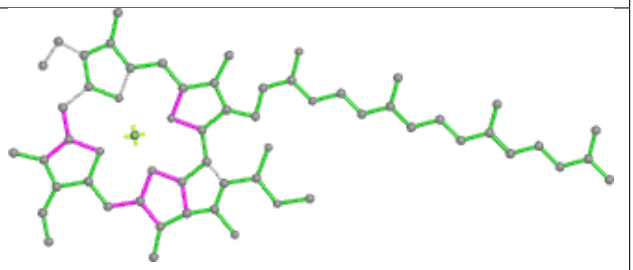
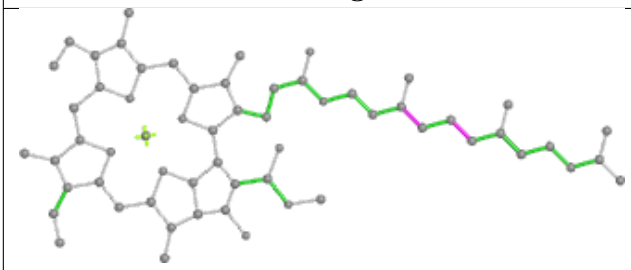
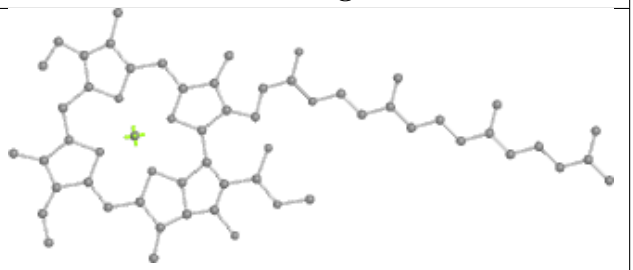


Bond angles

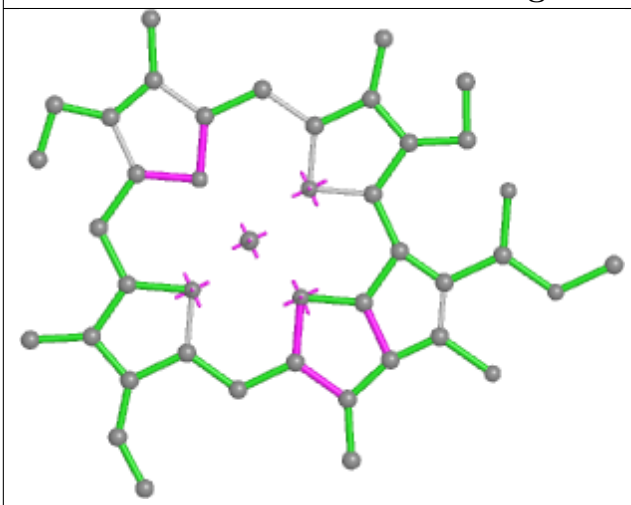


Torsions



Rings

Ligand CLA J 607



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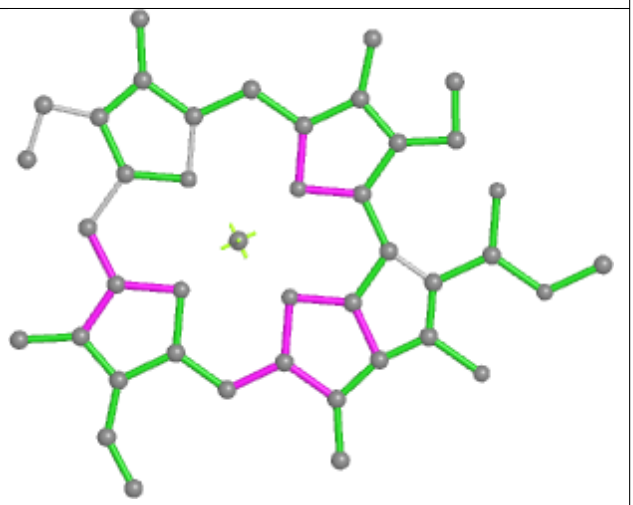
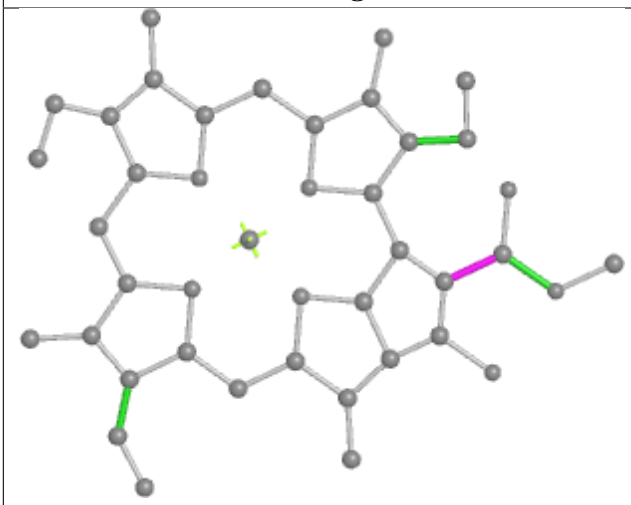


Bond angles



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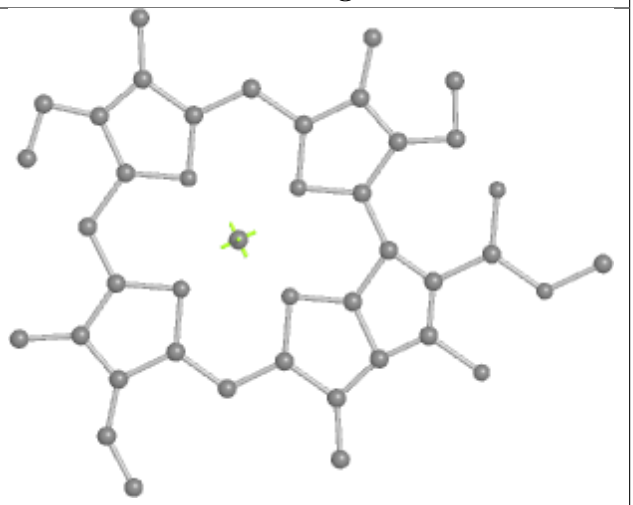
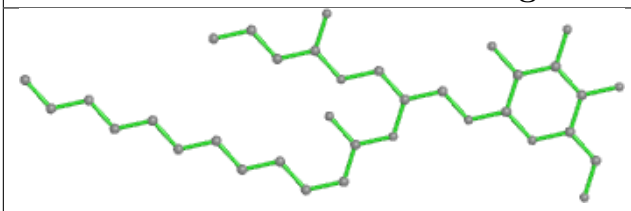


Rings

Ligand LMG D 618



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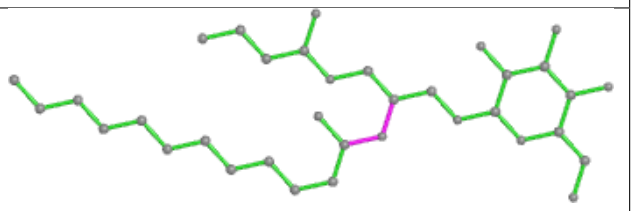
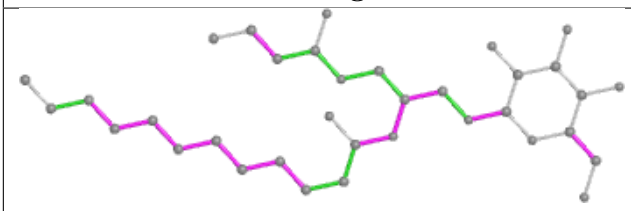
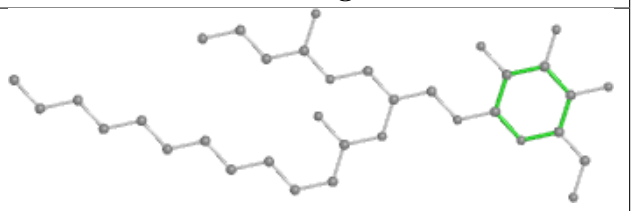


Bond angles

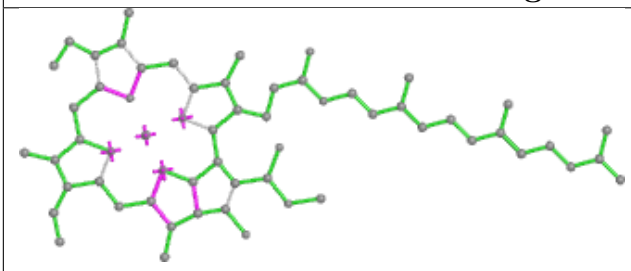


Torsions



Rings

Ligand CLA B 601



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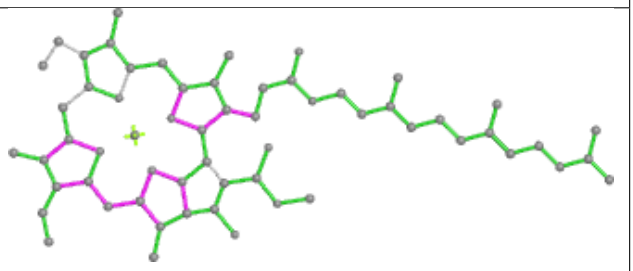
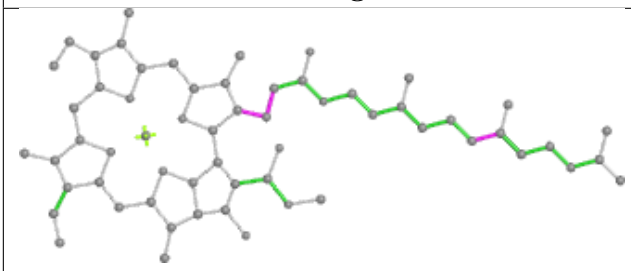
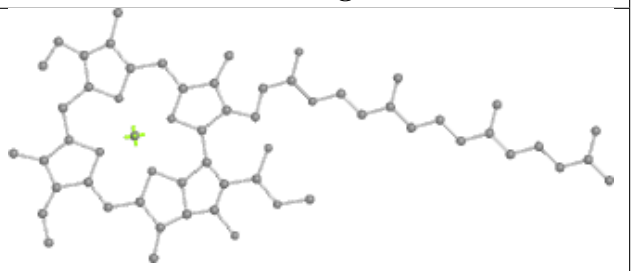


Bond angles

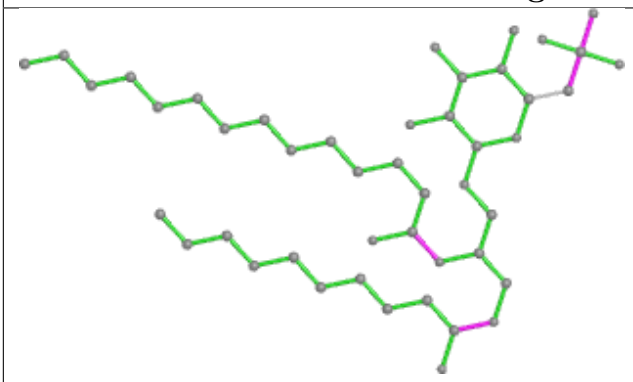


Torsions

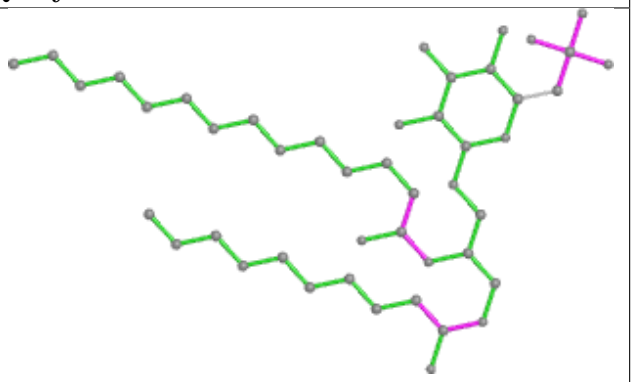


Rings

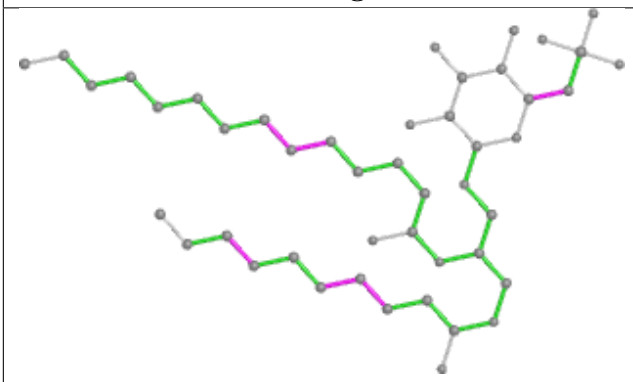
Ligand SQD y 301



Bond lengths



Bond angles



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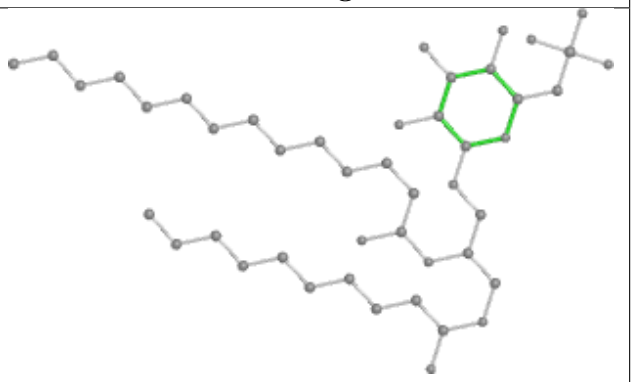
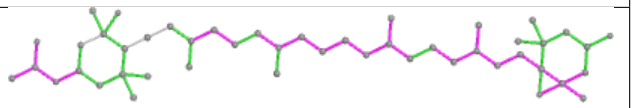


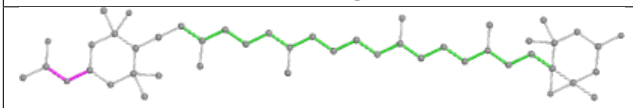
Rings

Ligand UIX H 317

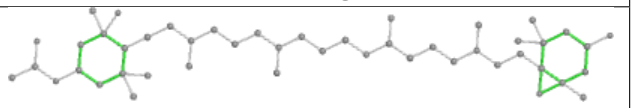
Bond lengths



Bond angles

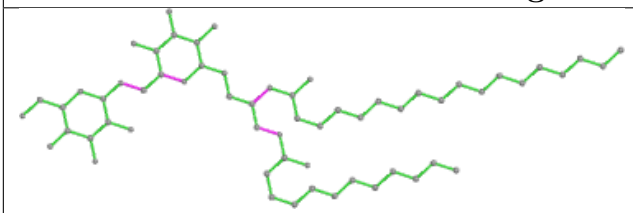


Torsions



Rings

Ligand DGD j 201



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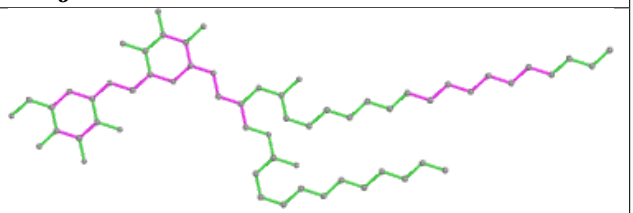

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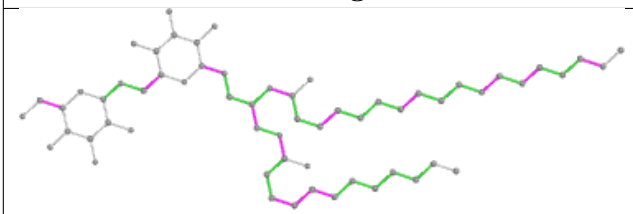
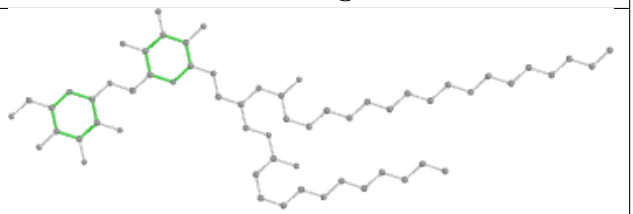
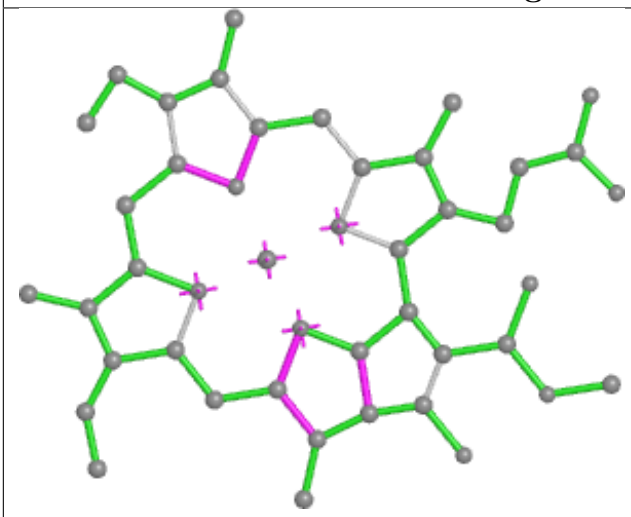


Torsions



Rings

Ligand CLA T 603



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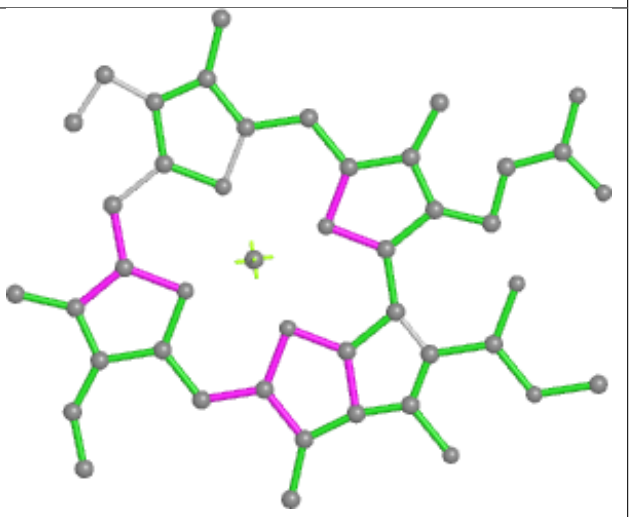

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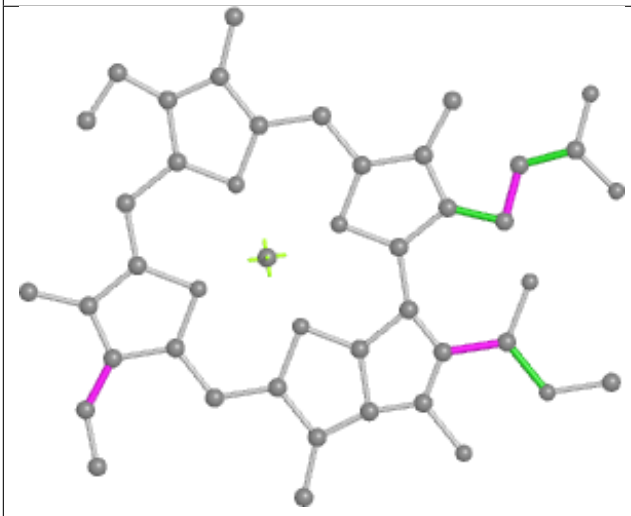

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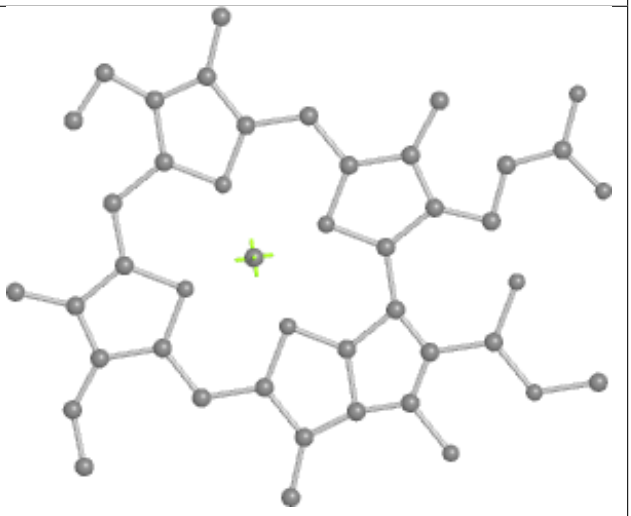
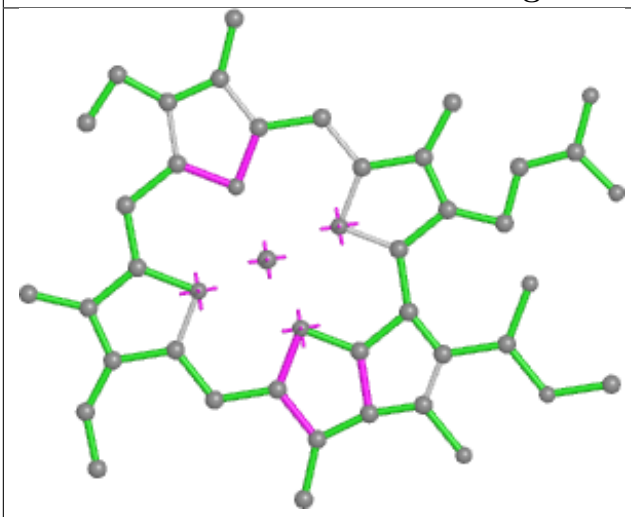


Rings

Ligand CLA G 611



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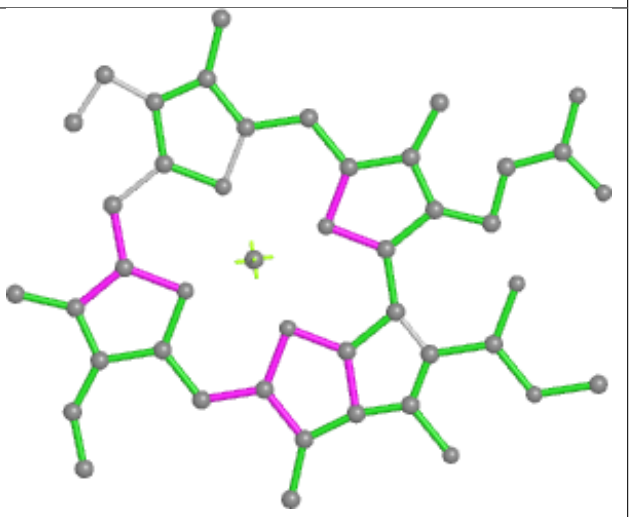

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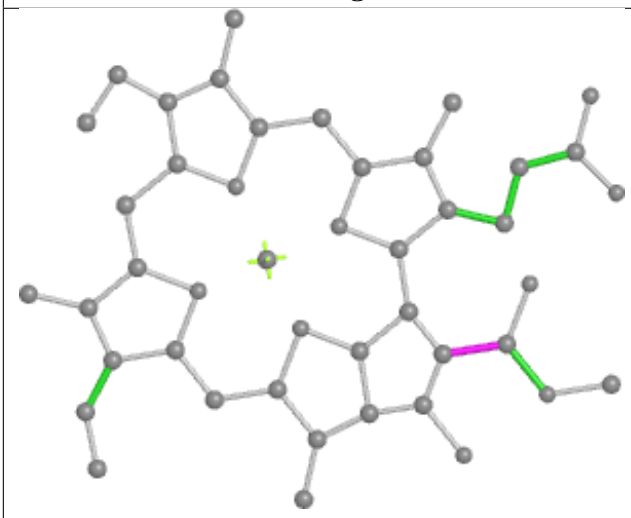

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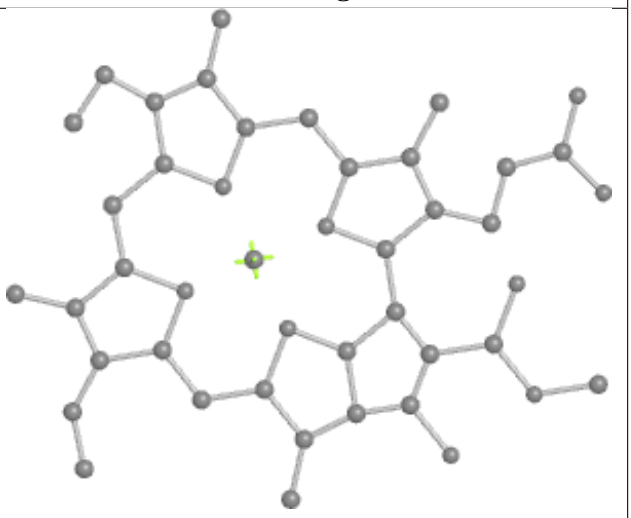
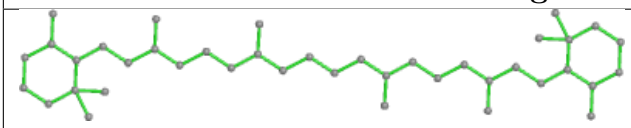


Rings

Ligand BCR l 413



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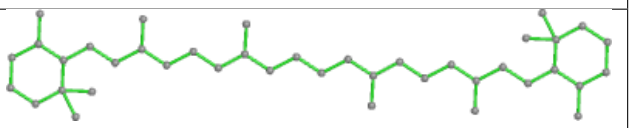

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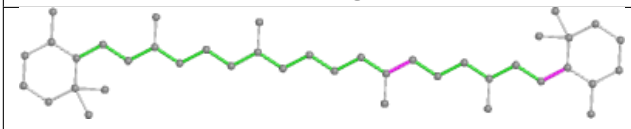
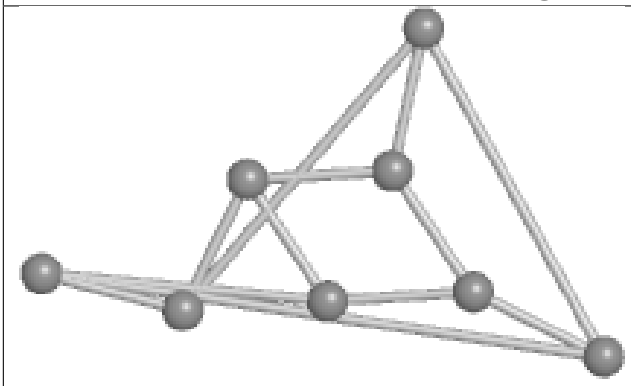


Torsions

Rings

Ligand SF4 a 838



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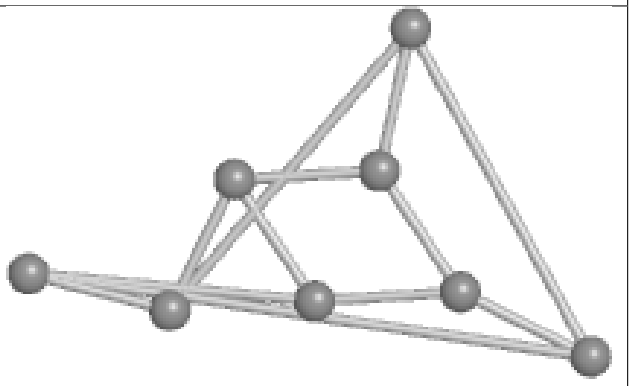

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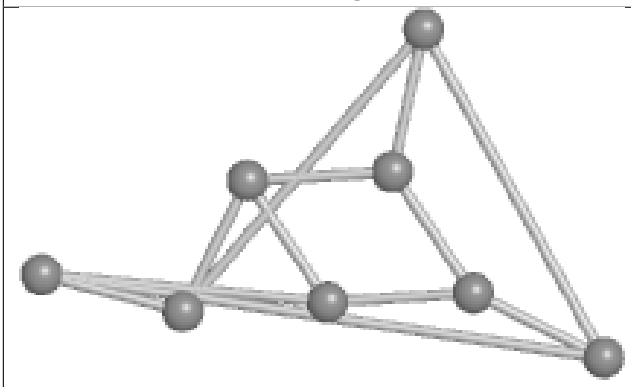

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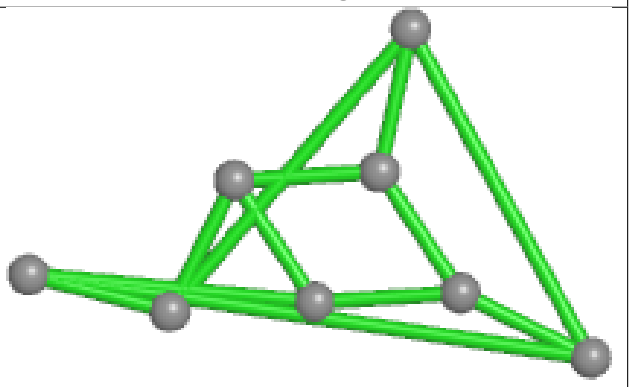
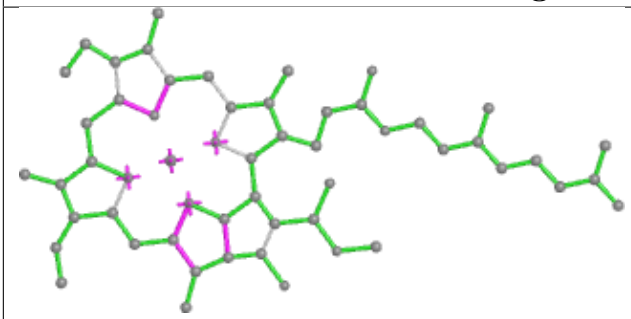


Rings

Ligand CLA I 602



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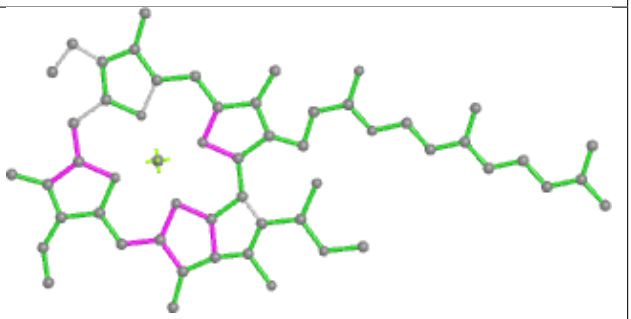

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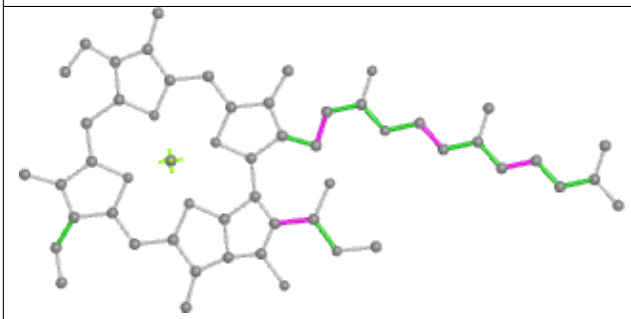

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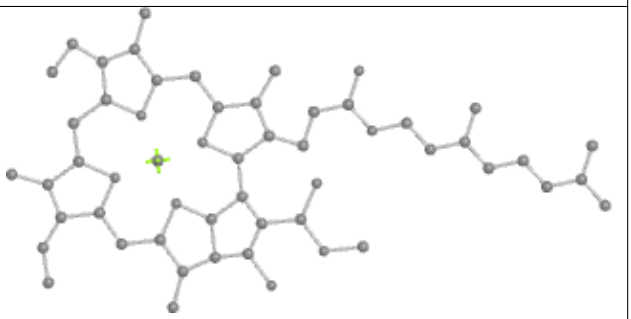
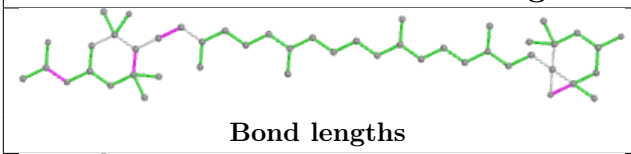


Rings

Ligand UIX T 612



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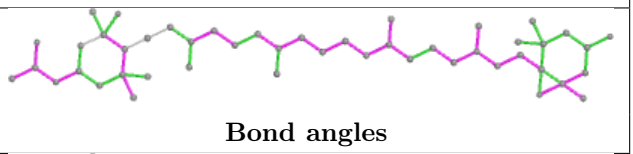

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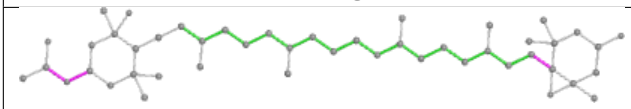
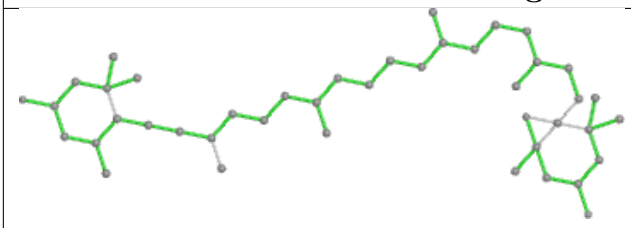


Torsions

Rings

Ligand DD6 B 614



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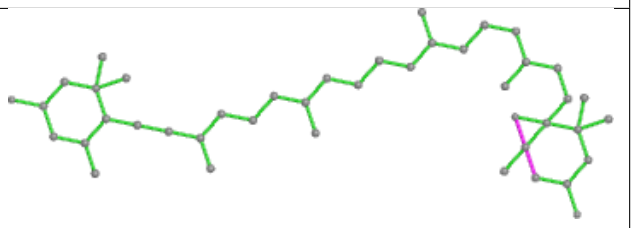

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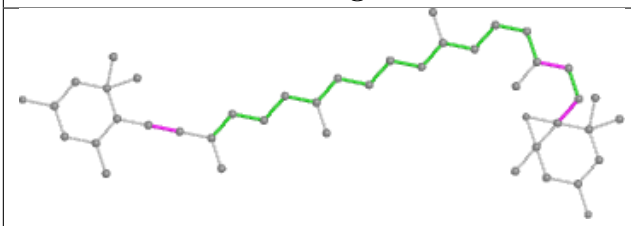
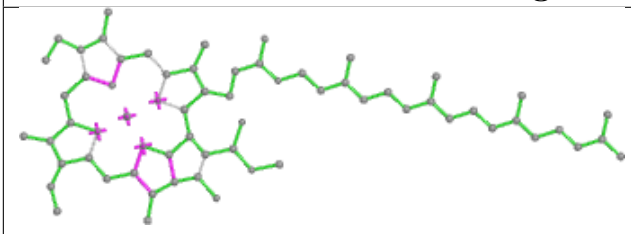


Torsions

Rings

Ligand CLA l 403



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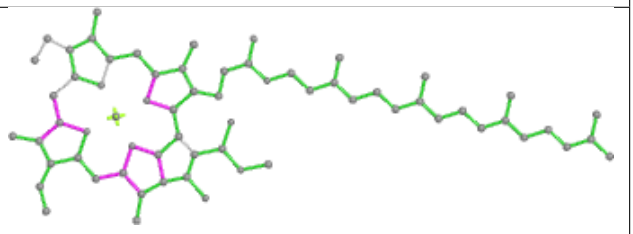

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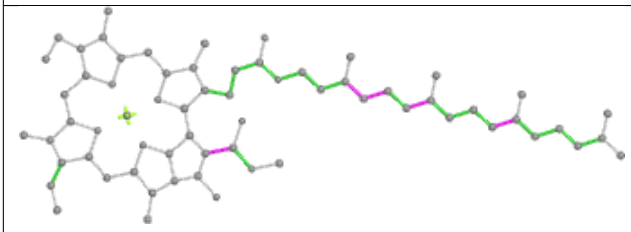

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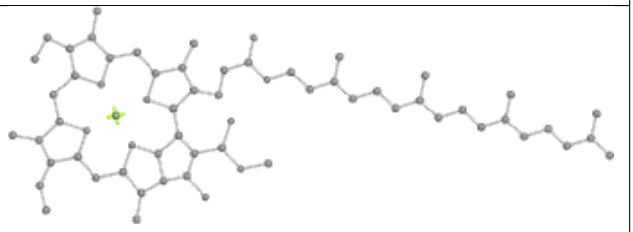
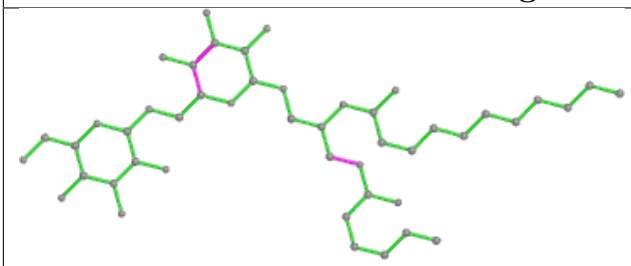


Rings

Ligand DGD K 614



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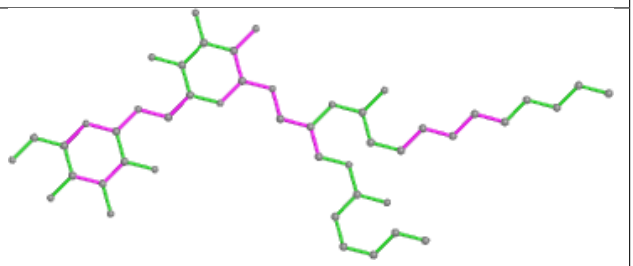

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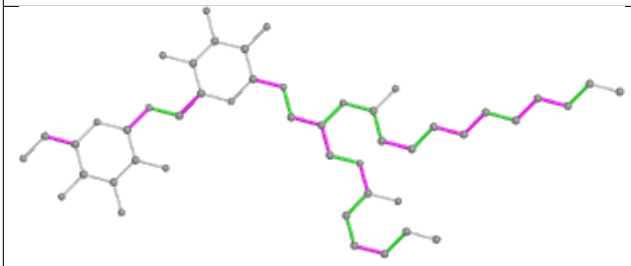

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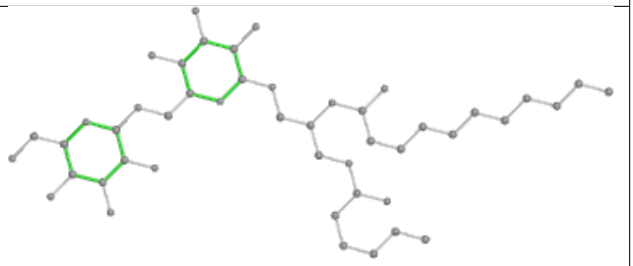
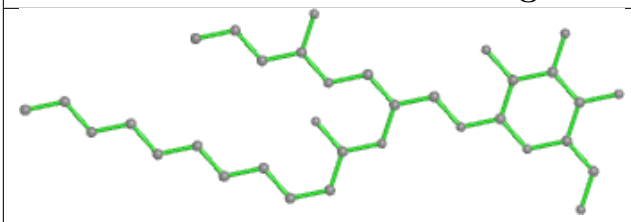


Rings

Ligand LMG C 217



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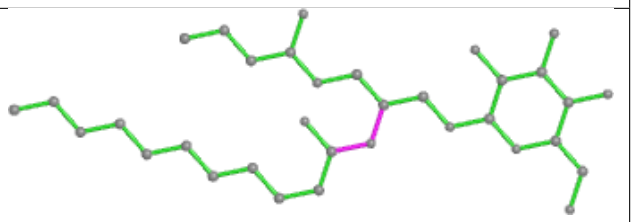

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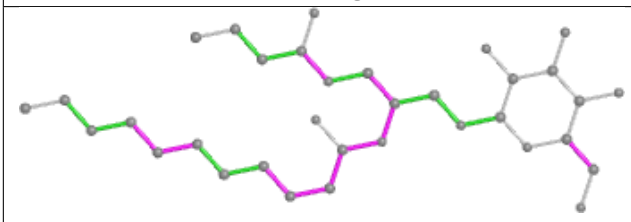

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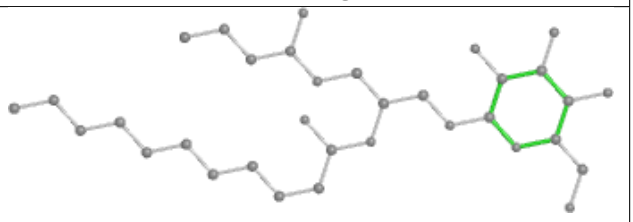
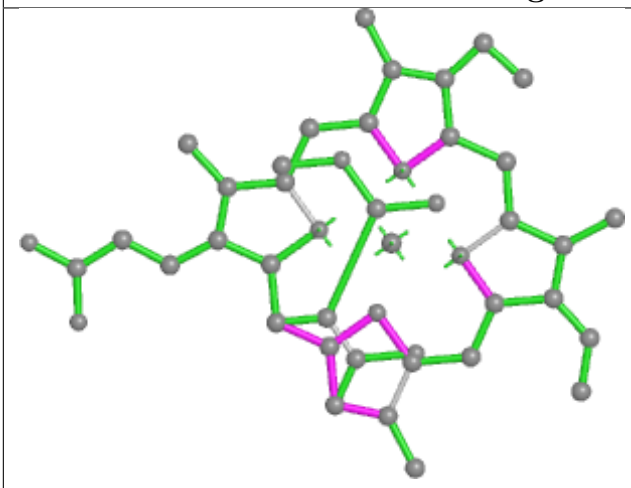


Rings

Ligand KC2 E 610



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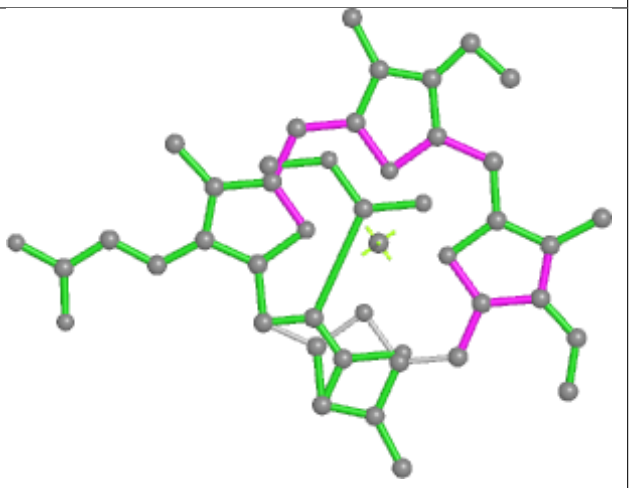
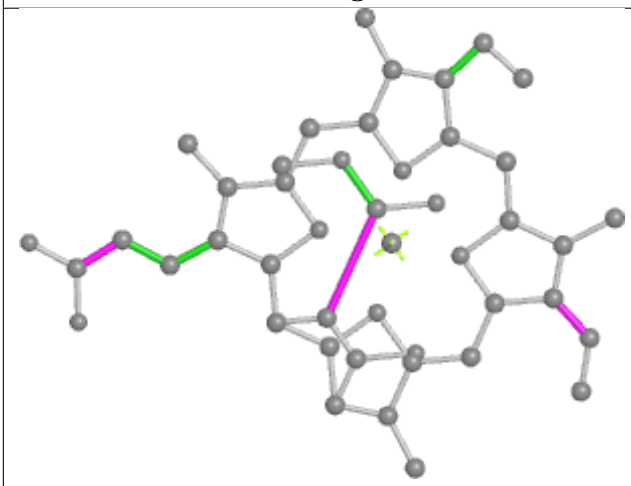


Bond angles



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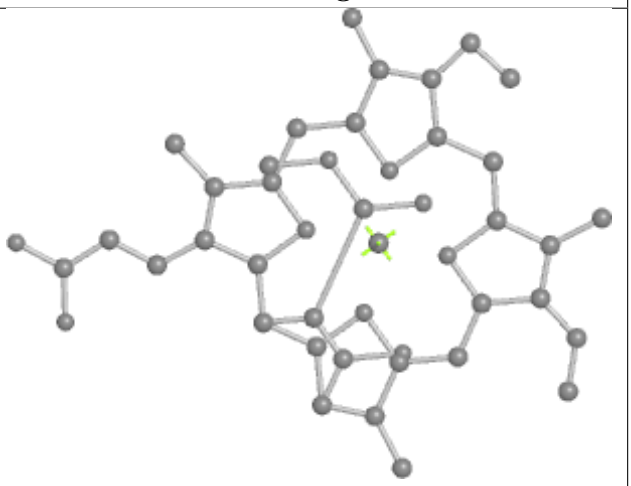
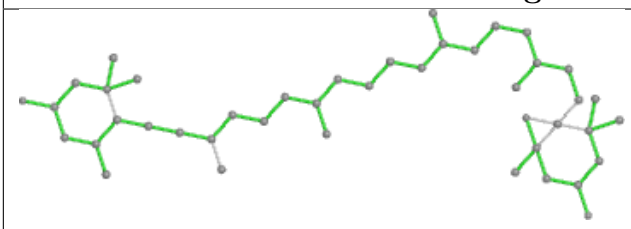


Rings

Ligand DD6 K 609



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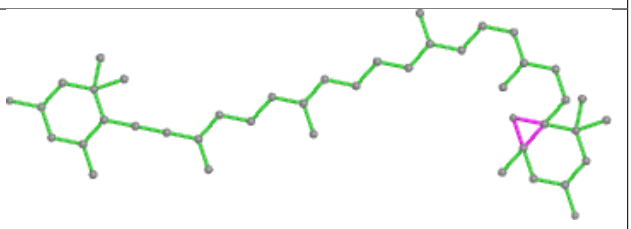
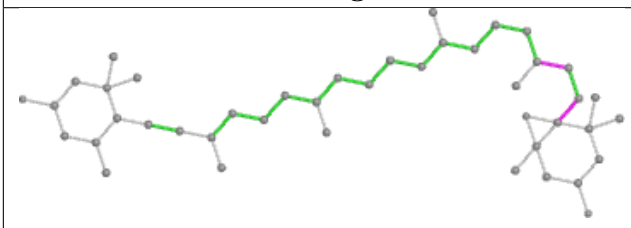


Bond angles



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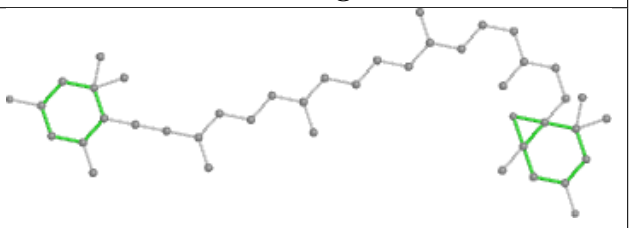
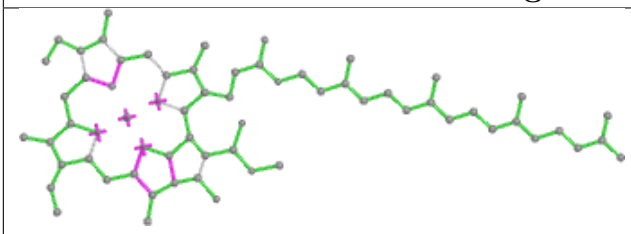


Rings

Ligand CLA C 203



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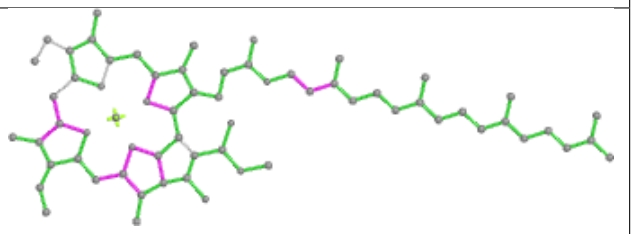
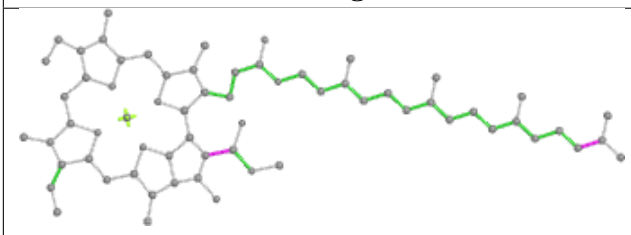


Bond angles



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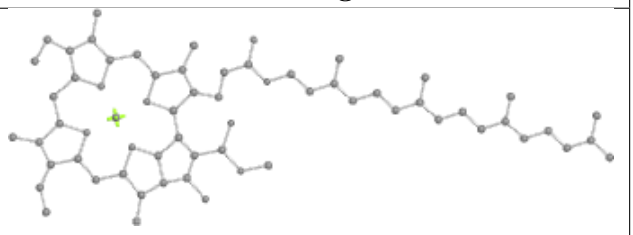
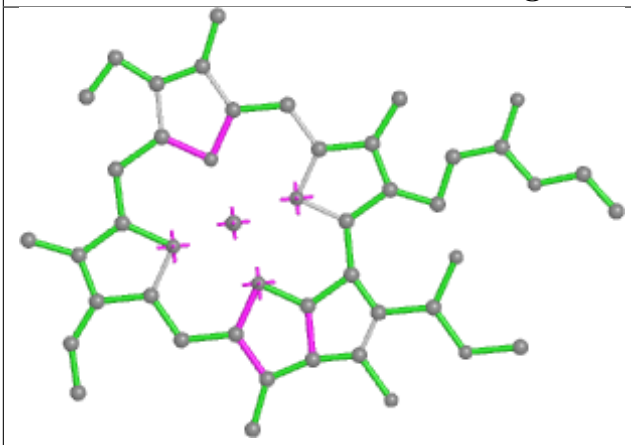
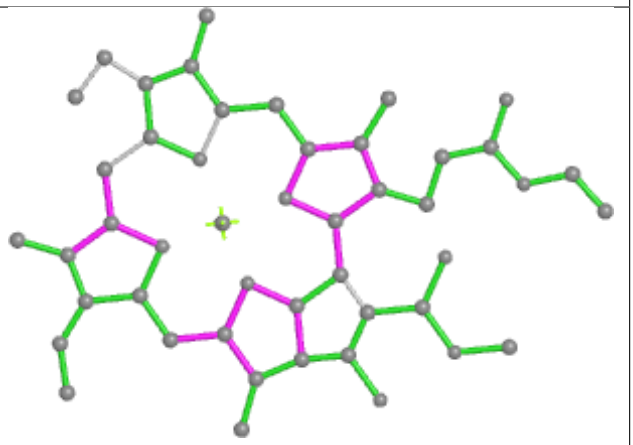


Rings

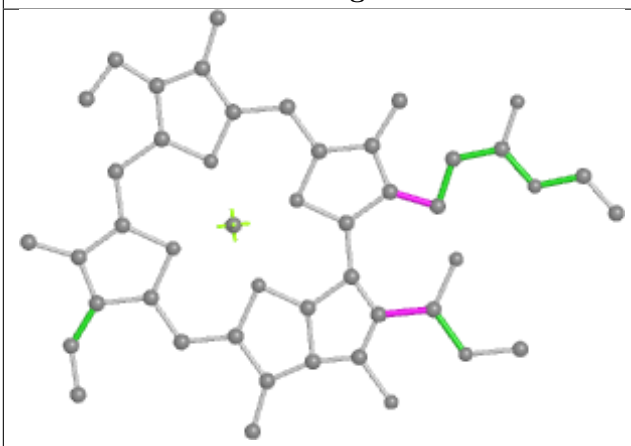
Ligand CLA A 612



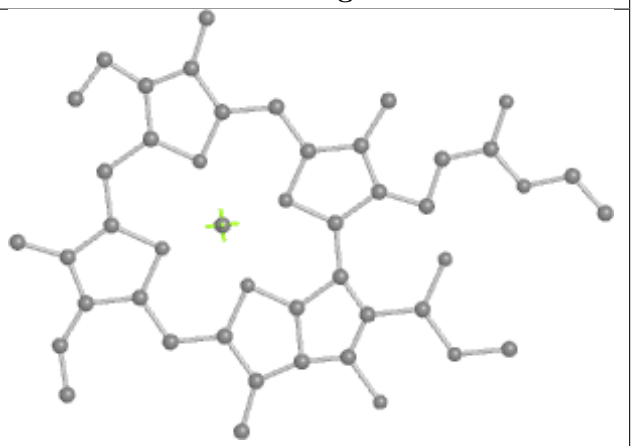
Bond lengths



Bond angles

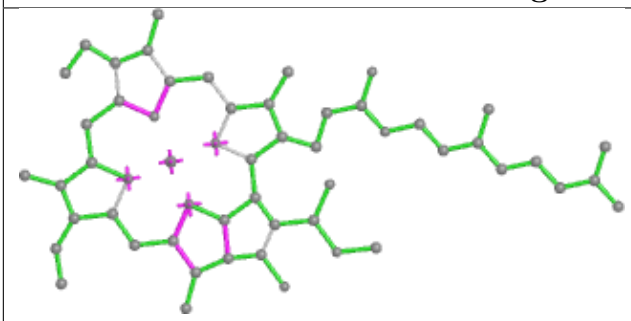


Torsions

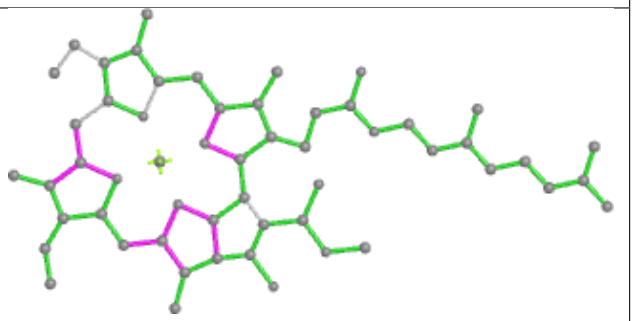


Rings

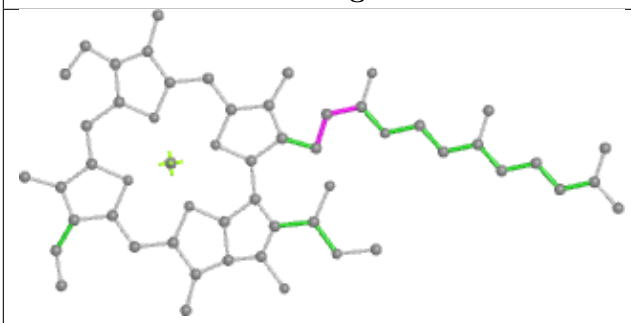
Ligand CLA I 606



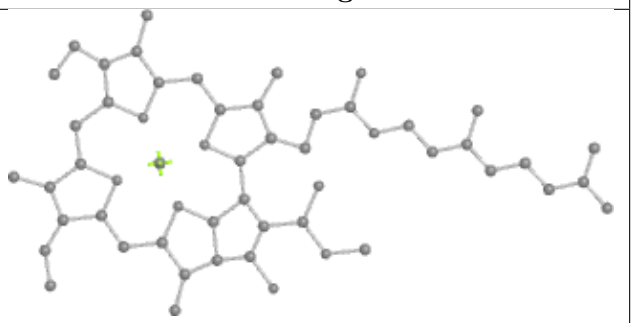
Bond lengths



Bond angles

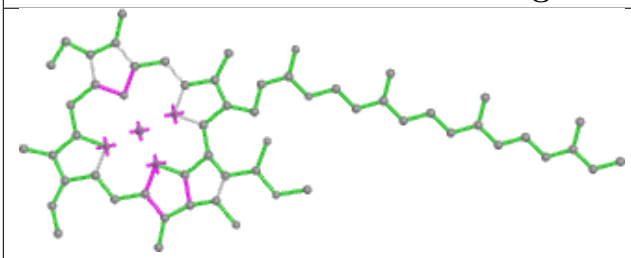


Torsions



Rings

Ligand CLA l 405



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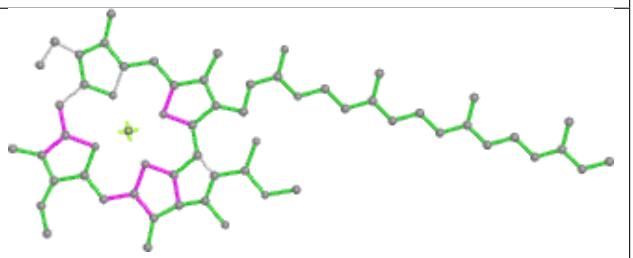
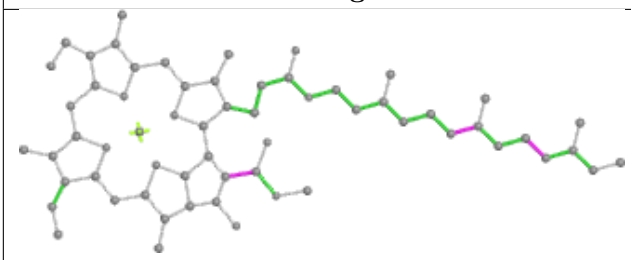


Bond angles



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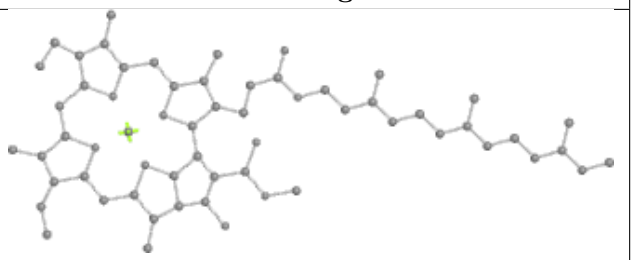
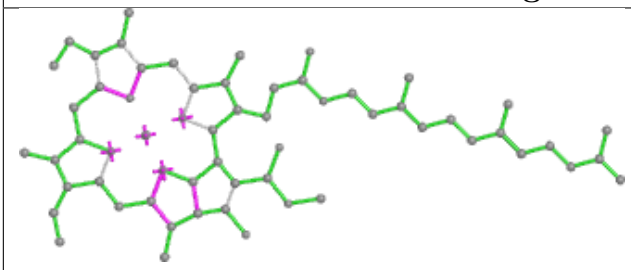


Rings

Ligand CLA G 605



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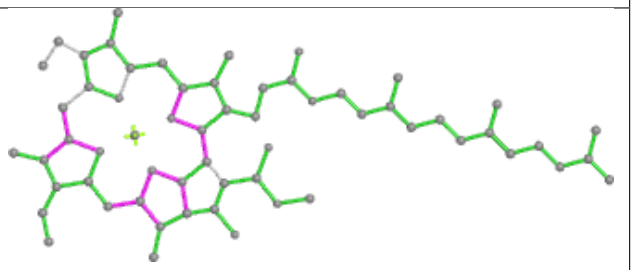

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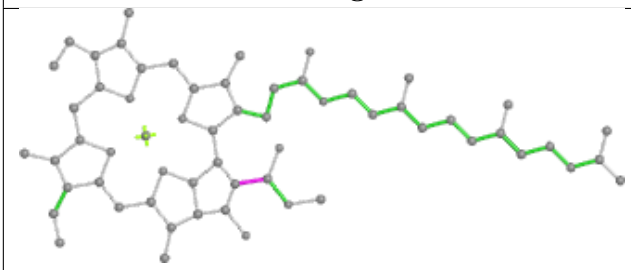
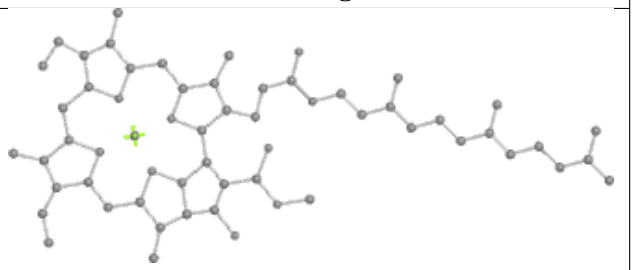
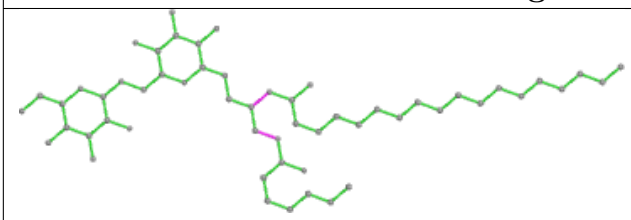


Torsions



Rings

Ligand DGD l 416



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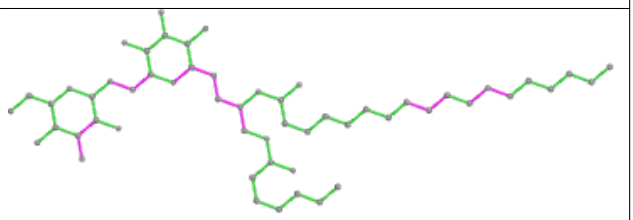
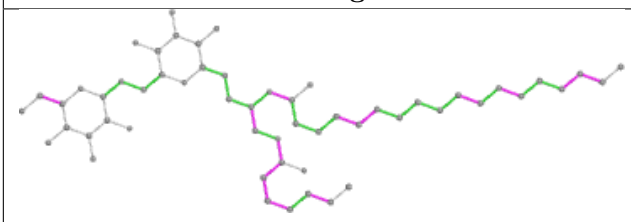


Bond angles



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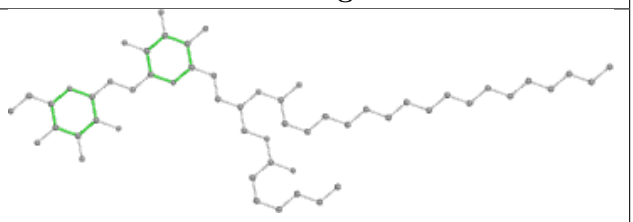
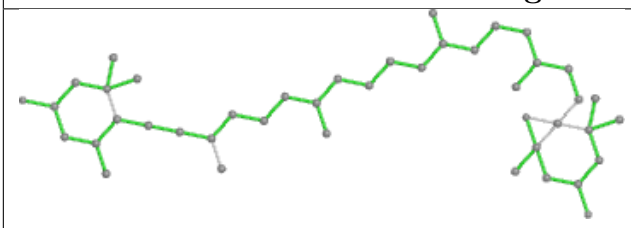


Rings

Ligand DD6 U 607



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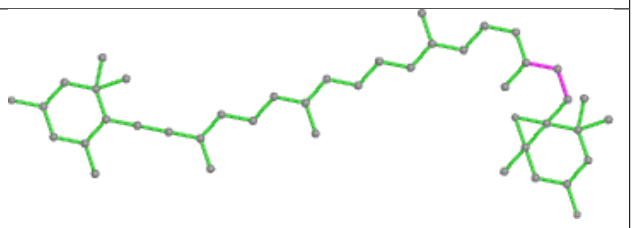
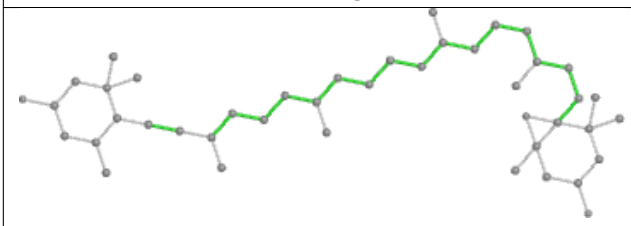


Bond angles



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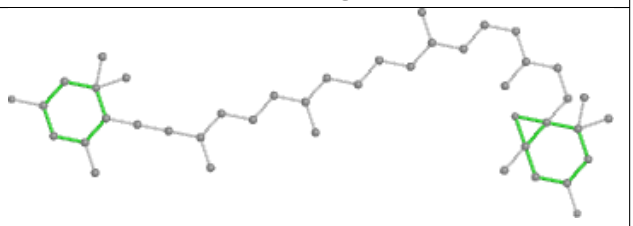
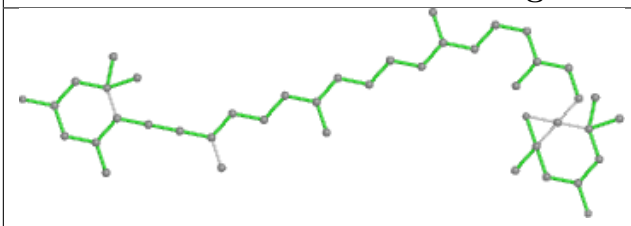


Rings

Ligand DD6 E 615



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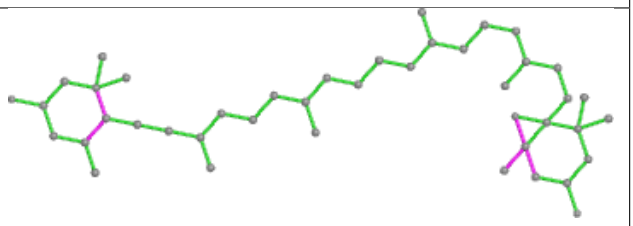
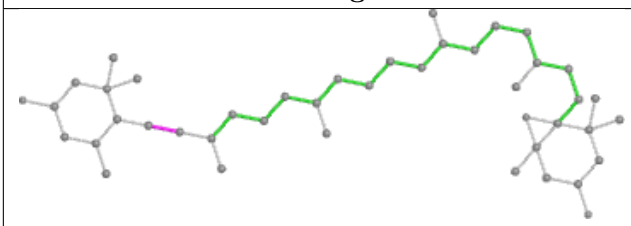


Bond angles



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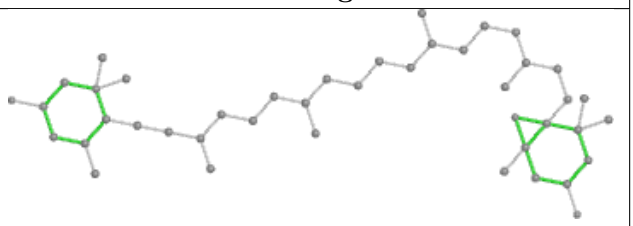
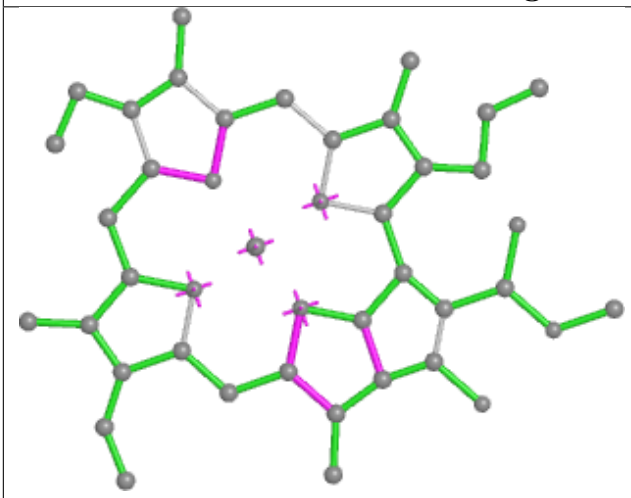


Rings

Ligand CLA U 601



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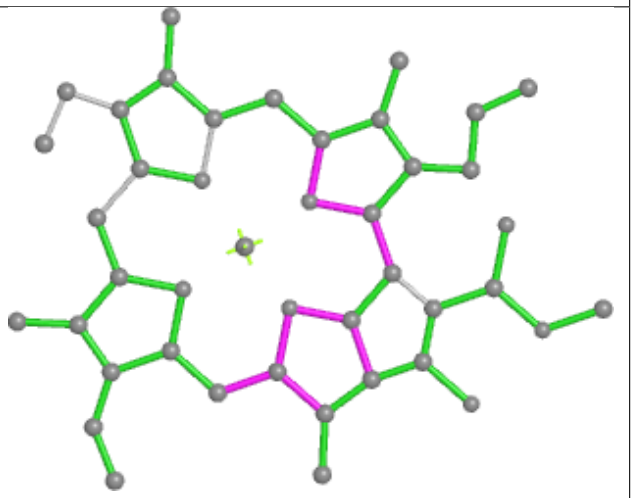

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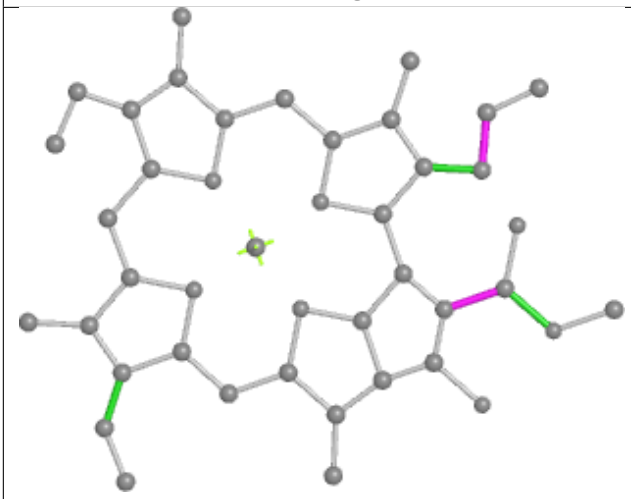

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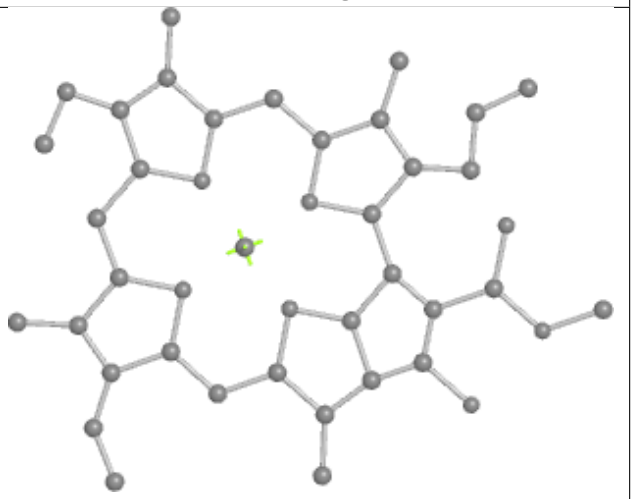

Rings

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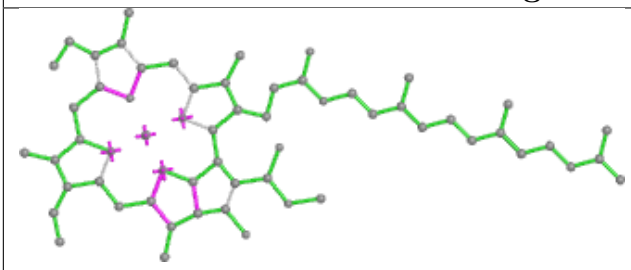

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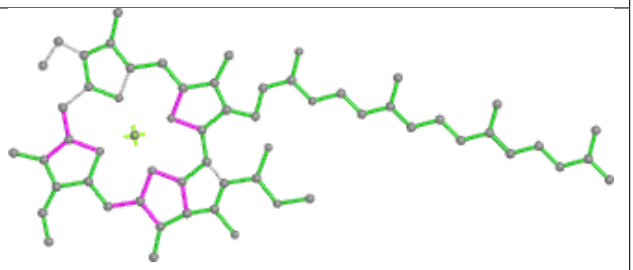
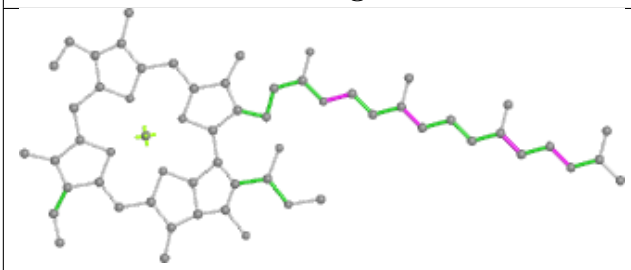


Bond angles



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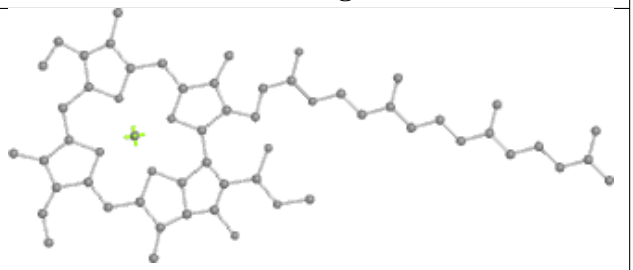
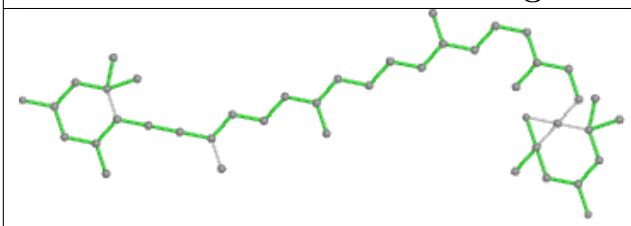


Rings

Ligand DD6 H 316



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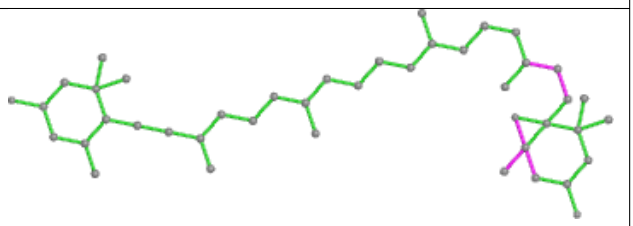
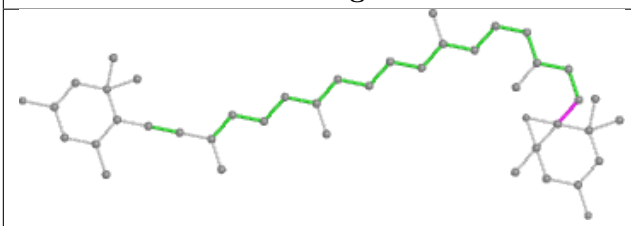


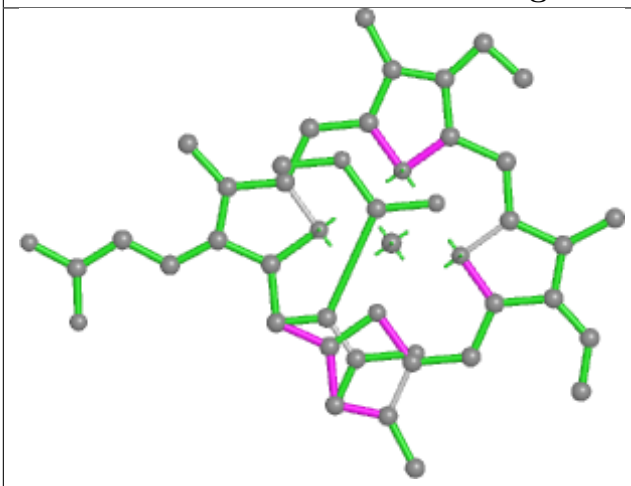
Bond angles



Torsions

Rings

Ligand KC2 J 606



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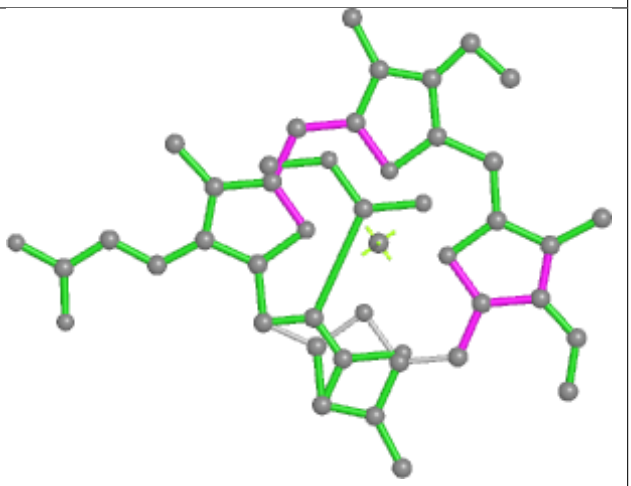
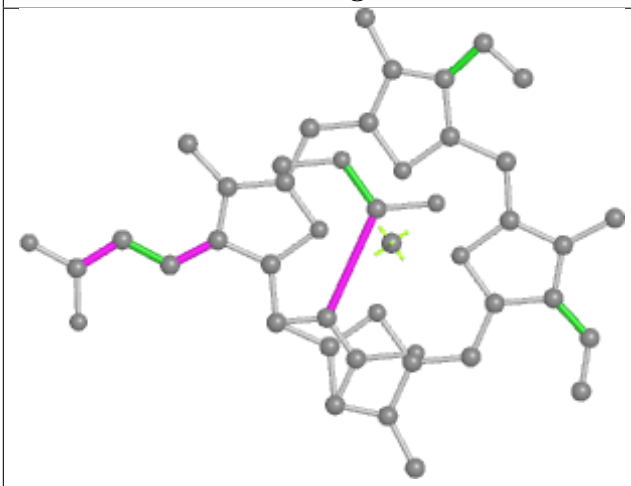


Bond angles



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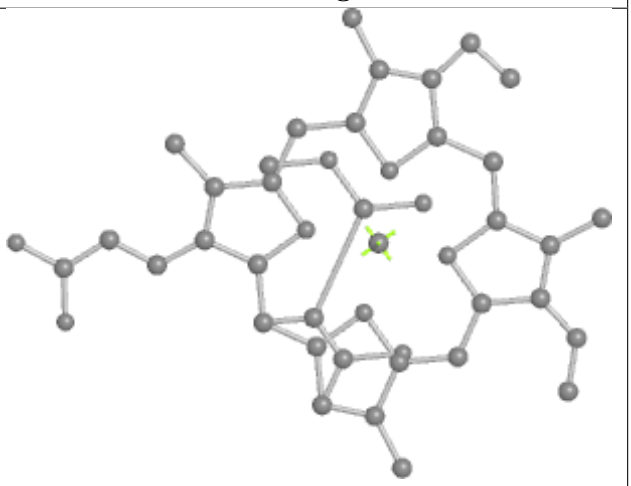
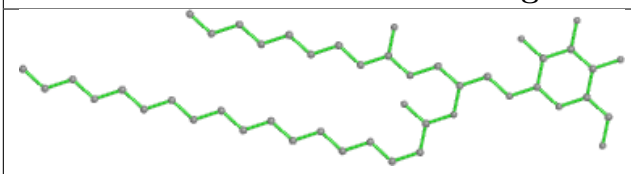


Rings

Ligand LMG F 616



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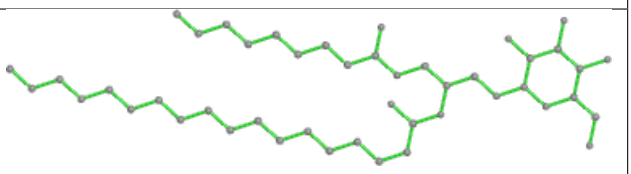
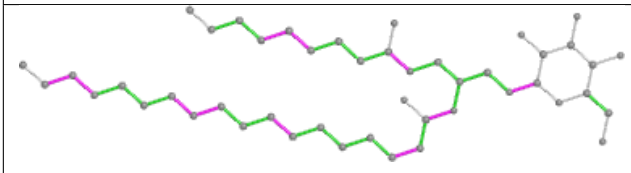


Bond angles



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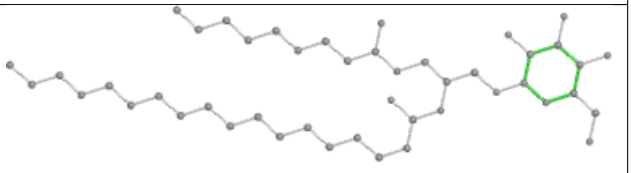
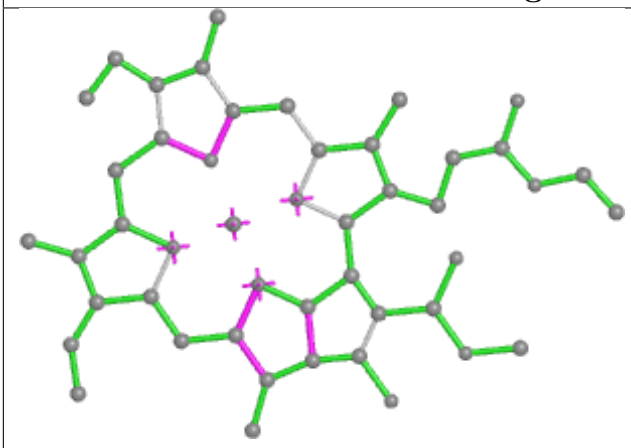


Rings

Ligand CLA T 601



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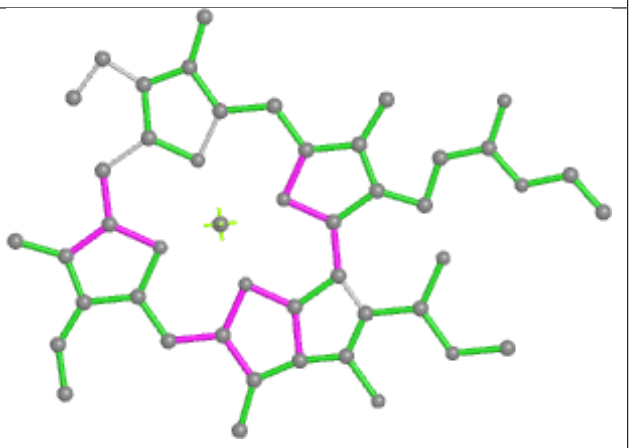
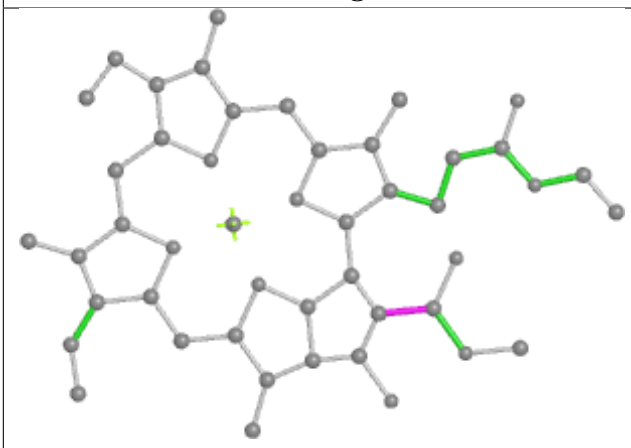


Bond angles



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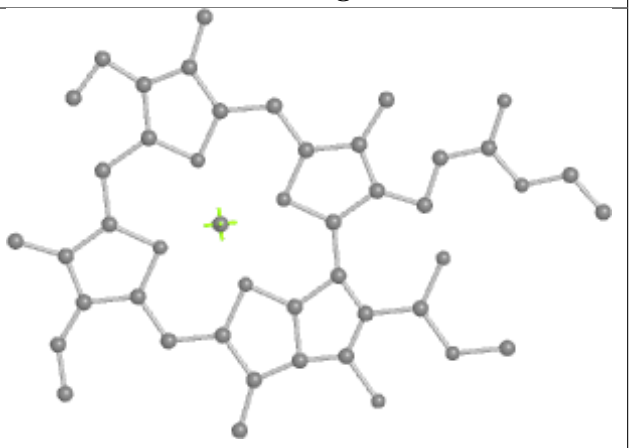
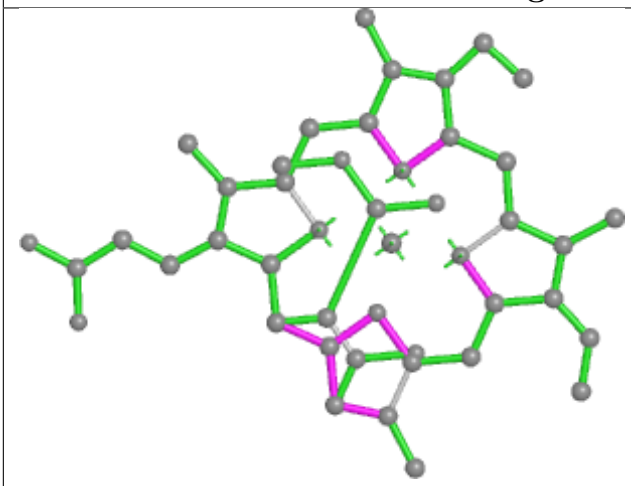
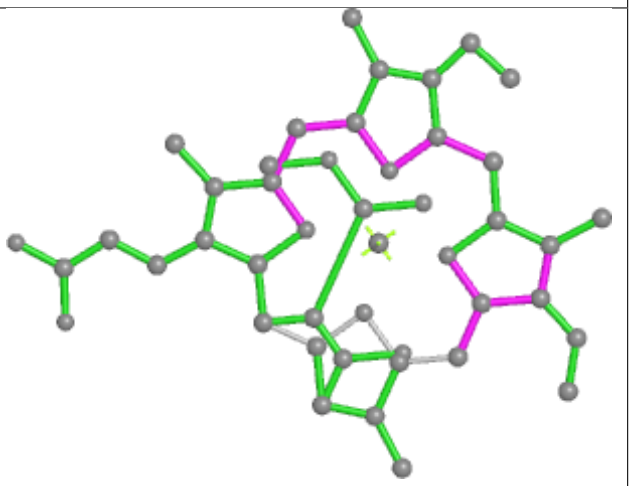


Rings

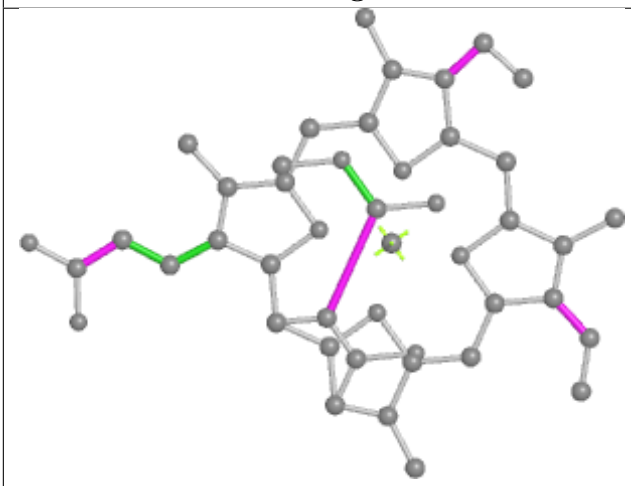
Ligand KC2 F 609



Bond lengths



Bond angles



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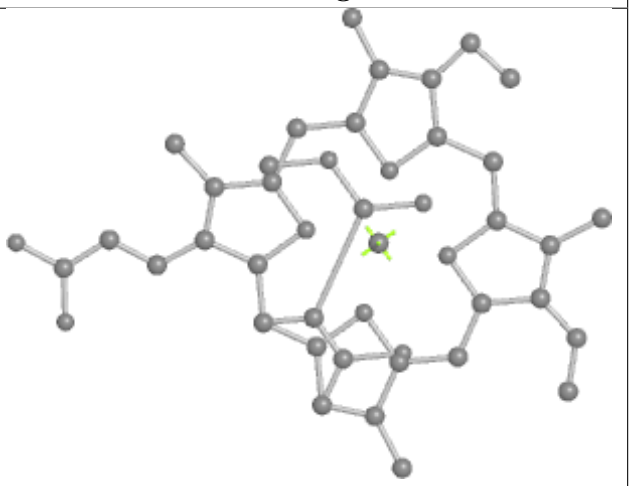
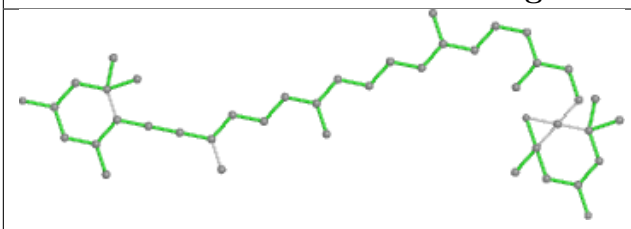
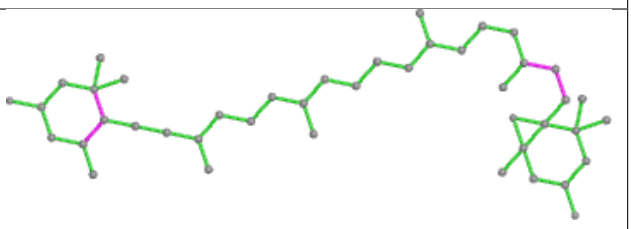


Rings

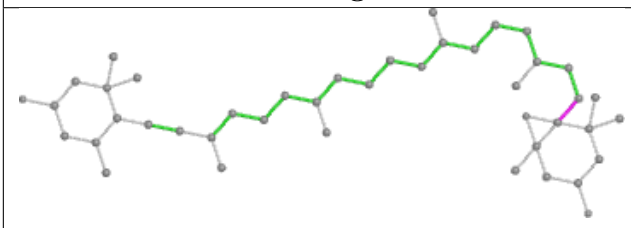
Ligand DD6 C 216



Bond lengths



Bond angles



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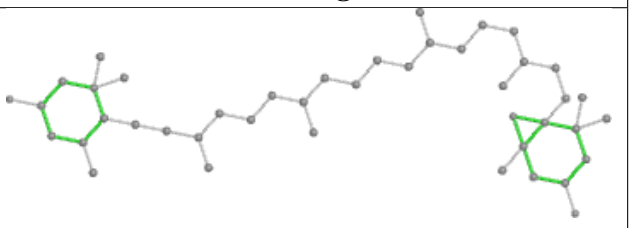
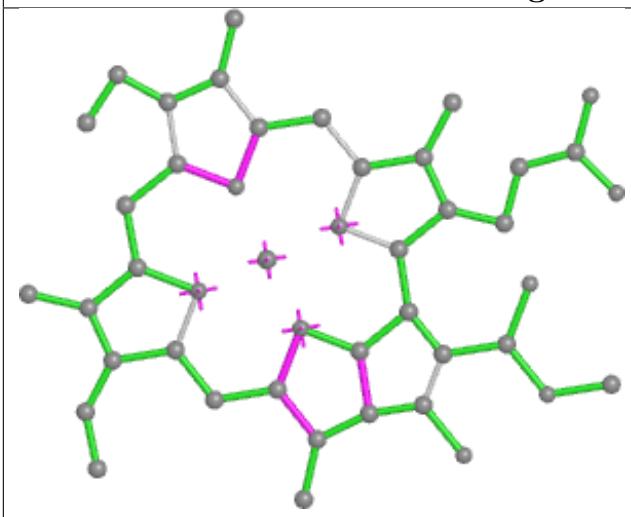
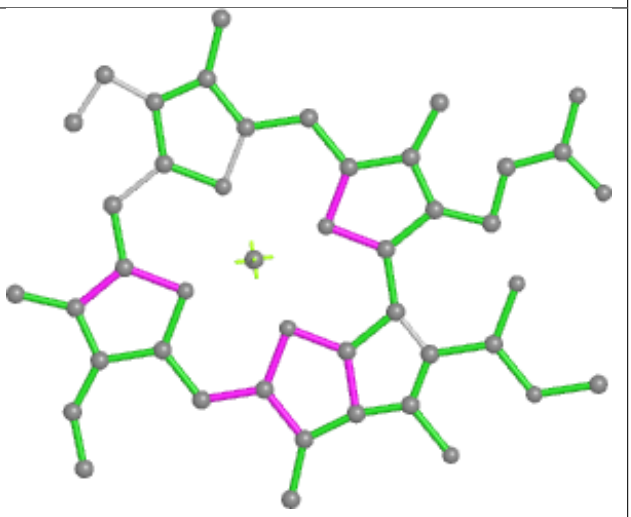


Rings

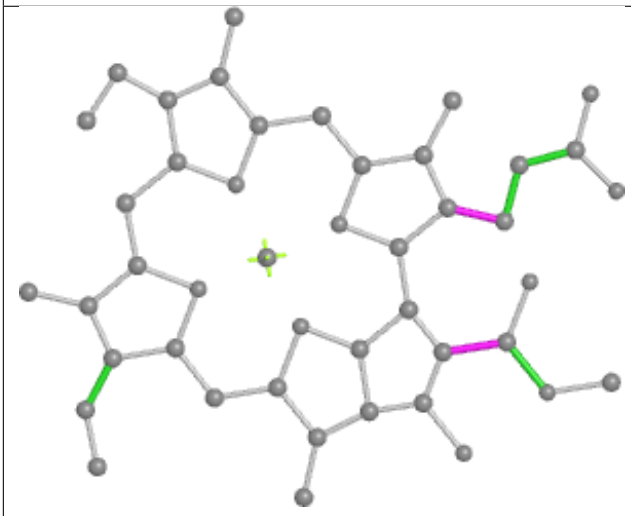
Ligand CLA J 601



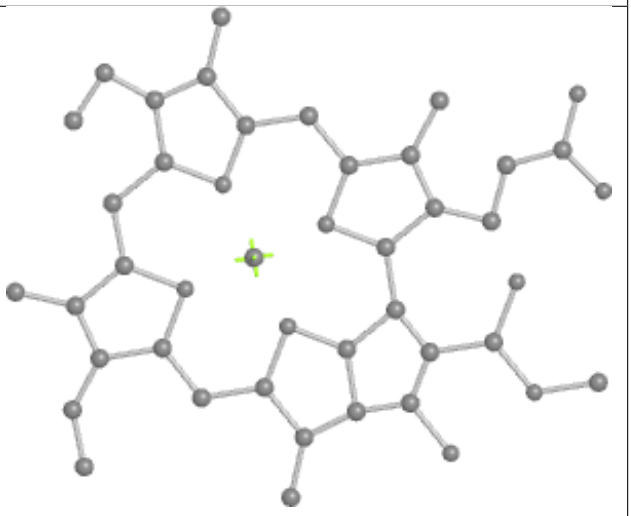
Bond lengths



Bond angles

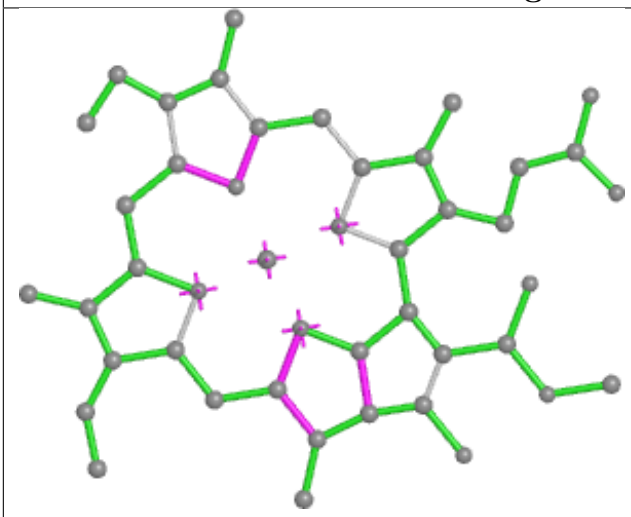


Torsions

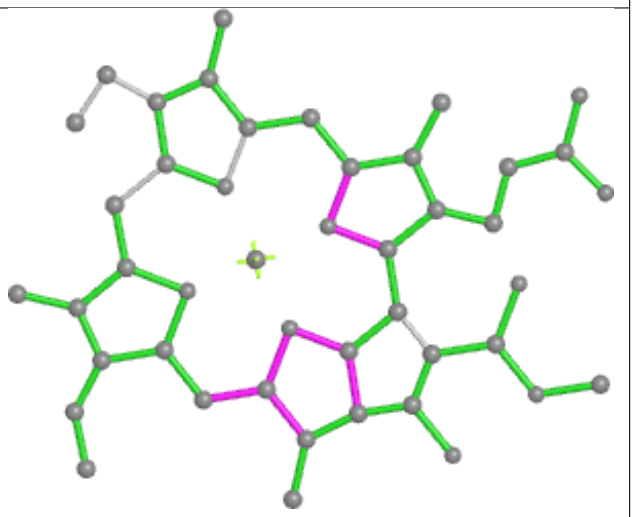


Rings

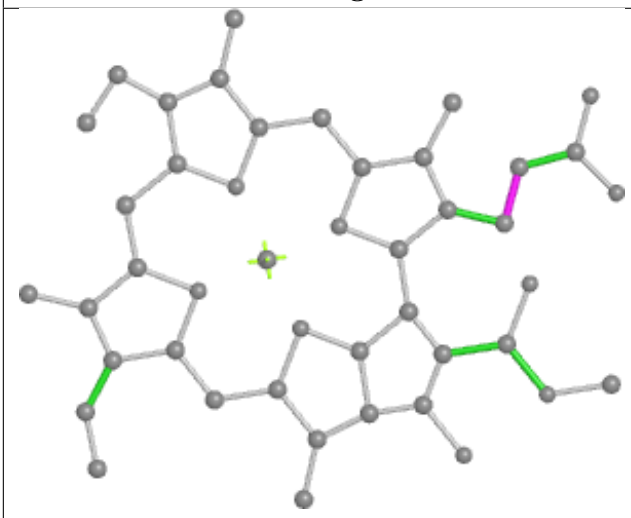
Ligand CLA T 606



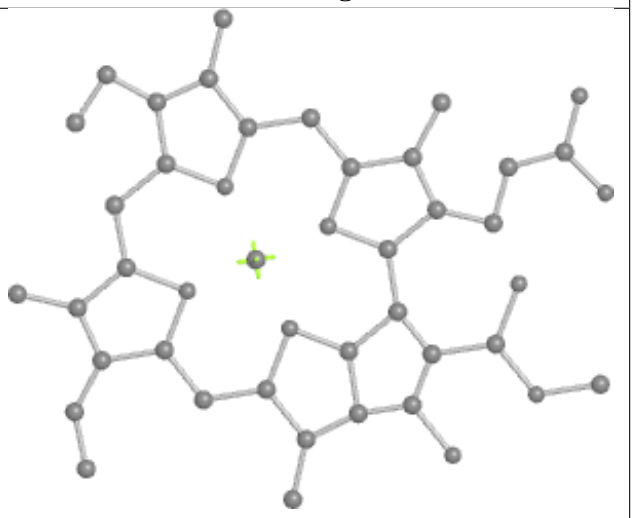
Bond lengths



Bond angles

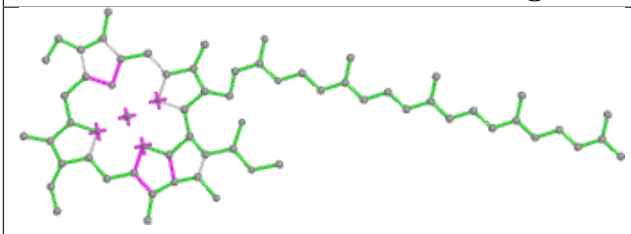


Torsions



Rings

Ligand CLA F 606



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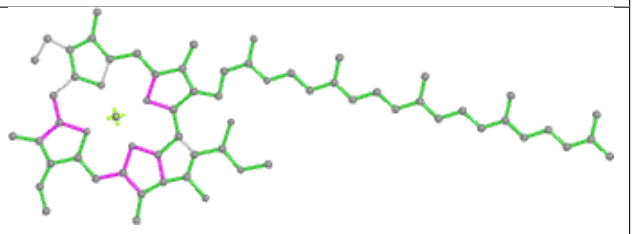
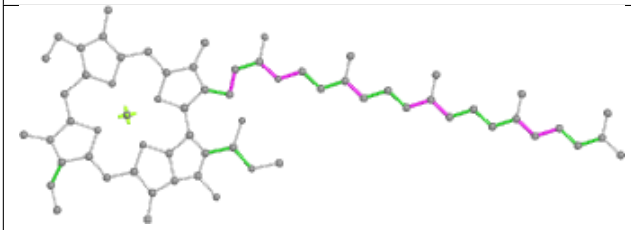


Bond angles



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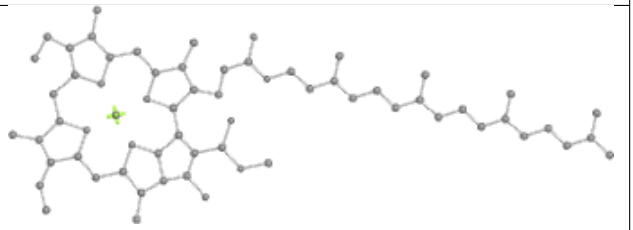
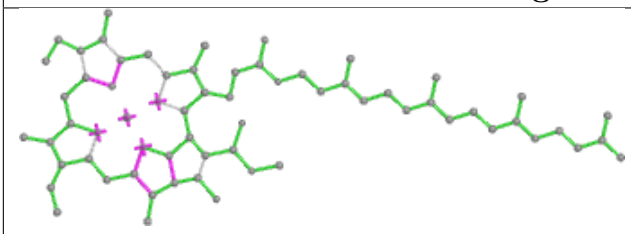


Rings

Ligand CLA l 406



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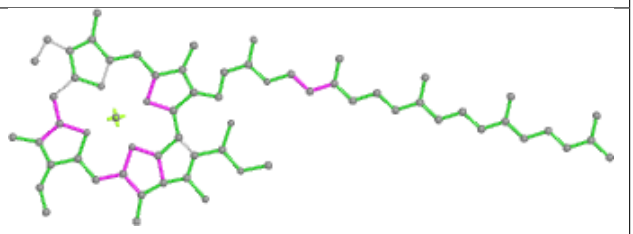
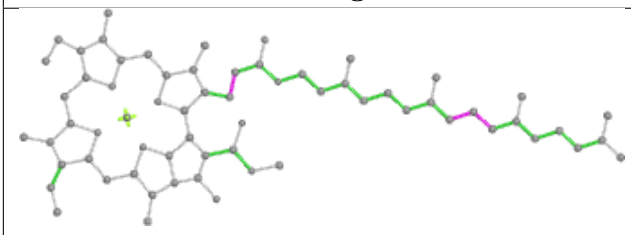


Bond angles



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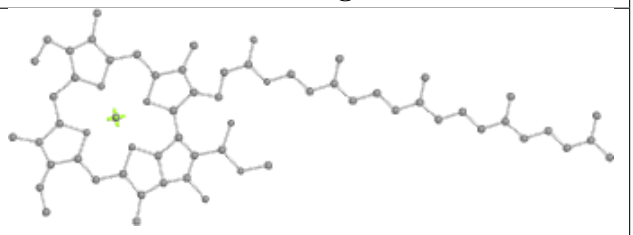
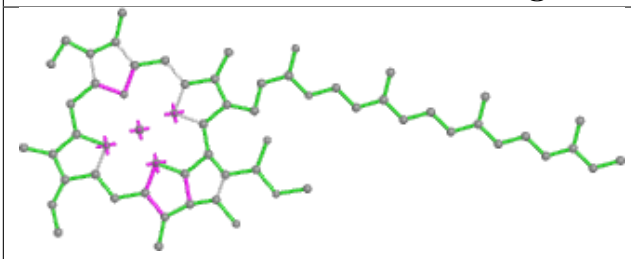


Rings

Ligand CLA a 839



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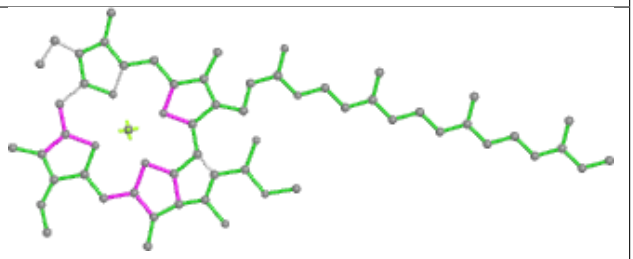
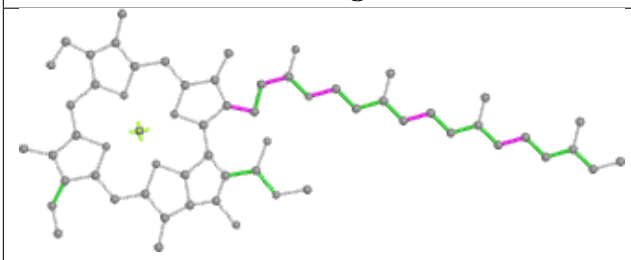


Bond angles



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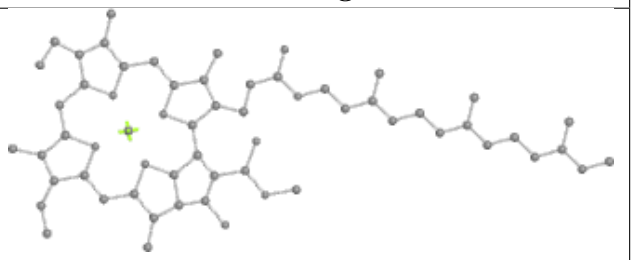
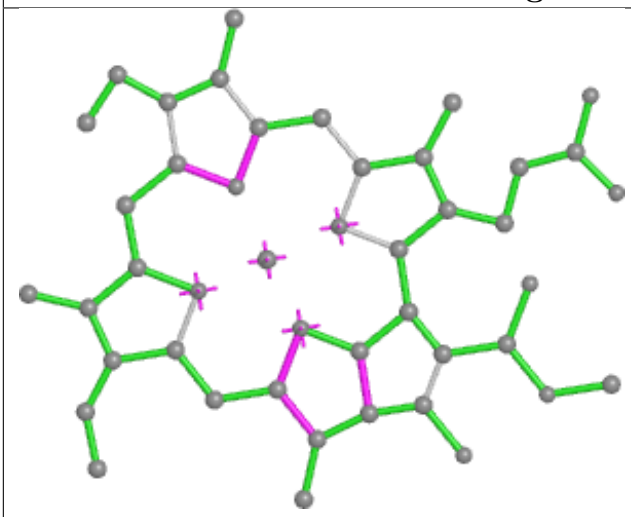


Rings

Ligand CLA F 607



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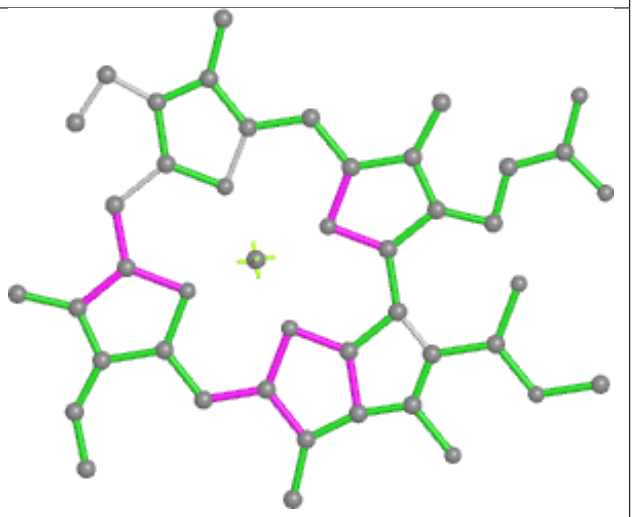

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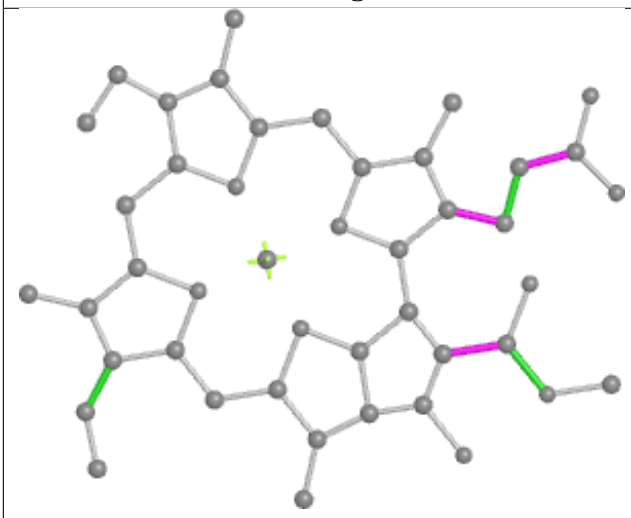

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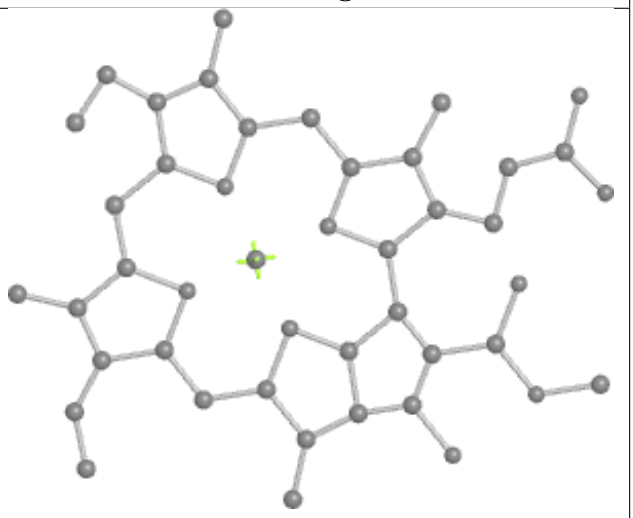
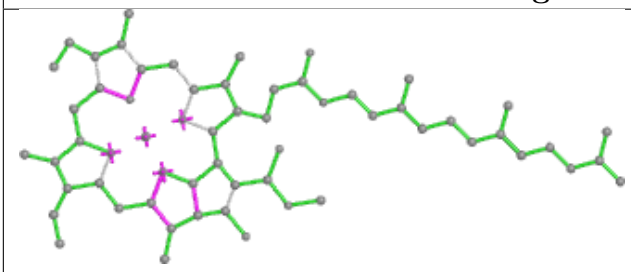


Rings

Ligand CLA l 402



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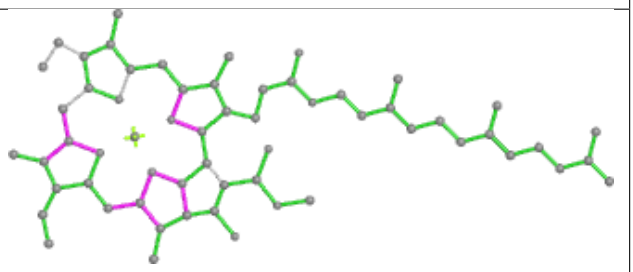
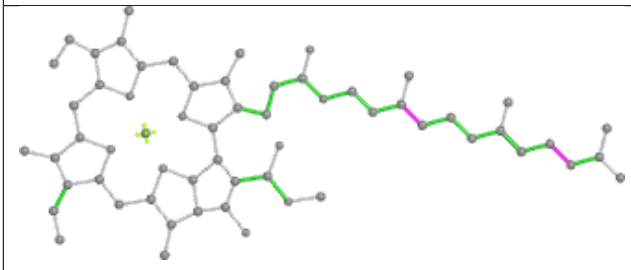


Bond angles



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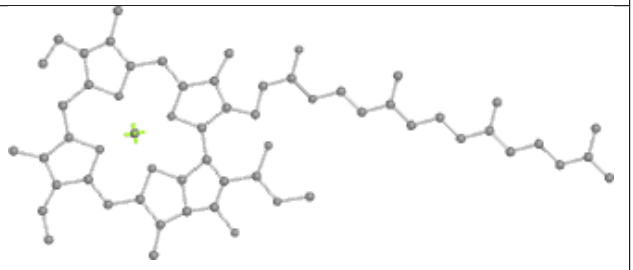
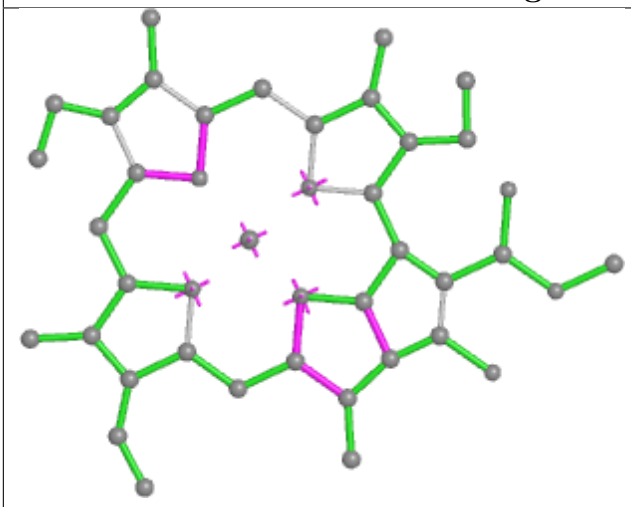


Rings

Ligand CLA C 201



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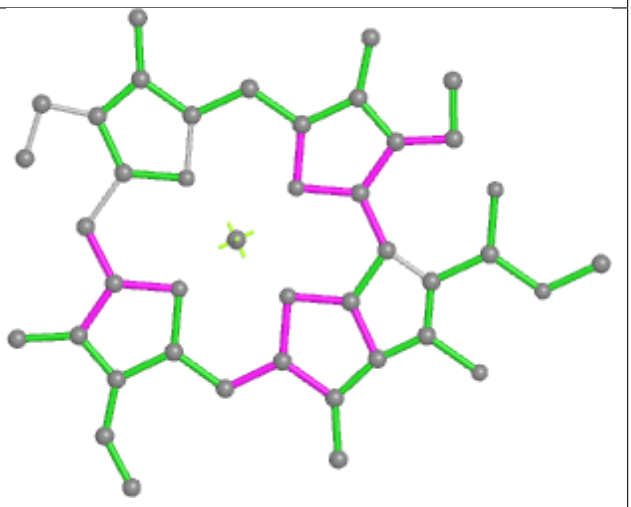
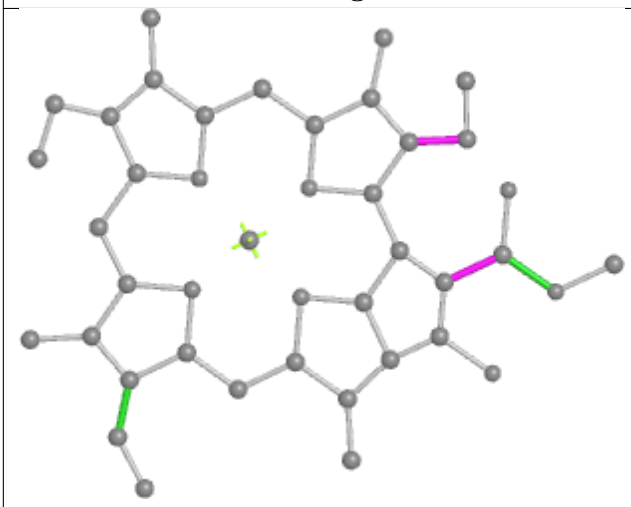


Bond angles



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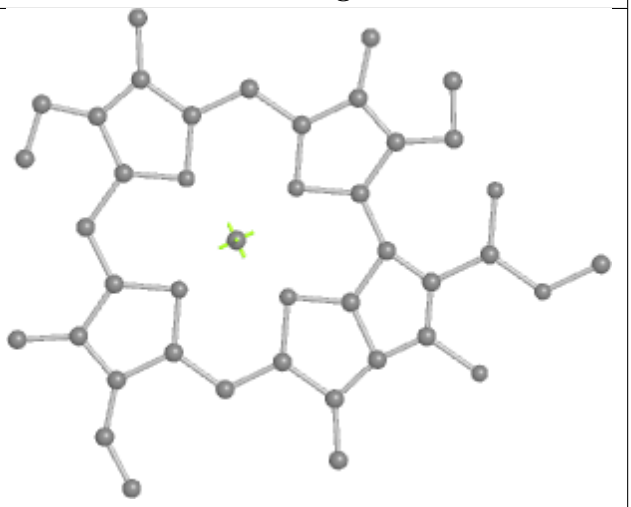
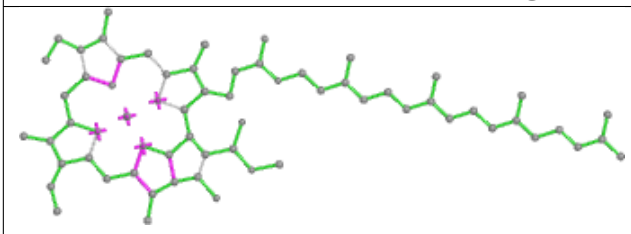


Rings

Ligand CLA H 319



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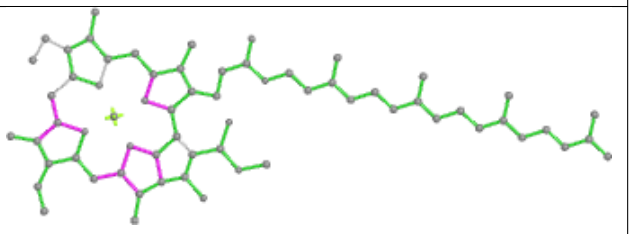
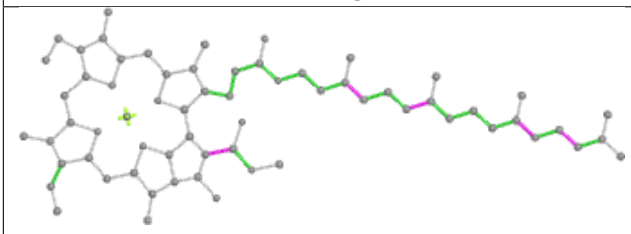


Bond angles



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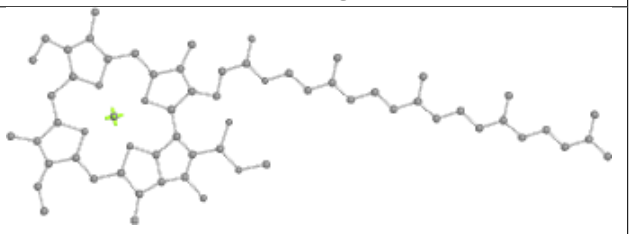
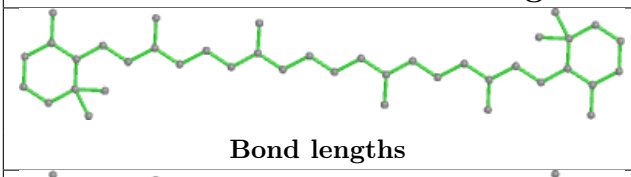
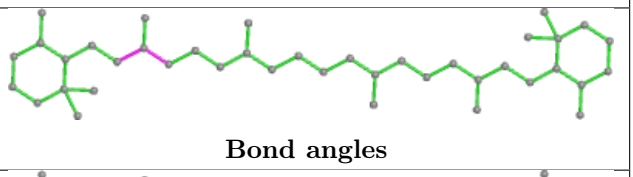


Rings

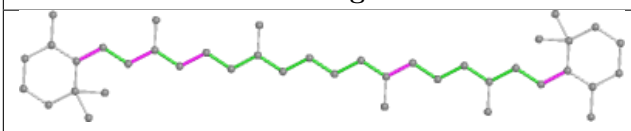
Ligand BCR b 731



Bond lengths



Bond angles



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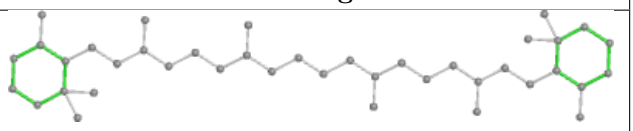
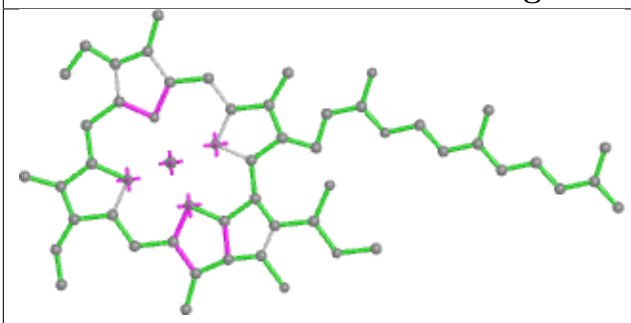


Rings

Ligand CLA A 603



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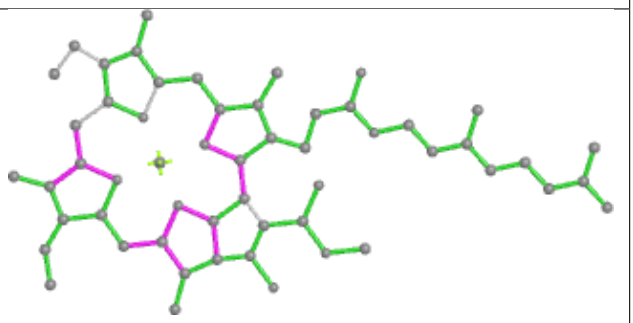
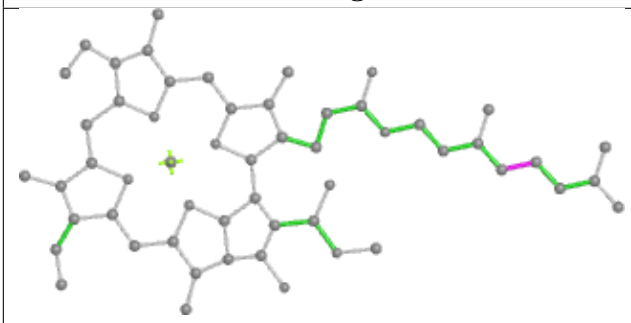


Bond angles



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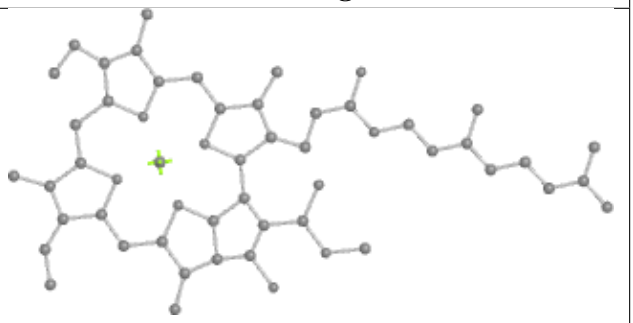
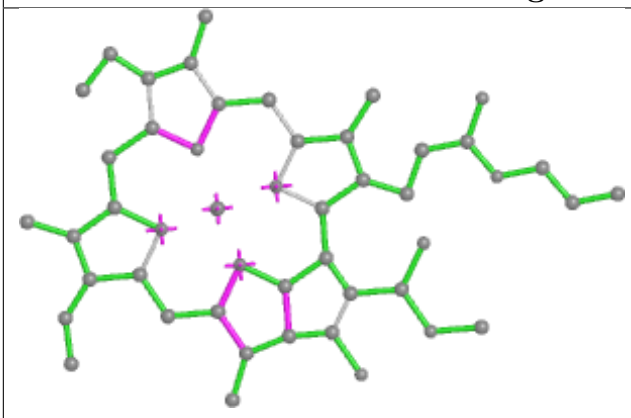


Rings

Ligand CLA b 720



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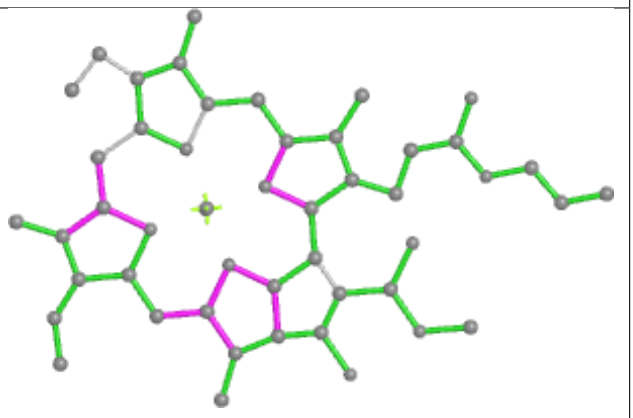
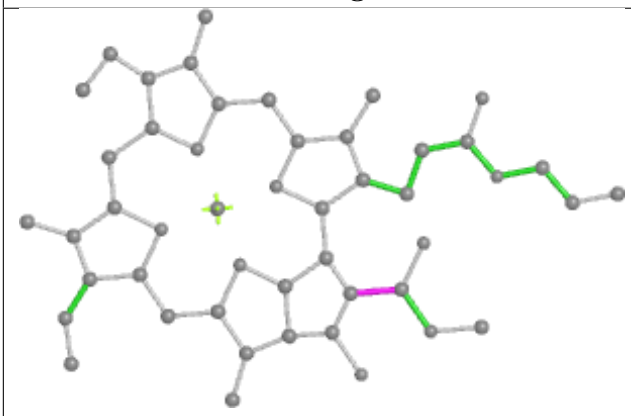


Bond angles



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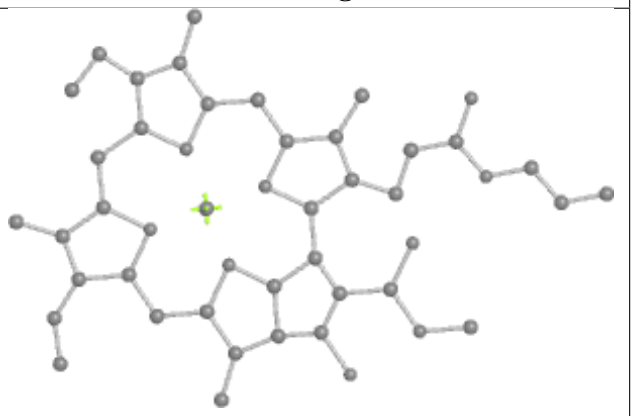
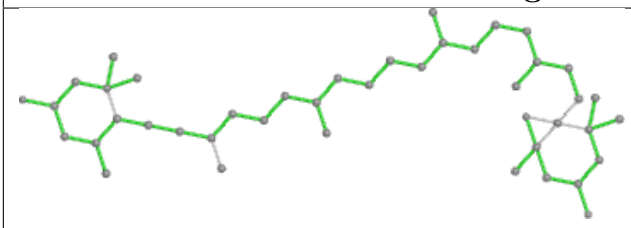


Rings

Ligand DD6 K 612



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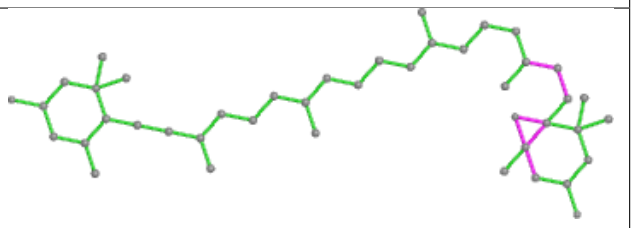
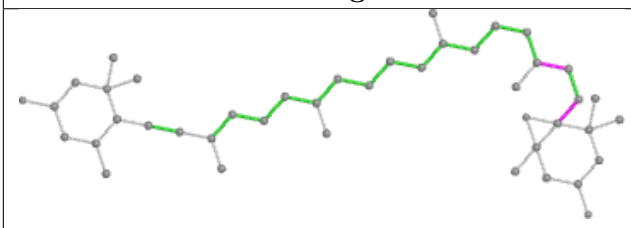


Bond angles



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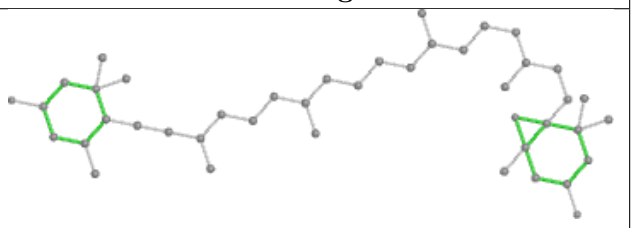
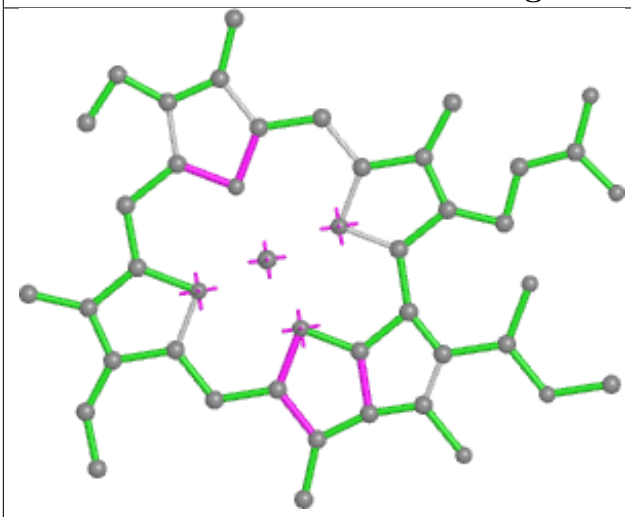
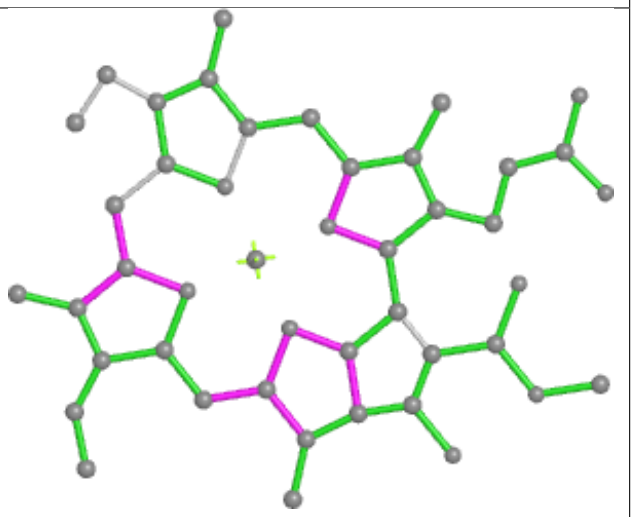


Rings

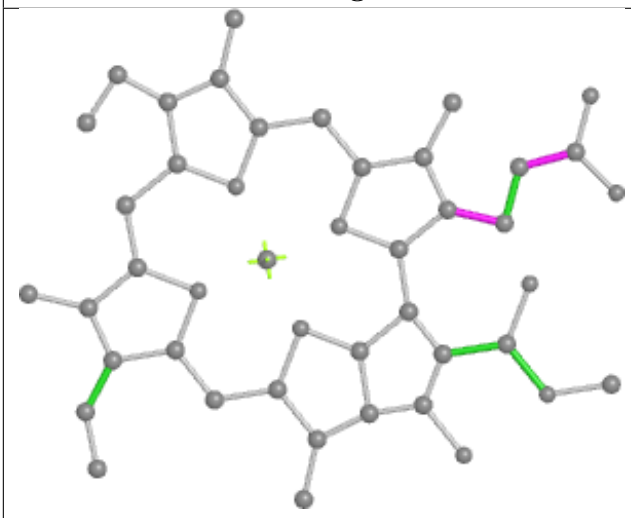
Ligand CLA T 607



Bond lengths



Bond angles



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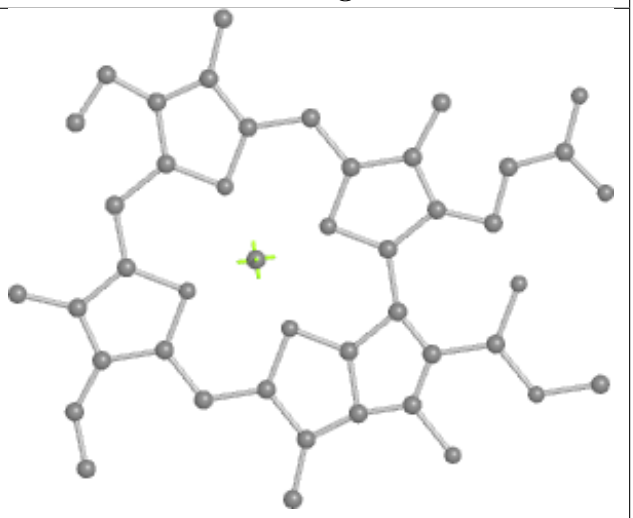
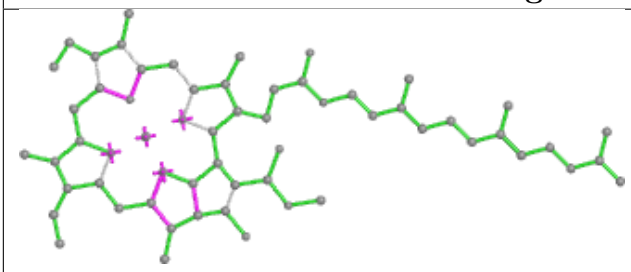
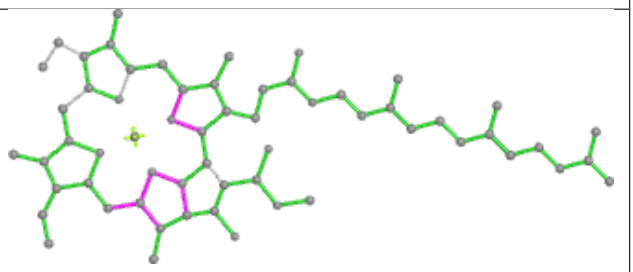


Rings

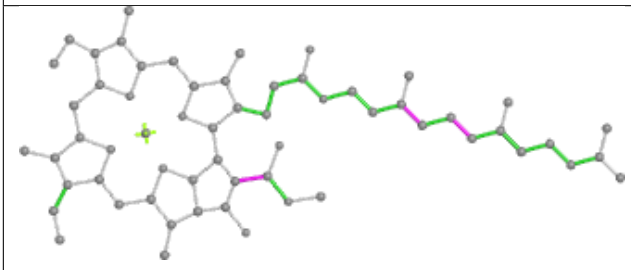
Ligand CLA E 608



Bond lengths



Bond angles



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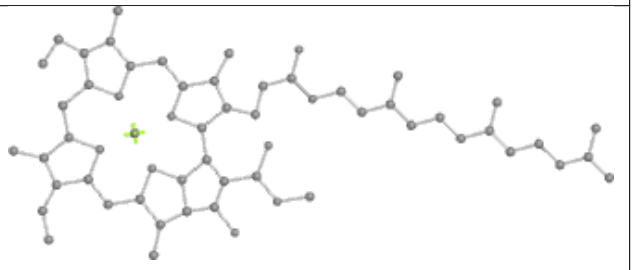
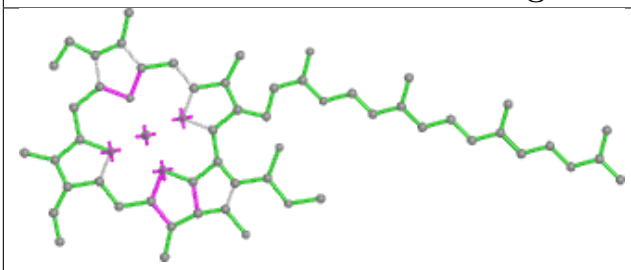
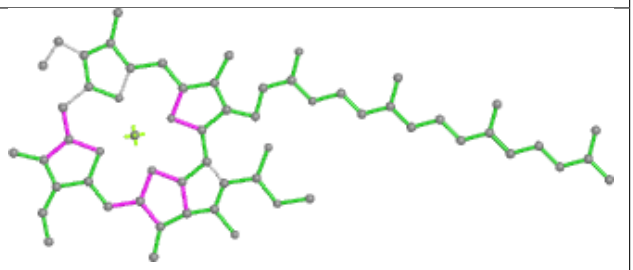


Rings

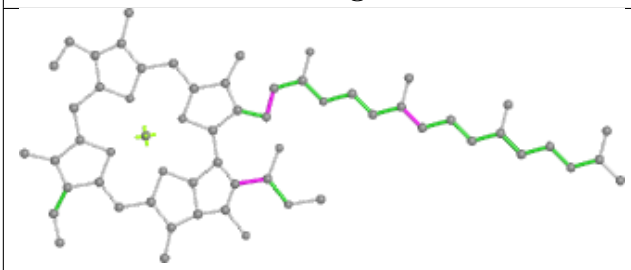
Ligand CLA b 726



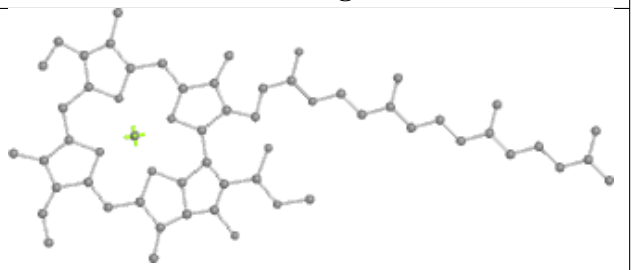
Bond lengths



Bond angles

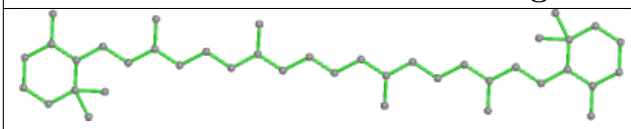


Torsions



Rings

Ligand BCR i 201



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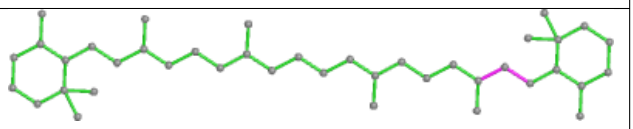
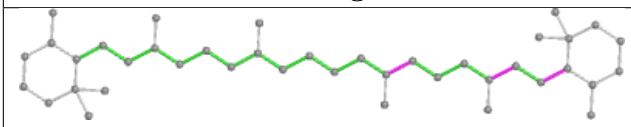


Bond angles



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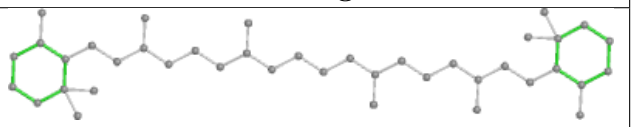
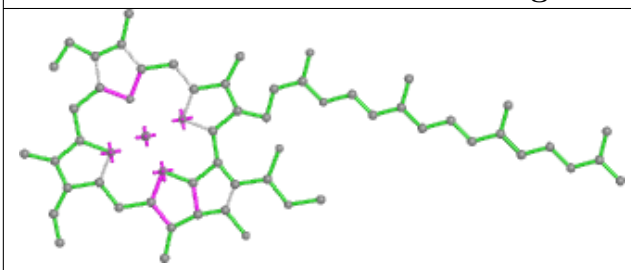


Rings

Ligand CLA I 608



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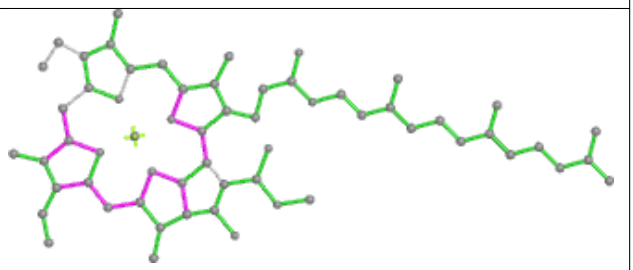
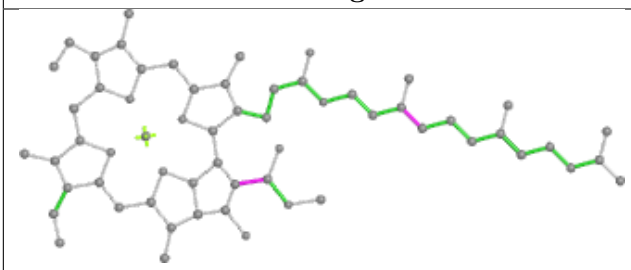


Bond angles



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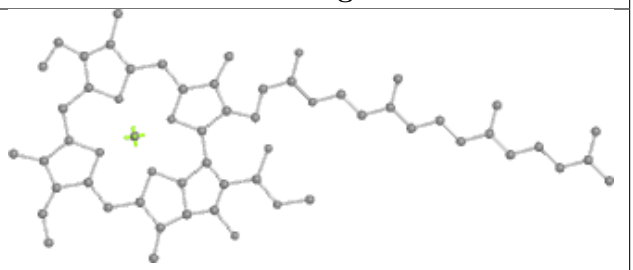
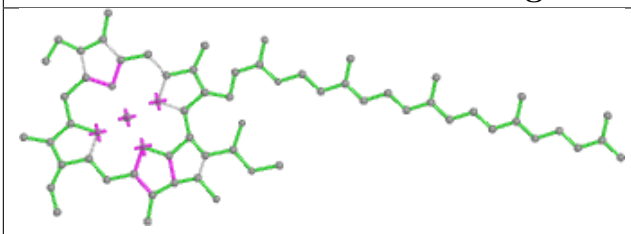
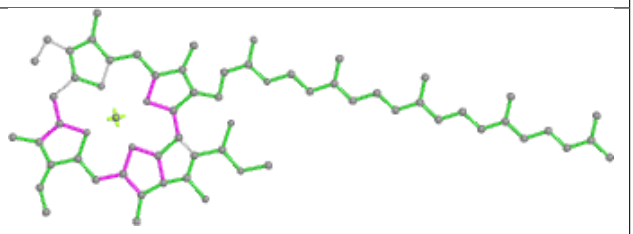
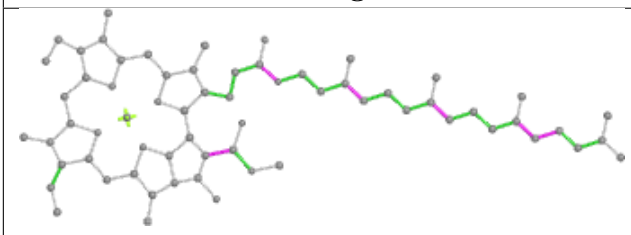
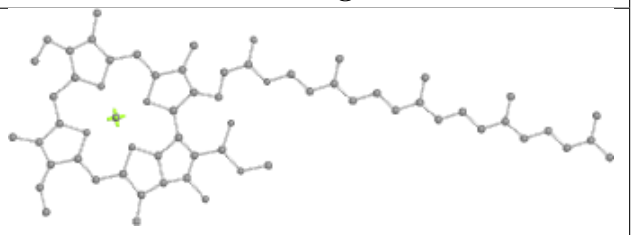
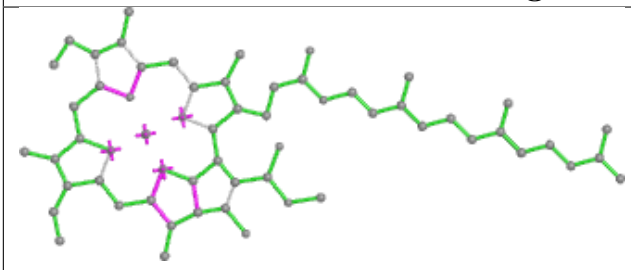
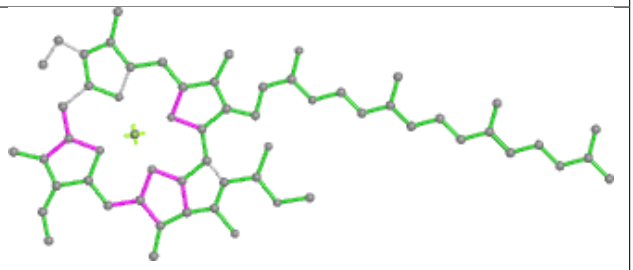
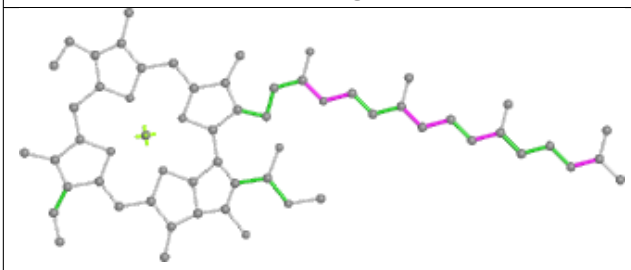
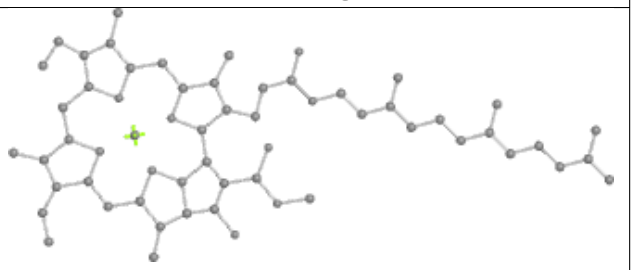
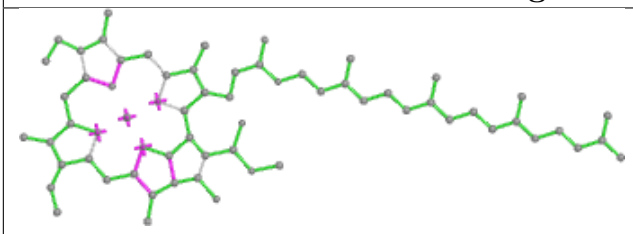


Rings

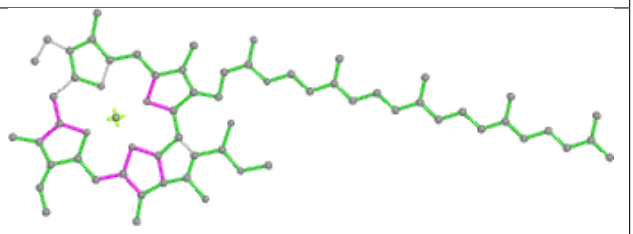
Ligand CLA E 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

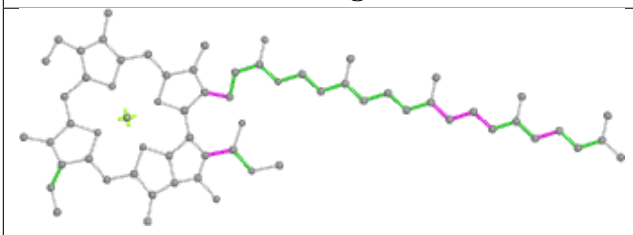
Ligand CLA a 821



Bond lengths



Bond angles



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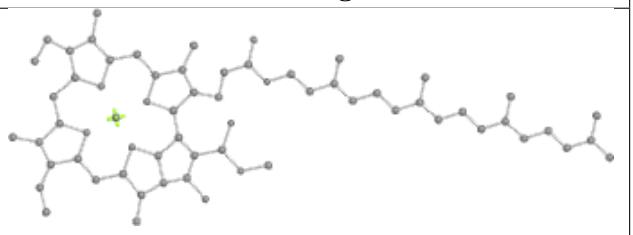
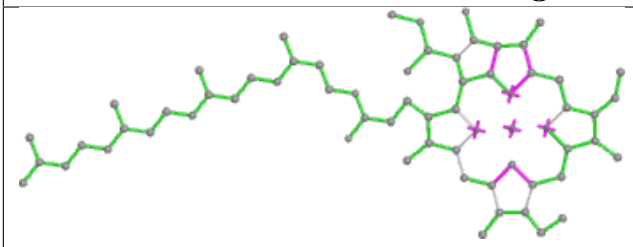


Rings

Ligand CLA I 603



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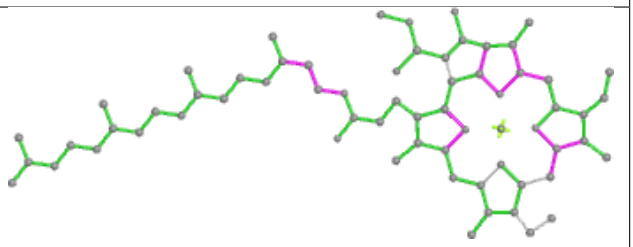
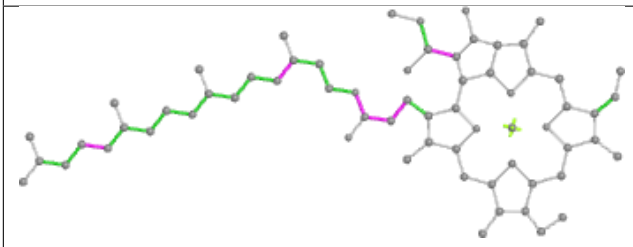


Bond angles



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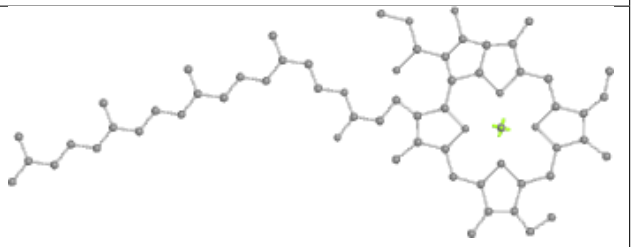
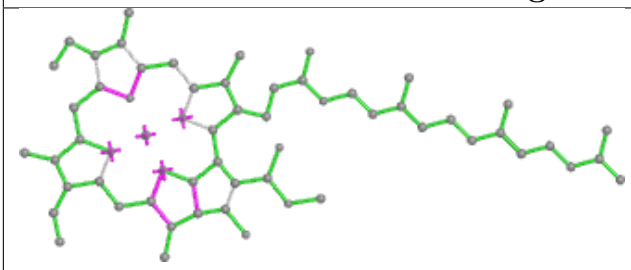


Rings

Ligand CLA a 822



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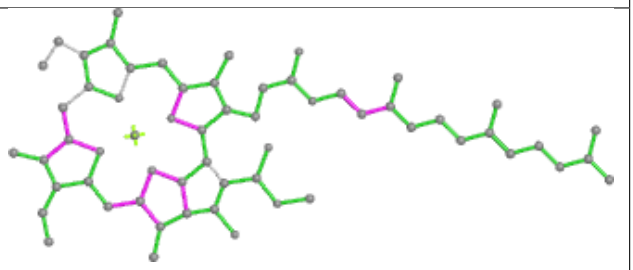
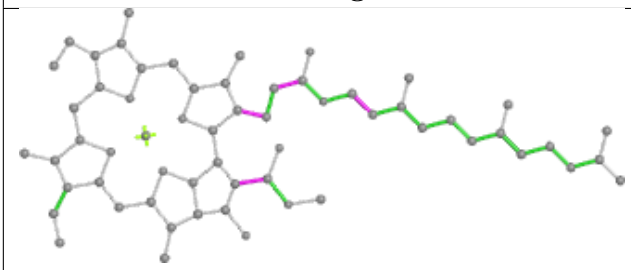


Bond angles



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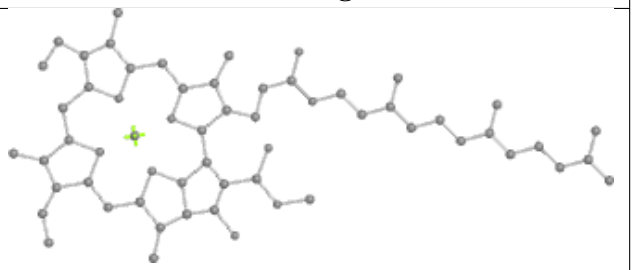
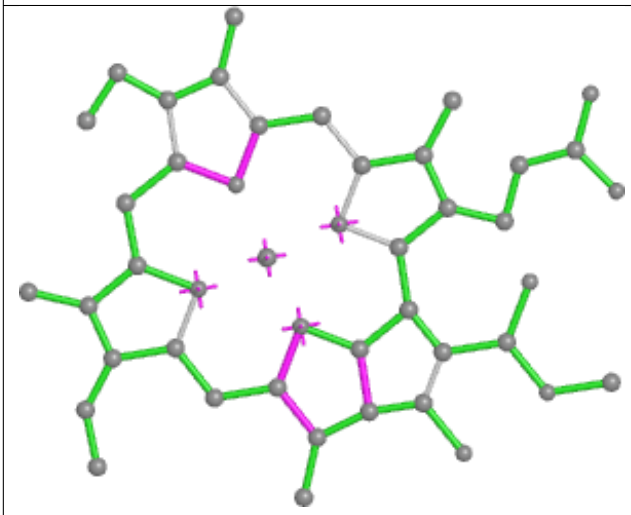
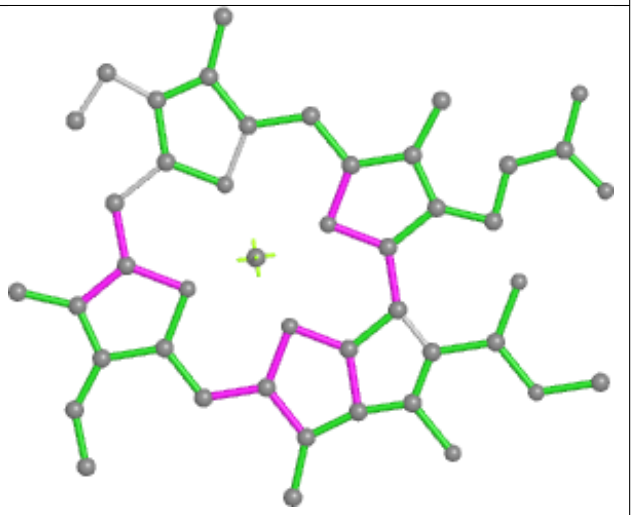


Rings

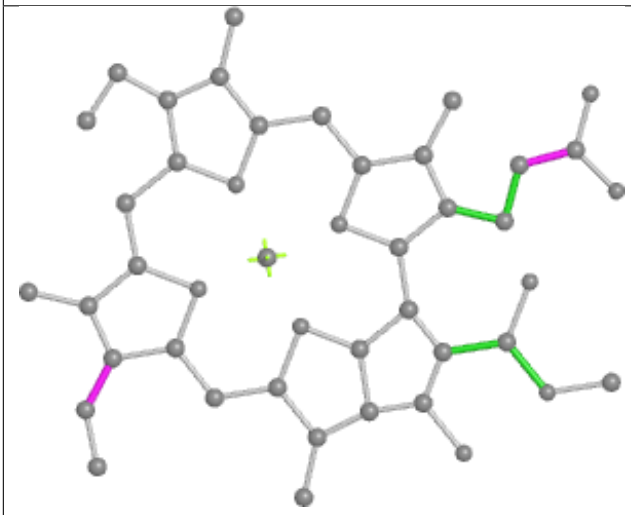
Ligand CLA F 604



Bond lengths



Bond angles



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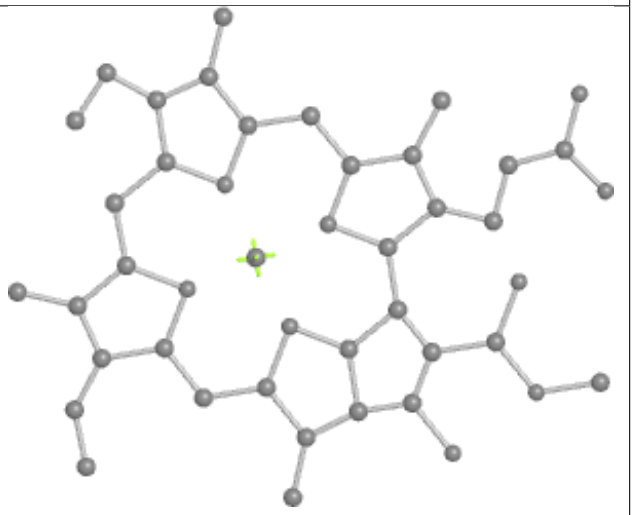
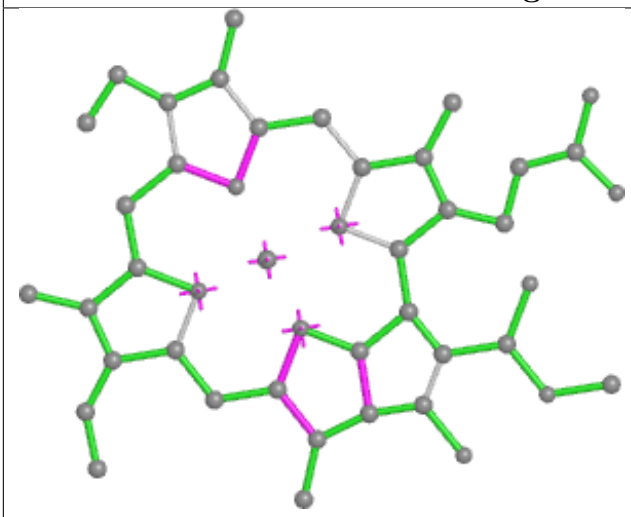
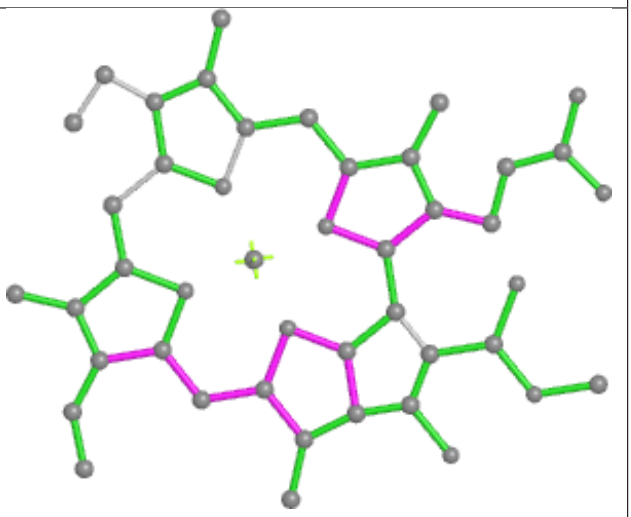


Rings

Ligand CLA G 607



Bond lengths



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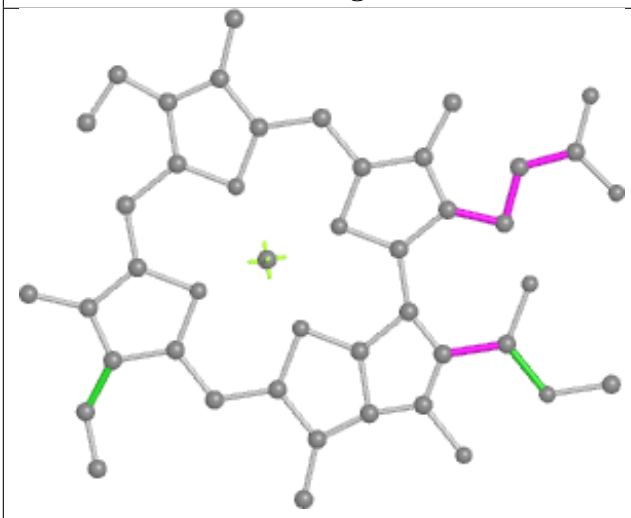

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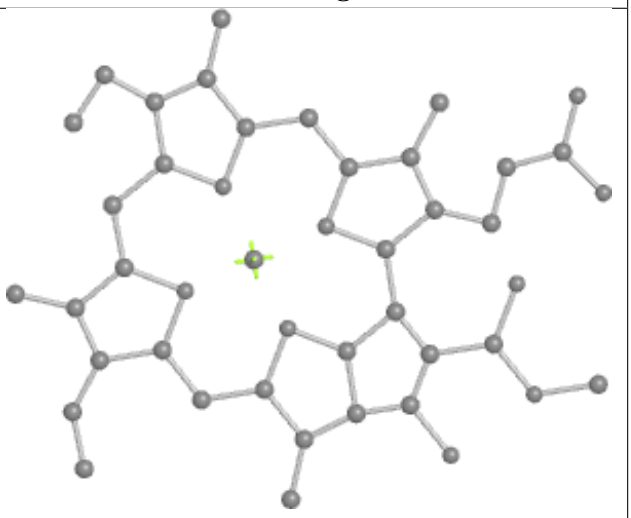
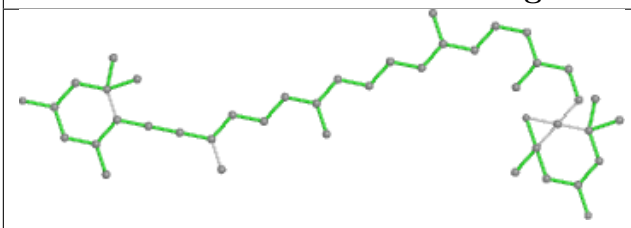


Rings

Ligand DD6 D 617



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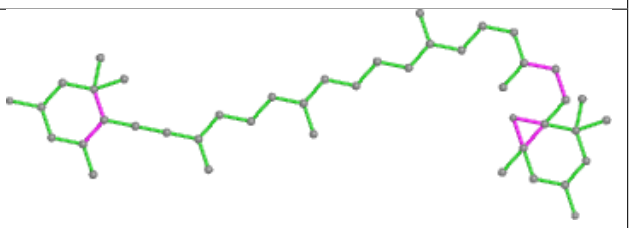
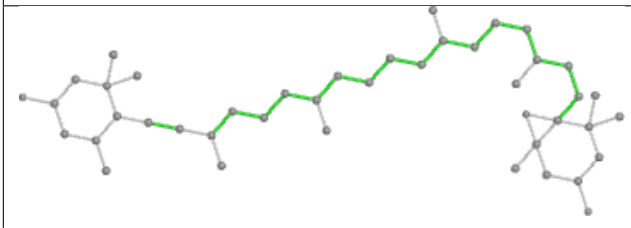


Bond angles



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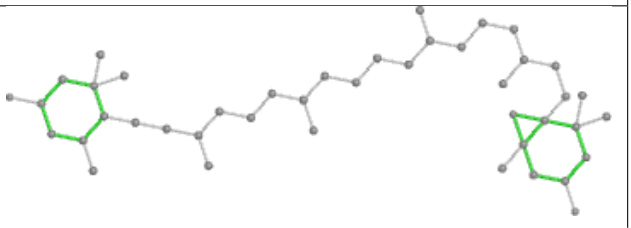
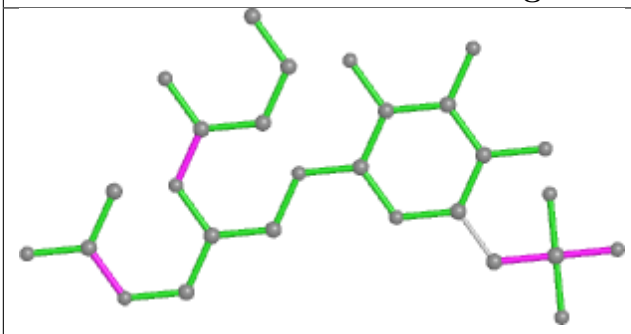


Rings

Ligand SQD A 618



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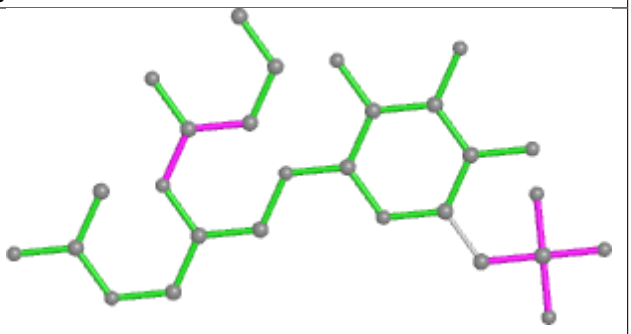
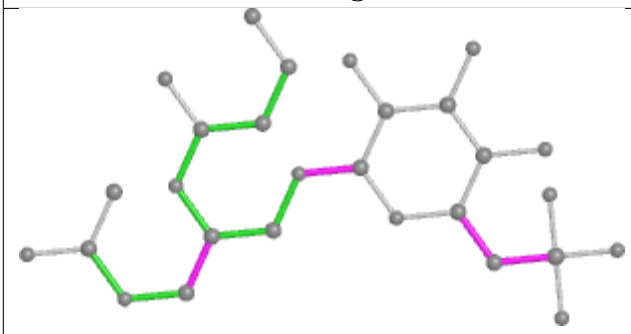


Bond angles



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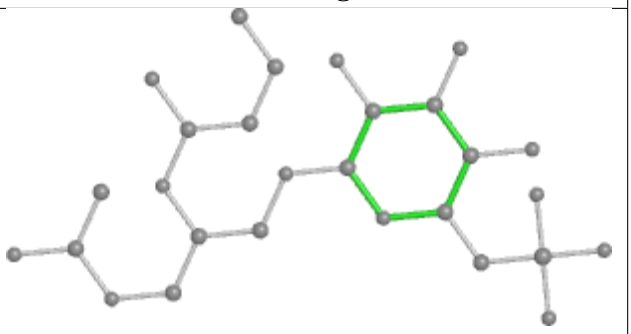
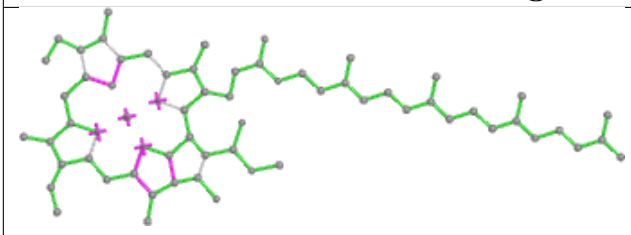


Rings

Ligand CLA b 707



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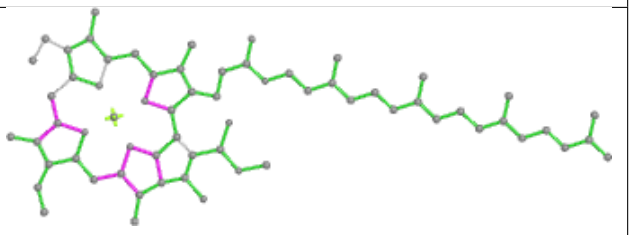
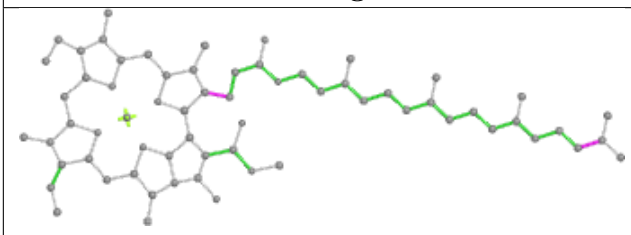
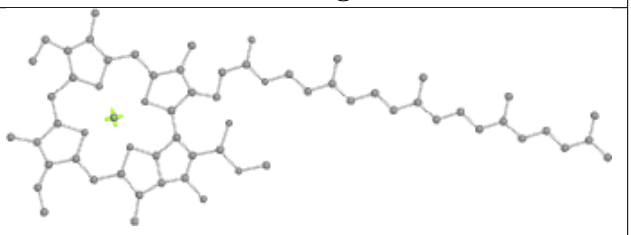


Bond angles

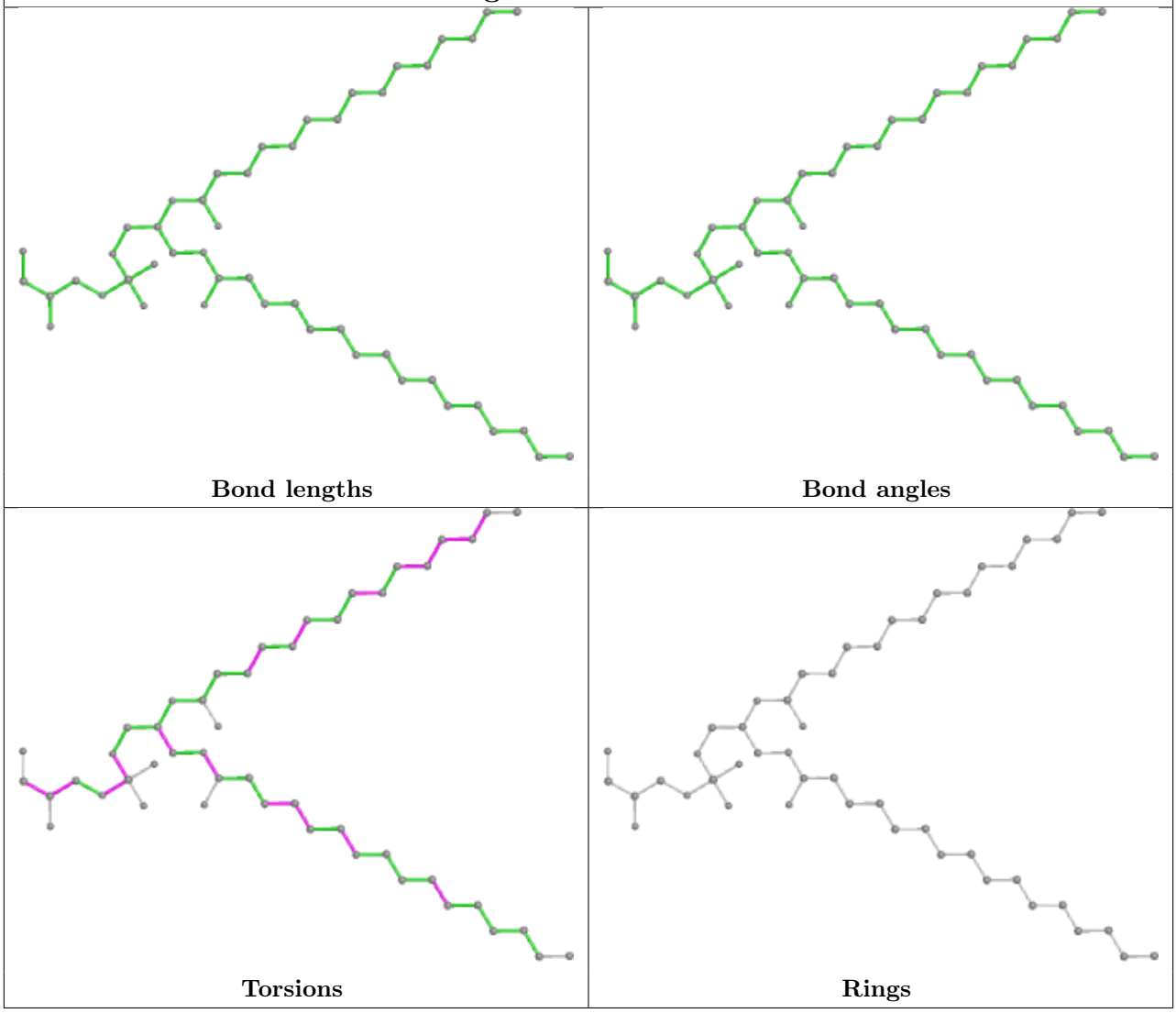


Torsions

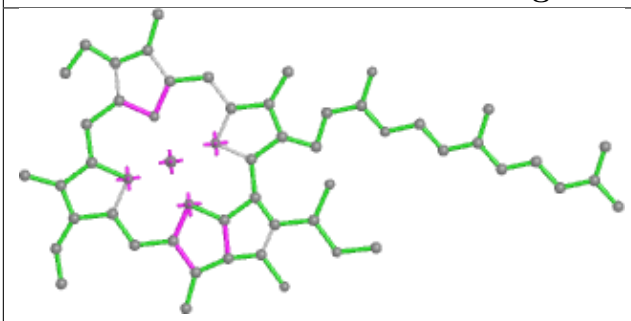


Rings

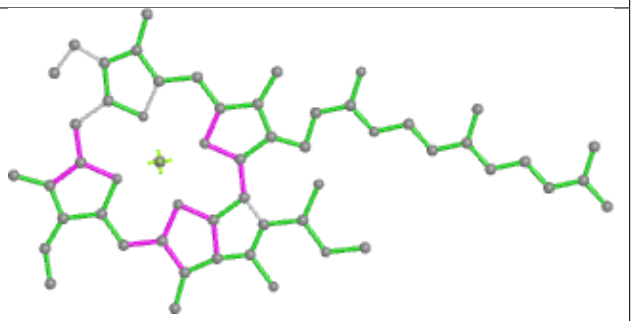
Ligand LHG a 835



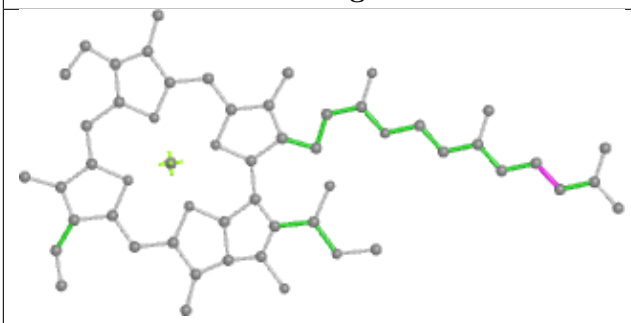
Ligand CLA l 404



Bond lengths



Bond angles



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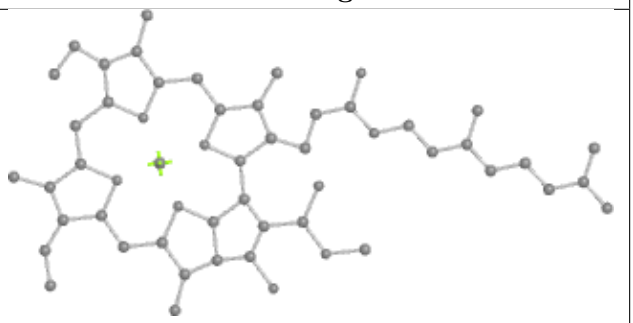
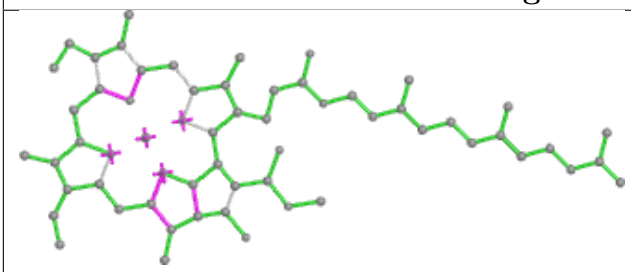
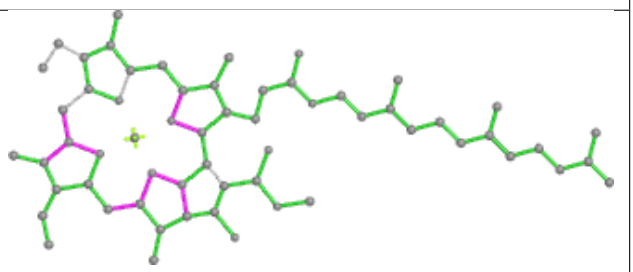


Rings

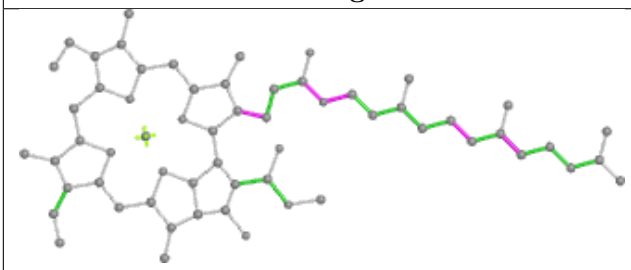
Ligand CLA K 605



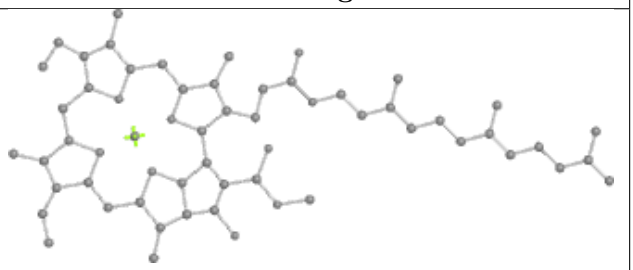
Bond lengths



Bond angles

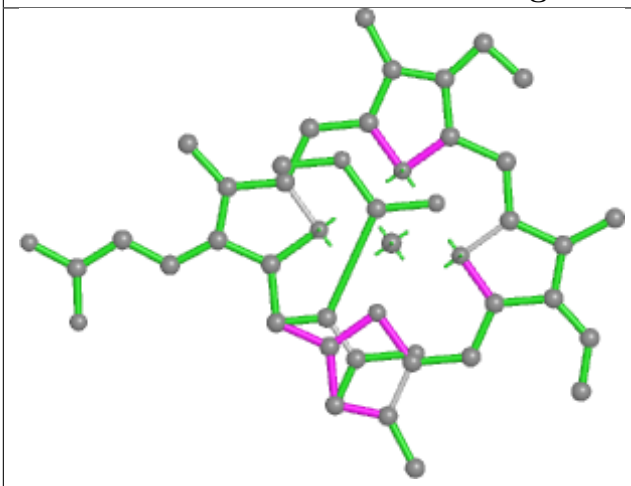


Torsions

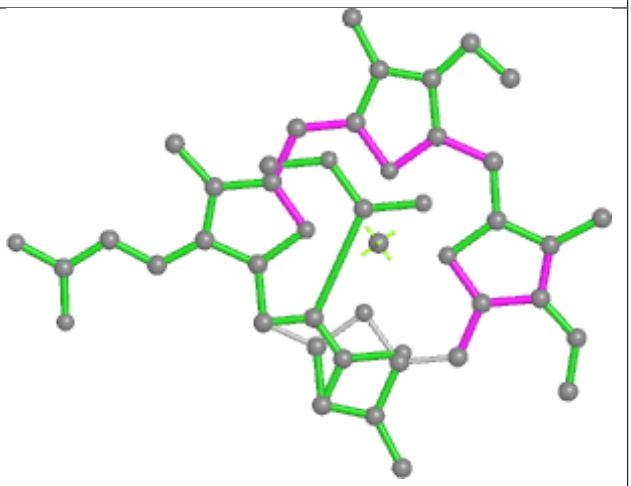


Rings

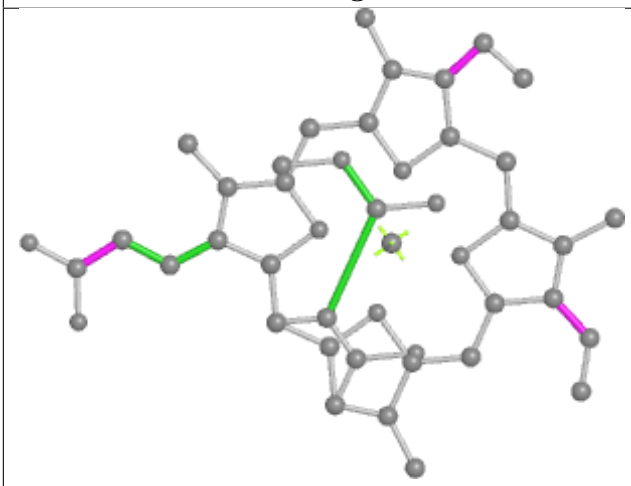
Ligand KC2 J 610



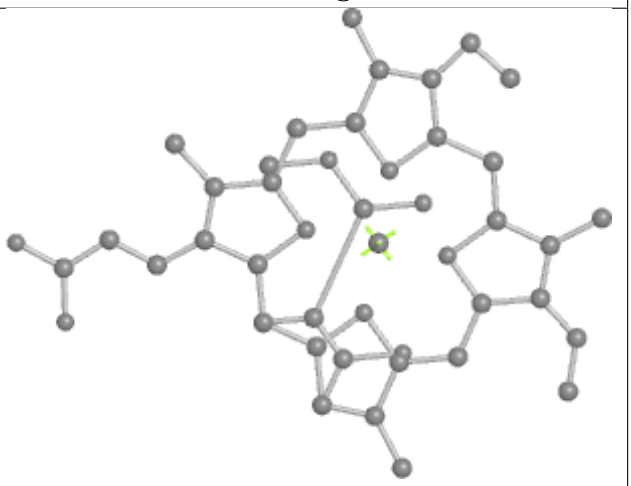
Bond lengths



Bond angles

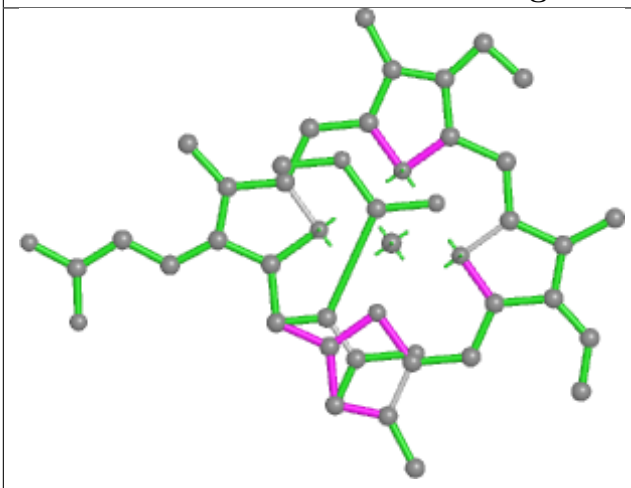


Torsions

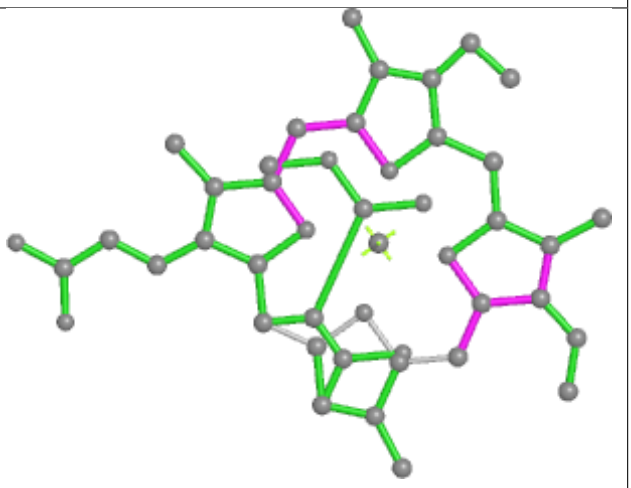


Rings

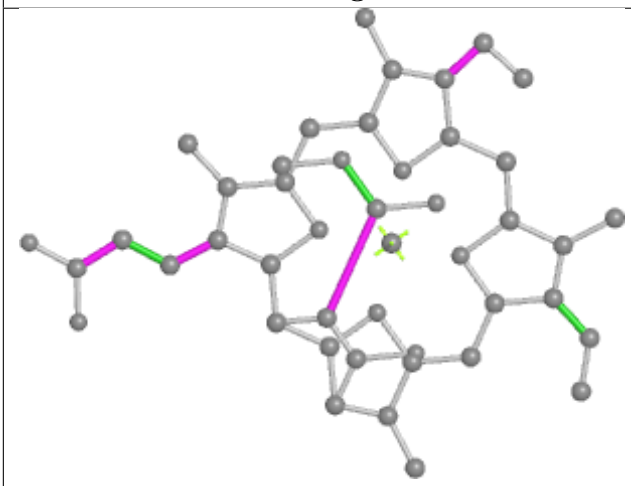
Ligand KC2 J 602



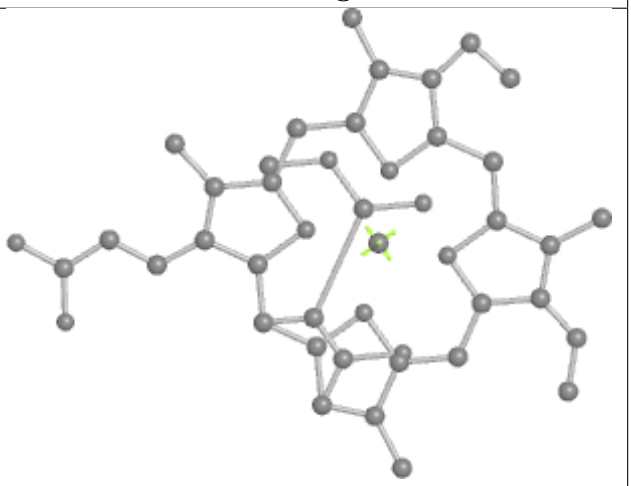
Bond lengths



Bond angles

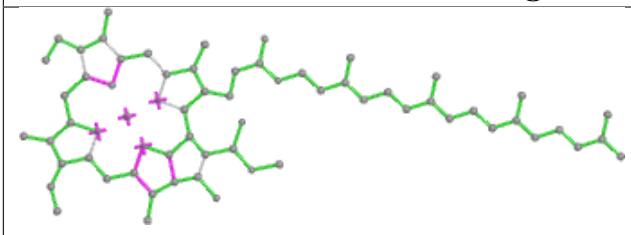


Torsions



Rings

Ligand CLA B 603



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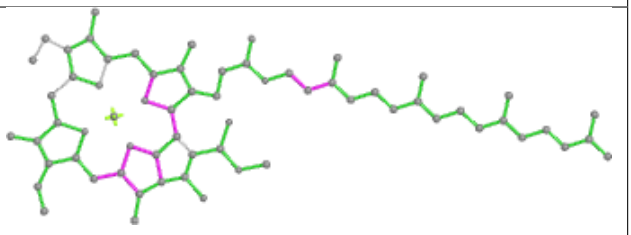
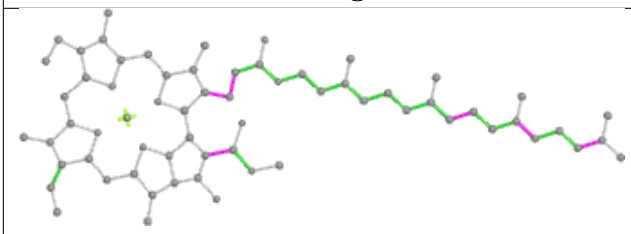
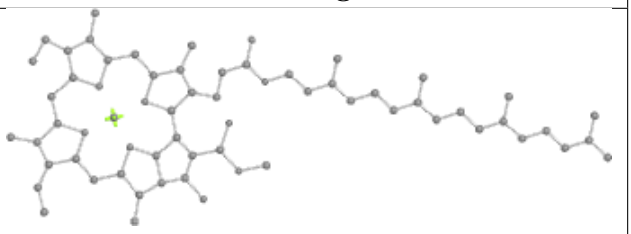


Bond angles

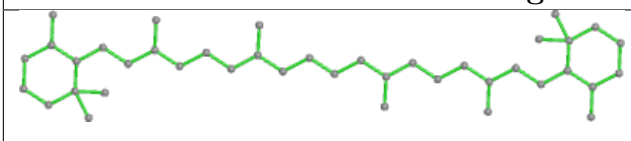


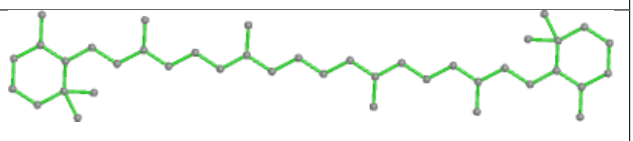
Torsions

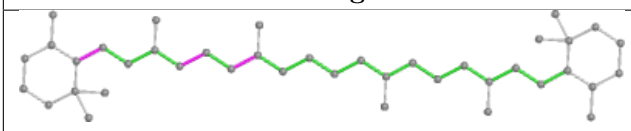


Rings

Ligand BCR a 834


Bond lengths


Bond angles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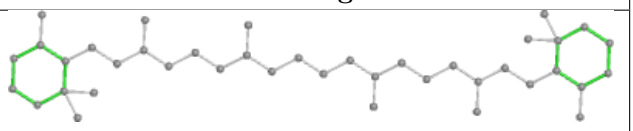
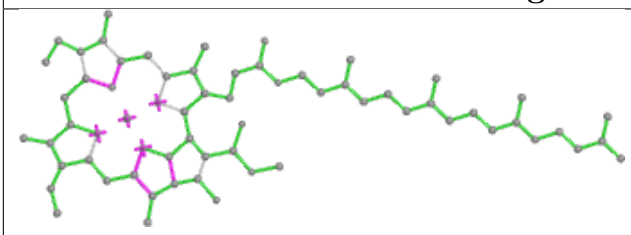
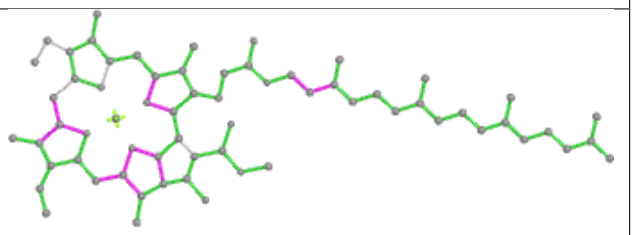
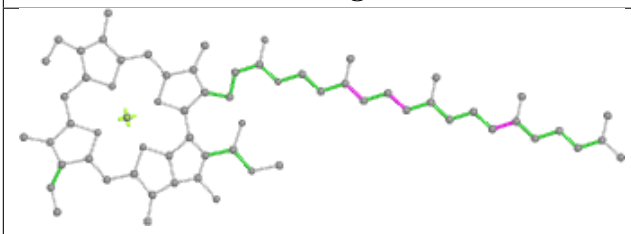
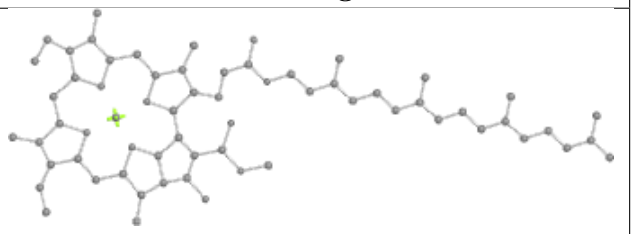

Rings

Ligand CLA b 725

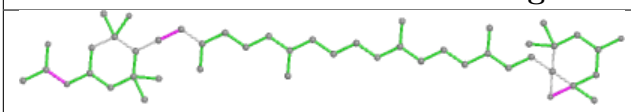

Bond lengths

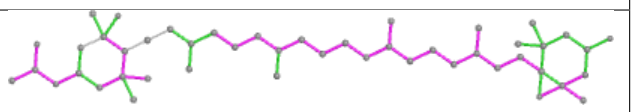

Bond angles

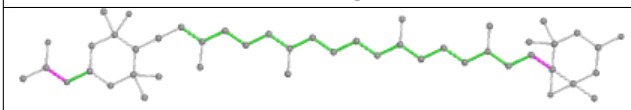

Torsions

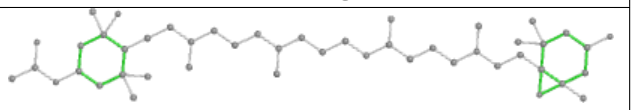

Rings

Ligand UIX C 215

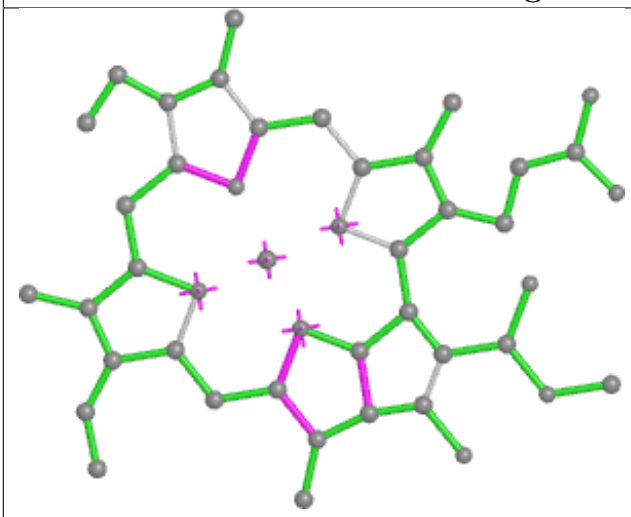

Bond lengths


Bond angles

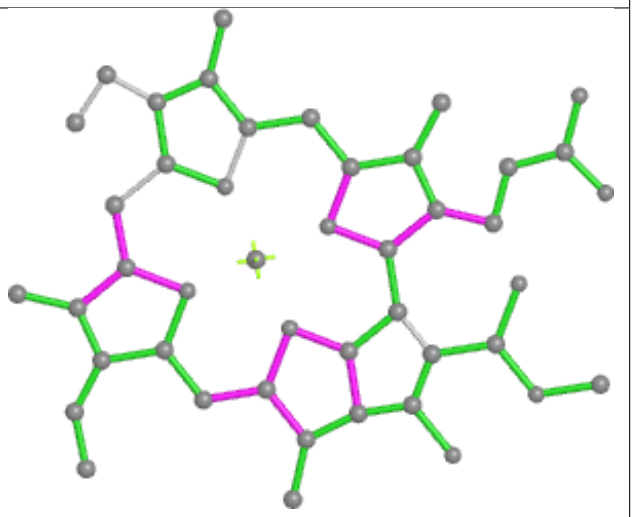

Torsions


Rings

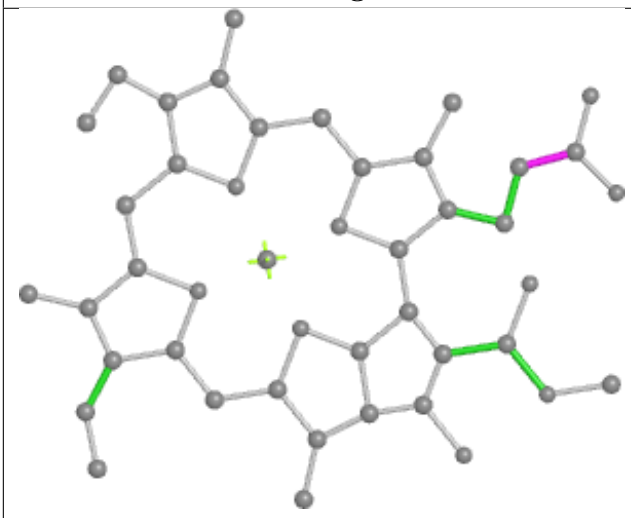
Ligand CLA C 209



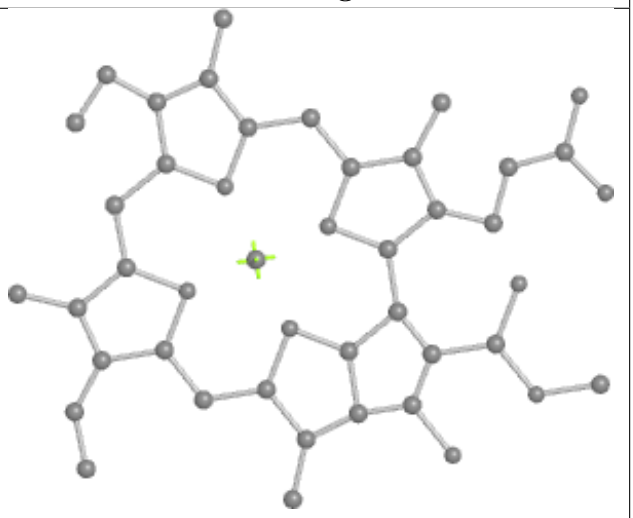
Bond lengths



Bond angles

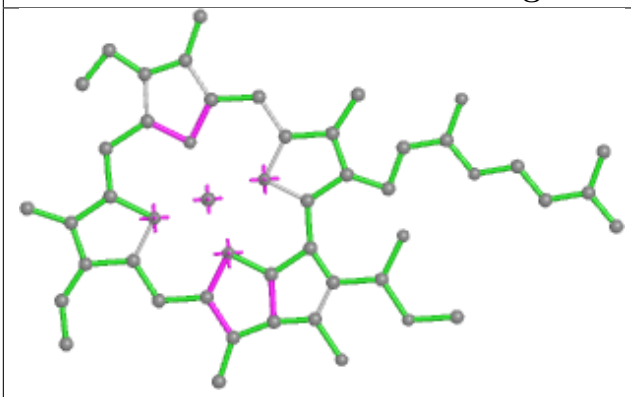


Torsions

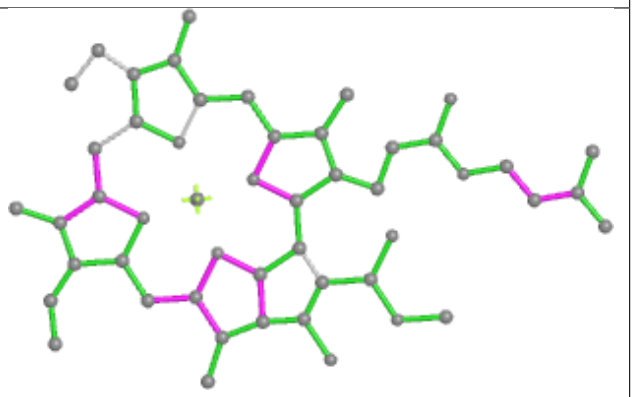


Rings

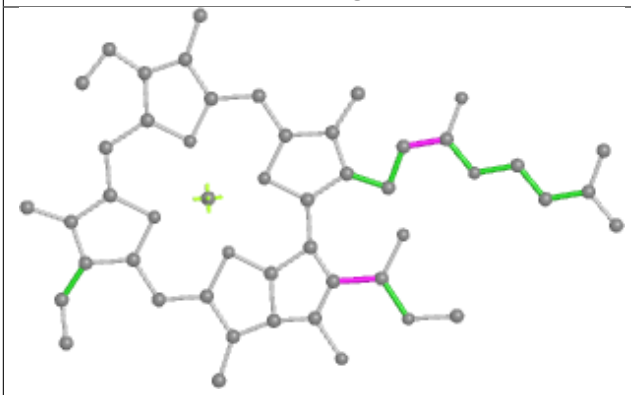
Ligand CLA G 603



Bond lengths



Bond angles



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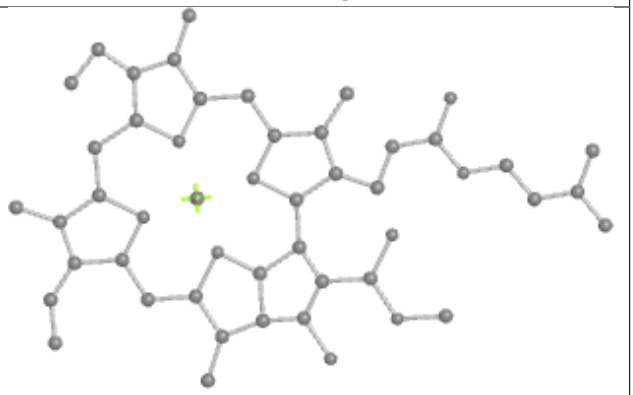
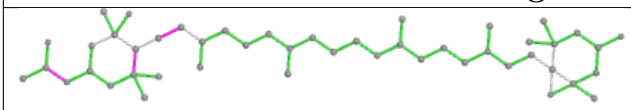
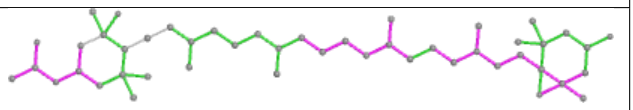


Rings

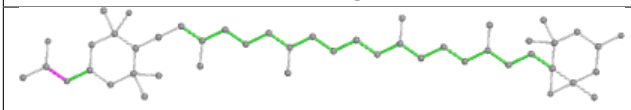
Ligand UIX C 213



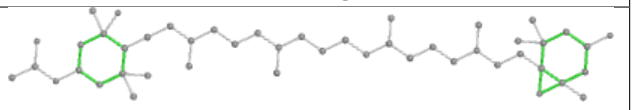
Bond lengths



Bond angles

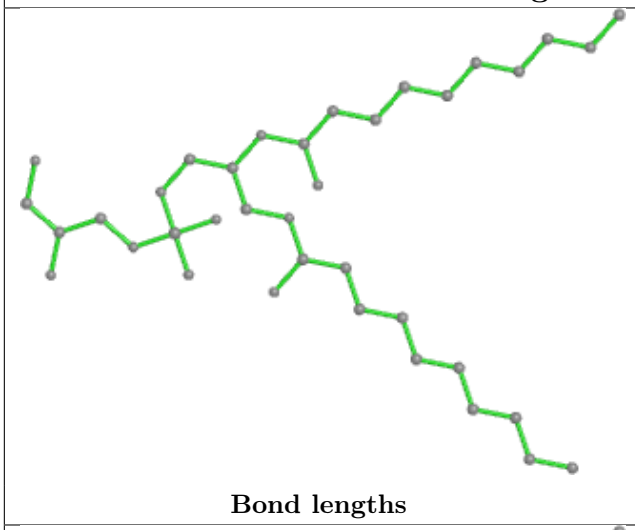


Torsions



Rings

Ligand LHG j 205



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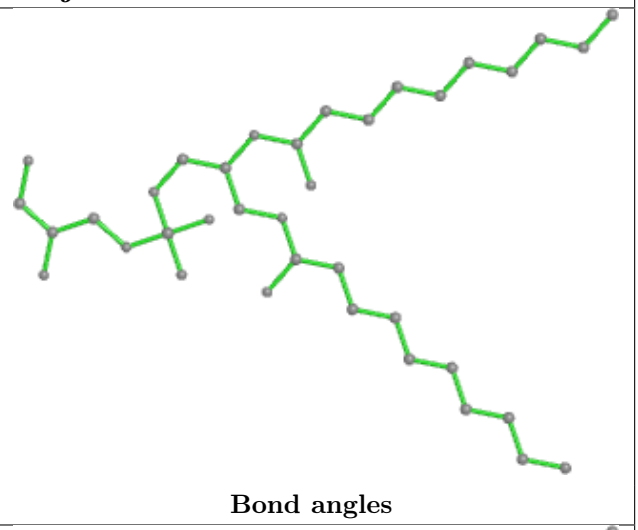
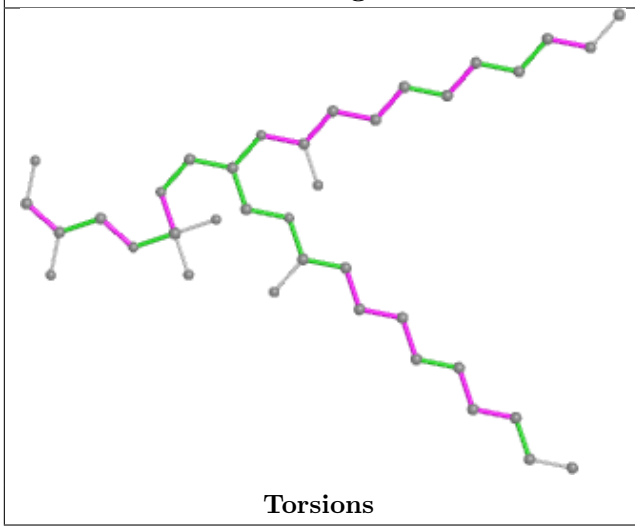
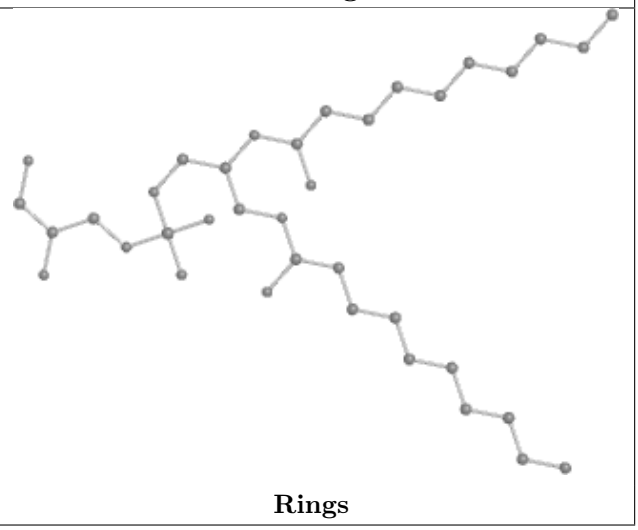


Bond angles

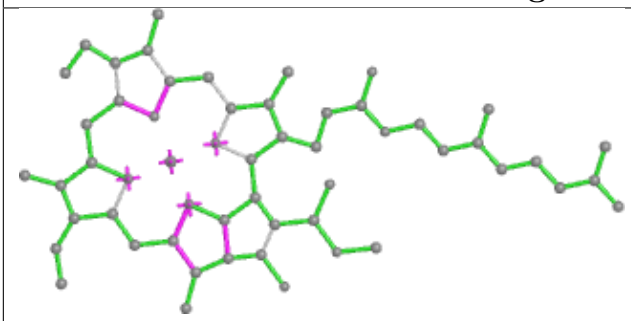


Torsions

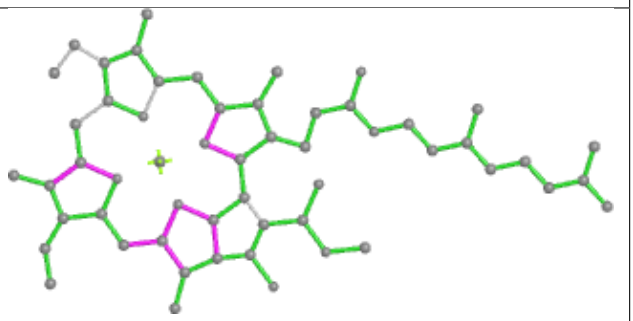


Rings

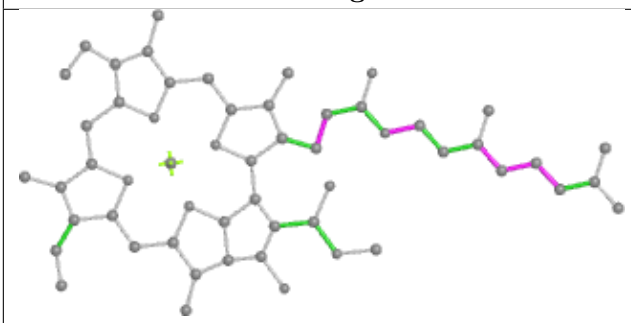
Ligand CLA a 818



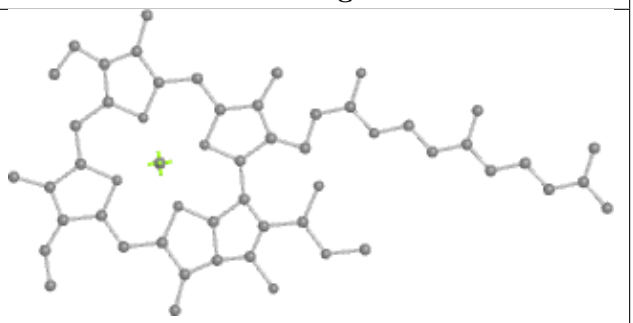
Bond lengths



Bond angles

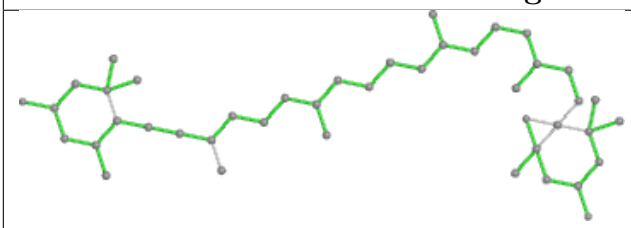


Torsions



Rings

Ligand DD6 D 621



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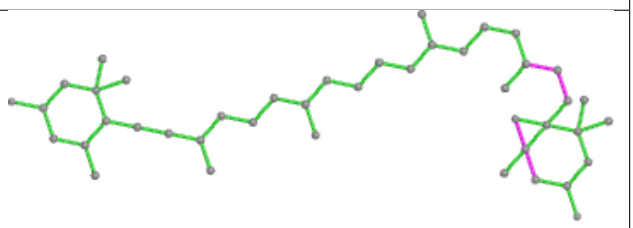
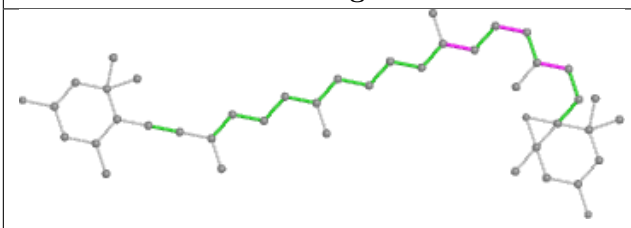
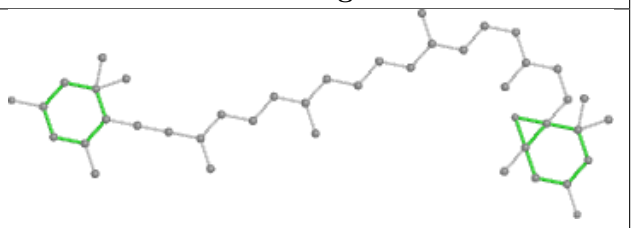


Bond angles

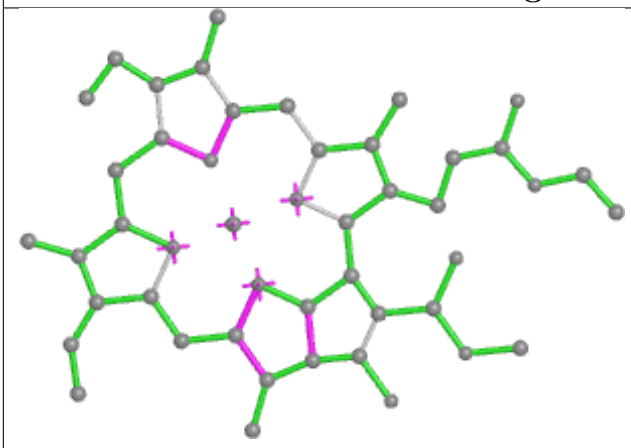


Torsions

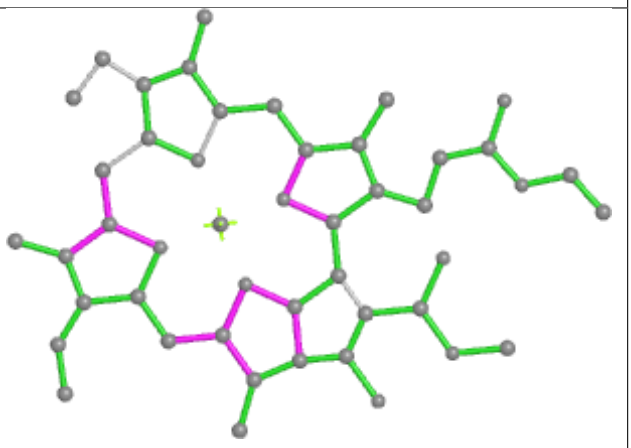


Rings

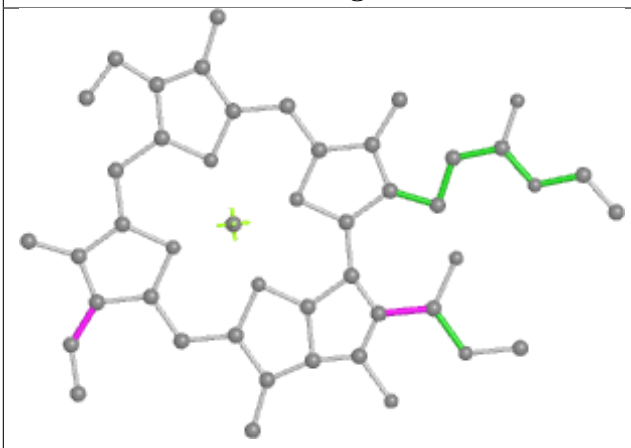
Ligand CLA B 610



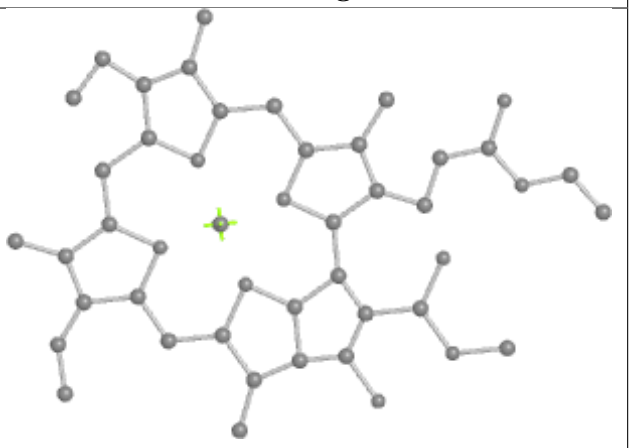
Bond lengths



Bond angles

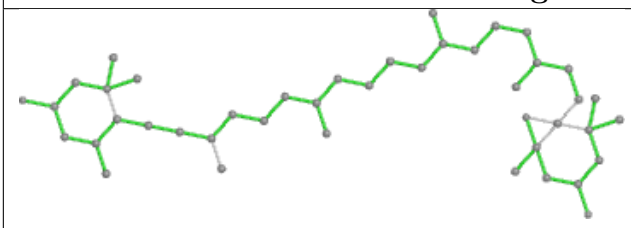


Torsions

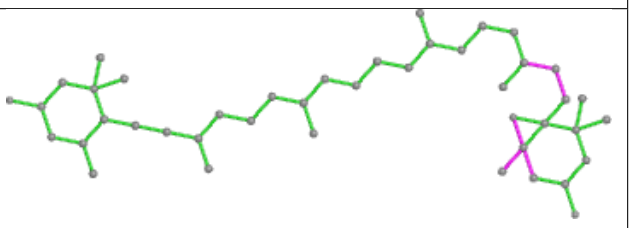


Rings

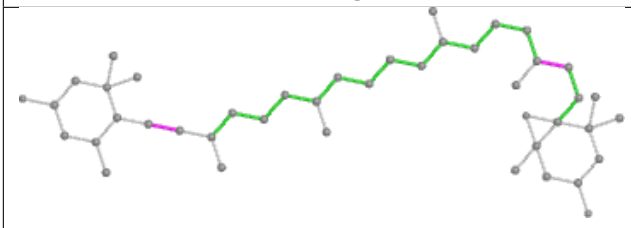
Ligand DD6 r 206



Bond lengths



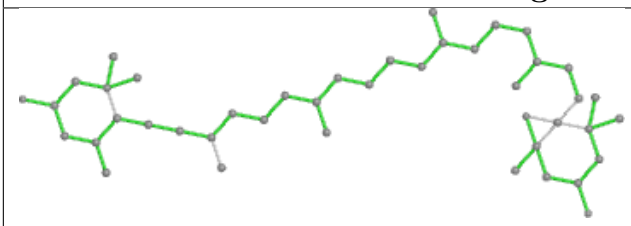
Bond angles



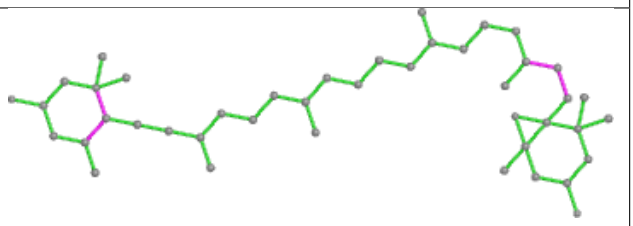
Torsions

Rings

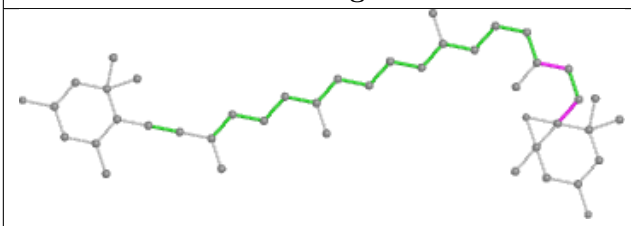
Ligand DD6 r 205



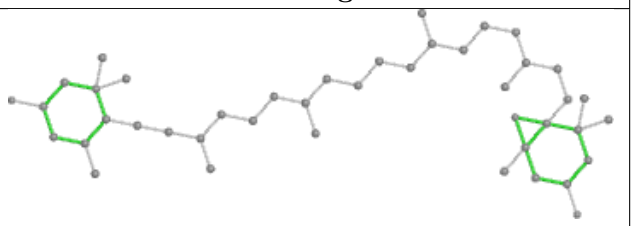
Bond lengths



Bond angles

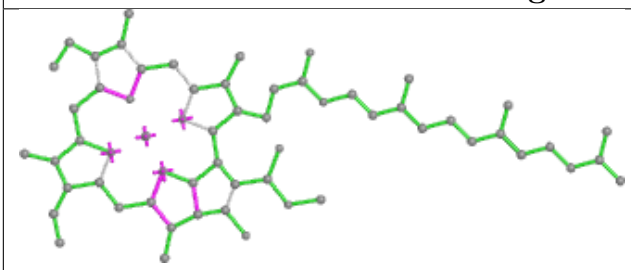


Torsions



Rings

Ligand CLA a 815



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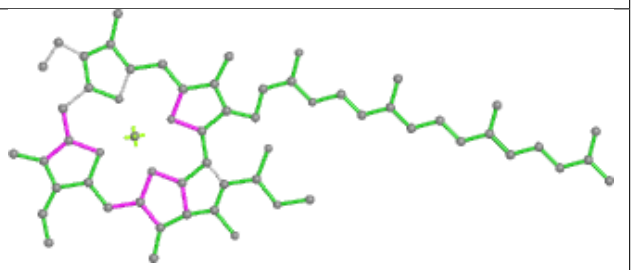
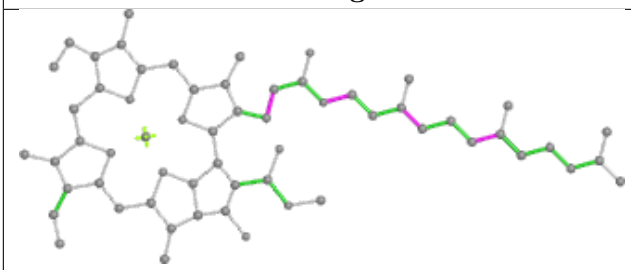
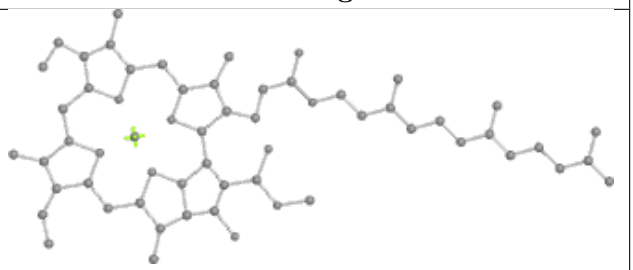


Bond angles

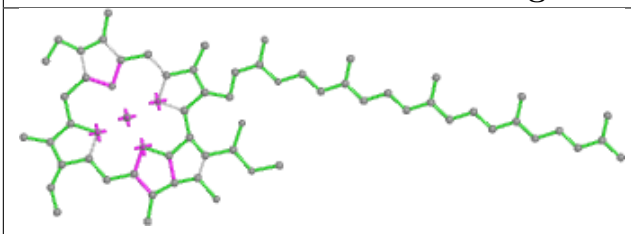


Torsions

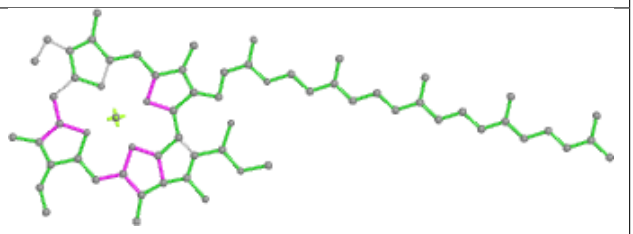


Rings

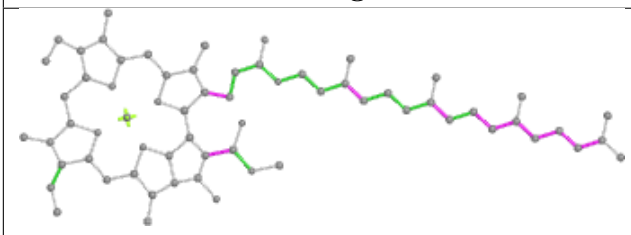
Ligand CLA a 829



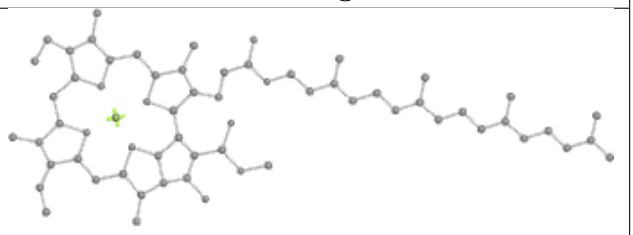
Bond lengths



Bond angles

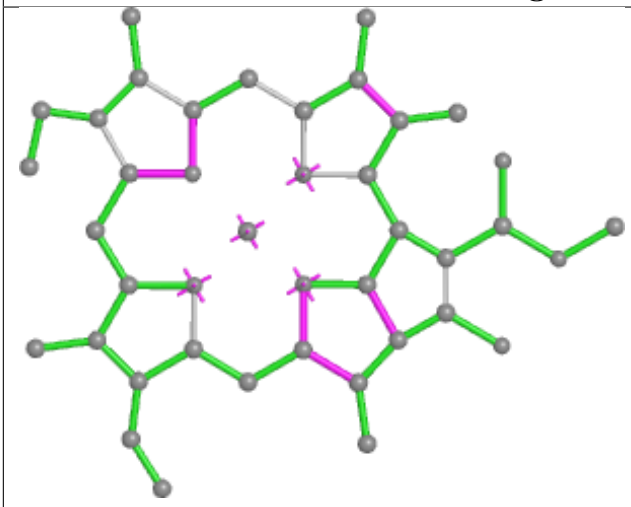


Torsions

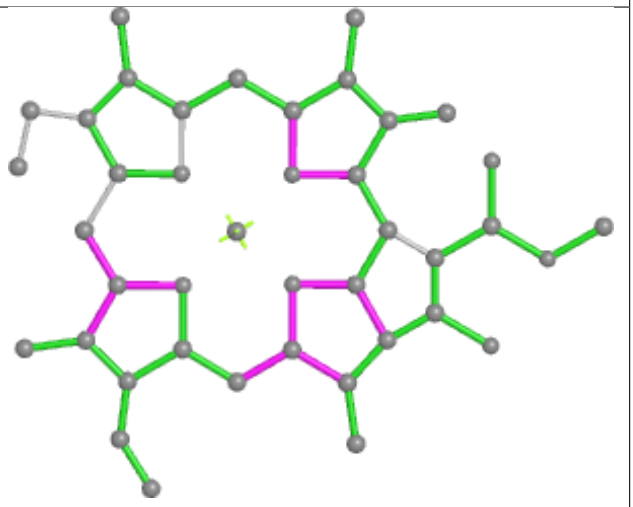


Rings

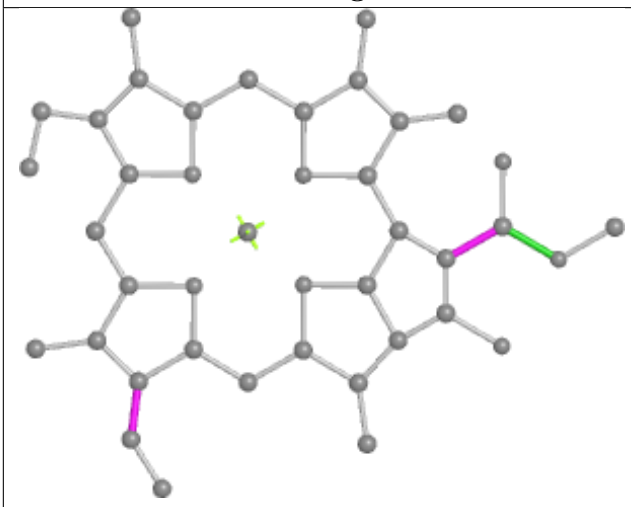
Ligand CLA J 609



Bond lengths



Bond angles



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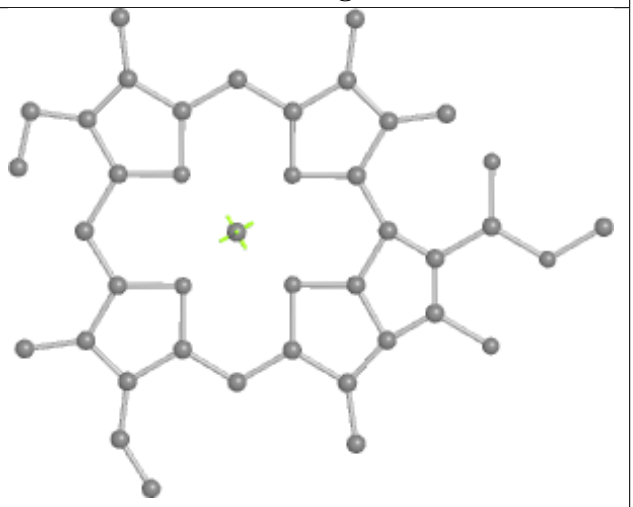
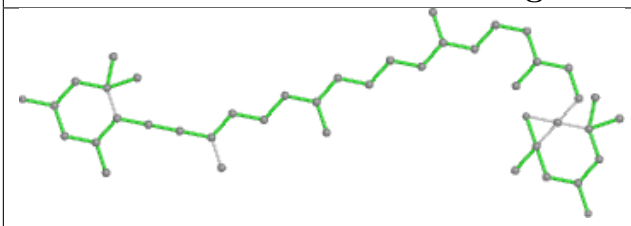


Rings

Ligand DD6 T 610



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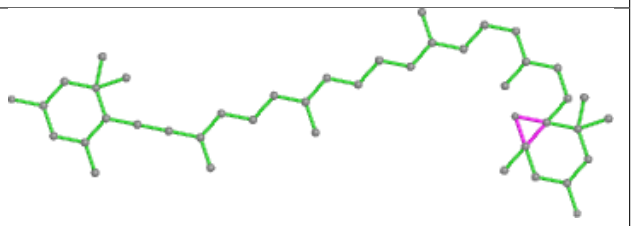
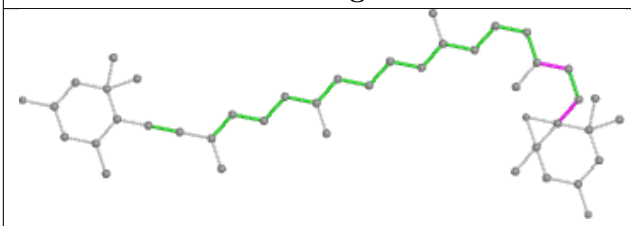


Bond angles



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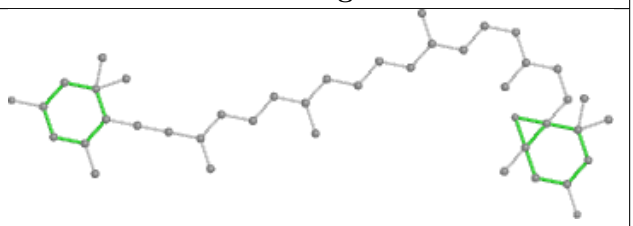
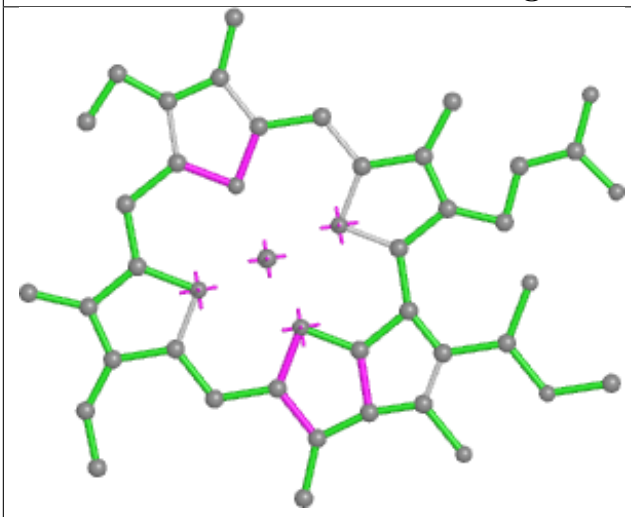


Rings

Ligand CLA K 608



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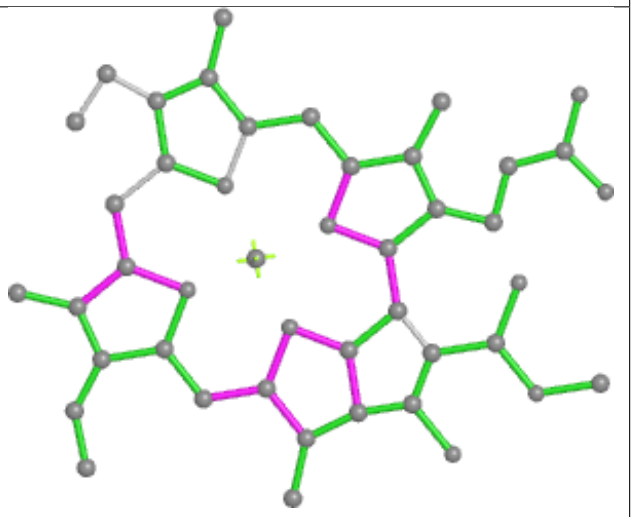
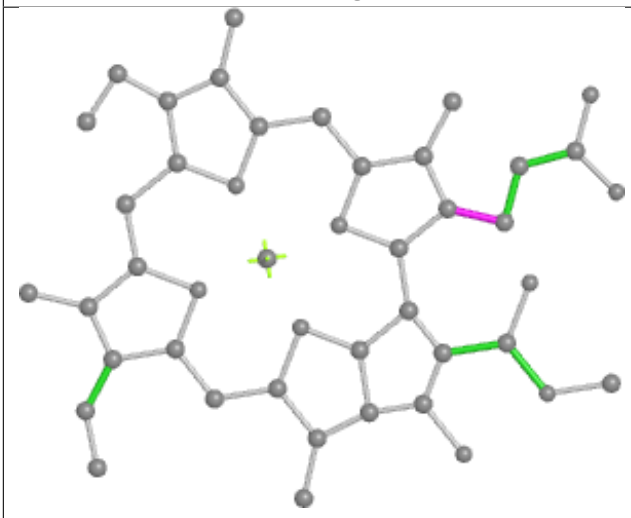


Bond angles



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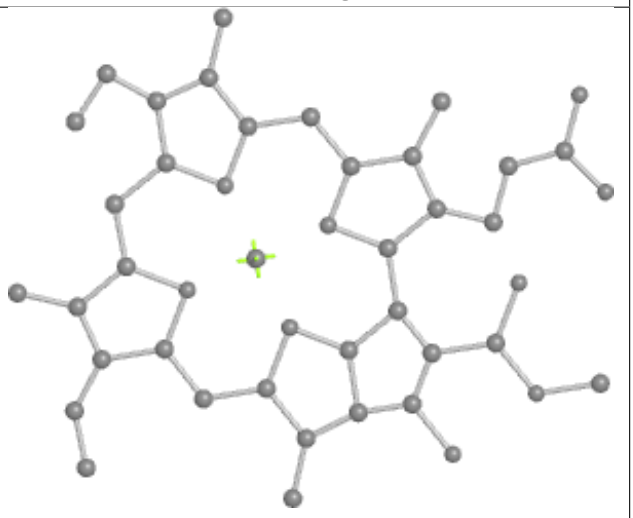
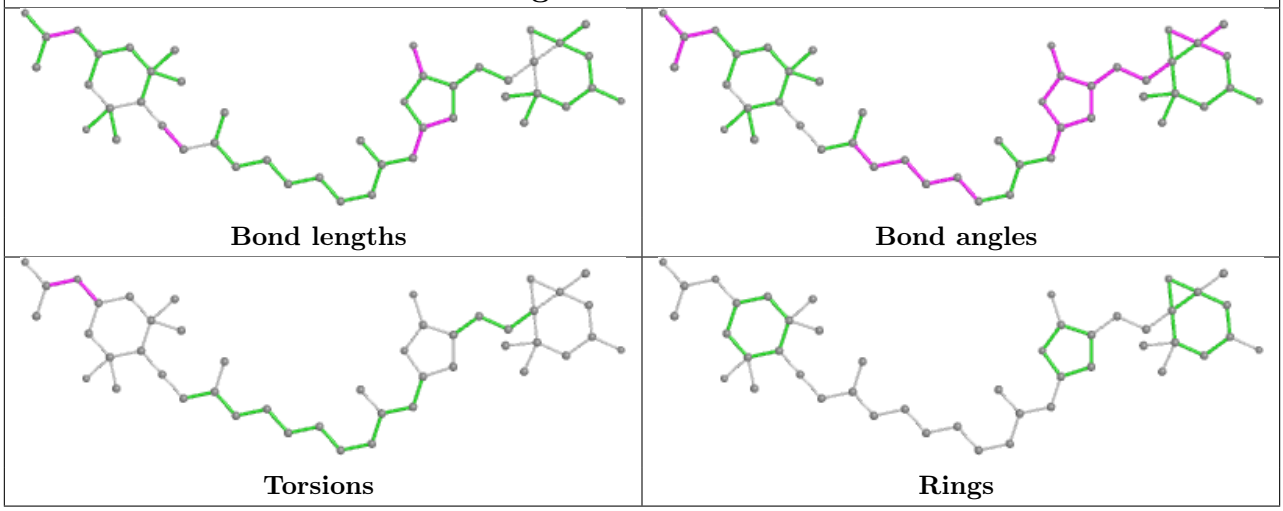
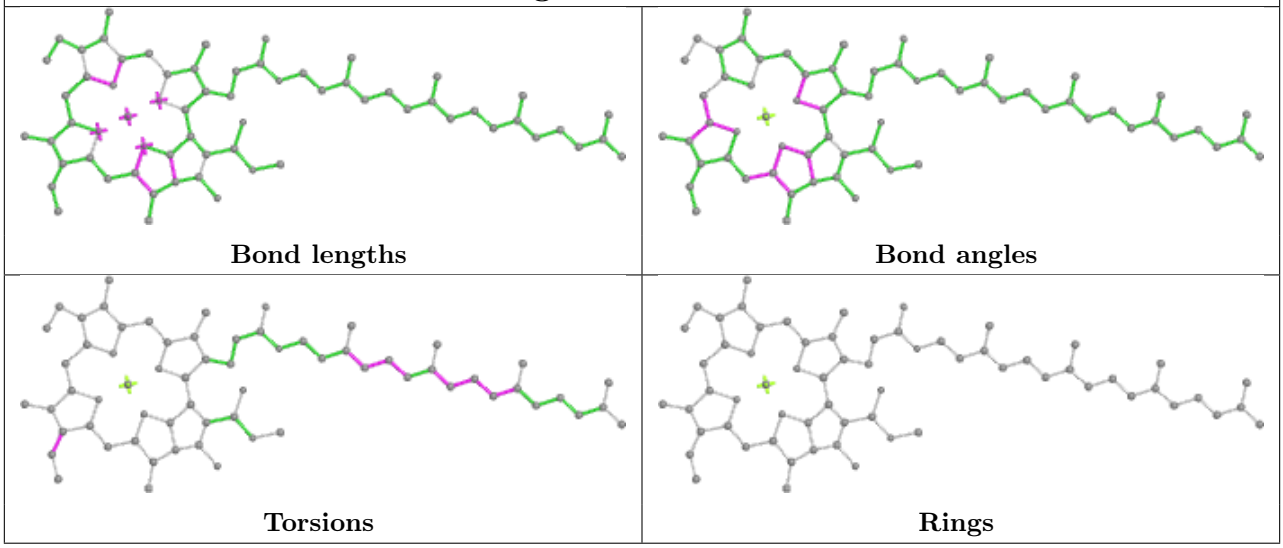


Rings

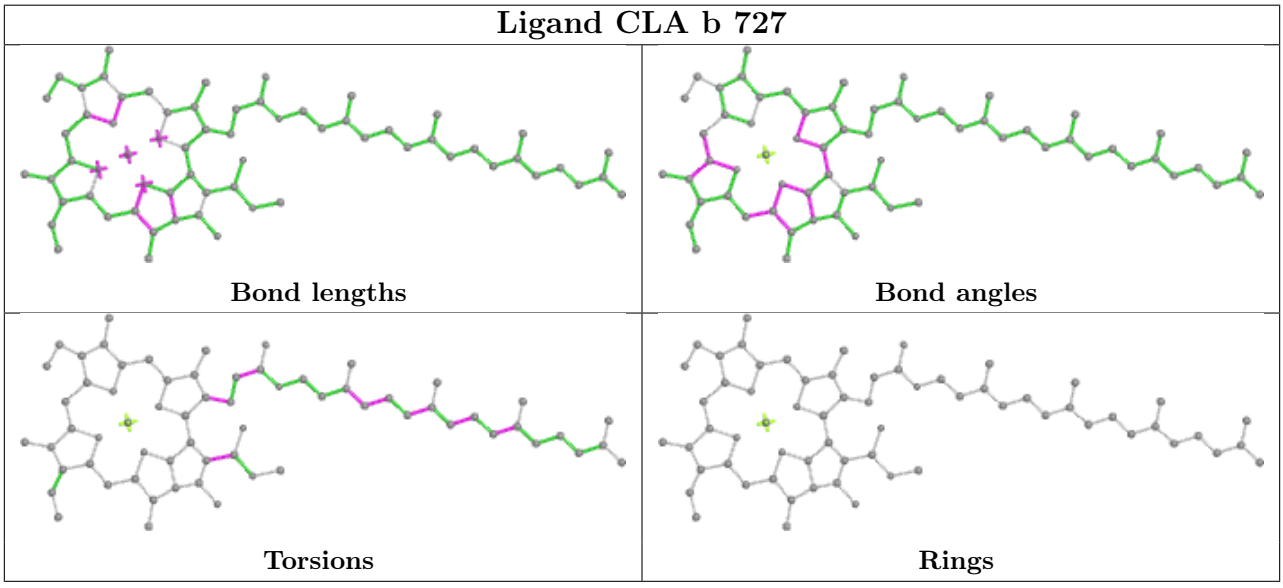
Ligand PID F 615



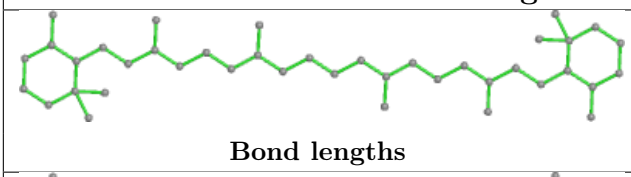
Ligand CLA l 409



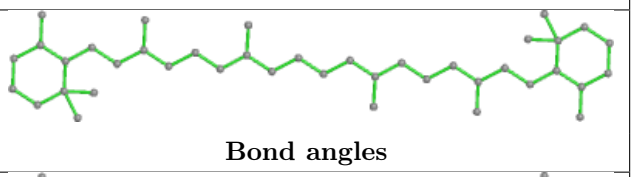
Ligand CLA b 727



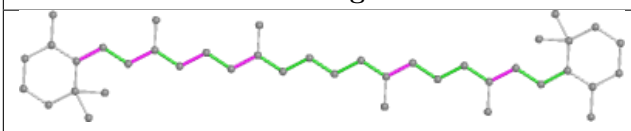
Ligand BCR m 201



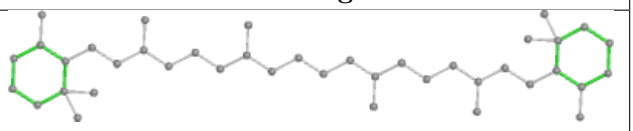
Bond lengths



Bond angles

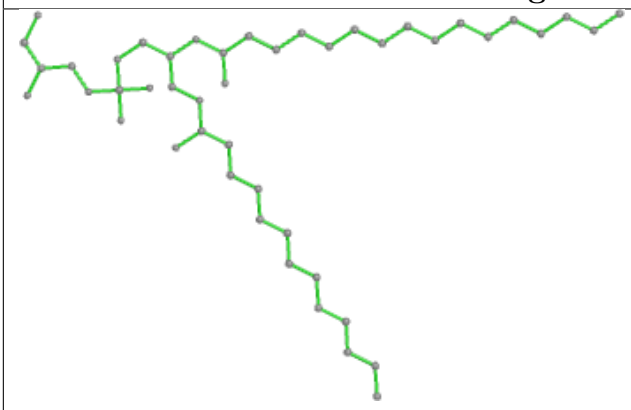


Torsions

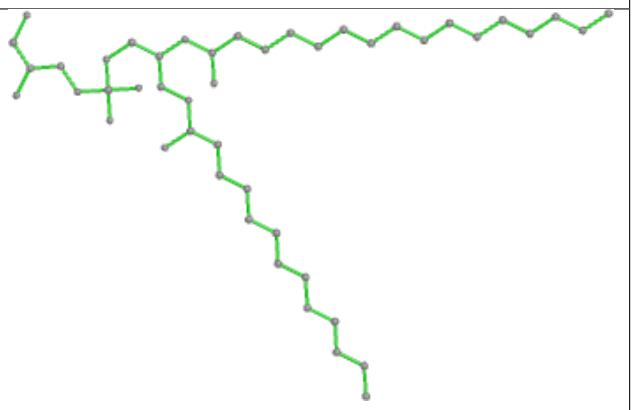


Rings

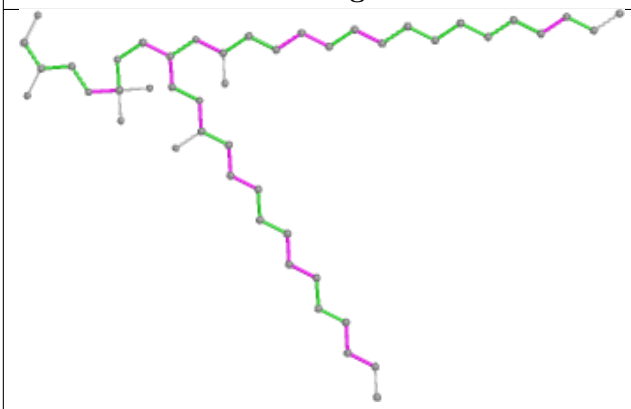
Ligand LHG r 202



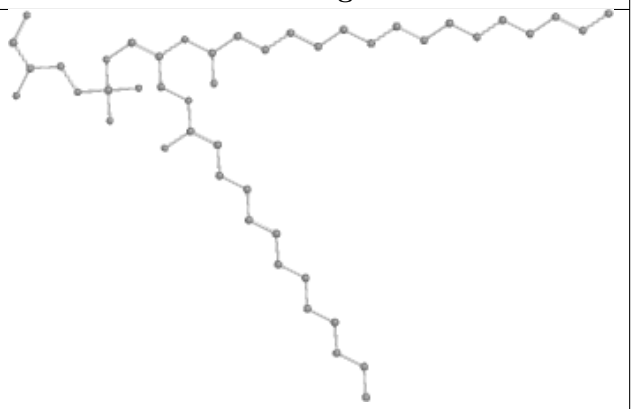
Bond lengths



Bond angles

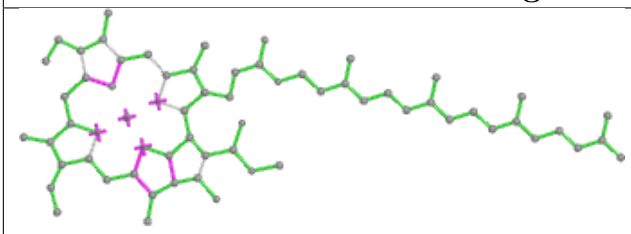


Torsions

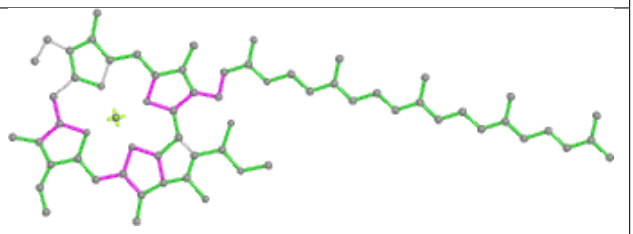


Rings

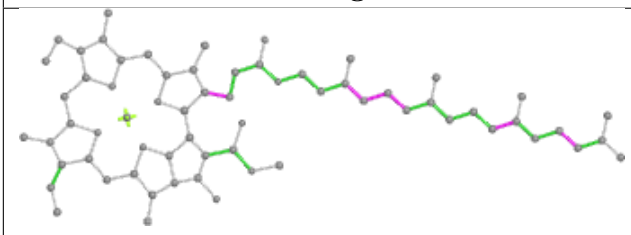
Ligand CLA G 606



Bond lengths



Bond angles



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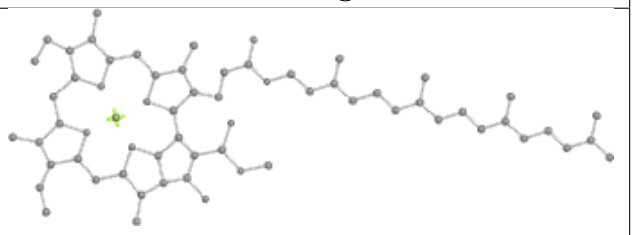
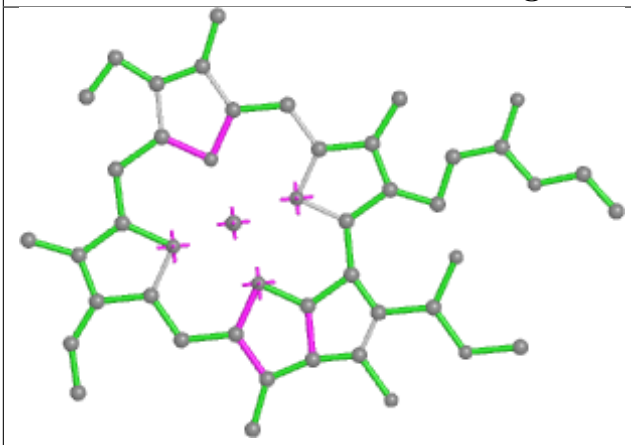
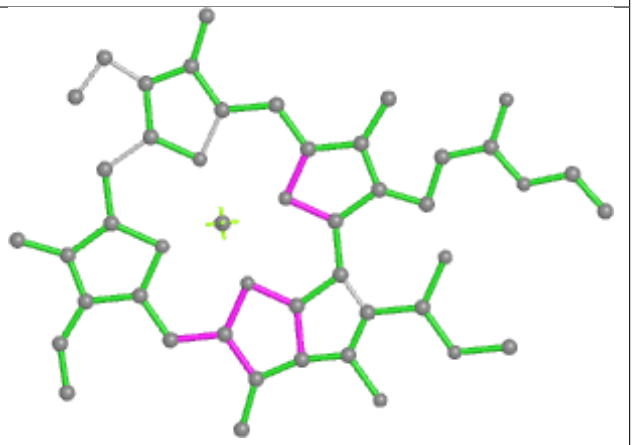


Rings

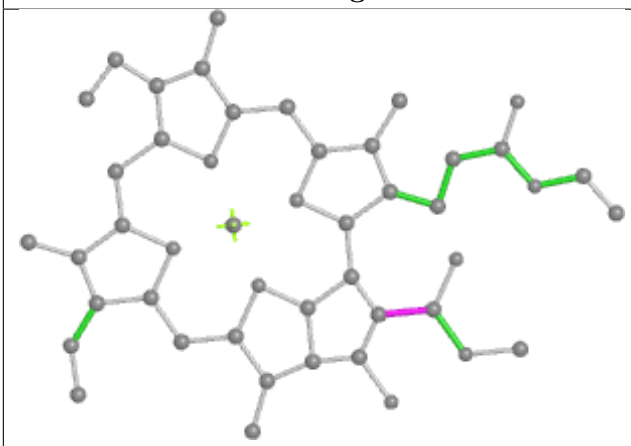
Ligand CLA G 604



Bond lengths



Bond angles



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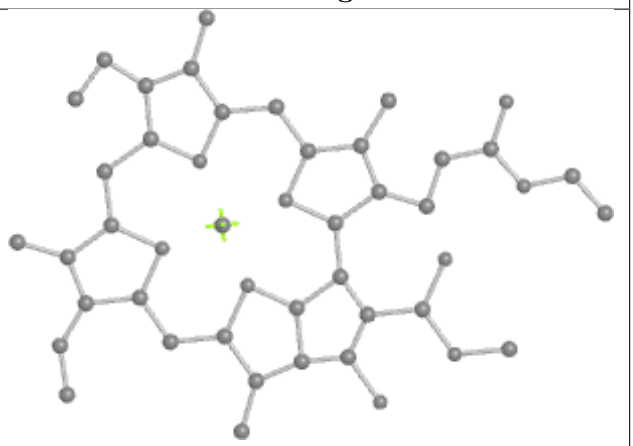
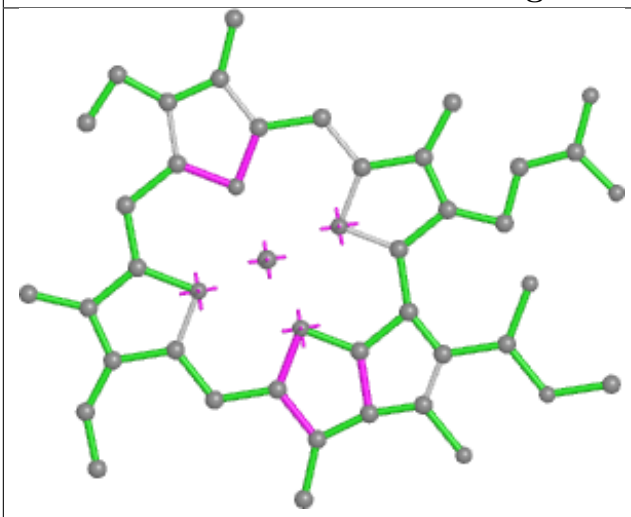


Rings

Ligand CLA F 605



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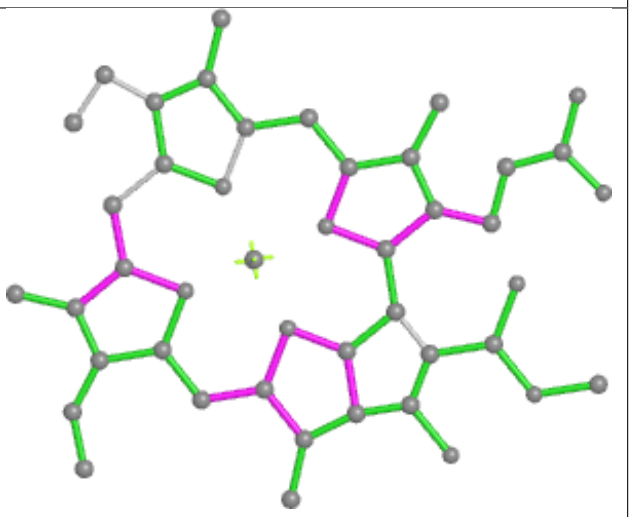
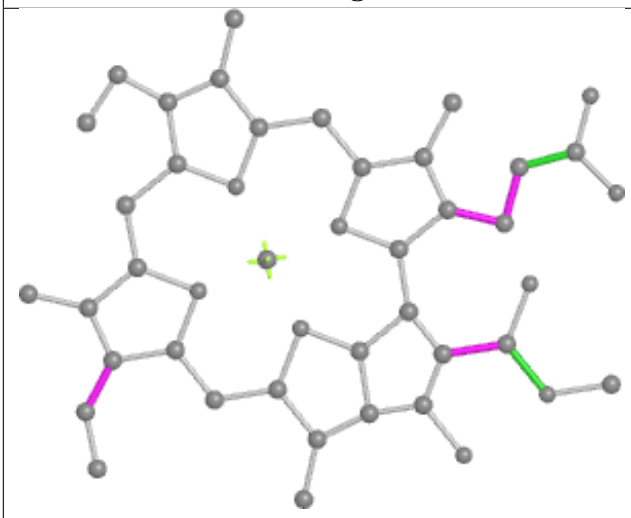
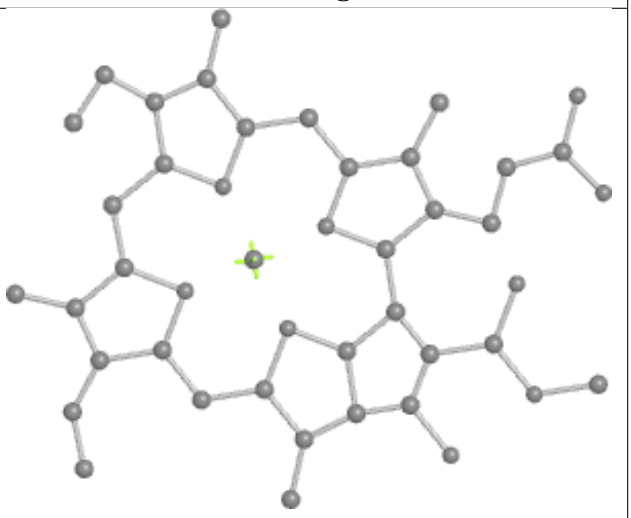


Bond angles

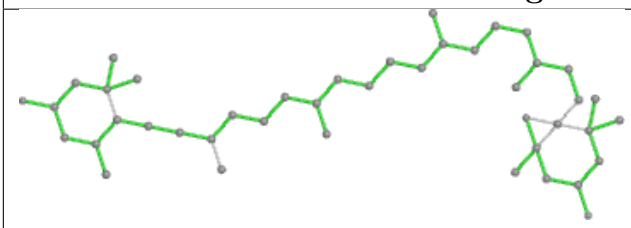


Torsions



Rings

Ligand DD6 T 611



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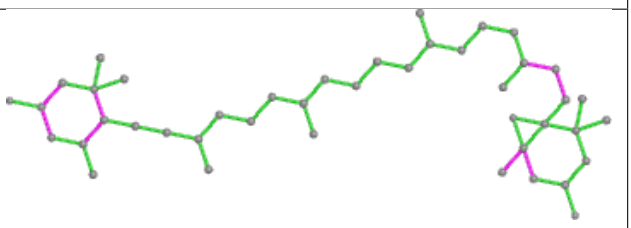
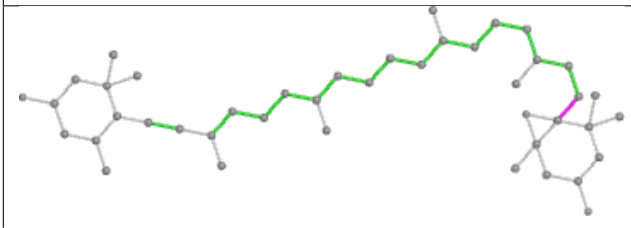
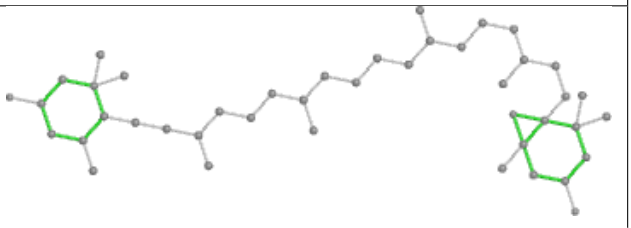


Bond angles

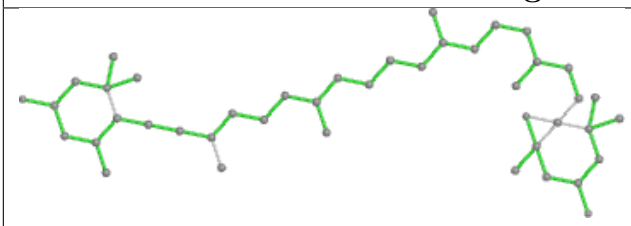


Torsions

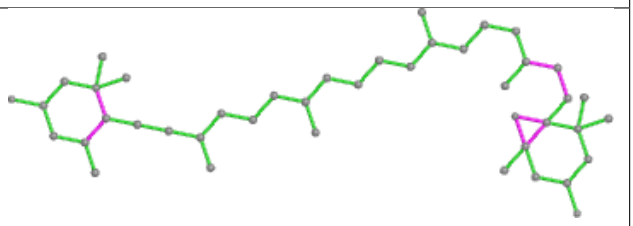


Rings

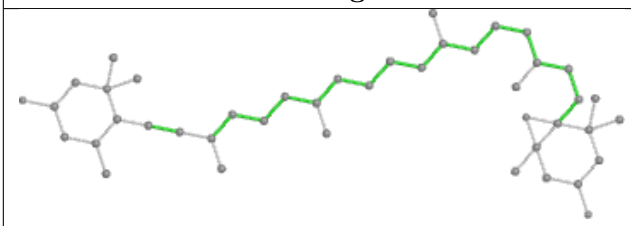
Ligand DD6 H 318



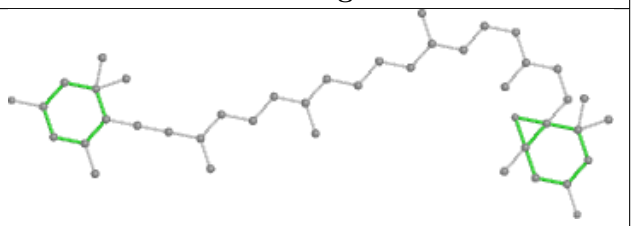
Bond lengths



Bond angles

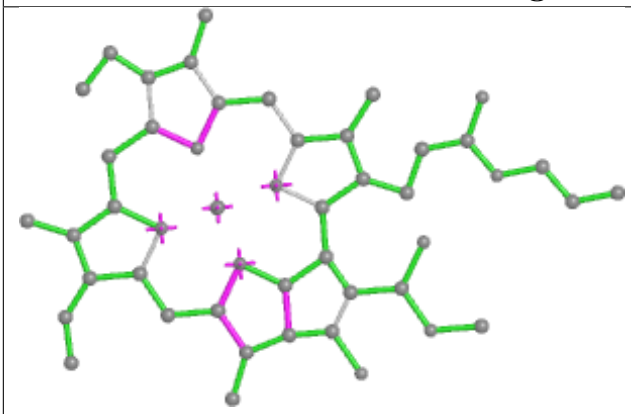


Torsions

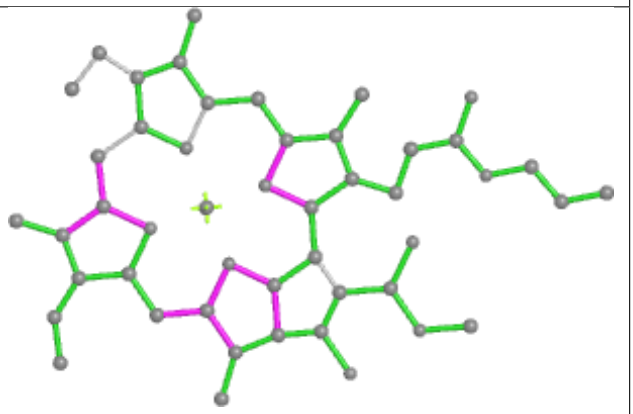


Rings

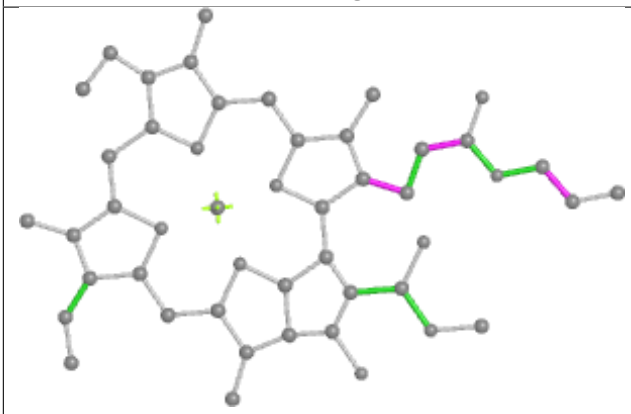
Ligand CLA a 813



Bond lengths



Bond angles



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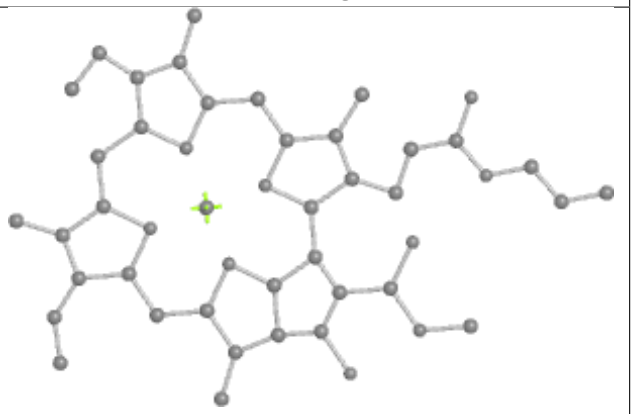
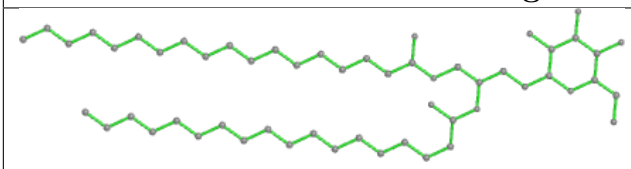
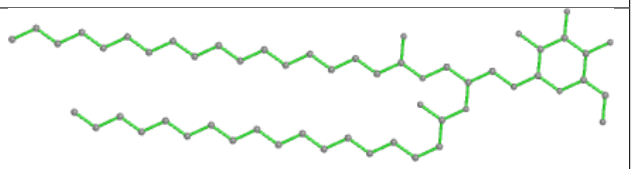


Rings

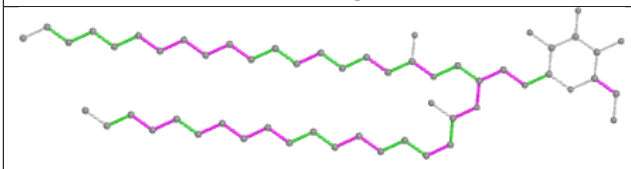
Ligand LMG b 733



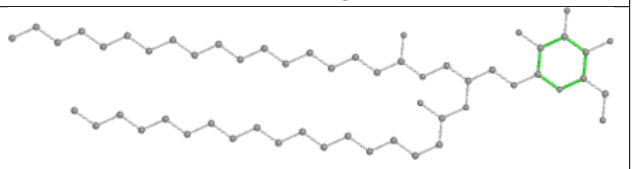
Bond lengths



Bond angles

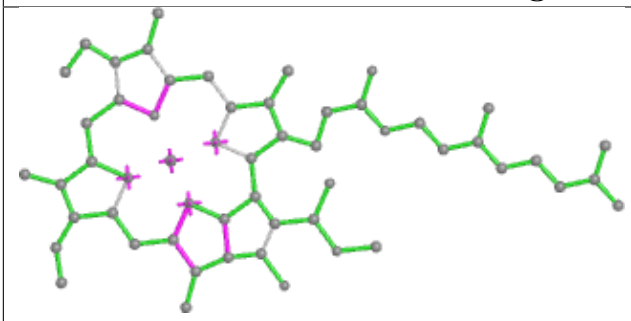


Torsions



Rings

Ligand CLA a 814



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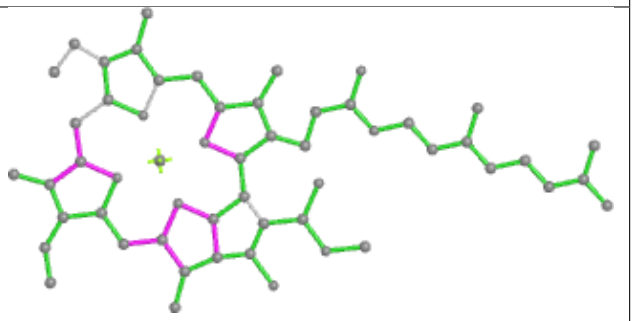
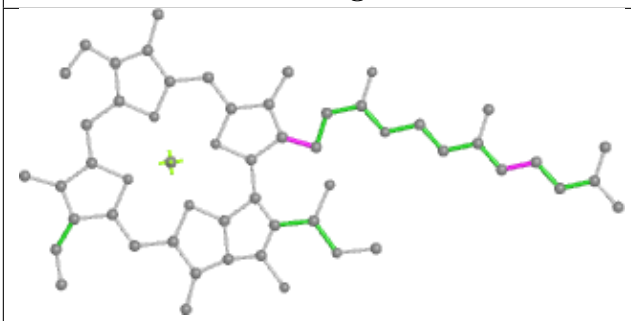


Bond angles



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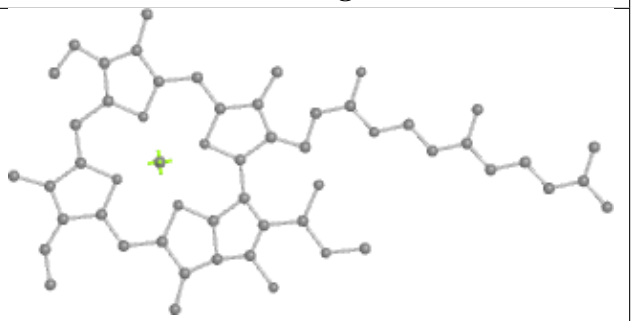
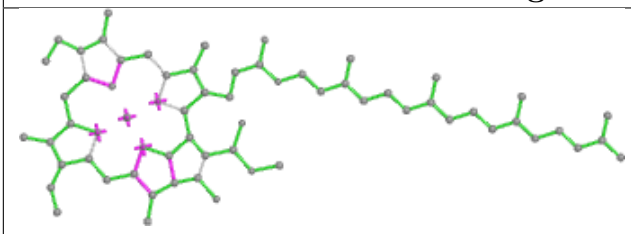


Rings

Ligand CLA b 724



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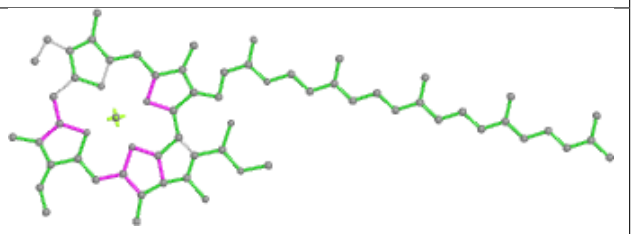
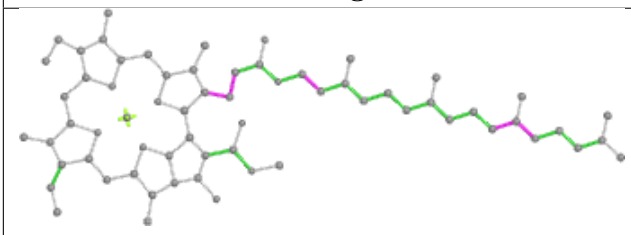


Bond angles



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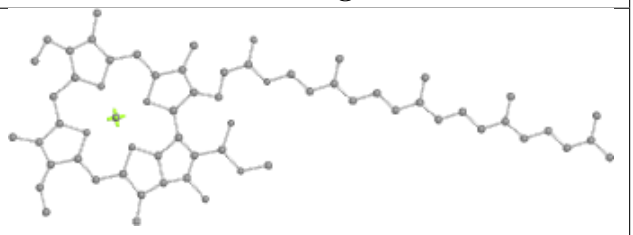
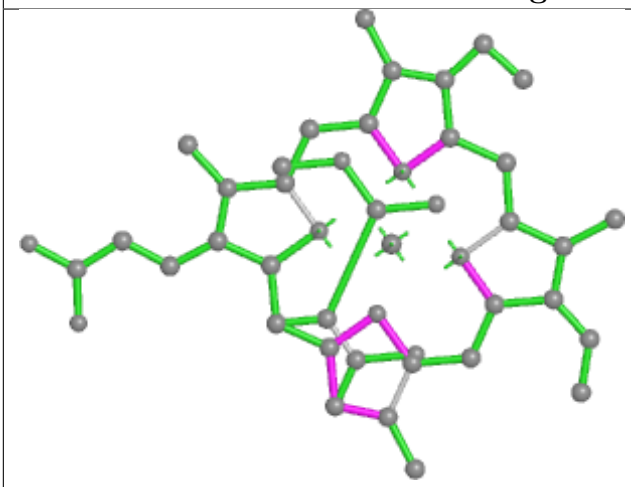


Rings

Ligand KC2 J 608



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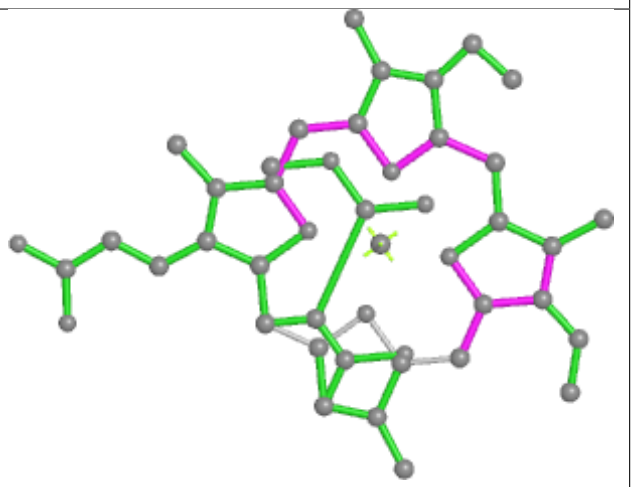
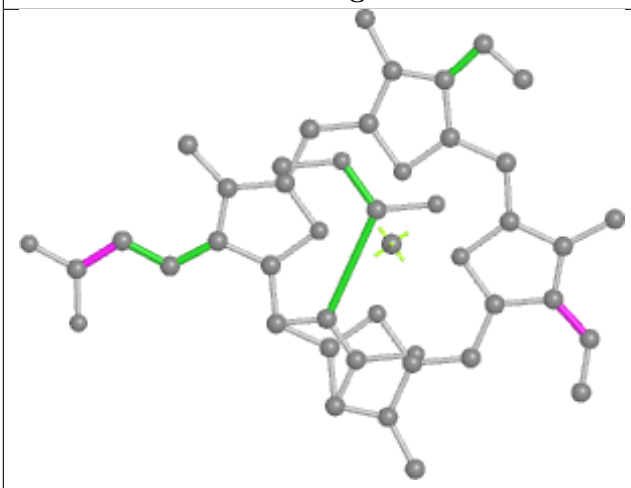


Bond angles



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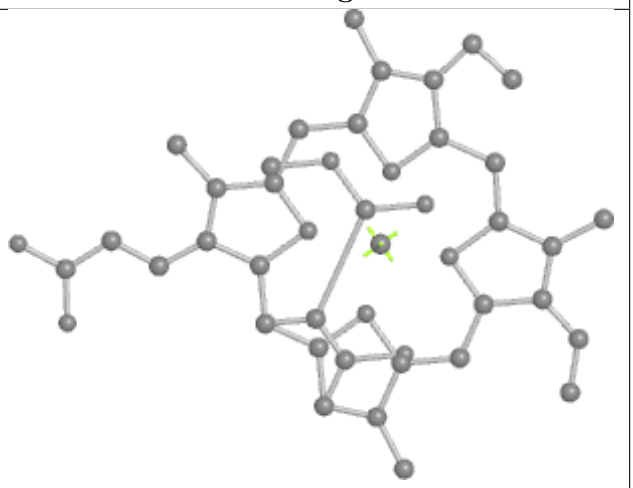
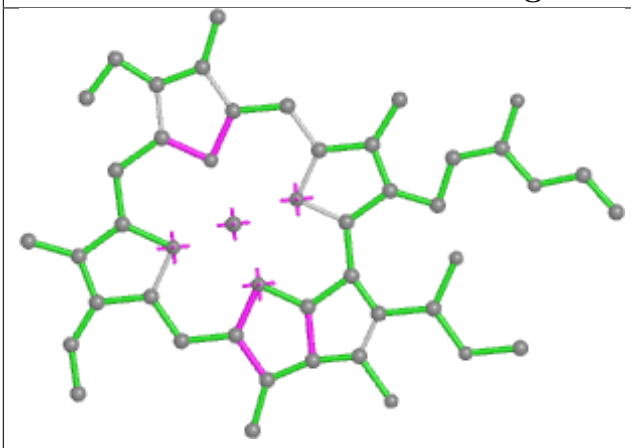


Rings

Ligand CLA C 211



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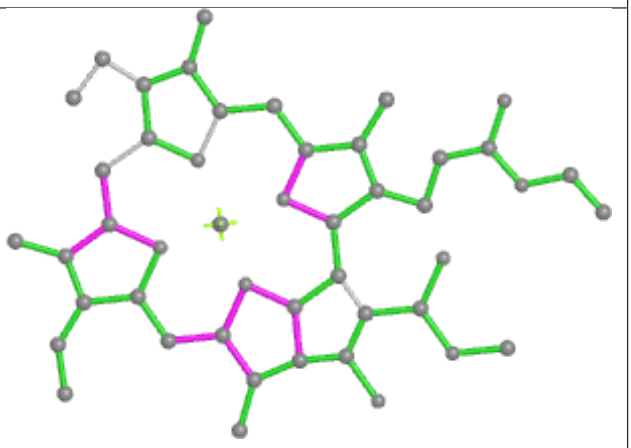
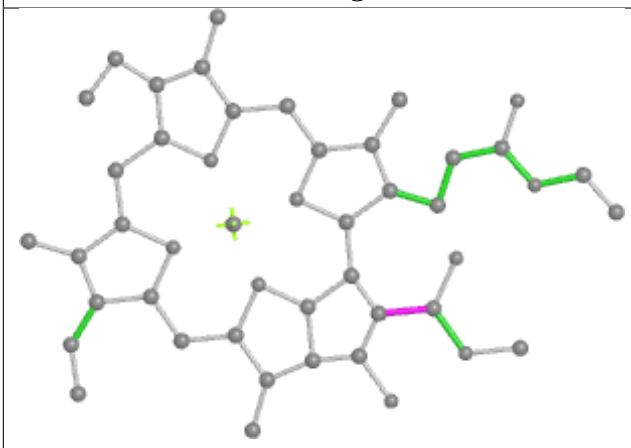


Bond angles



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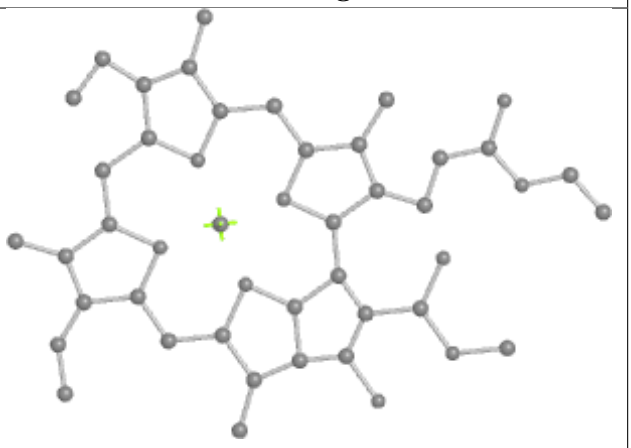
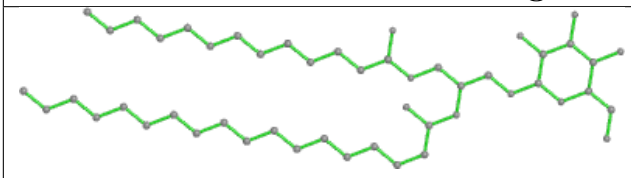


Rings

Ligand LMG l 417



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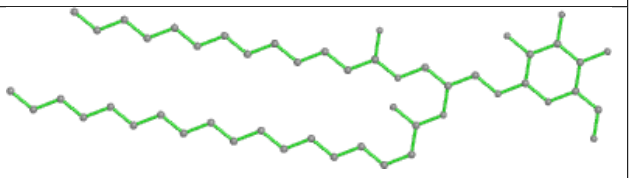

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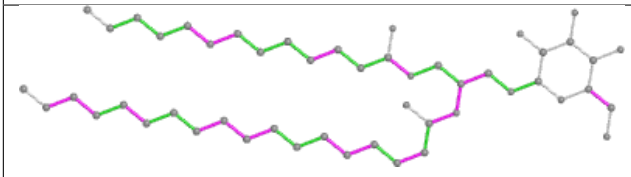

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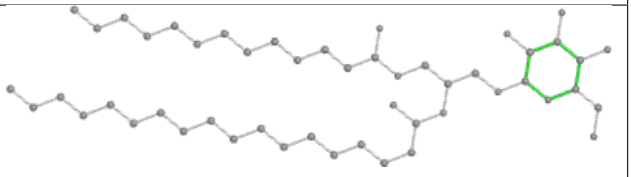
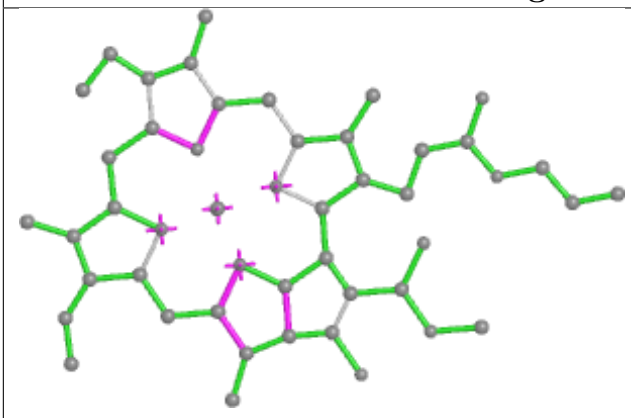


Rings

Ligand CLA a 828



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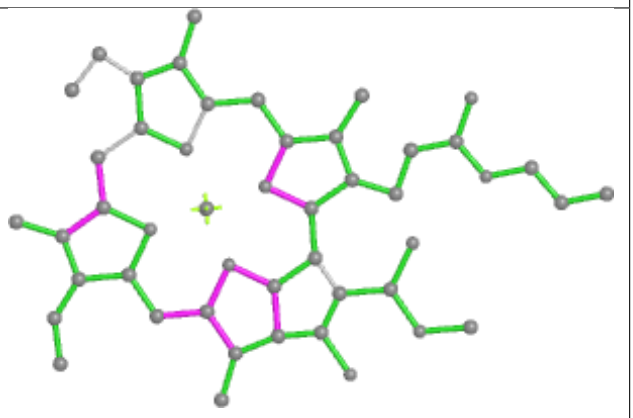
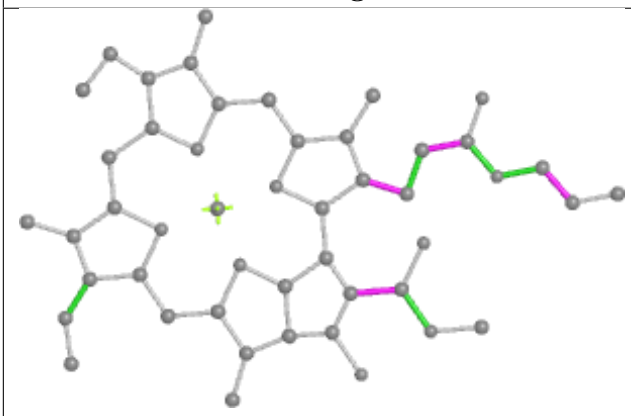


Bond angles



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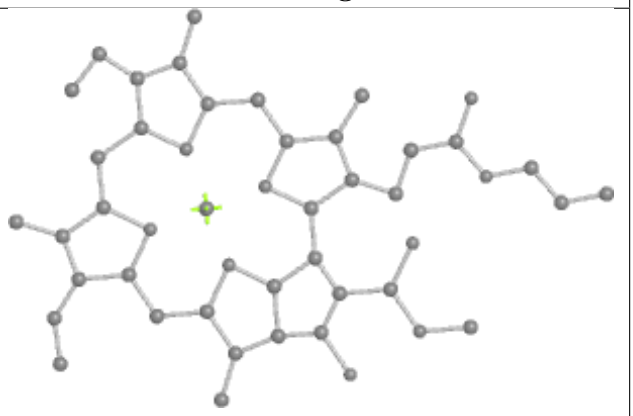
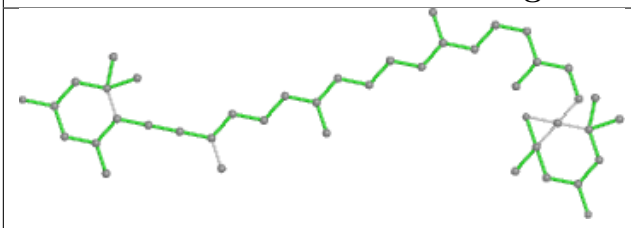


Rings

Ligand DD6 H 301



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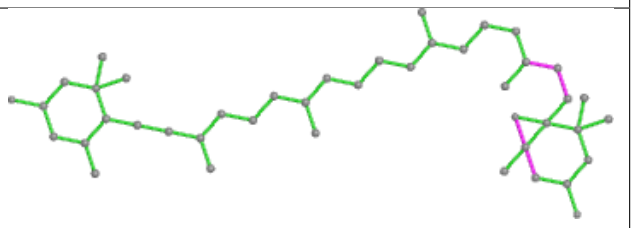
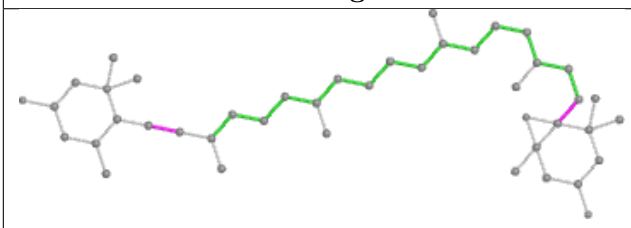


Bond angles



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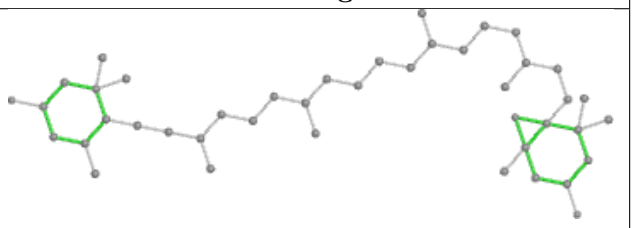
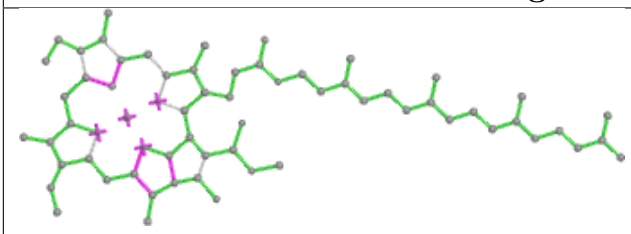
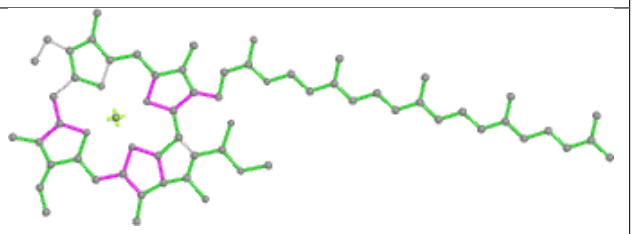


Rings

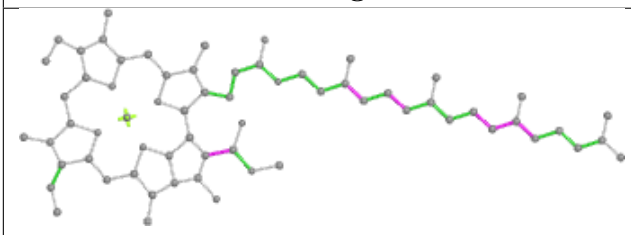
Ligand CLA a 824



Bond lengths



Bond angles



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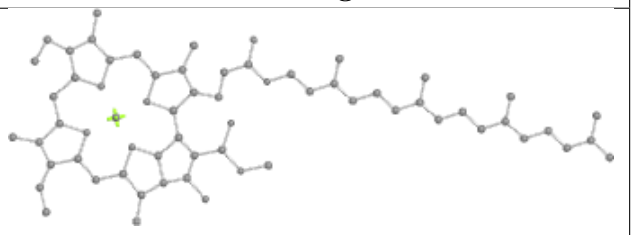
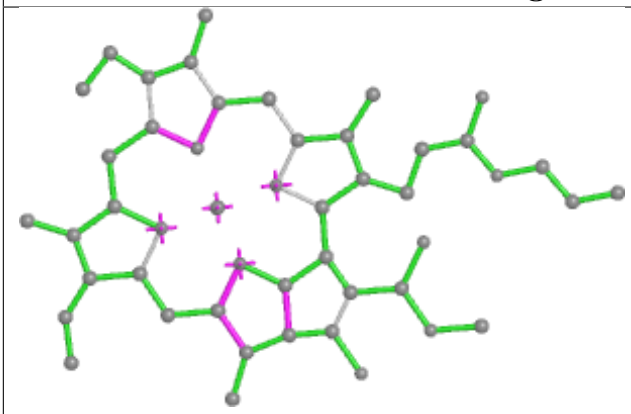


Rings

Ligand CLA b 722



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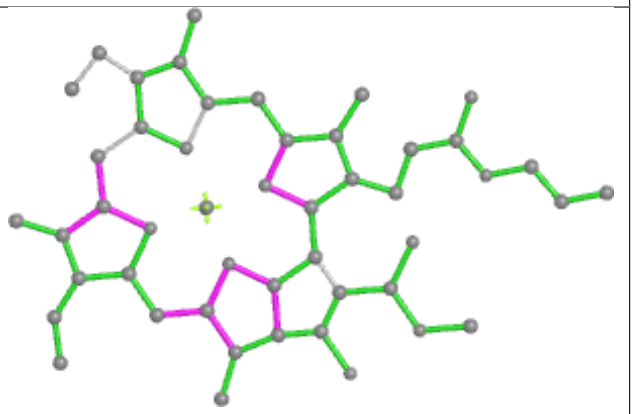
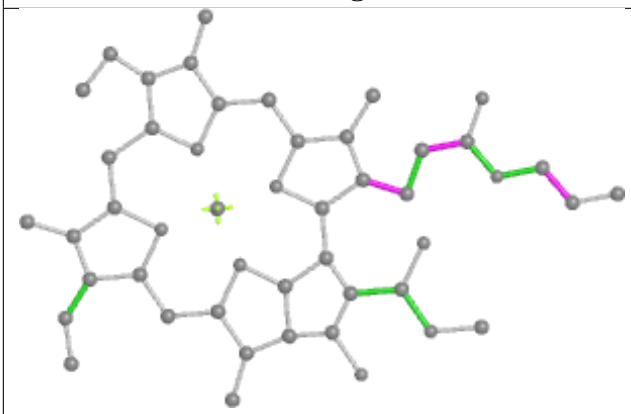


Bond angles



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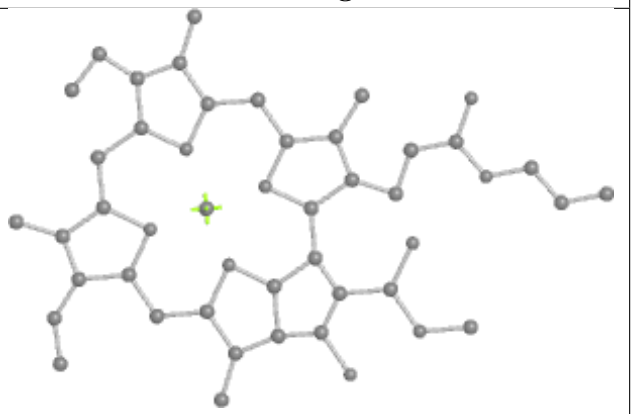
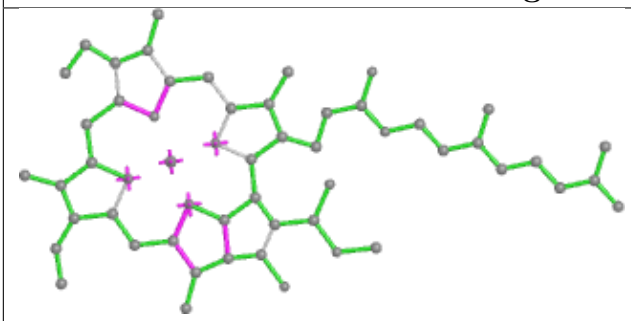


Rings

Ligand CLA D 603



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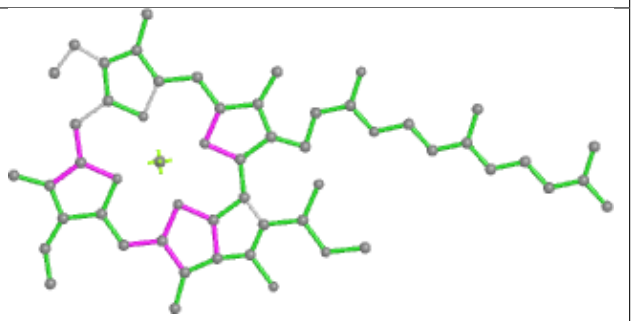
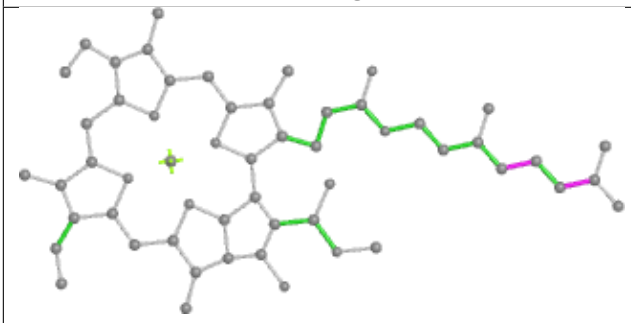


Bond angles



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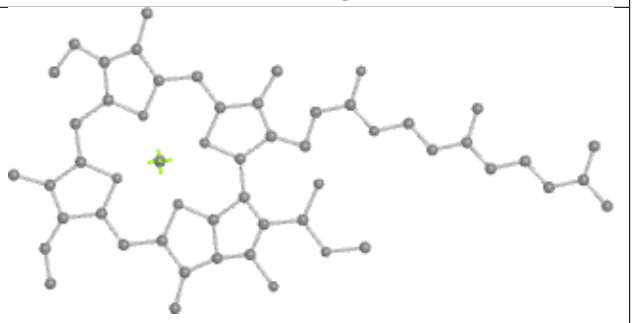
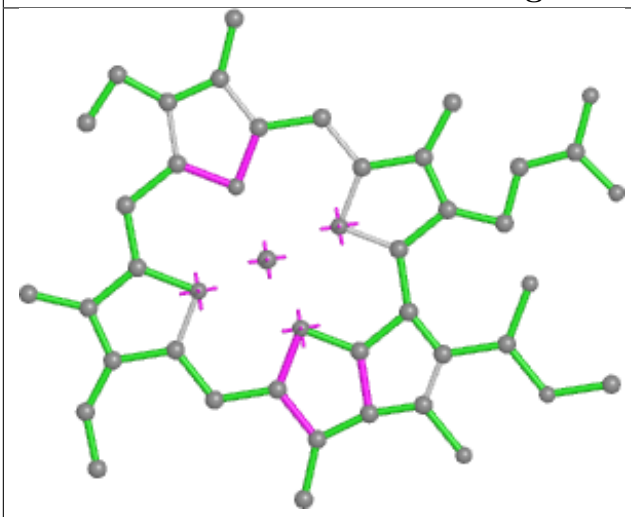


Rings

Ligand CLA E 609



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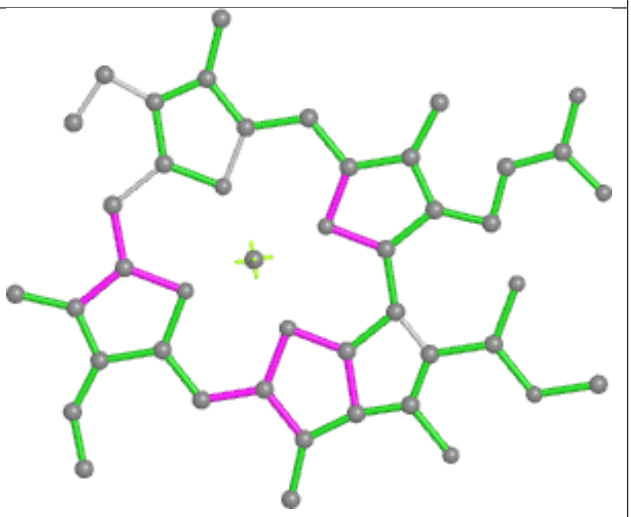
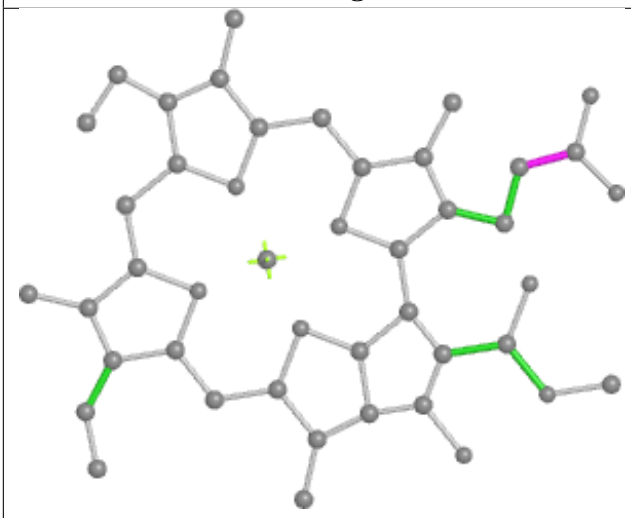


Bond angles



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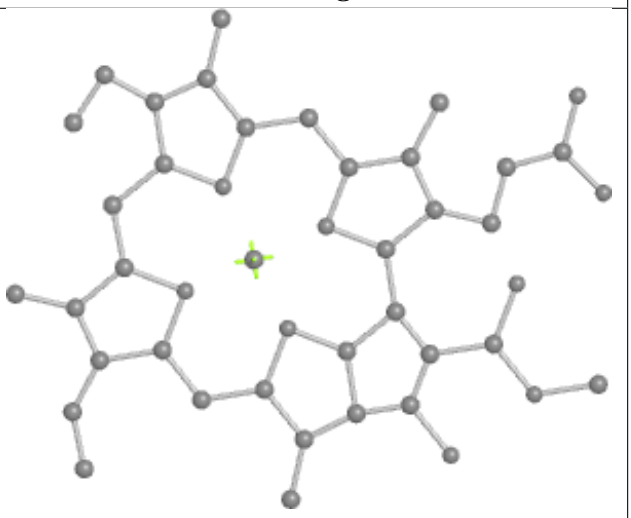
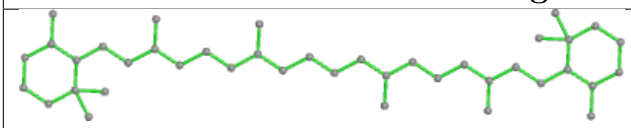


Rings

Ligand BCR l 414



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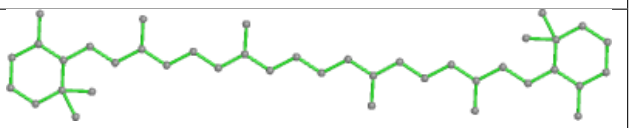
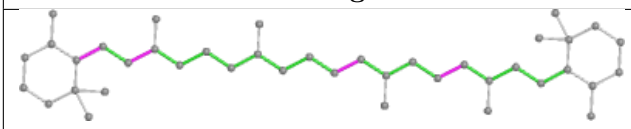


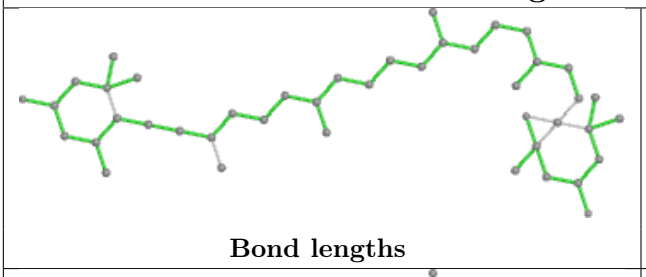
Bond angles



Torsions

Rings

Ligand DD6 J 612



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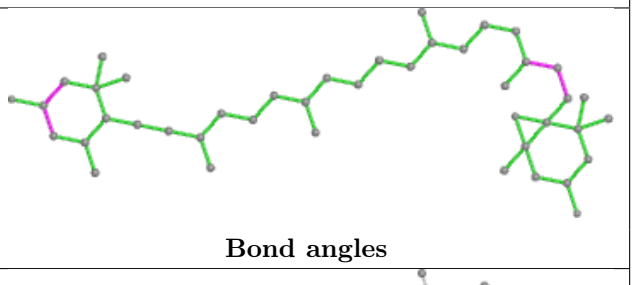
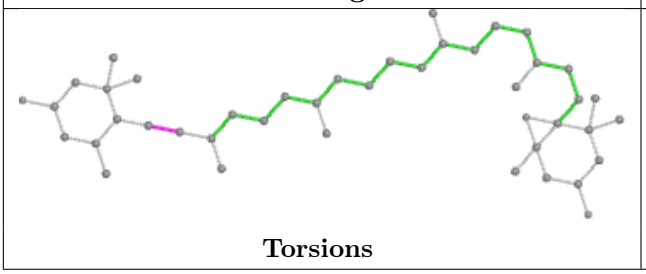
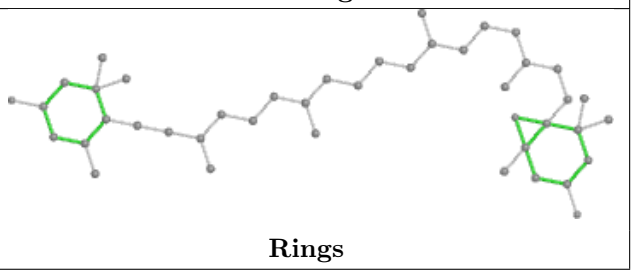


Bond angles

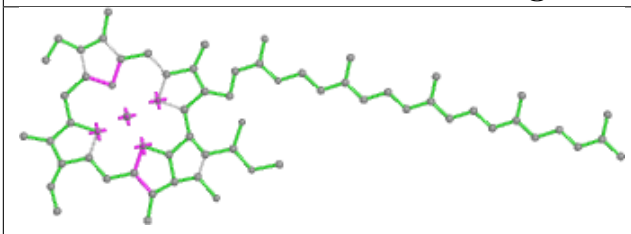


Torsions

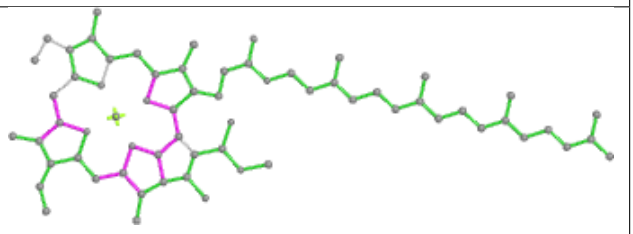


Rings

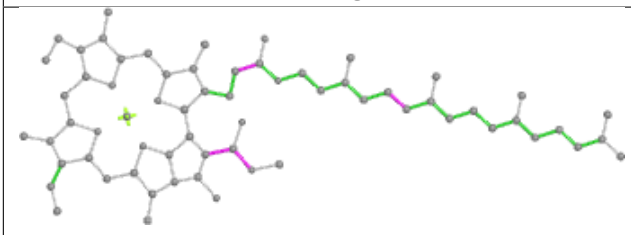
Ligand CLA a 801



Bond lengths



Bond angles



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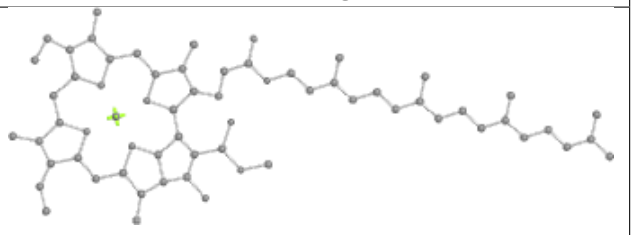
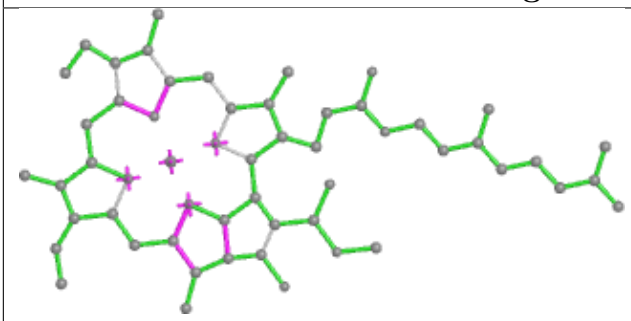
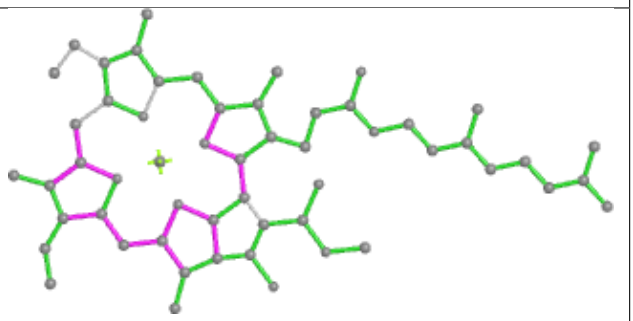


Rings

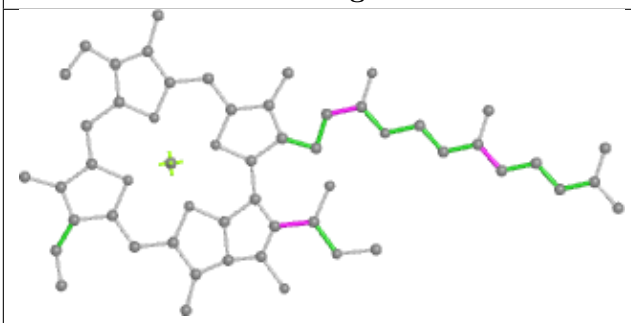
Ligand CLA G 609



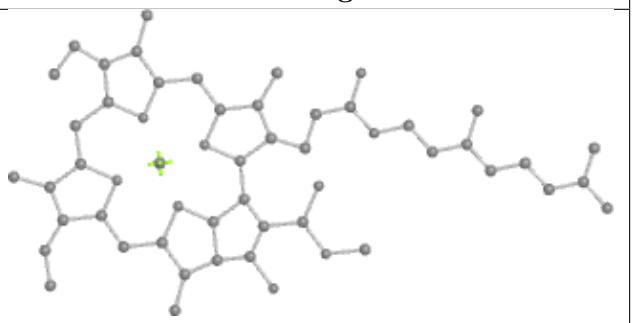
Bond lengths



Bond angles

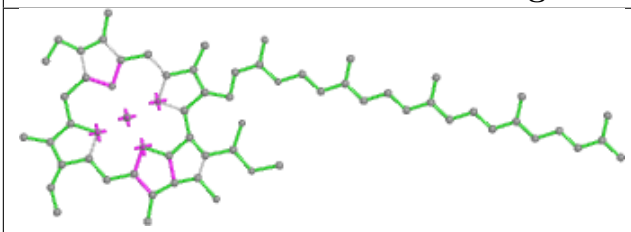


Torsions



Rings

Ligand CLA a 804



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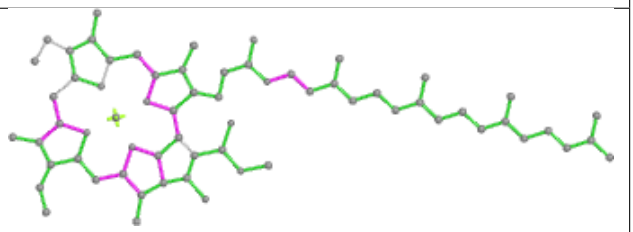
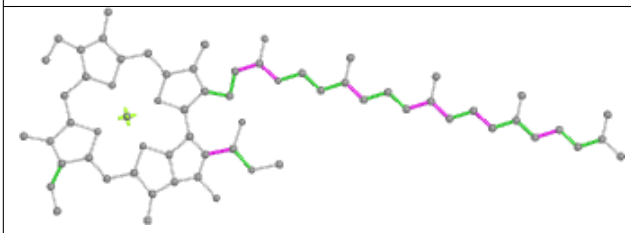


Bond angles



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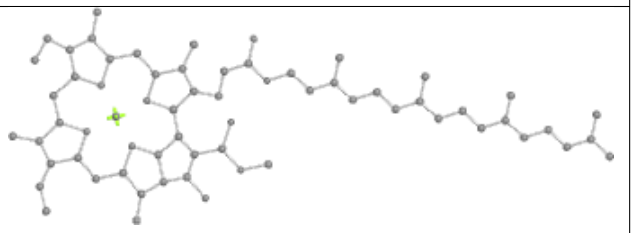
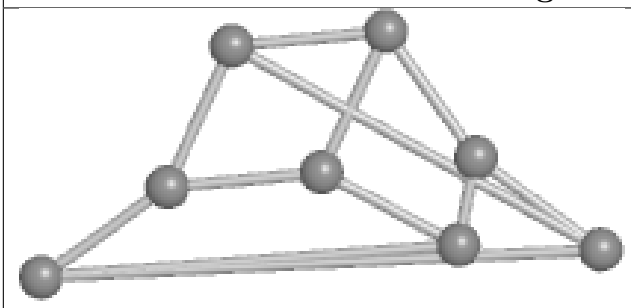


Rings

Ligand SF4 c 201



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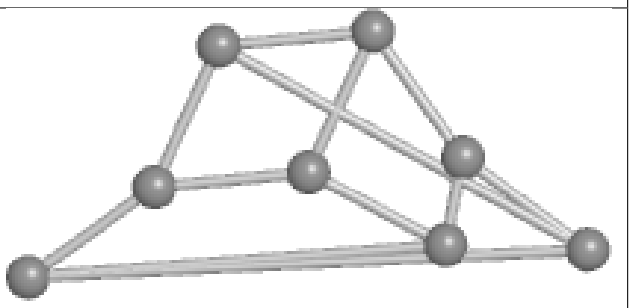
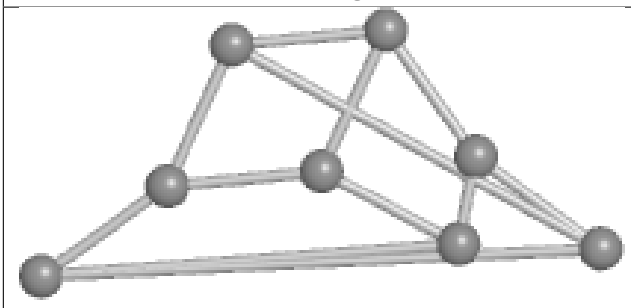


Bond angles



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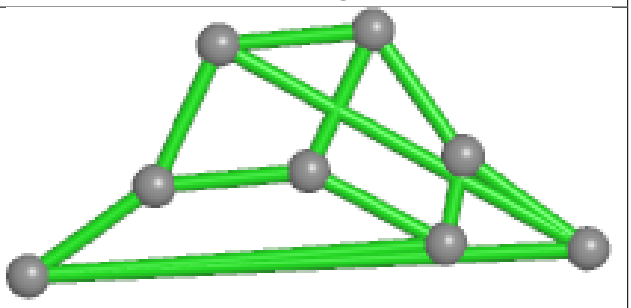
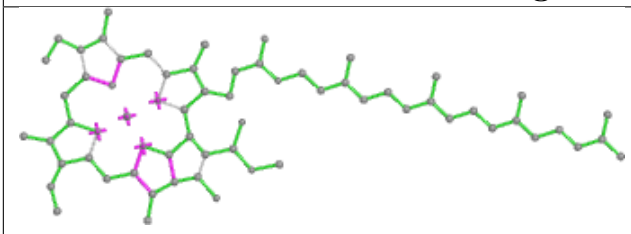


Rings

Ligand CLA l 412



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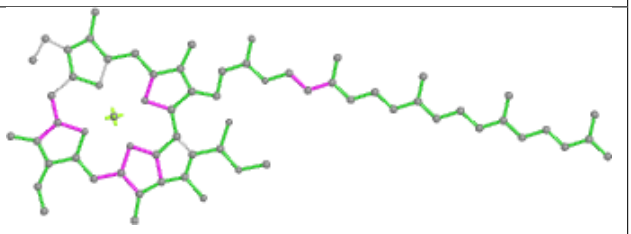
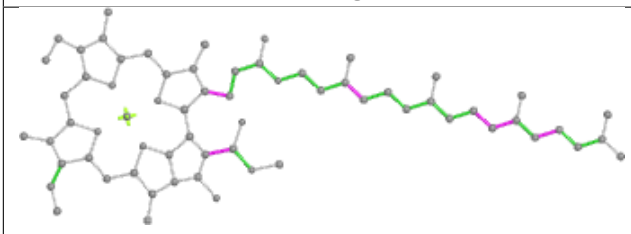


Bond angles



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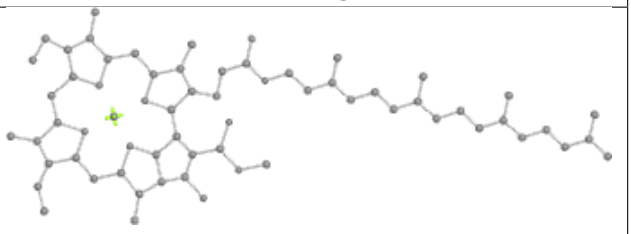
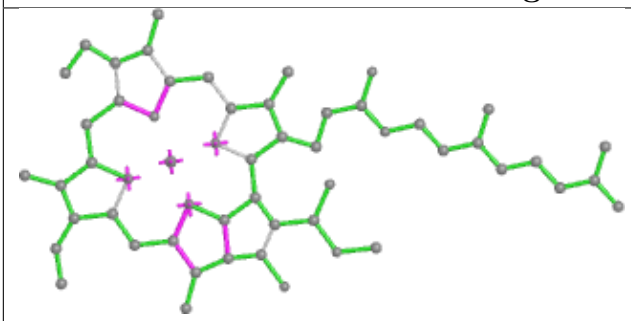


Rings

Ligand CLA G 602



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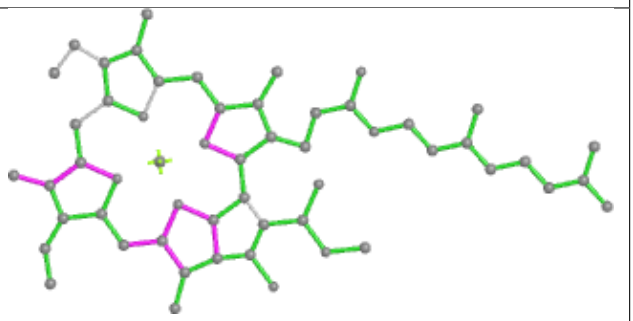
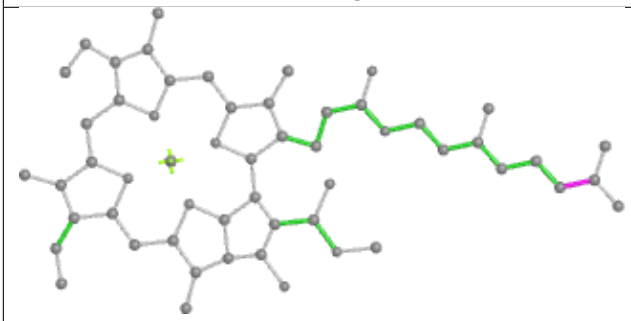


Bond angles



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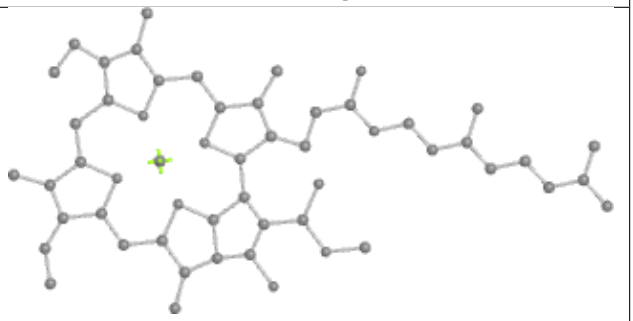
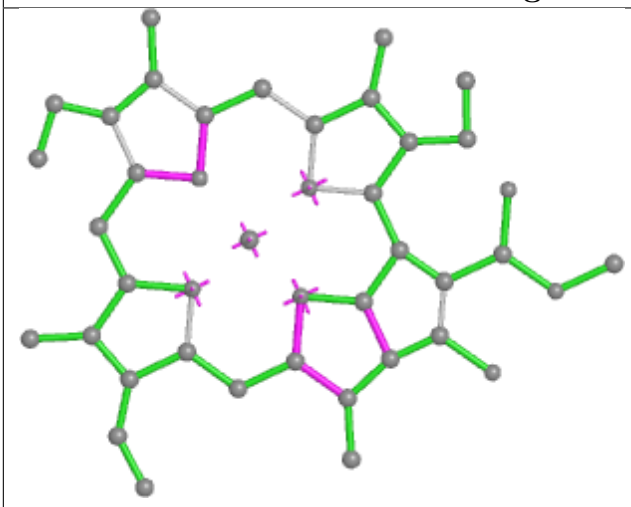


Rings

Ligand CLA A 601



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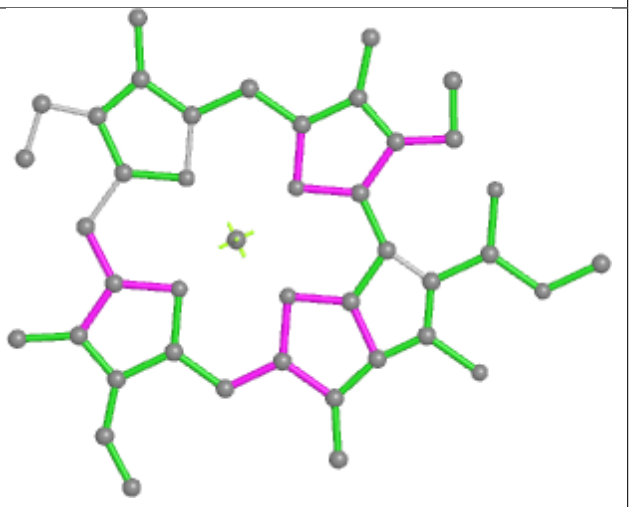
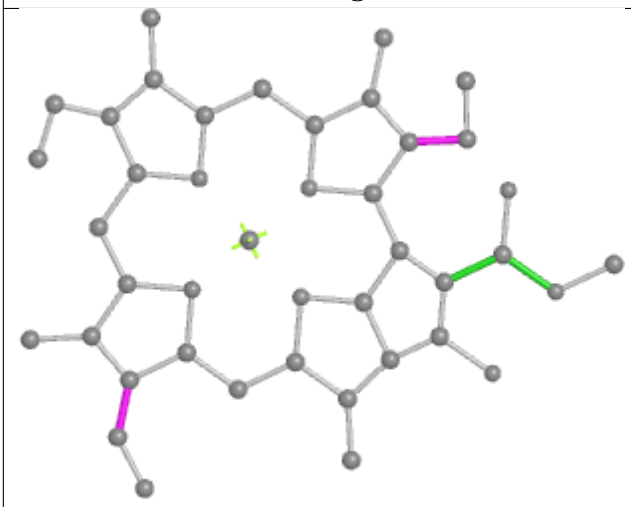


Bond angles



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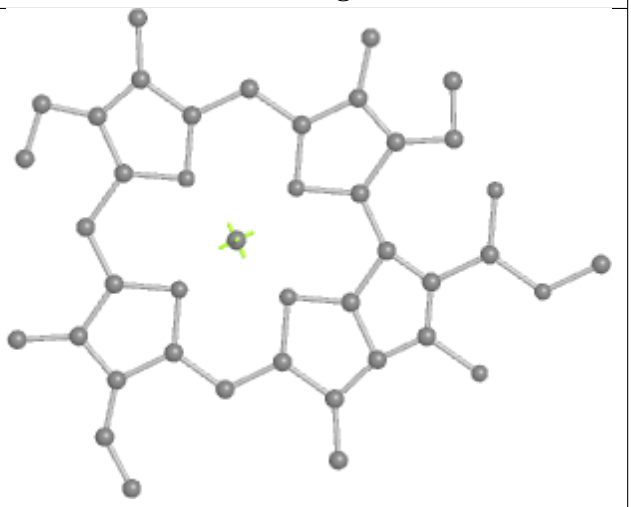
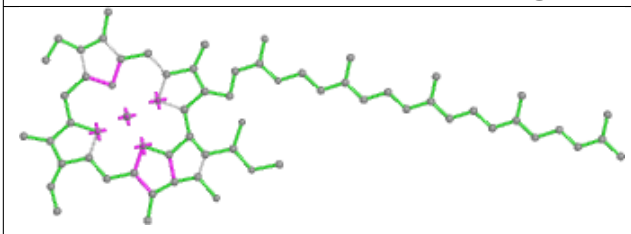


Rings

Ligand CLA I 616



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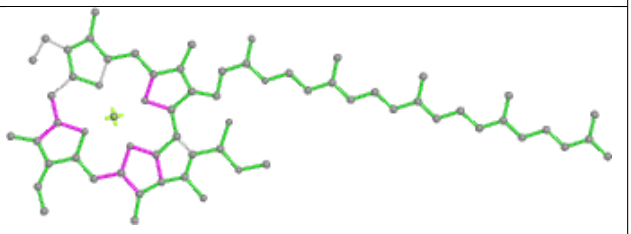
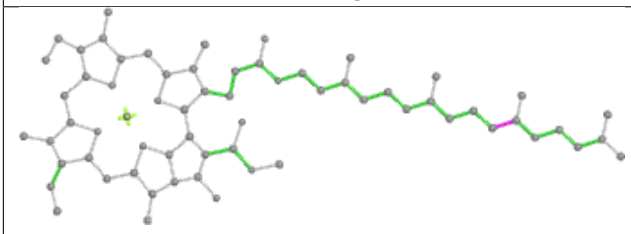


Bond angles



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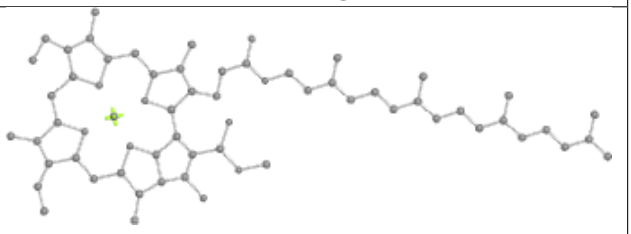
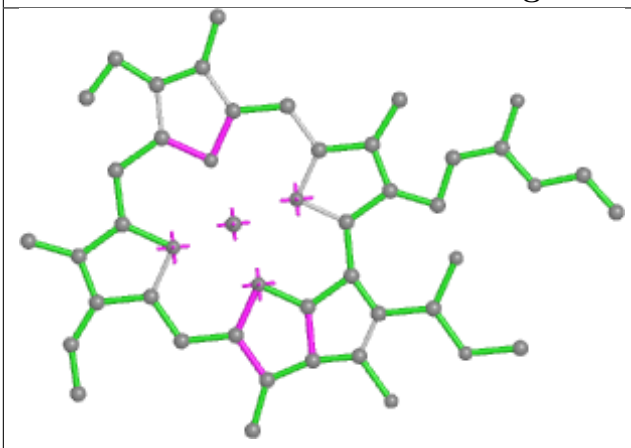


Rings

Ligand CLA G 610



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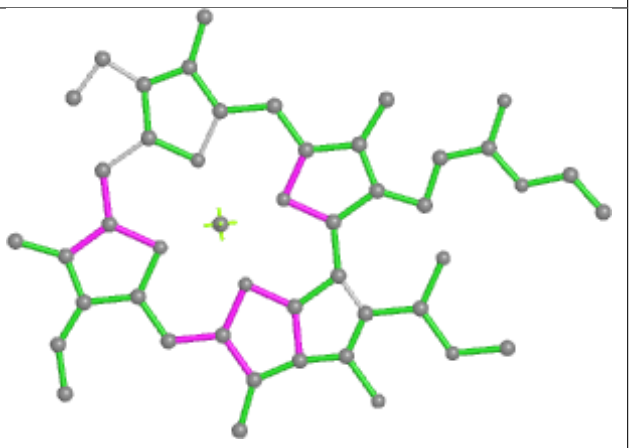
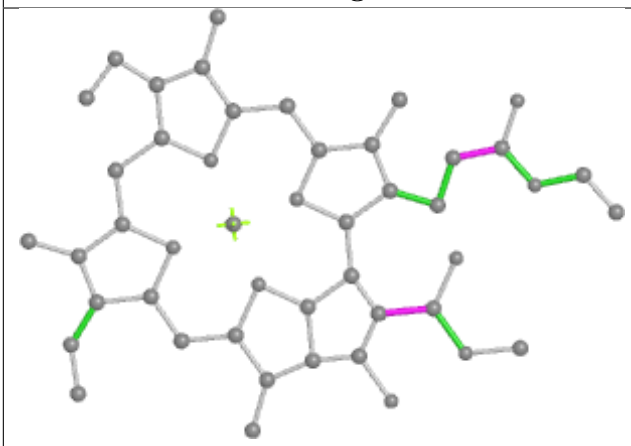


Bond angles



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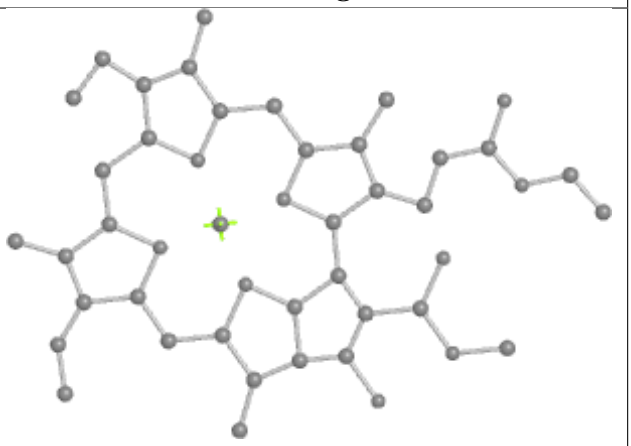
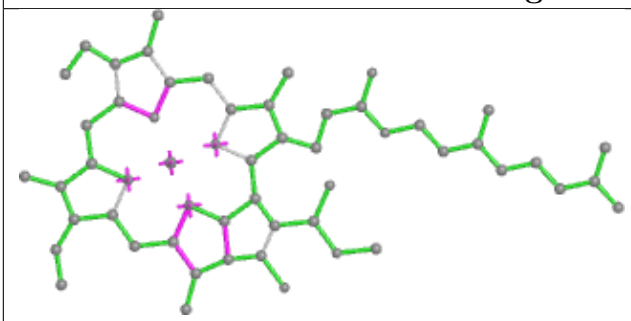


Rings

Ligand CLA E 604



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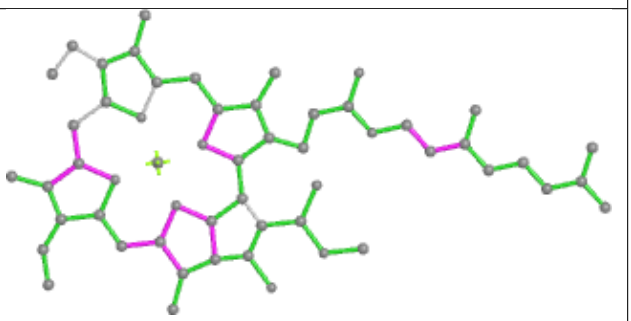
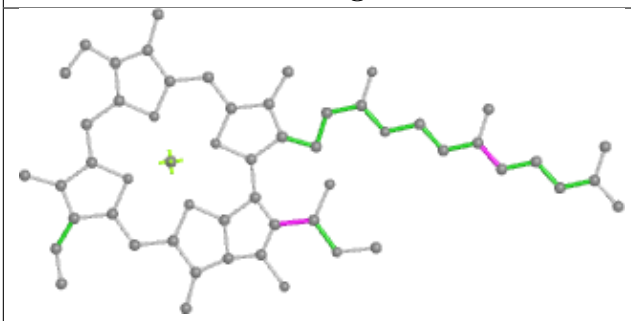


Bond angles



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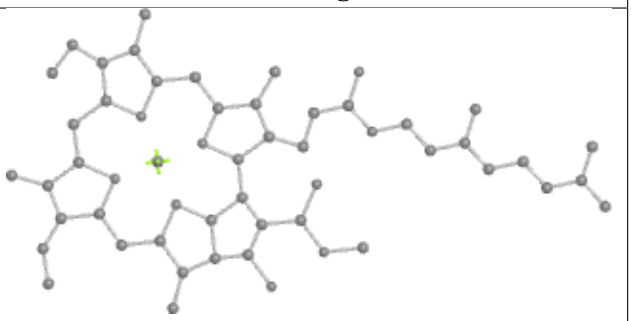
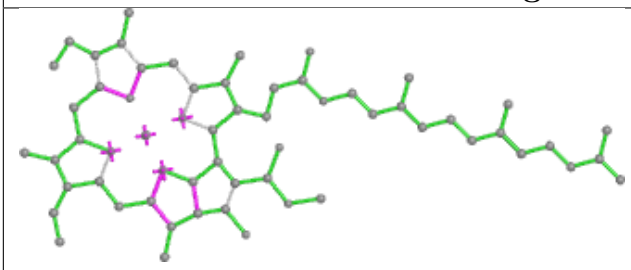


Rings

Ligand CLA D 611



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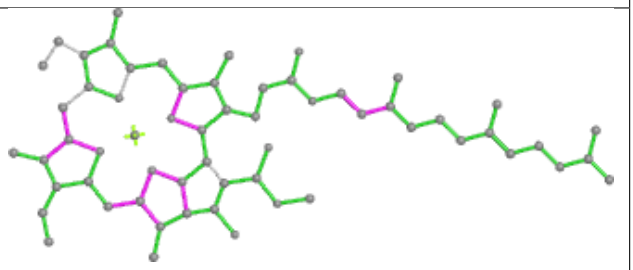

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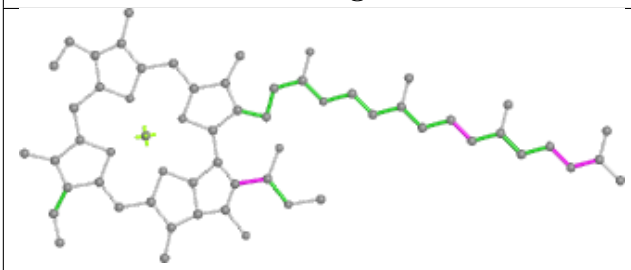

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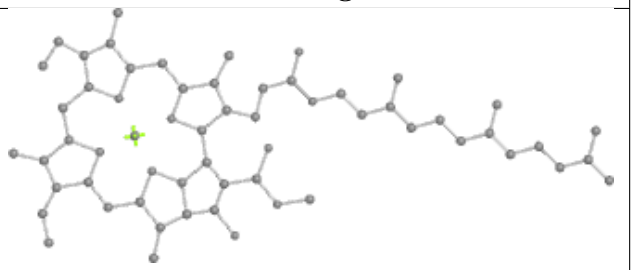
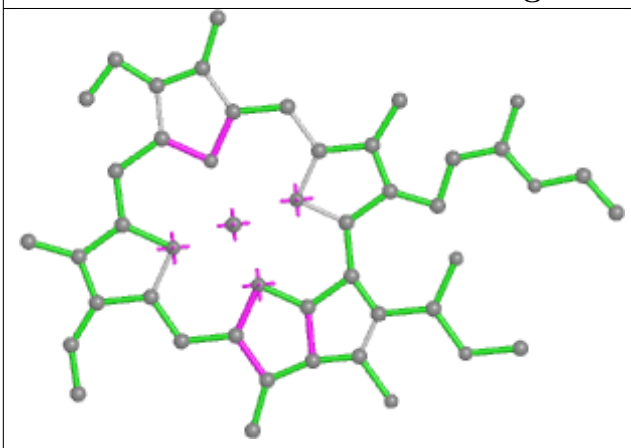


Rings

Ligand CLA A 606



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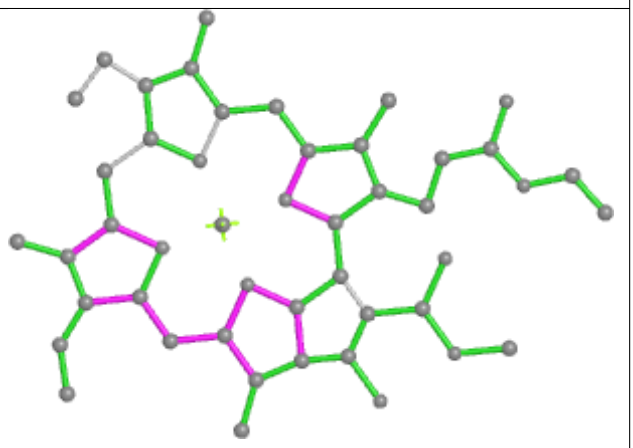

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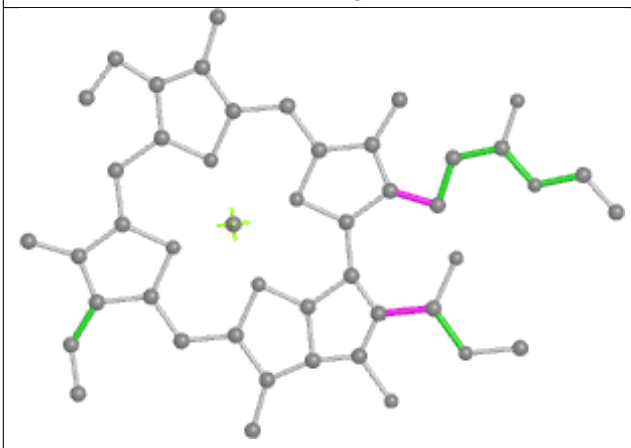

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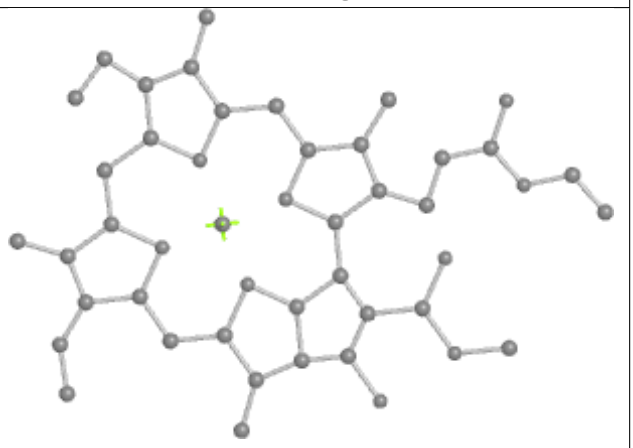
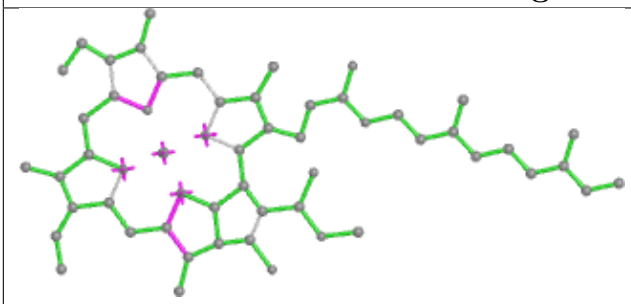


Rings

Ligand CLA j 202



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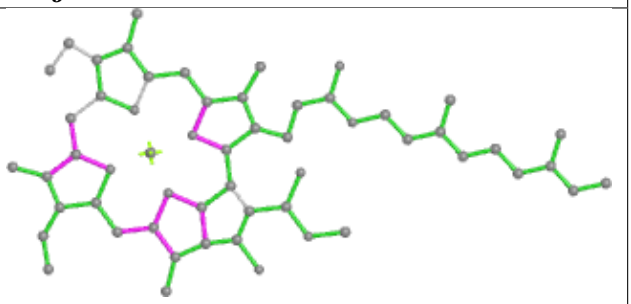
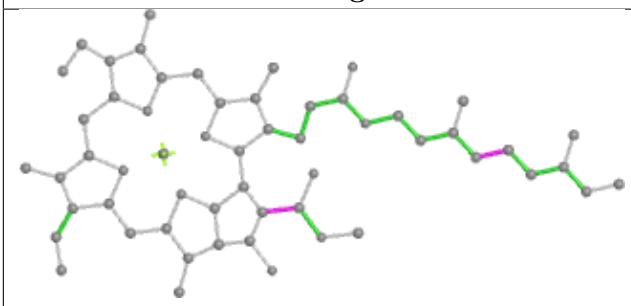


Bond angles



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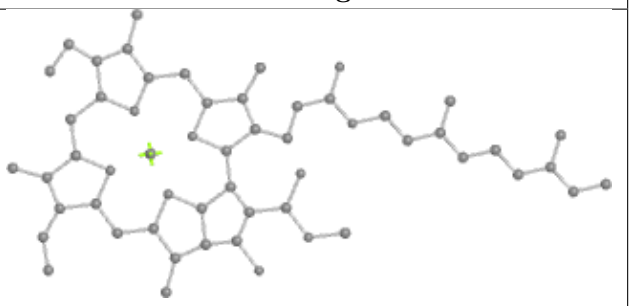
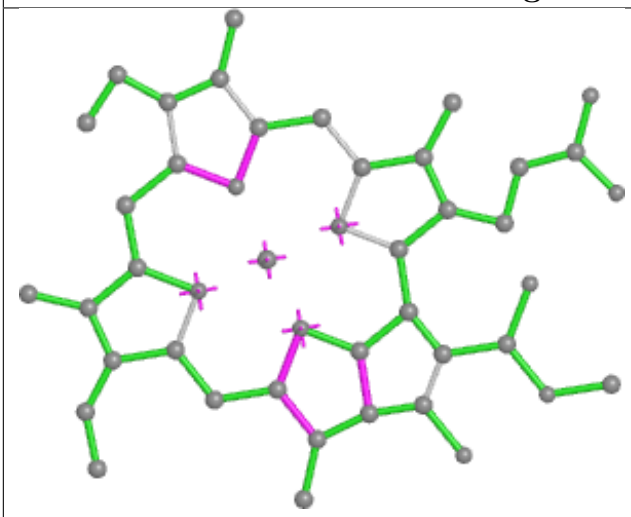


Rings

Ligand CLA D 601



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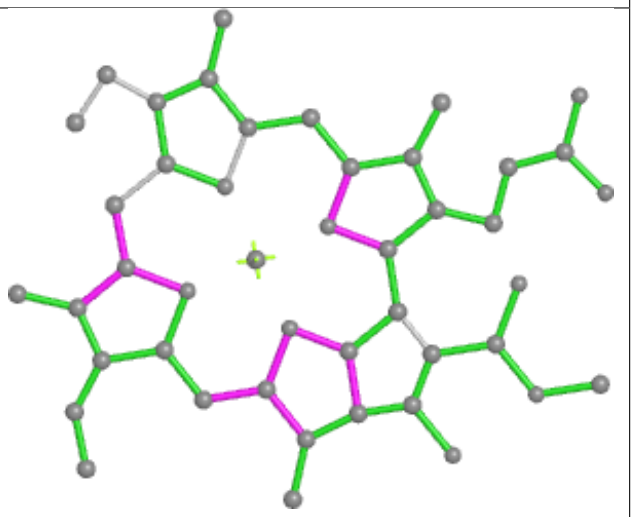
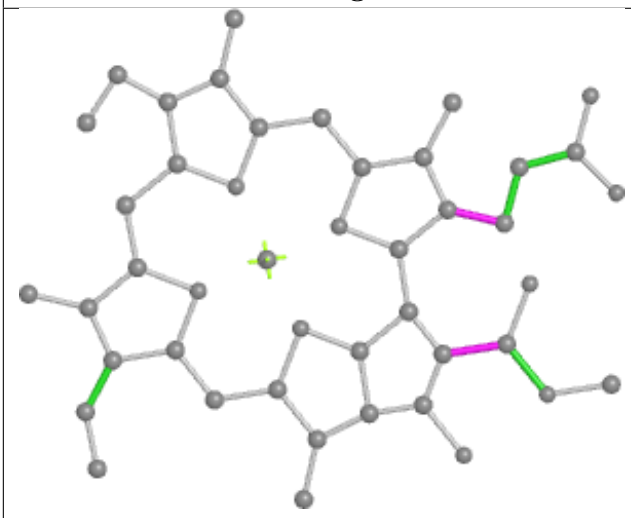


Bond angles



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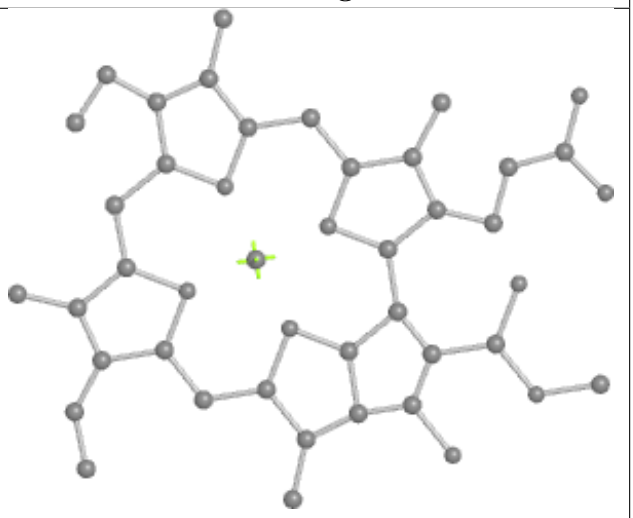
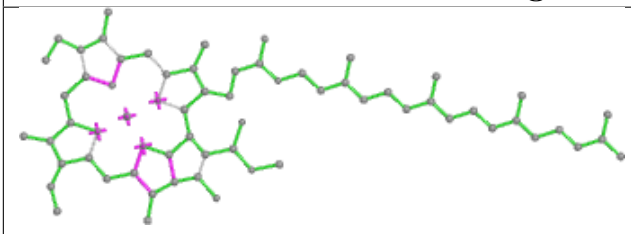


Rings

Ligand CLA b 704



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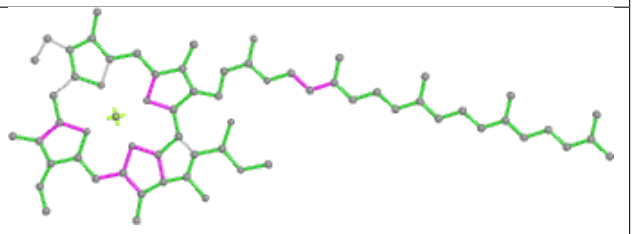
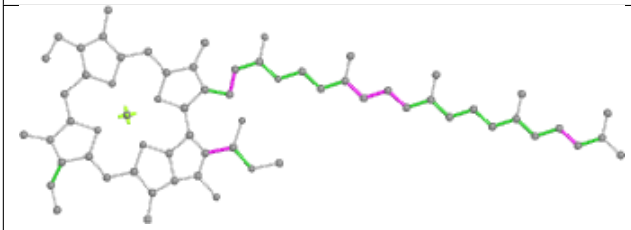


Bond angles



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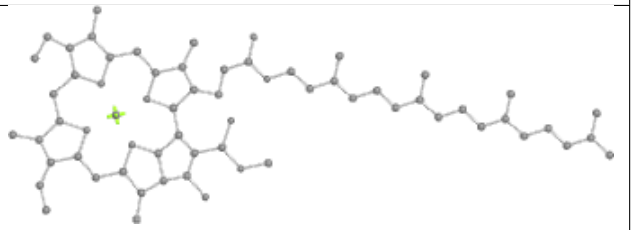
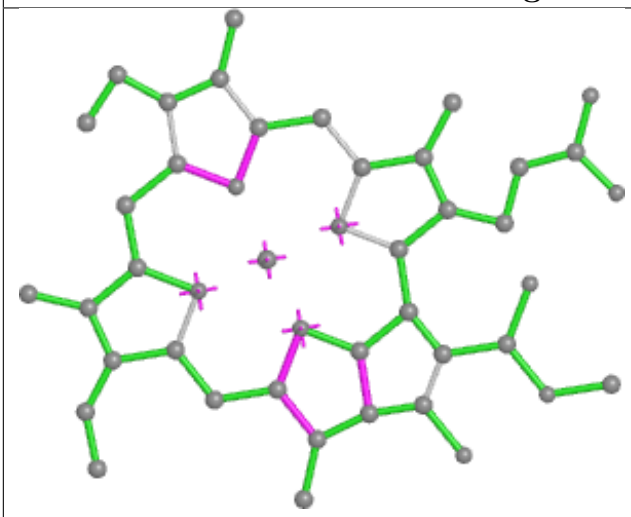
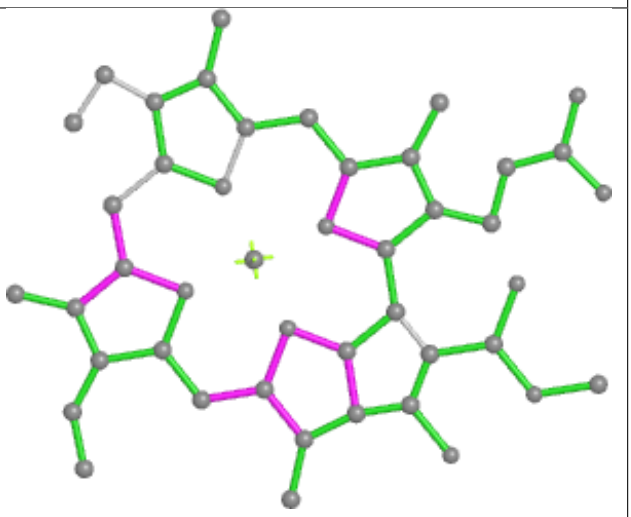


Rings

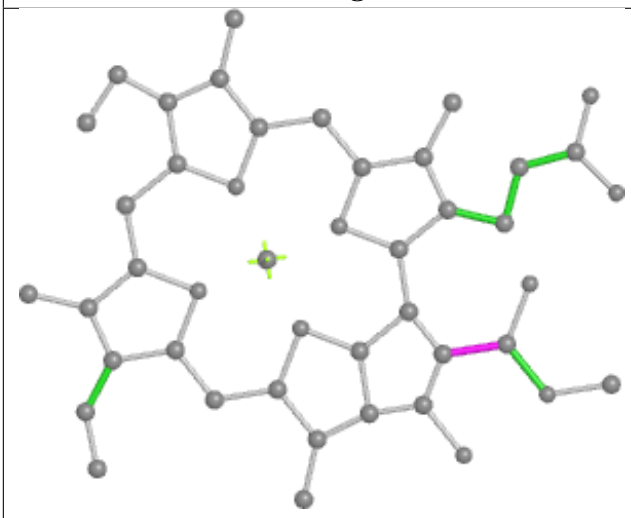
Ligand CLA D 606



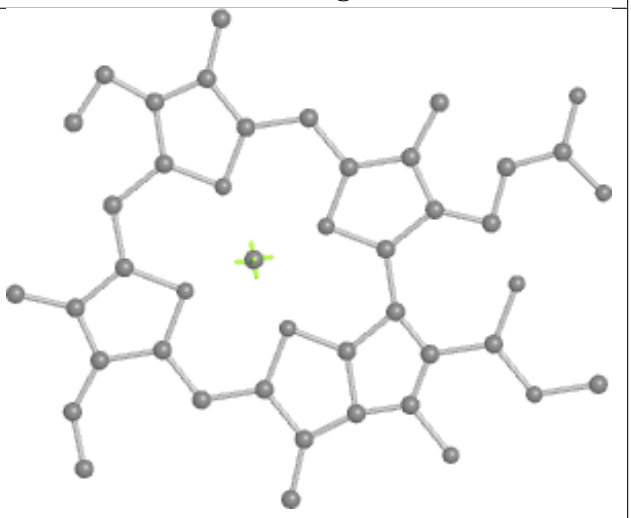
Bond lengths



Bond angles

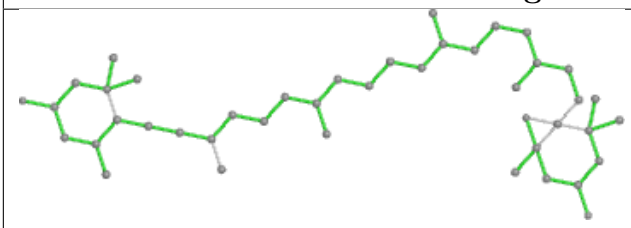


Torsions

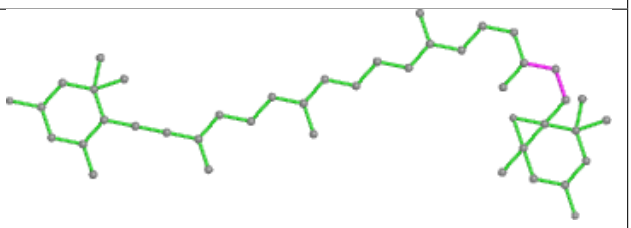


Rings

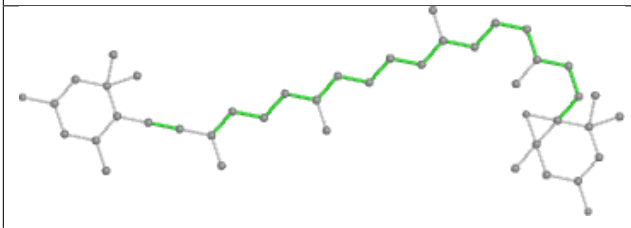
Ligand DD6 H 315



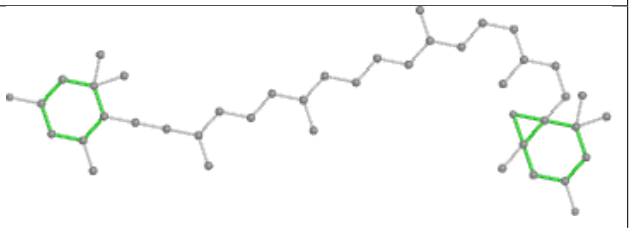
Bond lengths



Bond angles

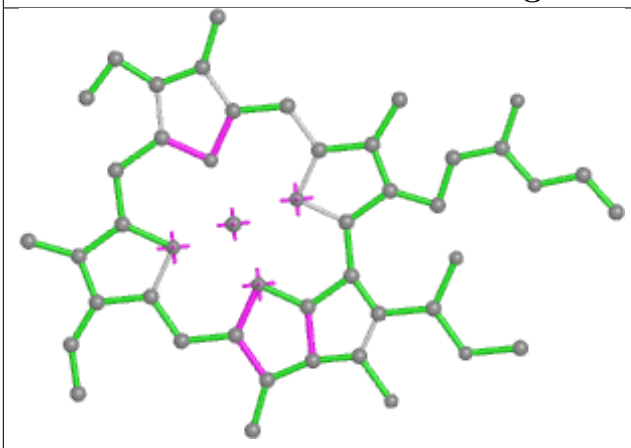


Torsions



Rings

Ligand CLA A 609



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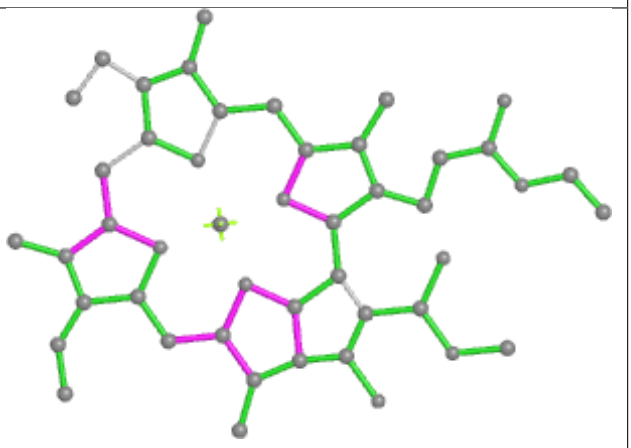
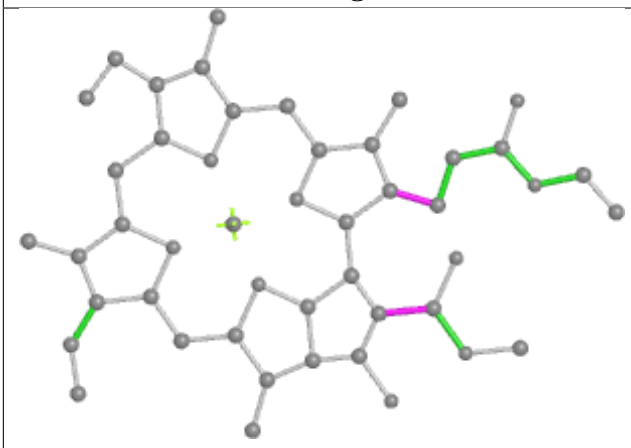
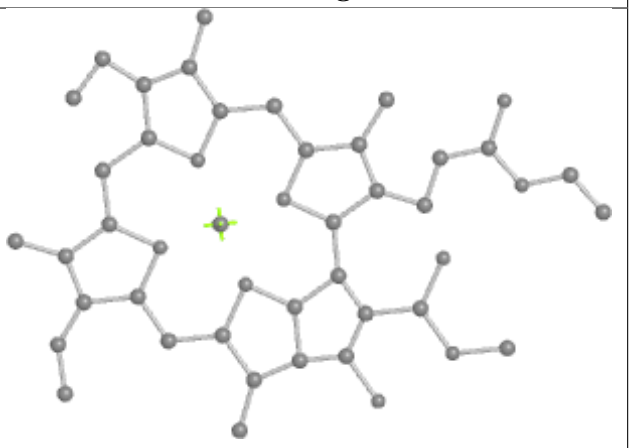


Bond angles

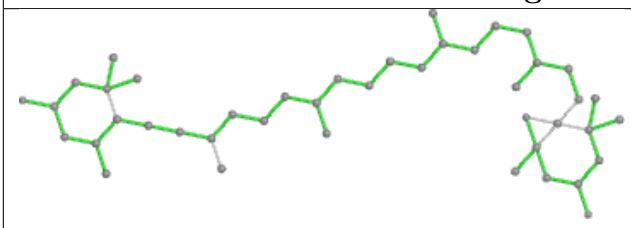


Torsions



Rings

Ligand DD6 A 614



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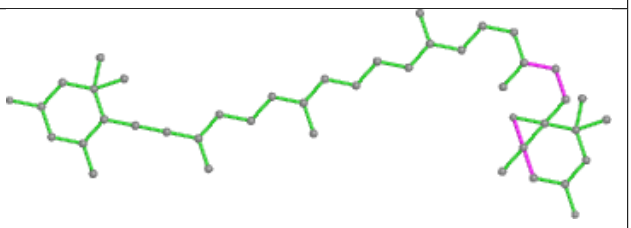
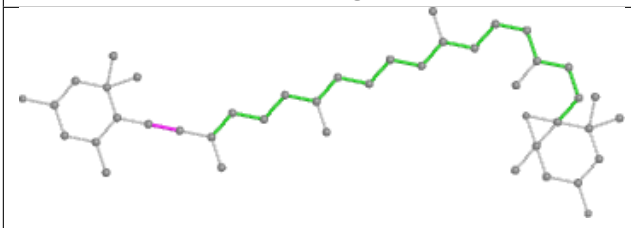


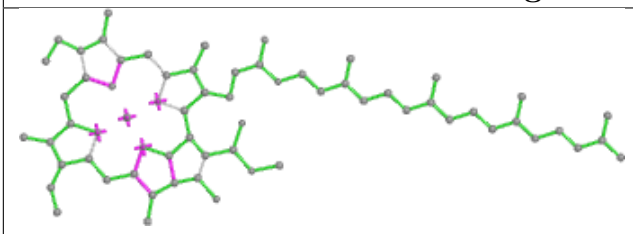
Bond angles



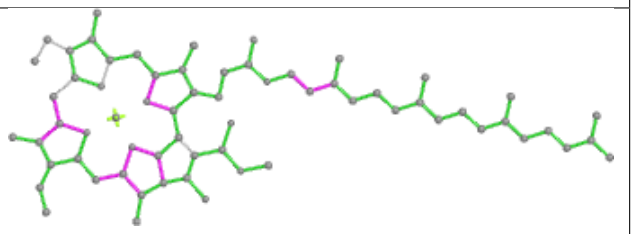
Torsions

Rings

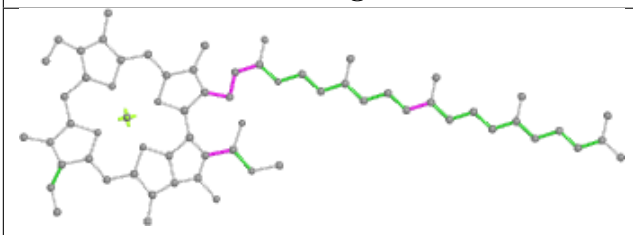
Ligand CLA C 204



Bond lengths



Bond angles



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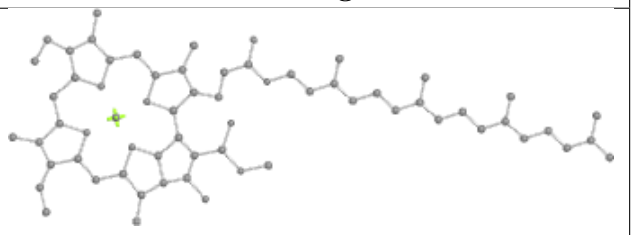
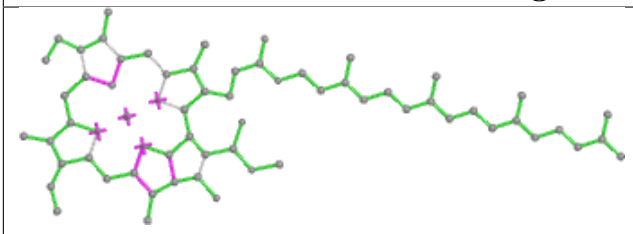


Rings

Ligand CLA I 601



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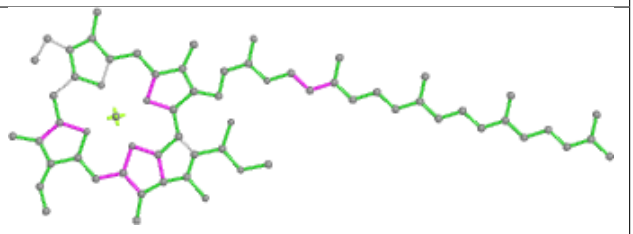
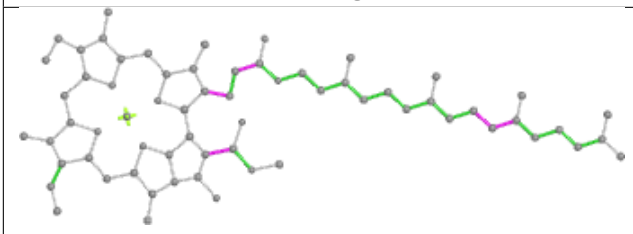


Bond angles



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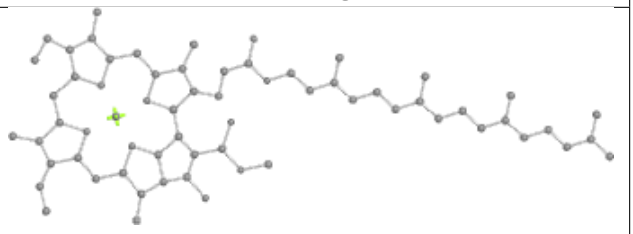
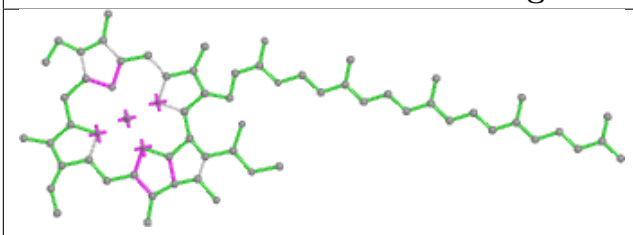


Rings

Ligand CLA b 709



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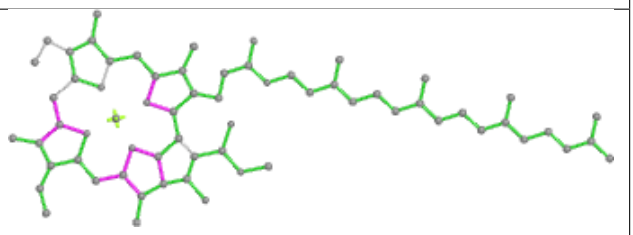
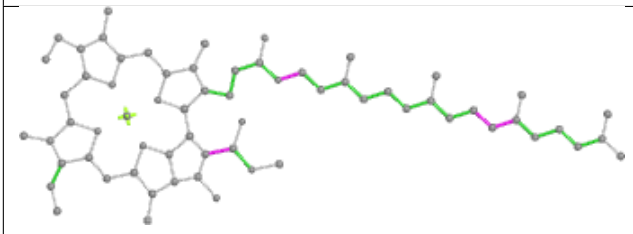


Bond angles



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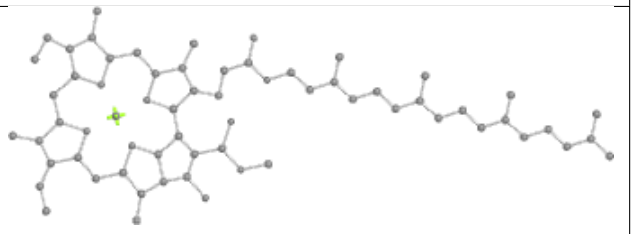
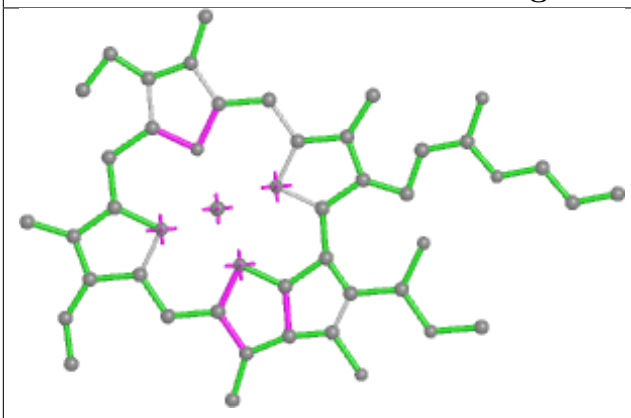


Rings

Ligand CLA r 203



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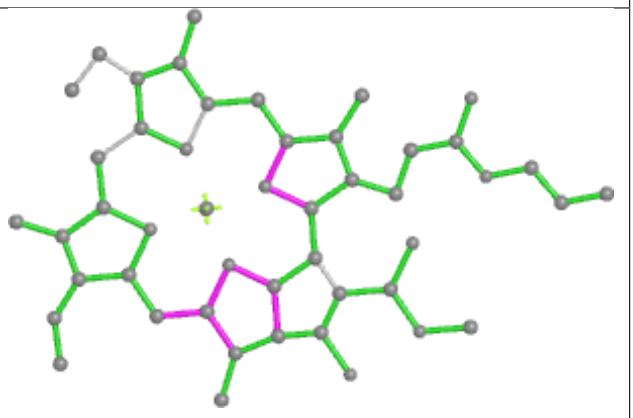
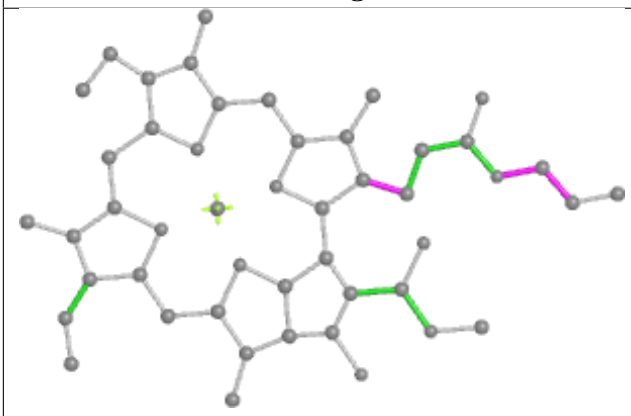


Bond angles



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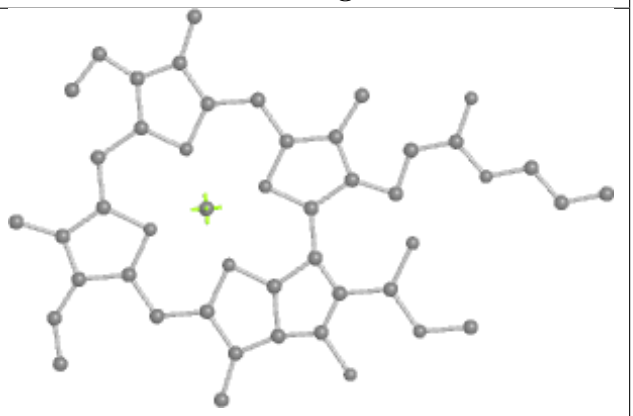
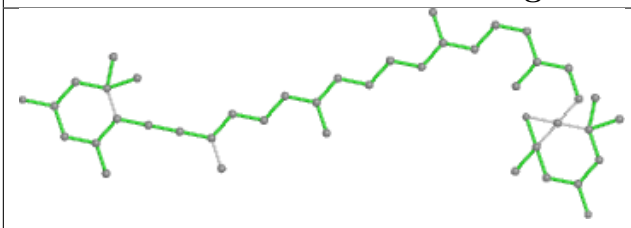


Rings

Ligand DD6 D 614



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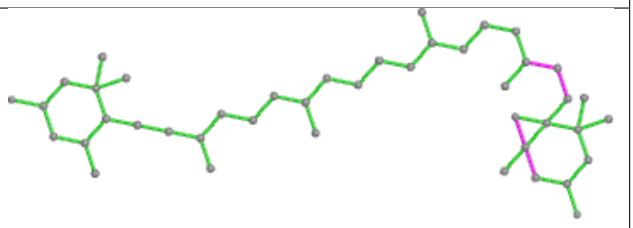
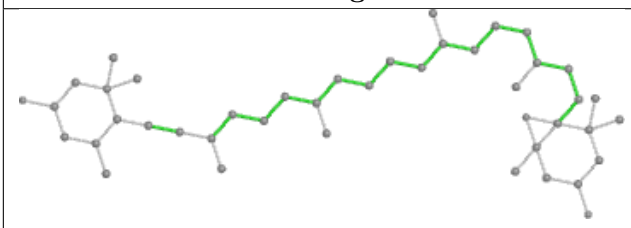


Bond angles



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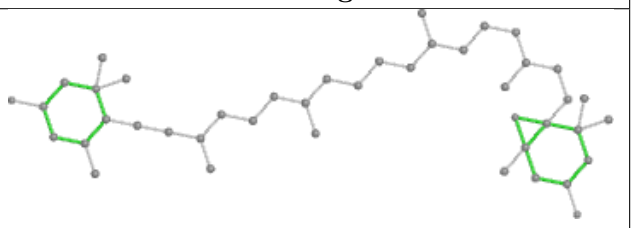
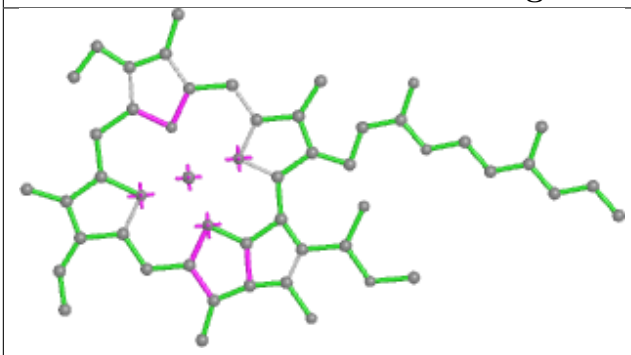


Rings

Ligand CLA F 603



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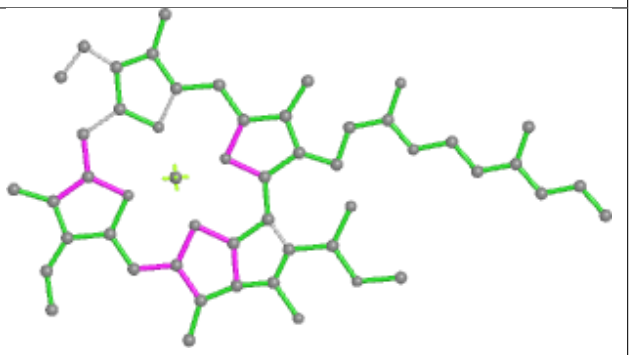
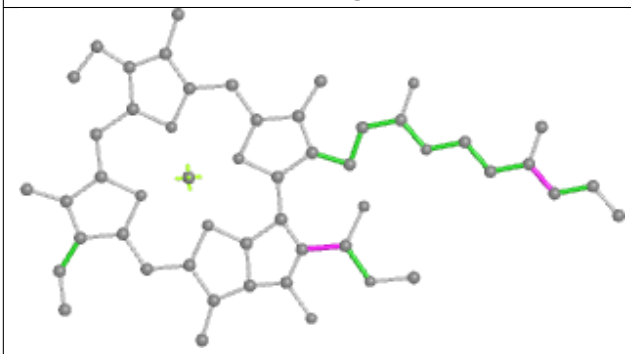


Bond angles



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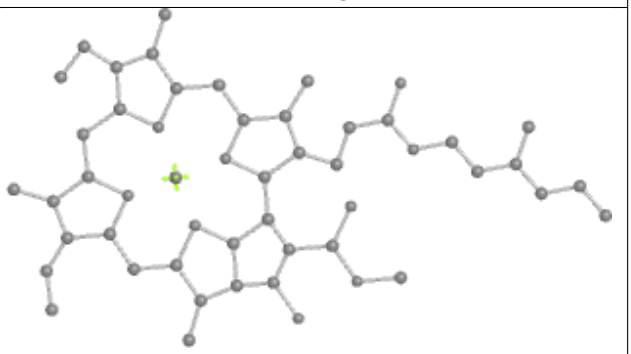
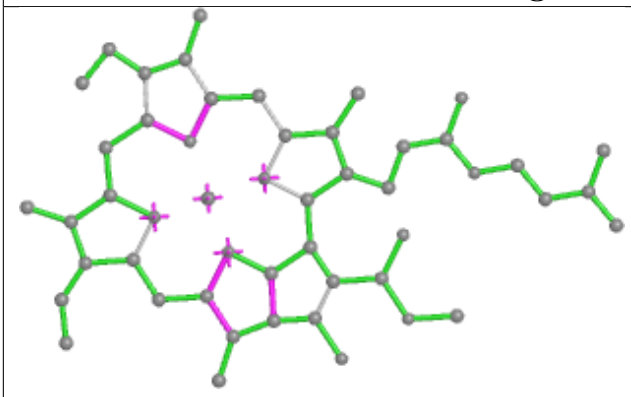


Rings

Ligand CLA a 812



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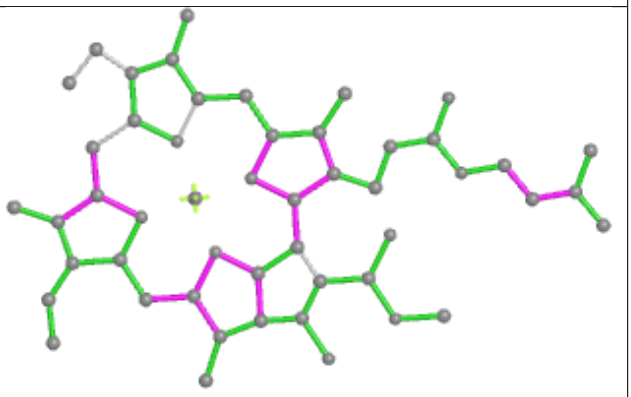
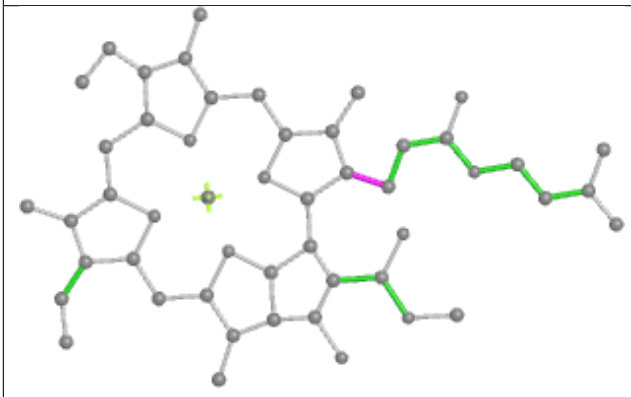


Bond angles



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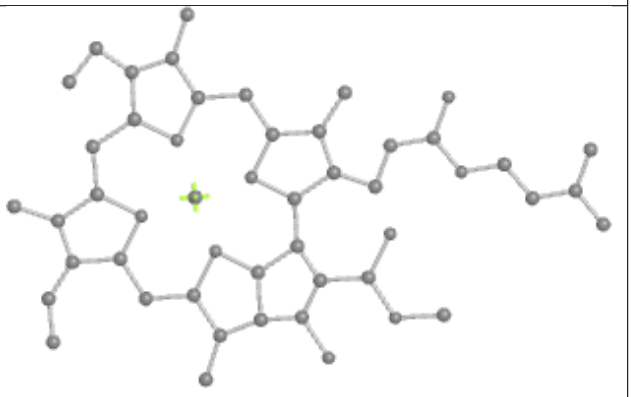
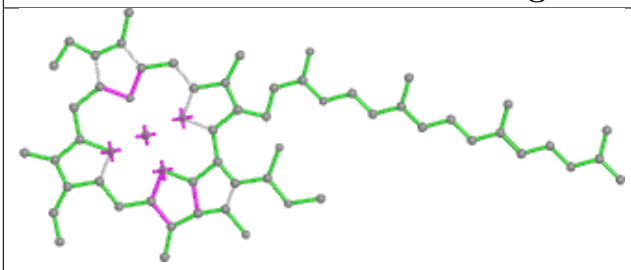


Rings

Ligand CLA a 819



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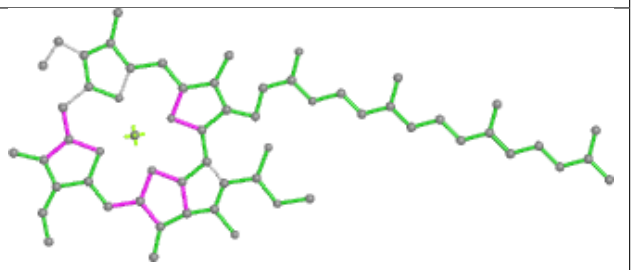
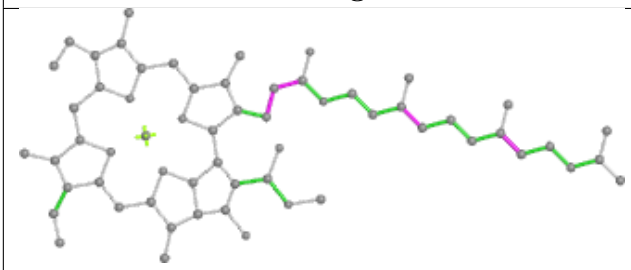


Bond angles



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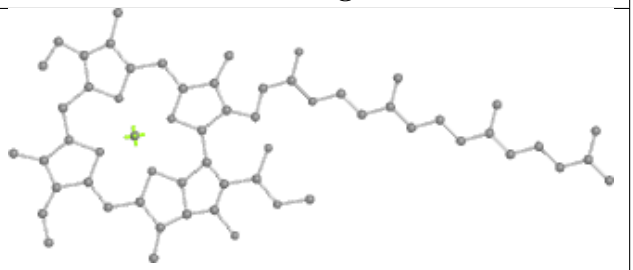
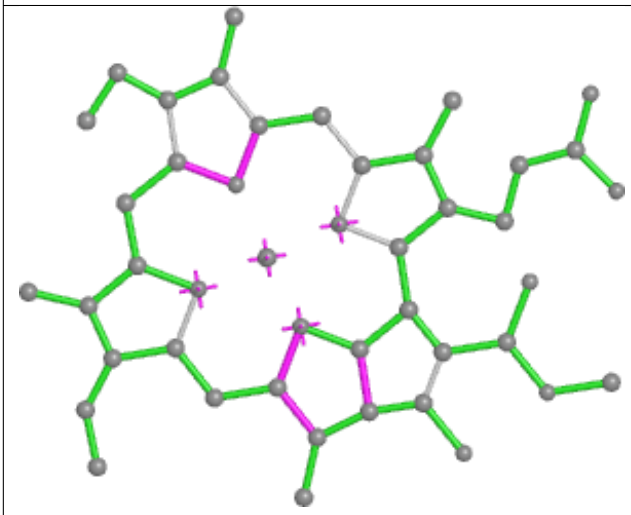


Rings

Ligand CLA I 609



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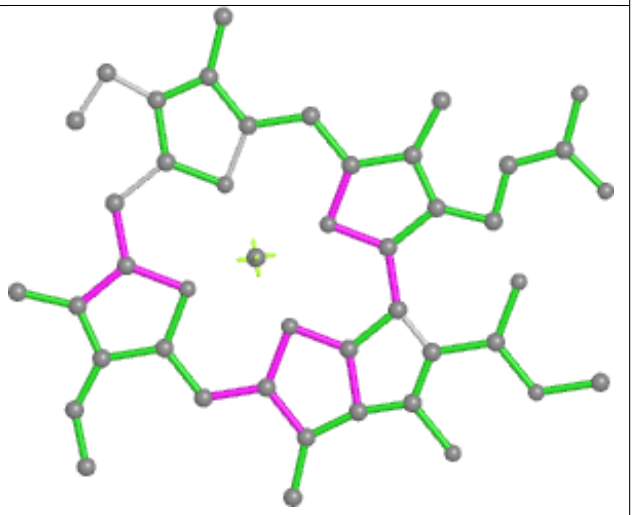

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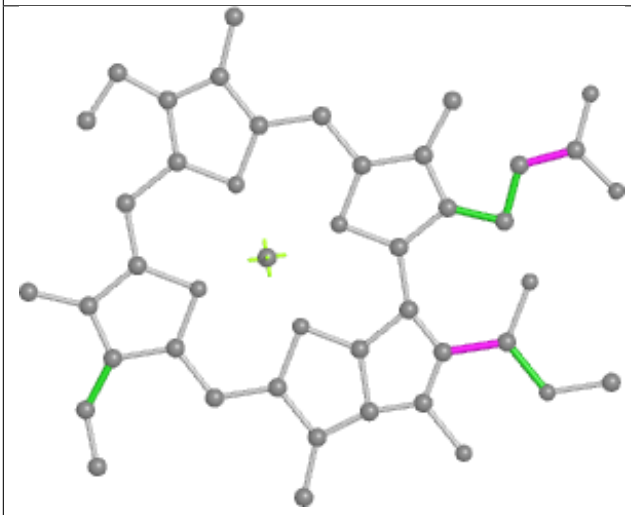

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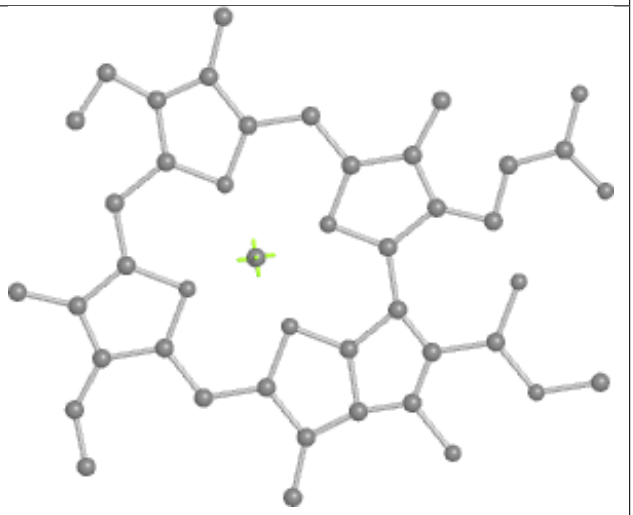
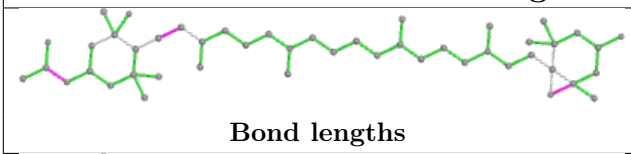


Rings

Ligand UIX F 613



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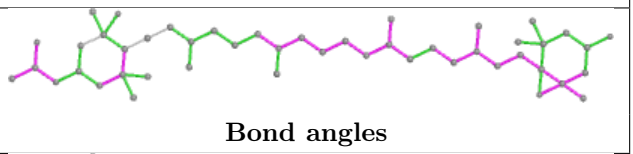
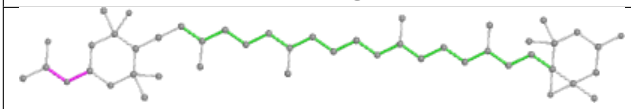


Bond angles

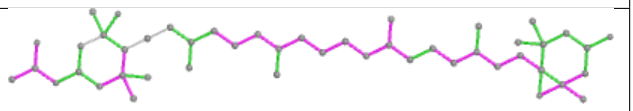


Torsions

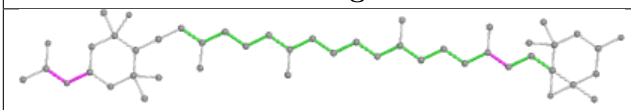
Rings

Ligand UIX D 616

Bond lengths



Bond angles



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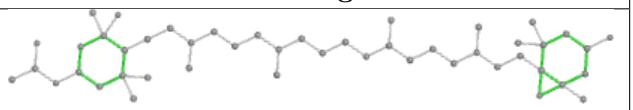
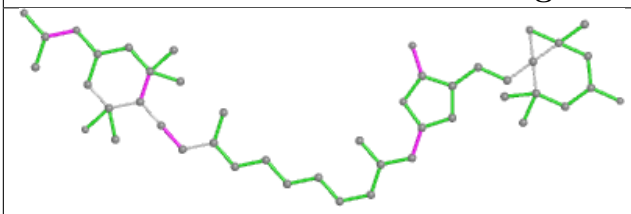


Rings

Ligand PID I 614



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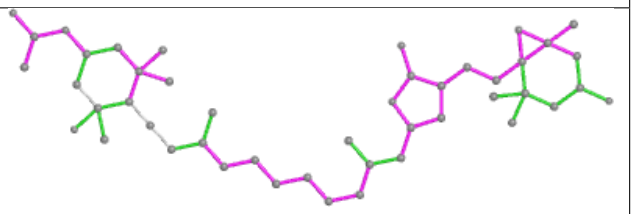
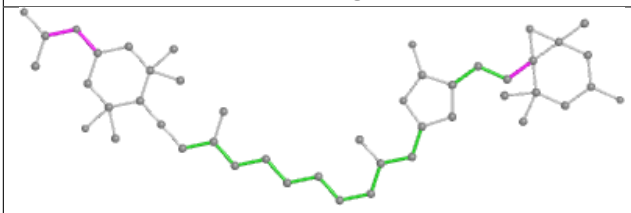
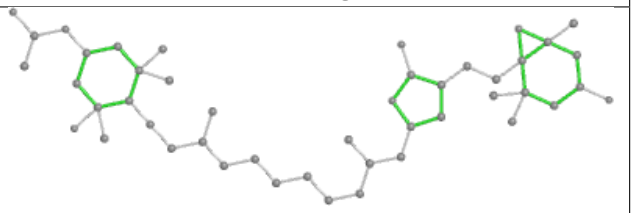


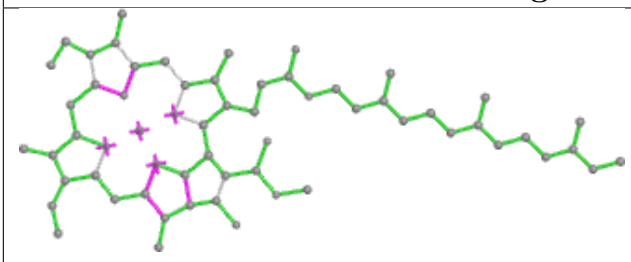
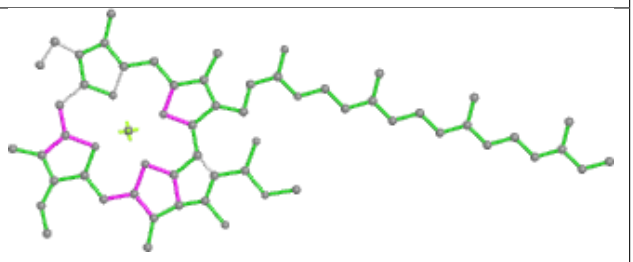
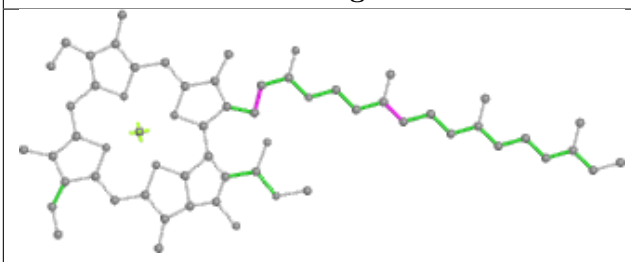
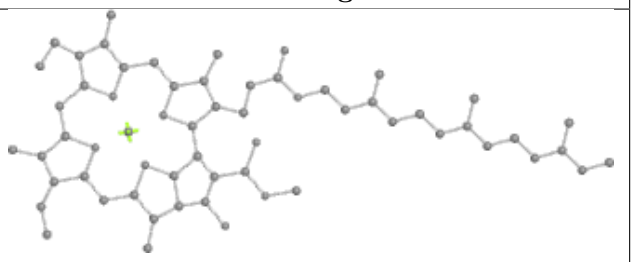
Bond angles

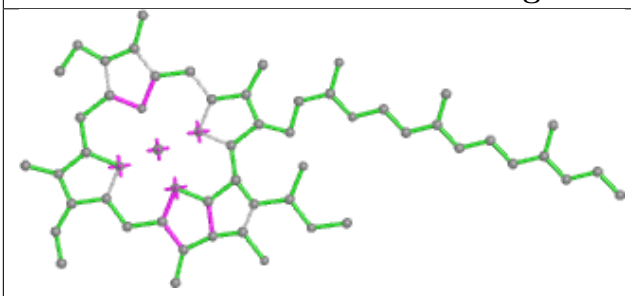
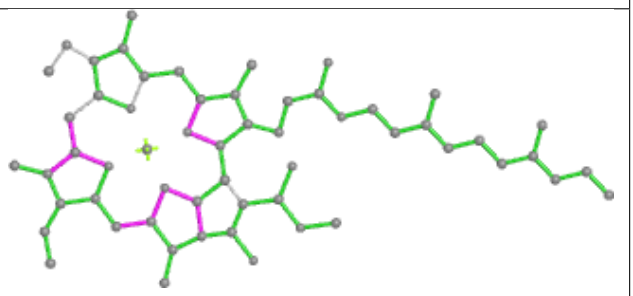
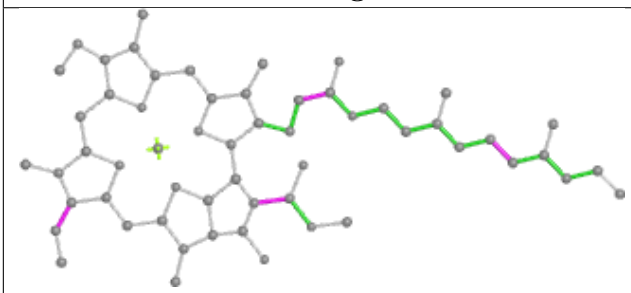
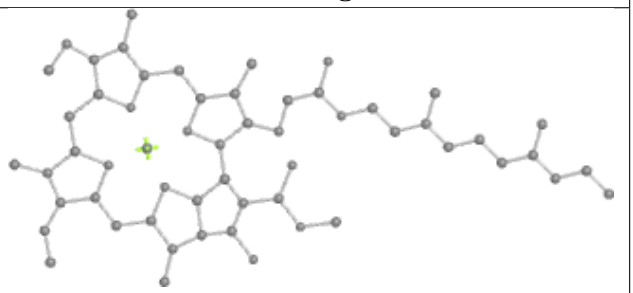


Torsions

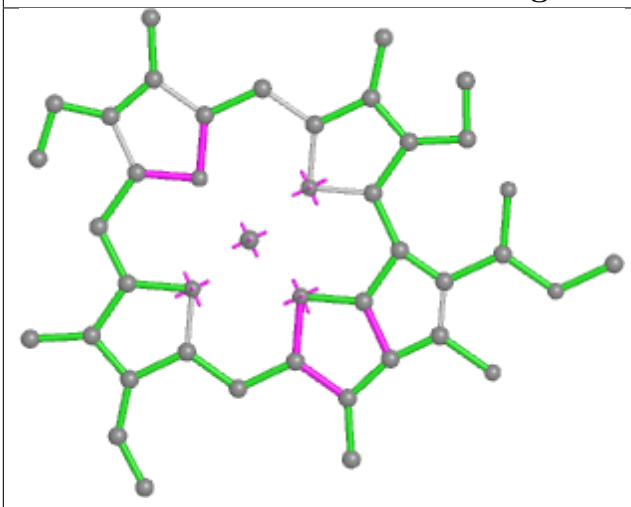


Rings

Ligand CLA I 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA I 611



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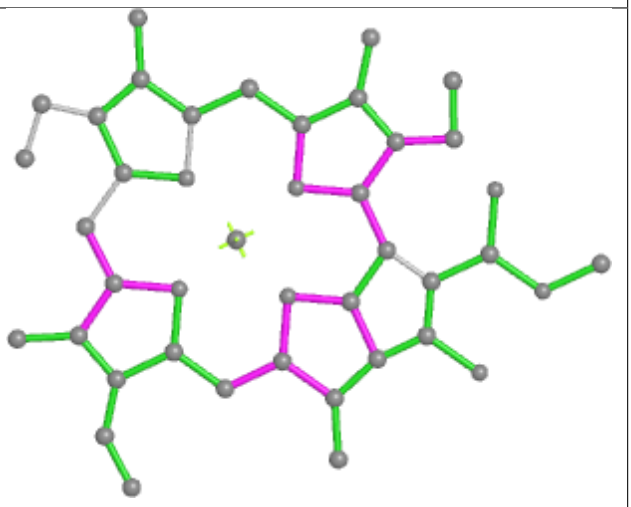
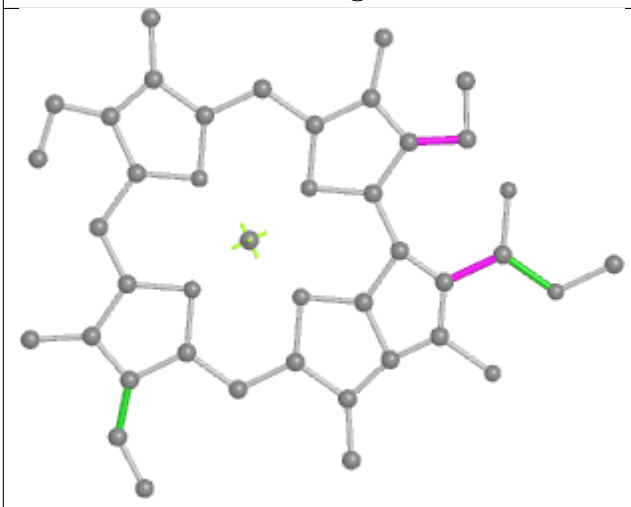


Bond angles



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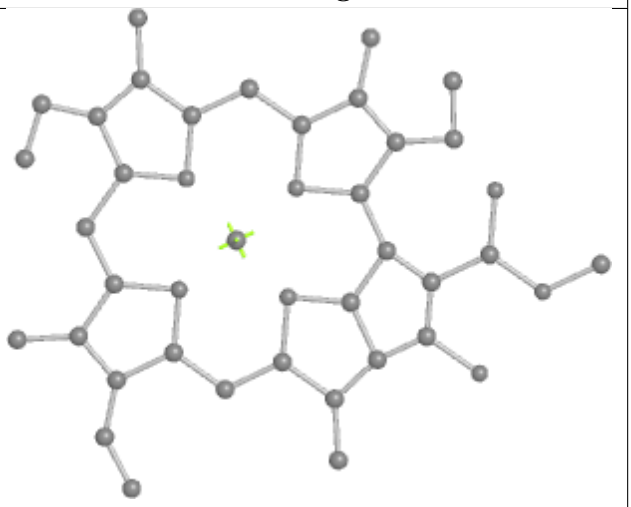
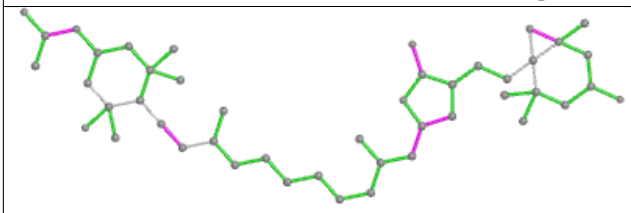


Rings

Ligand PID J 611



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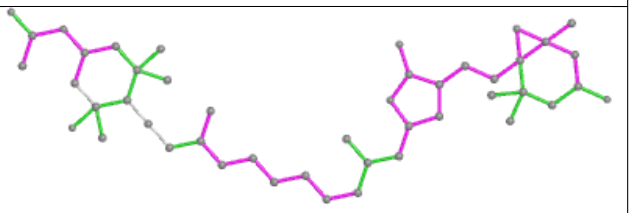
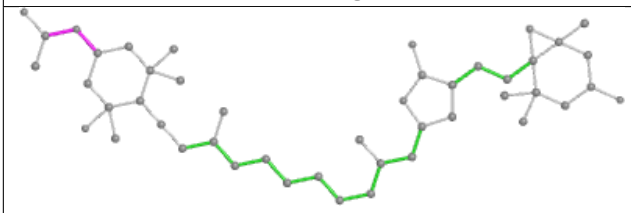


Bond angles



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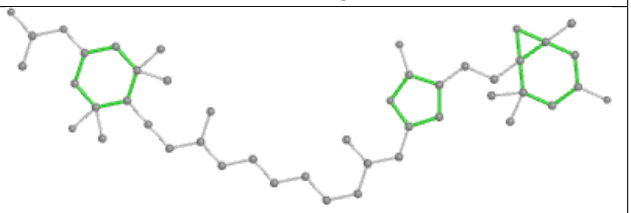
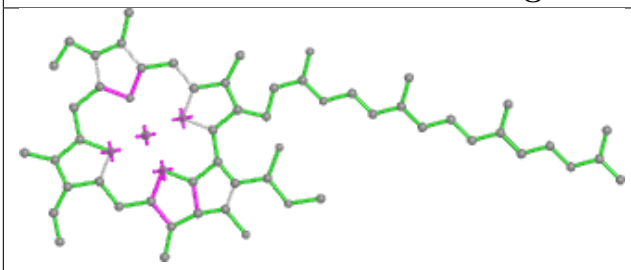
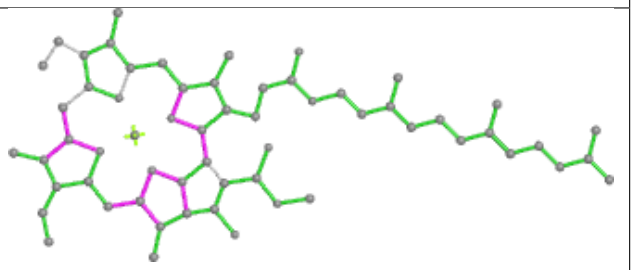
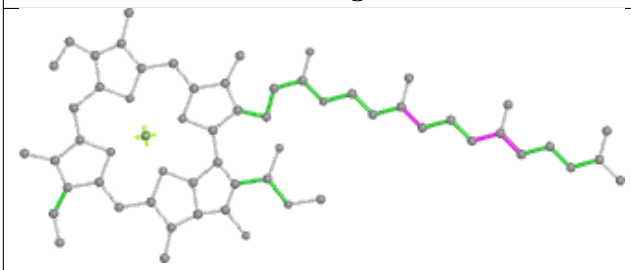
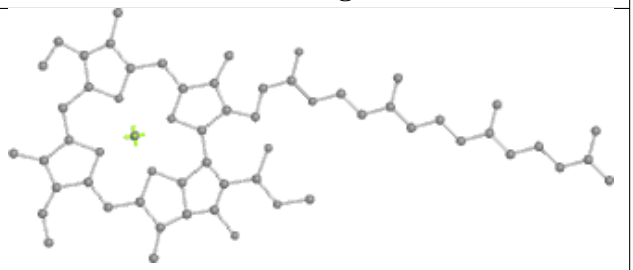
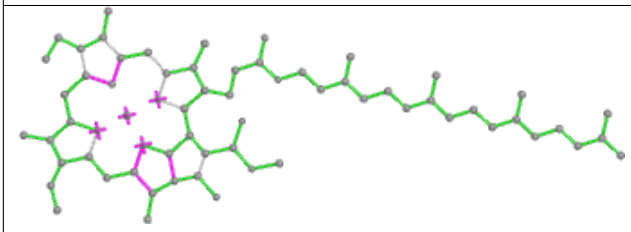
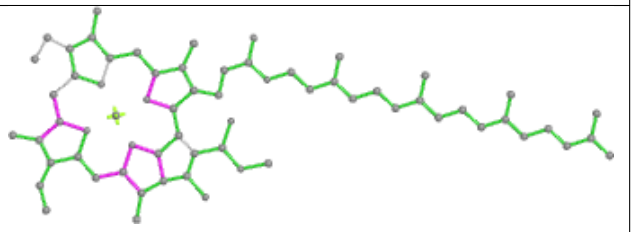
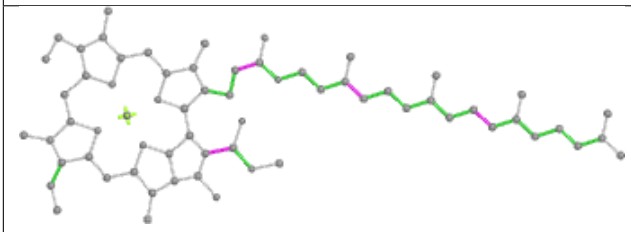
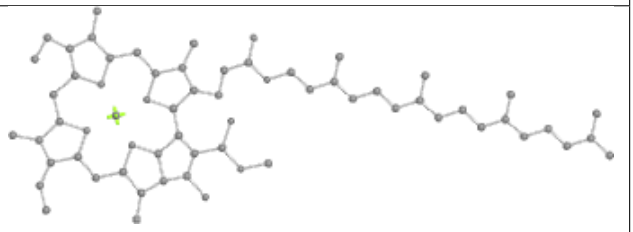
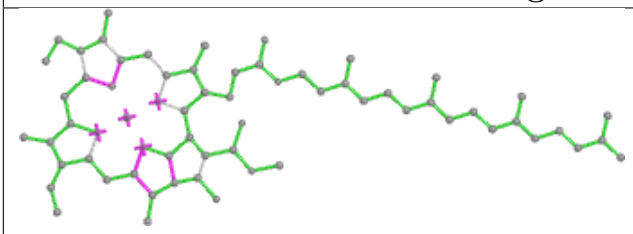


Rings

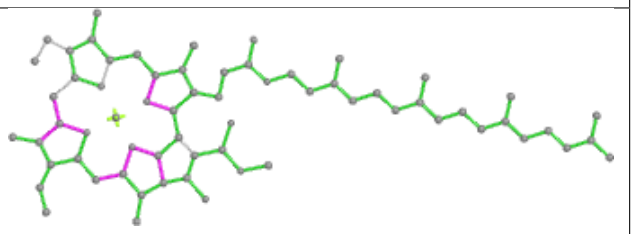
Ligand CLA C 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 708



Bond lengths



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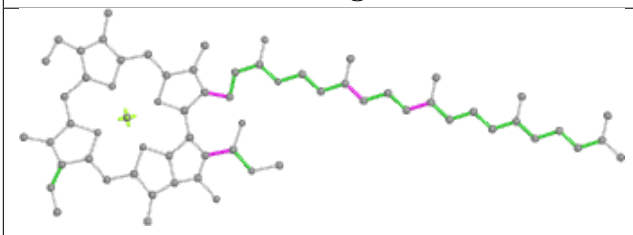
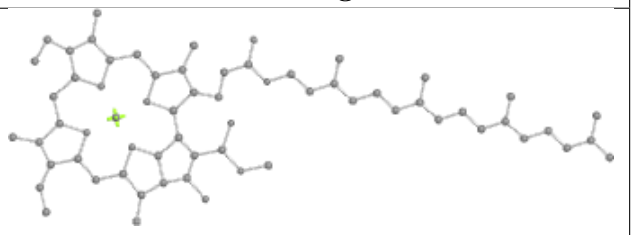
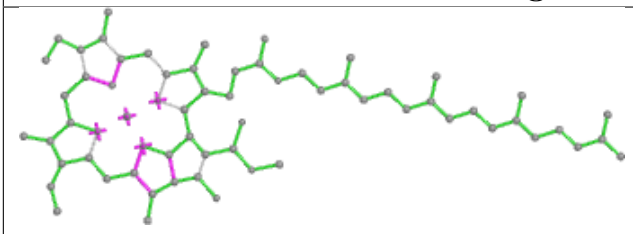


Torsions



Rings

Ligand CLA b 713



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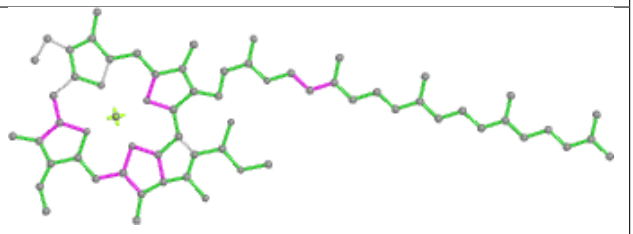
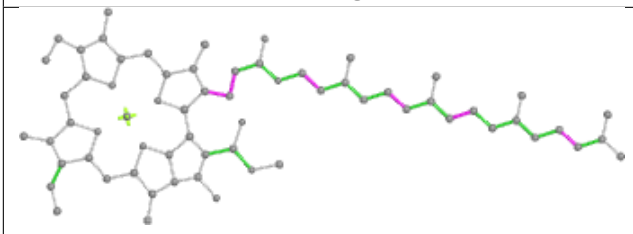


Bond angles



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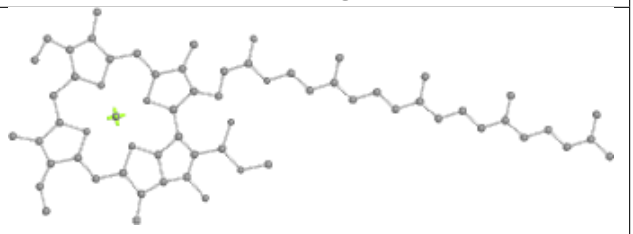
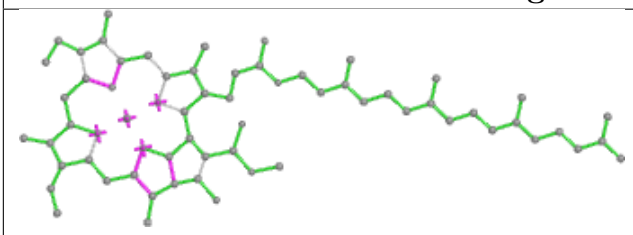


Rings

Ligand CLA b 705



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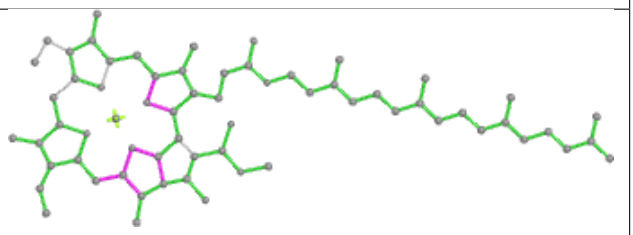
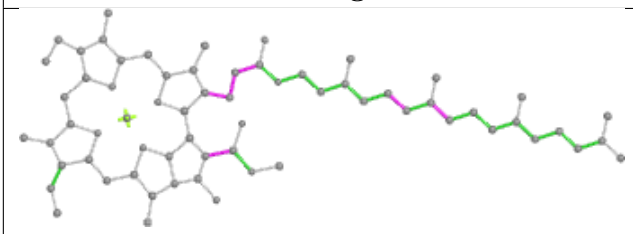


Bond angles



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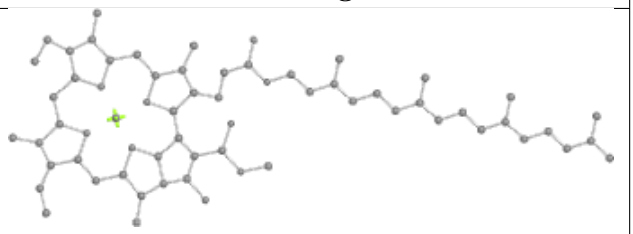
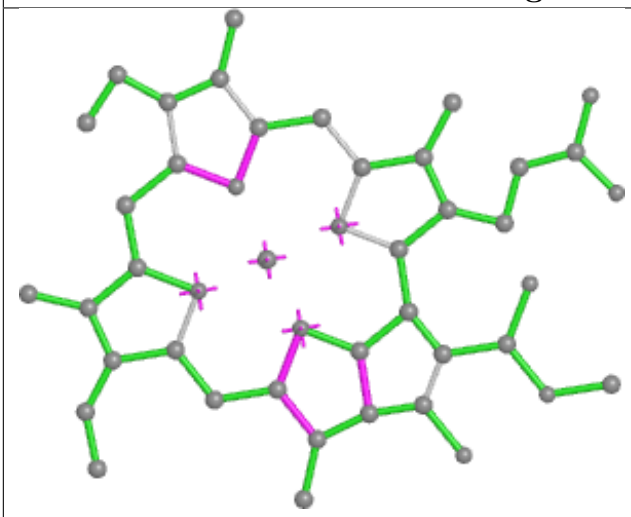


Rings

Ligand CLA E 612



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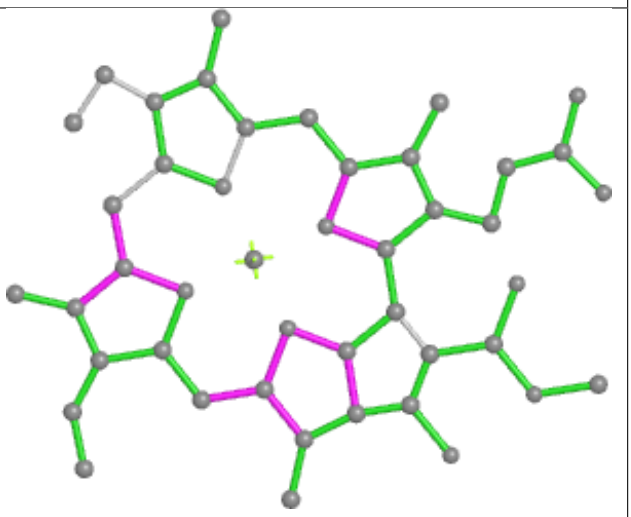
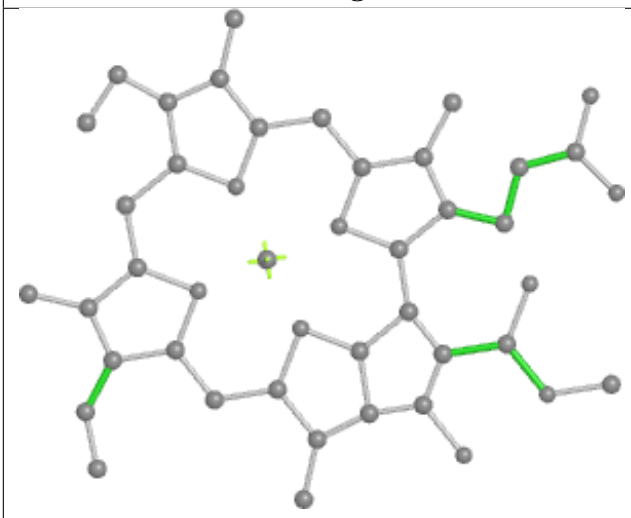


Bond angles



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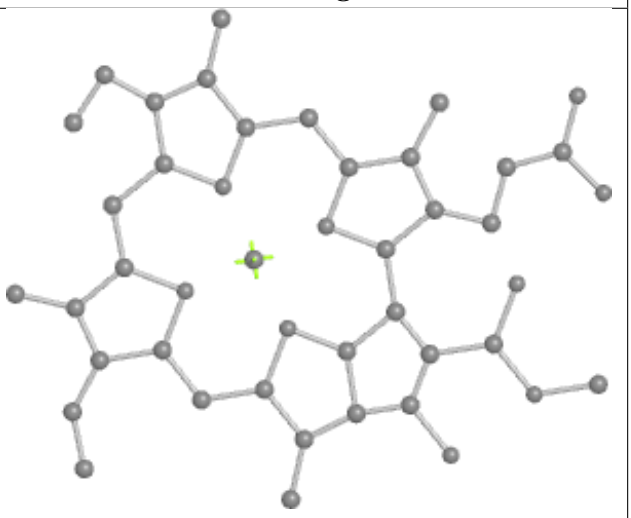
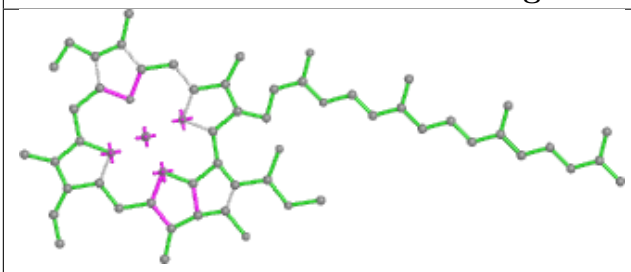


Rings

Ligand CLA H 305



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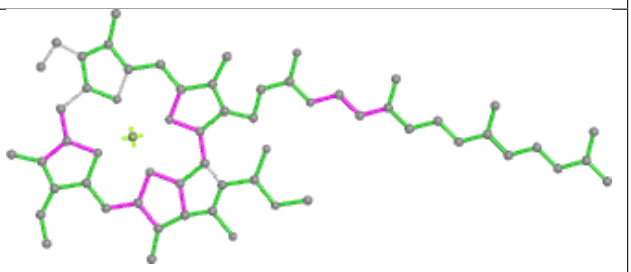

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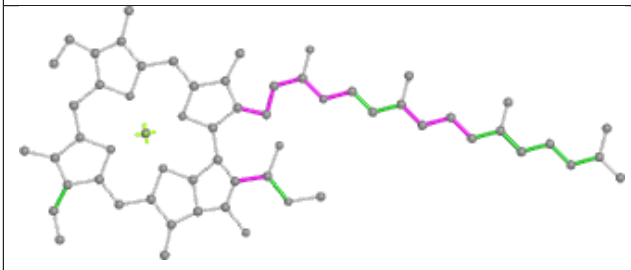

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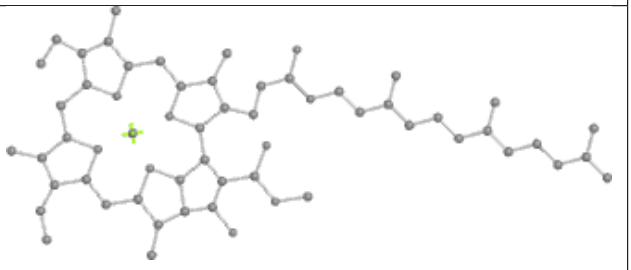
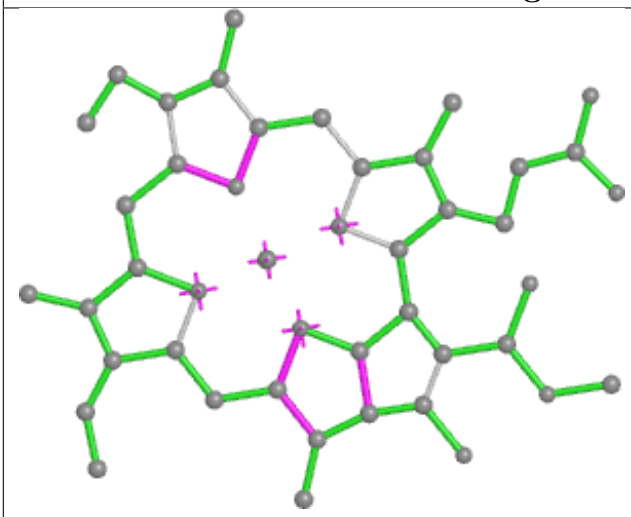


Rings

Ligand CLA A 611



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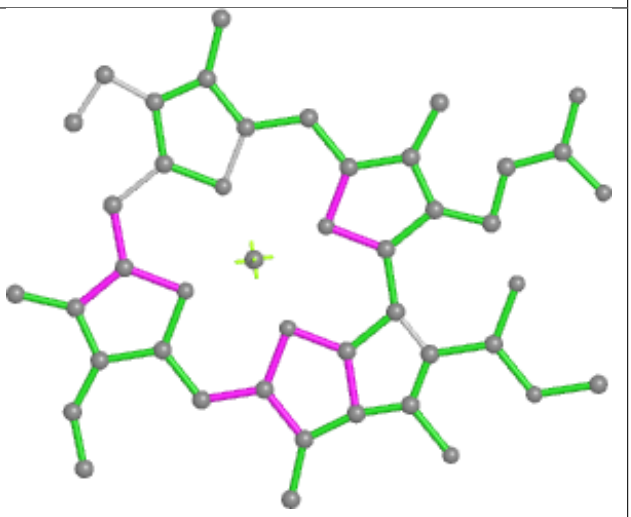
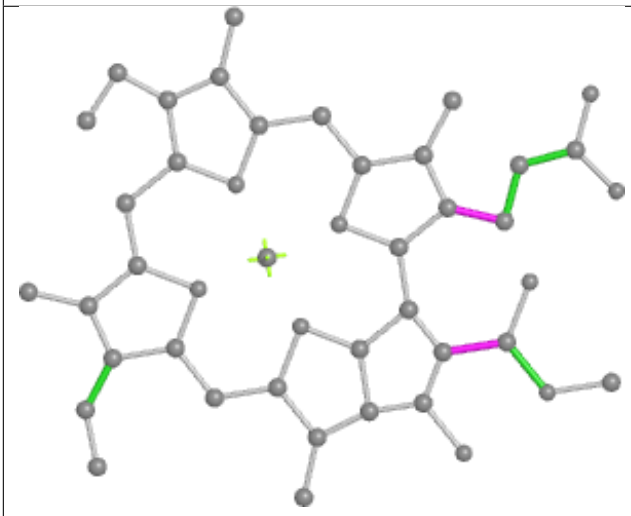


Bond angles



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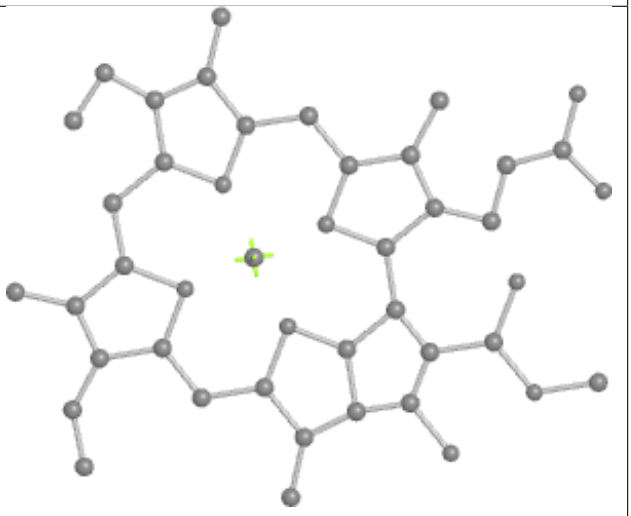
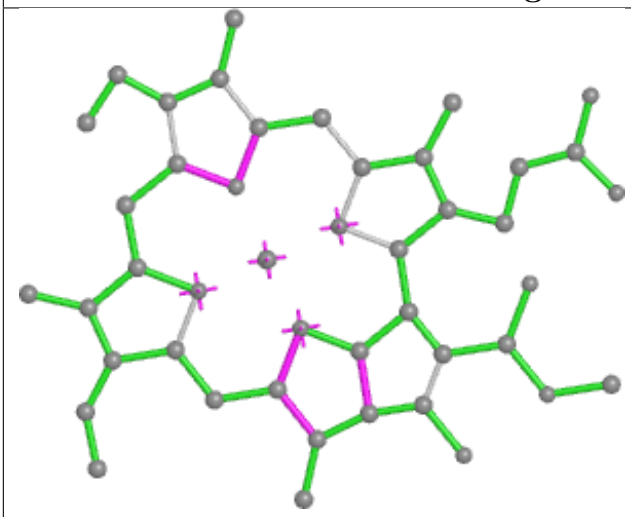


Rings

Ligand CLA B 605



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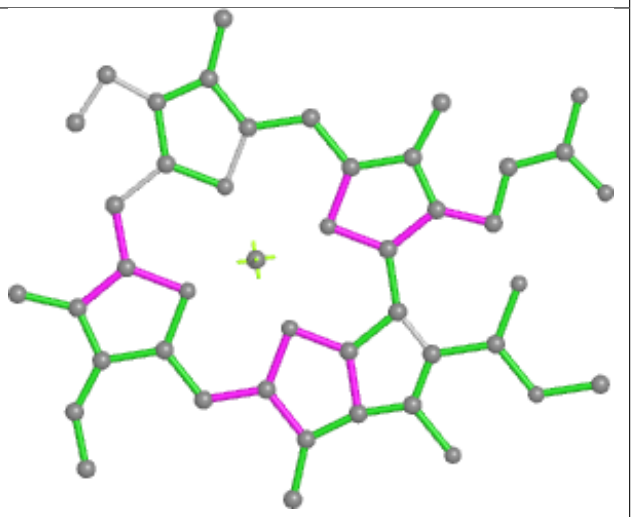
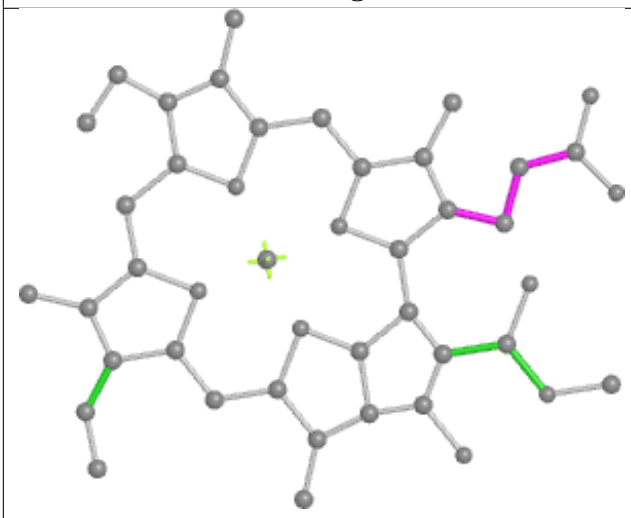


Bond angles



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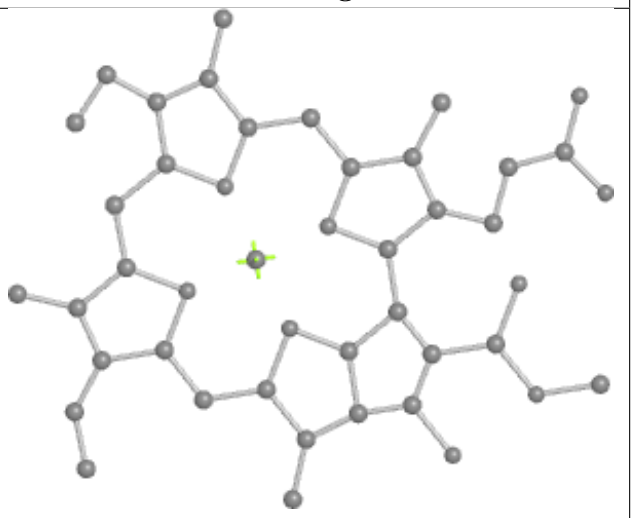
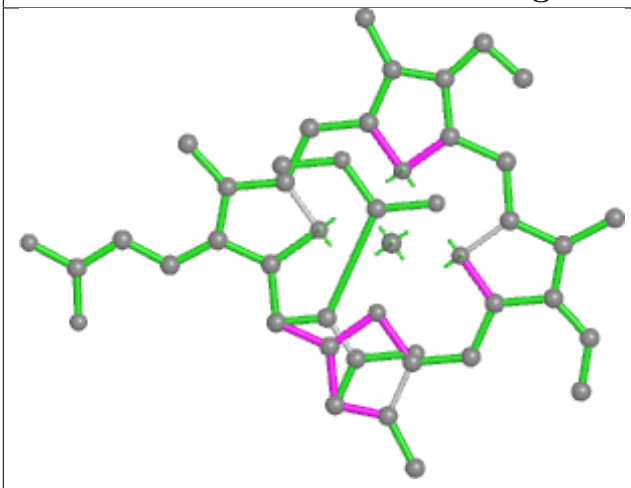
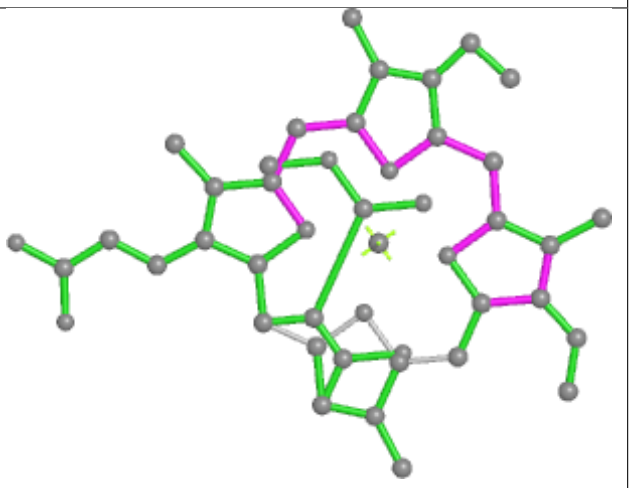


Rings

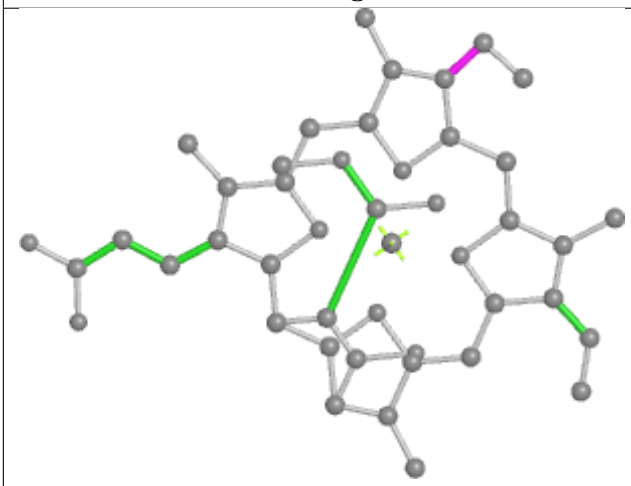
Ligand KC2 I 604



Bond lengths



Bond angles



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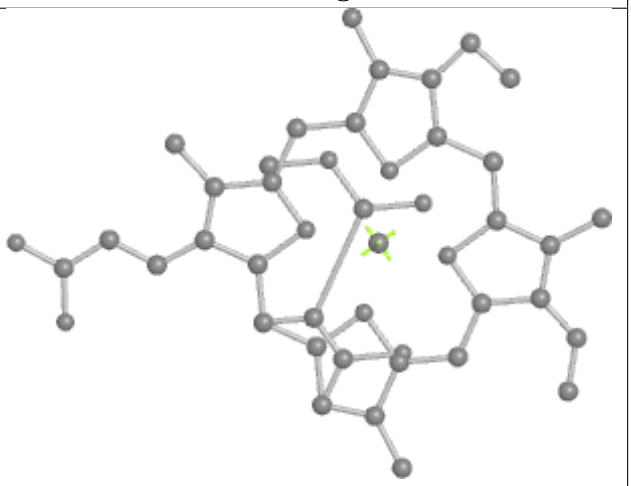
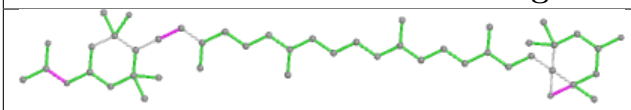
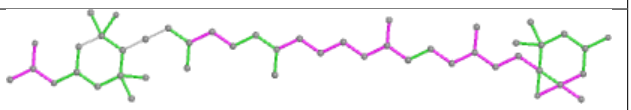


Rings

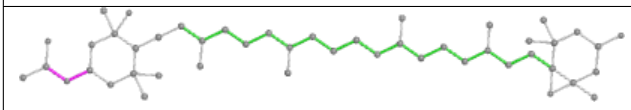
Ligand UIX J 616



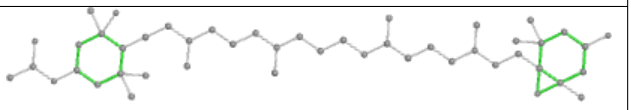
Bond lengths



Bond angles

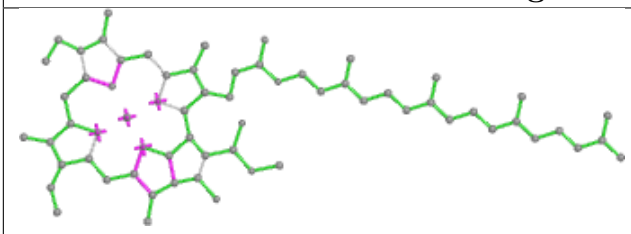


Torsions

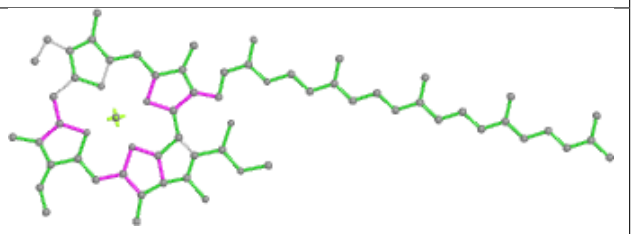


Rings

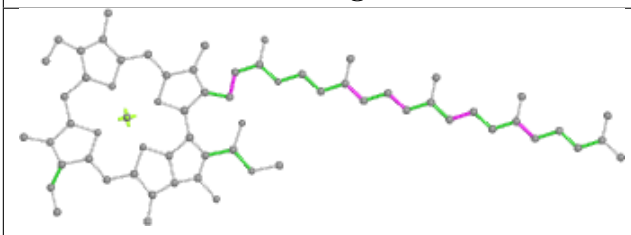
Ligand CLA b 715



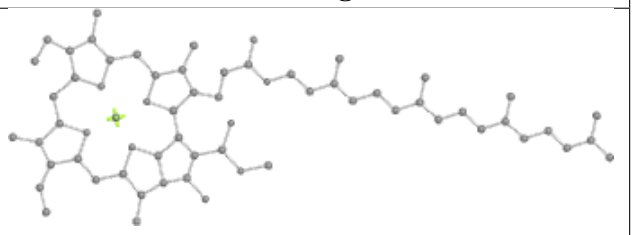
Bond lengths



Bond angles

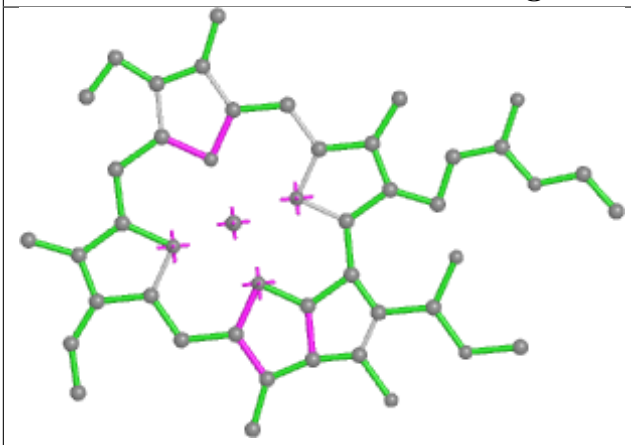


Torsions



Rings

Ligand CLA E 603



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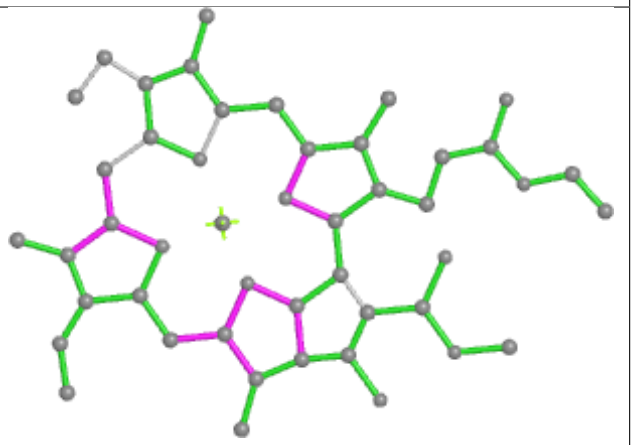
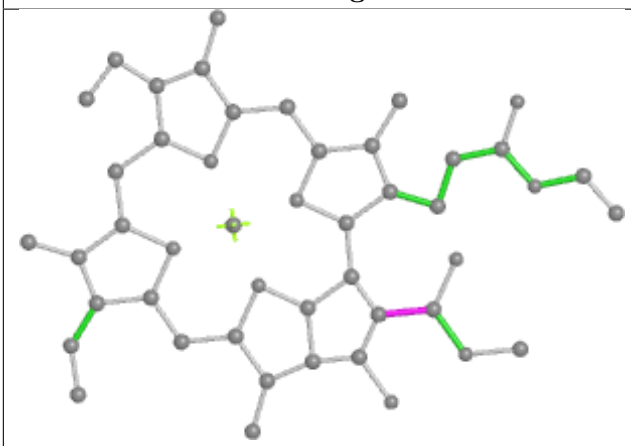
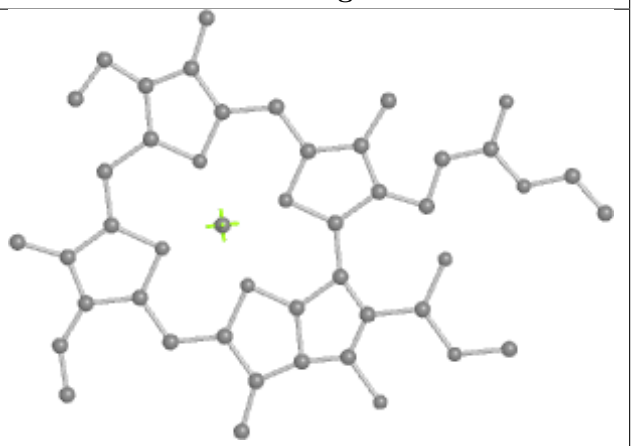


Bond angles

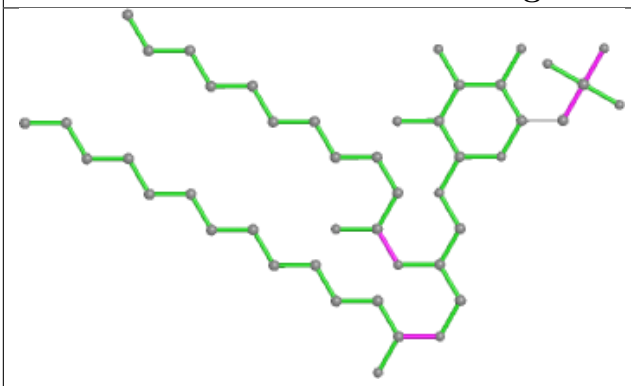


Torsions

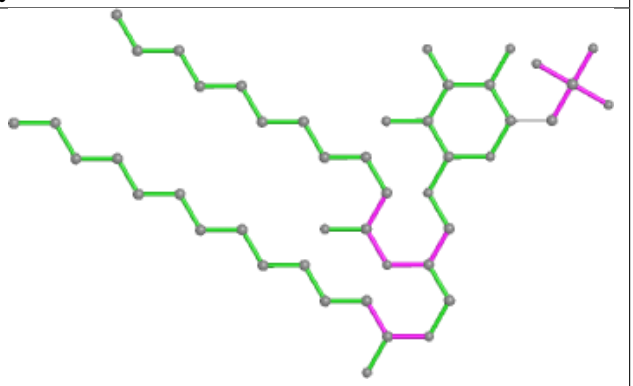


Rings

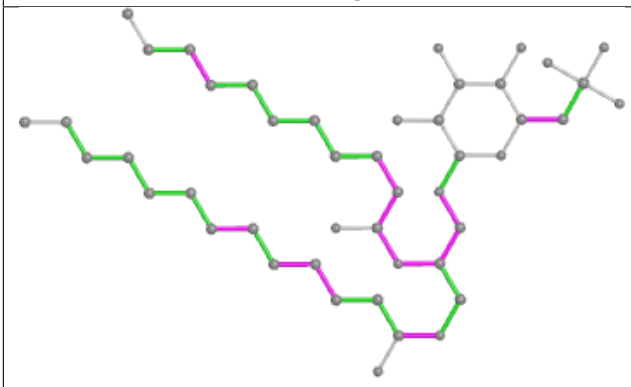
Ligand SQD H 320



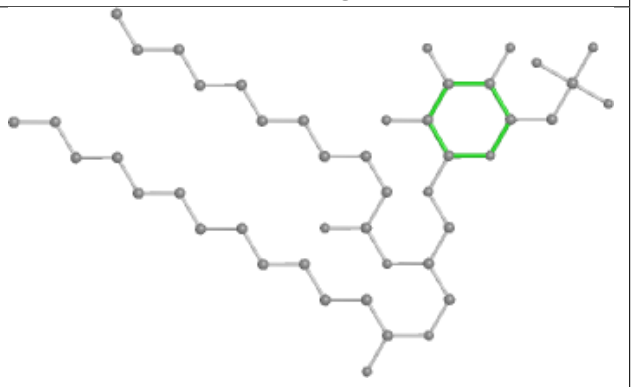
Bond lengths



Bond angles

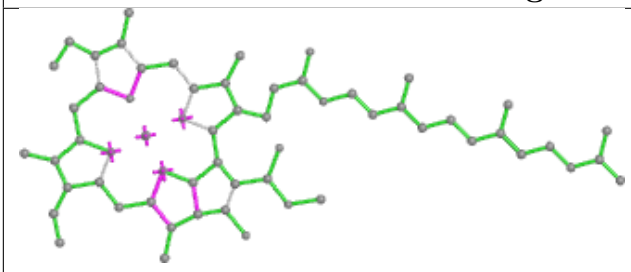


Torsions



Rings

Ligand CLA F 601



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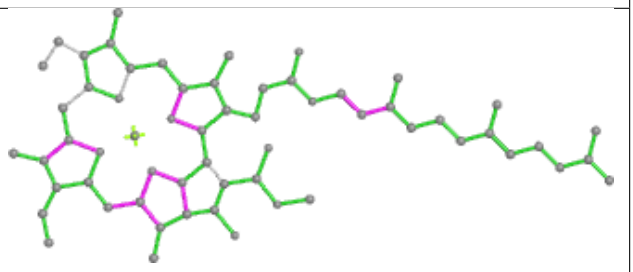
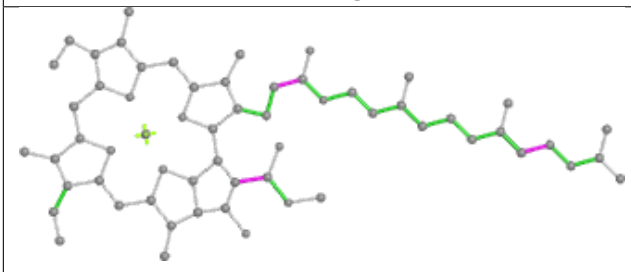


Bond angles



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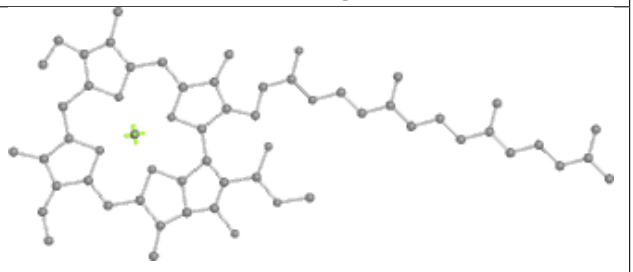
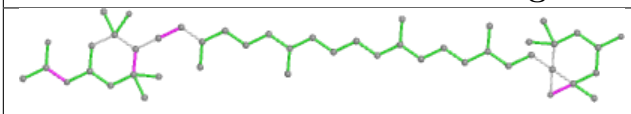


Rings

Ligand UIX E 616



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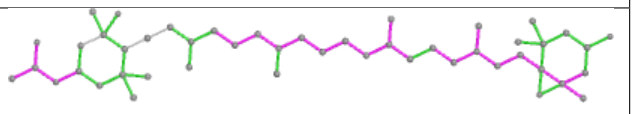

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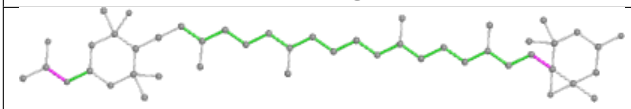
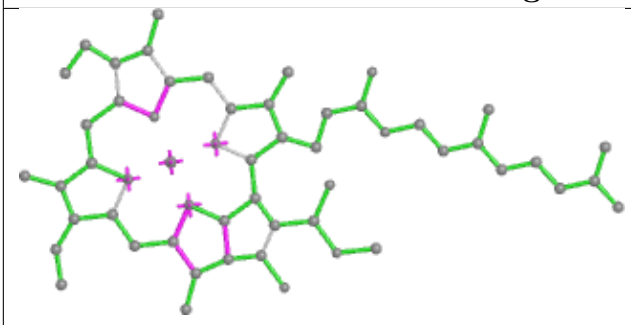


Torsions

Rings

Ligand CLA K 602



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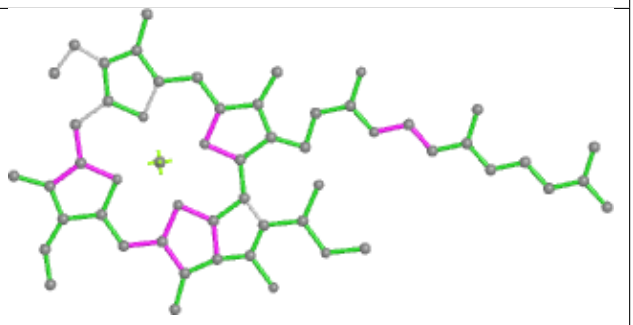
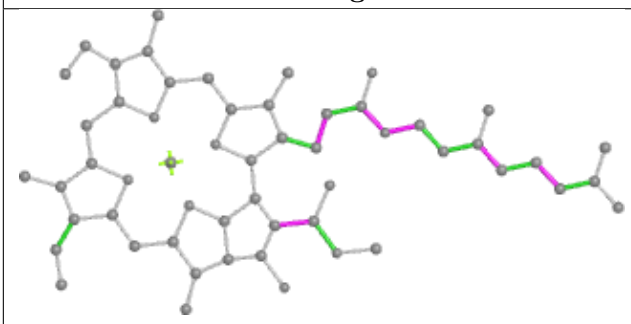


Bond angles



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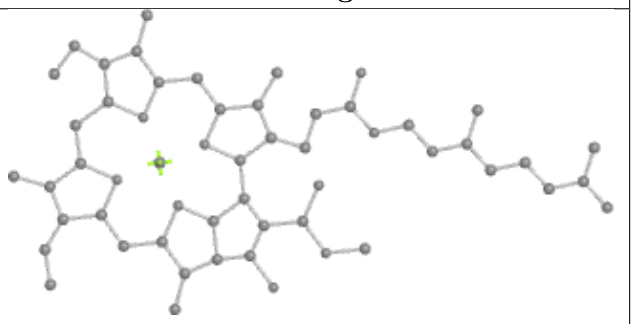
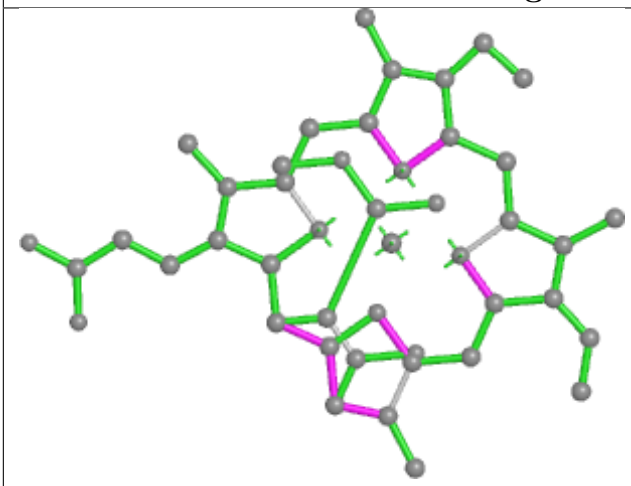


Rings

Ligand KC2 K 607



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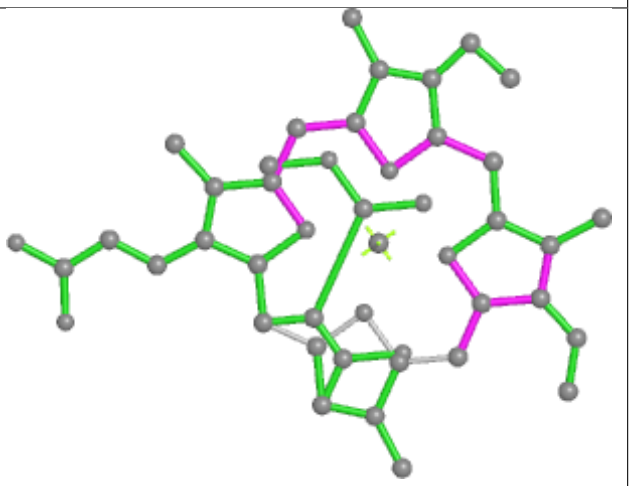

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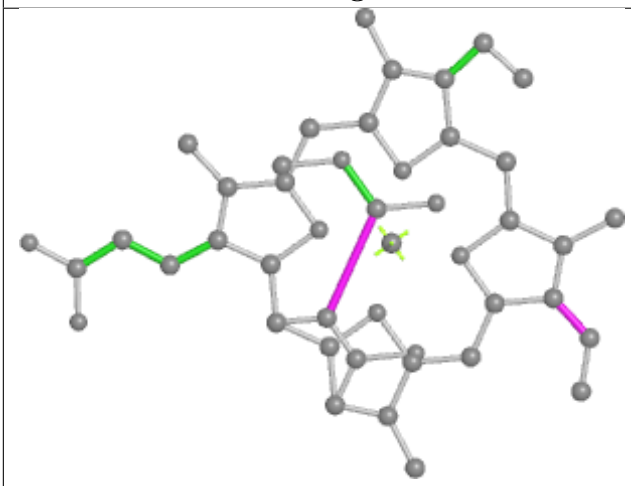

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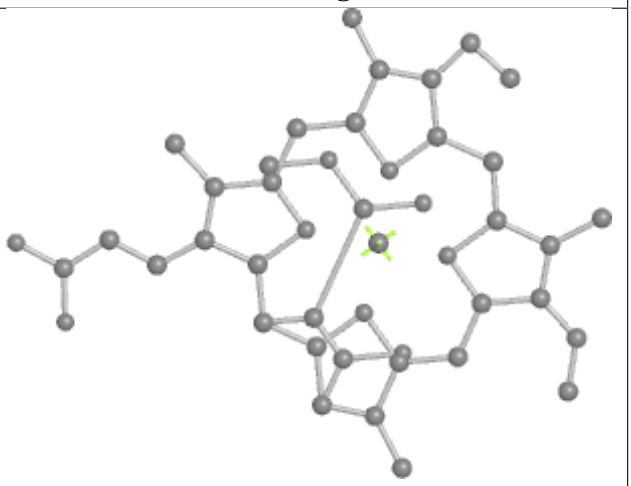
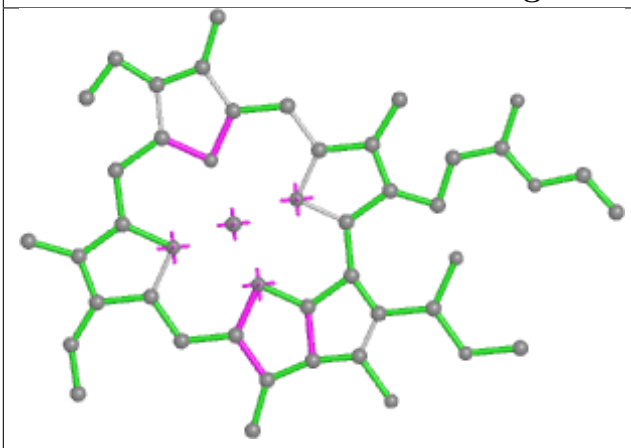


Rings

Ligand CLA D 610



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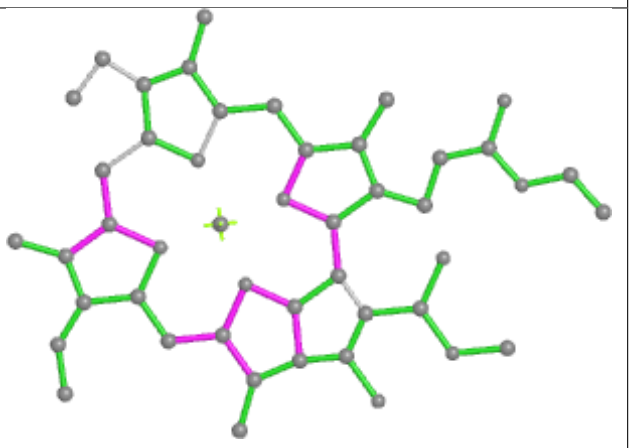

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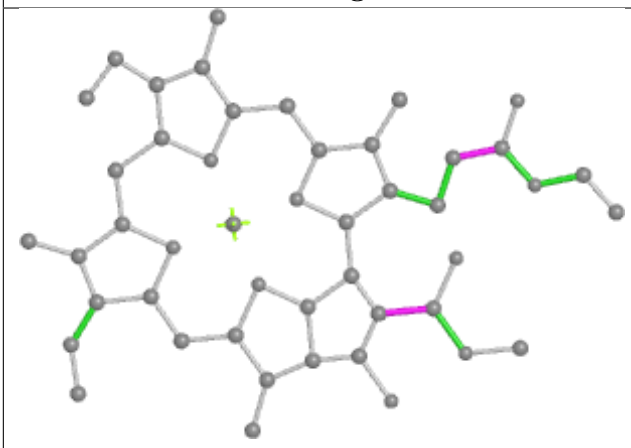

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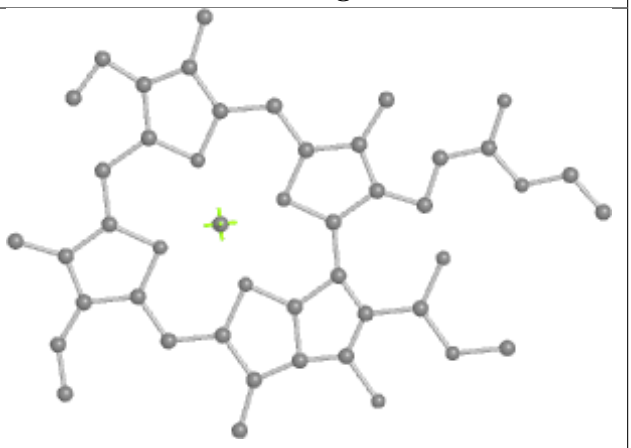
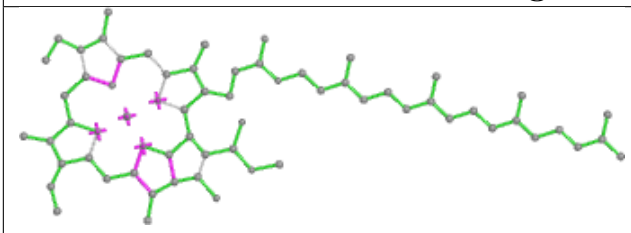
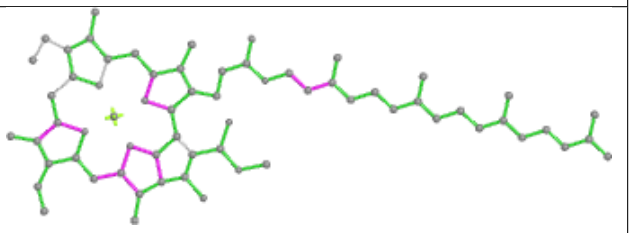


Rings

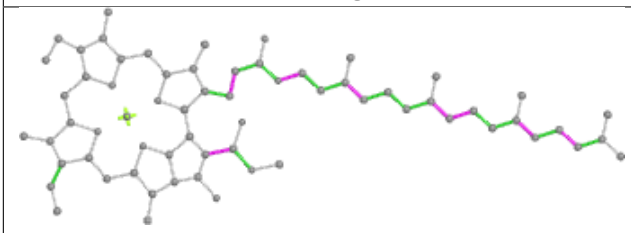
Ligand CLA a 830



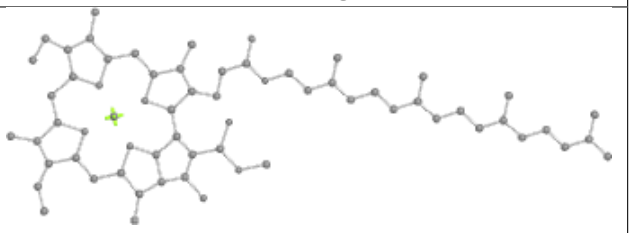
Bond lengths



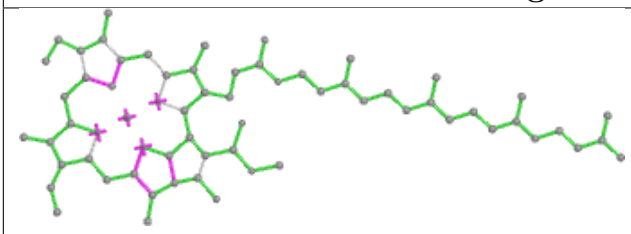
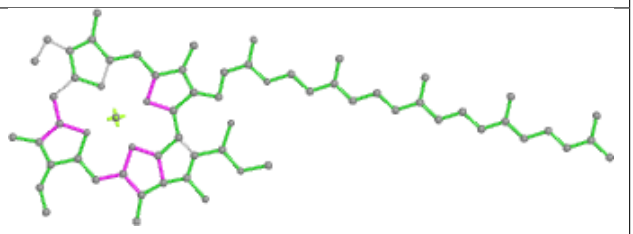
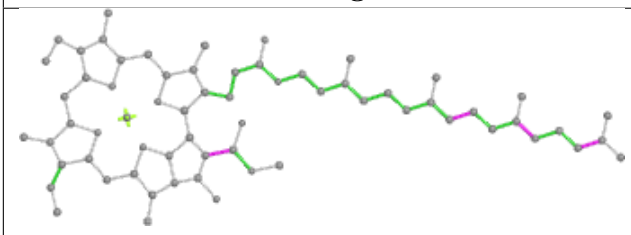
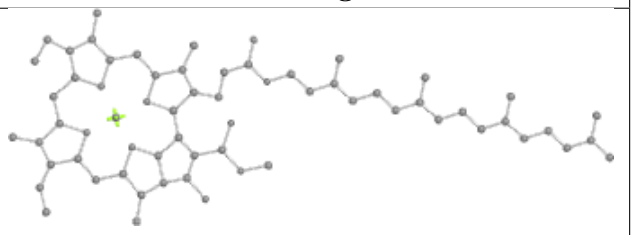
Bond angles

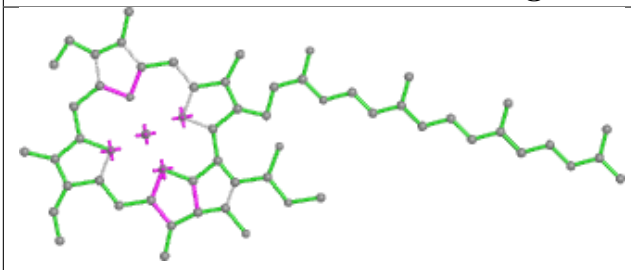
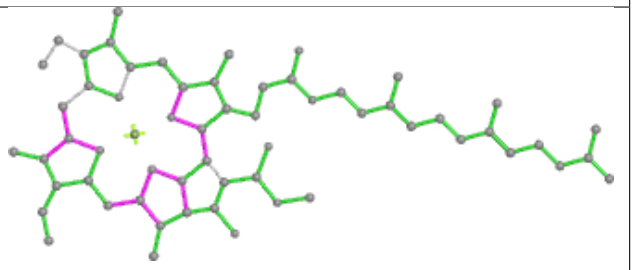
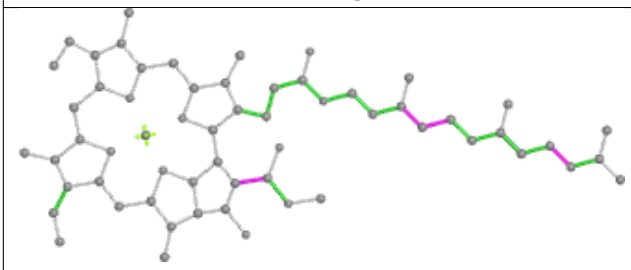
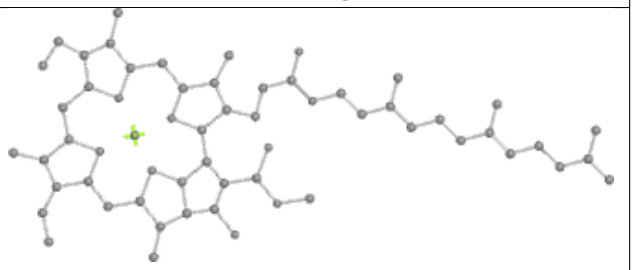


Torsions

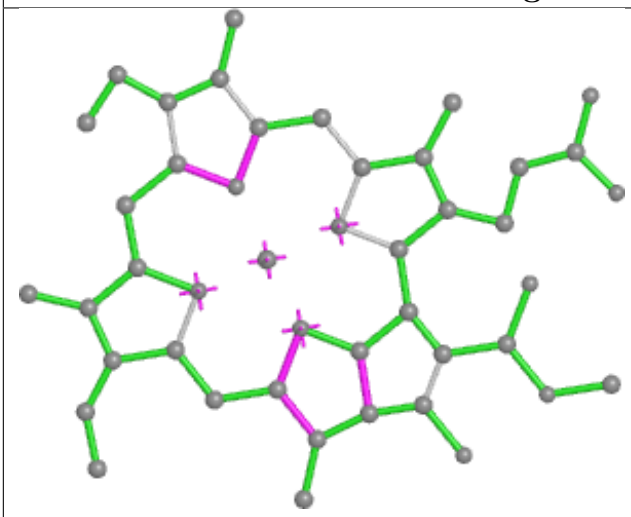


Rings

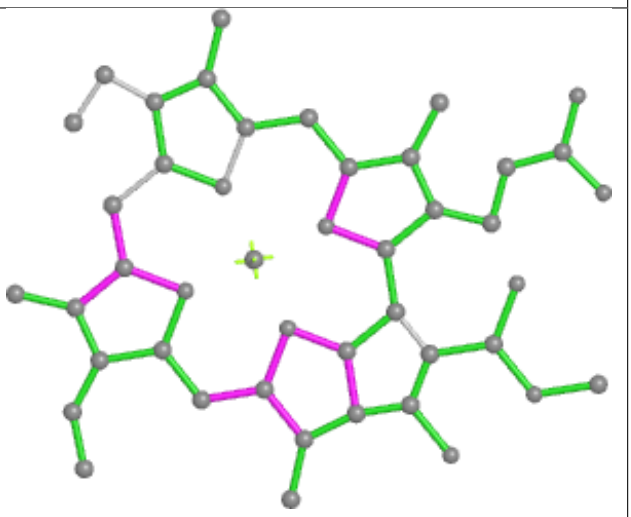
Ligand CLA b 716	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA E 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

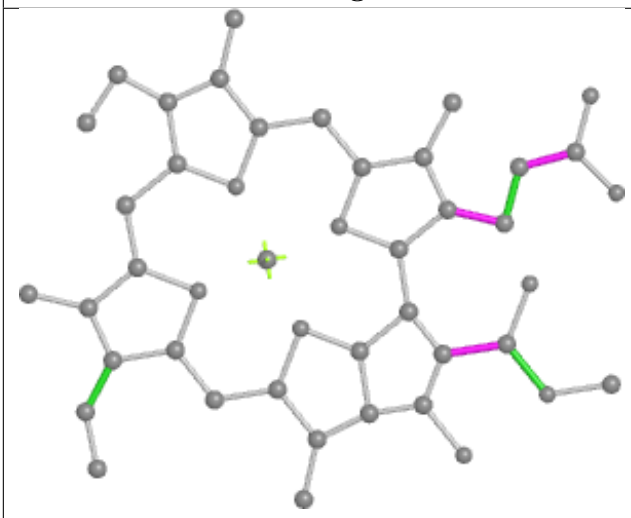
Ligand CLA U 606



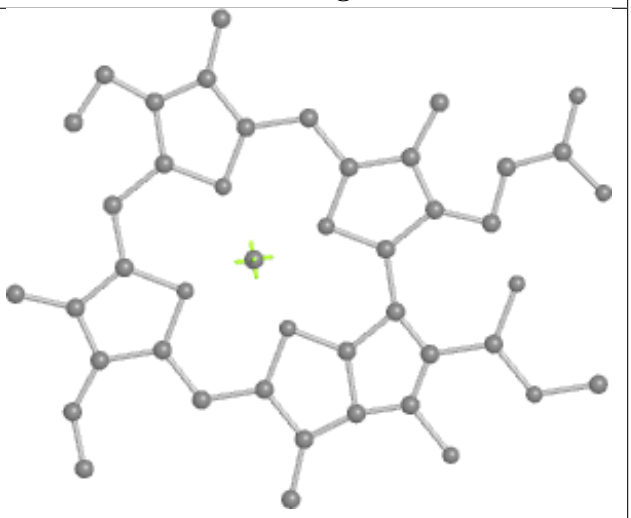
Bond lengths



Bond angles

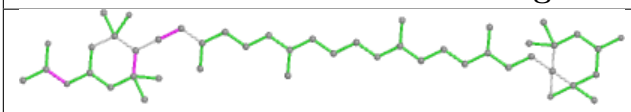


Torsions

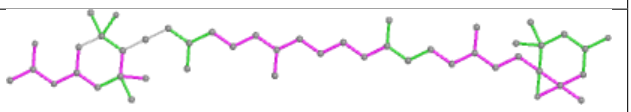


Rings

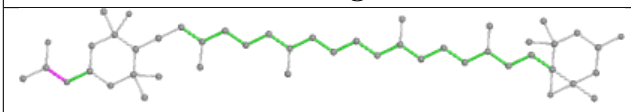
Ligand UIX I 612



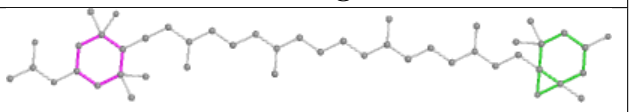
Bond lengths



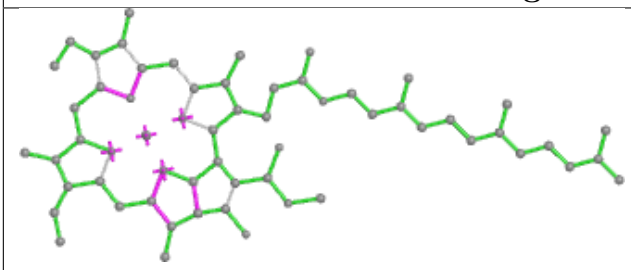
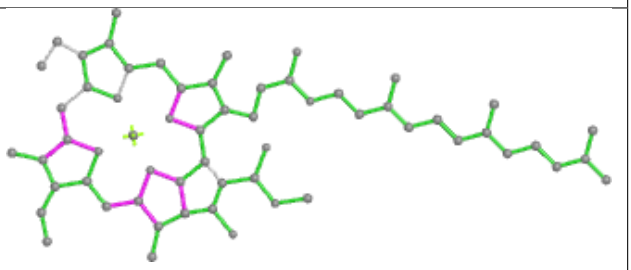
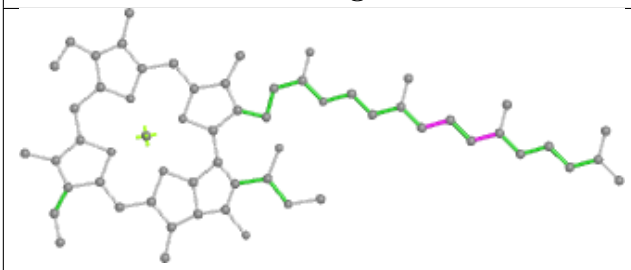
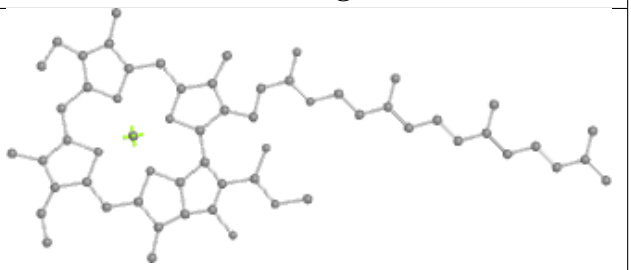
Bond angles

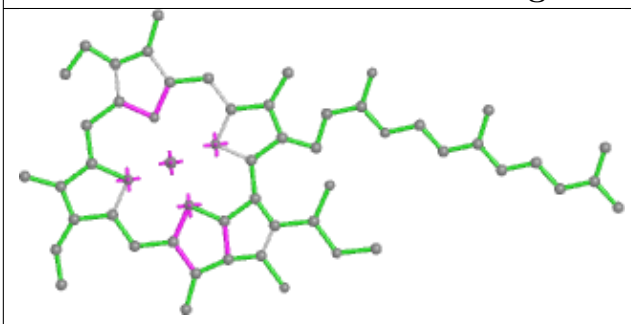
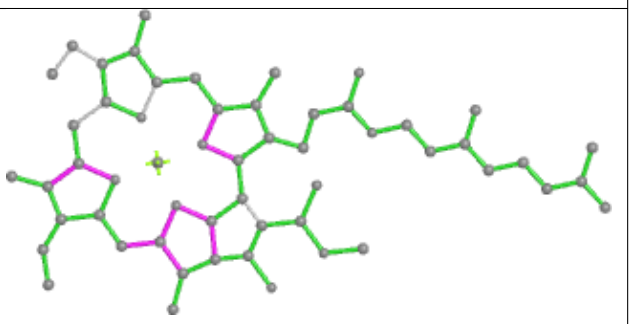
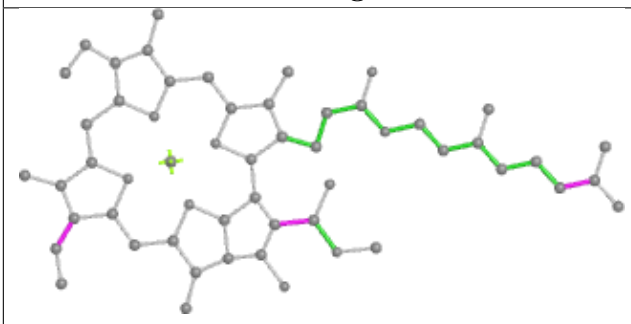
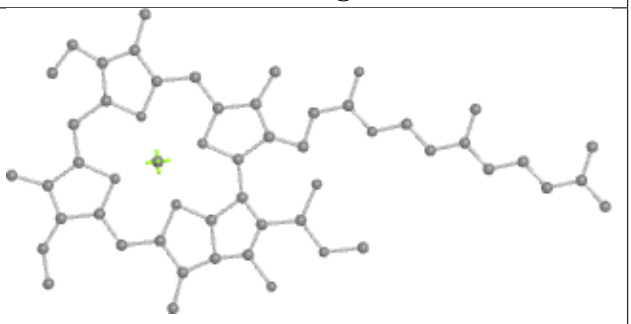


Torsions

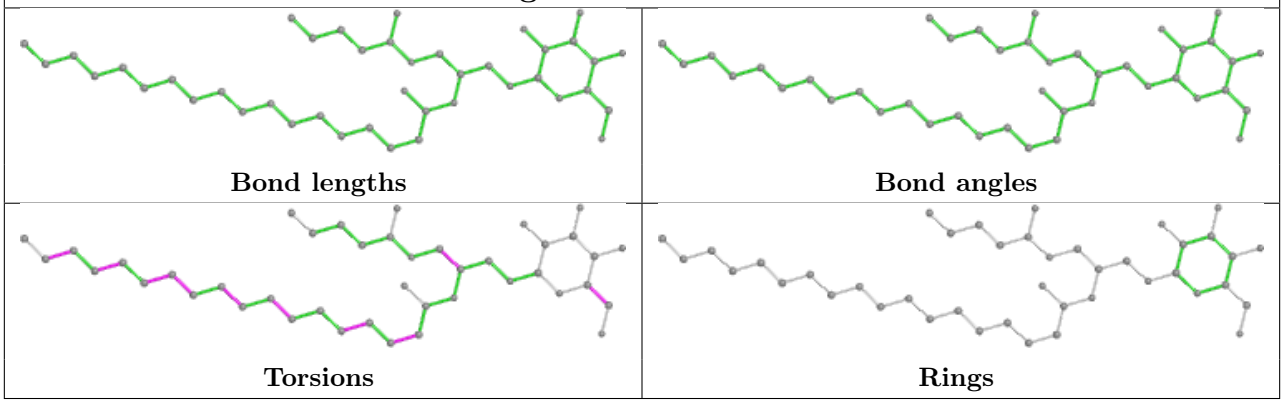


Rings

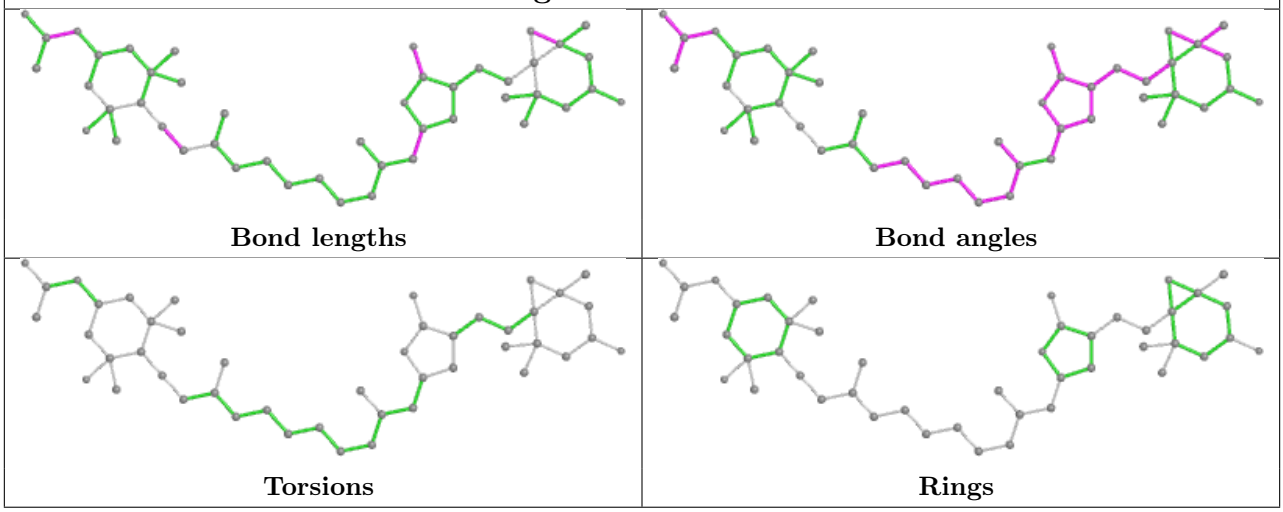
Ligand CLA H 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

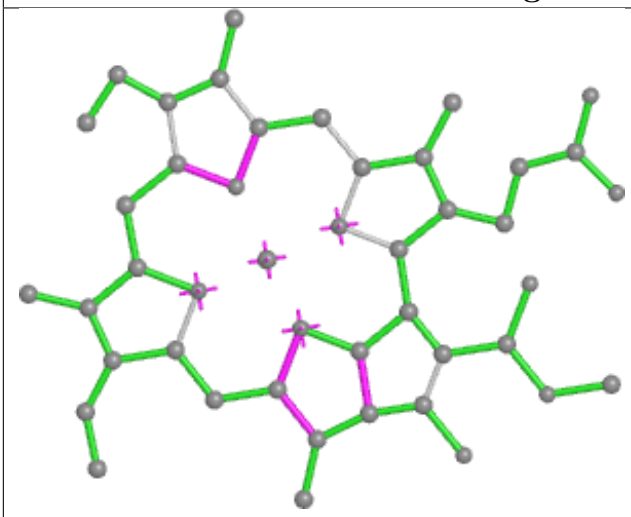
Ligand LMG K 613



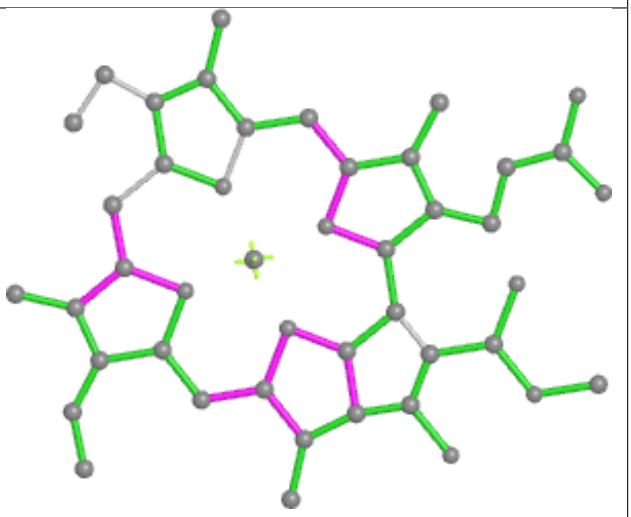
Ligand PID J 614



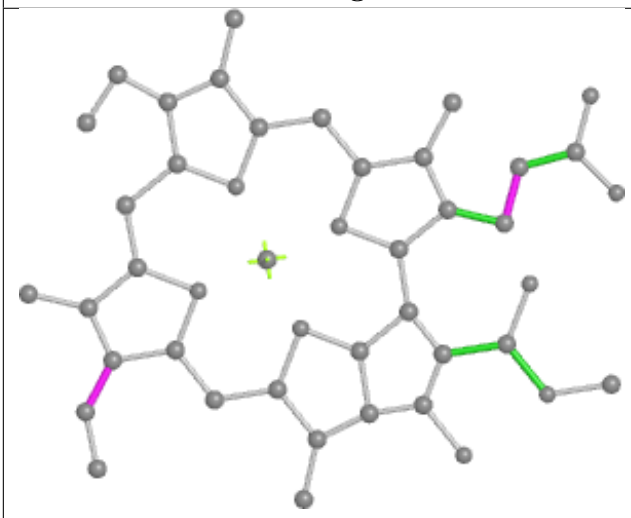
Ligand CLA H 306



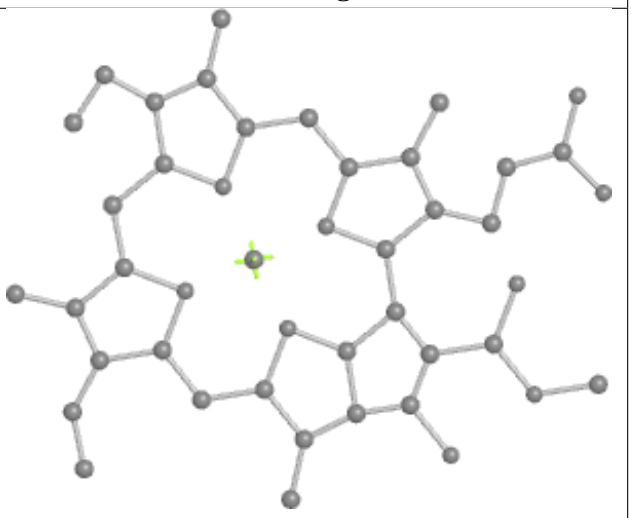
Bond lengths



Bond angles

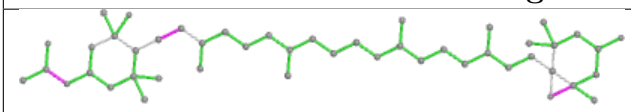


Torsions

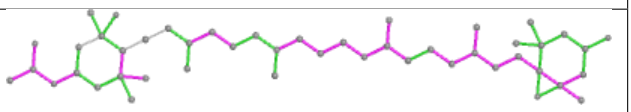


Rings

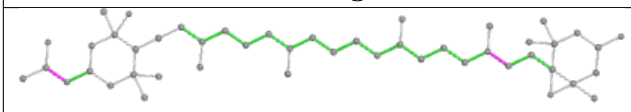
Ligand UIX G 615



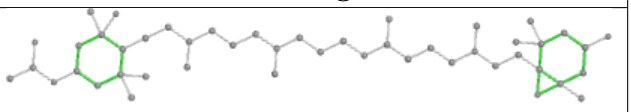
Bond lengths



Bond angles

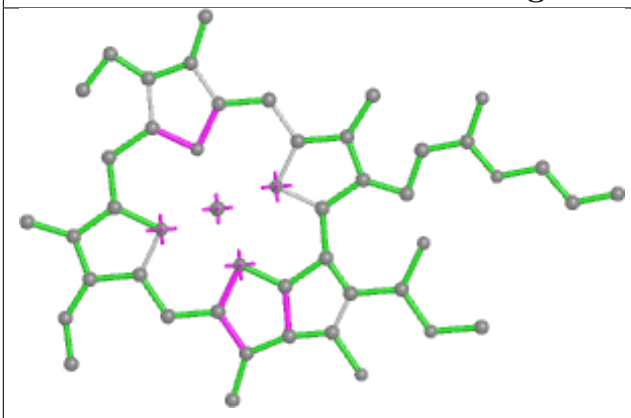


Torsions

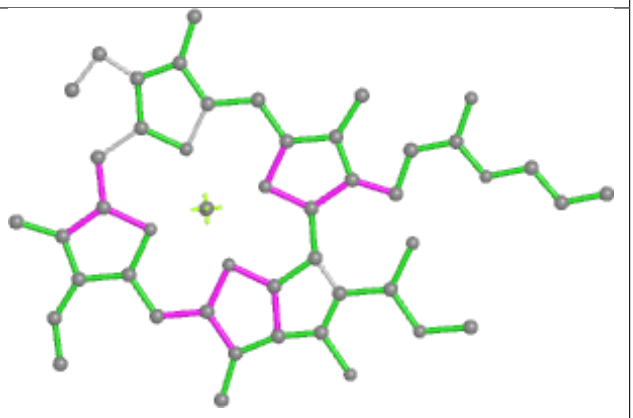


Rings

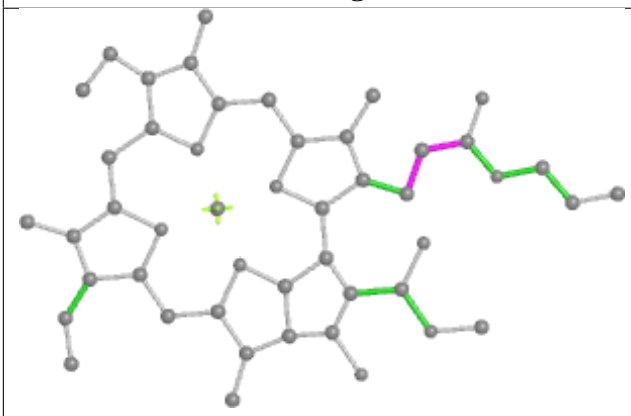
Ligand CLA b 712



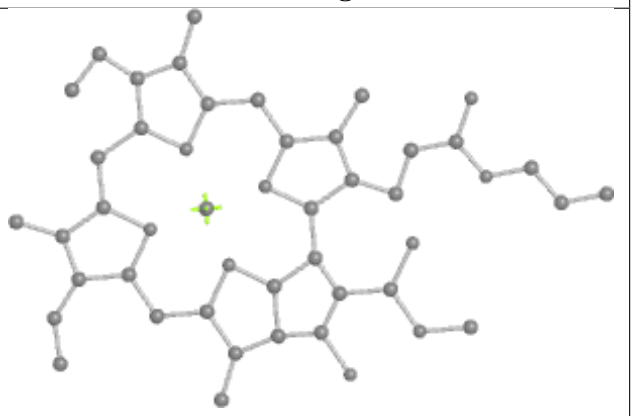
Bond lengths



Bond angles

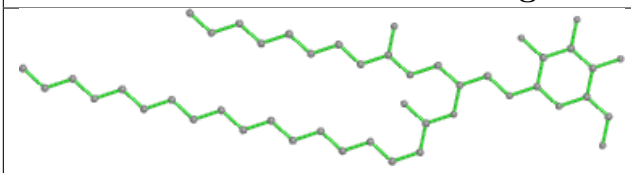


Torsions

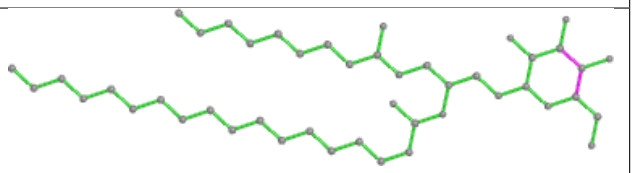


Rings

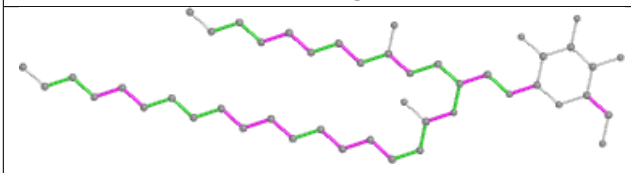
Ligand LMG D 619



Bond lengths



Bond angles



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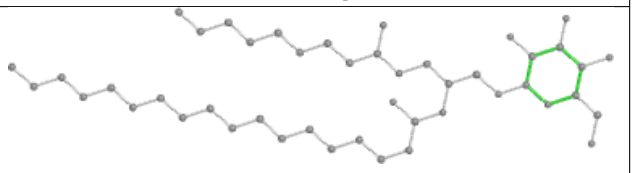
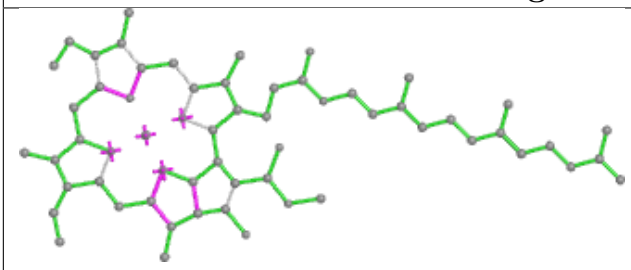
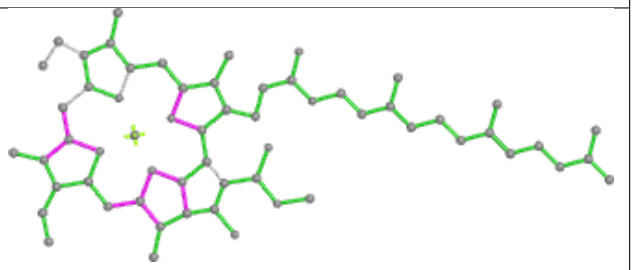


Rings

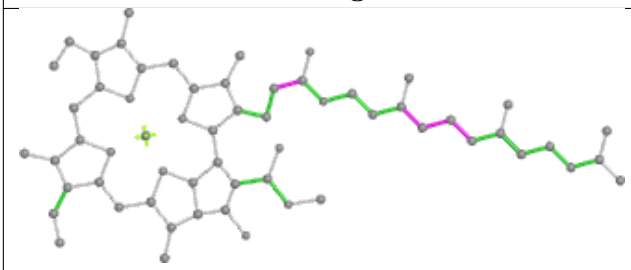
Ligand CLA J 605



Bond lengths



Bond angles



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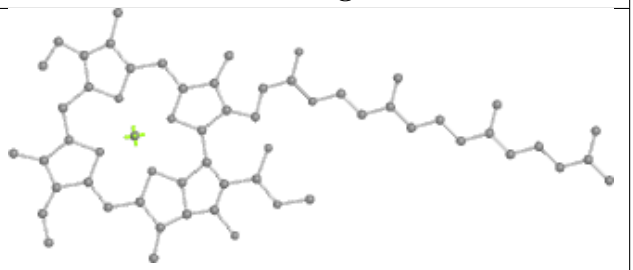
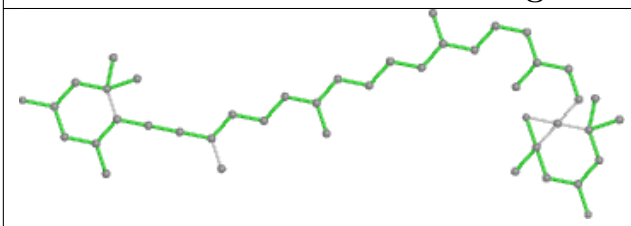
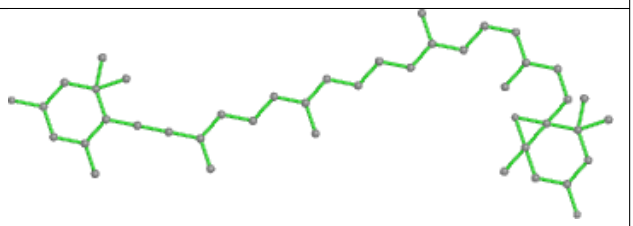


Rings

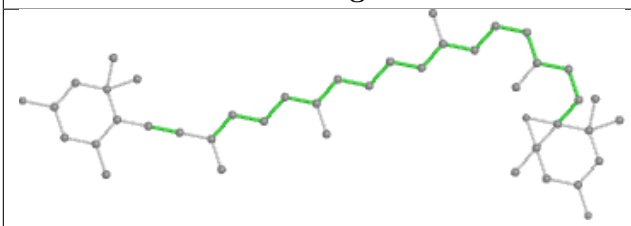
Ligand DD6 E 614



Bond lengths



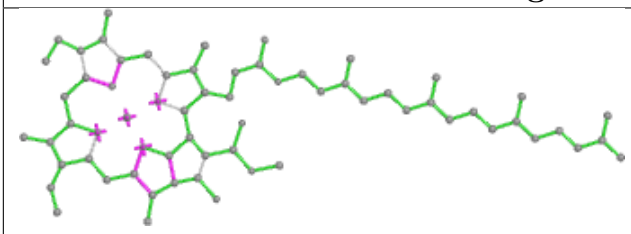
Bond angles



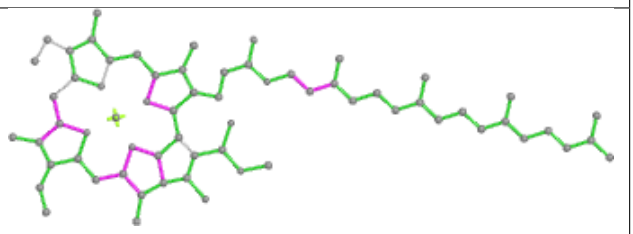
Torsions

Rings

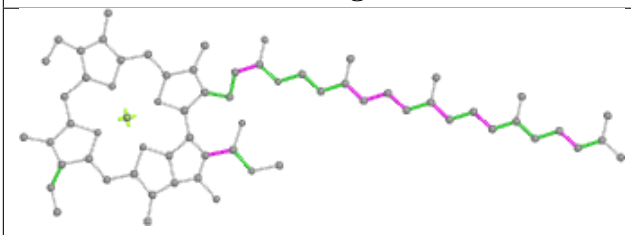
Ligand CLA b 706



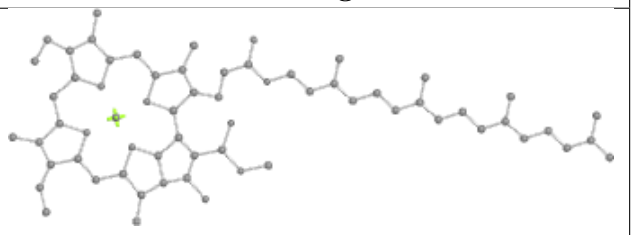
Bond lengths



Bond angles

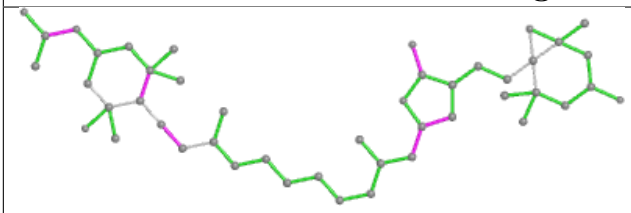


Torsions

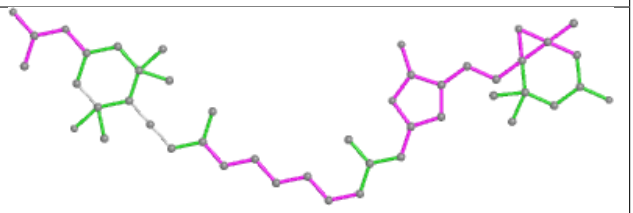


Rings

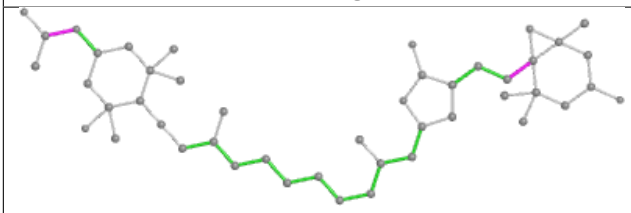
Ligand PID J 613



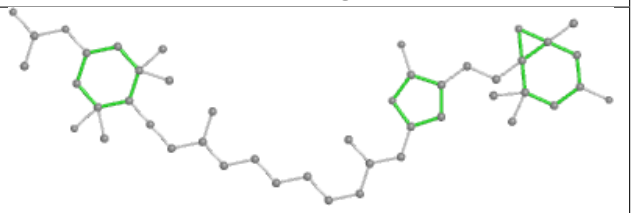
Bond lengths



Bond angles

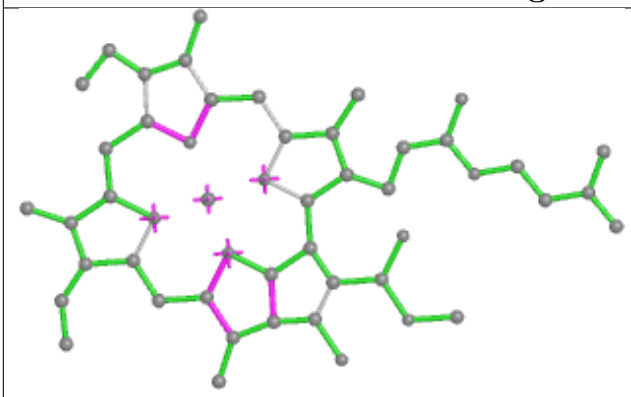


Torsions

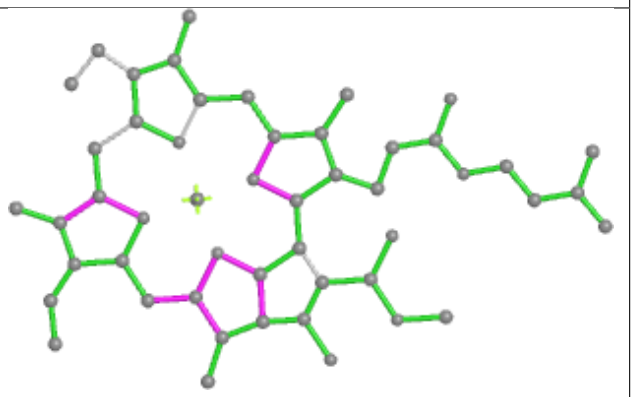


Rings

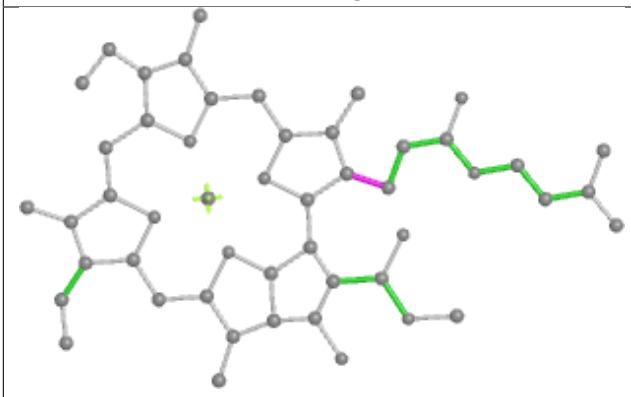
Ligand CLA a 803



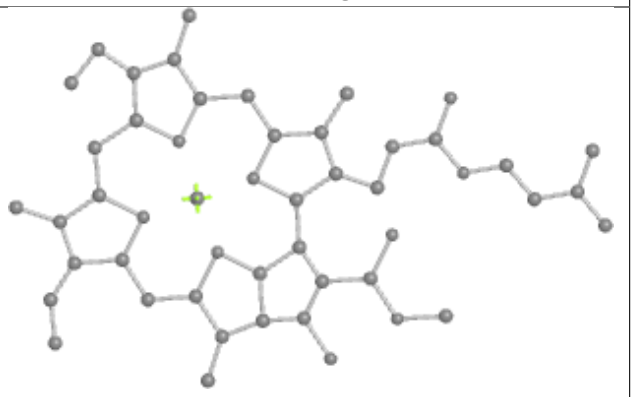
Bond lengths



Bond angles

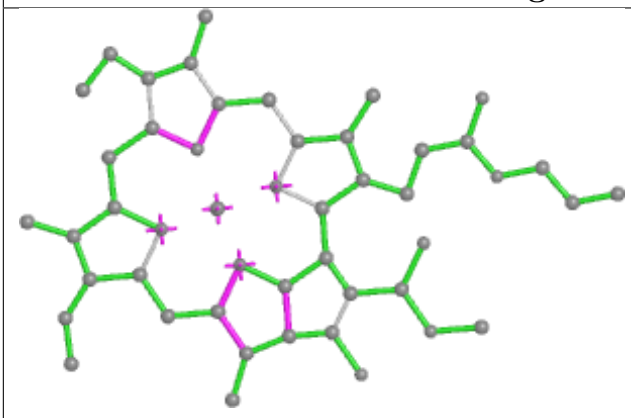


Torsions

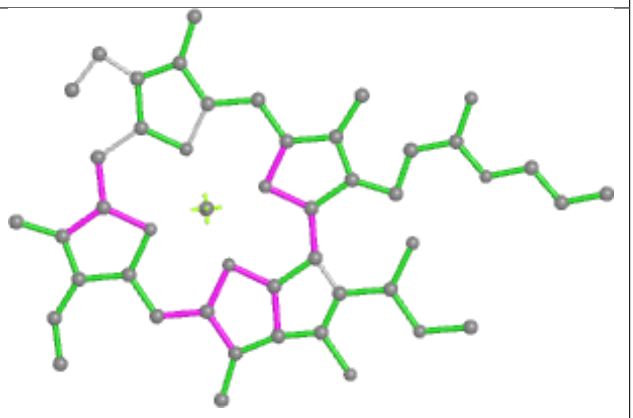


Rings

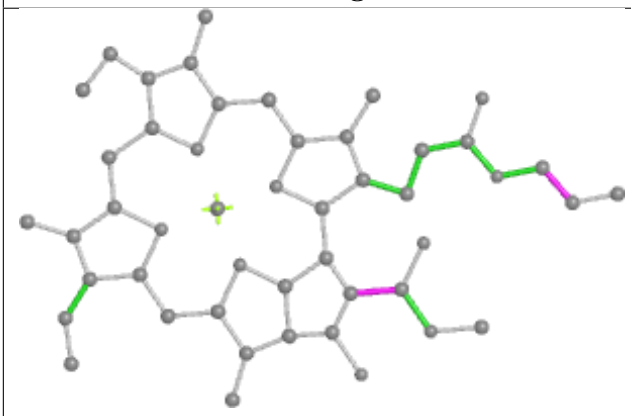
Ligand CLA a 811



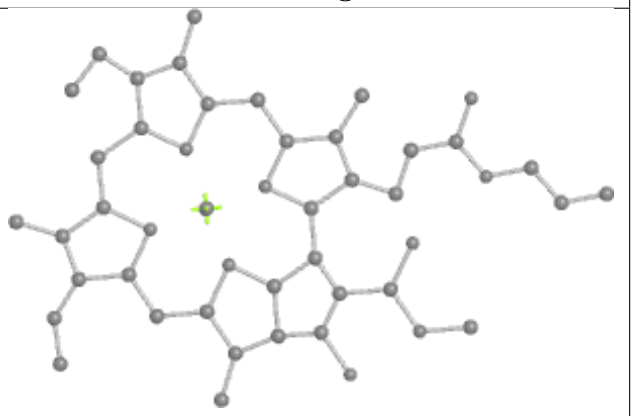
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

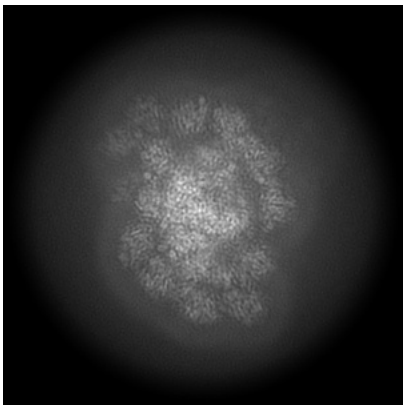
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36366. These allow visual inspection of the internal detail of the map and identification of artifacts.

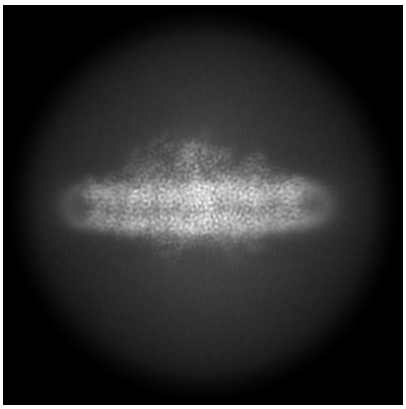
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

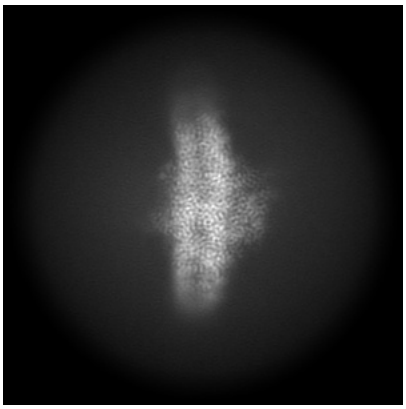
6.1.1 Primary map



X

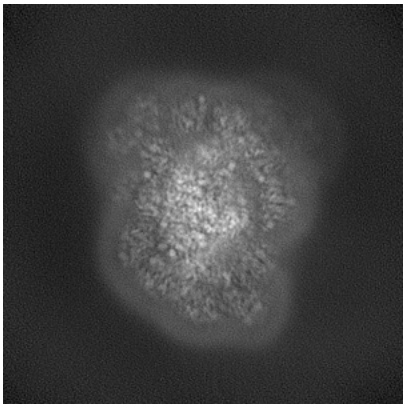


Y

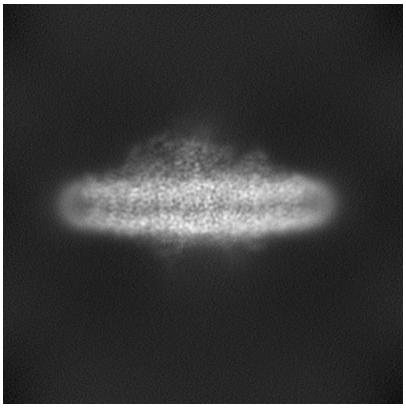


Z

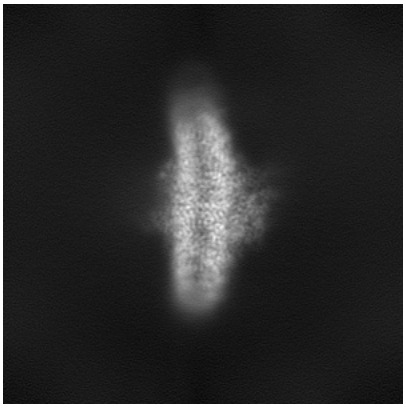
6.1.2 Raw map



X



Y

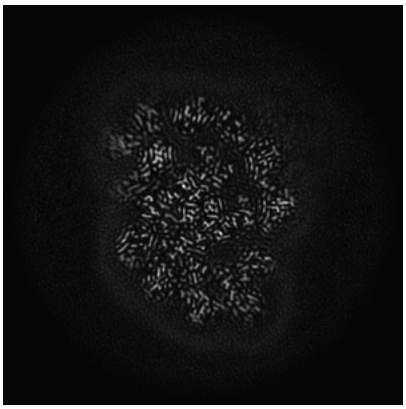


Z

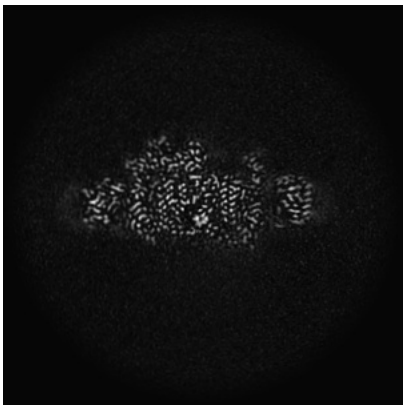
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

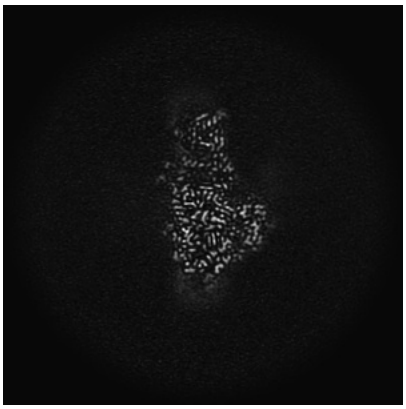
6.2.1 Primary map



X Index: 160

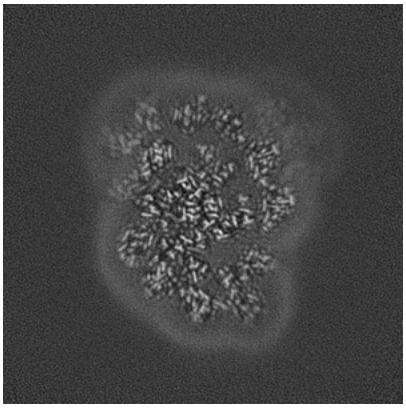


Y Index: 160

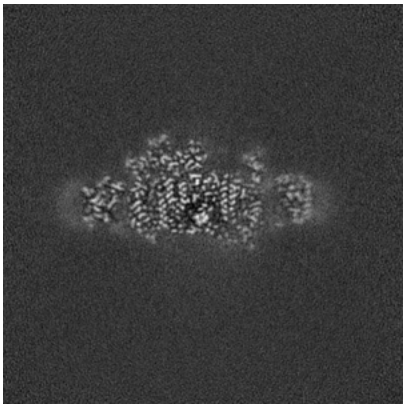


Z Index: 160

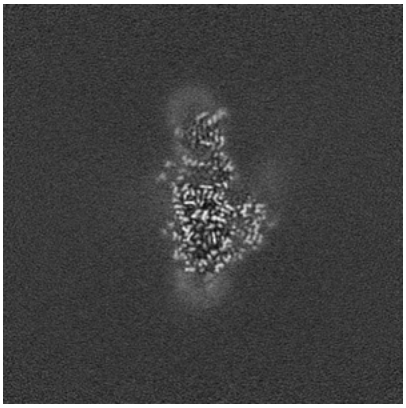
6.2.2 Raw map



X Index: 160



Y Index: 160

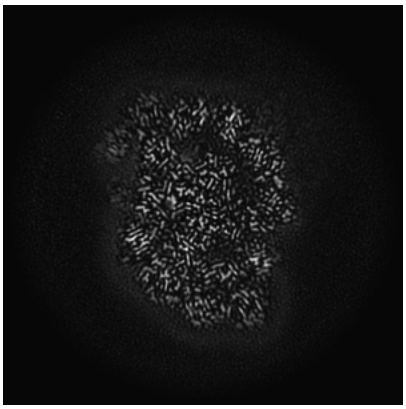


Z Index: 160

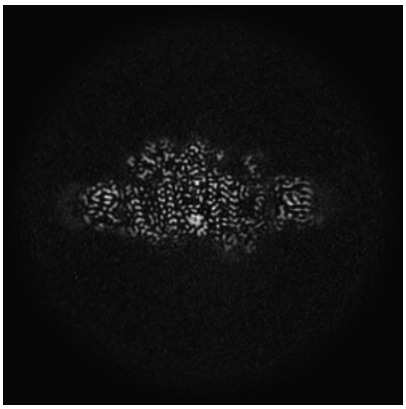
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

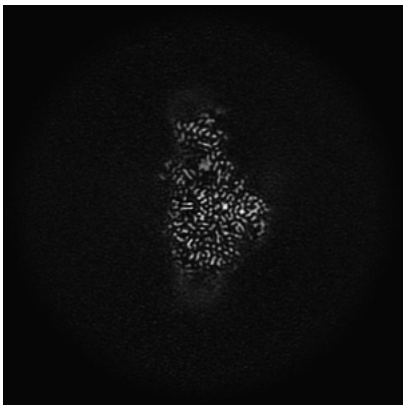
6.3.1 Primary map



X Index: 167

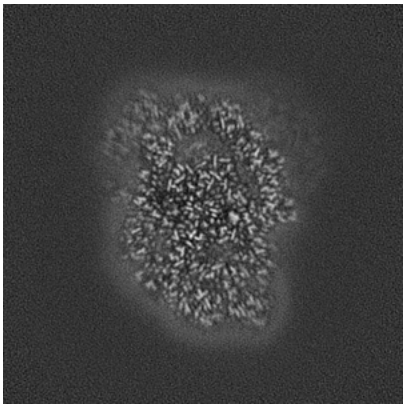


Y Index: 157

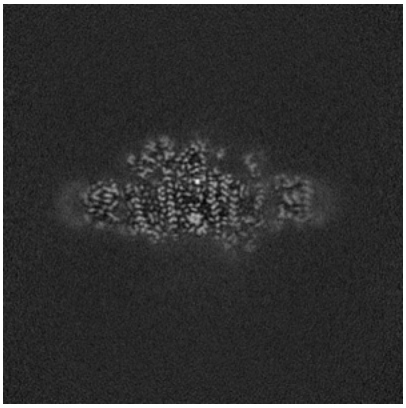


Z Index: 155

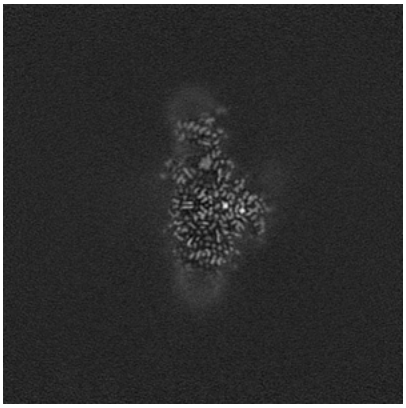
6.3.2 Raw map



X Index: 170



Y Index: 157

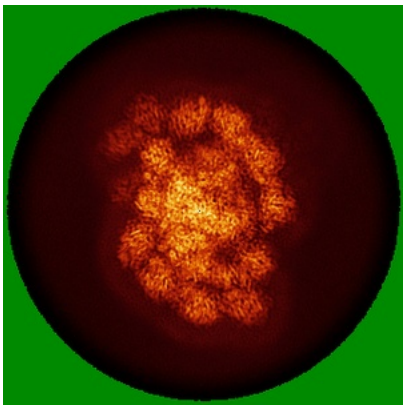


Z Index: 155

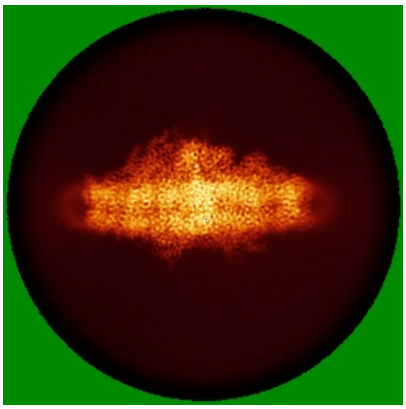
The images above show the largest variance slices of the map in three orthogonal directions.

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

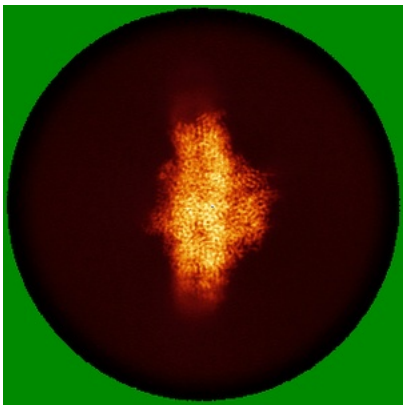
6.4.1 Primary map



X

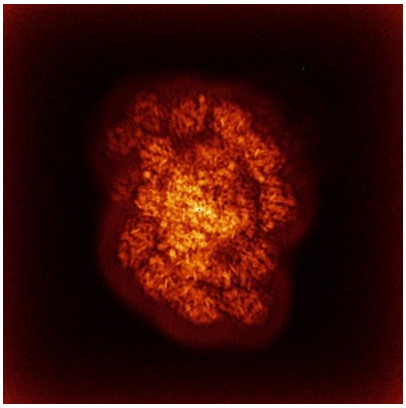


Y

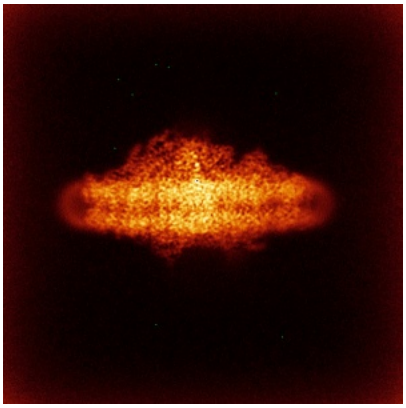


Z

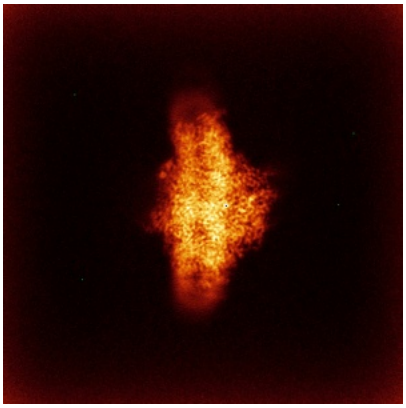
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

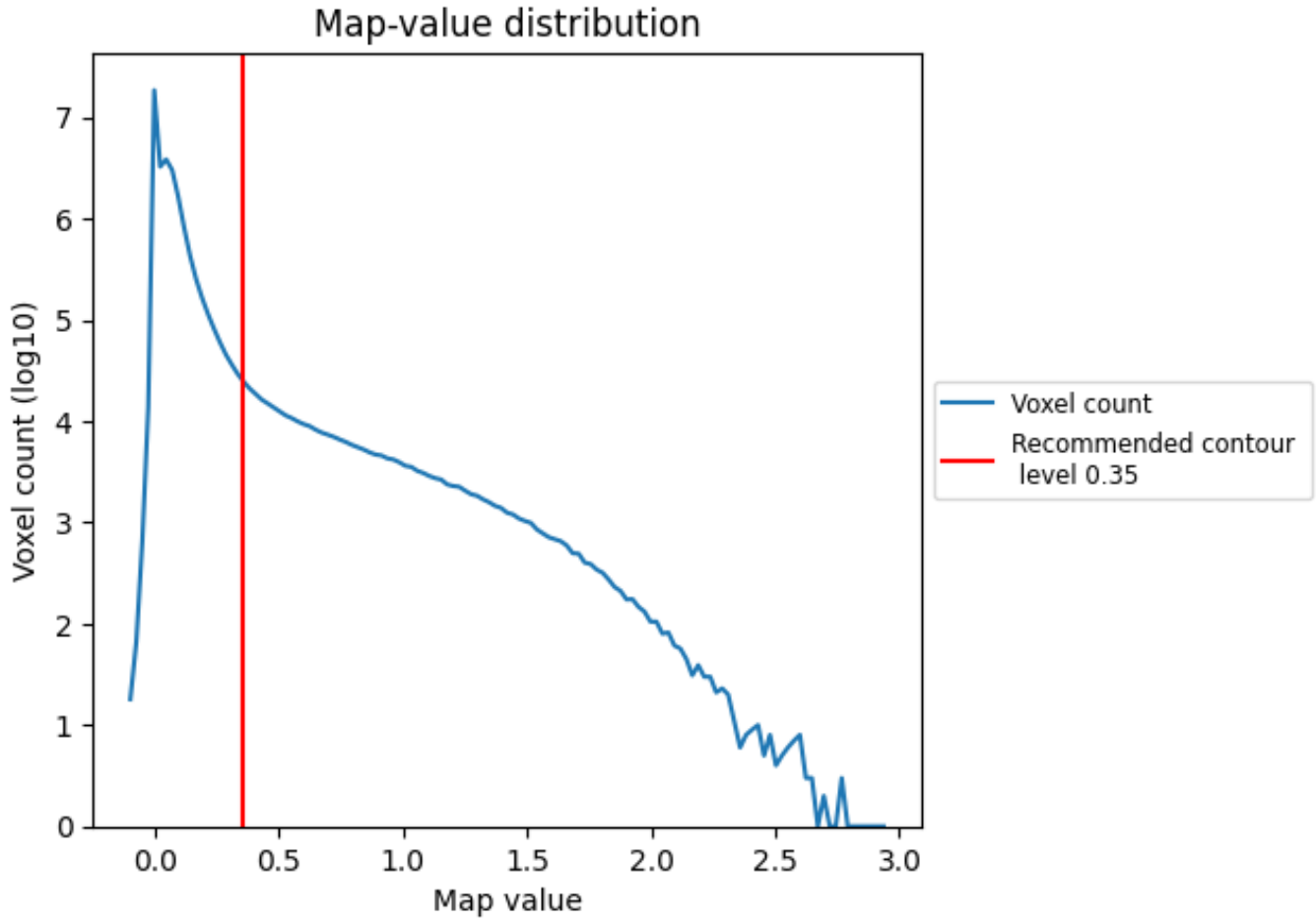
6.6 Mask visualisation (i)

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

7 Map analysis

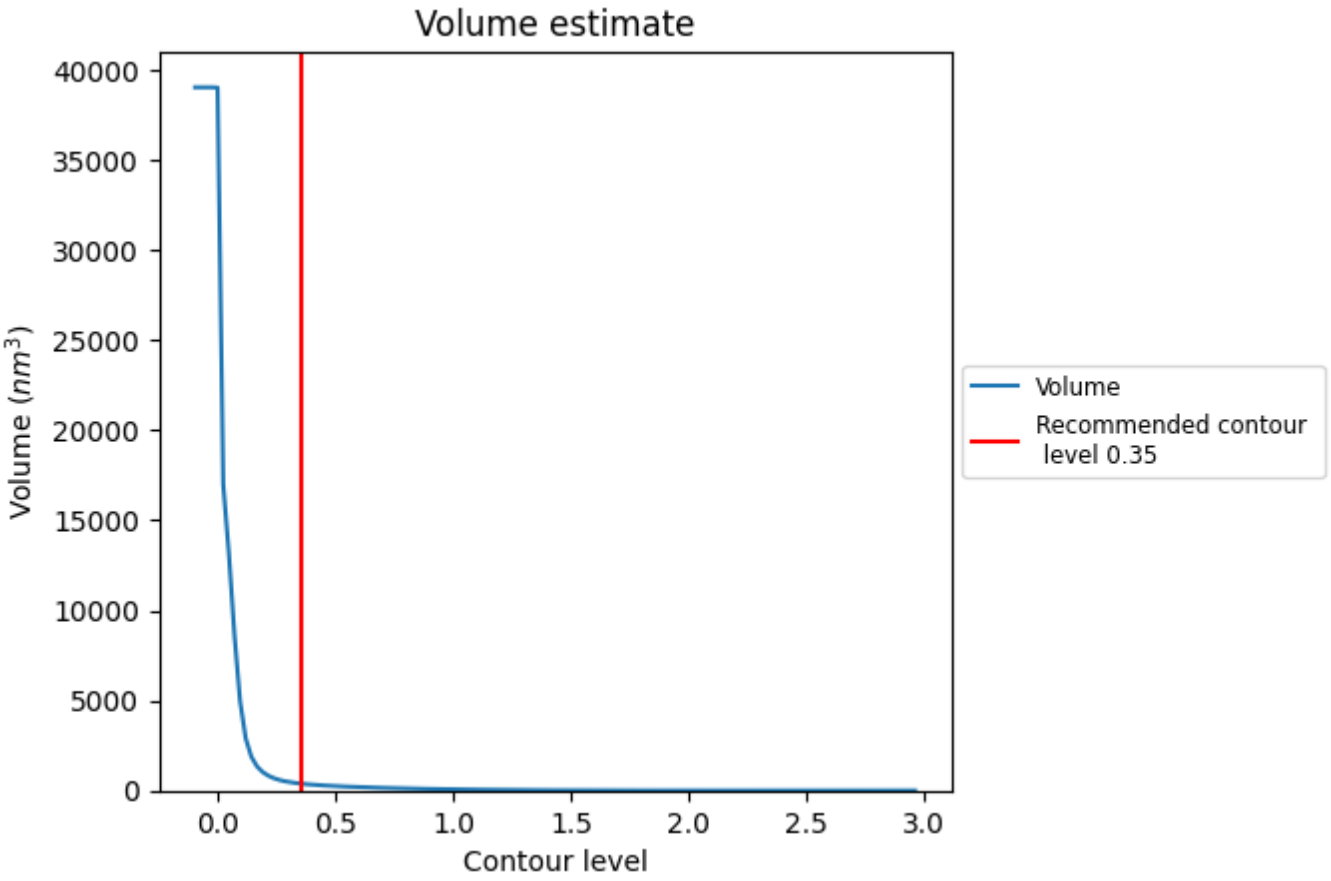
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

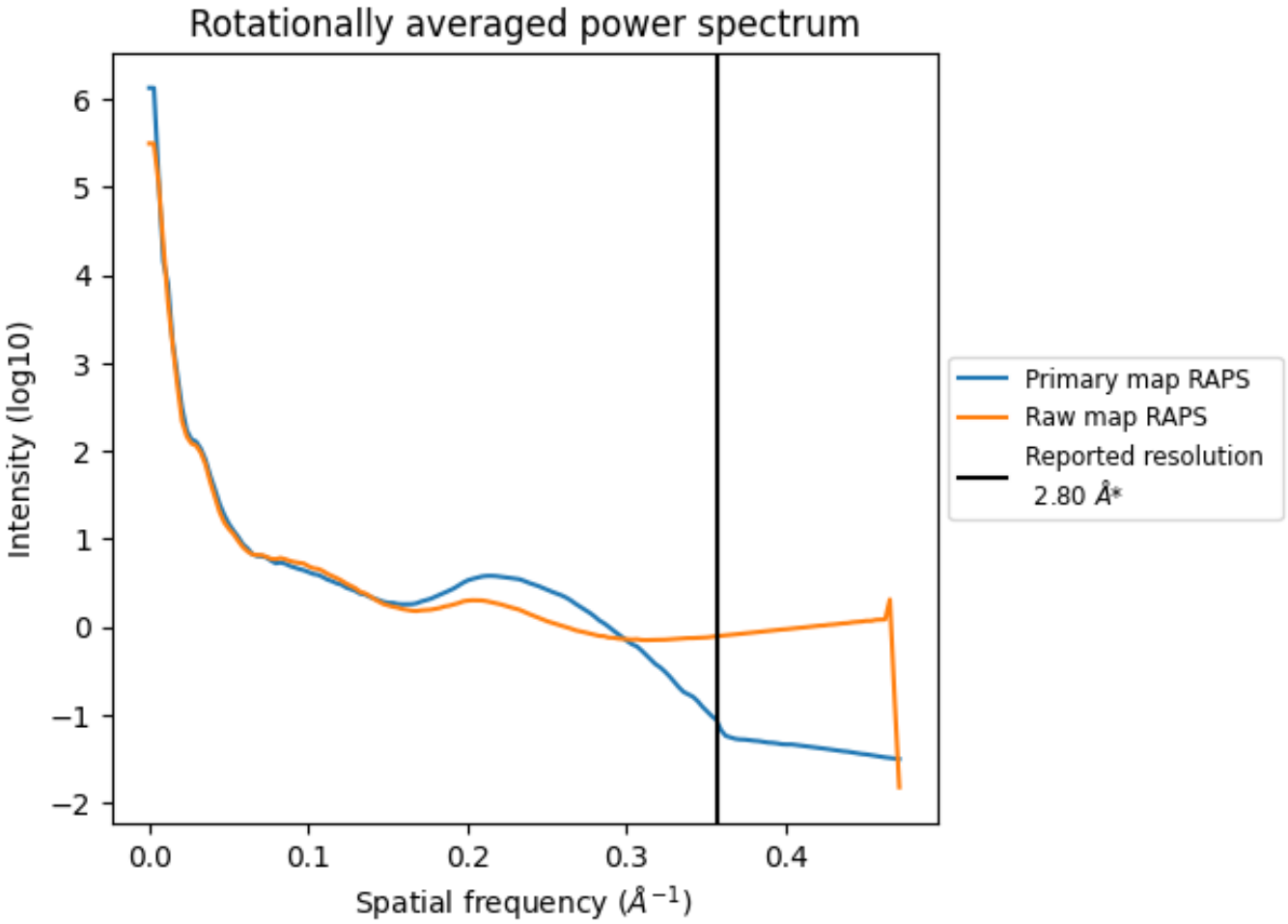
7.2 Volume estimate



The volume at the recommended contour level is 386 nm^3; this corresponds to an approximate mass of 349 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

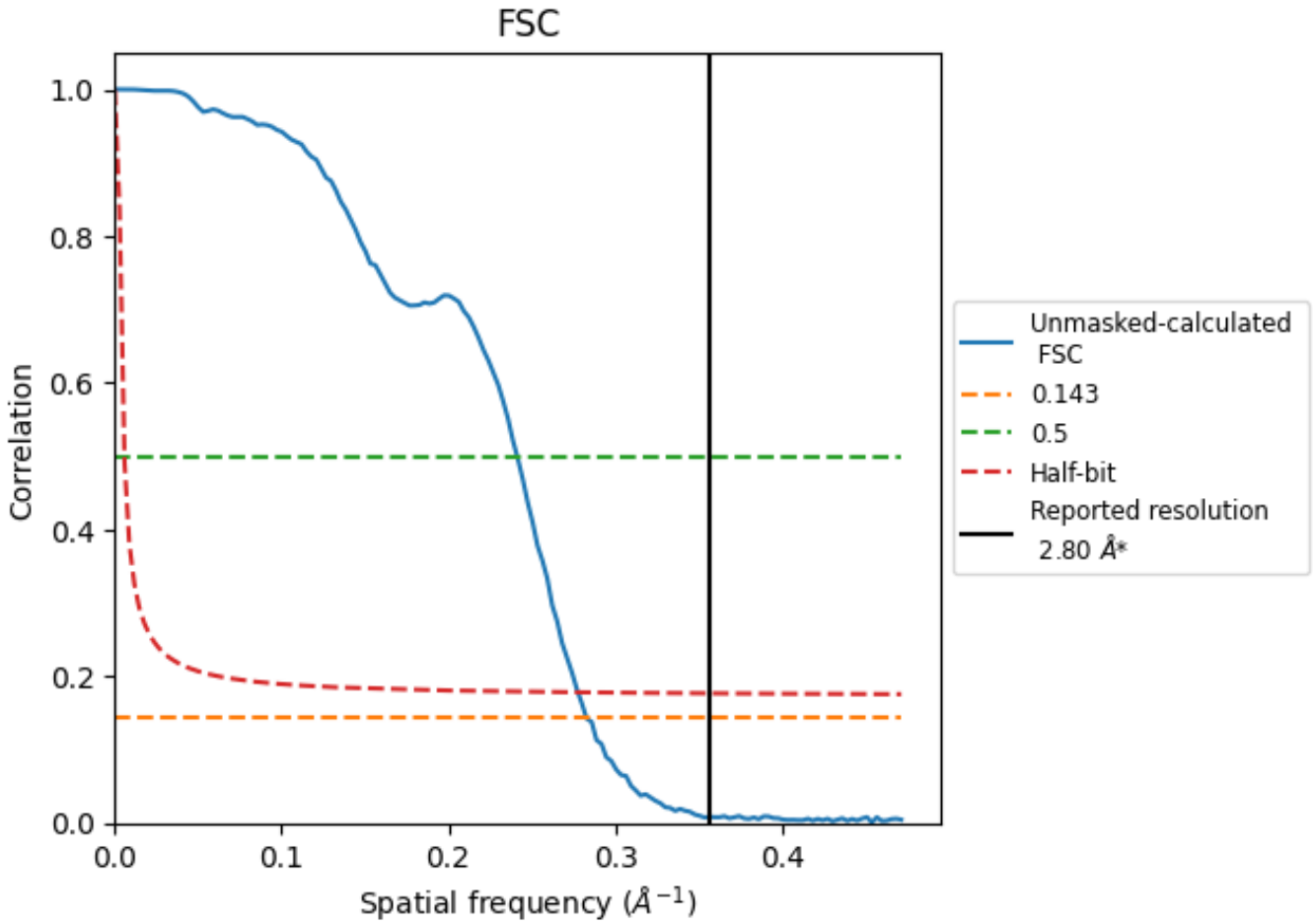


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

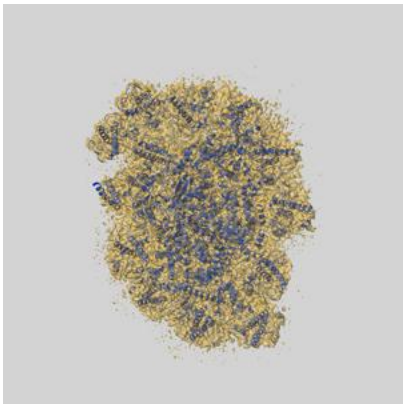
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.14	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.8 by more than 10 %

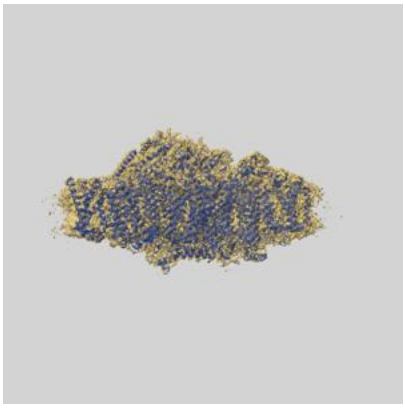
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36366 and PDB model 8JJR. Per-residue inclusion information can be found in section 3 on page 36.

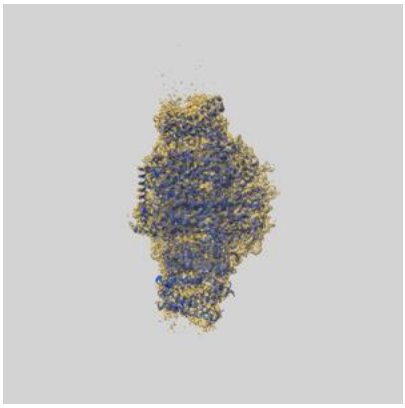
9.1 Map-model overlay



X



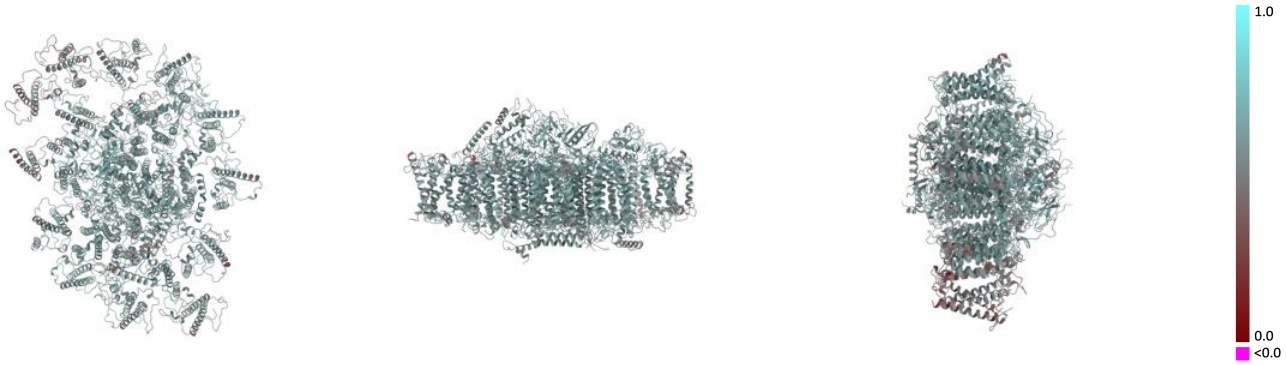
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

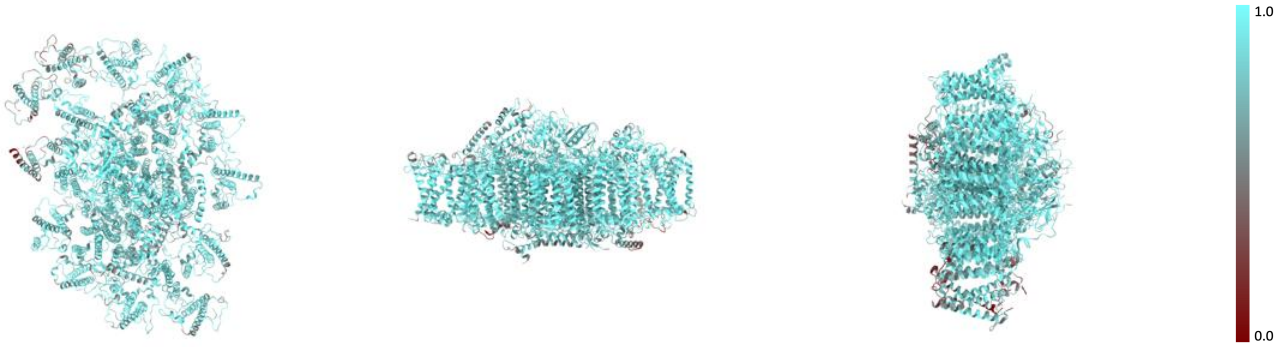
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

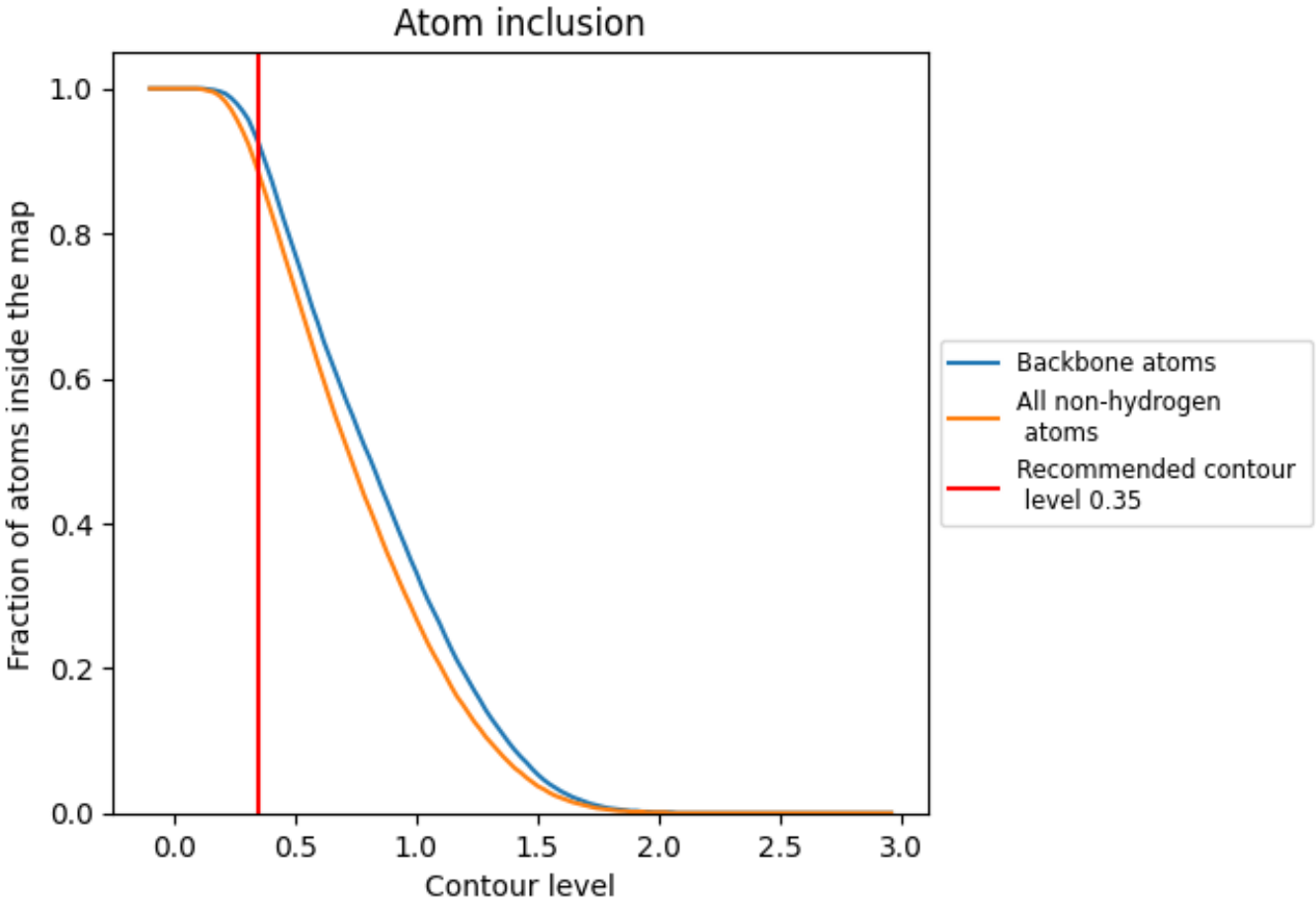
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.5750
A	0.8810	0.5710
B	0.9160	0.5810
C	0.8970	0.5880
D	0.9220	0.6000
E	0.9190	0.5760
F	0.8660	0.5680
G	0.8660	0.5410
H	0.9040	0.5730
I	0.8900	0.5700
J	0.8410	0.5450
K	0.6670	0.4810
T	0.6320	0.4260
U	0.6680	0.4840
a	0.9250	0.6020
b	0.9490	0.6130
c	0.9760	0.6000
d	0.9020	0.5800
e	0.9500	0.6090
f	0.8320	0.5850
i	0.8890	0.5790
j	0.8380	0.5740
l	0.9350	0.6010
m	0.9130	0.6000
r	0.9290	0.5780
x	0.9140	0.5860
y	0.7230	0.5400